Synthesis and Photophysical Properties of Two Diazaporphyrin-Porphyrin Hetero Dimers in Polar and Nonpolar Solutions

Two diazaporphyrin (DAP)-porphyrin hetero dimers, in β-meso and β-β configurations, were prepared to study their photoinduced intramolecular electron transfer properties. The two meso nitrogen atoms in the porphyrin ring of DAP change its redox potential, making DAP more easily reduced, compared to its porphyrin counterpart. A charge-transfer from porphyrin to DAP in both hetero dimers was verified by versatile optical spectroscopic methods. The steady-state fluorescence spectra indicated an efficient intramolecular exciplex formation for both dimers. For the β-meso dimer, ultrafast time-resolved spectroscopic methods revealed the subpicosecond formation of two types of primary short-living (1-18 ps) intramolecular exciplexes, which relaxed in toluene to form a long-living final exciplex (1.4 ns) followed by a longer-living charge transfer complex (>5 ns). However, in benzonitrile, the lifetime of the final exciplex was longer (660 ps) as was that of the charge transfer complex (180 ps). The β-β analogue formed similar short-living exciplexes in both solvents, but the final exciplex and the charge transfer state had significantly shorter lifetimes. The electrochemical redox potential measurements and density functional theory calculations supported the proposed mechanism.

General information

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Tampere Graduate School in Information Science and Engineering (TISE), Kyoto Women's University, Department of Molecular Engineering, Graduate School of Engineering, Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Kyoto University, Kyushu University, Niigata University
Contributors: Abou-Chahine, F., Fujii, D., Imahori, H., Nakano, H., Tkachenko, N. V., Matano, Y., Lemmetyinen, H.
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Original language: English
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Source: Scopus
Source ID: 84934905262
Research output: Contribution to journal › Article › Scientific › peer-review

Photoresponsive liquid-crystalline polymer films bilayered with an inverse opal structure

An inverse opal film was layered to a photodeformable film, and its photoresponsive behavior was investigated. This bilayer films composed of colorless photonic crystal using inverse opal structures and colored photoresponsive layers with azobenzene-containing CLCP.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tokyo Institute of Technology, Japan Science and Technology Agency
Contributors: Akamatsu, N., Aizawa, M., Tatsumi, R., Hisano, K., Priimägi, A., Shishido, A.
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Scopus rating (2016): CiteScore 1.5 SJR 0.3 SNIP 0.558
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ASJC Scopus subject areas: Organic Chemistry, Polymers and Plastics, Materials Chemistry
Keywords: Bragg diffraction, Inverse opal structure, Photoresponsive film
DOIs:

10.2494/photopolymer.29.145
Source: Scopus
Source ID: 84981200985
Research output: Contribution to journal › Article › Scientific › peer-review

The red, purple and blue modifications of polymeric unsymmetrical hydroxyalkadiynyl-N-arylcarbamate derivatives in Langmuir-Schaefer films

Solid topochemical photopolymerization (STP) of Langmuir-Schaefer films of a new class of unsymmetrical diynes, containing N-arylcarbamate groups in the hydrophobic part and hydroxymethylene groups in the hydrophilic part of the molecules was examined. In addition, the monomeric Langmuir monolayer formation was studied by Brewster angle microscopy and the surface morphology of monomer and polymer films on solid substrates were studied by scanning electron microscopy and atomic force microscopy. Three phases of polydiacetylene (PDA) (red, purple and blue) were observed after UV-light polymerization of above-mentioned films of alcohol diacetylene (DA) derivatives. The substitution of MeO group in the aryl ring substituent by hydrogen atom and the variation of the methylene group number in the hydrophobic part from 5 to 6 changed significantly the result of STP: instead of blue phase PDA observed for diynes with MeO group, the red phase PDA was observed for DA with H-atom from the very beginning of diyne film UV irradiation. For two other diynilic N-arylcarbamates of identical chemical structures except of the substituents in the aryl ring of hydrophobic parts of the molecules, no changes in the efficiency of polymerization or the position and shape of absorption bands were observed. This indicated the formation of the purple phase PDA. For these molecules, the number of methylene groups in hydrophobic and hydrophilic parts of the molecules was 9 and 2, respectively.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, A. M. Prokhorov General Physics Institute, Russian Academy of Sciences, Åbo Akademi University, St. Petersburg State University, NRC Kurchatov Institute, Russian Acad Sci, Russian Academy of Sciences, Kotelnikov Inst Radio Engn & Elect
Contributors: Alekseev, A., Ihalainen, P., Ivanov, A., Domnin, I., Klechkovskaya, V., Orekhov, A., Lemmetyinen, H., Vuorimaa-Laukkanen, E., Peltonen, J., Vyaz'min, S.
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ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Materials Chemistry, Metals and Alloys, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Langmuir monolayer, Langmuir-Schaefer film, Polydiacetylenes with urethane group, Solid topochemical photopolymerization
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Bibliographical note

EXT="Alekseev, Alexander"
Source: Scopus
Source ID: 84976884439
Research output: Contribution to journal › Article › Scientific › peer-review

Stable blue phase polymeric Langmuir-Schaefer films based on unsymmetrical hydroxyalkadiynyl N-arylcarbamate derivatives

Unsymmetrical diynes containing N-arylcarbamate groups in the hydrophobic part and hydroxymethylene groups in the hydrophilic part of the molecules were synthesized and studied. The Langmuir monolayer formation process was followed by Brewster angle microscopy (BAM). The Langmuir-Schaefer monolayer films, transferred on solid substrates (quartz or

Si), were investigated by absorption spectroscopy and atomic force microscopy (AFM). Four substances had 2 methylene groups in the hydrophilic part of the molecule (n) and 4 or 5 of these groups in the hydrophobic part (m). At the same time the aryl substituent had a hydrogen atom or a MeO group in the p-position of the benzene ring. After 20 min of UV irradiation the initially colorless monomeric films of all four compounds turned into stable blue phase polymeric films. The blue phase is unusual for alcoholic diacetylene derivatives. The BAM and AFM measurements demonstrated higher homogeneity of the films with a MeO group in the aryl substituent in comparison to the molecules with a hydrogen atom. The reasons for these different structural organizations as well as potential applications of stable blue phase polydiacetylene thin films are discussed.

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Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, A. M. Prokhorov General Physics Institute, Russian Academy of Sciences, Åbo Akademi University, St. Petersburg State University, Russian Academy of Science
Contributors: Alekseev, A., Ihalainen, P., Ivanov, A., Domnin, I., Rosqvist, E., Lemmetyinen, H., Vuorimaa-Laukkanen, E., Peltonen, J., Vyaz'min, S.
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ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
Keywords: Absorption spectroscopy, Blue phase polydiacetylenes, Brewster angle microscopy, Langmuir-Schaefer film, Photopolymerization
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Bibliographical note
EXT="Alekseev, Alexander"
Source: Scopus
Source ID: 85032302551
Research output: Contribution to journal › Article › Scientific › peer-review

Guanidinium Pairing Facilitates Membrane Translocation
Ab initio free energy calculations of guanidinium pairing in aqueous solution confirm the counterintuitive conjecture that the like-charge ion pair is thermodynamically stable. Transferring the guanidinium pair to the inside of a POPC lipid bilayer, like-charge ion pairing is found to occur also inside the membrane defect. It is found to contribute to the nonadditivity of ion transfer, thereby facilitating the presence of ions inside the bilayer. The effect is quantified by free energy decomposition and comparison with ammonium ions, which do not form a stable pair. The presence of two charges inside the center of the bilayer leads to the formation of a pore. Potential consequences for cell penetrating peptides and ion conduction are drawn.

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Universität Regensburg, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Bijenička Cesta 54
Contributors: Allolio, C., Baxova, K., Vazdar, M., Jungwirth, P.
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Bibliographical note
EXT="Vazdar, Mario"
Source: Scopus
Source ID: 84955271467
Research output: Contribution to journal › Article › Scientific › peer-review

Additive manufacturing of monolithic supercapacitors with biopolymer separator
In this paper, additive layer-by-layer fabrication of a fully screen printed monolithic supercapacitor exhibiting performance comparable with supercapacitors prepared using lamination is reported. A novel separator material improves the performance of the monolithic supercapacitor, is easily applicable using scalable processes such as screen and stencil printing, and is based on sustainable biomaterials. The additive monolithic manufacturing offers advantages for system integration and avoids the need of an additional alignment step as needed in the fabrication of laminated supercapacitors. Previously, the monolithically fabricated supercapacitors showed higher equivalent series resistance (ESR) and leakage current than the laminated ones. By using microfibrillated cellulose (MFC) and chitosan as separator materials ESR and leakage current were decreased. These disposable and non-toxic aqueous electrolyte supercapacitors are optimized for autonomous sensor systems, for example in Internet-of-Things (IoT) applications, with capacitance of 200–300 mF and ESR of about 10 Ω. The new composite separator material consisting of MFC and chitosan has good adhesion on the electrodes and the substrate, is easy to apply using printing and coating processes, and does not diffuse into the porous electrode. Graphic Abstract: [Figure not available: see fulltext.].

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Electrical Engineering, Automation Technology and Mechanical Engineering, BioMediTech, Abo Akademi University
Contributors: Arvani, M., Keskinen, J., Railanmaa, A., Siljander, S., Björkqvist, T., Tuukkanen, S., Lupo, D.
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Arvani2020_Article_AdditiveManufacturingOfMonolit
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Source: Scopus
Source ID: 85085106449
Research output: Contribution to journal › Article › Scientific › peer-review

Hydrolysis and drug release from poly(ethylene glycol)-modified lactone polymers with open porosity
The ability to release active agents from a porous scaffold structure in situ enables the simultaneous structural support for the cells proliferating and differentiating towards tissue as well as the stimulation of tissue regeneration. Due to the great potentiality of such approach, drug-releasing scaffolds were fabricated from hydrolytically degradable polymers. Three copolymers of poly(ethylene glycol), ε-caprolactone, L- and D,L-lactide were synthesized and blended with bone-growth

inducing active agents, dexamethasone (DM) and 2-phospho-L-ascorbic acid trisodium salt (AS). Porous scaffolds were prepared by means of super-critical carbon dioxide foaming. In the final scaffold structures, the particle size, location and the water solubility of the drug affected the release kinetics. As the large and water soluble AS particles were more exposed to the buffer solution compared to small DM particles, the AS release was burst-like whereas DM showed a long-term release. The material structure had a significant effect on the release kinetics as the porous scaffolds released active agents faster compared to the solid cylinders. Furthermore, this study showed the strong effect of polymer degradation and wettability on the release, which were more determinative than the pore architecture.

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MoE publication type: A1 Journal article-refereed
Organisations: BioMediTech, Aalto University, Orton Orthopaedic Hospital
Contributors: Asikainen, S., Paakinaho, K., Kyhkynen, A. K., Hannula, M., Malin, M., Ahola, N., Kellomäki, M., Seppälä, J.
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DOIs:

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Source: Scopus
Source ID: 85060767586
Research output: Contribution to journal › Article › Scientific › peer-review

Rapid and sensitive detection of norovirus antibodies in human serum with a biolayer interferometry biosensor
Here, we describe the use of a biolayer interferometry biosensor for the fast and sensitive detection of virus-specific antibodies from human serum samples. Norovirus-like particles and norovirus P-particles were used to functionalise the biosensor tip. The detection of antibodies directly from serum samples was challenging, but the addition of a metal chelator (DAB) combined with an anti-human horseradish peroxidase-tagged antibody enabled enhanced detection of virus-specific antibodies in serum dilutions up to 1:100,000. Biolayer interferometry provides results faster than an ELISA, with results in as little as 10-20 min when using pre-functionalised sensors. Therefore, biolayer interferometry combined with DAB enhancement offers an attractive method for quick and sensitive quantification of biomolecules from complicated sample matrices.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Fimlab Laboratories Ltd
Contributors: Auer, S., Koho, T., Uusi-Kerttula, H., Vesikari, T., Blazevic, V., Hytönen, V. P.
Number of pages: 8
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Peer-reviewed: Yes

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Journal: Sensors and Actuators B: Chemical
Volume: 221
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ASJC Scopus subject areas: Electrical and Electronic Engineering, Condensed Matter Physics, Electronic, Optical and Magnetic Materials, Metals and Alloys, Surfaces, Coatings and Films, Materials Chemistry, Instrumentation
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DOIs:
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http://www.scopus.com/inward/record.url?scp=84956972181&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84956972181
Research output: Contribution to journal › Article › Scientific › peer-review

Water-Responsive and Mechanically Adaptive Natural Rubber Composites by in Situ Modification of Mineral Filler Structures

A new biomimetic stimuli-responsive adaptive elastomeric material, whose mechanical properties are altered by a water treatment is reported in this paper. This material is a calcium sulphate ($CaSO_4$) filled composite with an epoxidized natural rubber (ENR) matrix. By exploiting various phase transformation processes that arise when $CaSO_4$ is hydrated, several different crystal structures of $CaSO_4 \cdot xH_2O$ can be developed in the cross-linked ENR matrix. Significant improvements in the mechanical and thermal properties are then observed in the water-treated composites. When compared with the untreated sample, there is approximately 100% increase in the dynamic modulus. The thermal stability of the composites is also improved by increasing the maximum degradation rate temperature by about 20 °C. This change in behavior results from an in situ development of hydrated crystal structures of the nanosized $CaSO_4$ particles in the ENR matrix, which has been verified using Raman spectroscopy, transmission electron microscopy, atomic force microscopy, and X-ray scattering. This work provides a promising and relatively simple pathway for the development of next generation of mechanically adaptive elastomeric materials by an eco-friendly route, which may eventually also be developed into an innovative biodegradable and biocompatible smart polymeric material.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Leibniz-Institut für Polymerforschung Dresden E.V., University of Massachusetts Lowell, Vodafone Department of Mobile Communications Systems, Queen Mary University of London
Contributors: Banerjee, S. S., Hait, S., Natarajan, T. S., Wießner, S., Stöckelhuber, K. W., Jehnichen, D., Janke, A., Fischer, D., Heinrich, G., Busfield, J. J., Das, A.
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ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry
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Source ID: 85067653290
Research output: Contribution to journal › Article › Scientific › peer-review

Temperature scanning stress relaxation behavior of water responsive and mechanically adaptive elastomer nanocomposites

The decrease of stress at constant strain, that is, the stress relaxation process as a function of temperature, is a central mechanical characteristics of elastomer nanocomposites for their potential applications. However, in the conventional stress relaxation test, the relaxation behavior is usually determined as a function of time at constant temperature. The present work reports the temperature scanning stress relaxation (TSSR) characteristics of a new kind of mechanically adaptive elastomer nanocomposite by monitoring the nonisothermal relaxation behavior as a function of temperature. This kind of adaptive elastomer nanocomposite was prepared by introducing calcium sulfate ($CaSO_4$), as the water-responsive phase into the hydrophilic elastomer matrix. The influence of water-induced structural changes on TSSR behavior was investigated. Water treatment had a strong effect on the shape of the relaxation spectrum of the nanocomposite. It was revealed that the in situ development of hydrated nano-rod crystal structures of $CaSO_4$ in the elastomer matrix was responsible for the changes in the mechanical relaxation behavior of the composites. Atomic force microscopy was used to verify this nano-rod crystal morphology in the elastomer matrix. The mechanism of water-induced mechanical reinforcement of the composite was explored from dynamic mechanical analysis of the material and correlated with its

stress relaxation behavior.

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Contributors: Banerjee, S. S., Natarajan, T. S., Subramani B., E., Wießner, S., Janke, A., Heinrich, G., Das, A.
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ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry
Keywords: adaptive elastomer nanocomposite, calcium sulphate, mechanical reinforcement, morphology, temperature scanning stress relaxation
DOIs:

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Source: Scopus
Source ID: 85070677934
Research output: Contribution to journal › Article › Scientific › peer-review

Compatibilization of natural rubber/nitrile rubber blends by sol–gel nano-silica generated by in situ method
Abstract: Controlled growth of in situ silica, into natural rubber (NR)/nitrile rubber (NBR) blend (40/60 composition by weight) following solution sol–gel method, results in a coherent blend morphology with enhanced composite properties. Similar composites, i.e., in situ silica-filled NR/NBR blend (40/60 by weight), showed better mechanical properties than any other composition that were prepared by soaking sol–gel method in earlier study. However, silica content in the rubber blend was limited to 20 phr (parts per hundred parts of rubber) and could not be increased under experimental condition following soaking sol–gel method. In the present work, silica content is increased (up to 30 phr) beyond that limit for the same blend composition. Accordingly, mechanical properties of the NR/NBR composites are improved. Use of a silane coupling agent, viz., bis-(3-triethoxysilylpropyl)-tetra sulfide, in the reactive sol–gel system during in situ silica generation brings in remarkable effect in silica distribution, rubber–filler interaction and mechanical properties of the composites. TEM micrographs of the selected composites reveal that silica is mostly grown at the interfacial region, when silane is used in particular. This results in further enhancement in mechanical properties and compatibility of the blend at the same silica content as evident from stress–strain and dynamic mechanical analysis studies. The reinforcement of effect in situ silica is assessed by Guth–Gold equation and modified form of Guth equation (with shape factor f = 2.53). The results are supported by the detailed studies on rheological, morphological, mechanical and viscoelastic properties of the composites. Graphical Abstract: [Figure not available: see fulltext.]

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Visvesvaraya National Institute of Technology, Indian Rubber Manufacturers Research Association, Department of Elastomers, Leibniz-Institut für Polymerforschung Dresden E.V., University of Kalyani
Contributors: Bansod, N. D., Kapgate, B. P., Das, C., Das, A., Basu, D., Debnath, S. C.
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Journal: JOURNAL OF SOL-GEL SCIENCE AND TECHNOLOGY
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ISSN (Print): 0928-0707
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ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Biomaterials, Ceramics and Composites, Electronic, Optical and Magnetic Materials, Materials Chemistry

Keywords: In situ silica, Reinforcement, Rubber blend, Rubber–filler interaction, Silane treatment, Sol–gel method
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Source ID: 84974817789
Research output: Contribution to journal › Article › Scientific › peer-review

Mechanical characterization of pore-graded bioactive glass scaffolds produced by robocasting

Since the discovery of 45S5 Bioglass® by Larry Hench, bioactive glasses have been widely studied as bone substitute materials and, in more recent years, have also shown great promise for producing three-dimensional scaffolds. The development of additive manufacturing techniques and their application in bone tissue engineering allows the design and fabrication of complex structures with controlled porosity. However, achieving strong and mechanically-reliable bioactive glass scaffolds is still a great challenge. Furthermore, there is a relative paucity of studies reporting an exhaustive assessment of other mechanical properties than compressive strength of glass-derived scaffolds. This research work aimed at determining key mechanical properties of silicate SiO_2-Na_2O-K_2OMgO-CaO-P_2O_5 glass scaffolds fabricated by robocasting and exhibiting a porosity gradient. When tested in compression, these scaffolds had a strength of 6 MPa, a Young's modulus around 340 MPa, a fracture energy of 93 kJ/m^3 and a Weibull modulus of 3, which provides a quantification of the scaffold reliability and reproducibility. Robocasting was a suitable manufacturing method to obtain structures with favorable porosity and mechanical properties comparable to those of the human cancellous bone, which is fundamental regarding osteointegration of bone implants.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: BioMediTech, Politecnico di Torino, McGill University
Contributors: Barberi, J., Nommeots-Nomm, A., Fiume, E., Verné, E., Massera, J., Baino, F.
Number of pages: 8
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Publication information

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ISSN (Print): 2299-3932
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Scopus rating (2019): CiteScore 2.9 SJR 0.39 SNIP 1.056
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Ceramics and Composites, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Bioactive glass, Mechanical properties, Robocasting, Scaffold
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DOIs:

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Bibliographical note

EXT="Nommeots-Nomm, Amy"
Source: Scopus
Source ID: 85078096149
Research output: Contribution to journal › Article › Scientific › peer-review

Unmodified LDH as reinforcing filler for XNBR and the development of flame-retardant elastomer composites

Layered double hydroxides (LDHs), inorganic clay materials with mixed metals present in the structure along with some interlayer cations, have immense potential for use as a filler in rubbers.Wereport the preparation and properties of a set of novel nanocomposites consisting of aLDHdispersed in carboxylic-acrylonitrile-butadiene rubber (XNBR).Wesucceed in obtaining significantly improved physical properties by altering the chemical structure of a LDH with Zn and Al ions (Zn-Al LDH). In particular, we discover a significant reinforcing effect. This occurs despite the size difference between the LDH and traditional reinforcing fillers such as precipitated silica and carbon black. Both the elastic modulus and tensile strength increase. This increase is a function of the LDH concentration and, reaches a maximum value when the LDH concentration is at 100 phr. Experimental evidence suggests that this reinforcing effect is due to direct ion-to-ion interaction between the filler and the matrix. In addition, we report that the presence of the nanofiller positively affects the

flame retardence and thermal decomposition of the nanocomposites. We attribute this effect to the presence of a layer formed by the nanofiller.

General information

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Organisations: Engineering materials science and solutions (EMASS), Vodafone Department of Mobile Communications Systems, Leibniz-Institut für Polymerforschung Dresden E.V., Technical University of Tampere, Rubber Research Institute of, IMDEA Materials Institute
Contributors: Basu, D., Das, A., Jacobgeorge, J., Wang, D. Y., Stöckelhuber, K., Wagenknecht, U., Leuteritz, A., Kutlu, B. , Reuter, U., Heinrich, G.
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ISSN (Print): 0035-9475
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Original language: English
ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry
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10.5254/rct.14.86920
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Source: Scopus
Source ID: 84907840430
Research output: Contribution to journal › Article › Scientific › peer-review

High-performance elastomeric strain sensors based on nanostructured carbon fillers for potential tire applications

For the development of intelligent vehicle tires, especially for future self-driving cars, suitable strain sensors are mandatory. The design of such a strain sensor must fulfil several criteria, most important of all, it must be easily mounted or implanted into the tire and the elastic nature of the sensors must be synchronized with the deformation behaviour of the tire. To our knowledge, we evaluate for the first time, the piezoresistive characteristics of a composite developed from tire rubber, taking into account the morphology (distribution and dispersion of the fillers), filler network structure, crosslinking density and the stiffness (hardness) of the rubber matrix. We use a commercially available synthetic solution polymerized styrene butadiene rubber (SSBR) which is widely used in modern car tire industries. As the internal structure of the filler particles can rearrange or alter during deformation, it is extremely important to study the piezo-resistive performance with respect to crosslinking density, hardness and modulus of the rubber composites in details. The present paper focusses on the development of strain sensors by exploiting conductive elastomeric composites based on SSBR with conducting carbon fillers like carbon black and carbon nanotubes. The sensors can be stretched to several hundred percent of their original length and a sensitivity could be achieved as much as ~1000 (gauge factor) in a given strain regime of ~100%, while maintaining the mechanical robustness. Some of the mechanical properties like tensile strength (~20 MPa), and modulus at 100% elongation are found to be quite satisfactory indicating the suitability of the materials for real applications.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Leibniz-Institut für Polymerforschung Dresden E.V., Vodafone Department of Mobile Communications Systems
Contributors: Bhagavatheswaran, E. S., Vaikuntam, S. R., Stöckelhuber, K. W., Wießner, S., Heinrich, G., Das, A.
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ASJC Scopus subject areas: Materials Science(all), Mechanics of Materials, Materials Chemistry
DOIs:

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Source: Scopus
Source ID: 85044867652
Research output: Contribution to journal › Article › Scientific › peer-review

Tribology of HVOF- and HVAF-sprayed WC-10Co4Cr hardmetal coatings: A comparative assessment

This paper provides a comprehensive assessment of the sliding and abrasive wear behaviour of WC-10Co4Cr hardmetal coatings, representative of the existing state-of-the-art. A commercial feedstock powder with two different particle size distributions was sprayed onto carbon steel substrates using two HVOF and two HVAF spray processes. Mild wear rates of $<10^{-7}$ mm^3/(Nm) and friction coefficients of ≈0.5 were obtained for all samples in ball-on-disk sliding wear tests at room temperature against Al_2O_3 counterparts. WC-10Co4Cr coatings definitely outperform a reference electrolytic hard chromium coating under these test conditions. Their wear mechanisms include extrusion and removal of the binder matrix, with the formation of a wavy surface morphology, and brittle cracking. The balance of such phenomena is closely related to intra-lamellar features, and rather independent of those properties (e.g. indentation fracture toughness, elastic modulus) which mainly reflect large-scale inter-lamellar cohesion, as quantitatively confirmed by a principal component analysis. Intra-lamellar dissolution of WC into the matrix indeed increases the incidence of brittle cracking, resulting in slightly higher wear rates. At 400°C, some of the hardmetal coatings fail because of the superposition between tensile residual stresses and thermal expansion mismatch stresses (due to the difference between the thermal expansion coefficients of the steel substrate and of the hardmetal coating). Those which do not fail, on account of lower residual stresses, exhibit higher wear rates than at room temperature, due to oxidation of the WC grains.The resistance of the coatings against abrasive wear, assessed by dry sand-rubber wheel testing, is related to inter-lamellar cohesion, as proven by a principal component analysis of the collected dataset. Therefore, coatings deposited from coarse feedstock powders suffer higher wear loss than those obtained from fine powders, as brittle inter-lamellar detachment is caused by their weaker interparticle cohesion, witnessed by their systematically lower fracture toughness as well.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Surface Engineering, Engineering materials science and solutions (EMASS), University West, Dipartimento di Ingegneria Enzo Ferrari, University of Modena and Reggio Emilia, Fraunhofer-Institut für Werkstoff- und Strahltechnik (IWS), Fraunhofer-Institut für Keramische Technologien und Systeme (IKTS), Institut für Korrosionsschutz Dresden GmbH
Contributors: Bolelli, G., Berger, L. M., Börner, T., Koivuluoto, H., Lusvarghi, L., Lyphout, C., Markocsan, N., Matikainen, V., Nylén, P., Sassatelli, P., Trache, R., Vuoristo, P.
Number of pages: 20
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Publication date: 15 Mar 2015
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Abrasive wear, Hardmetal, High velocity air-fuel (HVAF), High velocity oxy-fuel (HVOF), Sliding wear, WC-10Co4Cr
DOIs:

10.1016/j.surfcoat.2015.01.048
URLs:

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Source: Scopus
Source ID: 84925299473
Research output: Contribution to journal › Article › Scientific › peer-review

Sliding and abrasive wear behaviour of HVOF- and HVAF-sprayed Cr_3C_2-NiCr hardmetal coatings

This paper provides a comprehensive characterisation of HVOF- and HVAF-sprayed Cr_3C_2-25 wt.% NiCr hardmetal coatings. One commercial powder composition with two different particle size distributions was processed using five HVOF and HVAF thermal spray systems. All coatings contain less Cr_3C_2 than the feedstock powder, possibly due to the rebound of some Cr_3C_2-rich particles during high-velocity impact onto the substrate. Dry sand-rubber wheel abrasive wear testing causes both grooving and pull-out of splat fragments. Mass losses depend on inter- and intra-lamellar cohesion, being higher (≥70 mg after a wear distance of 5904 m) for the coatings deposited with the coarser feedstock powder or with one type of HVAF torch. Sliding wear at room temperature against alumina involves shallower abrasive grooving, small-scale delamination and carbide pull-outs, and it is controlled by intra-lamellar cohesion. The coatings obtained from the fine feedstock powder exhibit the lowest wear rates (≈5×10^{-6} mm^3/(Nm)). At 400 °C, abrasive grooving dominates the sliding wear behaviour; wear rates increase by one order of magnitude but friction coefficients decrease from ≈0.7 to ≈0.5. The thermal expansion coefficient of the coatings (11.08×10^{-6} $°C^{-1}$ in the 30-400 °C range) is sufficiently close to that of the steel substrate (14.23×10^{-6} $°C^{-1}$) to avoid macro-cracking.

General information

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Organisations: Department of Materials Science, Research group: Surface Engineering, University of Modena and Reggio Emilia, Fraunhofer Institut für Keramische Technologien und Systeme, Institut für Korrosionsschutz Dresden GmbH, University West, Fraunhofer Institut für Werkstoff- und Strahltechnik
Contributors: Bolelli, G., Berger, L. M., Börner, T., Koivuluoto, H., Matikainen, V., Lusvarghi, L., Lyphout, C., Markocsan, N., Nylén, P., Sassatelli, P., Trache, R., Vuoristo, P.
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces and Interfaces, Materials Chemistry, Surfaces, Coatings and Films, Mechanics of Materials
Keywords: Cermets, High temperature, Indentation, Sliding wear, Thermal spray coatings, Three-body abrasion
DOIs:

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Source: Scopus
Source ID: 84962802963
Research output: Contribution to journal › Article › Scientific › peer-review

Tribology of FeVCrC coatings deposited by HVOF and HVAF thermal spray processes

This work studies FeVCrC-based coatings as potential alternatives to conventional Ni- and Co-based alloys for wear protection. Specifically, the microstructure and tribological properties of the coatings are characterized as a function of the particle size distribution of the feedstock powder, of the deposition technique – High Velocity Oxygen-Fuel (HVOF) or High Velocity Air-Fuel (HVAF) spraying – and of specific processing parameters. HVOF-sprayed coatings obtained from fine feedstock powder exhibit numerous oxide inclusions, which provide high hardness (≈ 900 $HV_{0.3}$) but do not excessively impair fracture toughness, as determined through scratch testing techniques. HVAF-sprayed coatings obtained from the same feedstock powder contain much fewer oxide inclusions, and some of them possess simultaneously high hardness and high toughness. Defects (e.g. speckles) are instead formed in case unsuitable HVAF torch hardware is employed. A coarse feedstock powder always results in unmelted inclusions, which impair the cohesion of the coatings, particularly of the HVAF-sprayed ones. Most coatings anyway exhibit very low sliding wear rates < 3×10^{-6} mm^3/(N m); abrasive grooving and surface fatigue-induced pitting are the main wear mechanisms. Oxide inclusions do not affect negatively the response of HVOF coatings, whereas too many unmolten particles increase pitting under severe test conditions. Rubber-wheel abrasion testing produces comparatively more severe grooving.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Surface Engineering, Universita degli Studi di Modena e Reggio Emilia , ECOR Research SpA
Contributors: Bolelli, G., Bursi, M., Lusvarghi, L., Manfredini, T., Matikainen, V., Rigon, R., Sassatelli, P., Vuoristo, P.
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Publication date: 2018
Peer-reviewed: Yes
Early online date: 5 Nov 2017

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Journal: Wear
Volume: 394-395
ISSN (Print): 0043-1648
Ratings:

Scopus rating (2018): CiteScore 5.5 SJR 1.321 SNIP 2.035
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Coating: thermal spray coatings, Hardness, Sliding wear, Two-body abrasion
DOIs:

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Source: Scopus
Source ID: 85032352458
Research output: Contribution to journal › Article › Scientific › peer-review

Post operation inactivation of acidophilic bioleaching microorganisms using natural chloride-rich mine water
The H2020 BIOMOre project (www.biomore.info, Grant Agreement #642456) tests the feasibility of in situ bioleaching of copper in deep subsurface deposits in the Rudna mine, Poland. Copper is leached using biologically produced ferric iron solution, which is recycled back to the in situ reactor after re-oxidation by iron-oxidizing microorganisms. From a post operational point of view, it is important that the biological processes applied during the operation can be controlled and terminated. Our goal was to determine the possibility to use natural saline mine water for the inactivation of the introduced iron-oxidizing microorganisms remaining in the in situ reactor after completion of the leaching process of the ore block. Aerobic and anaerobic microcosms containing acid-leached (pH 2) sandstone or black shale from the Kupferschiefer in the Rudna mine were further leached with the effluent from a ferric iron generating bioreactor at 30 °C for 10 days to simulate the in situ leaching process. After the removal of the iron solution, residing iron-oxidizing microorganisms were inactivated by filling the microcosms with chloride-rich water (65 g L^{-1} Cl^-) originating from the mine. The chloride-rich water irreversibly inactivated the iron-oxidizing microorganisms and showed that the naturally occurring saline water of the mine can be used for long-term post process inactivation of bioleaching microorganisms

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, VTT Technical Research Centre of Finland
Contributors: Bomberg, M., Miettinen, H., Wahlström, M., Kaartinen, T., Ahoranta, S., Lakaniemi, A., Kinnunen, P.
Number of pages: 10
Pages: 236-245
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Peer-reviewed: Yes

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Journal: Hydrometallurgy
Volume: 180
ISSN (Print): 0304-386X
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Scopus rating (2018): CiteScore 5.7 SJR 1.014 SNIP 1.852
Original language: English
ASJC Scopus subject areas: Industrial and Manufacturing Engineering, Metals and Alloys, Materials Chemistry
Keywords: BIOMOre, in situ bioleaching, Inactivation, Iron-oxidizing bacteria, Quantitative PCR
DOIs:

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Source: Scopus
Source ID: 85051388591
Research output: Contribution to journal › Article › Scientific › peer-review

Porous polybutylene succinate films enabling adhesion of human embryonic stem cell-derived retinal pigment epithelial cells (hESC-RPE)
In the last decade, several studies have shown that polybutylene succinate (PBSu)has a high potential as a biomaterial enabling cell adhesion and growth. In this study, porous PBSu films have been prepared by the breath figure method (BF)and by particulate leaching (PL), and characterized in terms of thickness, surface properties, diffusion capacity and in

vitro stability. Because porous films are of high interest for tissue engineering of retinal pigment epithelium (RPE), the initial viability and adhesion of human embryonic stem cell-derived RPE onto the PBSu films was then evaluated. To the best of our knowledge, this is the first study on the adhesion behavior of hESC-RPE onto porous and biodegradable polymer surfaces. The results clearly demonstrated that the two manufacturing methods produced materials with very distinct properties. Films produced by BF expressively demonstrated the highest roughness and surface area, and the lowest water contact angle. These features likely contributed to increase the biocompatibility of the surface, particularly when coated with laminin and collagen IV, as observed by the improved cell viability, cell morphology, adhesion and production of extracellular matrix proteins. Altogether, our results showed not only that PBSu holds high potential in retinal tissue engineering, but also that the physical properties and biocompatibility of the material are highly dependent on the adopted casting method.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: BioMediTech, Tampere University, Tampere University Hospital
Contributors: Calejo, M. T., Haapala, A., Skottman, H., Kellomäki, M.
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Publication date: 1 Sep 2019
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Publication information
Journal: European Polymer Journal
Volume: 118
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Ratings:

Scopus rating (2019): CiteScore 6.1 SJR 0.864 SNIP 1.188
Original language: English
ASJC Scopus subject areas: Physics and Astronomy(all), Polymers and Plastics, Organic Chemistry, Materials Chemistry
Keywords: Biodegradable films, Breath figures, Cell adhesion, Polybutylene succinate, Retinal pigment epithelium
DOIs:

10.1016/j.eurpolymj.2019.05.041
URLs:

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Source: Scopus
Source ID: 85066269398
Research output: Contribution to journal › Article › Scientific › peer-review

Near-threshold high spin amplification in a 1300 nm GaInNAs spin laser

Using continuous-wave optical pumping of a spin-VCSEL at room temperature, we find high spin amplification of the pump close to threshold within the communications wavelength window, here at 1300 nm. This facilitates a strong switch from left to right circularly polarised light emission, which has potential applications in polarisation encoding for data communications. We use a simple spin flip model to fit the experimental results and discuss the VCSEL parameters that affect this amplification.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Photonics, Research group: ORC, Research group: Semiconductor Technology and Applications, University of Essex, University of Bristol
Contributors: Cemlyn, B., Adams, M., Harbord, E., Li, N., Henning, I. D., Oulton, R., Korpijärvi, V. M., Guina, M.
Publication date: 1 Aug 2018
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Issue number: 9
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Ratings:

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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Condensed Matter Physics, Electrical and Electronic Engineering, Materials Chemistry

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Source: Scopus
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Research output: Contribution to journal › Article › Scientific › peer-review

Role of fracture toughness in impact-abrasion wear

Two new low alloyed steels were developed with different fracture toughness values but at similar level of hardness with same composition and microstructural phase. The steels were subjected to impact-abrasion wear test. This work examines specifically the additional role of toughness during impact-abrasion wear, using a newly developed high toughness steel. Microstructural characterisation of the damaged samples revealed that better toughness helps resist both impact and abrasion damage.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Research group: Materials Characterization, Materials Science and Environmental Engineering, University of Cambridge, Tata Steel Ltd.
Contributors: Chintha, A. R., Valtonen, K., Kuokkala, V. T., Kundu, S., Peet, M. J., Bhadeshia, H. K.
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Abrasion, Fracture toughness, Impact-abrasion, Steel, Wear testing
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URLs:
http://urn.fi/URN:NBN:fi:tty-201906111888
Source: Scopus
Source ID: 85064619336
Research output: Contribution to journal › Article › Scientific › peer-review

Starch-poly(vinyl alcohol) barrier coatings for flexible packaging paper and their effects of phase interactions

Starch and poly(vinyl alcohol) based barrier coatings for flexible packaging papers were studied. Both octenyl succinate modified and hydroxypropylated corn and potato starches were blended with regular and ethylene modified poly(vinyl alcohol) to increase the water vapor barrier properties and enhance the flexibility of the starch coatings, in order to accomplish superior barrier performance. Phase separation between starch and poly(vinyl alcohol) was studied in detail, both in the solution and in dry draw-down coatings on paper. The barrier performance of the coated paper was evaluated with respect to water vapor transmission rate. Conditions for the creation of a thin surface layer consisting of only one of the pure polymers were identified and discussed in terms of phase separation in solution migration of poly(vinyl alcohol) to the uppermost surface layer. The phase separation promoted low water vapor transmission rates also with a rather high fraction of starch in the coatings.

General information

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MoE publication type: A1 Journal article-refereed

Organisations: Karlstad University
Contributors: Christophliemk, H., Ullsten, H., Johansson, C., Järnström, L.
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Ratings:

Scopus rating (2017): CiteScore 5.1 SJR 0.844 SNIP 1.334
Original language: English
ASJC Scopus subject areas: Chemical Engineering(all), Surfaces, Coatings and Films, Organic Chemistry, Materials Chemistry
Keywords: Barrier coating, PVOH, Starch, Turbidity, Viscosity, WVTR, XPS
DOIs:

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URLs:

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Source: Scopus
Source ID: 85019450052
Research output: Contribution to journal › Article › Scientific › peer-review

Oxygen and water vapor transmission rates of starch-poly(vinyl alcohol) barrier coatings for flexible packaging paper
Creating efficient water-borne dispersions based mainly on renewable materials for coating of flexible packaging paper was the aim of this study. The effects of an ethylene modified poly(vinyl alcohol) grade and a standard poly(vinyl alcohol) on the oxygen and water vapor barrier performance of corn starch and potato starch coatings was studied. The results showed that a coating composition with a high fraction of a renewable polymer was effective in keeping the oxygen barrier at a technically and commercially applicable level. An ethylene modified poly(vinyl alcohol) grade was found to provide lower oxygen transmission rates at high relative humidity, as compared to a standard poly(vinyl alcohol) grade. The oxygen barrier properties of blends of starch and poly(vinyl alcohol) were similar to that of the pure modified poly(vinyl alcohol) in the range from 0% starch to 60% starch. This was observed with both hydroxypropylated and octenyl succinate modified starch grades. The drying conditions of the mixed starch:poly(vinyl alcohol) coatings were based on drying trials with pure poly(vinyl alcohol) coatings. Drying at moderate temperatures indicated the possibility to slightly decrease water vapor transmission rate by higher drying temperature. Several secondary effects of increased drying temperature such as coating hold-out and formation of defects may also be of importance.

General information
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MoE publication type: A1 Journal article-refereed
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Contributors: Christophliemk, H., Johansson, C., Ullsten, H., Järnström, L.
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Original language: English
ASJC Scopus subject areas: Chemical Engineering(all), Surfaces, Coatings and Films, Organic Chemistry, Materials Chemistry
Keywords: Barrier coating, Drying, Oxygen transmission rate, Poly(vinyl alcohol), Starch, Water vapor transmission rate
DOIs:

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Research output: Contribution to journal › Article › Scientific › peer-review

Novel oxyfluorophosphate glasses and glass-ceramics

Effect of CaF_2 addition at the expense of CaO on the thermal, physical, optical and structural properties of glasses in the $NaPO_3$-CaO system was studied. The glasses were prepared by the conventional melt quenching method. For each glass, the thermal properties were studied by differential thermal analysis (DTA) and the optical properties by UV-Vis-NIR spectroscopy. The changes in the glass structure induced by the progressive replacement of CaO by CaF_2 were investigated using IR and Raman spectroscopies. The glasses were heat treated at 20 °C above their respective glass transition temperature for 17 h to form nuclei and then at their peak crystallization temperature for 1 h to grow the nuclei into crystals. An increase in the CaF_2 content increased the polymerization of the phosphate network leading to shift of the band gap to lower wavelength and reduced the crystallization tendency of the glasses. At least two crystalline phases precipitated in all the investigated glasses, the composition of which depended on the CaF_2 content. Finally, bulk crystallization was suspected to occur in the oxyfluorophosphate glasses.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Electronics and Communications Engineering, Research group: Biomaterials and Tissue Engineering Group, Abo Akademi University, University of Turku
Contributors: Cui, S., Massera, J., Lastusaari, M., Hupa, L., Petit, L.
Number of pages: 5
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Publication information

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Volume: 445-446
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Ceramics and Composites, Electronic, Optical and Magnetic Materials, Materials Chemistry
Keywords: Crystallization, Fluorophosphate glasses and glass-ceramics, Raman and IR spectroscopies, XRD
DOIs:

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Source: Scopus
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Research output: Contribution to journal › Article › Scientific › peer-review

Self-assembly of polystyrene-block-poly(4-vinylpyridine) block copolymer on molecularly functionalized silicon substrates: Fabrication of inorganic nanostructured etchmask for lithographic use

Block copolymers (BCPs) are seen as a possible cost effective complementary technique to traditional lithography currently used in the semiconductor industry. This unconventional approach has received increased attention in recent years as a process capable of facilitating the ever decreasing device size demanded. Control over microdomain orientation and enhancing long range order are key aspects for the utility of BCPs for future lithographic purposes. This paper provides an efficient route for the fabrication of highly ordered nanostructures suitable for such application. We investigate the significant effect of surface treatment regarding the self-assembly process of polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) by employing an ethylene glycol layer, producing well defined perpendicular P4VP cylinders with long range order over large surface areas. Nanopores are generated through surface reconstruction using a preferential solvent, which allows for the incorporation of an inorganic moiety. Treatment of this pattern with UV/Ozone leads to formation of well-ordered iron oxide nanodots with a pitch of ~26 nm. Furthermore, high aspect ratio silicon nanopillars result following pattern transfer (using Ar/O_2).

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Tyndall National Institute at National University of Ireland, Cork, Trinity College Dublin, University College Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN)
Contributors: Cummins, C., Borah, D., Rasappa, S., Chaudhari, A., Ghoshal, T., O'Driscoll, B. M. D., Carolan, P., Petkov, N., Holmes, J. D., Morris, M. A.
Number of pages: 11
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Volume: 1
Issue number: 47
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Materials Chemistry
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URLs:

http://www.scopus.com/inward/record.url?scp=84887902210&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84887902210
Research output: Contribution to journal › Article › Scientific › peer-review

A novel thermotropic elastomer based on highly-filled LDH-SSB composites
Elastomeric composites are prepared based on solution styrene butadiene elastomer and zinc-aluminium layered double hydroxides (LDH), using a conventional sulphur cure system. Up to 100 parts per hundred rubber of LDH are incorporated into the elastomer matrix. The composites exhibit an interesting phenomenon of thermoreversible transparency, i.e. the transparent sample becomes opaque at warm condition and restores the transparency at room temperature. The transparency is found to be increased as the amount of LDH was increased. The addition of LDH gradually improved the mechanical, dynamic mechanical performance and thermal stability of the base elastomer. These developped elastomers could be utilised as smart materials in different applications

General information
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Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V. , Vodafone Department of Mobile Communications Systems
Contributors: Das, A., George, J. J., Kutlu, B., Leuteritz, A., Wang, D. Y., Rooj, S., Jurk, R., Rajeshbabu, R., Stöckelhuber, K. W., Galiatsatos, V., Heinrich, G.
Number of pages: 6
Pages: 337-342
Publication date: 27 Feb 2012
Peer-reviewed: Yes

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Volume: 33
Issue number: 4
ISSN (Print): 1022-1336
Ratings:

Scopus rating (2012): CiteScore 7.9 SJR 2.096 SNIP 1.251
Original language: English
ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics
DOIs:

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URLs:

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Source: Scopus
Source ID: 84863149624
Research output: Contribution to journal › Article › Scientific › peer-review

Preparation of zinc oxide free, transparent rubber nanocomposites using a layered double hydroxide filler
A layered double hydroxide (LDH) mineral filler particle has been designed and employed in rubber vulcanization to prepare a more environmentally friendly rubber composite. The LDH delivers zinc ions in the vulcanization process as accelerators, stearate anions as activators and simultaneously the mineral sheets act as a nanofiller to reinforce the rubber matrix whilst totally replacing the separate zinc oxide (ZnO) and stearic acid conventionally used in the formulation of rubber. This method leads to a significant reduction (nearly 10 times) of the zinc level and yields excellent transparent properties in the final rubber product. The morphological characterization, rheometric curing behaviour, mechanical

properties and uniaxial multi-hysteresis behaviours of the resultant rubber/LDH nanocomposite are studied in this paper.

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MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V. , Durham University
Contributors: Das, A., Wang, D. Y., Leuteritz, A., Subramaniam, K., Greenwell, H. C., Wagenknecht, U., Heinrich, G.
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Source: Scopus
Source ID: 79955619174
Research output: Contribution to journal › Article › Scientific › peer-review

Naturally occurring amino acids: A suitable substitute of N-N/-di-phenyl guanidine (DPG) in silica tyre formulation?
N-N/-di-phenyl guanidine (DPG) in combination with cyclohexyl benzothiazole sulfenamide (CBS) is widely used as an accelerator for the vulcanization of silica filled solution styrene butadiene rubber (S-SBR). The vulcanizates thus obtained exhibit excellent mechanical properties, good dynamic properties and also good aging resistance property. However, the use of DPG is a bit restricted of late being reported to be a potent carcinogenic compound and, hence, the effective substitution for DPG by safe alternative has been extensively explored. In this study, we systematically study the effects of naturally occurring amino acid L-cystine (L-cys) and its derivative L-cystine dimethyl ester dihydrochloride (ELCH) as environmental friendly co-accelerators for the vulcanization of silicafilled S-SBR.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V.
Contributors: Debnath, S. C., Das, A., Basu, D., Heinrich, G.
Number of pages: 7
Pages: 25-31
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Publication information
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Volume: 66
Issue number: 1-2
ISSN (Print): 0948-3276
Ratings:

Scopus rating (2013): CiteScore 0.6 SJR 0.207 SNIP 0.487
Original language: English
ASJC Scopus subject areas: Mechanical Engineering, Industrial and Manufacturing Engineering, Materials Chemistry, Polymers and Plastics
Keywords: L-cystine, N-N/-di-phenyl guanidine, Silica, Solution styrene butadiene rubber, Vulcanization
URLs:

http://www.scopus.com/inward/record.url?scp=84874674495&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84874674495
Research output: Contribution to journal › Article › Scientific › peer-review

Novel borosilicate bioactive scaffolds with persistent luminescence

Persistent luminescent amorphous borosilicate scaffolds were successfully prepared, for the first time, with a porosity of >70% using the burn-off technique. The persistent luminescence was obtained by adding the $SrAl_2O_4:Eu^{2+},Dy^{3+}$ microparticles: i) in the glass melt or ii) in the glass crushed into powder prior to the sintering. The scaffolds prepared by adding the microparticles in the glass melt exhibits lower persistent luminescence and a slower reaction rate in simulated body fluid than the scaffolds prepared by adding the microparticles in the glass powder due to the release of strontium from the microparticles into the glass during the glass melting.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: BioMediTech, Research group: Biomaterials and Tissue Engineering Group, Physics, Research group: Photonics Glasses, Turun yliopisto
Contributors: Del Cerro, P. R., Teittinen, H., Norrbo, I., Lastusaari, M., Massera, J., Petit, L.
Number of pages: 9
Pages: 1-9
Publication date: 2020
Peer-reviewed: Yes

Publication information

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Issue number: 1
ISSN (Print): 2299-3932
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Ceramics and Composites, Surfaces, Coatings and Films, Materials Chemistry
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Electronic versions:

Novel borosilicate bioactive scaffolds 2020
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URLs:

http://urn.fi/URN:NBN:fi:tuni-202008066397

Bibliographical note

INT=phys,"Del Cerro, Paloma Roldan"
INT=bmte,"Teittinen, Henriikka"
Source: Scopus
Source ID: 85085038962
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of surface morphology of poly(ïµ-caprolactone) scaffolds on adipose stem cell adhesion and proliferation

Summary The effect of the surface morphology of flat poly(Ïµ- caprolactone) (PCL) scaffolds on human adipose stem cell (hASC) adherence and proliferation was studied. During fabrication of the scaffolds by phase inversion, the employment of different non-solvents (water (W), ethanol (EtOH) or isopropanol (IPA)) led to distinct surface morphologies. It was found that PCL scaffolds fabricated using IPA as a non-solvent had a higher roughness and porosity compared to the other groups. Moreover, during culturing of hASCs under static conditions, best cell attachment, spreading and growth were observed on the PCL scaffold. Our results show the potential of PCL scaffolds prepared using IPA as a non-solvent for especially soft tissue engineering applications.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), University of Twente, University of Groningen
Contributors: Diban, N., Haimi, S. P., Bolhuis-Versteeg, L., Teixeira, S., Miettinen, S., Poot, A. A., Grijpma, D. W., Stamatialis, D.
Number of pages: 7
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Original language: English
ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Condensed Matter Physics
Keywords: morphology, phase inversion, poly(Ìµ-caprolactone), roughness, scaffold porosity
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Research output: Contribution to journal › Article › Scientific › peer-review

Lubricated icephobic coatings prepared by flame spraying with hybrid feedstock injection
Lubricated icephobic coatings were fabricated by flame spraying with hybrid feedstock injection. In this one-step process, composite coatings were produced by spraying a matrix material from a combustion flame spray gun and a lubricating additive from an injector, externally to the flame. External injection avoided possible thermal degradation of the heat sensitive additive during spraying. Inexpensive and widely available feedstock materials were used, polyethylene as the matrix and solid cottonseed oil as the lubricating additive. The coating properties were investigated by thermal and chemical analyses, surface roughness and wettability measurements at room temperature and in cold conditions. The icephobic behaviour was evaluated by accreting ice from supercooled water droplets in the icing wind tunnel. Ice adhesion was measured by the centrifugal ice adhesion test. The results showed that lubricant addition improved the icephobic performance of the coatings. Moreover, cooling the flame temperature with compressed air addition reduced thermal degradation of polymers. This was beneficial for the icephobic behaviour, thus lowering the shear ice adhesion strength down to 23 kPa ± 6 kPa. In conclusion, lubricated icephobic coatings were successfully produced by combining the hybrid feedstock injection and the thorough optimization of process parameters. This approach provides a potential surface engineering solution for the industrial sectors facing icing problems.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Surface Engineering, Research group: Plastics and Elastomer Technology
Contributors: Donadei, V., Koivuluoto, H., Sarlin, E., Vuoristo, P.
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Surfaces and Interfaces, Materials Chemistry, Condensed Matter Physics
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URLs:

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Source ID: 85090860951
Research output: Contribution to journal › Article › Scientific › peer-review

First principles prediction of the solar cell efficiency of chalcopyrite materials $AgMX_2$(M=In, Al; X=S, Se, Te)

Using the spectroscopic limited maximum efficiency, and Shockley and Queisser predictor models, we compute the solar efficiency of the chalcopyrites $AgMX_2$(M = In, Al; X = S, Se, Te). The results presented are based on the estimation of the electronic and optical properties obtained from first principles density functional theory as well as the many-body perturbation theory calculations. The results from this report were consistent with the experimental data.The optical bandgap was accurately estimated from the absorption spectra, obtained by solving the Bethe and Salpeter equation. Fitting the Tauc's plot on the absorption spectra, we also predicted that the materials studied have a direct allowed optical transition. The theoretical estimations of the solar cell performance showed that the efficiencies from the Shockley and Queisser model are higher than those from the spectroscopic limited maximum efficiency model. This improvement is attributed to the absorption, the recombination processes and the optical transition accounted in the calculation of the efficiency.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Electrical Engineering, University of South Africa, University of Witwatersrand
Contributors: Dongho-Nguimdo, G. M., Igumbor, E., Zambou, S., Joubert, D. P.
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ISSN (Print): 2352-2143
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Scopus rating (2019): CiteScore 1.7 SJR 0.341 SNIP 0.706
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Materials Science (miscellaneous), Condensed Matter Physics, Materials Chemistry
Keywords: Chalcopyrites, First principles, Solar cell efficiency
DOIs:

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Electronic transport in n-type modulation-doped AlGaAs/GaAsBi quantum well structures: Influence of Bi and thermal annealing on electron effective mass and electron mobility

We investigate electronic transport properties of as-grown and annealed n-type modulation-doped $Al_{0.15}Ga_{0.85}As/GaAs_{1-x}Bi_x$ ($x = 0$ and 0.04) quantum well (QW) structures using magnetotransport measurements in the temperature range 4.2 K and 60 K and at magnetic fields up to 18 T. Thermal annealing process was applied at two different temperatures, 700 °C and 350 °C during 60 s and 180 s, respectively. We find that electron effective mass and 2D electron density in as-grown Bi-containing sample are slightly lower than that in Bi-free one. Furthermore, quantum electron mobility and quantum scattering time are observed to be decreased in Bi-containing samples. The annealing process at 700 °C causes a slight increase in electron effective mass and 2D electron density. A negligible decrease in electron effective mass and an increase in 2D electron density are determined following annealing at 350 °C. The observed change in electron effective mass following thermal annealing process is attributed to changing 2D electron density in the samples. No improvement on quantum electron mobility and quantum scattering time are observed following thermal annealing at both process temperatures. We determine that one electron subband (e1) for as-grown and annealed (at 700 °C for 60 s) Bi-containing QWs and two electron subbands (e1 and e2) for the annealed (at 350 °C for 180 s) GaAsBi QW sample and the Bi-free QW sample contribute to electronic transport. Our results reveal that there is no significant direct effect of Bi on effective electron mass, but an indirect effect, in which Bi can provoke changes in 2D electron density and hence causes not to observe actual band-edge electron mass but a deviation from its band-edge value. Therefore, it can be concluded that dispersion curve of conduction band does not change as an effect of Bi incorporation in GaAs.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Physics, Istanbul University, Eskişehir Technical University (ESTU), Istanbul University-Cerrahpasa
Contributors: Donmez, O., Aydin, M., Ardali, Yildirim, S., Tiraş, E., Nutku, F., Cetinkaya, C., okduygulular, E., Puustinen, J. , Hilska, J., Guina, M., Erol, A.
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Article number: 025009
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Condensed Matter Physics, Electrical and Electronic Engineering, Materials Chemistry
Keywords: bismuthindependent effective mass, Electron effective mass in GaAsBi, electron mobility in GaAsBi, electronic transport in GaAsBi, n-type GaAsBi
DOIs:
10.1088/1361-6641/ab5d8d
Source: Scopus
Source ID: 85082305824
Research output: Contribution to journal › Article › Scientific › peer-review

Power loss mechanisms in n-type modulation-doped AlGaAs/GaAsBi quantum well heterostructures
We report on the power loss mechanisms of hot electrons in as-grown and annealed n-type modulation-doped Al0.15Ga0.85As/GaAs1-xBix (x = 0 and 0.04) quantum well structures considering acoustic phonon interactions via the deformation potential (non-polar) and piezoelectric (polar) scatterings. The two-dimensional (2D) electron gas is heated by applying various electric fields under a steady-state magnetic field, and the effect of the applied electric field on the Shubnikov de Haas (SdH) oscillations is analyzed to investigate the power loss mechanism. The temperature of hot electrons (T e) has been obtained by comparing the lattice temperature and applied electric field dependencies of the SdH oscillation amplitude. The hot electron temperature is almost the same for both Bi-free and Bi-containing samples except for the sample annealed at a higher temperature (700 °C) than the growth temperature of GaAsBi. The electron temperature dependence of power loss is analyzed using current theoretical analytic models derived for 2D semiconductors. We find that energy relaxation occurs in the intermediate temperature regime, including mixing of piezoelectric and deformation potential scattering. The power loss of hot electrons is found to be proportional to (Teγ-TLγ) with γ in the range from 2.4 to 4.2, which indicates that the hot electron relaxation is due to acoustic phonon scatterings via unscreened deformation potential and piezoelectric scattering. It is found that deformation potential scattering is dominant over piezoelectric scattering in the Bi-free sample, while the incorporation of Bi into the GaAs lattice makes these processes comparable. After thermal annealing at lower than growth temperature (350 °C), the scattering mechanism switches from deformation potential to piezoelectric scattering. After thermal annealing at higher than growth temperature (700 °C), the theoretical model does not fit to the experimental results due to degradation of the sample.

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Organisations: Physics, Research group: ORC, Istanbul University, Eskişehir Technical University (ESTU)
Contributors: Donmez, O., Aydin, M., Ardali, Yildirim, S., Tiraş, E., Erol, A., Puustinen, J., Hilska, J., Guina, M.
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Article number: 095038
ISSN (Print): 0268-1242
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Condensed Matter Physics, Electrical and Electronic Engineering, Materials Chemistry
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Source: Scopus
Source ID: 85090446844
Research output: Contribution to journal › Article › Scientific › peer-review

Efficient photon upconversion at remarkably low annihilator concentrations in a liquid polymer matrix: when less is more
A green-to-blue triplet-triplet annihilation upconversion of 24.5% quantum yield was achieved at a remarkably low 600 μM annihilator concentration in a viscous polymer matrix. This was made possible by utilizing a ZnTPP-based photosensitizer with exceptionally long 11 ms phosphorescence lifetime. Higher 3 mM annihilator concentration resulted in lower 24%

upconversion quantum yield.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering
Contributors: Durandin, N. A., Isokuortti, J., Efimov, A., Vuorimaa-Laukkanen, E., Tkachenko, N. V., Laaksonen, T.
Number of pages: 4
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Publication date: 2018
Peer-reviewed: Yes

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Journal: Chemical Communications
Volume: 54
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ISSN (Print): 1359-7345
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Original language: English
ASJC Scopus subject areas: Catalysis, Electronic, Optical and Magnetic Materials, Ceramics and Composites, Chemistry(all), Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
Keywords: triplet-triplet annihilation, triplet-triplet energy transfer, triplet state lifetime, upconversion, triplet fusion
Electronic versions:

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Source: Scopus
Source ID: 85058301188
Research output: Contribution to journal › Article › Scientific › peer-review

PEGylated liposomes as carriers of hydrophobic porphyrins
Sterically stabilized liposomes (SSLs) (PEGylated liposomes) are applied as effective drug delivery vehicles. Understanding the interactions between hydrophobic compounds and PEGylated membranes is therefore important to determine the effectiveness of PEGylated liposomes for delivery of drugs or other bioactive substances. In this study, we have combined fluorescence quenching analysis (FQA) experiments and all-atom molecular dynamics (MD) simulations to study the effect of membrane PEGylation on the location and orientation of 5,10,15,20-tetrakis(4-hydroxyphenyl)porphyrin (p-THPP) that has been used in our study as a model hydrophobic compound. First, we consider the properties of p-THPP in the presence of different fluid phosphatidylcholine bilayers that we use as model systems for protein-free cell membranes. Next, we studied the interaction between PEGylated membranes and p-THPP. Our MD simulation results indicated that the arrangement of p-THPP within zwitterionic membranes is dependent on their free volume, and p-THPP solubilized in PEGylated liposomes is localized in two preferred positions: deep within the membrane (close to the center of the bilayer) and in the outer PEG corona (p-THPP molecules being wrapped with the polymer chains). Fluorescence quenching methods confirmed the results of atomistic MD simulations and showed two populations of p-THPP molecules as in MD simulations. Our results provide both an explanation for the experimental observation that PEGylation improves the drug-loading efficiency of membranes and also a more detailed molecular-level description of the interactions between porphyrins and lipid membranes.

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Organisations: Department of Physics, Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), University of Cambridge, Faculty of Physics and Chemistry, Helsinki University, University of Southern Denmark, Jagiellonian University, Centre for Drug Research, Faculty of Pharmacy
Contributors: Dzieciuch, M., Rissanen, S., Szydłowska, N., Bunker, A., Kumorek, M., Jamróz, D., Vattulainen, I., Nowakowska, M., Róg, T., Kepczynski, M.
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Issue number: 22
ISSN (Print): 1520-6106
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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
DOIs:

10.1021/acs.jpcb.5b01351
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Source ID: 84930960276
Research output: Contribution to journal › Article › Scientific › peer-review

Exploring the role of stearic acid in modified zinc aluminum layered double hydroxides and their acrylonitrile butadiene rubber nanocomposites

The proposed study attempted to explore the role of stearic acid modification on the properties of zinc-aluminum based layered double hydroxides (LDH) and their composites with acrylonitrile butadiene rubber (NBR). Three distinctive LDH systems were adapted for such comparison; an unmodified LDH and two stearic acid modified LDH. The use of zinc oxide and stearic acid in the rubber formulation was avoided as the modified LDH would be able to deliver the necessary activators for the vulcanization process. Emphasis was predominantly given to reconnoiter the merits of stearic acid modification on the increase in interlayer distance of the LDH. X-ray diffraction studies and transmission electron microscope morphological investigations of LDH powders indicated that modification with stearic acid increased the interlayer spacing which would favor the intercalation of NBR polymer chains into the layered space. However, stress-strain studies indicated better mechanical properties for composites with unmodified LDH. Composites with LDH showed higher crosslinking densities than conventionally sulfur cured control compounds using zinc oxide/stearic acid as activators. This was evident from equilibrium swelling method as well as statistical theory of rubber elasticity.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Vodafone Department of Mobile Communications Systems, Leibniz-Institut für Polymerforschung Dresden E.V., Technische Universität Dresden, Rubber Technology Centre, Indian Institute of Technology Kharagpur
Contributors: Eshwaran, S. B., Basu, D., Vaikuntam, S. R., Kutlu, B., Wiessner, S., Das, A., Naskar, K., Heinrich, G.
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Article number: 41539
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry
Keywords: crosslinking, elastomers, mechanical properties, properties and characterization, rubber
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Stearate Modified Zinc-Aluminum Layered Double Hydroxides and Acrylonitrile Butadiene Rubber Nanocomposites

The aim of this investigation is to highlight the potentials of layered double hydroxides (LDH) and to serve as a replacement for zinc oxide and stearic acid from the basic rubber formulation. This will eventually result in about a 10× significant reduction of Zn^{2+} ion concentration in the final compound. The unique advantage of stearate ion-modified LDH is the delivery of zinc ions to accelerate and stearate ions to activate the vulcanization process. Furthermore, it can also reinforce the rubber matrix by virtue of its layered structure as nanofiller.

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Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Vodafone Department of Mobile Communications Systems, Leibniz-Institut für Polymerforschung Dresden E.V., Rubber Technology Centre, Indian Institute of Technology Kharagpur
Contributors: Eshwaran, S. B., Basu, D., Kutlu, B., Leuteritz, A., Wagenknecht, U., Stöckelhuber, K. W., Naskar, K., Das, A., Heinrich, G.
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ASJC Scopus subject areas: Polymers and Plastics, Materials Science (miscellaneous), Chemical Engineering(all), Materials Chemistry
Keywords: Layered double hydroxide, Nitrile rubber, Sulfur vulcanization, Zinc oxide
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Sulfonated polyetheretherketone/polypropylene polymer blends for the production of photoactive materials
Sulfonated polyetheretherketone (SPEEK) was synthesized via a mono-substitution reaction of PEEK in concentrated sulphuric acid and was blended with polypropylene (PP) in 2-10%w/w concentration to be used for the production of photoactive thermoplastic products. SPEEK and SPEEK/PP blends were characterized using FTIR, DSC, TGA, NMR, rheology, SEM, and EPR. Under UV-Vis irradiation, stable benzophenone ketyl (BPK) radicals were generated by hydrogen extraction from PP. By increasing the amount of SPEEK in the polymer blend a linear increase in the BPK radicals was achieved according to the EPR data. DSC and TGA tests indicated weaknesses in the thermal stability of SPEEK but according to the rheological tests this should not have a major effect on processabililty. The optimal amount of SPEEK in the blend was obtained at 5%w/w. This concentration provided a good compromise between radical concentration, material processability, and cost.

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Organisations: Department of Materials Science
Contributors: Fatarelle, E., Mylläri, V., Ruzzante, M., Pogni, R., Baratto, M. C., Skrifvars, M., Syrjälä, S., Järvelä, P.
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ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)
Keywords: Blends, Photochemistry, Polyolefins
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Research output: Contribution to journal › Article › Scientific › peer-review

Structure and Dynamics of Thermosensitive pDNA Polyplexes Studied by Time-Resolved Fluorescence Spectroscopy

Combining multiple stimuli-responsive functionalities into the polymer design is an attractive approach to improve nucleic acid delivery. However, more in-depth fundamental understanding how the multiple functionalities in the polymer structures are influencing polyplex formation and stability is essential for the rational development of such delivery systems. Therefore, in this study the structure and dynamics of thermosensitive polyplexes were investigated by tracking the behavior of labeled plasmid DNA (pDNA) and polymer with time-resolved fluorescence spectroscopy using fluorescence resonance energy transfer (FRET). The successful synthesis of a heterofunctional poly(ethylene glycol) (PEG) macroinitiator containing both an atom transfer radical polymerization (ATRP) and reversible addition-fragmentation chain-transfer (RAFT) initiator is reported. The use of this novel PEG macroinitiator allows for the controlled polymerization of cationic and thermosensitive linear triblock copolymers and labeling of the chain-end with a fluorescent dye by maleimide-thiol chemistry. The polymers consisted of a thermosensitive poly(N-isopropylacrylamide) (PNIPAM, N), hydrophilic PEG (P), and cationic poly(2-(dimethylamino)ethyl methacrylate) (PDMAEMA, D) block, further referred to as NPD. Polymer block D chain-ends were labeled with Cy3, while pDNA was labeled with FITC. The thermosensitive NPD polymers were used to prepare pDNA polyplexes, and the effect of the N/P charge ratio, temperature, and composition of the triblock copolymer on the polyplex properties were investigated, taking nonthermosensitive PD polymers as the control. FRET was observed both at 4 and 37 °C, indicating that the introduction of the thermosensitive PNIPAM block did not compromise the polyplex structure even above the polymer's cloud point. Furthermore, FRET results showed that the NPD- and PD-based polyplexes have a less dense core compared to polyplexes based on cationic homopolymers (such as PEI) as reported before. The polyplexes showed to have a dynamic character meaning that the polymer chains can exchange between the polyplex core and shell. Mobility of the polymers allow their uniform redistribution within the polyplex and this feature has been reported to be favorable in the context of pDNA release and subsequent improved transfection efficiency, compared to nondynamic formulations.

General information

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Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials, Utrecht University, Helsinki University, Chemistry and Advanced Materials
Contributors: Fliervoet, L. A., Lisitsyna, E. S., Durandin, N. A., Kotsis, I., Maas-Bakker, R. F., Yliperttula, M., Hennink, W. E., Vuorimaa-Laukkanen, E., Vermonden, T.
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Source ID: 85073002500
Research output: Contribution to journal › Article › Scientific › peer-review

Biomimetic surface modification of polycarbonateurethane film via phosphorylcholine-graft for resisting platelet adhesion

Phosphorylcholine groups were covalently introduced onto a polycarbonateurethane (PCU) surface in order to create a biomimetic structure on the polymer surfaces. After introducing primary amine groups onto the polymer surface by 1,6-hexanediamine, phosphorylcholine groups were covalently linked onto the surface by the reductive amination between the amino group and the aldehyde group of phosphorylcholine glyceraldehyde (PCGA). The results of water contact angle

test, X-ray photoelectron spectroscopy (XPS), and X-ray fluorescence spectrometer (XRF) analysis of the modified films indicated that PCGA had already been covalently linked to the PCU surface. The topographies and surface roughnesses were both imaged and measured by atomic force microscopy (AFM). Scanning electron microscopy (SEM) observation of the PCU films after treatment with platelet-rich plasma demonstrated that platelets had rarely adhered to the surface of the PCGA-grafted PCU films but had mainly adhered to the surface of the blank PCU films. The platelet adhesion result indicated that the PC modified PCU films could resist platelet adhesion after grafting with PCGA, and that these PCGA-grafted PCU materials, potentially, might be applied as blood-contacting materials.

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MoE publication type: A1 Journal article-refereed
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Tianjin University, School of Chemical Engineering and Technology
Contributors: Gao, W., Feng, Y., Lu, J., Khan, M., Guo, J.
Number of pages: 7
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Peer-reviewed: Yes

Publication information
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Volume: 20
Issue number: 10
ISSN (Print): 1598-5032
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Original language: English
ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Chemical Engineering(all)
Keywords: Biomimetic, Phosphorylcholine glyceraldehydes, Platelet adhesion, Polycarbonateurethane, Surface modification
DOIs:

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Source: Scopus
Source ID: 84867230066
Research output: Contribution to journal › Article › Scientific › peer-review

Human adipose stem cells in chondrogenic differentiation medium without growth factors differentiate towards annulus fibrosus phenotype in vitro
Summary Intervertebral disc degeneration is the main cause of chronic back pain. Disc degeneration mainly leads to tearing of annulus fibrosus (AF), which is with current methods difficult to restore and impossible to regenerate. Stem cell technology offers a potential technique to repair the ruptured AF by enabling new matrix synthesis at the defect site. Previous studies have shown that human adipose stem cells (hASCs) are able to differentiate towards AF phenotype when treated with suitable growth factors. There are concerns about the use of growth factors in clinical applications because of their short half-lives, high costs and low effectiveness. The main aim of this research project was to regenerate AF tissue in vitro using hASCs and serum free chondrogenic medium without supplementation of growth factors. Differentiation of hASCs was induced by using the micromass culture technique. Human annulus fibrosus cell (hAFCs) cultured in commercial AF growth medium were used as positive control. Assessment of AF phenotype of hASCs and hAFCs was done at 14 and 21 days of culture. Quantification of sulphated glycosaminoglycan (GAG) content showed that hASCs cultured in chondrogenic medium expressed similar levels of sulphated GAGs as hAFCs. qRT-PCR confirmed the similarity of the differentiated hASCs with AF phenotype. Several markers for AF phenotype (aggrecan, collagen type I and glypican-3) were expressed in both hAFCs and differentiated hASCs. This is the first study that demonstrated that hASCs can be differentiated towards AF phenotype using serum free chondrogenic medium without growth factors. In a next step, scaffolds manufactured from biodegradable polymers will be used in combination with ASCs to find an optimal construct to repair AF defects.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), University of Twente, University of Groningen
Contributors: Gebraad, A. W. H., Miettinen, S., Grijpma, D. W., Haimi, S. P.
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Original language: English
ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Condensed Matter Physics
Keywords: adipose stem cells, annulus fibrosus, intervertebral disc, tissue engineering
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Source: Scopus
Source ID: 84890722713
Research output: Contribution to journal › Article › Scientific › peer-review

Proliferation and differentiation of adipose stem cells towards smooth muscle cells on poly(trimethylene carbonate) membranes
Summary Multipotent human adipose stem cells (hASCs) are an abundant and potential source of cells for vascular tissue engineering when combined with a suitable biomaterial scaffold. Poly(trimethylene carbonate) (PTMC) has been shown to be a useful biodegradable material for tissue engineered vascular grafts due to its flexibility, excellent biocompatibility and enzymatic degradation by surface erosion in vivo. The purpose of the current study was to evaluate the proliferation and differentiation of hASCs towards smooth muscle cells (SMCs) on gamma-crosslinked and photo-crosslinked PTMC membranes. PTMC macromers were functionalized with methacrylate end groups and crosslinked by UV initiated radical polymerization. High molecular weight linear PTMC was crosslinked by gamma irradiation. Cell viability, cell numbers and SMC differentiation of hASCs were evaluated on the differently crosslinked PTMC films at 7 and 14 days (d). On the photo-crosslinked membranes, homogenous monolayers of hASC were detected by live/dead assay. Consistently, cells on the photo-crosslinked membranes had significantly higher cell numbers compared to cells on the gamma-crosslinked membranes after 14 d of culture. SMC specific genes were expressed on both membranes at 14 d. Photo-crosslinked membranes showed higher expression of SMC specific proteins at 14 d compared to gamma-crosslinked membranes. These results suggest that especially the photo-crosslinked PTMC membranes are suitable for vascular tissue engineering applications when combined with hASCs.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Aachen University of Applied Sciences, University of Groningen
Contributors: German, S. J., Behbahani, M., Miettinen, S., Grijpma, D. W., Haimi, S. P.
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Keywords: adipose stem cell differentiation, poly (trimethylene carbonate), smooth muscle cells, tissue engineering
DOIs:

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Source: Scopus

Source ID: 84890729494
Research output: Contribution to journal › Article › Scientific › peer-review

Damage mechanisms and cracking behavior of thermal sprayed WC-CoCr coating under scratch testing

Evaluation of wear mechanisms of thick thermal sprayed cermet coatings is a challenging endeavor given the numerous process-induced structural and chemical changes as well as presence of residual stresses. In an effort to understand the damage processes under contact load and their sensitivity to the process induced microstructural attributes, controlled scratch testing was used. Detailed assessment of the resultant damage zone provided repeatable cracking patterns that are categorized as (i) Localized collapsing of material, (ii) angular cracks, (iii) primary semi-circular and developed semi-circular cracks and (iv) splat delamination. A correlation was established by linking observed damage mechanisms to the process induced microstructural descriptions including role of spray particle conditions and residual stresses. Quantitative correlations between delamination load for cracking and the process induced variable including particle properties as described by the non-dimensional melting index concept as well as residual stresses were established. Melting index captures the combined effect of particles[U+05F3] thermal and kinetic history and thus coating porosity and the process induced decarburization. The results highlight the critical role of coating density and stress evolution during the coating formation. The research points to scratch testing as a powerful evaluation method to characterize contact response of thick thermal spray cermet coatings including operative mechanisms.

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Organisations: Engineering materials science and solutions (EMASS), Thermal Spray Advance Research Team, VTT Technical Research Centre of Finland, Stony Brook University State University of New York, Center for Thermal Spray Research
Contributors: Ghabchi, A., Sampath, S., Holmberg, K., Varis, T.
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Original language: English
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Keywords: Damage mechanism, Scratch test, Sliding wear, Thermal spray coating
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Research output: Contribution to journal › Article › Scientific › peer-review

HVOF process control enabling strategies

Complexity in dynamics and mechanism of supersonic flame formation and effects of processing variables has made the understanding of interaction of particles and flame a difficult task. Lack of such understanding limits the possibilities of controlling the process to obtain desired in-flight particles temperature and velocity and consequent particles state. This problem is even more pronounced in TS systems with no dedicated decoupled temperature and velocity controlled regime. Different approaches based on total volume flow, back pressure and fuel to oxygen ratio have been examined to address the robustness of each approach to control the temperature and velocity. WC-CoCr material was used employing DJ-2600 torch. A guideline to control the in-flight particles temperature and velocity based on process variables is provided. A process map was developed to establish a correlation between process, in-flight particles state, microstructure, properties and performance.

General information

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MoE publication type: A4 Article in a conference publication
Organisations: Engineering materials science and solutions (EMASS), Thermal Spray Advance Research Team, VTT Technical Research Centre of Finland, Center for Thermal Spray Research

Contributors: Ghabchi, A., Varis, T., Holmberg, K., Sampath, S.
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ISBN (Print): 9781632666796
ASJC Scopus subject areas: Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces
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Source ID: 84907084172
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

Towards universal enrichment nanocoating for IR-ATR waveguides
Polymer multilayered nanocoating capable of concentrating various chemical substances at IR-ATR waveguide surfaces is described. The coating affinity to an analyte played a pivotal role in sensitivity enhancement of the IR-ATR measurements, since the unmodified waveguide did not show any analyte detection.

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MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Clemson University, School of Materials Science and Engineering/COMSET, University of Delaware, Massachusetts Institute of Technology
Contributors: Giammarco, J., Zdyrko, B., Petit, L., Musgraves, J. D., Hu, J., Agarwal, A., Kimerling, L., Richardson, K., Luzinov, I.
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Original language: English
ASJC Scopus subject areas: Catalysis, Electronic, Optical and Magnetic Materials, Ceramics and Composites, Chemistry(all), Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
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Source: Scopus
Source ID: 79961012632
Research output: Contribution to journal › Article › Scientific › peer-review

Better understanding of the role of SiO_2, P_2O_5 and Al_2O_3 on the spectroscopic properties of Yb^{3+} doped silica sol-gel glasses
Yb^{3+} doped silica sol-gel glass powders were prepared with different concentrations of SiO_2, Al_2O_3 and P_2O_5 in order to understand the impact of the glass composition on the Yb^{3+} emission properties. In this paper, we clearly show that not only the Al/P ratio but also the SiO_2 content have an impact on the Yb^{3+} spectroscopic properties. Our results provide new insight on the real impact of the composition on the spectroscopic properties of Yb^{3+} doped sol-gels: we demonstrate that an increase in the Al_2O_3 content at the expense of P_2O_5 leads to an increase in the intensity of the emission at 1000nm of the Yb^{3+} ions whereas an increase in the SiO_2 content decreases it. We clearly showed that the inexpensive sol-gel approach can be easily used when investigating new Yb^{3+} doped silica glasses.

General information
Publication status: Published

MoE publication type: A1 Journal article-refereed
Organisations: Photonics, Research group: Nanophotonics, Faculty of Biomedical Sciences and Engineering, Research group: Biomaterials and Tissue Engineering Group, Research group: Photonics Glasses, Institut de Chimie de la Matiere Condensee de Bordeaux, Turun Yliopisto/Turun Biomateriaalikeskus
Contributors: Glorieux, B., Salminen, T., Massera, J., Lastusaari, M., Petit, L.
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Ceramics and Composites, Condensed Matter Physics, Materials Chemistry
Keywords: Silica glass, Sol-gel, Spectroscopic properties, Yb doping
DOIs:

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Source: Scopus
Source ID: 85037629421
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of head group size on the photoswitching applications of azobenzene Disperse Red 1 analogues
We investigate the effect of the increased molecular bulk in the 'head' group for a class of newly synthesized azobenzene chromophores with a clickable ethynyl group para and a nitro group ortho to the azo bond on the distal benzene ring. This 'variable-head' functionalization provides a family of dyes with photophysical characteristics very similar to those of Disperse Red 1, one of the most commonly used azo dyes in materials science. Phenyl, naphthyl, and anthracyl derivatives were synthesized as small molecules, monomers, homopolymers, and copolymers in a rapid and facile manner using click chemistry, confirming the versatility of this parent chromophore. Photochemical and spectral studies indicate that this strategy is suitable to build a 'bulkiness series' of stimuli-responsive materials, as the various material derivatives retain the absorption and kinetic characteristics of the parent chromophore necessary for all optical patterning applications that DR1 dyes have been optimized for. In thin films, larger head group size was found to increase the stability of light-induced birefringence in copolymers. The homopolymers formed stable surface-relief gratings upon interference irradiation, whose grating depths correlate with head group size, demonstrating that this new class of polymers can also undergo tailored macroscopic photoinduced motions, which could have applications in all optical nano-patterning.

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MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Humboldt-Universität zu Berlin, McGill University, Aalto University
Contributors: Goulet-Hanssens, A., Corkery, T. C., Priimagi, A., Barrett, C. J.
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Volume: 2
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Materials Chemistry
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Source: Scopus
Source ID: 84906539664

The effects of laser patterning 10CeTZP-Al_2O_3 nanocomposite disc surfaces: Osseous differentiation and cellular arrangement in vitro

Customized square grid arrangements of different groove depths (1.0, 1.5 and 3.0 μm) and separations (10 and 30 μm) were successfully laser patterned, using a nanosecond pulsed fibre laser, on the surface of 10 mol% ceria-stabilized zirconia and alumina (10CeTZP-Al_2O_3) nanocomposite discs (diameter: 10 mm; thickness: 1.5 mm). The patterned surfaces and the in vitro biological response of osteoblasts (SAOS-2) towards them were thoroughly analysed. In terms of composition, the laser treatment was found to cause superficial monoclinic-tetragonal zirconia phase transformation and alumina evaporation. In vitro, the most effective grid configuration for osseous differentiation was found to be 1.5 μm groove depth and 10 μm groove separation, and confocal microscopy revealed that the cells show a tendency to be sorted as groove depth increases. It is thought that custom-made patterns could be produced to guide cell attachment in vivo, which could favour implant integration and reduce healing time.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Mechanical Engineering and Industrial Systems, Nanoker Research, Universidad de Oviedo
Contributors: Goyos-Ball, L., Prado, C., Díaz, R., Fernández, E., Ismailov, A., Kumpulainen, T., Levänen, E., Torrecillas, R., Fernández, A.
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ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Ceramics and Composites, Process Chemistry and Technology, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Alumina, Cellular arrangement, Ceramic nanocomposite, Laser patterning, Osseous differentiation, Zirconia
DOIs:

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Source ID: 85042621677
Research output: Contribution to journal › Article › Scientific › peer-review

Optical properties of $GaAs_{1-x}Bi_x$/GaAs quantum well structures grown by molecular beam epitaxy on (100) and (311)B GaAs substrates

In this work, the electronic bandstructure of $GaAs_{1-x}Bi_x$/GaAs single quantum well (QW) samples grown by molecular beam epitaxy is investigated by photomodulated reflectance (PR) measurements as a function of Bi content ($0.0065 \leq x \leq 0.0215$) and substrate orientation. The Bi composition is determined via simulation of high-resolution x-ray diffraction measurement and is found to be maximized in the 2.15%Bi and 2.1%Bi samples grown on (100) and (311)B GaAs substrates. However, the simulations indicate that the Bi composition is not only limited in the GaAsBi QW layer but extends out of the GaAsBi QW towards the GaAs barrier and forms a GaAsBi epilayer. PR spectra are fitted with the third derivative function form (TDFF) to identify the optical transition energies. We analyze the TDFF results by considering strain-induced modification on the conduction band (CB) and splitting of the valence band (VB) due to its interaction with the localized Bi level and VB interaction. The PR measurements confirm the existence of a GaAsBi epilayer via observed optical transitions that belong to GaAsBi layers with various Bi compositions. It is found that both Bi composition and substrate orientation have strong effects on the PR signal. Comparison between TDFF and calculated optical transition energies provides a bandgap reduction of 92 meV/%Bi and 36 meV/%Bi and an interaction strength of the isolated Bi atoms with host GaAs valence band (C_{BiM}) of 1.7 eV and 0.9 eV for (100) and (311)B GaAs substrates, respectively.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Photonics, Research group: ORC, Adana Science and Technology University, Istanbul University, University of Cukurova, University of Nottingham, Universidade Federal de São Carlos, Leibniz Institute for Crystal Growth

Contributors: Gunes, M., Ukelge, M. O., Donmez, O., Erol, A., Gumus, C., Alghamdi, H., Galeti, H. V., Henini, M., Schmidbauer, M., Hilska, J., Puustinen, J., Guina, M.
Publication date: 13 Nov 2018
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Condensed Matter Physics, Electrical and Electronic Engineering, Materials Chemistry
Keywords: high-index substrate, oriented GaAsBi, photomodulated reflectance, strained quantum well, type I band line-up
DOIs:

10.1088/1361-6641/aaea2e
Source: Scopus
Source ID: 85057810892
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of tempering on the impact-abrasive and abrasive wear resistance of ultra-high strength steels
Tempering is an essential part in the fabrication of ultra-high strength steels and it is also widely applied in the processing of wear-resistant steels. In this paper, the effects of different tempering temperatures on the impact-abrasive and abrasive wear properties of martensitic ultra-high strength steels were studied. A novel press-hardening steel with carbon content of 0.4 wt% was received in hot-rolled condition and further austenitized, water-quenched and tempered for 2 h at different temperatures (150–400 °C). Tensile strength values up to 2200MPa and hardness exceeding 650HV were measured. Wear testing was done with impact-abrasive impeller-tumbler and abrasive dry-pot application-oriented test methods simulating mining and mineral handling environments. A laboratory rolled 600HB steel and a commercial 500HB grade wear-resistant steel were included for comparison. The wear surfaces and cross-sections of the samples were thoroughly characterized. Both testing methods produced highly deformed surface layers and strong work-hardening. Wear performance was mainly controlled by the initial hardness of the steels, but differences were found in the highly work-hardened surfaces of the steels.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Univ of Oulu, SSAB
Contributors: Haiko, O., Valtonen, K., Kaijalainen, A., Uusikallio, S., Hannula, J., Liimatainen, T., Kömi, J.
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Abrasion, Impact-abrasion, Steel, Tempering, Wear testing
DOIs:

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http://urn.fi/URN:NBN:fi:tuni-202001231492. Embargo ends: 1/11/21
Source: Scopus
Source ID: 85074214509
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of prior austenite grain size on the abrasive wear resistance of ultra-high strength martensitic steels
Prior austenite grain size has a marked effect on the hardenability, strength, and impact toughness properties of steels. This study was conducted in order to understand the effect of prior austenite grain size and morphology on the mechanical

properties and abrasive wear performance of an ultra-high strength steel. A commercial quenched 500 HB grade wear-resistant steel was selected for the study: the steel was austenitized at two different temperatures and compared to the original, as-received quenched condition. The resulting mean prior austenite grain size was ranging from 14 μm to 34 μm. The decrease in grain size improved the low-temperature impact toughness properties. A high stress abrasive wear testing method with natural granite abrasives was utilized for the evaluation of abrasive wear resistance. The results suggest that decreasing the prior austenite grain size improves the abrasive wear resistance with similar hardness level martensitic steels. In addition, high-resolution electron backscatter diffraction measurements revealed formation of ultra-fine grain structures in the severely deformed regions of the wear surfaces.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Research group: Materials Characterization, Materials Science and Environmental Engineering, University of Oulu, Tampere Wear Center
Contributors: Haiko, O., Javaheri, V., Valtonen, K., Kaijalainen, A., Hannula, J., Kömi, J.
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ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Abrasion, Electron microscopy, Hardness, Steel, Wear testing
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Research output: Contribution to journal › Article › Scientific › peer-review

Characteristics of carbide-free medium-carbon bainitic steels in high-stress abrasive wear conditions
This study encompasses a comprehensive account of the abrasive wear properties of carbide-free, ultrahigh-strength bainitic steels processed through ausforming at three different temperatures well below the recrystallization stop temperature followed by bainitic transformation at temperatures close to the M_S temperature. Five medium-carbon, high-silicon compositions were designed for the study by suitably varying the alloying levels of carbon, vanadium, niobium, molybdenum, and aluminum. While ausforming at lower temperatures enabled a large number of nucleation sites leading to significant refinement of bainitic laths, the decomposition of austenite at relatively low transformation temperatures was accelerated due to the presence of a high dislocation density, thus enabling completion of bainitic transformation in a reasonable length of time. The steels were characterized in respect of microstructural features and mechanical properties, besides evaluation of wear resistance through a high-stress abrasive wear testing method with natural granite abrasives. The microstructures comprised different fractions of bainitic ferrite and/or granular bainite (56–68%), martensite (0–25%), besides a significant fraction of retained austenite (20–34%) manifesting as pools and also interlath films, depending on the ausforming conditions and subsequent cooling paths. A tensile strength of 1900 MPa level was achieved with hardness exceeding 500 HV for the medium-temperature ausformed steel containing a high carbon content that also showed lowest mass loss in the wear test. The hardness-to-mass loss ratio appeared highly promising with some of the carbide-free bainitic steels on par with or better than the reference martensitic steel. The high work-hardening capability as a consequence of the strain-induced austenite to martensite transformation was considered as the main factor for the superior abrasive wear resistance of the carbide-free bainitic steels.

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Contributors: Haiko, O., Kaikkonen, P., Somani, M., Valtonen, K., Kömi, J.
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Improved Stability of Atomic Layer Deposited Amorphous TiO_2 Photoelectrode Coatings by Thermally Induced Oxygen Defects

Amorphous titanium dioxide (a-TiO_2) combined with an electrocatalyst has shown to be a promising coating for stabilizing traditional semiconductor materials used in artificial photosynthesis for efficient photoelectrochemical solar-to-fuel energy conversion. In this study we report a detailed analysis of two methods of modifying an undoped thin film of atomic layer deposited (ALD) a-TiO_2 without an electrocatalyst to affect its performance in water splitting reaction as a protective photoelectrode coating. The methods are high-temperature annealing in ultrahigh vacuum and atomic hydrogen exposure. A key feature in both methods is that they preserve the amorphous structure of the film. Special attention is paid to the changes in the molecular and electronic structure of a-TiO_2 induced by these treatments. On the basis of the photoelectrochemical results, the a-TiO_2 is susceptible to photocorrosion but significant improvement in stability is achieved after heat treatment in vacuum at temperatures above 500 °C. On the other hand, the hydrogen treatment does not increase the stability despite the ostensibly similar reduction of a-TiO_2. The surface analysis allows us to interpret the improved stability to the thermally induced formation of O^- species within a-TiO_2 that are essentially electronic defects in the anionic framework.

General information

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Organisations: Photonics, Materials Science
Contributors: Hannula, M., Ali-Löytty, H., Lahtonen, K., Sarlin, E., Saari, J., Valden, M.
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Source: Scopus
Source ID: 85042704048
Research output: Contribution to journal › Article › Scientific › peer-review

Local Mechanical Properties at the Dendrite Scale of Ni-Based Superalloys Studied by Advanced High Temperature Indentation Creep and Micropillar Compression Tests

Chemical inhomogenities due to dendritic solidification of Ni-based superalloys result in different local microstructures with varying mechanical properties. New indentation creep test methods allow probing of the local creep properties at the

dendrite scale at high temperatures. The as-cast single crystalline Ni-based superalloy ERBO1A (a derivative alloy of CMSX–4) was investigated and electron-probe microanalysis (EPMA) measurements revealed strong segregation of, e.g., Re and W in the dendritic region and, e.g., Ta in the interdendritic region. Indentation creep experiments at 750 °C and micropillar compression tests at 785 °C were conducted in both regions, and a higher creep strength was found in the dendritic region compared to the interdendritic region. Theoretical models for solid solution hardening as well as γ′ precipitation hardening confirm these results, since they predict a higher strength in the dendritic region than in the interdendritic region. Compared with the fully heat treated state, a smaller difference in the local mechanical properties or even a reverse strength ratio of the dendritic and interdendritic region can be expected.

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MoE publication type: A4 Article in a conference publication
Organisations: Materials Science and Environmental Engineering, Research group: Materials Characterization, Friedrich-Alexander-Universität Erlangen-Nürnberg, Swiss Federal Laboratories for Materials Science and Technology, Fraunhofer Institut für Keramische Technologien und Systeme
Contributors: Haußmann, L., Neumeier, S., Kolb, M., Ast, J., Mohanty, G., Michler, J., Göken, M.
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Source ID: 85091283715
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Printable and flexible macroporous organosilica film with high protein adsorption capacity

An approach for creating a flexible and macroporous silsesquioxane film using phase separation method is described. The porous film was prepared by a simple coating method where sol-gel solution containing polyacrylic acid (PAA) and 1,6-bis(trimethoxysilyl)hexane in water was applied on boehmite silica coated polymethylmethacrylate (PMMA) film. After drying, the water soluble PAA template was removed by washing the film with water revealing the porous film. With certain ratios of PAA and water, fully co-continuous pore system with open surface was obtained. Porous films with 3-4 μm thickness were found to be highly flexible. The biocompatibility of the porous film was tested by immobilizing a high affinity biotin-binding chimeric avidin (ChiAVD(I117Y)) into the porous matrix The porous film was found to adsorb higher amounts of functional chimeric avidin compared to the pure PMMA film or a boehmite silica coated PMMA film.

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MoE publication type: A1 Journal article-refereed
Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Univ of Oulu, VTT Technical Research Centre of Finland, School of Management (JKK)
Contributors: Heikkinen, J. J., Kivimäki, L., Hytönen, V. P., Kulomaa, M. S., Hormi, O. E. O.
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ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
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Source: Scopus
Source ID: 84855940396
Research output: Contribution to journal › Article › Scientific › peer-review

Photocatalytic and antibacterial properties of ZnO films with different surface topographies on stainless steel substrate
Zinc oxide films with three types of topographies: needle-like and hexagonal rods and flakes, were prepared by hydrothermal synthesis on stainless steel substrates to investigate their photocatalytic and antibacterial properties. The photocatalytic activity was measured with a methylene blue (MB) discoloration test, whereas a method using bioluminescent whole cell bacterial biosensors enabling the constant monitoring of the amount of living cells on the surfaces was used here to study the antibacterial properties. The results showed that photocatalytic activity was clearly influenced by the surface area, which is in turn dependent on the topography. Moreover, it was found that all the examined films decreased notably the amount of Staphylococcus aureus and Escherichia coli on the surfaces. Despite significant differences in the surface areas of the studied samples that led to different zinc dissolution rate in aqueous environment, no notable differences in antibacterial activity between the films with different morphologies could be detected. These results are presented and discussed in this paper.

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Ceramic materials, Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, VTT Technical Research Centre of Finland
Contributors: Heinonen, S., Kannisto, M., Nikkanen, J., Huttunen-Saarivirta, E., Karp, M., Levänen, E.
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ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
Keywords: Antibacterial, Biosensor cell, Hydrothermal synthesis, Photocatalytic activity, Zinc oxide
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Source: Scopus
Source ID: 84991648557
Research output: Contribution to journal › Article › Scientific › peer-review

Investigation of long-term chemical stability of structured ZnO films in aqueous solutions of varying conditions
Nanostructured zinc oxide, ZnO, films feature attractive functional properties, but their long-term stability needs further investigation. Here, ZnO thin films with well-aligned rod-like structure were grown on stainless steel substrate. The long-term chemical stability of the ZnO films was investigated in solutions with varying pH values (3 − 11) to enhance knowledge about the durability of films in acidic and basic environments. The solubility and stability of the films in the

solutions were investigated using atomic absorption spectrophotometry, scanning electron microscopy imaging and energy-dispersive X-ray spectroscopy analyses, as well as by monitoring changes in water contact angle of the films and in the pH values of the solutions. The ZnO film was found to be most stable at highest pH value, with the amount of dissolved zinc being lowest among the studied pH values and the changes observed with other characterization methods being minor compared to the samples immersed to other solutions. At the lowest pH, the film was removed rapidly from the substrate by dissolution. In solutions featuring pH values 5 and 9, the measured pH was unstable and changed constantly until it reached the value 7.2–7.6, i.e., until the equilibrium of different chemical species in the solution was achieved. These results are presented and discussed in this paper from the viewpoint of applicability of the ZnO films.

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Organisations: Materials Science, Research group: Ceramic materials, VTT Technical Research Centre of Finland
Contributors: Heinonen, S., Nikkanen, J., Huttunen-Saarivirta, E., Levänen, E.
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ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
Keywords: Chemical stability, Hydrothermal synthesis, pH, Solubility, Thin film, Zinc oxide
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Source: Scopus
Source ID: 85027885831
Research output: Contribution to journal › Article › Scientific › peer-review

Aryl end-capped quaterthiophenes applied as anode interfacial layers in inverted organic solar cells
Four aryl end-capped quaterthiophene derivatives were synthesized and their material properties were studied by computational, spectroscopic, electrochemical, and thermoanalytical methods. Compounds were applied as interfacial layers between the bulk heterojunction active layer and Ag anode in inverted organic solar cells. Results show that p-cyanophenyl end-capped quaterthiophene with hexyl side chains increases both the short circuit current density and power conversion efficiency notably compared to reference interlayer material, tris-(8-hydroxyquinoline)aluminum. The improved cell performance was attributed to the optimal positions of the highest occupied molecular orbital and the lowest unoccupied molecular orbital (LUMO) of this material, relative to those of the photoactive electron donor poly(3-hexylthiophene) and Ag anode, and evenly distributed LUMO. In addition, the use of these materials as an anode interfacial layer increases the absorption of the solar cell, which could contribute to the formation of excitons and additional current production by the cell.

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Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, University of Oulu, Department of Chemistry and Mathematics, Faculty of Petroleum and Mining Engineering, Suez University
Contributors: Heiskanen, J. P., Manninen, V. M., Pankov, D., Omar, W. A. E., Kastinen, T., Hukka, T. I., Lemmetyinen, H. J., Hormi, O. E. O.
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Materials Chemistry, Metals and Alloys, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Anode interfacial layer, Bulk heterojunction, Computational research, Inverted organic solar cell, Oligothiophene, Spectroscopy, Suzuki-Miyaura
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Source: Scopus
Source ID: 84921286591
Research output: Contribution to journal › Article › Scientific › peer-review

Urea and guanidinium induced denaturation of a Trp-cage miniprotein
Using a combination of experimental techniques (circular dichroism, differential scanning calorimetry, and NMR) and molecular dynamics simulations, we performed an extensive study of denaturation of the Trp-cage miniprotein by urea and guanidinium. The experiments, despite their different sensitivities to various aspects of the denaturation process, consistently point to simple, two-state unfolding process. Microsecond molecular dynamics simulations with a femtosecond time resolution allow us to unravel the detailed molecular mechanism of Trp-cage unfolding. The process starts with a destabilizing proline shift in the hydrophobic core of the miniprotein, followed by a gradual destruction of the hydrophobic loop and the α-helix. Despite differences in interactions of urea vs guanidinium with various peptide moieties, the overall destabilizing action of these two denaturants on Trp-cage is very similar.

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MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, University of Leeds
Contributors: Heyda, J., Kožíšek, M., Bednárova, L., Thompson, G., Konvalinka, J., Vondrášek, J., Jungwirth, P.
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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
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Research output: Contribution to journal › Article › Scientific › peer-review

Epitaxial phases of high Bi content GaSbBi alloys
GaSbBi alloys have recently emerged as attractive materials for mid-infrared optoelectronics owing to strong band gap reduction enabled by Bi incorporation into the GaSb matrix. The fundamental understanding of the epitaxial process required to demonstrate high quality crystals is in an early-developmental phase. From this perspective, we report on the key role played by the Sb/Ga flux ratio in controlling the structural quality and incorporation of high Bi content GaSbBi (up to 14.5%-Bi), revealing three distinct epitaxial phases. The first phase (below stoichiometric Sb/Ga) exhibits Ga-Bi compound droplets, low crystal quality, and reduced Bi content. At the second phase (above stoichiometric Sb/Ga), the crystal exhibits smooth surfaces and excellent crystallinity with efficient Bi incorporation. The last phase corresponds to exceeding a Sb/Ga threshold that leads to reduced Bi incorporation, Bi droplets and degraded crystallinity. This threshold

value that defines the optimal growth window is controlled by the temperature as well as the Bi/Ga ratio. Increasing temperature increases the threshold, albeit simultaneously reducing Bi incorporation. Conversely, increasing the Bi/Ga flux ratio increases Bi incorporation, while narrowing down and ultimately closing the window. This study provides a general framework enabling development of high quality GaSbBi heterostructures for emerging mid-infrared optoelectronics.

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Organisations: Physics, Research group: ORC
Contributors: Hilska, J., Koivusalo, E., Puustinen, J., Suomalainen, S., Guina, M.
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Release of halide ions from the buried active site of the haloalkane dehalogenase LinB revealed by stopped-flow fluorescence analysis and free energy calculations
Release of halide ions is an essential step of the catalytic cycle of haloalkane dehalogenases. Here we describe experimentally and computationally the process of release of a halide anion from the buried active site of the haloalkane dehalogenase LinB. Using stopped-flow fluorescence analysis and umbrella sampling free energy calculations, we show that the anion binding is ion-specific and follows the ordering $I^- > Br^- > Cl^-$. We also address the issue of the protonation state of the catalytic His272 residue and its effect on the process of halide release. While deprotonation of His272 increases binding of anions in the access tunnel, we show that the anionic ordering does not change with the switch of the protonation state. We also demonstrate that a sodium cation could relatively easily enter the active site, provided the His272 residue is singly protonated, and replace thus the missing proton. In contrast, Na^+ is strongly repelled from the active site containing the doubly protonated His272 residue. Our study contributes toward understanding of the reaction mechanism of haloalkane dehalogenase enzyme family. Determination of the protonation state of the catalytic histidine throughout the catalytic cycle remains a challenge for future studies.

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Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Masaryk University
Contributors: Hladilkova, J., Prokop, Z., Chaloupkova, R., Damborsky, J., Jungwirth, P.
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Research output: Contribution to journal › Article › Scientific › peer-review

Hydration of hydroxyl and amino groups examined by molecular dynamics and neutron scattering

Neutron diffraction with isotopic substitution was performed on aqueous solutions of isopropyl alcohol and isopropylamine. The difference between these two measurements primarily contains information about the different hydration of the alcohol and amino group. This data is used as a test of the accuracy of molecular dynamic simulations of the same systems. Having established the level of accuracy of the modeling, it is employed as an interpretive tool for the experimental data. Even though the alcohol and the amine possess comparable hydrogen bonding capabilities, consisting respectively of either two hydrogen bond acceptors and one donor, or two hydrogen bond donors and one acceptor, we find significant differences in the hydration of the hydroxyl and amino groups.

General information

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Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Institut Laue-Langevin
Contributors: Hladílková, J., Fischer, H. E., Jungwirth, P., Mason, P. E.
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Source ID: 84930682015
Research output: Contribution to journal › Article › Scientific › peer-review

Transparent Yb^{3+} doped phosphate glass-ceramics

Yb^{3+} doped oxyfluorophosphate glasses with the composition (98.75) [90$NaPO_3$-(10-x) Na_2O-xNaF] - 1.25Yb_2O_3 (in mol%) with x = 0, 2.5, 5, 7.5 and 10 were prepared using a standard melting process. The progressive replacement of Na_2O by NaF leads to an increase in the number of Q^2 units at the expense of the Q^1 units. This increase in the polymerization of the glass network leads to a shift of the optical band gap to lower wavelength, to a slight increase in the intensity of the emission at 1000 nm and more importantly to a change in the glass crystallization process. Indeed, both surface and bulk crystallization were observed in the glass with x = 0 while surface crystallization only occurs when NaF is added in the phosphate network. The heat treatment leads to the precipitation of at least three crystalline phases: as x increases, the $NaPO_3$ phase grows at the expense of $Na_5P_3O_{10}$. All glasses precipitate the Yb containing crystal, $NaYbP_2O_7$ which leads to an increase in the intensity of the emission at 1000 nm compared to the emission at 975 nm. We show for the first time to the best of our knowledge that transparent Yb^{3+} doped phosphate glass-ceramics can be obtained within this glass system when free of NaF.

General information

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Organisations: Physics, Fondazione LINKS – Leading Innovation & Knowledge for Society, CNRS, Université de Bordeaux, ICMCB
Contributors: Hongisto, M., Veber, A., Boetti, N. G., Danto, S., Jubera, V., Petit, L.

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Source: Scopus
Source ID: 85077933290
Research output: Contribution to journal › Article › Scientific › peer-review

Dissolution behavior of the bioactive glass S53P4 when sodium is replaced by potassium, and calcium with magnesium or strontium
The initial dissolution behavior of glasses based on bioactive glass S53P4 was studied with a dynamic measurement setup in a Tris-buffered solution. The glass composition was modified systematically on a molar basis by replacing sodium oxide with potassium oxide (0-100% K) and calcium oxide with magnesium (0-18% Mg) or strontium oxide (0-100% Sr). The concentrations of the ions dissolving from the glasses were measured continuously on-line in the fluid flow for 15 to 25 min using an inductively coupled plasma emission optical spectrometer. This method enabled attainment of detailed information on the initial dissolution mechanisms without the, for bioactive glasses typical, interference of apatite layer formation. The results showed that initial dissolutions of sodium and potassium were markedly higher from the mixed alkali oxide glasses than from the compositions containing only one alkali oxide. Introducing MgO in S53P4 caused a minor decrease in the dissolution rates of all ions. The glass containing 3 mol% of MgO showed the best chemical durability. In contrast, replacing CaO gradually with SrO increased the dissolution rates of all ions. The glasses with the highest replacement of CaO with SrO showed rapid release of both Sr and Na ions. The results corroborate the overall knowledge of glass durability and can be utilized to design bioactive glasses with controlled ion release rate for tissue engineering applications.

General information
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Organisations: Department of Electronics and Communications Engineering, Research group: Biomaterials and Tissue Engineering Group, Johan Gadolin Process Chemistry Centre, Abo Akademi University, Paroc Group Oy, Åbo Akademi University
Contributors: Hupa, L., Fagerlund, S., Massera, J., Björkvik, L.
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ASJC Scopus subject areas: Condensed Matter Physics, Ceramics and Composites, Electronic, Optical and Magnetic Materials, Materials Chemistry
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Aligned Poly(ε-caprolactone) Nanofibers Guide the Orientation and Migration of Human Pluripotent Stem Cell-Derived Neurons, Astrocytes, and Oligodendrocyte Precursor Cells In Vitro
Stem cell transplantations for spinal cord injury (SCI) have been studied extensively for the past decade in order to replace the damaged tissue with human pluripotent stem cell (hPSC)-derived neural cells. Transplanted cells may, however, benefit from supporting and guiding structures or scaffolds in order to remain viable and integrate into the host tissue.

Biomaterials can be used as supporting scaffolds, as they mimic the characteristics of the natural cellular environment. In this study, hPSC-derived neurons, astrocytes, and oligodendrocyte precursor cells (OPCs) are cultured on aligned poly(ε-caprolactone) nanofiber platforms, which guide cell orientation to resemble that of spinal cord in vivo. All cell types are shown to efficiently spread over the nanofiber platform and orient according to the fiber alignment. Human neurons and astrocytes require extracellular matrix molecule coating for the nanofibers, but OPCs grow on nanofibers without additional treatment. Furthermore, the nanofiber platform is combined with a 3D hydrogel scaffold with controlled thickness, and nanofiber-mediated orientation of hPSC-derived neurons is also demonstrated in a 3D environment. In this work, clinically relevant materials and substrates for nanofibers, fiber coatings, and hydrogel scaffolds are used and combined with cells suitable for developing functional cell grafts for SCI repair.

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Organisations: Materials Science, Research group: Materials Characterization
Contributors: Hyysalo, A., Ristola, M., Joki, T., Honkanen, M., Vippola, M., Narkilahti, S.
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Research output: Contribution to journal › Article › Scientific › peer-review

Systematic analysis of coating-substrate interactions in the presence of flow localization
Localized deformation and cracking in a system of thermally sprayed hard metal coating overlaid on a low alloy steel is studied by means of bend testing. In-situ digital image correlation measurements are used to characterize material strain field near the coating/substrate interface. The studied substrate undergoes softening upon yielding which manifests itself as narrow bands of localized shear deformation. The measurements show that the coating cracks and the substrate shear bands interact. When the coating starts cracking during the elastic loading of the substrate, the formed cracks function as nucleation points for the shear bands. In contrast, if the coating resists cracking until the yielding of the substrate, the coating cracks and substrate shear bands form simultaneously. Based on the experiments, continuum-scale finite element model of the system is developed, validated and then used for a systematic numerical analysis of the effects of substrate shear banding on the measurement of coating properties. Based on the results of this work, three main effects can be identified. Firstly, the flow localization in the substrate can increase the measured apparent (macroscopic) surface strain of the coating, if not accounted for by using microscopic techniques. Secondly, substrate shear bands increase the interfacial loading, which may cause unexpected delamination of the coating and thus affect the evaluation of the interfacial strength. Finally, substrate shear bands affect the stress state within the coating and may thus affect the cracking morphology in the coating. Therefore, based on the results of this study, if the coating and interfacial strengths are of similar magnitude with the substrate yield strength, the possible tendency of the substrate towards flow localization should be taken into account in the analysis of the coating behavior.

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Contributors: Isakov, M., Matikainen, V., Koivuluoto, H., May, M.
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ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
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Measuring optical anisotropy in poly(3,4-ethylene dioxythiophene): poly(styrene sulfonate) films with added graphene

Abstract Graphene is a 2D nanomaterial having a great potential for applications in electronics and optoelectronics. Composites of graphene with conducting polymers have shown high performance in practical devices and their solution-processability enables low-cost and high-throughput mass manufacturing using printing techniques. Here we measure the effect of incorporation of graphene into poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) to the optical anisotropy, absorbance and conductivity of the film. Uniaxial anisotropy in PEDOT:PSS films has been thought to be caused by the spin-coating process used in fabrication. We have characterized spray- and spin-coated films using ellipsometry and total internal reflection spectroscopy, the latter especially for films too thick and uneven for ellipsometry, and show that spray-coating, similar to inkjet printing, also produces consistently anisotropic properties even in very thick and uneven films. Possible plasmonic excitations related to graphene are not seen in the films. The optical and electrical anisotropy of graphene/PEDOT:PSS enables routes to high performance devices for electronics, photonics and optoelectronics.

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Automation Science and Engineering, Research area: Microsystems, Research area: Measurement Technology and Process Control, Integrated Technologies for Tissue Engineering Research (ITTE), Miktech Oy, University of Jyväskylä
Contributors: Isoniemi, T., Tuukkanen, S., Cameron, D. C., Simonen, J., Toppari, J. J.
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ASJC Scopus subject areas: Biomaterials, Electronic, Optical and Magnetic Materials, Materials Chemistry, Electrical and Electronic Engineering, Chemistry(all), Condensed Matter Physics
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Corrosion mechanisms of sintered Nd-Fe-B magnets in the presence of water as vapour, pressurised vapour and liquid

Corrosion behaviour of three commercial sintered Nd-Fe-B magnets exposed to environments containing water as vapour, pressurised vapour, and liquid was investigated in order to understand their overall corrosion performance under a range of conditions. Two types of heat humidity exposure tests, namely the 85/85 and pressure cooker test, and the immersion test combined with electrochemical measurements were used as corrosion tests. It was observed that varying the temperature, pressure, and the prevailing state of water in the exposure tests, different corrosion mechanisms were detected on the surface of Nd-Fe-B magnets. The surface finish of the magnet had an effect on the initiation of corrosion in mild heat-humidity exposure. Immersion in liquid water resulted in a corrosion topography where the Nd-rich grain-boundary phase did not corrode selectively as in the other accelerated corrosion tests but was retained intact while the matrix phase underwent corrosion. These results and the dominant corrosion mechanisms of sintered Nd-Fe-B magnets in different environments are presented and discussed in this paper.

General information

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Organisations: Department of Materials Science, Research group: Ceramic materials, Research group: Materials Characterization, Engineering materials science and solutions (EMASS), Prizztech Magnet Technology Centre, VTT Technical Research Centre of Finland
Contributors: Isotahdon, E., Huttunen-Saarivirta, E., Heinonen, S., Kuokkala, V. T., Paju, M.
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Source: Scopus
Source ID: 84920283616
Research output: Contribution to journal › Article › Scientific › peer-review

Characterization of the microstructure and corrosion performance of Ce-alloyed Nd-Fe-B magnets

Expensive rare-earth elements used in neodymium-iron-boron permanent magnets can be partly replaced by a more abundant cerium without significantly compromising the magnetic properties. In this study, we investigated the effects that cerium addition has on the corrosion resistance of Nd-Fe-B magnets. The cerium-alloyed magnet grade was compared to two Ce-free magnet materials, a standard-grade Nd-Fe-B and a Co-alloyed magnet grade, with respect to microstructure and corrosion behaviour. The microstructure of the magnets was characterized by scanning electron microscopy, with the location of Ce being of primary interest. The magnets were exposed to electrochemical measurements and accelerated corrosion tests. Although the amount of the corrosion-sensitive grain-boundary phase was higher in the Ce-alloyed magnets than in the other two magnet grades, the overall corrosion behaviour was in many ways comparable to that of the Co-alloyed grade magnet, e.g., showing a slight increase in open circuit potential as compared to the standard grade magnet. In accelerated tests, corrosion of the Fe-rich phase was equal to the other magnet grades. Pulverization of the Ce-alloyed magnet was not detected during the accelerated tests, similarly to the Co-alloyed grade.

General information

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MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Materials Characterization, VTT Technical Research Centre of Finland
Contributors: Isotahdon, E., Huttunen-Saarivirta, E., Kuokkala, V.
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Research output: Contribution to journal › Article › Scientific › peer-review

Influence of heat treatment on the abrasive wear resistance of a Cr_3C_2NiCr coating deposited by an ethene-fuelled HVOF spray process

This work reveals the influence of heat treatments on the microstructure, mechanical properties and abrasive wear behaviour of a Cr_3C_2NiCr coating deposited by an ethene-fuelled high-velocity oxygen-fuel spray process using an agglomerated-and-sintered feedstock powder. The wear resistance of an as-sprayed and heat treated (8 h at 800 °C) coating was evaluated in low- and high-stress abrasion regimes, the latter in a temperature range up to 800 °C. Precipitation of secondary carbides from the supersaturated as-sprayed binder matrix is at the core of the observed changes in the coatings wear resistance upon heat treating. This aging process renders the binder matrix softer and more ductile, as was probed by means of nanoindentation, and thereby improves its resistance against micro-cracking which is identified as an important wear mechanism in high-stress abrasion conditions.

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Organisations: Department of Materials Science, AC2T Research GmbH, Fraunhofer Institut für Werkstoff- und Strahltechnik, Fraunhofer Institut für Keramische Technologien und Systeme
Contributors: Janka, L., Norpoth, J., Trache, R., Berger, L. M.
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Source: Scopus
Source ID: 84960192258
Research output: Contribution to journal › Article › Scientific › peer-review

HVOF- and HVAF-Sprayed Cr_3C_2-NiCr Coatings Deposited from Feedstock Powders of Spherical Morphology: Microstructure Formation and High-Stress Abrasive Wear Resistance Up to 800 °C

Chromium carbide-based coatings are commonly applied to protect surfaces against wear at high temperatures. This work discusses the influence of feedstock powder and spray torch selection on the microstructure and high-stress abrasion resistance of thermally sprayed Cr_3C_2-NiCr coatings. Four commercial feedstock powders with spherical morphology and different microstructures were deposited by different high-velocity spray processes, namely third-generation gas- and liquid-fueled HVOF torches and by the latest generation HVAF torch. The microstructures of the coatings were studied in the as-sprayed state and after various heat treatments. The high-stress abrasion resistance of as-sprayed and heat-treated coatings was tested at room temperature and at 800 °C. The study reveals that the selection of the spray torch mainly affects the room temperature abrasion resistance of the as-sprayed coatings, which is due to differences in the embrittlement of the binder phase generated by carbide dissolution. At elevated temperatures, precipitation and growth of secondary carbides yields a fast equalization of the various coatings microstructures and wear properties.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Viktor-Kaplan-Straße 2/C, Fraunhofer Institut für Werkstoff- und Strahltechnik, Fraunhofer Institut für Keramische Technologien und Systeme
Contributors: Janka, L., Norpoth, J., Trache, R., Thiele, S., Berger, L. M.
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Source: Scopus
Source ID: 85027972309
Research output: Contribution to journal › Article › Scientific › peer-review

Improving the high temperature abrasion resistance of thermally sprayed Cr_3C_2-NiCr coatings by WC addition

Two experimental agglomerated and sintered (a&s) feedstock powders were prepared, in order to reveal the role of WC addition on the microstructure, hardness, and the abrasion resistance of HVOF-sprayed Cr_3C_2-NiCr coatings. These powders contained 10 wt.% of sub-micron WC, 20 or 10 wt.% of nickel binder, and Cr_3C_2 as balance. Experimental coatings were deposited by a liquid fueled high velocity oxygen-fuel (HVOF) spray process and subsequently heat treated at 800 °C for 8 h to simulate elevated temperature service conditions. The microstructures of the powders and coatings were studied by SEM and X-ray diffraction, and the hardnesses of coatings were probed by means of micro and nanoindentation. In addition, the high stress abrasion resistance was tested in a temperature range from room temperature up to 800 °C. The microstructural characterization of the coatings displayed the presence of WC and tungsten containing Cr_3C_2 grains. The coating hardness increased after heat treatment, which stemmed from precipitation of secondary carbides and solid solution strengthening of the binder by tungsten. In addition, the study revealed that both experimental coatings have high wear resistance at room and elevated temperatures.

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Organisations: Materials Science, Research group: Surface Engineering, Viktor-Kaplan-Straße 2/C, Fraunhofer Institut für Keramische Technologien und Systeme, Fraunhofer Institut für Werkstoff- und Strahltechnik, Treibacher Industrie AG
Contributors: Janka, L., Berger, L. M., Norpoth, J., Trache, R., Thiele, S., Tomastik, C., Matikainen, V., Vuoristo, P.
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
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Active packaging by paper coating

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MoE publication type: A4 Article in a conference publication
Organisations: Department of Materials Science, Research group: Paper Converting and Packaging, Umea University, BillerudKorsnäs, Karlstad University
Contributors: Jarnstrom, L., Johansson, K., Kuusipalo, J., Jonsson, L.
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Two cations, two mechanisms: Interactions of sodium and calcium with zwitterionic lipid membranes
Adsorption of metal cations onto a cellular membrane changes its properties, such as interactions with charged moieties or the propensity for membrane fusion. It is, however, unclear whether cells can regulate ion adsorption and the related functions via locally adjusting their membrane composition. We employed fluorescence techniques and computer simulations to determine how the presence of cholesterol - a key molecule inducing membrane heterogeneity - affects the adsorption of sodium and calcium onto zwitterionic phosphatidylcholine bilayers. We found that the transient adsorption of sodium is dependent on the number of phosphatidylcholine head groups, while the strong surface binding of calcium is determined by the available surface area of the membrane. Cholesterol thus does not affect sodium adsorption and only plays an indirect role in modulating the adsorption of calcium by increasing the total surface area of the membrane. These observations also indicate how lateral lipid heterogeneity can regulate various ion-induced processes including adsorption of peripheral proteins, nanoparticles, and other molecules onto membranes.

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MoE publication type: A1 Journal article-refereed
Organisations: Physics, University of Helsinki, J. Heyrovský Institute of Physical Chemistry, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
Contributors: Javanainen, M., Melcrová, A., Magarkar, A., Jurkiewicz, P., Hof, M., Jungwirth, P., Martinez-Seara, H.
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Original language: English
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Rotational Diffusion of Membrane Proteins in Crowded Membranes

Membrane proteins travel along cellular membranes and reorient themselves to form functional oligomers and protein-lipid complexes. Following the Saffman-Delbrück model, protein radius sets the rate of this diffusive motion. However, it is unclear how this model, derived for ideal and dilute membranes, performs under crowded conditions of cellular membranes. Here, we study the rotational motion of membrane proteins using molecular dynamics simulations of coarse-grained membranes and 2-dimensional Lennard-Jones fluids with varying levels of crowding. We find that the Saffman-Delbrück model captures the size-dependency of rotational diffusion under dilute conditions where protein-protein interactions are negligible, whereas stronger scaling laws arise under crowding. Together with our recent work on lateral diffusion, our results reshape the description of protein dynamics in native membrane environments: The translational and rotational motions of proteins with small transmembrane domains are rapid, whereas larger proteins or protein complexes display substantially slower dynamics.

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Contributors: Javanainen, M., Ollila, O. H., Martinez-Seara, H.
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EXT="Ollila, O. H.Samuli"
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Compounding and characterization of recycled multilayer plastic films

Mechanical recycling of multilayer plastic films from food packages was investigated. The multilayer films were manually separated from municipal solid waste, washed, grinded, and finally compounded at 0–100 wt% concentrations with virgin low-density polyethylene (PE-LD). Polyethylene grafted with maleic anhydride (PE-g-MA) compatibilizer was used in two of the compounds to replace 2 and 5 wt% of the PE-LD to study its effect as well. PE-g-MA is expected to improve the mechanical properties of the compounds by promoting the adhesion between incompatible polymer phases. The composition of the compounds was characterized with Fourier-transform infrared spectroscopy and differential scanning calorimetry and their properties were studied with tensile testing and rotational rheometer measurements. All tested compounds had relatively good mechanical properties and processability. This indicates that recycled multilayer films could replace at least part of the virgin PE-LD in applications where high-thermal stability or good visual appearance is not required. The PE-g-MA compatibilizer did not have a significant effect on the mechanical properties of the compounds.

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Organisations: Research group: Tribology and Machine Elements, Materials Science and Environmental Engineering, Research group: Plastics and Elastomer Technology, Arcada, Fortum Waste Solutions Oy
Contributors: Jönkkäri, I., Poliakova, V., Mylläri, V., Anderson, R., Andersson, M., Vuorinen, J.
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ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry
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Source ID: 85079375444
Research output: Contribution to journal › Article › Scientific › peer-review

Reversible photodoping of TiO2 nanoparticles
Observations on strong photochromic effect of crystalline TiO2 quantum dots (mean size ≈ 4 nm) are presented. The synthesized quantum dots consist of irregularly shaped anatase TiO2 nanoparticles (NPs) and are dispersed in butanol (8 % by mass). Obtained NPs exhibit a dramatic photo-response to UV light, enabling effective transmittance modula-tion of in a broad wavelength range extending from visible to near-infrared region, and even the thermal black body radiation regime beyond 10 μm. The exceptional photo-response is attributed to hole-scavenging by butanol, TiO2 self-reduction, injection of electrons to the conduction band, and consequent localized surface plasmon resonances in NPs. Observed optical effect is reversible and the initial high transmittance state can be restored simply by exposing the NPs to air. Applied NP synthesis route is economic and can be easily scaled for applications such as smart window technol-ogies.

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Contributors: Joost, U., Sutka, A., Oja, M., Smits, K., Doebelin, N., Loot, A., Järvekülg, M., Hirsimäki, M., Valden, M., Nommiste, E.
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Avoiding the initial adhesive friction peak in fretting

An initial friction peak typically occurs in a dry self-mated quenched and tempered steel fretting contact in gross sliding conditions. The peak is related to adhesive friction and wear, which causes non-Coulomb friction. An early surface degradation including cracks may occur. To avoid such a peak, different media were studied using a flat-on-flat fretting test device with a large annular contact. All the media decreased the initial friction peak in comparison to the dry reference case, and in one series the peak was completely removed. The peak could often be delayed by lubrication. The steady-state coefficient of friction values mostly remained at similar levels to those of the dry contact, but decreased when oil was applied. Nevertheless, some surface damage occurred in every test, with varying amounts of wear.

General information

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Contributors: Juoksukangas, J., Hintikka, J., Lehtovaara, A., Mäntylä, A., Vaara, J., Frondelius, T.
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Research output: Contribution to journal › Article › Scientific › peer-review

Chemical and bacterial leaching of metals from a smelter slag in acid solutions

The purpose of this study was to assess the dissolution of Si, Fe, Cu and Zn from a smelter slag sample under acidic chemical and bacterial leaching conditions. The Cu-containing solid phases were Cu-sulfides (57% distribution), fayalite (18%) and metallic Cu (16%). Zn was mostly associated with fayalite, magnetite and Na-silicate phases (Σ94%). Two mixed cultures (HB1 and HB2) were enriched from samples taken from the slag lagoon site at the smelter location. Comparable results of metal dissolution were obtained with the two mixed cultures. The enrichment culture HB1 was characterized further by denaturing gradient gel electrophoresis (DGGE) of polymerase chain reaction amplified 16S rRNA genes. Based on the 16S rRNA gene sequences, culture HB1 contained at least Acidithiobacillus ferrivorans and Alicyclobacillus cycloheptanicus, with sequences of three DGGE bands matching distantly with Alicyclobacillus tolerans and Alicyclobacillus herbarium in the database. Alicyclobacillus spp. have not been previously associated with slag lagoons or slag bioleaching. Approximately 80% Cu and 25% Zn were dissolved from the slag (10% pulp) in shake flasks when S^0 was provided for the bacteria to produce H_2SO_4. Bioleaching in stirred tanks was conducted at controlled pH values and was practiced at pH levels promoting metal dissolution and suppressing iron and silicate solubilization from fayalite and Na-silicate. Chemical leaching at pH 2.3-4.0 did not yield substantial dissolution of valuable metals.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, CSIRO Land and Water Flagship, Boliden Harjavalta Oy, Department of Microbiology, Ohio State University
Contributors: Kaksonen, A. H., Särkijärvi, S., Puhakka, J. A., Peuraniemi, E., Junnikkala, S., Tuovinen, O. H.
Pages: 46-53
Publication date: 2016

Peer-reviewed: Yes
Early online date: 2015

Publication information
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Scopus rating (2016): CiteScore 4.1 SJR 1.154 SNIP 1.801
Original language: English
ASJC Scopus subject areas: Industrial and Manufacturing Engineering, Materials Chemistry, Metals and Alloys
Keywords: Acidithiobacillus, Alicyclobacillus, Bacterial leaching, Bioleaching, Chemical leaching, Smelter slag
DOIs:

10.1016/j.hydromet.2015.10.032
Source: Scopus
Source ID: 84946882317
Research output: Contribution to journal › Article › Scientific › peer-review

Recent progress in biohydrometallurgy and microbial characterisation
Since the discovery of microbiological metal dissolution, numerous biohydrometallurgical approaches have been developed to use microbially assisted aqueous extractive metallurgy for the recovery of metals from ores, concentrates, and recycled or residual materials. Biohydrometallurgy has helped to alleviate the challenges related to continually declining ore grades by transforming uneconomic ore resources to reserves. Engineering techniques used for biohydrometallurgy span from above ground reactor, vat, pond, heap and dump leaching to underground in situ leaching. Traditionally biohydrometallurgy has been applied to the bioleaching of base metals and uranium from sulfides and the biooxidation of sulfidic refractory gold ores and concentrates before cyanidation. More recently the interest in using bioleaching for oxide ore and waste processing, as well as extracting other commodities such as rare earth elements has been growing. Bioprospecting, adaptation, engineering and storing of microorganisms has increased the availability of suitable biocatalysts for biohydrometallurgical applications. Moreover, the advancement of microbial characterisation methods has increased the understanding of microbial communities and their capabilities in the processes. This paper reviews recent progress in biohydrometallurgy and microbial characterisation.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, CSIRO Land and Water, School of Biomedical Sciences, University of Western Australia, CSIRO Mineral Resources, Murdoch University
Contributors: Kaksonen, A. H., Boxall, N. J., Gumulya, Y., Khaleque, H. N., Morris, C., Bohu, T., Cheng, K. Y., Usher, K. M., Lakaniemi, A.
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Pages: 7-25
Publication date: 1 Sep 2018
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Volume: 180
ISSN (Print): 0304-386X
Ratings:

Scopus rating (2018): CiteScore 5.7 SJR 1.014 SNIP 1.852
Original language: English
ASJC Scopus subject areas: Industrial and Manufacturing Engineering, Metals and Alloys, Materials Chemistry
Keywords: Biohydrometallurgy, Bioleaching, Biooxidation, Characterisation, Microbiology
DOIs:

10.1016/j.hydromet.2018.06.018

Bibliographical note
EXT="Kaksonen, Anna H."
Source: Scopus
Source ID: 85049805480
Research output: Contribution to journal › Article › Scientific › peer-review

How conformational flexibility stabilizes the hyperthermophilic elongation factor G-domain
Proteins from thermophilic organisms are stable and functional well above ambient temperature. Understanding the molecular mechanism underlying such a resistance is of crucial interest for many technological applications. For some

time, thermal stability has been assumed to correlate with high mechanical rigidity of the protein matrix. In this work we address this common belief by carefully studying a pair of homologous G-domain proteins, with their melting temperatures differing by 40 K. To probe the thermal-stability content of the two proteins we use extensive simulations covering the microsecond time range and employ several different indicators to assess the salient features of the conformational landscape and the role of internal fluctuations at ambient condition. At the atomistic level, while the magnitude of fluctuations is comparable, the distribution of flexible and rigid stretches of amino-acids is more regular in the thermophilic protein causing a cage-like correlation of amplitudes along the sequence. This caging effect is suggested to favor stability at high T by confining the mechanical excitations. Moreover, it is found that the thermophilic protein, when folded, visits a higher number of conformational substates than the mesophilic homologue. The entropy associated with the occupation of the different substates and the thermal resilience of the protein intrinsic compressibility provide a qualitative insight on the thermal stability of the thermophilic protein as compared to its mesophilic homologue. Our findings potentially open the route to new strategies in the design of thermostable proteins.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Laboratoire de Biochimie Théorique, Université Paris Diderot, Centro S3
Contributors: Kalimeri, M., Rahaman, O., Melchionna, S., Sterpone, F.
Number of pages: 11
Pages: 13775-13785
Publication date: 7 Nov 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B
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Issue number: 44
ISSN (Print): 1520-6106
Ratings:

Scopus rating (2013): CiteScore 6.3 SJR 1.504 SNIP 1.195
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
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Bibliographical note
EXT="Kalimeri, Maria"
Source: Scopus
Source ID: 84887752230
Research output: Contribution to journal › Article › Scientific › peer-review

Are coarse-grained models apt to detect protein thermal stability? the case of OPEP force field
We present the first investigation of the kinetic and thermodynamic stability of two homologous thermophilic and mesophilic proteins based on the coarse-grained model OPEP. The object of our investigation is a pair of G-domains of relatively large size, 200 amino acids each, with an experimental stability gap of about 40 K. The OPEP force field is able to maintain stable the fold of these relatively large proteins within the hundred-nanosecond time scale without including external constraints. This makes possible to characterize the conformational landscape of the folded protein as well as to explore the unfolding. In agreement with all-atom simulations used as a reference, we show that the conformational landscape of the thermophilic protein is characterized by a larger number of substates with slower dynamics on the network of states and more resilient to temperature increase. Moreover, we verify the stability gap between the two proteins using replica-exchange simulations and estimate a difference between the melting temperatures of about 23 K, in fair agreement with experiment. The detailed investigation of the unfolding thermodynamics allows to gain insight into the mechanism underlying the enhanced stability of the thermophile relating it to a smaller heat capacity of unfolding.

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Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Laboratoire de Biochimie Théorique, Institut Universitaire de France
Contributors: Kalimeri, M., Derreumaux, P., Sterpone, F.
Number of pages: 8
Pages: 494-501

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Publication information
Journal: Journal of Non-Crystalline Solids
Volume: 407
ISSN (Print): 0022-3093
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Ceramics and Composites, Electronic, Optical and Magnetic Materials, Materials Chemistry
Keywords: Coarse-grained force field, Conformational substates network, Molecular dynamics, Protein thermodynamic stability, Thermophilic proteins
DOIs:

10.1016/j.jnoncrysol.2014.07.005
URLs:

http://www.scopus.com/inward/record.url?scp=84922435805&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84922435805
Research output: Contribution to journal › Article › Scientific › peer-review

Evaluation of crushing strength of spray-dried MgAl2O4 granule beds
The crushing strengths of four different experimental magnesium aluminate spinel (MgAl2O4) granule beds were monitored with the axial die pressing test after heat treatments. Precursor, magnesium hydroxide (Mg(OH)2) and magnesium oxide (MgO) as Mg precursor and aluminium oxide hydroxide Al(O)OH and α-Al2O3 as Al precursor, were used for experimental granules, which were manufactured via a dispersion manufacturing and spray-drying process. After spray-drying, granules were heat treated in air at 1000, 1100, 1200, 1300 and 1400 °C. In order to understand the potential effect of precursor, phase structure, morphology, particle size distribution and density of granules on crushing strength behaviour, scanning X-ray diffraction (XRD) was used together with electron microscopy (SEM) and laser diffraction (LDPA) for characterisation. All precursor mixtures formed spherical granules during the spray-drying process and pure spinel phase structure during heat treatment. The crushing strength test results indicated that the Al precursor clearly affected the crushing strength behaviour of experimental granule beds. The highest strength was observed for granule beds with Al(O)OH) as Al and Mg(OH)2 as Mg precursor.

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Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland
Contributors: Kanerva, U., Suhonen, T., Lagerbom, J., Levänen, E.
Number of pages: 7
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Peer-reviewed: Yes

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ISSN (Print): 0272-8842
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Scopus rating (2015): CiteScore 4 SJR 0.823 SNIP 1.353
Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Process Chemistry and Technology, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Axial pressing, Granule, MgAl<inf>2</inf>O<inf>4</inf> spinel, The crushing strength
DOIs:

10.1016/j.ceramint.2015.03.056
URLs:

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Bibliographical note
EXT="Lagerbom, Juha"
EXT="Kanerva, Ulla"

Source: Scopus
Source ID: 84929271760
Research output: Contribution to journal › Article › Scientific › peer-review

Chemical synthesis of WC-Co from water-soluble precursors: The effect of carbon and cobalt additions to WC synthesis
The chemical synthesis of WC-Co from water-soluble precursors and the effect of carbon content and cobalt addition were studied. Ammonium metatungstate AMT as tungsten source, glycine as a carbon source and cobalt acetate $Co(C_2H_3O_2)_2$ as a cobalt source was dissolved in water and spray-dried, and thermal synthesis in Ar atmosphere was performed. In order to understand the effects of carbon content and cobalt addition on synthesis steps, and the chemical and phase structure, thermogravimetry (TGA) with Differential Scanning Calorimetry (DCS) and mass spectrometry was used together with X-ray diffractometry and chemical analysis. The results reveal that carbon content mainly affected reduction temperatures and cobalt addition to reaction route and solid state synthesis temperature. This presented manufacturing route with water-soluble raw materials was a potential way of preparing nanostructural WC-Co composition with the correct phase structure and chemical composition.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Materials Characterization, VTT Technical Research Centre of Finland
Contributors: Kanerva, U., Karhu, M., Lagerbom, J., Kronlöf, A., Honkanen, M., Turunen, E., Laitinen, T.
Number of pages: 7
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Peer-reviewed: Yes

Publication information
Journal: International Journal of Refractory Metals and Hard Materials
Volume: 56
ISSN (Print): 0958-0611
Ratings:
Scopus rating (2016): CiteScore 4.3 SJR 1.065 SNIP 1.736
Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Materials Chemistry, Metals and Alloys, Mechanical Engineering , Mechanics of Materials
Keywords: Nano-sized WC-Co synthesis, Spray drying, Water soluble precursors
DOIs:
10.1016/j.ijrmhm.2015.11.014

Bibliographical note
EXT="Kanerva, Ulla"
EXT="Lagerbom, Juha"
Source: Scopus
Source ID: 84952359921
Research output: Contribution to journal › Article › Scientific › peer-review

Antibacterial polymer fibres by rosin compounding and melt-spinning
The antibacterial features of natural pine/spruce rosin are well established, yet the functionality in various thermoplastics has not been surveyed. This work focuses on the processing of industrial grade purified rosin mixed with polyethylene (PE), polypropylene (PP), polylactic acid (PLA), polyamide (PA)and corn starch based biopolymer (CS). Homopolymer masterbatches were extrusion-compounded and melt-spun to form fibres for a wide range of products, such as filters, reinforcements, clothing and medical textiles. Due to the versatile chemical structure of rosin, it was observed compatible with all the selected polymers. In general, the rosin-blended systems were shear-thinning in a molten condition. The doped fibres spun of PE and PP indicated adequate melt-spinning capability and proper mechanical properties in terms of ultimate strength and Young's modulus. The antibacterial response was found dependent on the selected polymer. Especially PE with a 10 wt% rosin content showed significant antibacterial effects against Escherichia coli DH5α and Staphylococcus aureus ATCC 12598 when analysed in the Ringer's solution for 24 h.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Plastics and Elastomer Technology, Department of Microbiology, Bundesanstalt für Materialforschung und -prüfung (BAM), Premix Oy, Aalto University, COMP Centre of Excellence, University of Helsinki

Contributors: Kanerva, M., Puolakka, A., Takala, T. M., Elert, A. M., Mylläri, V., Jönkkäri, I., Sarlin, E., Seitsonen, J., Ruokolainen, J., Saris, P., Vuorinen, J.
Publication date: Sep 2019
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Publication information
Journal: Materials Today Communications
Volume: 20
Article number: 100527
ISSN (Print): 2352-4928
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Scopus rating (2019): CiteScore 2.8 SJR 0.599 SNIP 0.917
Original language: English
ASJC Scopus subject areas: Materials Science(all), Mechanics of Materials, Materials Chemistry
Keywords: Antibacterial, Fibre, Melt spinning, Thermoplastics
Electronic versions:

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DOIs:

10.1016/j.mtcomm.2019.05.003
URLs:

http://urn.fi/URN:NBN:fi:tty-201906201900

Bibliographical note
EXT="Mylläri, V."
Source: Scopus
Source ID: 85066275027
Research output: Contribution to journal › Article › Scientific › peer-review

Reinforced chloroprene rubber by in situ generated silica particles: Evidence of bound rubber on the silica surface
Nano silica is generated in situ inside the uncrosslinked chloroprene rubber (CR) by the sol-gel reaction of tetraethoxysilane (TEOS). This results in appreciable improvement in mechanical properties of the CR composites at relatively low filler content. Furthermore, exploitation of reactive organosilanes, γ-aminopropyltrimethoxysilane (γ-APS) in particular, in the silica synthesis process facilitates growing of spherical silica particles with a size distribution in the range of 20-50 nm. The silica particles are found to be uniformly dispersed and they do not suffer from filler-filler interaction. Additionally, it is observed that the silica particles are coated by silane and rubber chains together which are popularly known as bound rubber. The existence of the bound rubber on silica surface has been supported by the detailed investigations with transmission electron microscopy (TEM), energy filtered transmission electron microscopy (EFTEM) and energy dispersive X-ray spectroscopy (EDAX). The interaction between rubber and silica, via bi-functionality of the γ-APS, has been explored by detailed FTIR studies.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Visvesvaraya National Institute of Technology, Leibniz-Institut für Polymerforschung Dresden E.V., Institut für Werkstoffwissenschaft
Contributors: Kapgate, B. P., Das, C., Das, A., Basu, D., Wiessner, S., Reuter, U., Heinrich, G.
Publication date: 10 Aug 2016
Peer-reviewed: Yes

Publication information
Journal: Journal of Applied Polymer Science
Volume: 133
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Article number: 43717
ISSN (Print): 0021-8995
Ratings:

Scopus rating (2016): CiteScore 3.9 SJR 0.588 SNIP 0.815
Original language: English
ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)
Keywords: bound rubber, in situ silica and silane treatment, transmission electron microscopy
DOIs:

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Source: Scopus
Source ID: 84964925986

Research output: Contribution to journal › Article › Scientific › peer-review

Effect of silane integrated sol-gel derived in situ silica on the properties of nitrile rubber

Nitrile rubber/silica composites are prepared by a sol-gel process using tetraethoxysilane as precursor in the presence of γ- mercaptopropyltrimethoxysilane as a silane coupling agent. Here, we follow a novel processing route where the silica particles are generated inside the rubber matrix before compounding with vulcanizing ingredients. The effect of in situ generated silanized silica on the properties of the rubber composite has been evaluated by studying curing characteristics, morphology, mechanical and dynamic mechanical properties. Enhanced rubber-filler interaction of these composites is revealed from stress-strain studies and dynamic mechanical analysis. Excessive use of silane shows an adverse effect on mechanical properties of the composites. Due to finer dispersed state of the in situ silica and enhanced rubber-filler interaction, the mechanical properties and thermal stability of the composites are improved compared to corresponding ex situ processed composite.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Visvesvaraya National Institute of Technology, Vodafone Department of Mobile Communications Systems, Leibniz-Institut für Polymerforschung Dresden E.V.
Contributors: Kapgate, B. P., Das, C., Basu, D., Das, A., Heinrich, G., Reuter, U.
Publication date: 5 Aug 2014
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Publication information

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Volume: 131
Issue number: 15
Article number: 40531
ISSN (Print): 0021-8995
Ratings:

Scopus rating (2014): CiteScore 3.2 SJR 0.664 SNIP 0.98
Original language: English
ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)
Keywords: elastomers, mechanical properties, morphology, rheology, structure-property relations
DOIs:

10.1002/app.40531
URLs:

http://www.scopus.com/inward/record.url?scp=84900485659&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84900485659
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of sol-gel derived in situ silica on the morphology and mechanical behavior of natural rubber and acrylonitrile butadiene rubber blends

Silica particles were generated and grown in situ by sol-gel method into rubber blends comprised of natural rubber (NR) and acrylonitrile butadiene rubber (NBR) at various blend ratios. Silica formed into rubber matrix was amorphous in nature. Amount of in situ silica increased with increase in natural rubber proportion in the blends during the sol-gel process. Morphology studies showed that the generated in situ silica were nanoparticles of different shapes and sizes mostly grown into the NR phase of the blends. In situ silica filled NR/NBR blend composites showed improvement in the mechanical and dynamic mechanical behaviors in comparison to those of the unfilled and externally filled NR/ NBR blend composites. For the NR/NBR blend at 40/60 composition, in particular, the improvement was appreciable where size and dispersion of the silica particles into the rubber matrix were found to be more uniform. Dynamic mechanical analysis revealed a strong rubber-in situ silica interaction as indicated by a positive shift of the glass transition temperature of both the rubber phases in the blends.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Visvesvaraya National Institute of Technology, Leibniz-Institut für Polymerforschung Dresden E.V.
Contributors: Kapgate, B. P., Das, C., Das, A., Basu, D., Reuter, U., Heinrich, G.
Number of pages: 9
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Peer-reviewed: Yes

Publication information
Journal: JOURNAL OF SOL-GEL SCIENCE AND TECHNOLOGY
Volume: 63
Issue number: 3
ISSN (Print): 0928-0707
Ratings:

Scopus rating (2012): CiteScore 2.8 SJR 0.732 SNIP 1.133
Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Biomaterials, Ceramics and Composites, Electronic, Optical and Magnetic Materials, Materials Chemistry
Keywords: In situ silica, Reinforcement, Rubber blend, Rubber-filler interaction, Sol-gel
DOIs:

10.1007/s10971-012-2812-9
URLs:

http://www.scopus.com/inward/record.url?scp=84875426374&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84875426374
Research output: Contribution to journal › Article › Scientific › peer-review

Mining tailings as raw materials for reaction-sintered aluminosilicate ceramics: Effect of mineralogical composition on microstructure and properties

This paper presents studies on the utilization of aluminosilicate-based mining tailings as raw materials for mullite-based ceramics. Based on the 3:2 stoichiometric composition, mullite was synthesised by reactive sintering with a series of powder mixtures with alumina additions. X-ray diffractometry and scanning electron microscopy analyses revealed that, at the specific mineralogical composition, mullite structure formed surrounded by an amorphous glass phase in reaction-sintered powder mixtures. Results demonstrated that the chemical and mineralogical composition of mining tailings do have an effect on mullite formation possibilities and, only with the particular mineralogical composition, the mullite formation is possible regardless of the correct Al:Si ratio in tailings. Physical and mechanical properties of the formed ceramics were defined, showing comparable values to 3:2 mullite reference. Mullite structure formation enables a better thermal resistance up to above 1450 °C of the formed tailings-based ceramics compared to other aluminosilicates, reflecting their utilization potential for refractory ceramic applications.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Materials Characterization, VTT Technical Research Centre of Finland , Geologian tutkimuskeskus
Contributors: Karhu, M., Lagerbom, J., Solismaa, S., Honkanen, M., Ismailov, A., Räisänen, M. L., Huttunen-Saarivirta, E. , Levänen, E., Kivikytö-Reponen, P.
Pages: 4840-4848
Publication date: Mar 2019
Peer-reviewed: Yes
Early online date: 2018

Publication information
Journal: Ceramics International
Volume: 45
Issue number: 4
ISSN (Print): 0272-8842
Ratings:

Scopus rating (2019): CiteScore 6.1 SJR 0.891 SNIP 1.31
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Ceramics and Composites, Process Chemistry and Technology, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Mining tailings, Mullite, Reaction sintering, Refractory ceramics, Utilization
DOIs:

10.1016/j.ceramint.2018.11.180

Bibliographical note
EXT="Lagerbom, Juha"
Source: Scopus
Source ID: 85057276435
Research output: Contribution to journal › Article › Scientific › peer-review

Mining tailings as a raw material for glass-bonded thermally sprayed ceramic coatings: Microstructure and properties
Magnesium aluminate, $MgAl_2O_4$, spinel powders for thermal spraying, were synthesized from secondary raw materials by spray drying and subsequent reaction sintering. Talc ore mining tailings and aluminium hydroxide precipitate from aluminium anodizing process were studied. A stoichiometric $MgAl_2O_4$ spinel coating was prepared as a reference using pure raw materials. Atmospheric plasma spraying resulted in the formation of ceramic coatings. Microstructural investigations revealed that the reference coatings exhibited crystalline lamellar microstructure of $MgAl_2O_4$ but secondary coatings contained amorphous areas between the crystalline $MgAl_2O_4$ clusters. Abrasive wear test results revealed considerably lower wear rate for secondary coatings. It is suggested that the different structure of coatings, particularly the high degree of amorphous phase between the isolated crystalline $MgAl_2O_4$ clusters caused the higher abrasive wear resistance by changing the wear mechanism. The dielectric breakdown strength of the secondary coatings were at the same level, 24 V/μm, as compared to reference coating, 23 V/μm.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Research group: Materials Characterization, Materials Science and Environmental Engineering, Research group: Surface Engineering, VTT Technical Research Centre of Finland, Geologian tutkimuskeskus
Contributors: Karhu, M., Lagerbom, J., Honkanen, M., Huttunen-Saarivirta, E., Kiilakoski, J., Vuoristo, P., Solismaa, S., Kivikytö-Reponen, P.
Number of pages: 11
Pages: 4111-4121
Publication date: 2020
Peer-reviewed: Yes

Publication information
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Volume: 40
Issue number: 12
ISSN (Print): 0955-2219
Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Materials Chemistry
Keywords: Ceramic coating, Circular economy, MgAlO spinel, Mining tailings, Thermal spray
DOIs:
10.1016/j.jeurceramsoc.2020.04.038
Source: Scopus
Source ID: 85084507525
Research output: Contribution to journal › Article › Scientific › peer-review

Oxidation of cholesterol does not alter significantly its uptake into high-density lipoprotein particles
Using replica exchange umbrella sampling we calculated free energy profiles for uptake of cholesterol and one of its oxysterols (7-ketocholesterol) from an aqueous solution into a high-density lipoprotein particle. These atomistic molecular dynamics simulations show that both sterols are readily taken up from the aqueous solution with comparable free energy minima at the surface of the particle of-17 kcal/mol for cholesterol and-14 kcal/mol for 7-ketocholesterol. Moreover, given its preferred position at the particle surface, 7-ketocholesterol is expected to be able to participate directly in biological signaling processes.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), University of Southern Denmark, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
Contributors: Karilainen, T., Timr, Š., Vattulainen, I., Jungwirth, P.
Number of pages: 7
Pages: 4594-4600
Publication date: 2 Apr 2015
Peer-reviewed: Yes

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Volume: 119
Issue number: 13
ISSN (Print): 1520-6106
Ratings:

Scopus rating (2015): CiteScore 5.9 SJR 1.335 SNIP 1.058
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
DOIs:

10.1021/acs.jpcb.5b00240
URLs:

http://www.scopus.com/inward/record.url?scp=84926433475&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84926433475
Research output: Contribution to journal › Article › Scientific › peer-review

Soft hydrazone crosslinked hyaluronan- and alginate-based hydrogels as 3D supportive matrices for human pluripotent stem cell-derived neuronal cells

Regenerative medicine, especially cell therapy combined with a supportive biomaterial scaffold, is considered to be a potential treatment for various deficits in humans. Here, we have produced and investigated the detailed properties of injectable hydrazone crosslinked hyaluronan-polyvinyl alcohol (HA-PVA) and alginate-polyvinyl alcohol (AL-PVA) hydrogels to be used as a supportive biomaterial for 3D neural cell cultures. To the best of our knowledge, this is the first time the polymerization and properties of hydrazone crosslinked AL-PVA hydrogel have been reported. The effect of the degree of substitution and molecular weight of the polymer components as well as the polymer concentration of the hydrogel on the swelling, degradation and mechanical properties of the hydrogels is reported. Furthermore, we studied the effect of the above parameters on the growth of human pluripotent stem cell-derived neuronal cells. The most neural cell supportive HA-PVA hydrogel was composed of high molecular weight HA component with brain-mimicking mechanical properties and decreased polymer concentration. AL-PVA hydrogel, with stiffness quite similar to brain tissue, was also shown to be similarly supportive. Neuronal spreading and 3D network formation was enhanced inside the softest hydrogels.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Faculty of Biomedical Sciences and Engineering, Research group: Biomaterials and Tissue Engineering Group, BioMediTech Institute and Faculty of Medicine and Life Sciences
Contributors: Karvinen, J., Joki, T., Ylä-Outinen, L., Koivisto, J. T., Narkilahti, S., Kellomäki, M.
Number of pages: 11
Pages: 29-39
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Publication information

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Ratings:

Scopus rating (2018): CiteScore 4.9 SJR 0.712 SNIP 0.92
Original language: English
ASJC Scopus subject areas: Chemistry(all), Environmental Chemistry, Biochemistry, Chemical Engineering(all), Polymers and Plastics, Materials Chemistry
Keywords: 3D neuronal culture, Alginate, Hyaluronan, Hydrazone, Hydrogel
DOIs:

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Source: Scopus
Source ID: 85040229275
Research output: Contribution to journal › Article › Scientific › peer-review

Stability and Function at High Temperature. What Makes a Thermophilic GTPase Different from Its Mesophilic Homologue

Comparing homologous enzymes adapted to different thermal environments AIDS to shed light on their delicate stability/function trade-off. Protein mechanical rigidity was postulated to secure stability and high-temperature functionality of thermophilic proteins. In this work, we challenge the corresponding-state principle for a pair of homologous GTPase domains by performing extensive molecular dynamics simulations, applying conformational and kinetic clustering, as well as exploiting an enhanced sampling technique (REST2). While it was formerly shown that enhanced protein flexibility and high temperature stability can coexist in the apo hyperthermophilic variant, here we focus on the holo states of both homologues by mimicking the enzymatic turnover. We clearly show that the presence of the ligands affects the conformational landscape visited by the proteins, and that the corresponding state principle applies for some functional

modes. Namely, in the hyperthermophilic species, the flexibility of the effector region ensuring long-range communication and of the P-loop modulating ligand binding are recovered only at high temperature.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research area: Computational Physics, Laboratoire de Biochimie Théorique
Contributors: Katava, M., Kalimeri, M., Stirnemann, G., Sterpone, F.
Number of pages: 10
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Publication information
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Ratings:

Scopus rating (2016): CiteScore 6.1 SJR 1.345 SNIP 1.023
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
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Source: Scopus
Source ID: 84961282502
Research output: Contribution to journal › Article › Scientific › peer-review

The effect of carbon and nickel additions on the precursor synthesis of Cr_3C_2-Ni nanopowder

Decreasing crystal size to nanoscale is a proven method to enhance material properties. In this study, nanosize Cr_3C_2 and Cr_3C_2-Ni were synthetized and the reaction sequence was studied. Aqueous precursors using only water-soluble raw materials with varying carbon contents and a nickel addition were spray-dried. Glycine was used as a carbon source and chromium acetate hydroxide as a chromium source in the precursor solutions. Nickel nitrate hexahydrate was introduced as a nickel source to yield a metallic binder into the carbide nanopowder.Resulting powders were heat-treating to identify an applicable precursor composition producing the targeted Cr_3C_2 phase with crystal size of tens of nanometers. Thermal synthesis tests of the precursor powders to yield Cr_3C_2 took place at a temperature between 900 and 1300 °C under an Argon atmosphere. The synthesis of nanosize Cr_3C_2-Ni powder was successful at 1000 °C in 30 min, in a case of the best precursor. In order to produce the carbide phase with no residual oxide traces, relative carbon load has to be 48 wt%, while the stoichiometric amount of carbon in Cr_3C_2 is 13 wt%. When also introducing the nickel source into the precursor, an even higher carbon load was required. The carbon surplus needed to enable the Cr_3C_2 synthesis attributes to the non-homogeneity of the precursor composition.The chemical synthesis starting from water-soluble raw materials is a promising way of preparing nanosize Cr_3C_2-Ni with the targeted phase configuration.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Materials Characterization, VTT Technical Research Centre of Finland
Contributors: Kaunisto, K., Kotilainen, M., Karhu, M., Lagerbom, J., Vuorinen, T., Honkanen, M., Vippola, M., Turunen, E.
Pages: 9338-9346
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Early online date: 2018

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ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Ceramics and Composites, Process Chemistry and Technology, Surfaces, Coatings and Films, Materials Chemistry
Keywords: A. Nanosize CrC synthesis, A. Powders: chemical preparation, B. Grain size, D. Carbides, E. Wear parts
DOIs:

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Bibliographical note
EXT="Vuorinen, Tommi"
EXT="Lagerbom, Juha"
EXT="Kaunisto, Kimmo"
Source: Scopus
Source ID: 85042300396
Research output: Contribution to journal › Article › Scientific › peer-review

Spectroscopic study of a DNA brush synthesized in situ by surface initiated enzymatic polymerization
We used a combination of synchrotron-based X-ray photoelectron spectroscopy (XPS) and angle-resolved near-edge X-ray absorption fine structure (NEXAFS) spectroscopy to study the chemical integrity, purity, and possible internal alignment of single-strand (ss) adenine deoxynucleotide (poly(A)) DNA brushes. The brushes were synthesized by surface-initiated enzymatic polymerization (SIEP) on a 25-mer of adenine self-assembled monolayer (SAM) on gold (A25-SH), wherein the terminal 3′-OH of the A25-SH serve as the initiation sites for SIEP of poly(A). XPS and NEXAFS spectra of poly(A) brushes were found to be almost identical to those of A25-SH initiator, with no unambiguous traces of contamination. Apart from the well-defined chemical integrity and contamination-free character, the brushes were found to have a high degree of orientational order, with an upright orientation of individual strands, despite their large thickness up to ~55 nm, that corresponds to a chain length of at least several hundred nucleotides for individual ssDNA molecules. The orientational order exhibited by these poly(A) DNA brushes, mediated presumably by base stacking, was found to be independent of the brush thickness as long as the packing density was high enough. The well-defined character and orientational ordering of the ssDNA brushes make them a potentially promising system for different applications.

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MoE publication type: A1 Journal article-refereed
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Universitat Heidelberg, Duke University
Contributors: Khan, M. N., Tjong, V., Chilkoti, A., Zharnikov, M.
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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
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Source: Scopus
Source ID: 84883395998
Research output: Contribution to journal › Article › Scientific › peer-review

Ultrafast Photochemistry of the $[Cr(NCS)_6]^{3-}$ Complex in Dimethyl Sulfoxide and Dimethylformamide upon Excitation into Ligand-Field Electronic State
The ultrafast photochemistry of the $[Cr(NCS)_6]^{3-}$ complex upon excitation to the $^4T_2$ ligand-field (LF) state was studied in dimethyl sulfoxide (DMSO) and N,N-dimethylformamide (DMF) in a wide temporal range (100 fs to 9 ms) by a combination of femtosecond and nanosecond transient absorption spectroscopy techniques and supported by quantum-chemical DFT/TD-DFT calculations. The initially excited $^4T_2$ state undergoes intersystem crossing to the vibrationally hot ^2E state with time constants of 1.1 ± 0.2 and 1.8 ± 0.1 ps in DMSO and DMF, respectively. Vibrational relaxation occurs in the same time scale and takes 1-5 ps. A major part of the $[Cr(NCS)_6]^{3-}$ complex in the ^2E state undergoes intersystem crossing to the ground state with time constants of 65 ± 5 and 85 ± 5 ns in DMSO and DMF, respectively. A minor part of electronically excited $[Cr(NCS)_6]^{3-}$ undergoes irreversible photochemical decomposition. In DMSO, the photolysis of the $[Cr(NCS)_6]^{3-}$ complex results in single or double isothiocyanate ion release followed by the coordination of the solvent molecules with a time constant of 1 ± 0.2 ms.

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials, St. Petersburg State University, Russian Academy of Science
Contributors: Khvorost, T. A., Beliaev, L. Y., Potalueva, E., Laptenkova, A. V., Selyutin, A. A., Bogachev, N. A., Skripkin, M. Y., Ryazantsev, M. N., Tkachenko, N., Mereshchenko, A. S.
Number of pages: 10
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Peer-reviewed: Yes

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ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry
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Source: Scopus
Source ID: 85084379376
Research output: Contribution to journal › Article › Scientific › peer-review

Characterization of High-Velocity Single Particle Impacts on Plasma-Sprayed Ceramic Coatings
High-velocity impact wear can have a significant effect on the lifetime of thermally sprayed coatings in multiple applications, e.g., in the process and paper industries. Plasma-sprayed oxide coatings, such as Cr_2O_3- and TiO_2-based coatings, are often used in these industries in wear and corrosion applications. An experimental impact study was performed on thermally sprayed ceramic coatings using the High-Velocity Particle Impactor (HVPI) at oblique angles to investigate the damage, failure, and deformation of the coated structures. The impact site was characterized by profilometry, optical microscopy, and scanning electron microscopy (SEM). Furthermore, the connection between the microstructural details and impact behavior was studied in order to reveal the damage and failure characteristics at a more comprehensive level. Differences in the fracture behavior were found between the thermally sprayed Cr_2O_3 and TiO_2 coatings, and a concept of critical impact energy is presented here. The superior cohesion of the TiO_2 coating inhibited interlamellar cracking while the Cr_2O_3 coating suffered greater damage at high impact energies. The HVPI experiment has proven to be able to produce valuable information about the deformation behavior of coatings under high strain rates and could be utilized further in the development of wear-resistant coatings.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Materials Characterization
Contributors: Kiilakoski, J., Lindroos, M., Apostol, M., Koivuluoto, H., Kuokkala, V., Vuoristo, P.
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Pages: 1127-1137
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Volume: 25
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films
Keywords: electron microscopy, fracture, impact wear, thermal spray coatings, wear testing
Electronic versions:

Kiilakoski et al JTST 2016_Accepted
DOIs:

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URLs:

http://urn.fi/URN:NBN:fi:tty-201801161083

Source: Scopus
Source ID: 84976320961
Research output: Contribution to journal › Article › Scientific › peer-review

Evaluating the toughness of APS and HVOF-sprayed Al_2O_3-ZrO_2-coatings by in-situ- and macroscopic bending

Thermally-sprayed ceramic coatings are commonly used in applications where high wear and corrosion resistance are essential. However, their inherently low toughness and resistance to impacts often limit their use. In bulk ceramics, the toughening effect of ZrO_2 has been successfully implemented in different compositions of Al_2O_3-ZrO_2. Successful toughening leads to increased wear resistance and higher reliability. In this study, APS- and HVOF-sprayed Al_2O_3-40ZrO_2 coatings were characterized with SEM and XRD techniques. The toughness of the coatings was evaluated by measuring their strain tolerance with in-situ (SEM) three-point-bending and macroscopic four-point bending with acoustic emission instrumentation. The APS-coatings had a higher strain-to-fracture but failed abruptly. In HVOF-coatings, the cracking commenced earlier but proceeded slower with more crack deflections. The observed behaviour is likely to derive from the coarser microstructure of the APS-coatings, which allows strain distribution in a larger area unlike the finer structure with a lesser melting degree of the HVOF-coatings.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Surface Engineering, Institute of Plasma Physics, Academy of Sciences of the Czech Republic
Contributors: Kiilakoski, J., Musalek, R., Lukac, F., Koivuluoto, H., Vuoristo, P.
Pages: 1908-1918
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Peer-reviewed: Yes
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Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Materials Chemistry
Keywords: AlO-ZrO, Fracture, Mechanical testing, Thermal spray, Toughening
Electronic versions:

Kiilakoski et al. JECS 2017_Accepted version. Embargo ended: 2/12/19
DOIs:

10.1016/j.jeurceramsoc.2017.11.056
URLs:

http://urn.fi/URN:NBN:fi:tty-201801161085. Embargo ended: 2/12/19
Source: Scopus
Source ID: 85035355737
Research output: Contribution to journal › Article › Scientific › peer-review

Characterizing the micro-impact fatigue behavior of APS and HVOF-sprayed ceramic coatings

The fatigue life of thermally sprayed Al_2O_3- and Cr_2O_3-based coatings has been studied under low-energy (0.7–5 mJ) impact conditions. A threshold impact energy and amount of repetitions the coatings can endure with said energy before catastrophic failure was obtained. The catastrophic failure was determined to occur when the fracture mode of the coating switched from brittle cone cracking to quasi-plastic radial cracking. The results are examined relative to the microstructural features along with other properties of the coatings - hardness and cavitation resistance. The experiment provided a new approach for a straightforward comparison of the micro-scale impact fatigue life of thermally sprayed coatings unachievable with previous methods.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Université Bourgogne Franche-Comté - ICB - UTBM - LERMPS
Contributors: Kiilakoski, J., Langlade, C., Koivuluoto, H., Vuoristo, P.
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Original language: English
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Keywords: Ceramic coating, Characterization, Fracture, Impact test, Surface fatigue, Thermal spray
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10.1016/j.surfcoat.2018.10.097
URLs:

http://urn.fi/URN:NBN:fi:tty-201812202888
Source: Scopus
Source ID: 85055977332
Research output: Contribution to journal › Article › Scientific › peer-review

Characterization of Powder-Precursor HVOF-Sprayed Al_2O_3-YSZ/ZrO_2 Coatings

Thermal spraying using liquid feedstock can produce coatings with very fine microstructures either by utilizing submicron particles in the form of a suspension or through in situ synthesis leading, for example, to improved tribological properties. The focus of this work was to obtain a bimodal microstructure by using simultaneous hybrid powder-precursor HVOF spraying, where nanoscale features from liquid feedstock could be combined with the robustness and efficiency of spraying with powder feedstock. The nanostructure was achieved from YSZ and ZrO_2 solution-precursors, and a conventional Al_2O_3 spray powder was responsible for the structural features in the micron scale. The microstructures of the coatings revealed some clusters of unmelted nanosized YSZ/ZrO_2 embedded in a lamellar matrix of Al_2O_3. The phase compositions consisted of γ- and α-Al_2O_3 and cubic, tetragonal and monoclinic ZrO_2. Additionally, some alloying of the constituents was found. The mechanical strength of the coatings was not optimal due to the excessive amount of the nanostructured YSZ/ZrO_2 addition. An amount of 10 vol.% or 7 wt.% 8YSZ was estimated to result in a more desired mixing of constituents that would lead to an optimized coating architecture.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, ELCOGEN OY, Univ of Oulu
Contributors: Kiilakoski, J., Puranen, J., Heinonen, E., Koivuluoto, H., Vuoristo, P.
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Publication date: Jan 2019
Peer-reviewed: Yes
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Volume: 28
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Scopus rating (2019): CiteScore 4.7 SJR 0.71 SNIP 1.281
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
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DOIs:

10.1007/s11666-018-0816-x
URLs:

http://urn.fi/URN:NBN:fi:tty-201901081028
Source: Scopus
Source ID: 85058214735
Research output: Contribution to journal › Article › Scientific › peer-review

Process Parameter Impact on Suspension-HVOF-Sprayed Cr_2O_3 Coatings

Chromium oxide (Cr_2O_3) is commonly used as an atmospheric plasma-sprayed (APS) coating from powder feedstock in applications requiring resistance to sliding wear and corrosion, as well as amenability to texturing, e.g., in anilox rolls. Recently, high-velocity oxy-fuel spray methods involving suspension feedstock have been considered an extremely promising alternative to produce denser and more homogeneous chromium oxide coatings with lower as-sprayed surface roughness, higher hardness and potentially superior wear performance compared to conventional APS-sprayed coatings. In this study, the impact of process parameters namely auxiliary air cleaning nozzles and a transverse air curtain on suspension high-velocity oxy-fuel-sprayed Cr_2O_3 suspensions is presented. The produced coatings are characterized for their microstructure, mechanical properties and wear resistance by cavitation erosion. The results reveal the importance of optimized air nozzles and air curtain to achieve a vastly improved coating structure and performance.

General information

Publication status: E-pub ahead of print
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Surface Engineering, Treibacher Industrie AG, University West
Contributors: Kiilakoski, J., Trache, R., Björklund, S., Joshi, S., Vuoristo, P.
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ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
Keywords: CrO, influence of spray parameters, mechanical properties, SHVOF, suspension spraying
Electronic versions:

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DOIs:

10.1007/s11666-019-00940-7
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Source: Scopus
Source ID: 85074710199
Research output: Contribution to journal › Article › Scientific › peer-review

Accurate description of calcium solvation in concentrated aqueous solutions

Calcium is one of the biologically most important ions; however, its accurate description by classical molecular dynamics simulations is complicated by strong electrostatic and polarization interactions with surroundings due to its divalent nature. Here, we explore the recently suggested approach for effectively accounting for polarization effects via ionic charge rescaling and develop a new and accurate parametrization of the calcium dication. Comparison to neutron scattering and viscosity measurements demonstrates that our model allows for an accurate description of concentrated aqueous calcium chloride solutions. The present model should find broad use in efficient and accurate modeling of calcium in aqueous environments, such as those encountered in biological and technological applications.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
Contributors: Kohagen, M., Mason, P. E., Jungwirth, P.
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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films, Medicine(all)
DOIs:

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Source: Scopus
Source ID: 84904581115
Research output: Contribution to journal › Article › Scientific › peer-review

Novel Online Diagnostic Analysis for In-Flight Particle Properties in Cold Spraying

In cold spraying, powder particles are accelerated by preheated supersonic gas stream to high velocities and sprayed on a substrate. The particle velocities depend on the equipment design and process parameters, e.g., on the type of the process gas and its pressure and temperature. These, in turn, affect the coating structure and the properties. The particle velocities in cold spraying are high, and the particle temperatures are low, which can, therefore, be a challenge for the diagnostic methods. A novel optical online diagnostic system, HiWatch HR, will open new possibilities for measuring particle in-flight properties in cold spray processes. The system employs an imaging measurement technique called S-PTV (sizing-particle tracking velocimetry), first introduced in this research. This technique enables an accurate particle size measurement also for small diameter particles with a large powder volume. The aim of this study was to evaluate the velocities of metallic particles sprayed with HPCS and LPCS systems and with varying process parameters. The measured in-flight particle properties were further linked to the resulting coating properties. Furthermore, the camera was able to provide information about variations during the spraying, e.g., fluctuating powder feeding, which is important from the process control and quality control point of view.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Surface Engineering, Oseir Ltd.
Contributors: Koivuluoto, H., Matikainen, V., Larjo, J., Vuoristo, P.
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Ratings:

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ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
Keywords: cold spraying, diagnostics, in-flight properties, particle size, particle velocity
DOIs:

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Source ID: 85040347243
Research output: Contribution to journal › Article › Scientific › peer-review

Cold-Sprayed Al6061 coatings: Online spray monitoring and influence of process parameters on coating properties

Process optimization and quality control are important issues in cold spraying and coating development. Because the cold spray processing is based on high kinetic energy by high particle velocities, online spray monitoring of particle inflight properties can be used as an assisting process tool. Particle velocities, their positions in the spray jet, and particle size measurements give valuable information about spraying conditions. This, in turn, improves reproducibility and reliability of coating production. This study focuses on cold spraying of Al6061 material and the connections between particle inflight properties and coating characteristics such as structures and mechanical properties. Furthermore, novel 2D velocity scan maps done with theHWCS2 online spray monitoring system are presented as an advantageous powder and spray condition controlling tool. Cold spray processing conditions were similar using different process parameters, confirmed with the online spray monitoring prior to coating production. Higher particle velocities led to higher particle deformation and

thus, higher coating quality, denser structures, and improved adhesions. Also, deposition efficiency increased significantly by using higher particle velocities.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Surface Engineering, Oseir Ltd., Sapienza University
Contributors: Koivuluoto, H., Larjo, J., Marini, D., Pulci, G., Marra, F.
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Peer-reviewed: Yes

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Article number: 348
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ASJC Scopus subject areas: Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
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Electronic versions:

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Source: Scopus
Source ID: 85083845948
Research output: Contribution to journal › Article › Scientific › peer-review

Calculated electronic density of states and structural properties of tetrahedral amorphous carbon

A series of tetrahedral amorphous carbon structures with different microscopic mass densities was generated by calculations based on the density functional theory with a local density approximation and using a method of melting-cooling cycles. A detailed investigation of the properties of the simulated structures has been carried out. Particularly, the short-range order, nearest neighbour distances, fractions of sp^1, sp^2 and sp^3 sites, average C-C-C bond angles and electronic density of states have been analyzed. The simulated structures and calculated properties are in good agreement with those obtained by others and with the experimental data. An unexpected observation is the presence of planar structures, which are typical for graphite, in the sample with low density. In addition, the nearest neighbour distance in the sample with mass density 3.54 g/cm^3 is different from those reported previously. Possibilities to compare the density of states obtained from the simulations with the experimental results from scanning tunnelling spectroscopy and X-ray near edge spectrum are discussed.

General information

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Organisations: University of Oulu, Department of Physical Sciences
Contributors: Koivusaari, K. J., Rantala, T. T., Leppävuori, S.
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Peer-reviewed: Yes

Publication information

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Issue number: 3
ISSN (Print): 0925-9635
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Scopus rating (2000): SJR 1.393 SNIP 0.943
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces
DOIs:

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Source ID: 0033748066
Research output: Contribution to journal › Article › Scientific › peer-review

Both zundel and eigen isomers contribute to the IR spectrum of the gas-phase H9O4 + cluster

The "Eigen cation", $H_3O^+(H_2O)_3$, is the most prevalent protonated water structure in the liquid phase and the most stable gas-phase isomer of the $H^+(H_2O)_4$ cluster. Nevertheless, its 50 K argon predissociation vibrational spectrum contains unexplainable low frequency peak(s). We have simulated the IR spectra of 10 gas-phase $H^+(H_2O)_4$ isomers, that include zero to three argon ligands, using dipole autocorrelation functions from ab initio molecular dynamics with the CP2K software. We have also tested the effect of elevated temperature and dispersion correction. The Eigen isomers describe well the high frequency portion of the spectrum but do not agree with experiment below 2000 cm^{-1}. Most notably, they completely lack the "proton transfer bands" observed at 1050 and 1750 cm^{-1}, which characterize Zundel-type (H_5O_2+) isomers. In contrast, linear isomers with a Zundel core, although not the lowest in energy, show very good agreement with experiment, particularly at low frequencies. Peak assignments made with partial velocity autocorrelation functions verify that the 1750 cm^{-1} band does not originate with the Eigen isomer but is rather due to coupled proton transfer/water bend in the Zundel isomer.

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MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Tallinn Technical University, Institute of Chemistry, Hebrew University of Jerusalem
Contributors: Kulig, W., Agmon, N.
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Source: Scopus
Source ID: 84892594412
Research output: Contribution to journal › Article › Scientific › peer-review

Microphase mechanism of "superquenching" of luminescent probes in aqueous solutions of DNA and some other polyelectrolytes

A new approach in terms of microphase model of aqueous solutions of polyelectrolytes is proposed for explanation of a very strong quenching of luminescent probes ("superquenching") in these solutions. This phenomenon is used in literature for creation of extremely sensitive chemical and biosensors and was attributed predominantly to efficient energy or electron transfer. Microphase approach considers this phenomenon in terms of local concentrations of both the luminescent compound and of the quencher in microphase, formed by DNA and other polyelectrolytes, which can be several (4-10) orders of magnitude greater than their apparent concentrations in solution. Large local concentrations of the light absorbing centers in the microphase also provide conditions for aggregation of these centers and efficient energy transfer, which provides a significant increase in quenching constants (~10^2-10^5). Microphase approach provides good quantitative description of all the features of the superquenching, new possibilities for analysis and control of kinetics of DNA reactions, and for improvement of the sensitivity of luminescent sensors. It reveals nonspecific localization of the luminescent centers and of Au_n nanoparticles in different positions of DNA molecules that hinders from the simultaneous use of optical methods and electron or tunneling microscopy for the combined study of the structure of DNA.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Moscow State University, Emanuel' Institute of Biochemical Physics, Russian Academy of Sciences
Contributors: Kuzmin, M. G., Soboleva, I. V., Durandin, N. A., Lisitsyna, E. S., Kuzmin, V. A.
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Source: Scopus
Source ID: 84899003075
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of Phosphatidic Acid on Biomembrane: Experimental and Molecular Dynamics Simulations Study
We consider the impact of phosphatidic acid (namely, 1,2-dioleoyl-sn-glycero-3-phosphate, DOPA) on the properties of a zwitterionic (1,2-dipalmitoyl-sn-glycero-3-phosphocholine, DPPC) bilayer used as a model system for protein-free cell membranes. For this purpose, experimental measurements were performed using differential scanning calorimetry and the Langmuir monolayer technique at physiological pH. Moreover, atomistic-scale molecular dynamics (MD) simulations were performed to gain information on the mixed bilayer's molecular organization. The results of the monolayer studies clearly showed that the DPPC/DOPA mixtures are nonideal and the interactions between lipid species change from attractive, at low contents of DOPA, to repulsive, at higher contents of that component. In accordance with these results, the MD simulations demonstrated that both monoanionic and dianionic forms of DOPA have an ordering and condensing effect on the mixed bilayer at low concentrations. For the DOPA monoanions, this is the result of both (i) strong electrostatic interactions between the negatively charged oxygen of DOPA and the positively charged choline groups of DPPC and (ii) conformational changes of the lipid acyl chains, leading to their tight packing according to the so-called umbrella model, in which large headgroups of DPPC shield the hydrophobic part of DOPA (the conical shape lipid) from contact with water. In the case of the DOPA dianions, cation-mediated clustering was observed. Our results provide a detailed molecular-level description of the lipid organization inside the mixed zwitterionic/PA membranes, which is fully supported by the experimental data.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Computational Science X (CompX), Jagiellonian University, Faculty of Chemistry
Contributors: Kwolek, U., Kulig, W., Wydro, P., Nowakowska, M., Róg, T., Kepczynski, M.
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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
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Source: Scopus
Source ID: 84938696964
Research output: Contribution to journal › Article › Scientific › peer-review

Gas atomized thermal spray powders of various metals and alloys

Thermal spraying is a group of methods which are used to produce for example wear and corrosion resistant coatings on different surfaces. Fine powder of material is fed to high temperature gas flow. The particles accelerate, partially melt and hit to the surface to form a coating. Thermal spraying sets some requirements for the powder. The powder should be able to be fed with constant feed rate and the particle size distribution should be quite narrow to achieve even melt fraction of the particles. For metal alloys gas atomization is the optimum method to produce thermal spray powders. In this paper, results of some powders prepared by laboratory scale medium/high pressure gas atomizer are discussed. Motivation of this work was to study if thermal spray powders could be atomized in suitable particle size without major post processing. Copper and different stainless steels were atomized. Characterization of particle size and morphology were tested. Different aspects of atomization and post processing to increase thermal spray powder quality are discussed.

General information

Publication status: Published
MoE publication type: A4 Article in a conference publication
Organisations: Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland
Contributors: Lagerbom, J., Ritvonen, T., Suhonen, T., Varis, T.
Publication date: 2011

Host publication information

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Publisher: European Powder Metallurgy Association (EPMA)
ISBN (Print): 9781899072200
ASJC Scopus subject areas: Mechanics of Materials, Ceramics and Composites, Materials Chemistry, Metals and Alloys, Condensed Matter Physics
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http://www.scopus.com/inward/record.url?scp=84902181974&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
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Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

Improved properties for packaging materials by nanoscale surface modification and ALD barrier coating

General information

Publication status: Published
MoE publication type: A4 Article in a conference publication
Organisations: Department of Materials Science, Research group: Paper Converting and Packaging, Metsä Board, Bemis , LUT Energy, Masaryk University
Contributors: Lahti, J., Lavonen, J., Lahtinen, K., Johansson, P., Seppänen, T., Cameron, D. C.
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ISBN (Electronic): 9781510828001
ASJC Scopus subject areas: Biotechnology, Biomaterials, Materials Chemistry, Surfaces, Coatings and Films
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Source: Scopus
Source ID: 84992694476
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

Effect of rubber polarity on selective wetting of carbon nanotubes in ternary blends

Based on atomic force microscopy (AFM) and Fourier transform infrared spectroscopy (FTIR) analysis of the rubber-filler gel (wetting concept) the kinetics of selective wetting of carbon nanotubes (CNTs) in ternary styrene butadiene rubber (SBR)/butadiene rubber (BR)/natural rubber (NR) blends was qualitatively and quantitatively characterized. Almost all

CNTs are found to be wetted by the non-polar NR but not by the other non-polar rubber like BR or weakly polar SBR. It was proposed that phospholipids, which are linked to the α-terminal of NR can interact with the CNT surface through cation-π interactions forming strong bonding between NR and CNTs. Using the corrected surface tension value of NR, which involves the effect of phospholipids found in our previous work the selective wetting of CNTs in ternary rubber blends can be well predicted using the Z-model for a thermodynamic equilibrium state. By replacing the non-polar BR by a polar rubber like nitrile butadiene rubber (NBR) as a blend component CNTs are wetted by NBR slightly more than by NR thanks to the strong interaction between CNTs and nitrile groups of NBR. SBR remains unbound to CNTs in both blends.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Institut für Polymerwerkstoffe E.V., Martin-Luther-University Halle-Wittenberg, Fraunhofer IWM, Vodafone Department of Mobile Communications Systems, Leibniz-Institut für Polymerforschung Dresden E.V., Vietnamese Academy of Science and Technology Institute of Chemistry, Polymer Service GmbH Merseburg
Contributors: Le, H. H., Parsaker, M., Sriharish, M. N., Henning, S., Menzel, M., Wießner, S., Das, A., Do, Q. K., Heinrich, G., Radusch, H. J.
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Original language: English
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Keywords: Carbon nanotubes, Manocomposites, Rubber blends, Selective filler wetting
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Source ID: 84940868023
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of non-rubber components of NR on the carbon nanotube (CNT) localization in SBR/NR blends

Carbon nanotubes (CNTs) are mixed into SBR/NR and SBR/IR blends using a wet mixing process. The phase specific localization of CNTs in rubber blends is predicted theoretically using surface energy data of blend components and determined experimentally by means of the wetting concept. Almost all CNTs are found to be localized in the SBR matrix of SBR/IR blends due to the better affinity of CNTs to SBR than to IR. In contrast, a high CNT loading localized in the NR phase of SBR/NR blends results from the presence of phospholipids in NR. Electrical and mechanical properties of the rubber blends depend strongly on CNT localization. A lower CNT loading in SBR matrix of SBR/NR blends imparts a better wet grip and lower rolling resistance to tire tread compounds.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Martin-Luther-University Halle-Wittenberg, Styron Deutschland GmbH, Fraunhofer IWM, Leibniz-Institut für Polymerforschung Dresden E.V., Dau Mot University, Tribhuvan University, Vodafone Department of Mobile Communications Systems
Contributors: Le, H. H., Parsekar, M., Ilisch, S., Henning, S., Das, A., Stöckelhuber, K. W., Beiner, M., Ho, C. A., Adhikari, R., Wießner, S., Heinrich, G., Radusch, H. J.
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Keywords: carbon nanotubes, filler localization, nanocomposites, rubber blends
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Source ID: 84899990693
Research output: Contribution to journal › Article › Scientific › peer-review

Detection of gaseous species during KCl-induced high-temperature corrosion by the means of CPFAAS and CI-APi-TOF
Two different analytical approaches—collinear photofragmentation and atomic absorption spectroscopy (CPFAAS) and chemical ionization atmospheric pressure interface time-of-flight mass spectrometer (CI-APi-TOF)—were applied to detect and identify the online gaseous KOH and HCl formed in the addressed high-temperature reactions. Samples of pure KCl, KCl+Cr, KCl+Fe, and KCl+316 L were studied at 550°C under dry and humid conditions with varying oxygen concentrations. The goal was to shed more light on the gas-phase chemistry during KCl-induced corrosion under conditions relevant to biomass combustion. CI-APi-TOF proved to be a valuable tool for high-temperature corrosion studies: HCl was identified to have formed during the reactions under humid conditions. On the contrary, despite the known sensitivity of CPFAAS, the formation of KOH could not be verified in any of the performed measurements.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Research area: Aerosol Physics, Research group: The Instrumentation, Emissions, and Atmospheric Aerosols Group, Physics, Research group: Applied Optics, Åbo Akademi University
Contributors: Lehmusto, J., Olin, M., Viljanen, J., Kalliokoski, J., Mylläri, F., Toivonen, J., Dal Maso, M., Hupa, L.
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ASJC Scopus subject areas: Environmental Chemistry, Mechanics of Materials, Mechanical Engineering, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
Keywords: CI-APi-TOF, CPFAAS, gaseous KCl, HCl formation, high-temperature corrosion
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Research output: Contribution to journal › Article › Scientific › peer-review

Cold gas spraying of a high-entropy CrFeNiMn equiatomic alloy
Cold gas spraying was used to make a coating from an equiatomic CrFeNiMn high-entropy alloy. This four-component alloy was chosen because it is Co-free, thus allowing application in nuclear industries as a possible replacement of currently used stainless steel coatings. The feedstock material was gas atomized powder with a particle size distribution from 20 to 45 μm. A number of parameters were tested, such as the powder feed rate and gas feed pressure, in order to obtain as dense a coating as possible with nitrogen as the process gas. Spraying was performed using a gas preheating temperature of 1000 °C, gas feed pressure ranging from 50 to 60 bar, and two powder feeding rates. The coating thicknesses ranging from 230 to 490 m and porosities ranging from 3% to 10% were obtained depending on the powder feed rate and gas feed pressure. The hardness of the cross-section of the coating was usually lower than that of the surface. The highest coating hardness obtained was above 300 $HV_{0.3}$ for both the surface and the cross-section. The as-atomized powder consisted of a face-centered cubic (FCC) phase with a minute amount of body-centered cubic (BCC) phase, which was no longer detectable in the coatings. The microstructure of the coating was highly stressed due to the high degree of deformation occurring in cold gas spraying. The deformation leads to strain hardening and induces a pronounced texture in the coating. The 111 planes tend to align along the coating surface, with deformation and texturing

concentrating mainly on particle boundaries. A high-entropy alloy (HEA) coating was successfully sprayed for the first time using nitrogen as a process gas. The coating has the potential to replace stainless steel coatings in nuclear industry applications.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Surface Engineering, Aalto University
Contributors: Lehtonen, J., Koivuluoto, H., Ge, Y., Juselius, A., Hannula, S. P.
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ASJC Scopus subject areas: Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
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Source: Scopus
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Research output: Contribution to journal › Article › Scientific › peer-review

Erosive wear of various stainless steel grades used as impeller blade materials in high temperature aqueous slurry
Two austenitic stainless steel grades, 316L and 904L, and three duplex stainless steel grades, LDX 2101, 2205, and 2507, were erosion tested as impeller blade materials for hydrometallurgical applications. Samples were attached to the pressure and suction sides of an impeller and were tested for 72. h at 80. °C and 95. °C in a small-scale reactor using quartz sand slurry. Based on the mass losses measured, the steel grades could be ranked into two distinct categories; LDX 2101 and 2507 comprising the category with the better erosion resistance. The categories were the same for the pressure and suction side tests even though the erosion mechanism differed. In most cases, erosion was more severe in the suction side samples, which has practical implications for wear protection design. In the pressure side samples, the variation in the erosion mass loss with different experimental parameters was in line with earlier reported findings. In contrast, in the suction side samples, under some experimental conditions, increasing tip speed and increasing particle size were found to reduce erosion mass loss. This emphasizes the fact that the erosivity of particles for the impeller suction side cannot be deduced solely based on particle size. The reasons for the observed behavior are discussed.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Engineering materials science and solutions (EMASS), Outotec Research Center
Contributors: Lindgren, M., Suihkonen, R., Vuorinen, J.
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces and Interfaces, Materials Chemistry, Surfaces, Coatings and Films, Mechanics of Materials

Keywords: Erosion, Impellers, Mixing, Slurry, Stainless steels, Wear
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Source: Scopus
Source ID: 84926200934
Research output: Contribution to journal › Article › Scientific › peer-review

Erosion–corrosion resistance of various stainless steel grades in high-temperature sulfuric acid solution
Two austenitic stainless steel grades, 316L and 904L, and three duplex stainless steel grades, LDX 2101, 2205, and 2507, were erosion–corrosion tested as impeller blade materials for hydrometallurgical applications. Samples were attached to the pressure and suction sides of an impeller and were tested in 50 g/l H_2SO_4 and 0.5 g/l $Fe_2(SO_4)_3$ for 72 h at 80°C and 95 °C in a small-scale reactor using quartz sand slurry. The results showed that under lower erosion intensity the ranking of the grades was similar to that in pure erosion. Under higher erosion intensity the ranking of the grades changed completely: lean alloys LDX 2101 and 316L suffered from the highest mass losses followed by 2205, 2507, and 904L. To clarify this behavior, the ability of the grades to repassivate was investigated with scratch tests. It was found that the ranking could be explained by the repassivation rates. The only exception was that 2507 showed a similar repassivation rate to 904L but its erosion–corrosion mass loss under higher erosion intensity was larger. One contributing factor to this was found to be the selective dissolution of the austenite phase of all the tested duplex grades. The prerequisites for the galvanic coupling between the phases that was responsible for the selective dissolution are discussed.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Outotec Research Center, VTT Technical Research Centre of Finland
Contributors: Lindgren, M., Siljander, S., Suihkonen, R., Pohjanne, P., Vuorinen, J.
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Ratings:
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces and Interfaces, Materials Chemistry, Surfaces, Coatings and Films, Mechanics of Materials
Keywords: Erosion–corrosion, Slurry, Stainless steels, Sulfuric acid, Wear
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EXT="Lindgren, M."
Source: Scopus
Source ID: 84975744612
Research output: Contribution to journal › Article › Scientific › peer-review

Barkhausen noise response of three different welded duplex stainless steels
An investigation was made into the Barkhausen noise responses of three duplex grades: a lean alloy LDX 2101, a conventional duplex 2205 and a super duplex 2507, in welded conditions. The aim was to study the influence of alloy chemistry and microstructure on the Barkhausen noise response. In addition, the residual stresses of the grades were measured by X-ray diffraction and the microstructure and hardness of the base materials and welds were determined. It was observed that the Barkhausen noise responses in the rolling direction and in the transverse direction were governed by the phase morphology of the materials. Only the root mean square of the Barkhausen noise burst seemed to be additionally dependent on the alloy chemistry through the hardness of the materials. Furthermore, the relationships between various characteristics of the Barkhausen noise burst measured in the rolling direction and the transverse

direction and microstructural features are discussed.

General information
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Contributors: Lindgren, M., Santa-aho, S., Vippola, M.
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Keywords: Barkhausen, Stainless steel, Welds
DOIs:

10.1784/insi.2016.58.9.480
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The effect of impact conditions on the wear and deformation behavior of wear resistant steels
The deformation and wear behavior of four high strength wear resistant steels were studied in various impact conditions to evaluate their performance in applications involving heavy impacts and impact-abrasion. In the normal direction impacts, the studies were conducted with single and repeated (multiple) drop tests. To better simulate the actual application conditions, the samples were positioned at an angle relative to the impact direction in the tests with the high velocity particle impactor (HVPI) device. The effect of strain rate was investigated using constant size projectiles made from materials with different density but keeping the impact energy constant by varying the incident projectile velocity. The effect of surface hardening on the wear resistance of the high strength steels was determined by impacting the same surface area multiple times at a constant velocity using spherical high velocity projectiles. Regardless of the rather similar hardness of the studied three martensitic steel grades, the impact behavior showed differences in wear rate and damage mechanisms in each case due to the microstructural characteristics of the materials. The adiabatic shear bands forming in the martensitic steels at higher loading rates were found to increase the wear rate. Moreover, the carbide reinforced steel performed in general better than the martensitic grades but showed more brittle behavior and generation of crack networks that can affect the wear performance of the material.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Materials Characterization, Computational Science X (CompX), Engineering materials science and solutions (EMASS), AC2T Research GmbH, VTT Technical Research Centre of Finland
Contributors: Lindroos, M., Ratia, V., Apostol, M., Valtonen, K., Laukkanen, A., Molnar, W., Holmberg, K., Kuokkala, V. T.
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Keywords: Adiabatic shear bands (ASB), High strength steel, High velocity impact, Wear testing

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Source: Scopus
Source ID: 84924069828
Research output: Contribution to journal › Article › Scientific › peer-review

Time-Resolved Fluorescence Spectroscopy Reveals Fine Structure and Dynamics of Poly(l-lysine) and Polyethylenimine Based DNA Polyplexes

Structural dynamics of the polyethylenimine-DNA and poly(l-lysine)-DNA complexes (polyplexes) was studied by steady-state and time-resolved fluorescence spectroscopy using the fluorescence resonance energy transfer (FRET) technique. During the formation of the DNA polyplexes, the negative phosphate groups (P) of DNA are bound by the positive amine groups (N) of the polymer. At N/P ratio 2, nearly all of the DNA's P groups are bound by the polymer N groups: These complexes form the core of the polyplexes. The excess polymer, added to this system to increase the N/P ratio to the values giving efficient gene delivery, forms a positively charged shell around the core polyplex. We investigated whether the exchange between the core and shell regions of PEI and PLL polyplexes takes place. Our results demonstrated a clear difference between the two studied polymers. Shell PEI can replace PEIs previously attached to DNA in the polyplex core, while PLL cannot. Such a dynamic structure of PEI polyplexes compared to a more static one found for PLL polyplexes partially explains the observed difference in the DNA transfection efficiency of these polyplexes. Moreover, the time-resolved fluorescence spectroscopy revealed additional details on the structure of PLL polyplexes: In between the core and shell, there is an intermediate layer where both core and shell PLLs or their parts overlap.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Centre for Drug Research, University of Helsinki, Ita-Suomen yliopisto, Universita degli Studi di Padova, Italy
Contributors: Lisitsyna, E. S., Ketola, T., Morin-Picardat, E., Liang, H., Hanzlíková, M., Urtti, A., Yliperttula, M., Vuorimaa-Laukkanen, E.
Number of pages: 11
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Publication date: 7 Dec 2017
Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry B
Volume: 121
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ISSN (Print): 1520-6106
Ratings:

Scopus rating (2017): CiteScore 6 SJR 1.331 SNIP 0.993
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry
DOIs:

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Source: Scopus
Source ID: 85037731381
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of the addition of Al_2O_3, TiO_2 and ZnO on the thermal, structural and luminescence properties of Er^{3+}-doped phosphate glasses

Er-doped phosphate glasses were fabricated by melt-quenching technique. The changes in their thermal, structural and luminescence properties with the addition of Al_2O_3, TiO_2 or ZnO were studied. Physical and thermal properties were investigated through density measurement and differential thermal analysis. Structural characterization was performed using the Raman and Infrared spectroscopy. In order to study the influence of the composition on the luminescence properties of the glasses, the refractive index, the luminescence spectra and the lifetime values were measured. The results show that with the addition of Al_2O_3 and TiO_2 the phosphate network becomes more connected increasing the glass transition temperature, whereas the addition of ZnO does not show significant changes in the optical, thermal and structural properties but it leads to a larger emission cross-section at 1540 nm as compared to the other glasses. As the site of the Er^{3+} is not strongly affected by the change in the glass composition, we think that the emission properties of the glasses depend on the glass structure connectivity, which has an impact on the Er^{3+} ions solubility.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Photonics, Faculty of Biomedical Sciences and Engineering, Research group: Biomaterials and Tissue Engineering Group, Politecnico di Torino, Istituto Superiore Mario Boella, CSMFO Lab.
Contributors: Lopez-Iscoa, P., Petit, L., Massera, J., Janner, D., Boetti, N. G., Pugliese, D., Fiorilli, S., Novara, C., Giorgis, F., Milanese, D.
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Publication date: 15 Mar 2017
Peer-reviewed: Yes

Publication information
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Volume: 460
ISSN (Print): 0022-3093
Ratings:

Scopus rating (2017): CiteScore 4 SJR 0.722 SNIP 1.178
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Ceramics and Composites, Condensed Matter Physics, Materials Chemistry
Keywords: Er luminescence property, Infrared spectroscopy, Phosphate glass, Raman spectroscopy
DOIs:

10.1016/j.jnoncrysol.2017.01.030
Source: Scopus
Source ID: 85010441113
Research output: Contribution to journal › Article › Scientific › peer-review

Design, processing, and characterization of an optical core-bioactive clad phosphate fiber for biomedical applications
The aim of this study was to fabricate a bioactive optical fiber able to monitor “in situ” its reaction with the body through changes in its optical properties. Core and cladding preforms were prepared with the composition (97.25*(0.50P_2O_5-0.40SrO-0.10Na_2O)-2.5ZnO-0.25Er_2O_3) and (98.25*(0.50P_2O_5-0.40SrO-0.10Na_2O)-1.75ZnO) (in mol%), respectively, and successfully drawn into a multimode core/clad optical fiber. Optical and near-Infrared images assessed the proper light guiding properties of the fiber. The fibers favor the precipitation of a Ca-P reactive layer at its surface concomitant with a reduction in the fiber diameter, when immersed in SBF, often assigned as a sign of bioactivity. It is clearly shown here that the bio-response of the fiber upon immersion in SBF can be tracked from the decrease in the intensity of the Er^{3+} ions emission at 1.5 μm. This confirms that the newly developed optical fiber, which combines good optical properties with a suitable bioactive behavior, is a promising platform for the development of novel biomedical devices for biophotonic and photomedical applications. Finally, the successful splicing of the newly developed fiber with commercial optical fibers was an evidence of the possibility to integrate the newly developed phosphate fiber within existing components used in the field of biomedicine.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Physics, BioMediTech, Politecnico di Torino, Fondazione LINKS – Leading Innovation & Knowledge for Society, UMR CNRS 6226 Sciences Chimiques de Rennes, University of Parma, Photonics Laboratory
Contributors: Lopez-Iscoa, P., Ojha, N., Pugliese, D., Mishra, A., Gumenyuk, R., Boetti, N. G., Janner, D., Troles, J., Bureau, B., Boussard-Plédel, C., Massera, J., Milanese, D., Petit, L.
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: JOURNAL OF THE AMERICAN CERAMIC SOCIETY
ISSN (Print): 0002-7820
Ratings:

Scopus rating (2019): CiteScore 5.4 SJR 0.902 SNIP 1.222
Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Materials Chemistry
Keywords: bioactivity, Er luminescence property, optical fiber, phosphate glass
DOIs:

10.1111/jace.16553
Source: Scopus
Source ID: 85066458189
Research output: Contribution to journal › Article › Scientific › peer-review

DFT simulations and microkinetic modelling of 1-pentyne hydrogenation on Cu_{20} model catalysts

Adsorption and dissociation of H_2 and hydrogenation of 1-pentyne on neutral and anionic Cu_{20} clusters have been investigated using the density functional theory and microkinetic modelling. Molecular adsorption of H_2 is found to occur strictly at atop sites. The H_2 dimer is activated upon adsorption, and the dissociation occurs with moderate energy barriers. The dissociated H atoms reside preferentially on 3-fold face and 2-fold edge sites. Based on these results, the reaction paths leading to the partial and total hydrogenation of 1-pentyne have been studied step-by-step. The results suggest that copper clusters can display selective activity on the hydrogenation of alkyne and alkene molecules. The hydrogenated products are more stable than the corresponding initial reactants following an energetic staircase with the number of added H atoms. Stable semi-hydrogenated intermediates are formed before the partial (1-pentene) and total (pentane) hydrogenation stages of 1-pentyne. The microkinetic model analysis shows that C_5H_{10} is the dominant product. Increasing the reactants (C_5H_8/H_2) ratio enhances the formation of products (C_5H_{10} and C_5H_{12}).

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Aalto University, COMP Centre of Excellence, Department of Applied Physics, Aalto University
Contributors: Ma, L., Melander, M., Weckman, T., Lipasti, S., Laasonen, K., Akola, J.
Number of pages: 10
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Publication information

Journal: Journal of Molecular Graphics and Modelling
Volume: 65
ISSN (Print): 1093-3263
Ratings:

Scopus rating (2016): CiteScore 3.1 SJR 0.524 SNIP 0.731
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Spectroscopy, Computer Graphics and Computer-Aided Design, Materials Chemistry
Keywords: Adsorption and dissociation, Cluster model, Density functional theory, Heterogeneous catalysis, Hydrogenation
DOIs:

10.1016/j.jmgm.2016.02.007

Bibliographical note

INT=fys,"Ma, Li"
Source: Scopus
Source ID: 84961675623
Research output: Contribution to journal › Article › Scientific › peer-review

Membrane bound COMT isoform is an interfacial enzyme: General mechanism and new drug design paradigm

The enzyme catechol-O-methyltransferase (COMT) has water soluble (S-COMT) and membrane associated (MB-COMT), bitopic, isoforms. Of these MB-COMT is a drug target in relation to the treatment of Parkinson's disease. Using a combination of computational and experimental protocols, we have determined the substrate selection mechanism specific to MB-COMT. We show: (1) substrates with preferred affinity for MB-COMT over S-COMT orient in the membrane in a fashion conducive to catalysis from the membrane surface and (2) binding of COMT to its cofactor ADOMET induces conformational change that drives the catalytic surface of the protein to the membrane surface, where the substrates and Mg^{2+} ions, required for catalysis, are found. Bioinformatics analysis reveals evidence of this mechanism in other proteins, including several existing drug targets. The development of new COMT inhibitors with preferential affinity for MB-COMT over S-COMT is now possible and insight of broader relevance, into the function of bitopic enzymes, is provided.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Physics, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Universite de Geneve
Contributors: Magarkar, A., Parkkila, P., Viitala, T., Lajunen, T., Mobarak, E., Licari, G., Cramariuc, O., Vauthey, E., Róg, T., Bunker, A.
Number of pages: 4
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Peer-reviewed: Yes

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Scopus rating (2018): CiteScore 11.6 SJR 2.177 SNIP 1.145
Original language: English
ASJC Scopus subject areas: Catalysis, Electronic, Optical and Magnetic Materials, Ceramics and Composites, Chemistry(all), Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
DOIs:

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Source: Scopus
Source ID: 85044968200
Research output: Contribution to journal › Article › Scientific › peer-review

Azobenzene photomechanics: Prospects and potential applications
The change in shape inducible in some photo-reversible molecules using light can effect powerful changes to a variety of properties of a host material. This class of reversible light-switchable molecules includes molecules that photodimerize, such as coumarins and anthracenes; those that allow intra-molecular photo-induced bond formation, such as fulgides, spiro-pyrans, and diarylethenes; and those that exhibit photo-isomerization, such as stilbenes, crowded alkenes, and azobenzenes. The most ubiquitous natural molecule for reversible shape change, however, and perhaps the inspiration for all artificial bio-mimics, is the rhodopsin/retinal protein system that enables vision, and this is the quintessential reversible photo-switch for performance and robustness. Here, the small retinal molecule embedded in a cage of rhodopsin helices isomerizes from a cis geometry to a trans geometry around a C=C double bond with the absorption of just a single photon. The modest shape change of just a few angstroms is quickly amplified and sets off a cascade of larger shape and chemical changes, eventually culminating in an electrical signal to the brain of a vision event, the energy of the input photon amplified many thousands of times in the process. Complicated biochemical pathways then revert the trans isomer back to cis, and set the system back up for another cascade upon subsequent absorption. The reversibility is complete, and many subsequent cycles are possible. The reversion mechanism back to the initial cis state is complex and enzymatic, hence direct application of the retinal/rhodopsin photo-switch to engineering systems is difficult. Perhaps the best artificial mimic of this strong photo-switching effect however in terms of reversibility, speed, and simplicity of incorporation, is azobenzene. Trans and cis states can be switched in microseconds with low-power light, reversibility of 10^5 and 10^6 cycles is routine before chemical fatigue, and a wide variety of molecular architectures is available to the synthetic materials chemist, permitting facile anchoring and compatibility, as well as chemical and physical amplification of the simple geometric change. This review article focuses on photo-mechanical effect taking place in various material systems incorporating azobenzene. The photo-mechanical effect can be defined as reversible change in shape by absorption of light, which results in a significant macroscopic mechanical deformation, and reversible mechanical actuation, of the host material. Thus, we exclude simple thermal expansion effects, reversible but non-mechanical photo-switching or photo-chemistry, as well as the wide range of optical and electro-optical switching effects for which good reviews exist elsewhere. Azobenzene-based material systems are also of great interest for light energy harvesting applications across much of the solar spectrum, yet this emerging field is still in an early enough stage of research output as to not yet warrant review, but we hope that some of the ideas put forward here toward promising future directions of research, will help guide the field.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, McGill University, Brookhaven National Laboratory, Tokyo Institute of Technology, Aalto University
Contributors: Mahimwalla, Z., Yager, K. G., Mamiya, J. I., Shishido, A., Priimagi, A., Barrett, C. J.
Number of pages: 40
Pages: 967-1006
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Peer-reviewed: Yes

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Journal: Polymer Bulletin
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Issue number: 8
ISSN (Print): 0170-0839
Ratings:

Scopus rating (2012): CiteScore 2.2 SJR 0.559 SNIP 1.027

Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Polymers and Plastics, Materials Chemistry
Keywords: Azobenzene, Light harvesting, Liquid crystals, Photochemistry, Photomechanics, Thin films
DOIs:

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URLs:

http://www.scopus.com/inward/record.url?scp=84868637316&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84868637316
Research output: Contribution to journal › Article › Scientific › peer-review

Carbon nanotubes-filled thermoplastic polyurethane-urea and carboxylated acrylonitrile butadiene rubber blend nanocomposites

This article reports the preparation and characterization of multiwalled carbon nanotubes (MWCNTs)-filled thermoplastic polyurethane-urea (TPUU) and carboxylated acrylonitrile butadiene rubber (XNBR) blend nanocomposites. The dispersion of the MWCNTs was carried out using a laboratory two roll mill. Three different loadings, that is, 1, 3, and 5 wt % of the MWCNTs were used. The electron microscopy image analysis proves that the MWCNTs are evenly dispersed along the shear flow direction. Through incorporation of the nanotubes in the blend, the tensile modulus was increased from 9.90 ± 0.5 to 45.30 ± 0.3 MPa, and the tensile strength at break was increased from 25.4 ± 2.5 to 33.0 ± 1.5 MPa. The wide angle X-ray scattering result showed that the TPUU:XNBR blends were arranged in layered structures. These structures are formed through chemical reactions of -NH group from urethane and urea with the carboxylic group on XNBR. Furthermore, even at a very low loading, the high degree of nanotubes dispersion results in a significant increase in the electrical percolation threshold. © 2014 Wiley Periodicals, Inc. J. Appl. Polym. Sci. 2014, 131, 40341.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), COMSATS Institute of Information Technology Lahore, Leibniz-Institut für Polymerforschung Dresden E.V., Institut für Polymerwerkstoffe, Vodafone Department of Mobile Communications Systems
Contributors: Mahmood, N., Khan, A. U., Stöckelhuber, K. W., Das, A., Jehnichen, D., Heinrich, G.
Publication date: 5 Jun 2014
Peer-reviewed: Yes

Publication information

Journal: Journal of Applied Polymer Science
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Issue number: 11
ISSN (Print): 0021-8995
Ratings:

Scopus rating (2014): CiteScore 3.2 SJR 0.664 SNIP 0.98
Original language: English
ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)
Keywords: blends, elastomers, graphene and fullerenes, nanotubes, polyurethanes, rubber
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URLs:

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Source: Scopus
Source ID: 84897664169
Research output: Contribution to journal › Article › Scientific › peer-review

Vacancy-type defect distributions near argon sputtered Al(100) surface studied by variable-energy positrons and molecular dynamics simulations

A beam of variable-energy positrons, whose back-diffusion probability is measured as a function of positron implantation energy, is applied to studies of depth distribution of sputtering damage in aluminum. The defects are produced by argon ion bombardment of an Al(110) surface in ultra-high vacuum. We have varied the Ar^+ energy, incident angle and dose, as well as sputtering and annealing temperatures. The extracted defect profiles have typically a narrow peak at the surface with a width of 10-20 A and a broader tail extending down to 50-100 Å. The shape of the defect profile varies only slightly with the sputtering energy and angle. Defect production at less than 1 keV Ar^+ energies is typically 1-5 vacancies per incident ion. The defect profiles become fluence-independent at about 2×10^{16} Ar^+ cm^{-2}. The defect density at the outer atomic layers saturates at high argon fluences to a few at%, depending on sputtering conditions. The sputtering temperature (below or above the vacancy migration stage at 250 K) has little effect on vacancy profiles. Defects anneal out gradually between 100 °C and 400 °C. Sputtering damage was also evaluated with the molecular dynamics technique. The shape and depth scale of the simulated collision cascades are in agreement with the experimentally extracted

quantities.

General information
Publication status: Published
MoE publication type: Not Eligible
Organisations: Department of Physics, Electrical Engineering, Laboratory of Physics, Aalto University, Jyväskylän yliopisto
Contributors: Mäkinen, J., Vehanen, A., Hautojärvi, P., Huomo, H., Lahtinen, J., Nieminen, R. M., Valkealahti, S.
Number of pages: 30
Pages: 385-414
Publication date: 2 Sep 1986
Peer-reviewed: Yes

Publication information
Journal: Surface Science
Volume: 175
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ISSN (Print): 0039-6028
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
DOIs:

10.1016/0039-6028(86)90242-6
Source: Scopus
Source ID: 0008385516
Research output: Contribution to journal › Article › Scientific › peer-review

Equipment for obtaining polimeric nanofibres by electrospinning technology: II. The obtaining of polimeric nanofibers
The computerized technologies and equipment for obtaining nanofibers impose high training, a large interdisciplinary substantiation, capacity for data storage, memorizing, easy usage, selectivity, fiability, stability, reduced time for analizing/processing of the technological parameters. That is why the computerized electrospinning equipment and technologies for obtaining nanofibers are possible candidates to carry out these requirements owing to the fact that they present both the proper selectivity/sensibility and the increased processing/determining/intervening speed by using the computerized control. This paper aims to present the operation and aplication of equipment for obtaining polimeric nanofibers by electrospinning technology. The designing and accomplishing of the suggested electrospinning equipment has been aimed to obtain a modular system which should allow the control of the technological parameters by means of the computer. Thus, the multitude of the parameters which influence the process of electrospinning, can be independently and automatically varied. The obtained nanofibers were studied by scanning electron microscope.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Computational Science X (CompX), Gheorghe Asachi Technical University Iasi, Faculty of Textile and Leather Engineering and Industrial Management, Centre of Competence in Electrostatics and Electrotechnologies, Alexandru Ioan Cuza University of Iasi, ARHEOINVEST Interdisciplinary Platform, Romanian Inventors Forum, IT Center for Science and Technology, 25 Av. Radu Beller, Bucharest, Romania
Contributors: Manea, L. R., Cramariuc, B., Popescu, V., Cramariuc, R., Sandu, I., Cramariuc, O.
Number of pages: 6
Pages: 180-185
Publication date: 1 Jun 2015
Peer-reviewed: Yes

Publication information
Journal: Materiale Plastice
Volume: 52
Issue number: 2
ISSN (Print): 0025-5289
Ratings:

Scopus rating (2015): CiteScore 1.1 SJR 0.28 SNIP 0.788
Original language: English
ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Chemistry(all), Mechanics of Materials
Keywords: Electrospinning, Equipment, Modular conception, Nanofibers, Technology
URLs:

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Bibliographical note

EXT="Cramariuc, Bogdan"
Source: Scopus
Source ID: 84931827044
Research output: Contribution to journal › Article › Scientific › peer-review

Accurate description of aqueous carbonate ions: An effective polarization model verified by neutron scattering

The carbonate ion plays a central role in the biochemical formation of the shells of aquatic life, which is an important path for carbon dioxide sequestration. Given the vital role of carbonate in this and other contexts, it is imperative to develop accurate models for such a high charge density ion. As a divalent ion, carbonate has a strong polarizing effect on surrounding water molecules. This raises the question whether it is possible to describe accurately such systems without including polarization. It has recently been suggested the lack of electronic polarization in nonpolarizable water models can be effectively compensated by introducing an electronic dielectric continuum, which is with respect to the forces between atoms equivalent to rescaling the ionic charges. Given how widely nonpolarizable models are used to model electrolyte solutions, establishing the experimental validity of this suggestion is imperative. Here, we examine a stringent test for such models: a comparison of the difference of the neutron scattering structure factors of K_2CO_3 vs KNO_3 solutions and that predicted by molecular dynamics simulations for various models of the same systems. We compare standard nonpolarizable simulations in SPC/E water to analogous simulations with effective ion charges, as well as simulations in explicitly polarizable POL3 water (which, however, has only about half the experimental polarizability). It is found that the simulation with rescaled charges is in a very good agreement with the experimental data, which is significantly better than for the nonpolarizable simulation and even better than for the explicitly polarizable POL3 model.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
Contributors: Mason, P. E., Wernersson, E., Jungwirth, P.
Number of pages: 9
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Publication date: 19 Jul 2012
Peer-reviewed: Yes

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Issue number: 28
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Ratings:

Scopus rating (2012): CiteScore 6.7 SJR 1.943 SNIP 1.243
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
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10.1021/jp3008267
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Source: Scopus
Source ID: 84863696122
Research output: Contribution to journal › Article › Scientific › peer-review

Processing and characterization of phosphate glasses containing CaAl2O4:Eu2+,Nd3+ and SrAl2O4:Eu2+,Dy3+ microparticles

In this paper, phosphate based glasses with persistent luminescence properties were processed using standard melting process in air by adding SrAl2O4:Eu2+,Dy3+ or CaAl2O4:Eu2+,Nd3+ in the glass batch before melting. All produced glasses were characterized using SEM/EDXA, Raman spectroscopy and photoluminescence. We discuss the effect of melting conditions (temperature and duration of the melting) on the persistent luminescence properties of the microparticles containing glasses. It is demonstrated that the melting in air allows for the preparation of glasses with persistent luminescence if the melting conditions are carefully controlled.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Electronics and Communications Engineering, Research group: Biomaterials and Tissue Engineering Group, Frontier Photonics, Integrated Technologies for Tissue Engineering Research (ITTE), Turun Yliopisto/Turun Biomateriaalikeskus, Johan Gadolin Process Chemistry Centre, Åbo Akademi University, University of Turku, Institute of Low Temperature and Structure Research Polish Academy of Sciences, Wroclaw, Poland, Turku

University Centre for Materials and Surfaces (MatSurf), Turku, Finland
Contributors: Massera, J., Gaussiran, M., Gluchowski, P., Lastusaari, M., Hupa, L., Petit, L.
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Pages: 3863-3871
Publication date: 1 Nov 2015
Peer-reviewed: Yes

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Journal: Journal of the European Ceramic Society
Volume: 35
Issue number: 14
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Ratings:

Scopus rating (2015): CiteScore 5.4 SJR 1.135 SNIP 1.859
Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Materials Chemistry
Keywords: Persistent luminescence, Phosphate glasses, SrAl<inf>2</inf>O<inf>4</inf>:Eu²⁺,Dy³⁺ and CaAl<inf>2</inf>O<inf>4</inf>:Eu²⁺,Nd³⁺ microparticles
DOIs:

10.1016/j.jeurceramsoc.2015.06.031
Source: Scopus
Source ID: 84939253464
Research output: Contribution to journal › Article › Scientific › peer-review

Crystallization mechanism of the bioactive glasses, 45S5 and S53P4
The crystallization kinetics of the two commercial bioactive glasses, 45S5 and S53P4, was studied using differential thermal analysis (DTA), optical microscopy, and scanning electron microscopy (SEM). The thermal properties, the activation energy of crystallization, and the Johnson-Mehl-Avrami (JMA) exponent were determined for two glass fractions: fine powder (2content. The nucleation temperature range of these two glasses together with DTA data makes it possible to develop guidelines for tailoring thermal treatment parameters to achieve desired glass-to-crystal ratios.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Johan Gadolin Process Chemistry Centre, Abo Akademi University
Contributors: Massera, J., Fagerlund, S., Hupa, L., Hupa, M.
Number of pages: 7
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Publication date: Feb 2012
Peer-reviewed: Yes

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Journal: JOURNAL OF THE AMERICAN CERAMIC SOCIETY
Volume: 95
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Scopus rating (2012): CiteScore 3.9 SJR 1.271 SNIP 1.493
Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Materials Chemistry
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10.1111/j.1551-2916.2011.05012.x
URLs:

http://www.scopus.com/inward/record.url?scp=84856543605&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84856543605
Research output: Contribution to journal › Article › Scientific › peer-review

Sliding wear behaviour of HVOF and HVAF sprayed Cr_3C_2-based coatings
Thermally sprayed tungsten carbide (WC) and chromium carbide (Cr_3C_2) based hard metal coatings are commonly applied on component surfaces as corrosion and wear resistant layers. Typically, WC-Co/Ni with optional Cr addition and Cr_3C_2-25NiCr powders are sprayed with high velocity oxy-fuel (HVOF) or high velocity air-fuel (HVAF) processes. Due to the poor oxidation resistance of the WC particles, Cr_3C_2-25NiCr composition is typically selected for high temperature

environments, up to 800-900°C. In this study, two distinct Cr_3C_2-based compositions of Cr_3C_2-50NiCrMoNb and Cr_3C_2-37WC-18NiCoCr were selected as interesting alternatives to conventional Cr_3C_2-25NiCr. Sliding wear behavior of the coatings sprayed with HVOF and HVAF processes were tested with a ball-on-disk configuration against an Al_2O_3 ball at room temperature and at 700°C. It was found that both alternative materials had comparable coefficients of friction with the Cr_3C_2-25NiCr coatings. The Cr_3C_2-37WC-18NiCoCr coatings provided improved wear resistance at room temperature conditions, but at 700°C the wear rate was increased to the level of the Cr_3C_2-50NiCrMoNb coatings. Cr_3C_2-25NiCr coatings experienced the lowest wear rates at elevated temperatures, which was even lower than at room temperature.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Surface Engineering, Universita degli Studi di Modena e Reggio Emilia
Contributors: Matikainen, V., Bolelli, G., Koivuluoto, H., Sassatelli, P., Lusvarghi, L., Vuoristo, P.
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Early online date: 6 Apr 2017

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Ratings:

Scopus rating (2017): CiteScore 4.4 SJR 1.386 SNIP 2.227
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: CrC, HVAF, HVOF, Sliding wear, Thermal spray coatings
Electronic versions:

WEAR Sliding wear behaviour of HVOF and HVAF sprayed Cr3C2-based coatings. Embargo ended: 10/09/19
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URLs:

http://urn.fi/URN:NBN:fi:tty-201712082311. Embargo ended: 10/09/19
Source: Scopus
Source ID: 85017474688
Research output: Contribution to journal › Article › Scientific › peer-review

A Study of Cr_3C_2-Based HVOF- and HVAF-Sprayed Coatings: Microstructure and Carbide Retention
The research on high-velocity air-fuel (HVAF)-sprayed Cr_3C_2-based materials has mostly focused on conventional Cr_3C_2-25NiCr composition. In this paper, two alternative compositions (Cr_3C_2-50NiCrMoNb and Cr_3C_2-37WC-18NiCoCrFe) were sprayed with high-velocity oxy-fuel (HVOF) and HVAF spray processes to evaluate the material behavior during spraying and to provide characterization of the microstructures and mechanical properties of the coatings. For comparison, coatings from the Cr_3C_2-25NiCr composition were sprayed with both processes. Spray diagnostics were carried out to obtain average particle velocity and temperature for each material and process combinations. The measured average in-flight particle data were 1800 °C and 700 m/s for HVOF process, and 1450 °C and 900 m/s for HVAF process. Characterization of the coating microstructures was carried out by scanning electron microscopy and X-ray diffraction. In addition, the carbon content of the feedstock powders and sprayed coatings was measured with carbon analyzer. The results show that carbide rebounding or selective deposition of particles with higher metal matrix content is the dominating reason for carbide loss during HVAF spraying, while carbide dissolution is an additional source for the HVOF spraying. Higher particle velocities and controlled temperature measured for the HVAF process produced dense coatings with improved toughness and more homogenous coating structure.

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Materials Characterization, Research group: Surface Engineering, Universita degli Studi di Modena e Reggio Emilia
Contributors: Matikainen, V., Bolelli, G., Koivuluoto, H., Honkanen, M., Vippola, M., Lusvarghi, L., Vuoristo, P.
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ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
Keywords: chromium carbide, diagnostics, HVAF, HVOF, image analysis
Electronic versions:

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DOIs:

10.1007/s11666-017-0578-x
URLs:

http://urn.fi/URN:NBN:fi:tty-201712082310. Embargo ended: 12/06/18
Source: Scopus
Source ID: 85020726840
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of nozzle geometry on the microstructure and properties of hvaf-sprayed wc-10co4cr and cr3c2-25nicr coatings
Thermally sprayed hard metal coatings are the industrial standard solution for numerous demanding applications to improve wear resistance. In the aim of improving coating quality by utilising finer particle size distributions, several approaches have been studied to control the spray temperature. The most viable solution is to use the modern high velocity air-fuel (HVAF) spray process, which has already proven to produce high-quality coatings with dense structures. In HVAF spray process, the particle heating and acceleration can be efficiently controlled by changing the nozzle geometry. In this study, fine WC-10Co4Cr and Cr_3C_2-25NiCr powders were sprayed with three nozzle geometries to investigate their effect on the particle temperature, velocity and coating microstructure. The study demonstrates that the particle melting and resulting carbide dissolution can be efficiently controlled by changing the nozzle geometry from cylindrical to convergent–divergent. Moreover, the average particle velocity was increased from 780 to over 900 m/s. The increase in particle velocity significantly improved the coating structure and density. Further evaluation was carried out to resolve the effect of particle in-flight parameters on coating structure and cavitation erosion resistance, which was significantly improved in the case of WC-10Co4Cr coatings with the increasing average particle velocity.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Surface Engineering, VZÚ Plzeň - Research and Testing Institute, University of West Bohemia
Contributors: Matikainen, V., Koivuluoto, H., Vuoristo, P., Schubert, J., Houdková
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Publication date: 1 Apr 2018
Peer-reviewed: Yes

Publication information
Journal: Journal of Thermal Spray Technology
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Issue number: 4
ISSN (Print): 1059-9630
Ratings:

Scopus rating (2018): CiteScore 3.6 SJR 0.694 SNIP 1.117
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
Keywords: cavitation erosion < properties, chromium carbide < feedstock, diagnostics < processing, HP/HVOF < processing, HVAF < processing, HVOF < processing, WC-CO-Cr < feedstock
DOIs:

10.1007/s11666-018-0717-z
Source: Scopus
Source ID: 85045088095
Research output: Contribution to journal › Article › Scientific › peer-review

Erosion wear performance of WC-10Co4Cr and Cr_3C_2-25NiCr coatings sprayed with high-velocity thermal spray processes

Thermally sprayed hardmetal coatings are widely used to protect components and surfaces against wear in various applications. Hard and wear resistant coatings increase the component lifetime and can generate significant savings promoting ecological manufacturing. This study focuses on the performance of tungsten carbide (WC-10Co4Cr)and chromium carbide (Cr $_3$C $_2$-25NiCr)based hardmetal coatings sprayed with gaseous and liquid fuelled high-velocity oxygen-fuel (HVOF)spray processes and a modern high-velocity air-fuel (HVAF)spray process. The coating characterisation revealed reduced carbide dissolution with decreasing process temperature and denser feedstock powder particles. Smaller carbide size in the Cr $_3$C $_2$-25NiCr material significantly reduced the carbide rebounding leading to higher carbide content in the sprayed coating and improved erosion wear resistance. Most significant improvements were observed in cavitation erosion for HVAF sprayed WC-10Co4Cr coatings (0.4 μm/h)compared to the HVOF sprayed coatings (1.5–3.7 μm/h). The cavitation erosion resistance of the HVAF sprayed coatings was almost at the level of the WC-10Co sintered bulk (0.2 μm/h).

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Tampere University, VZÚ Plzeň - Research and Testing Institute
Contributors: Matikainen, V., Rubio Peregrina, S., Ojala, N., Koivuluoto, H., Schubert, J., Houdková, Vuoristo, P.
Number of pages: 17
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Cavitation erosion, Coating, Hardmetal, Slurry erosion, Thermal spray
DOIs:

10.1016/j.surfcoat.2019.04.067

Bibliographical note

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Research output: Contribution to journal › Article › Scientific › peer-review

A study of Cr_3C_2-based HVOF- and HVAF-sprayed coatings: Abrasion, dry particle erosion and cavitation erosion resistance

Material and spray process selection are the key factors in the tailoring of thermal sprayed coatings for demanding industrial applications. In this study, four commercial Cr_3C_2-based feedstock materials were sprayed with gas-fuelled high-velocity oxygen-fuel (HVOF) and modern high-velocity air-fuel (HVAF) spray processes. Two materials with standard Cr_3C_2–25NiCr composition (porous and dense), a Cr_3C_2–50NiCrMoNb and Cr_3C_2–37WC–18NiCoCr materials were sprayed in addition to the reference WC-10Co4Cr material. The Cr_3C_2–50NiCrMoNb had a higher content of the Ni-based metal matrix compared to standard Cr_3C_2–25NiCr composition for added corrosion resistance, while the Cr_3C_2–37WC–18NiCoCr material contained additional tungsten carbide (WC) particles to improve the wear resistance. In abrasion and dry particle erosion, the Cr_3C_2–50NiCrMoNb coatings showed a higher degree of plastic deformation and increased material loss, whereas the Cr_3C_2–37WC–18NiCoCr coating had wear resistance between the standard Cr_3C_2–25NiCr and reference WC-10Co4Cr coatings. In cavitation erosion, the lower carbide content of Cr_3C_2–50NiCrMoNb coatings turned out to improve the resistance against fatigue wear due to higher fracture toughness. Overall, the HVAF sprayed coatings had higher elastic modulus, higher fracture toughness, equal or higher abrasion and erosion resistance, and higher cavitation erosion resistance compared to the HVOF sprayed counterparts.

General information

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Contributors: Matikainen, V., Koivuluoto, H., Vuoristo, P.

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Journal: Wear
Volume: 446-447
Article number: 203188
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Abrasion, Cavitation erosion, Coating, Erosion, Hardmetal, HVAF
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Source: Scopus
Source ID: 85077986604
Research output: Contribution to journal › Article › Scientific › peer-review

Accurate Binding of Sodium and Calcium to a POPC Bilayer by Effective Inclusion of Electronic Polarization
Binding affinities and stoichiometries of Na^+ and Ca^{2+} ions to phospholipid bilayers are of paramount significance in the properties and functionality of cellular membranes. Current estimates of binding affinities and stoichiometries of cations are, however, inconsistent due to limitations in the available experimental and computational methods. In this work, we improve the description of the binding details of Na^+ and Ca^{2+} ions to a 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) bilayer by implicitly including electronic polarization as a mean field correction, known as the electronic continuum correction (ECC). This is applied by scaling the partial charges of a selected state-of-the-art POPC lipid model for molecular dynamics simulations. Our improved ECC-POPC model reproduces not only the experimentally measured structural parameters for the ion-free membrane, but also the response of lipid headgroup to a strongly bound cationic amphiphile, as well as the binding affinities of Na^+ and Ca^{2+} ions. With our new model, we observe on the one side negligible binding of Na^+ ions to POPC bilayer, while on the other side stronger interactions of Ca^{2+} primarily with phosphate oxygens, which is in agreement with the previous interpretations of the experimental spectroscopic data. The present model results in Ca^{2+} ions forming complexes with one to three POPC molecules with almost equal probabilities, suggesting more complex binding stoichiometries than those from simple models used to interpret the NMR data previously. The results of this work pave the way to quantitative molecular simulations with realistic electrostatic interactions of complex biochemical systems at cellular membranes.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Physics, Research group: Biological Physics and Soft Matter, Research area: Computational Physics, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Department of Physical Chemistry, University of Helsinki Institute of Biotechnology
Contributors: Melcr, J., Martinez-Seara, H., Nencini, R., Kolafa, J., Jungwirth, P., Ollila, O. H. S.
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Peer-reviewed: Yes

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ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry
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Bibliographical note
EXT=”Martinez-Seara, Hector”
EXT="Ollila, O. H. Samuli"
Source: Scopus
Source ID: 85046019210

Quench absorption coils: A quench protection concept for high-field superconducting accelerator magnets

A quench protection concept based on coupled secondary coils is studied for inductively transferring energy out of a quenching superconducting dipole and thus limiting the peak hotspot temperature. So-called 'quench absorption coils' are placed in close proximity to the superconducting coils and are connected in series with a diode for the purpose of preventing current transformation during regular operation. During a quench, current is then transformed into the quench absorption coils so that a significant fraction of the stored magnetic energy is dissipated in the these coils. Numerical calculations are performed to determine the impact of such a concept and to evaluate the dimensions of the quench absorption coils needed to obtain significant benefits. A previously constructed 15 T Nb_3Sn block coil is taken as a reference layout. Finite-element calculations are used to determine the combined inductive and thermal response of this system and these calculations are validated with a numerical model using an adiabatic approximation. The calculation results indicate that during a quench the presence of the quench absorption coils reduces the energy dissipated in the superconducting coils by 45% and reduces the hotspot temperature by over 100 K. In addition, the peak resistive voltage over the superconducting coils is significantly reduced. This suggests that this concept may prove useful for magnet designs in which the hotspot temperature is a design driver.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Electrical Energy Engineering, Research area: Electromagnetics, Research area: Power engineering, Research group: Modelling and superconductivity, European Organization for Nuclear Research
Contributors: Mentink, M., Salmi, T.
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Volume: 30
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ISSN (Print): 0953-2048
Ratings:

Scopus rating (2017): CiteScore 5 SJR 1.036 SNIP 1.519
Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Condensed Matter Physics, Metals and Alloys, Materials Chemistry, Electrical and Electronic Engineering
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http://urn.fi/URN:NBN:fi:tty-201712182395. Embargo ended: 3/05/18
Source: Scopus
Source ID: 85019572277
Research output: Contribution to journal › Article › Scientific › peer-review

Flip-chip Wafer-fused OP-VECSELs emitting 3.65 W at the 1.55-μm waveband

Optically-pumped vertical external cavity surface emitting lasers (VECSELs) based on flip-chip gain mirrors emitting at the 1.55-μm wavelength range are reported. The gain mirrors employ wafer-fused InAlGaAs/InP quantum well heterostructures and GaAs/AlAs distributed Bragg reflectors fixed on a diamond heat-sink substrate in a flip-chip geometry, incorporated in a V-cavity configuration. A maximum output power of 3.65 W was achieved for a heat sink temperature of 11°C and employing a 2.2% output coupler. The laser exhibited circular beam profiles for the full emission power range. This demonstration represents more than 5-fold increase of the output power compared to state-of-the-art flip-chip VECSELs previously reported at the 1.55 μm wavelength range. It opens new perspectives for developing practical VECSEL-based laser systems operating at a wavelength range widely used in many applications.

General information

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Organisations: Physics, CRPP, LakeDiamond SA
Contributors: Mereuta, A., Nechay, K., Caliman, A., Suruceanu, G., Rudra, A., Gallo, P., Guina, M., Kapon, E.
Publication date: 2019

Peer-reviewed: Yes

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Journal: IEEE Journal of Selected Topics in Quantum Electronics
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ISSN (Print): 0792-1233
Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Atomic and Molecular Physics, and Optics, Materials Chemistry, Electrical and Electronic Engineering
Keywords: diode pumped, Flip-chip devices, Heating systems, Lasers, Mirrors, Optical pumping, Power generation, Semiconductor lasers, Temperature measurement, Vertical cavity surface emitting lasers, Vertical emitting lasers
DOIs:

10.1109/JSTQE.2019.2922819
Source: Scopus
Source ID: 85067801249
Research output: Contribution to journal › Article › Scientific › peer-review

Hierarchical Self-Assembly of Halogen-Bonded Block Copolymer Complexes into Upright Cylindrical Domains
Self-assembly of block copolymers into well-defined, ordered arrangements of chemically distinct domains is a reliable strategy for preparing tailored nanostructures. Microphase separation results from the system, minimizing repulsive interactions between dissimilar blocks and maximizing attractive interactions between similar blocks. Supramolecular methods have also achieved this separation by introducing small-molecule additives binding specifically to one block by noncovalent interactions. Here, we use halogen bonding as a supramolecular tool that directs the hierarchical self-assembly of low-molecular-weight perfluorinated molecules and diblock copolymers. Microphase separation results in a lamellar-within-cylindrical arrangement and promotes upright cylindrical alignment in films upon rapid casting and without further annealing. Such cylindrical domains with internal lamellar self-assemblies can be cleaved by solvent treatment of bulk films, resulting in separated and segmented cylindrical micelles stabilized by halogen-bond-based supramolecular crosslinks. These features, alongside the reversible nature of halogen bonding, provide a robust modular approach for nanofabrication.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, VTT Technical Research Centre of Finland, Aalto University, Politecnico di Milano, Italian Institute of Technology, Università del Salento
Contributors: Milani, R., Houbenov, N., Fernandez-Palacio, F., Cavallo, G., Luzio, A., Haataja, J., Giancane, G., Saccone, M., Priimägi, A., Metrangolo, P., Ikkala, O.
Number of pages: 10
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Journal: CheM
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Scopus rating (2017): CiteScore 6.7 SJR 5.295 SNIP 2.265
Original language: English
ASJC Scopus subject areas: Chemistry(all), Chemical Engineering(all), Biochemistry, Environmental Chemistry, Materials Chemistry, Biochemistry, medical
Keywords: block copolymers, halogen bond, hierarchical self-assembly, nanofabrication, supramolecular complexes
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URLs:

http://urn.fi/URN:NBN:fi:tty-201703281227
Source: Scopus
Source ID: 85014778403
Research output: Contribution to journal › Article › Scientific › peer-review

Influence of the Spray Gun Type on Microstructure and Properties of HVAF Sprayed Fe-Based Corrosion Resistant Coatings

The aim of this study is to evaluate the microstructural details and corrosion properties of novel Fe-based coatings prepared using two different generations of HVAF spray guns. These two generations of HVAF guns are Activated Combustion HVAF (AC-HVAF, 2nd generation) M2 gun and Supersonic Air Fuel HVAF (SAF, 3rd generation) M3 gun. Structural details were analysed using x-ray diffractometry and field-emission scanning electron microscope. Higher denseness with homogeneous microstructure was achieved for Fe-based coating deposited by the M3 process. Such coatings exhibit higher particle deformation and lower oxide content compared to coatings manufactured with M2 gun. Corrosion properties were studied by open-cell potential measurements and electrochemical impedance spectroscopy. The lower porosity and higher interlamellar cohesion of coating manufactured with M3 gun prevent the electrolyte from penetrating through the coating and arriving to the substrate, enhancing the overall corrosion resistance. This can be explained by the improved microstructures and coating performance.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Surface Engineering, Engineering materials science and solutions (EMASS)
Contributors: Milanti, A., Koivuluoto, H., Vuoristo, P.
Number of pages: 11
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Publication date: 2015
Peer-reviewed: Yes

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Ratings:

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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films
Keywords: corrosion behavior, Fe-based coatings, HVAF, structure
DOIs:

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URLs:

http://www.scopus.com/inward/record.url?scp=84941340669&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84944279959
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of spraying parameters on the microstructural and corrosion properties of HVAF-sprayed Fe-Cr-Ni-B-C coatings

Thermally sprayed Fe-based coatings have been extensively studied as future solution in order to replace more expensive, harmful and environmentally dangerous Ni- and WC-based coatings for several industrial applications where high corrosion and wear resistance are required. The aim of the present study is to investigate the effect of spraying parameters on the microstructure and the corrosion resistance of Fe-based coatings manufactured with the High Velocity Air Fuel (HVAF) thermal spray process. Six sets of thermal spraying parameters have been chosen and their effect on the overall quality of coatings was investigated. All HVAF coatings showed comparably dense microstructure with near-zero oxidation, proving the high quality of the deposition process. However, higher anti-corrosion and mechanical properties were achieved by increasing the spraying air pressure and decreasing the particle feeding rate without altering the thickness and the overall deposition rate. Powder feeding rate was reported to have a remarkable effect on microstructure and corrosion properties. Coatings with beneficial compressive residual stresses were successfully obtained by increasing air pressure during spraying which resulted in improved microstructural and corrosion properties.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Surface Engineering, Engineering materials science and solutions (EMASS), University of Modena and Reggio Emilia, Department of Engineering Enzo Ferrari
Contributors: Milanti, A., Matikainen, V., Koivuluoto, H., Bolelli, G., Lusvarghi, L., Vuoristo, P.
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Corrosion behaviour, Fe-based coating, HVAF, Structure
DOIs:

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http://www.scopus.com/inward/record.url?scp=84939782846&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84939782846
Research output: Contribution to journal › Article › Scientific › peer-review

Microstructure and Sliding Wear Behavior of Fe-Based Coatings Manufactured with HVOF and HVAF Thermal Spray Processes
The microstructure and micromechanical behavior of thermally sprayed Fe-based coatings manufactured with high-velocity oxygen fuel (HVOF) and high-velocity air fuel (HVAF) processes were investigated. Fe-Cr-Ni-Si-B-C and Fe-Cr-Ni-Mo-Si-B-C powders were used as the feedstock materials. The coatings showed a highly dense microstructure with near-zero oxidation. The microstructure of the feedstock powders was better retained when sprayed with HVAF process. Differential scanning calorimetry revealed two small exothermic peaks at about 600 °C for the HVOF-sprayed coatings, without any increase in weight in thermogravimetric analysis. It suggested the re-precipitation of carbides that were dissolved during spraying due to the higher particle temperature reported by spray diagnostics system during the HVOF process (≈1800 °C) compared to the HVAF one (≈1400 °C). Micro- and nano-indentations helped to show the difference in inter-lamellar cohesive strength and, in turn, in the particle deposition mechanism. Coatings sprayed with Fe-Cr-Ni-Mo-Si-B-C composition possessed higher sliding wear resistance than that of Fe-Cr-Ni-Si-B-C due to higher nano-hardness. More specifically, HVOF-sprayed Fe-Cr-Ni-Mo-Si-B-C coating showed the largest intra-lamellar hardness, the largest elasticity, and high quality of particle interfaces which resulted in lower sliding wear rate.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Surface Engineering
Contributors: Milanti, A., Matikainen, V., Bolelli, G., Koivuluoto, H., Lusvarghi, L., Vuoristo, P.
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films
Keywords: iron alloys, protective coatings, wear resistant coatings
DOIs:

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Research output: Contribution to journal › Article › Scientific › peer-review

Electromagnetic interference shielding effectiveness of MWCNT filled poly(ether sulfone) and poly(ether imide) nanocomposites
Multiwalled carbon nanotube (MWCNT) filled poly(ether sulfone) (PES) and poly(ether imide) (PEI) composites were prepared with different MWCNT weight fractions (0.5-5wt%) by a solution mixing technique. Their electrical conductivities,

electromagnetic interference (EMI), shielding effectiveness (SE), return loss (RL), and absorption loss (AL) were investigated. Morphologies of the fracture surfaces of nanocomposites studied by scanning electron and transmission electron microscopy showed relatively good MWCNT dispersion and distribution. The electrical conductivity of compression molded samples measured at room temperature indicated that the electrical percolation network was achieved already at 0.5% loading. The measurements of shielding effectiveness (SE) carried out in the frequency range of 8 to 12 GHz (X-band range) showed that SE increases with measurement frequency and with filler loading, whereby no significant differences could be observed between PES and PEI as matrices. The nanocomposites based on both matrices with 5 wt% loading of MWCNT exhibited shielding levels at 8 GHz between 42 and 45 dB in comparison with the pure polymers which showed value in the range of 1 to 2 dB. RL and AL showed significantly lower values for the composites as compared to unfilled polymers, but no systematic trends were observed on frequency.

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MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Materials Science Centre, Indian Institute of Technology, Department of Applied Science, Symbiosis International University, Leibniz Institute of Polymer Research Dresden (IPF)
Contributors: Mohanty, A. K., Ghosh, A., Sawai, P., Pareek, K., Banerjee, S., Das, A., Pötschke, P., Heinrich, G., Voit, B.
Number of pages: 11
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ISSN (Print): 0032-3888
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Polymers and Plastics, Materials Chemistry
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10.1002/pen.23804
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http://www.scopus.com/inward/record.url?scp=84907865840&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84907865840
Research output: Contribution to journal › Article › Scientific › peer-review

The 5th international workshop on numerical modelling of high temperature superconductors

General information
Publication status: Published
MoE publication type: B1 Article in a scientific magazine
Organisations: Electrical Energy Engineering, University of Bologna, University of Cambridge, Karlsruhe Institute of Technology, Campus North
Contributors: Morandi, A., Ainslie, M. D., Grilli, F., Stenvall, A.
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Ratings:

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ASJC Scopus subject areas: Ceramics and Composites, Condensed Matter Physics, Metals and Alloys, Materials Chemistry, Electrical and Electronic Engineering
DOIs:

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Source: Scopus
Source ID: 85029536672
Research output: Contribution to journal › Editorial › Scientific

The effects of UV irradiation to polyetheretherketone fibres: Characterization by different techniques

The effects of UV irradiation on polyetheretherketone (PEEK) fibres were investigated in this study. PEEK fibres were manufactured with a melt spinning system and then artificially aged with simulated solar UV light. Fibres were then characterized by mechanical tests, Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), rheology, thermogravimetric analysis (TGA) and scanning electron microscopy (SEM). PEEK, best known for its excellent thermal stability, suffered greatly from the effects of UV irradiation. The low UV stability manifested as embrittlement of the fibres in the mechanical tests, increased crosslinking rate in the rheological tests, formation of carbonyl and hydroxyl groups and changes in the nature of the carbon-hydrogen bonds in the FTIR, diminished thermal properties in TGA, and transverse cracks in the SEM photos. DSC was found to be an inaccurate technique for estimating the degradation level of PEEK fibres, whereas the carbonyl index measured by FTIR was found to be the most convenient technique.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tampere University of Technology
Contributors: Mylläri, V., Ruoko, T. P., Järvelä, P.
Number of pages: 7
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Original language: English
ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry, Mechanics of Materials, Condensed Matter Physics
Keywords: PEEK, Fibre, Ultraviolet, Rheology, POLY(ETHER ETHER KETONE), STRUCTURE/DEGRADABILITY RELATIONSHIPS, SCANNING CALORIMETRY, THERMAL-DEGRADATION, POLYPROPYLENE, PHOTODEGRADATION, POLYMERS, PHOTOOXIDATION, CRYSTALLINITY
Electronic versions:

The_effects_of_UV_irradiation_pre-print
DOIs:

10.1016/j.polymdegradstab.2014.08.003
URLs:

http://urn.fi/URN:NBN:fi:tty-201612024839
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http://www.scopus.com/inward/record.url?scp=84907310748&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note

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Contribution: organisation=keb,FACT2=0.2
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Publisher name: Elsevier Ltd
Source: researchoutputwizard
Source ID: 1117
Research output: Contribution to journal › Article › Scientific › peer-review

Production of sulfonated polyetheretherketone/polypropylene fibers for photoactive textiles

New photocatalytic fibers made of sulfonated polyetheretherketone (SPEEK)/polypropylene (PP) are melt compounded and melt spun, first on laboratory scale and then on a semi-industrial scale. Fiber spinnability is optimized and the fibers are characterized using mechanical testing, electron paramagnetic resonance (EPR) spectroscopy, and scanning electron microscopy (SEM). According to the results, the fiber spinnability remains at a good level up to 10 wt % SPEEK concentration. Optimal processing temperature is 200C due to the thermal degradation at higher temperatures. EPR measurements show good and long-lasting photoactivity after the initial irradiation but also decay in the radical intensity during several irradiation cycles. Mechanical tenacity of the SPEEK/PP 5:95 fiber is approximately 20% lower than for otherwise similar PP fiber. The fiber is a potential alternative to compete against TiO2-based products but more research needs to be done to verify the real-life performance.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Department of Mechanical Engineering and Industrial Systems, Research area: Sustainable Machine Systems, University College of Borås, Högskolan i Borås, Next Technology Tecnotessile Società Nazionale di Ricerca S.r.l., Department of Biotechnology , Chemistry and Pharmacy, University of Siena
Contributors: Mylläri, V., Fatarella, E., Ruzzante, M., Pogni, R., Baratto, M. C., Skrifvars, M., Syrjälä, S., Järvelä, P.
Publication date: 1 Oct 2015
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ISSN (Print): 0021-8995
Ratings:

Scopus rating (2015): CiteScore 3.6 SJR 0.587 SNIP 0.846
Original language: English
ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)
Keywords: blends, fibers, functionalization of polymers, photochemistry, textiles
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ORG=mol,0.5
ORG=mei,0.5
EXT="Skrifvars, Mikael"
Source: Scopus
Source ID: 84937636904
Research output: Contribution to journal › Article › Scientific › peer-review

A comparison of rheology and FTIR in the study of polypropylene and polystyrene photodegradation
Rheology and FTIR spectroscopy are compared as methods to study the degree of photodegradation in polypropylene (PP) and polystyrene (PS) sheets. The materials are hot pressed, artificially photo-aged with fluorescent lights for 4-2048 h and then measured with a rotational rheometer and FTIR. Both materials show a tendency for chain scission which can be seen as a reduction in viscosity. Changes in PP can be observed with both methods after 256 h of irradiation. Changes in PS become significant in rheology after 64 h but in FTIR only after 1024 h of irradiation. Due to the different chemical nature of the materials, the degradation of PS is rather linear with exposure, whereas the degradation of PP is more exponential. Using the zero shear viscosities obtained through extrapolations of the Cole-Cole and Carreau-Yasuda models, relative molecular weights are estimated with the aid of the power-law relationship between these two. These results are compared with the carbonyl indices determined from the FTIR spectra. Rheology is found to be a viable alternative for FTIR in certain situations.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research area: Sustainable Machine Systems, Department of Mechanical Engineering and Industrial Systems, Tampere Univ Technol, Tampere University of Technology, Dept Chem & Bioengn
Contributors: Mylläri, V., Ruoko, T., Syrjälä, S.
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Article number: 42246
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Scopus rating (2015): CiteScore 3.6 SJR 0.587 SNIP 0.846
Original language: English
ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Surfaces, Coatings and Films, Chemistry(all)
Keywords: aging, degradation, rheology, thermoplastics, PHOTOOXIDATION, FILMS, PHOTOLYSIS
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DOIs:

10.1002/app.42246
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Bibliographical note
ORG=mol,0.7
ORG=keb,0.2
ORG=mei,0.1
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Source ID: 84928363110
Research output: Contribution to journal › Article › Scientific › peer-review

Characterization of thermally aged polyetheretherketone fibres: Mechanical, thermal, rheological and chemical property changes

This paper investigates the effects of thermal degradation on polyetheretherketone (PEEK) fibres. PEEK samples were aged at a constant temperature of 250 °C for 1-128 days and characterized with mechanical tests, FTIR (Fourier Transform Infrared Spectroscopy), DSC (Differential Scanning Calorimetry), rheology, TGA (Thermogravimetric Analysis), SEM (Scanning Electron Microscopy), and UV-Vis diffuse reflectance spectroscopy. The short-term thermal annealing had a positive effect on the mechanical properties, due to the formation and growth of secondary crystals. Crosslinking in the material was verified by rheological inspections. The crosslinking increased the mechanical strength and modulus but reduced the elongation at break of the fibres. FTIR tests showed that carbonyl and hydroxyl groups were slowly formed on the surface of the fibres while ring opening reactions took place. The thermal ageing reduced the thermal stability of PEEK. The decreased stability was observed in the decomposition onset temperature after 8 d and in the melting point and the glass transition temperature after 32 d. The first signs of degradation, crosslinking, embrittlement, and reduced thermal stability, were visible roughly after 8 d of ageing, whereas the deterioration in general usability occurred after 64 d.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Engineering materials science and solutions (EMASS)
Contributors: Mylläri, V., Ruoko, T., Vuorinen, J., Lemmetyinen, H.
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ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry, Mechanics of Materials, Condensed Matter Physics
Keywords: Fibre, PEEK, Thermal degradation
Electronic versions:

Characterization of thermally aged polyetheretherketone fibres_pre-print
DOIs:

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ORG=keb,0.25
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Research output: Contribution to journal › Article › Scientific › peer-review

Detergent impurity effect on recycled HDPE: Properties after repetitive processing
High density polyethylene (rHDPE) is extruded 1 to 8 times, with and without detergent, to simulate the effects of impurities on the material and on the artificial ageing process. The mechanical properties, thermal stability, rheology, Fourier transform infrared spectroscopy (FTIR), and volatile organic compound (VOC) emissions are measured. According to the results, ageing of rHDPE increases tensile strength, reduces elongation, and enhances side chain branching of the material and thus causes rheological changes. The addition of detergent reduces changes in mechanical properties and rheological behavior but accelerates thermal degradation. VOC and FTIR measurements of the samples with detergent addition show generation of harmful 1,4-dioxane. The amount of total emission, as well as emissions of important perfumes limonene and 1R-α-pinene, decreases during multiple extrusion cycles. Heating of the plastics is found to be a major factor in the VOC emission reduction. Impurities have a notable effect on the artificial ageing results.

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, University of Helsinki, Ekokem
Contributors: Mylläri, V., Hartikainen, S., Poliakova, V., Anderson, R., Jönkkäri, I., Pasanen, P., Andersson, M., Vuorinen, J.
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry
Keywords: Ageing, Degradation, Polyolefins, Recycling
DOIs:
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Source: Scopus
Source ID: 84992303578
Research output: Contribution to journal › Article › Scientific › peer-review

Dielectric Breakdown Strength of Thermally Sprayed Ceramic Coatings: Effects of Different Test Arrangements
Dielectric properties (e.g., DC resistivity and dielectric breakdown strength) of insulating thermally sprayed ceramic coatings differ depending on the form of electrical stress, ambient conditions, and aging of the coating, however, the test arrangements may also have a remarkable effect on the properties. In this paper, the breakdown strength of high velocity oxygen fuel-sprayed alumina coating was studied using six different test arrangements at room conditions in order to study the effects of different test and electrode arrangements on the breakdown behavior. In general, it was shown that test arrangements have a considerable influence on the results. Based on the results, the recommended testing method is to use embedded electrodes between the voltage electrode and the coating at least in DC tests to ensure a good contact with the surface. With and without embedded electrodes, the DBS was 31.7 and 41.8 V/μm, respectively. Under AC excitation, a rather good contact with the sample surface is, anyhow, in most cases acquired by a rather high partial discharge activity and no embedded electrodes are necessarily needed (DBS 29.2 V/μm). However, immersion of the sample in oil should strongly be avoided because the oil penetrates quickly into the coating affecting the DBS (81.2 V/μm).

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Electrical Engineering, Research area: Power engineering, Smart Energy Systems (SES), VTT Technical Research Centre of Finland
Contributors: Niittymäki, M., Lahti, K., Suhonen, T., Metsäjoki, J.
Number of pages: 10
Pages: 542-551
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Scopus rating (2015): CiteScore 3 SJR 0.735 SNIP 0.989
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films
Keywords: AlO, breakdown strength, coating, dielectric, HVOF, thermal spraying
Electronic versions:

Dielectric Breakdown Strength of Thermally 2015
DOIs:

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URLs:

http://urn.fi/URN:NBN:fi:tuni-202005225567

Bibliographical note
EXT="Metsäjoki, Jarkko"
Source: Scopus
Source ID: 84925536197
Research output: Contribution to journal › Article › Scientific › peer-review

Luminescence of Er^{3+} doped oxyfluoride phosphate glasses and glass-ceramics
Glasses with the composition (75 $NaPO_3$-(25-x) CaO-xCaF_2) (in mol %) were prepared with 0.15 mol% of Er_2O_3. The effect of the glass composition and of heat treatment on the spectroscopic properties of the newly developed glasses is reported. With the progressive replacement of CaO by CaF_2, the Er^{3+}:$^4I_{13/2}$ lifetime and the intensity of the upconversion emission increase whereas the intensity of the emission at 1.5 μm decreases due to the decrease in the phonon energy in the as-prepared glasses. The glasses were heat treated at 20 °C above their respective glass transition temperature for 17 h to form nuclei and then at their crystallization temperature from 15min to 1 h to grow the nuclei into crystals. The heat treatment leads to the precipitation of crystalline phases, the composition of which depends upon the glass composition. As the Er^{3+}:$^4I_{13/2}$ lifetime increases and the intensity of the upconversion increases for the glass with x = 0 after heat treatment, the Er^{3+} ions are expected to be incorporated into the phosphate-based crystals. However, as the shape of the emission band at 1.5 μm remains unchanged and the intensity of the upconversion decreases significantly after heat treatment of the glasses with x > 10, the crystals found in the glass-ceramics with x > 10 are thought to free of Er^{3+} ions. Although Er^{3+} ions entered in the CaF_2 crystals precipitating in aluminosilicate glass, the Er^{3+} ions are believed to remain in the amorphous phosphate part of the glass-ceramic containing CaF_2 crystals.

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Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Faculty of Biomedical Sciences and Engineering, Faculty of Engineering Sciences, Research group: Biomaterials and Tissue Engineering Group, Materials Science, Photonics, Istituto Superiore Mario Boella
Contributors: Nommeots-Nomm, A., Boetti, N. G., Salminen, T., Massera, J., Hokka, M., Petit, L.
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Journal: Journal of Alloys and Compounds
Volume: 751
ISSN (Print): 0925-8388
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Original language: English
ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Metals and Alloys, Materials Chemistry
Keywords: CaF crystals in glass, Er luminescence, Oxyfluoride phosphate glasses and glass-ceramics
DOIs:

10.1016/j.jallcom.2018.04.101
Source: Scopus
Source ID: 85045405038
Research output: Contribution to journal › Article › Scientific › peer-review

Powering of an HTS dipole insert-magnet operated standalone in helium gas between 5 and 85 K

This paper describes the standalone magnet cold testing of the high temperature superconducting (HTS) magnet Feather-M2.1-2. This magnet was constructed within the European funded FP7-EUCARD2 collaboration to test a Roebel type HTS cable, and is one of the first high temperature superconducting dipole magnets in the world. The magnet was operated in forced flow helium gas with temperatures ranging between 5 and 85 K. During the tests a magnetic dipole field of 3.1 T was reached inside the aperture at a current of 6.5 kA and a temperature of 5.7 K. These values are in agreement with the self-field critical current of the used SuperOx cable assembled with Sunam tapes (low-performance batch), thereby confirming that no degradation occurred during winding, impregnation, assembly and cool-down of the magnet. The magnet was quenched many tens of times by ramping over the critical current and no degradation nor training was evident. During the tests the voltage over the coil was monitored in the microvolt range. An inductive cancellation wire was used to remove the inductive component, thereby significantly reducing noise levels. Close to the quench current, drift was detected both in temperature and voltage over the coil. This drifting happens in a time scale of minutes and is a clear indication that the magnet has reached its limit. All quenches happened approximately at the same average electric field and thus none of the quenches occurred unexpectedly.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Electrical Energy Engineering, European Organization for Nuclear Research, University of Twente, French Atomic Energy Commission (CEA) Saclay, Karlsruhe Institute of Technology, Insitute for Technical Physics, Germany, SuperOx, Victoria University of Wellington, Bruker HTS, University of Southampton
Contributors: Nugteren, J. V., Kirby, G., Bajas, H., Bajko, M., Ballarino, A., Bottura, L., Chiuchiolo, A., Contat, P. A., Dhallé, M., Durante, M., Fazilleau, P., Fontalva, A., Gao, P., Goldacker, W., Kate, H. T., Kario, A., Lahtinen, V., Lorin, C., Markelov, A., Mazet, J., Molodyk, A., Murtomäki, J., Long, N., Perez, J., Petrone, C., Pincot, F., Rijk, G. D., Rossi, L., Russenschuck, S., Ruuskanen, J., Schmitz, K., Stenvall, A., Usoskin, A., Willering, G., Yang, Y.
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Ratings:

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Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Condensed Matter Physics, Metals and Alloys, Electrical and Electronic Engineering, Materials Chemistry
Keywords: cold testing, high temperature superconductors, superconducting accelerator magnets, superconducting magnets
DOIs:

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Bibliographical note

EXT="Murtomäki, J."
Source: Scopus
Source ID: 85046942716
Research output: Contribution to journal › Article › Scientific › peer-review

Effects of composition and microstructure on the abrasive wear performance of quenched wear resistant steels

Wear resistant steels are commonly categorized by their hardness, and in the case of quenched wear resistant steels, their Brinell hardness grades are widely considered almost as standards. In this study, the abrasive wear performance of 15 commercially available 400 HB grade quenched wear resistant steels from all over the world were tested with granite gravel in high stress conditions. The aim was to evaluate the real wear performance of nominally similar steels. Also

properties such as hardness, hardness profiles, microstructures and chemical compositions of the steels were studied and reasons for the differences in their wear performance further discussed. In terms of mass loss, over 50% differences were recorded in the abrasive wear performance of the studied steels. Variations in the chemical compositions were linked to the auto-tempered microstructures of the steels, and the microstructural characteristics were further linked to their ultimate wear behavior.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Materials Characterization, Tampere University of Technology, Metso Minerals, Inc.
Contributors: Ojala, N., Valtonen, K., Heino, V., Kallio, M., Aaltonen, J., Siitonen, P., Kuokkala, V. T.
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Issue number: 1-2
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Ratings:
Scopus rating (2014): CiteScore 4.1 SJR 1.711 SNIP 2.302
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces and Interfaces, Materials Chemistry, Surfaces, Coatings and Films, Mechanics of Materials
Keywords: Abrasion, Hardness, Microstructure, Mineral processing, Steel, Wear testing
Electronic versions:
Paper for WEAR_Niko Ojala_for open access. Embargo ended: 15/09/16
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URLs:
http://www.scopus.com/inward/record.url?scp=84903144175&partnerID=8YFLogxK (Link to publication in Scopus)

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Contribution: organisation=mol,FACT1=1
Portfolio EDEND: 2014-11-28
Publisher name: Elsevier
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Source ID: 1185
Research output: Contribution to journal › Article › Scientific › peer-review

Influence of the phosphate glass melt on the corrosion of functional particles occurring during the preparation of glass-ceramics

We report our findings on the impact of the glass composition on the corrosion of microparticles occurring during the preparation of glass-ceramics using the direct doping method. Microparticles (MPs) with the composition $Sr_4Al_{14}O_{25}:Eu^{2+},Dy^{3+}$ with blue-green persistent luminescence were chosen as the changes in their spectroscopic properties can be related to the MPs' corrosion. The MPs were added in phosphate-based glasses with different compositions. When using the same doping parameters, the glass system with the composition $90NaPO_3$-$10Na_2O$ (mol%) was found to be the least corrosive on the MPs whereas the glass system with the composition $90NaPO_3$-10NaF (mol%) is the most corrosive on the MPs probably due to their different viscosity at 575 °C, the temperature at which the MPs are added in the glass melts.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Photonics, Research group: Nanophotonics, Turun Yliopisto/Turun Biomateriaalikeskus, Laboratory of Photonics
Contributors: Ojha, N., Laihinen, T., Salminen, T., Lastusaari, M., Petit, L.
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Journal: Ceramics International
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ISSN (Print): 0272-8842
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Ceramics and Composites, Process Chemistry and Technology, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Corrosion, Direct doping method, Glass melt, Phosphate glass-ceramics, SrAlO:Eu, Dy microparticles
DOIs:

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Source: Scopus
Source ID: 85044921933
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Effect of heat-treatment on the upconversion of $NaYF_4:Yb^{3+}$, Er^{3+} nanocrystals containing silver phosphate glass

Novel $NaYF_4:Yb^{3+}$, Er^{3+} nanocrystals containing phosphate glass with composition $83.25NaPO_3$–9.25NaF-5ZnO-2.5Ag_2O (in mol%) was prepared by adding the $NaYF_4:Yb^{3+}$, Er^{3+} nanocrystals in the glass using the direct doping method. The optical and luminescence properties of this new glass are presented and discussed. The newly developed glass exhibits visible emission under 980 nm pumping with high intensity confirming the presence of the $NaYF_4:Yb^{3+}$, Er^{3+} nanocrystals in the glass. From the absorption spectrum of the as-prepared glass, it is showed that the as-prepared glasses contains already Ag nanoparticles which are thought to precipitate due to the decomposition of some of the $NaYF_4:Yb^{3+}$, Er^{3+} nanocrystals occurring during the glass preparation. A heat treatment of the glass was found to lead to the migration of Ag species at the surface of the glass as evidenced using SEM and to a decrease of the intensity of the upconversion mostly due to an increase of the inter defects in the $NaYF_4:Yb^{3+}$, Er^{3+} nanocrystals due to the heat treatment.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Physics, Technical University of Cluj-NapocaUniversitatea Tehnica din Cluj-Napoca
Contributors: Ojha, N., Bogdan, M., Galatus, R., Petit, L.
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Article number: 120243
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Ceramics and Composites, Condensed Matter Physics, Materials Chemistry
Keywords: Absorption, Luminescence, NaYF:Yb, Er nanocrystals, Phosphate glass, Silver nanoparticles
DOIs:

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Source: Scopus
Source ID: 85086450328
Research output: Contribution to journal › Article › Scientific › peer-review

Mechanical performance and CO2 uptake of ion-exchanged zeolite A structured by freeze-casting

Zeolite 4A has been freeze-cast into highly porous monoliths with a cylindrical shape. The brittle monoliths, with lamellar or columnar pores and wall thicknesses between 8 and 35μm, show a compressive mechanical response along the main pore axis that could be modeled by a buckling behavior. The failure strength is proportional to the density and the amount of transverse bridging across lamella, which was shown to be related to the pore cross-sectional aspect ratio. Monoliths with highly anisotropic pores with a cross-sectional aspect ratio higher than 3 yielded sequentially from the top surface, whereas monoliths with a pore aspect ratio lower than 3 were found to delaminate into longitudinal splinters. The freeze-cast monoliths show a sharp gas breakthrough front with a 1:9 mixture of CO<inf>2</inf> and N<inf>2</inf>, indicating rapid uptake kinetics of the lamellar structures.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Ceramic materials, Department of Signal Processing, Engineering materials science and solutions (EMASS), Workshop for Research in Artistic Technologies, RATS, Stockholm University, Sweden, Luleå University of Technology, Department of Materials and Environmental Chemistry, Berzelii

Center EXSELENT on Porous Materials, Division of Materials Science
Contributors: Ojuva, A., Järveläinen, M., Bauer, M., Keskinen, L., Valkonen, M., Akhtar, F., Levänen, E., Bergström, L.
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Peer-reviewed: Yes

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Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Materials Chemistry
Keywords: Freeze-casting, Laminate, Mechanical strength, Porous ceramics, Zeolite A
DOIs:

10.1016/j.jeurceramsoc.2015.03.001

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ORG=sgn,0.5
Source: Scopus
Source ID: 84933679506
Research output: Contribution to journal › Article › Scientific › peer-review

Performance testing of iron based thermally sprayed HVOF coatings in a biomass-fired fluidised bed boiler
Managing high temperature corrosion problems in biomass firing boilers has been challenging especially due to high amounts of chemically active compounds, in particular alkali chlorides. Thermally sprayed coatings with high chromium content can offer a solution for protecting low alloyed substrate materials in locations prone to high temperature corrosion. Two thermally sprayed (HVOF - high velocity oxy-fuel) iron based coatings (Fe-27Cr-11Ni-4Mo and Fe-19Cr-9W-7Nb-4Mo) were exposed to biomass boiler conditions for two years. The fluidised bed boiler for district heating used mainly wood-based fuels mixed with small amounts of peat. The coated tubes were located at the hot economiser of the boiler, where the estimated material temperature was about 200. °C maximum. After the exposure the coatings and the carbon steel St35.8 substrate material were analysed with SEM-EDX. It was detected that corrosion due to elements such as chlorine, potassium, zinc, lead and copper had caused severe material wastage in the biomass boiler with relatively low heat exchanger surface temperatures. The low alloyed boiler tubes had suffered severely with a corrosion rate as high as 2. mm/year, whereas dense thermal spray coatings offered excellent protection during the exposure.

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Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland
Contributors: Oksa, M., Varis, T., Ruusuvuori, K.
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Pages: 191-200
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Peer-reviewed: Yes

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Scopus rating (2014): CiteScore 3.7 SJR 0.983 SNIP 1.652
Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Biomass, Chlorine corrosion, Corrosion protection, High temperature corrosion, HVOF, Thermal spray coating
DOIs:

10.1016/j.surfcoat.2014.04.025
URLs:

http://www.scopus.com/inward/record.url?scp=84901601150&partnerID=8YFLogxK (Link to publication in Scopus)

Source: Scopus
Source ID: 84901601150
Research output: Contribution to journal › Article › Scientific › peer-review

Increased lifetime for biomass and waste to energy power plant boilers with HVOF coatings: High temperature corrosion testing under chlorine-containing molten salt

Heat exchanger surfaces of waste to energy and biomass power plant boilers experience often severe corrosion due to very aggressive components in the used fuels. High velocity oxy-fuel (HVOF) coatings offer excellent protection for boiler tubes against high temperature corrosion due to their high density and good adherence to the substrate material. Several thermal spray coatings with high chromium content were sprayed with HVOF technique. Their mechanical properties and high temperature corrosion resistance were tested and analyzed. The coating materials included NiCr, IN625, Ni-21Cr-10W-9Mo-4Cu, and iron-based partly amorphous alloy SHS9172 (Fe-25Cr-15W-12Nb-6Mo). High temperature corrosion testing was performed in NaCl-KCl-Na_2SO_4 salt with controlled H_2O atmosphere at 575 and 625 C. The corrosion test results of the coatings were compared to corrosion resistance of tube materials (X20, Alloy 263 and Sanicro 25).

General information

Publication status: Published
MoE publication type: A2 Review article in a scientific journal
Organisations: Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland
Contributors: Oksa, M., Tuurna, S., Varis, T.
Number of pages: 14
Pages: 783-796
Publication date: Jun 2013
Peer-reviewed: Yes

Publication information

Journal: Journal of Thermal Spray Technology
Volume: 22
Issue number: 5
ISSN (Print): 1059-9630
Ratings:

Scopus rating (2013): CiteScore 3 SJR 0.933 SNIP 1.366
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
Keywords: biofuel, CJS, coating characteristics, corrosion protection coating, high temperature corrosion, HVOF, molten salt, process optimization, waste to energy
DOIs:

10.1007/s11666-013-9928-5
URLs:

http://www.scopus.com/inward/record.url?scp=84878627004&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84878627004
Research output: Contribution to journal › Review Article › Scientific › peer-review

Comparison of laboratory rolling-sliding wear tests with in-service wear of nodular cast iron rollers against wire ropes

The present work describes the wear behaviour of nodular cast iron in rolling-sliding contact with steel wire ropes and steel wires in laboratory and in-service conditions. In each of the studied examples, the wear had proceeded through a surface fatigue process, in which inter-nodular crack propagation and simultaneous deformation in a thin sub-surface zone had resulted in the formation of ferrous scales consisting of material from the metal matrix of the cast iron. The scale layers of the wear surface were oriented towards the direction of the sliding component of the motion, and the spalling of the scales was identified as the dominating mechanism for material removal from the wear surface. The initiation behaviour of the inter-nodular cracks was analysed by crack measurements and statistical analysis of the depths and initiation angles of the cracks in relation to the wear surface. The initiation depths of the cracks increased with increasing contact pressure. Roller samples from in-service and from the component wear tests showed closely similar distributions of the crack depths and crack initiation angles. The sample from the twin-disc test showed aspects of cracking behaviour that were typical of both the rolling and the sliding direction of the roller samples.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Research group: Materials Characterization, Department of Materials Science, Tampere University of Technology, Research group: Tribology and Machine Elements, Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland
Contributors: Oksanen, V., Valtonen, K., Andersson, P., Vaajoki, A., Laukkanen, A., Holmberg, K., Kuokkala, V. T.

Number of pages: 9
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Publication date: 15 Oct 2015
Peer-reviewed: Yes

Publication information
Journal: Wear
Volume: 340-341
ISSN (Print): 0043-1648
Ratings:

Scopus rating (2015): CiteScore 4.2 SJR 1.512 SNIP 2.027
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces and Interfaces, Materials Chemistry, Surfaces, Coatings and Films, Mechanics of Materials
Keywords: Contact mechanics, Nodular cast iron, Rolling contact fatigue, Rolling-sliding, Wear testing, Wire rope
DOIs:

10.1016/j.wear.2015.07.006
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http://www.scopus.com/inward/record.url?scp=84939528862&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84939528862
Research output: Contribution to journal › Article › Scientific › peer-review

Load capacity of lubricated bismuth bronze bimetal bearing under elliptical sliding motion
Leaded tin bronze alloys are widely used in heavy machinery bearings operating in boundary and mixed lubrication regions due to the excellent dry lubrication properties of lead. However, restrictions on the use of lead have created an increasing demand for lead-free or low-lead bearing materials. In the present study, suitability of a novel bismuth bronze bimetal material for possible substitution of leaded tin bronze was studied with a special thrust bearing test device, which simulates the contact conditions in the main thrust bearing of mineral crushers. The oil-lubricated test bearings have a flat-on-flat type contact with oil grooves and a constant eccentric motion against a case hardened steel counter plate under a periodically increased axial pressure. The test was continued until a sudden rise in friction, which indicates bearing failure and risk of an imminent seizure. The bismuth bronze showed a load capacity of the same level with the reference material, continuously cast CuSn10Pb10. Characterization by electron microscopy showed that the dry-lubricating bismuth precipitations had a fine grain size and an even distribution, which explains the good load carrying capacity. It was concluded that the bismuth bronze has potential for substituting the leaded tin bronzes in the studied operating conditions.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Tribology and Machine Elements, Metso Minerals, Inc.
Contributors: Oksanen, V. T., Lehtovaara, A. J., Kallio, M. H.
Pages: 72-80
Publication date: 2017
Peer-reviewed: Yes
Early online date: 4 May 2017

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Journal: Wear
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Ratings:

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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Bearings, Bimetals, Lead substitution, Non-ferrous metals, Solid lubricants
Electronic versions:

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10.1016/j.wear.2017.05.001
URLs:

http://urn.fi/URN:NBN:fi:tty-201802091207. Embargo ended: 4/05/19
Source: Scopus
Source ID: 85019077732

PIP2 and Talin Join Forces to Activate Integrin

Integrins are major players in cell adhesion and migration, and malfunctions in controlling their activity are associated with various diseases. Nevertheless, the details of integrin activation are not completely understood, and the role of lipids in the process is largely unknown. Herein, we show using atomistic molecular dynamics simulations that the interplay of phosphatidylinositol 4,5-bisphosphate (PIP2) and talin may directly alter the conformation of integrin αIIbβ3. Our results provide a new perspective on the role of PIP2 in integrin activation and indicate that the charged PIP2 lipid headgroup can perturb a clasp at the cytoplasmic face of the integrin heterodimer.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Tampere University of Technology, Research group: Biological Physics and Soft Matter, BioMediTech, Computational Science X (CompX), Multi-scaled biodata analysis and modelling (MultiBAM), BioMediTech, Department of Physics and Chemistry, University of Southern Denmark, Fimlab Laboratories Ltd
Contributors: Orlowski, A., Kukkurainen, S., Pöyry, A., Rissanen, S., Vattulainen, I., Hytönen, V. P., Róg, T.
Number of pages: 9
Pages: 12381-12389
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Early online date: 26 Aug 2015

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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
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Bibliographical note

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Research output: Contribution to journal › Article › Scientific › peer-review

Biomimetic zinc chlorin-poly(4-vinylpyridine) assemblies: Doping level dependent emission-absorption regimes

To develop biomimetic dye-polymers for photonics, two different types of Zn chlorin-poly(4-vinylpyridine) (P4VP) assemblies were prepared by varying Zn pyro-pheophorbide a methylester (ZnPPME) and Zn 3^1-OH-pyro- pheophorbide a methylester (Zn-3^1-OH-PPME) doping levels. ^{1}H NMR spectroscopy and diffusion ordered NMR spectroscopy (DOSY) studies revealed that a coordinative interaction between Zn chlorin and P4VP was predominant in solution (d_5-nitrobenzene). Small angle X-ray scattering (SAXS) and transmission electron microscopy (TEM) characterization of bulk samples of polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) doped with variable amounts of Zn chlorin showed that the pigment doping transformed the native cylindrical block copolymer nanostructures to lamellar morphologies. The result indicates that the pyridine moiety-Zn chlorin coordination is stronger than the aggregation tendency between the pigment molecules even in the solid state. UV-Vis absorption spectroscopy studies of a Zn chlorin-P4VP thin film showed characteristic monomeric chlorin spectra, while steady-state fluorescence spectroscopy displayed quenching of fluorescence and time-resolved studies indicated shortening of fluorescence lifetimes with an increasing chlorin doping level. Notably, time-resolved fluorescence spectroscopy revealed that the lifetime decay changed from monoexponential to biexponential above 0.5 wt% (ca. 0.001 equiv.) loadings. The Förster analysis implies that excitonic chlorin-chlorin interactions are observed in the thin films when the distance between the pigment molecules is approximately 50 Å. The Zn chlorin-P4VP solid films emit strongly up to 1 wt% (ca. 0.002 equiv.) doping level above which the chlorin-chlorin interactions start to linearly dominate with an increase of doping level, while with 10 wt% (ca. 0.02 equiv.) loading less than 10% of fluorescence remains. Doping levels up to 300 wt% (0.5 equiv.) can be used in absorbing materials without the formation of chlorin aggregates. These defined optical response regions pave the way for photonic materials based on biopigment assemblies.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Aalto University, University of Helsinki, Department of Applied Physics
Contributors: Pale, V., Nikkonen, T., Vapaavuori, J., Kostiainen, M., Kavakka, J., Selin, J., Tittonen, I., Helaja, J.
Number of pages: 8
Pages: 2166-2173
Publication date: 21 Mar 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Materials Chemistry C
Volume: 1
Issue number: 11
ISSN (Print): 2050-7534
Ratings:

Scopus rating (2013): CiteScore 1.1
Original language: English
ASJC Scopus subject areas: Chemistry(all), Materials Chemistry
DOIs:

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Source: Scopus
Source ID: 84875847322
Research output: Contribution to journal › Article › Scientific › peer-review

DNA lesion can facilitate base ionization: Vertical ionization energies of aqueous 8-oxoguanine and its nucleoside and nucleotide
8-Oxoguanine is one of the key products of indirect radiation damage to DNA by reactive oxygen species. Here, we describe ionization of this damaged nucleobase and the corresponding nucleoside and nucleotide in aqueous phase, modeled by the nonequilibrium polarizable continuum model, establishing their lowest vertical ionization energies of 6.8-7.0 eV. We thus confirm that 8-oxoguanine has even lower ionization energy than the parental guanine, which is the canonical nucleobase with the lowest ionization energy. Therefore, it can act as a trap for the cationic hole formed by ionizing radiation and thus protect DNA from further radiation damage. We also model using time-dependent density functional theory and measure by liquid jet photoelectron spectroscopy the valence photoelectron spectrum of 8-oxoguanine in water. We show that the calculated higher lying ionization states match well the experiment which, however, is not sensitive enough to capture the electron signal corresponding to the lowest ionization process due to the low solubility of 8-oxoguanine in water.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Helmholtz Center Berlin
Contributors: Palivec, V., Pluharová, E., Unger, I., Winter, B., Jungwirth, P.
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Publication information
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ISSN (Print): 1520-6106
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Scopus rating (2014): CiteScore 5.9 SJR 1.449 SNIP 1.13
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films, Medicine(all)
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Source: Scopus

Source ID: 84915764488
Research output: Contribution to journal › Article › Scientific › peer-review

Development in additive methods in aramid fiber surface modification to increase fiber-matrix adhesion: A review
This review article highlights and summarizes the recent developments in the field of surface modification methods for aramid fibers. Special focus is on methods that create a multifunctional fiber surface by incorporating nanostructures and enabling mechanical interlocking. To give a complete picture of adhesion promotion with aramids, the specific questions related to the challenges in aramid-matrix bonding are also shortly presented. The main discussion of the surface modification approaches is divided into sections according to how material is added to the fiber surface; (1) coating, (2) grafting and (3) growing. To provide a comprehensive view of the most recent developments in the field, other methods with similar outcomes, are also shortly reviewed. To conclude, future trends and insights are discussed.

General information
Publication status: Published
MoE publication type: A2 Review article in a scientific journal
Organisations: Materials Science and Environmental Engineering, Research group: Plastics and Elastomer Technology, University of Twente
Contributors: Palola, S., Vuorinen, J., Noordermeer, J. W., Sarlin, E.
Number of pages: 31
Publication date: 1 Jun 2020
Peer-reviewed: Yes

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Journal: Coatings
Volume: 10
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ASJC Scopus subject areas: Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Adhesion, Aramid fiber, Mechanical interlocking, Multifunctional fiber surface, Nanostructures, Surface modification
Electronic versions:

coatings-10-00556-v2
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URLs:

http://urn.fi/URN:NBN:fi:tuni-202008276710
Source: Scopus
Source ID: 85087483658
Research output: Contribution to journal › Review Article › Scientific › peer-review

How well can we predict cluster fragmentation inside a mass spectrometer?
Fragmentation of molecular clusters inside mass spectrometers is a significant source of uncertainty in a wide range of chemical applications. We have measured the fragmentation of sulfuric acid clusters driving atmospheric new-particle formation, and developed a novel model, based on first principles calculations, capable of quantitatively predicting the extent of fragmentation.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: University of Helsinki, Beijing University of Chemical Technology, CNRS, Centre National de la Recherche Scientifique (CNRS), Universite de Bordeaux - PRES, Lab Bordelais Rech Informat, PICTURA Res Grp, UMR 5800
Contributors: Passananti, M., Zapadinsky, E., Zanca, T., Kangasluoma, J., Myllys, N., Rissanen, M. P., Kurtén, T., Ehn, M. , Attoui, M., Vehkamäki, H.
Number of pages: 4
Pages: 5946-5949
Publication date: 2019
Peer-reviewed: Yes

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Volume: 55
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Original language: English
ASJC Scopus subject areas: Catalysis, Electronic, Optical and Magnetic Materials, Ceramics and Composites, Chemistry(all), Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
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http://www.scopus.com/inward/record.url?scp=85065980333&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 85065980333
Research output: Contribution to journal › Article › Scientific › peer-review

Reversal of the hofmeister series: Specific ion effects on peptides

Ion-specific effects on salting-in and salting-out of proteins, protein denaturation, as well as enzymatic activity are typically rationalized in terms of the Hofmeister series. Here, we demonstrate by means of NMR spectroscopy and molecular dynamics simulations that the traditional explanation of the Hofmeister ordering of ions in terms of their bulk hydration properties is inadequate. Using triglycine as a model system, we show that the Hofmeister series for anions changes from a direct to a reversed series upon uncapping the N-terminus. Weakly hydrated anions, such as iodide and thiocyanate, interact with the peptide bond, while strongly hydrated anions like sulfate are repelled from it. In contrast, reversed order in interactions of anions is observed at the positively charged, uncapped N-terminus, and by analogy, this should also be the case at side chains of positively charged amino acids. These results demonstrate that the specific chemical and physical properties of peptides and proteins play a fundamental role in ion-specific effects. The present study thus provides a molecular rationalization of Hofmeister ordering for the anions. It also provides a route for tuning these interactions by titration or mutation of basic amino acid residues on the protein surface.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Pennsylvania State University, Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Texas A and M University
Contributors: Paterová, J., Rembert, K. B., Heyda, J., Kurra, Y., Okur, H. I., Liu, W. R., Hilty, C., Cremer, P. S., Jungwirth, P.
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Publication date: 11 Jul 2013
Peer-reviewed: Yes

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Issue number: 27
ISSN (Print): 1520-6106
Ratings:
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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
DOIs:
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http://www.scopus.com/inward/record.url?scp=84880155215&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84880155215
Research output: Contribution to journal › Article › Scientific › peer-review

Ab initio study of the surface properties of austenitic stainless steel alloys

Using ab initio calculations we investigated the surface energies of paramagnetic $Fe_{1-c-n}Cr_cNi_n$ random alloys within the concentration range of $0.12 \leq c \leq 0.32$ and $0.04 \leq n \leq 0.32$. These alloys crystallize mainly in the face centred cubic (fcc) structure and constitute the main building blocks of austenitic stainless steels. It is shown that all alloys have the lowest surface energies along the most close packed crystal orientation, namely the fcc (111) surfaces. The amount of Ni seems to have little effect on the surface energy, while almost all composition-driven change may be attributed to the changes in the Cr content. Within the studied compositional range, the change of the surface energy with the composition

is of the order of 10%. Trends of the surface energy can be related to the magnetic structure of surfaces. Using the total energy as a function of the concentration, we determine the effective chemical potentials in bulk and at the surface, which can be used to estimate the surface segregation energies.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Lappeenranta University of Technology, Aalto University, Fritz Haber Institute of the Max Planck Society, Department of Physics and Astronomy, University of Turku, Turun Yliopisto/Turun Biomateriaalikeskus, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences
Contributors: Pitkänen, H., Alatalo, M., Puisto, A., Ropo, M., Kokko, K., Vitos, L.
Number of pages: 5
Pages: 190-194
Publication date: Mar 2013
Peer-reviewed: Yes

Publication information

Journal: Surcface Science
Volume: 609
ISSN (Print): 0039-6028
Ratings:

Scopus rating (2013): CiteScore 3.3 SJR 0.829 SNIP 0.787
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Alloy surface, Austenitic, FeCrNi, First-principles calculation, Stainless steel, Surface energy
DOIs:

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Source: Scopus
Source ID: 84873060451
Research output: Contribution to journal › Article › Scientific › peer-review

Transforming anion instability into stability: Contrasting photoionization of three protonation forms of the phosphate ion upon moving into water

We use photoelectron emission spectroscopy with vacuum microjet technique and quantum chemistry calculations to investigate electronic structure and stability of aqueous phosphate anions. On the basis of the measured photoelectron spectra of sodium phosphates at different pH, we report the lowest vertical ionization energies of monobasic (9.5 eV), dibasic (8.9 eV), and tribasic (8.4 eV) anions. Electron binding energies were in tandem modeled with ab initio methods, using a mixed dielectric solvation model together with up to 64 explicitly solvating water molecules. We demonstrate that two solvation layers of explicit water molecules are needed to obtain converged values of vertical ionization energies (VIEs) within this mixed solvation model, leading to very good agreement with experiment. We also show that the highly charged PO_4^{3-} anion, which is electronically unstable in the gas phase, gains the electronic stability with about 16 water molecules, while only 2-3 water molecules are sufficient to stabilize the doubly charged phosphate anion. We also investigate the effect of ion pairing on the vertical ionization energy. In contrast to protonation (leading to a formation of covalent O-H bond), sodiation (leading to an anion$\cdots Na^+$ ion pair) has only a weak effect on the electron binding energy.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Department of Physical Chemistry, University of Southern California, Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, J. Heyrovský Institute of Physical Chemistry
Contributors: Pluhařová, E., Ončák, M., Seidel, R., Schroeder, C., Schroeder, W., Winter, B., Bradforth, S. E., Jungwirth, P., Slavíček, P.
Number of pages: 11
Pages: 13254-13264
Publication date: 8 Nov 2012
Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry Part B
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Issue number: 44
ISSN (Print): 1520-6106
Ratings:

Scopus rating (2012): CiteScore 6.7 SJR 1.943 SNIP 1.243
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
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10.1021/jp306348b
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http://www.scopus.com/inward/record.url?scp=84868554130&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84868554130
Research output: Contribution to journal › Article › Scientific › peer-review

Ionization of purine tautomers in nucleobases, nucleosides, and nucleotides: From the gas phase to the aqueous environment

We have simulated ionization of purine nucleic acid components in the gas phase and in a water environment. The vertical and adiabatic ionization processes were calculated at the PMP2/aug-cc-pVDZ level with the TDDFT method applied to obtain ionization from the deeper lying orbitals. The water environment was modeled via microsolvation approach and using a nonequilibrium polarizable continuum model. We have characterized a set of guanine tautomers and investigated nucleosides and nucleotides in different conformations. The results for guanine, i.e., the nucleic acid base with the lowest vertical ionization potential, were also compared to those for the other purine base, adenine. The main findings of our study are the following: (i) Guanine remains clearly the base with the lowest ionization energy even upon aqueous solvation. (ii) Water solvent has a strong effect on the ionization energetics of guanine and adenine and their derivatives; the vertical ionization potential (VIP) is lowered by about 1 eV for guanine while it is ~1.5 eV higher in the nucleotides, overall resulting in similar VIPs for GMP^-, guanosine and guanine in water. (iii) Water efficiently screens the electrostatic interactions between nucleic acid components. Consequently, ionization in water always originates from the base unit of the nucleic acid and all the information about conformational state is lost in the ionization energetics. (iv) The energy splitting between ionization of the two least bound electrons increases upon solvation. (v) Tautomerism does not contribute to the width of the photoelectron spectra in water. (vi) The effect of specific short-range interactions with individual solvent molecules is negligible for purine bases, compared to the long-range dielectric effects of the aqueous medium.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Department of Physical Chemistry, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, University of Southern California
Contributors: Pluhařová, E., Jungwirth, P., Bradforth, S. E., Slavíček, P.
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Pages: 1294-1305
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Peer-reviewed: Yes

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ISSN (Print): 1520-6106
Ratings:

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Original language: English
ASJC Scopus subject areas: Surfaces, Coatings and Films, Physical and Theoretical Chemistry, Materials Chemistry
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10.1021/jp110388v
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Source: Scopus
Source ID: 79952844542
Research output: Contribution to journal › Article › Scientific › peer-review

Improvement of actuation performance of dielectric elastomers by barium titanate and carbon black fillers

Dielectric elastomers are promising materials for actuators resembling human muscle. Among elastomers, acrylic rubbers (ACM) have shown good actuation performance but its use is limited by the high operating voltages required. The present

work demonstrates that simultaneous incorporation of nanostructured carbon black and dielectric fillers offers an increase in a dielectric permittivity and a suitable modulus of the elastomers matrix, enabling an improved electro-mechanical actuation performance at low voltages. By the use of reinforcing carbon black and barium titanate in an acrylic elastomer matrix a sixfold increase in the dielectric permittivity was realized. A fine tuning of the actuation stress and, consequently, actuation strain can be done by a judicial selection of the different filler concentrations in the soft rubber matrix. Finally, a synergistic effect of the fillers was observed in the improved actuation performance of the developed materials. This work may pave the way to design dielectric elastomers for actuator fabrication.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Leibniz-Institut für Polymerforschung Dresden E.V.
Contributors: Poikelispää, M., Shakun, A., Das, A., Vuorinen, J.
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Peer-reviewed: Yes

Publication information

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Article number: 44116
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Ratings:

Scopus rating (2016): CiteScore 3.9 SJR 0.588 SNIP 0.815
Original language: English
ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry
Keywords: actuators, dielectric properties, elastomers
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Source ID: 84982792344
Research output: Contribution to journal › Article › Scientific › peer-review

Vegetable fillers for electric stimuli responsive elastomers

Dielectric elastomer actuators (DEAs) have been studied widely in recent years for artificial muscle applications, but their implementation into production is limited due to high operating voltages required. The actuation behavior of dielectric elastomer under an applied electric field is predicted by Maxwell's pressure and thickness strain equations. According to these equations, the best electromechanical response is achieved when the relative permittivity is high and elastic modulus is low. The potential source for additives increasing the relative permittivity of rubbers can be vegetable powders that have much higher dielectric constant than common elastomers. In the present research, the dielectric and actuation properties of polyacrylate rubber (ACM) were studied after the addition of different vegetable-based fillers such as potato starch, corn starch, garlic, and paprika. The results were compared to ACM filled with barium titanate. The compounds containing vegetable fillers showed higher relative dielectric permittivity at 1 Hz frequency than the compounds containing barium titanate due to higher interfacial polarization. The actuation studies showed that lower electric fields are required to generate certain actuation forces when the starches and garlic are used in the rubber instead of barium titanate. Therefore, the vegetable-based fillers can be used to improve actuation performance of DEAs.

General information

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Organisations: Materials Science, Research group: Plastics and Elastomer Technology, Department of Elastomers, Leibniz-Institut für Polymerforschung Dresden E.V.
Contributors: Poikelispää, M., Shakun, A., Sarlin, E., Das, A., Vuorinen, J.
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Keywords: biomaterials, dielectric properties, elastomers, mechanical properties, sensors and actuators
DOIs:

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Bibliographical note
INT=mol,"Poikelispää, Minna"
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Research output: Contribution to journal › Article › Scientific › peer-review

Phase-change material: Natural rubber composites for heat storage applications
Global warming and environmental awareness in general have increased the research into thermal energy storage fields. Phase-change materials (PCMs) are efficient in storing thermal energy because of their high latent heat during the phase change. As the phase change is often based on the melting of the PCM, they need to be encapsulated, for example, by dispersing the PCM to a polymer matrix. In this study, the feasibility of the use of paraffin-natural rubber composites in applications requiring both the good ability to store heat energy and good vibration-damping properties is studied. This includes studies on PCM concentration and the microencapsulation of the PCM. It was found that the heat storage capacity increases with increasing PCM content, although the theoretical maximum capacity is not achieved because the PCM is released during vulcanization and the paraffin blooms. In addition, the loss factor was found to be increased at elevated temperatures, indicating improved damping properties. The encapsulation of PCM is found to have a positive influence on the heat storage capacity and the mechanical and damping properties of the rubber compound.

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Contributors: Poikelispää, M., Ruokangas, S., Honkanen, M., Vippola, M., Sarlin, E.
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Original language: English
ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry
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Bibliographical note
INT=msee,"Ruokangas, Sasu"
Source: Scopus
Source ID: 85084943612
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of carbon nanotubes and nanodiamonds on the heat storage ability of natural rubber composites
Phase change materials are utilized in heat storage applications, as they have high latent heat during the phase transition. In addition, high thermal conductivity is required from the heat storage materials to achieve high energy efficiency. In this study, the effect of carbon nanotubes (CNTs) and nanodiamonds (NDs) on the thermal conductivity and the heat storage capacity of the paraffin–natural rubber composites was studied. It was found that the CNTs work better than NDs in such composites. They increase thermal conductivity significantly and thus improve the heat transfer rate of the composite. They were also found to prevent the migration of paraffin out of the rubber during the vulcanization process, which increases the lifetime of the composite.

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MoE publication type: A1 Journal article-refereed
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Contributors: Poikelispää, M., Honkanen, M., Vippola, M., Sarlin, E.
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ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry
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Electronic versions:

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Source: Scopus
Source ID: 85086857766
Research output: Contribution to journal › Article › Scientific › peer-review

Structurally Controlled Dynamics in Azobenzene-Based Supramolecular Self-Assemblies in Solid State
Light-responsive supramolecular self-assemblies exhibit interplay between order and dynamics of the self-assembling motifs, through which the thermal isomerization rate of azobenzene chromophores can be tuned by orders of magnitude. By using supramolecular complexes of 4-(4-alkylphenylazo)phenols hydrogen-bonded to poly(4-vinylpyridine) as model systems, we demonstrate that the thermal isomerization rate of the hydroxyazobenzene derivatives increases 5700-fold when the material undergoes a transformation from a disordered, low-azobenzene-concentration state to a high-concentration state exhibiting lamellar, smectic-like self-assembly. Drastically smaller thermal isomerization rates are observed in disordered structures. This allows us to attribute the change to a combination of increased number density of the hydroxyazobenzenes inducing plasticization, and cooperativity created by the chromophore-chromophore interactions through self-assembled molecular order and alignment. Our results pinpoint the importance of molecular self-assembly and intermolecular interactions in modifying the dynamics in supramolecular complexes in a controlled manner. We foresee this to be important in light-controlled dynamic materials.

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Aalto University
Contributors: Poutanen, M., Ikkala, O., Priimägi, A.
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Electronic versions:

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http://urn.fi/URN:NBN:fi:tuni-202005145301
Source: Scopus
Source ID: 84975044511
Research output: Contribution to journal › Article › Scientific › peer-review

Thermal Isomerization of Hydroxyazobenzenes as a Platform for Vapor Sensing

Photoisomerization of azobenzene derivatives is a versatile tool for devising light-responsive materials for a broad range of applications in photonics, robotics, microfabrication, and biomaterials science. Some applications rely on fast isomerization kinetics, while for others, bistable azobenzenes are preferred. However, solid-state materials where the isomerization kinetics depends on the environmental conditions have been largely overlooked. Herein, an approach to utilize the environmental sensitivity of isomerization kinetics is developed. It is demonstrated that thin polymer films containing hydroxyazobenzenes offer a conceptually novel platform for sensing hydrogen-bonding vapors in the environment. The concept is based on accelerating the thermal cis-trans isomerization rate through hydrogen-bond-catalyzed changes in the thermal isomerization pathway, which allows for devising a relative humidity sensor with high sensitivity and quick response to relative humidity changes. The approach is also applicable for detecting other hydrogen-bonding vapors such as methanol and ethanol. Employing isomerization kinetics of azobenzenes for vapor sensing opens new intriguing possibilities for using azobenzene molecules in the future.

General information

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Organisations: Chemistry and Bioengineering, Aalto University
Contributors: Poutanen, M., Ahmed, Z., Rautkari, L., Ikkala, O., Priimägi, A.
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Original language: English
ASJC Scopus subject areas: Organic Chemistry, Polymers and Plastics, Inorganic Chemistry, Materials Chemistry
Electronic versions:
82E3E980-7E4D-4608-8C73-F2F0ADCB6EEA
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10.1021/acsmacrolett.8b00093
URLs:
http://urn.fi/URN:NBN:fi:tty-201901111060
Source: Scopus
Source ID: 85044222959
Research output: Contribution to journal › Article › Scientific › peer-review

Exciton localization and structural disorder of $GaAs_{1-x}Bi_x$/GaAs quantum wells grown by molecular beam epitaxy on (311)B GaAs substrates

In this work, we have investigated the structural and optical properties of $GaAs_{(1-x)}Bi_x$/GaAs single quantum wells (QWs) grown by molecular beam epitaxy on GaAs (311)B substrates using x-ray diffraction, atomic force microscopy, Fourier-transform Raman (FT-Raman) and photoluminescence spectroscopy techniques. The FT-Raman results revealed a decrease of the relative intensity ratio of transverse and longitudinal optical modes with the increase of Bi concentration, which indicates a reduction of the structural disorder with increasing Bi incorporation. In addition, the PL results show an enhancement of the optical efficiency of the structures as the Bi concentration is increased due to important effects of exciton localization related to Bi defects, nonradiative centers and alloy disorder. These results provide evidence that Bi is incorporated effectively into the QW region. Finally, the temperature dependence of the PL spectra has evidenced two distinct types of defects related to the Bi incorporation, namely Bi clusters and pairs, and alloy disorder and potential fluctuation.

General information

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MoE publication type: A1 Journal article-refereed

Organisations: Photonics, Research group: ORC, Universidade Federal de São Carlos, University of Nottingham, Adana Science and Technology University, University of São Paulo
Contributors: Prando, G. A., Orsi Gordo, V., Puustinen, J., Hilska, J., Alghamdi, H. M., Som, G., Gunes, M., Akyol, M., Souto, S., Rodrigues, A. D., Galeti, H. V., Henini, M., Gobato, Y. G., Guina, M.
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Condensed Matter Physics, Electrical and Electronic Engineering, Materials Chemistry
Keywords: dilute bismide, exciton localization, photoluminescence, structural disorder
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Source ID: 85051332383
Research output: Contribution to journal › Article › Scientific › peer-review

Recent twists in photoactuation and photoalignment control
The design of functional and stimuli-responsive materials is among the key goals of modern materials science. The structure and properties of such materials can be controlled via various stimuli, among which light is often times the most attractive choice. Light is ubiquitous and a gentle energy source and its properties can be optimized for a specific target remotely, with high spatial and temporal resolution. Light-control over molecular alignment has in recent years attracted particular interest, for potential applications such as reconfigurable photonic elements and optical-to-mechanical energy conversion. Herein, we bring forward some recent examples and emerging trends in this exciting field of research, focusing on liquid crystals, liquid-crystalline polymers and photochromic organic crystals, which we believe serve to highlight the immense potential of light-responsive materials to a wide variety of current and future high-tech applications in photonics, energy harvesting and conversion. This journal is

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Contributors: Priimagi, A., Barrett, C. J., Shishido, A.
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Materials Chemistry
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Source ID: 84906079173
Research output: Contribution to journal › Article › Scientific › peer-review

Azopolymer-based micro- and nanopatterning for photonic applications

Azopolymers comprise a unique materials platform, in which the photoisomerization reaction of azobenzene molecules can induce substantial material motions at molecular, mesoscopic, and even macroscopic length scales. In particular, amorphous azopolymer films can form stable surface relief patterns upon exposure to interfering light. This allows obtaining large-area periodic micro- and nanostructures in a remarkably simple way. Herein, recent progress in the development of azopolymer-based surface-patterning techniques for photonic applications is reviewed. Starting with a thin azopolymer layer, one can create a variety of photonic elements, such as diffraction gratings, microlens arrays, plasmonic sensors, antireflection coatings, and nanostructured light-polarization converters, either by using the azopolymer surface patterns themselves as optical elements or by utilizing them to microstructure or nanostructure other materials. Both of these domains are covered, with the aim of triggering further research in this fascinating field of science and technology that is far from being harnessed. © 2013 Wiley Periodicals, Inc. J. Polym. Sci., Part B: Polym. Phys. 2014, 52, 163-182
The aim of this review is to cover the existing research and trigger future research on the development of azopolymer-based micro- and nanopatterning techniques for applications in photonics. These techniques exploit a remarkably simple inscription of large-area surface relief gratings on azopolymer films. Starting with such an azopolymer pattern, one can create a variety of photonic elements, including diffraction gratings, distributed Bragg reflectors, microlens arrays, plasmonic sensors, antireflection coatings, and nanostructured converters of light polarization.

General information

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Contributors: Priimagi, A., Shevchenko, A.
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Physical and Theoretical Chemistry, Polymers and Plastics, Materials Chemistry
Keywords: azo polymers, isomer/isomerization, lithography, nanotechnology, periodic arrays, photonics; surface-relief grating
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Source: Scopus
Source ID: 84890653328
Research output: Contribution to journal › Article › Scientific › peer-review

Location of the Azobenzene moieties within the cross-linked liquid-crystalline polymers can dictate the direction of photoinduced bending

We present a simple way to control the photoinduced bending direction of azobenzene-containing cross-linked liquidcrystalline polymers. By changing the location of the photoactive azobenzene moieties from cross-links to side-chains, the bending direction of the sample is reversed under identical irradiation conditions. In addition to providing a versatile route toward directionality control of the photoinduced macroscopic motions, this observation highlights the complicated nature of the photomechanical response of azobenzene-containing cross-linked liquidcrystalline polymers, showing that the photomobile behavior can be determined by seemingly small details on the materials design.

General information

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Organisations: Frontier Photonics, Aalto University, Tokyo Institute of Technology, University of Hyogo, Kobe, Tohoku University, Chuo University
Contributors: Priimagi, A., Shimamura, A., Kondo, M., Hiraoka, T., Kubo, S., Mamiya, J. I., Kinoshita, M., Ikeda, T., Shishido, A.
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Pages: 96-99

Publication date: 2012
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Journal: ACS Macro Letters
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ISSN (Print): 2161-1653
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Original language: English
ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Inorganic Chemistry
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Source: Scopus
Source ID: 84861898337
Research output: Contribution to journal › Article › Scientific › peer-review

Analysis of GaAsBi growth regimes in high resolution with respect to As/Ga ratio using stationary MBE growth
The control of Bi incorporation and material properties in III-V-Bi alloys has proved challenging due to their high sensitivity to the epitaxial growth parameters. Here, we present a methodology for determining the variation in the Ga, As, and Bi fluxes and the temperature across a stationary substrate in molecular beam epitaxy. By correlating the flux distributions with material properties, we identify distinct regimes for epitaxy of GaAsBi. In particular, we devise a detailed image of the interplay between Bi incorporation and structural properties of a bulk $GaAs_{0.96}Bi_{0.04}$ layer grown on GaAs(1 0 0) with respect to the As/Ga ratio. The influence of As/Ga is analyzed with high resolution over the important stoichiometric range (i.e. As/Ga = 0.6–1.6). Growth outside the near-stoichiometric As/Ga regime leads to decreased Bi incorporation, decreased structural quality and the formation of Ga, Ga/Bi or Bi droplets. On the other hand, growth at As/Ga = 1.00–1.17 leads to maximized material quality. For this regime, the surface roughness is further optimized by fine-tuning the As/Ga ratio to suppress surface mounding to a value of 0.5 nm. The results reveal the extreme sensitivity of GaAsBi growth to small variations in the As/Ga ratio, and demonstrate the applicability of stationary growth in studying these effects.

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Organisations: Physics, Research group: ORC
Contributors: Puustinen, J., Hilska, J., Guina, M.
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Inorganic Chemistry, Materials Chemistry
Keywords: A3. Molecular beam epitaxy, B1. Bismuth compounds, B2. Semiconducting III-V materials, B2. Semiconducting ternary compounds
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URLs:

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Source: Scopus
Source ID: 85060893423
Research output: Contribution to journal › Article › Scientific › peer-review

Role of Internal Water on Protein Thermal Stability: The Case of Homologous G Domains
In this work, we address the question of whether the enhanced stability of thermophilic proteins has a direct connection with internal hydration. Our model systems are two homologous G domains of different stability: the mesophilic G domain

of the elongation factor thermal unstable protein from E. coli and the hyperthermophilic G domain of the EF-1α protein from S. solfataricus. Using molecular dynamics simulation at the microsecond time scale, we show that both proteins host water molecules in internal cavities and that these molecules exchange with the external solution in the nanosecond time scale. The hydration free energy of these sites evaluated via extensive calculations is found to be favorable for both systems, with the hyperthermophilic protein offering a slightly more favorable environment to host water molecules. We estimate that, under ambient conditions, the free energy gain due to internal hydration is about 1.3 kcal/mol in favor of the hyperthermophilic variant. However, we also find that, at the high working temperature of the hyperthermophile, the cavities are rather dehydrated, meaning that under extreme conditions other molecular factors secure the stability of the protein. Interestingly, we detect a clear correlation between the hydration of internal cavities and the protein conformational landscape. The emerging picture is that internal hydration is an effective observable to probe the conformational landscape of proteins. In the specific context of our investigation, the analysis confirms that the hyperthermophilic G domain is characterized by multiple states and it has a more flexible structure than its mesophilic homologue. (Figure Presented).

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Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), Université Paris Diderot, Laboratoire de Biochimie Théorique, Sapienza University
Contributors: Rahaman, O., Kalimeri, M., Melchionna, S., Hénin, J., Sterpone, F.
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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
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Source: Scopus
Source ID: 84937843946
Research output: Contribution to journal › Article › Scientific › peer-review

Configurational Disorder of Water Hydrogen-Bond Network at the Protein Dynamical Transition

We introduce a novel strategy to quantify the disorder of extended water-water hydrogen-bond (HB) networks sampled in particle-based computer simulations. The method relies on the conformational clustering of the HB connectivity states. We successfully applied it to unveil the fine relationship among the protein dynamical transition in hydrated powder, which marks the activation of protein flexibility at $T_d \approx 240$ K, and the sudden increase in the configurational disorder of the water HB network enveloping the proteins. Our finding links, in the spirit of the Adam-Gibbs relationship, the diffusivity of protein atoms, as quantified by the hydrogen mean-square displacements, and the thermodynamic solvent configurational entropy.

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MoE publication type: A1 Journal article-refereed
Organisations: Physics, Bauhaus-Universitt Weimar, Université Paris Diderot, Universite di Perugia
Contributors: Rahaman, O., Kalimeri, M., Katava, M., Paciaroni, A., Sterpone, F.
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ASJC Scopus subject areas: Surfaces, Coatings and Films, Physical and Theoretical Chemistry, Materials Chemistry
DOIs:
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Source ID: 85025646989
Research output: Contribution to journal › Article › Scientific › peer-review

Modification of epoxy resin by silane-coupling agent to improve tensile properties of viscose fabric composites

The modification of epoxy resin by 3-aminopropyltriethoxysilane (APTES) to improve the tensile properties of warp knitted viscose fabric composites is reported in this study. The study evaluates the efficiency of modification methods adopted to modify the epoxy resin and the influence of the resin modification on various properties of the cured castings. The influence of matrix resin modification on the tensile properties of viscose fabric composite is compared to those prepared from chemically modified fibre. The efficiency of the modification was determined through titration method to determine the epoxide content of epoxy resin, viscosity measurement and FTIR. The effect of APTES modification on various properties of cured castings is studied through differential scanning calorimeter, contact angle measurement and tensile testing. The addition of APTES into the epoxy resin decreased the epoxide content in the resin as evident from the titration method. The tensile strength of cured castings decreased after the resin modification. The tensile strength and elongation at break of the viscose fabric composites prepared from modified resin, increased up to 14 and 41%, respectively. The improved adhesion of APTES-modified epoxy resin to the viscose fibre is confirmed from SEM analysis of tensile fracture surface.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Plastics and Elastomer Technology, Centria University of Applied Sciences, Royal Commission Yanbu Colleges and Institutes, Swerea IVF AB, Jozef Stefan Institute, Swedish Centre for Resource Recovery, University of Borås
Contributors: Rajan, R., Rainosalo, E., Thomas, S. P., Ramamoorthy, S. K., Zavašnik, J., Vuorinen, J., Skrifvars, M.
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ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Polymers and Plastics, Materials Chemistry
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Electronic versions:
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http://urn.fi/URN:NBN:fi:tty-201706051574. Embargo ended: 20/04/18

Bibliographical note

EXT="Skrifvars, Mikael"
Source: Scopus
Source ID: 85018515485
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Mechanical, thermal, and burning properties of viscose fabric composites: Influence of epoxy resin modification

The influence of epoxy resin modification by 3-aminopropyltriethoxysilane (APTES) on various properties of warp knitted viscose fabric is reported in this study. Dynamic mechanical, impact resistance, flexural, thermal properties, and burning behavior of the epoxy/viscose fabric composites are studied with respect to varying content of silane coupling agent. The results obtained for APTES-modified epoxy resin based composites reinforced with unmodified viscose fabric composites

are compared to unmodified epoxy resin based composites reinforced with APTES-modified viscose fabric. The dynamic mechanical behavior of the APTES-modified resin based composites indicates improved interfacial adhesion. The composites prepared from modified epoxy resin exhibited a twofold increase in impact resistance. The improved adhesion between the fiber and modified resin was also visible from the scanning electron microscope analysis of the impact fracture surface. There was less influence of resin modification on the flexural properties of the composites. The 5% APTES modification induced early degradation of composites compared to all other composites. The burning rate of all the composites under study is rated to be satisfactory for use in automotive interior applications.

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Centria University of Applied Sciences, University of Borås, Yanbu Industrial College, Jozef Stefan Institute, Swedish Centre for Resource Recovery
Contributors: Rajan, R., Rainosalo, E., Ramamoorthy, S. K., Thomas, S. P., Zavašnik, J., Vuorinen, J., Skrifvars, M.
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Bibliographical note
EXT="Skrifvars, Mikael"
Source: Scopus
Source ID: 85049105961
Research output: Contribution to journal › Article › Scientific › peer-review

A Finite Cluster Approach to the Electron-Hole Pair Damping of the Adsorbate Vibration: CO Adsorbed on Cu(100)
Abstract: A finite cluster method is applied to describe the energy transfer from the adsorbate vibrations to the electron-hole pair excitations. For CO stretch vibration on Cu(100) surface a value of 0.5 meV is found for the consequent damping (corresponding to the lifetime of $1.3 \cdot 10^{-12}$ s) in an agreement with a recently measured vibrational line width. The mechanism behind the electron-hole pair excitations is found to be charge oscillations between the molecular $2\pi^*$ resonance and the substrate, caused by the molecular vibration. Cluster size effects have been found to be negligible.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Chalmers University of Technology, University of California, Santa Barbara
Contributors: Rantala, T. T., Rosén, A., Hellsing, B.
Number of pages: 9
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Publication date: 1986
Peer-reviewed: Yes

Publication information
Journal: Studies in Surface Science and Catalysis
Volume: 26
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ISSN (Print): 0167-2991
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Catalysis, Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
DOIs:

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Source: Scopus
Source ID: 77956976821
Research output: Contribution to journal › Article › Scientific › peer-review

Rapid, Brushless Self-assembly of a PS-b-PDMS Block Copolymer for Nanolithography

Block copolymers (BCP) are highly promising self-assembling precursors for scalable nanolithography. Very regular BCP nanopatterns can be used as on-chip etch masks. The first step in the processing of BCP thin films is usually the chemical modification of the substrate surface, typically by grafting of a brush layer that renders the surface energy neutral relative to the constituent blocks. We provide here a first study on rapid, low temperature self-assembly of PS-. b-PDMS (polystyrene-. block-polydimethylsiloxane) on silicon substrates without a brush layer. We show that it forms line and antidot patterns after short solvo-thermal annealing. Unlike previous reports on this system, low temperature and short annealing time provide self-assembly in homogeneous thin films covering large substrate areas. This on-chip mask was then used for pattern transfer to the underlying silicon substrate. SEM (scanning electron microscope) images reveal silicon nanowires relative to the PDMS patterns of the BCP mask.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Department of Micro and Nanotechnology, Danmarks Tekniske Universitet, DTU Informatik, Center for Nanostructured Graphene, Trinity College Dublin
Contributors: Rasappa, S., Schulte, L., Borah, D., Morris, M. A., Ndoni, S.
Number of pages: 5
Pages: 1-5
Publication date: 1 Oct 2014
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Publication information

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Volume: 2
ISSN (Print): 2215-0382
Ratings:

Scopus rating (2014): CiteScore 0.2
Original language: English
ASJC Scopus subject areas: Biotechnology, Colloid and Surface Chemistry, Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
Keywords: Aspect ratio, Brushless, Dry etching, Lines and antidots, Pattern transfer, PS-b-PDMS, Self-assembly, Silicon nanostructures, Soft mask template, Solvo-thermal annealing
DOIs:

10.1016/j.colcom.2014.07.001
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http://www.scopus.com/inward/record.url?scp=84919650698&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84919650698
Research output: Contribution to journal › Article › Scientific › peer-review

Block copolymer lithography: Feature size control and extension by an over-etch technique

Block copolymer lithography based on block copolymer (BCP) self-assembly can be used to develop soft mask nanoscale templates for subsequent pattern transfer to generate substrate features. Self-assembly of lamellar polystyrene-b-polymethylmethacrylate BCP of varying molecular weights to generate silicon nanoscale features is reported here. It has also been demonstrated that the feature size can be controlled by a plasma over-etch process and discussed.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Materials Chemistry and Analysis Group, University College Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Tyndall National Institute at National University of Ireland, Cork, Collinstown Industrial Estate
Contributors: Rasappa, S., Borah, D., Senthamaraikannan, R., Faulkner, C. C., Shaw, M. T., Gleeson, P., Holmes, J. D., Morris, M. A.
Number of pages: 6
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Publication date: 1 Nov 2012
Peer-reviewed: Yes

Publication information
Journal: Thin Solid Films
Volume: 522
ISSN (Print): 0040-6090
Ratings:

Scopus rating (2012): CiteScore 3.3 SJR 0.897 SNIP 1.153
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Materials Chemistry, Metals and Alloys, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Block copolymer, Lithography, Over-etching, Plasma etching, Polystyrene-b-polymethylmethacrylate, Self-assembly, Silicon nanowires
DOIs:

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URLs:

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Source: Scopus
Source ID: 84868593394
Research output: Contribution to journal › Article › Scientific › peer-review

Solvent Welding and Imprinting Cellulose Nanofiber Films Using Ionic Liquids
Cellulose nanofiber films (CNFF) were treated via a welding process using ionic liquids (ILs). Acid-base-conjugated ILs derived from 1,5-diazabicyclo[4.3.0]non-5-ene [DBN] and 1-ethyl-3-methylimidazolium acetate ([emim][OAc]) were utilized. The removal efficiency of ILs from welded CNFF was assessed using liquid-state nuclear magnetic resonance (NMR) spectroscopy and Fourier transform infrared spectroscopy (FTIR). The mechanical and physical properties of CNFF indicated surface plasticization of CNFF, which improved transparency. Upon treatment, the average CNFF toughness increased by 27%, and the films reached a Young's modulus of ~5.8 GPa. These first attempts for IL "welding" show promise to tune the surfaces of biobased films, expanding the scope of properties for the production of new biobased materials in a green chemistry context. The results of this work are highly relevant to the fabrication of CNFFs using ionic liquids and related solvents.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Paper Converting and Packaging, Universidad Del Bío-Bío, Aalto University
Contributors: Reyes, G., Borghei, M., King, A. W. T., Lahti, J., Rojas, O. J.
Pages: 502-514
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Journal: Biomacromolecules
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ISSN (Print): 1525-7797
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Scopus rating (2019): CiteScore 10 SJR 1.61 SNIP 1.276
Original language: English
ASJC Scopus subject areas: Bioengineering, Biomaterials, Polymers and Plastics, Materials Chemistry
DOIs:

10.1021/acs.biomac.8b01554
Source: Scopus
Source ID: 85059629357
Research output: Contribution to journal › Article › Scientific › peer-review

Polyarginine Interacts More Strongly and Cooperatively than Polylysine with Phospholipid Bilayers
The interactions of two highly positively charged short peptide sequences with negatively charged lipid bilayers were explored by fluorescence binding assays and all-atom molecular dynamics simulations. The bilayers consisted of mixtures of phosphatidylglycerol (PG) and phosphatidylcholine (PC) lipids as well as a fluorescence probe that was sensitive to the interfacial potential. The first peptide contained nine arginine repeats (Arg_9), and the second one had nine lysine repeats (Lys_9). The experimentally determined apparent dissociation constants and Hill cooperativity coefficients demonstrated that the Arg_9 peptides exhibited weakly anticooperative binding behavior at the bilayer interface at lower PG concentrations, but this anticooperative effect vanished once the bilayers contained at least 20 mol % PG. By contrast, Lys_9 peptides showed strongly anticooperative binding behavior at all PG concentrations, and the dissociation constants with

Lys_9 were approximately 2 orders of magnitude higher than with Arg_9. Moreover, only arginine-rich peptides could bind to the phospholipid bilayers containing just PC lipids. These results along with the corresponding molecular dynamics simulations suggested two important distinctions between the behavior of Arg_9 and Lys_9 that led to these striking differences in binding and cooperativity. First, the interactions of the guanidinium moieties on the Arg side chains with the phospholipid head groups were stronger than for the amino group. This helped facilitate stronger Arg_9 binding at all PG concentrations that were tested. However, at PG concentrations of 20 mol % or greater, the Arg_9 peptides came into sufficiently close proximity with each other so that favorable like-charge pairing between the guanidinium moieties could just offset the long-range electrostatic repulsions. This led to Arg_9 aggregation at the bilayer surface. By contrast, Lys_9 molecules experienced electrostatic repulsion from each other at all PG concentrations. These insights may help explain the propensity for cell penetrating peptides containing arginine to more effectively cross cell membranes in comparison with lysine-rich peptides.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Texas A and M University, Pennsylvania State University, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Division of Organic Chemistry and Biochemistry, Bijenička Cesta 54
Contributors: Robison, A. D., Sun, S., Poyton, M. F., Johnson, G. A., Pellois, J. P., Jungwirth, P., Vazdar, M., Cremer, P. S.
Number of pages: 10
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Publication date: 8 Sep 2016
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B
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Issue number: 35
ISSN (Print): 1520-6106
Ratings:
Scopus rating (2016): CiteScore 6.1 SJR 1.345 SNIP 1.023
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry
DOIs:
10.1021/acs.jpcb.6b05604
Source: Scopus
Source ID: 84986593892
Research output: Contribution to journal › Article › Scientific › peer-review

Highly exfoliated natural rubber/Clay composites by "propping-open procedure": The influence of fatty-acid chain length on exfoliation

A high degree of exfoliation of MMT in NR is achieved by using the so-called "propping-open approach" in which a stepwise expansion of the interlayer spacing of MMT takes place. The nanostructure is characterized by WAXD and TEM which indicate different extents of clay dispersion depending on the fatty-acid chain length. Curing kinetics of different nanocomposites is studied and interestingly low activation energies of the vulcanization process are observed in the case of NR/EMMT nanocomposites. The incorporation of EMMT dramatically affects composite properties whereas DMA indicates significant reduction of tan δ peak height and the tensile strength approximately doubles from 14 to 30 MPa with only 5 phr EMMT.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V. , Vodafone Department of Mobile Communications Systems
Contributors: Rooj, S., Das, A., Stöckelhuber, K. W., Reuter, U., Heinrich, G.
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Pages: 369-383
Publication date: Apr 2012
Peer-reviewed: Yes

Publication information
Journal: Macromolecular Materials and Engineering
Volume: 297
Issue number: 4

ISSN (Print): 1438-7492
Ratings:
Scopus rating (2012): CiteScore 3.7 SJR 0.963 SNIP 1.187
Original language: English
ASJC Scopus subject areas: Chemical Engineering(all), Organic Chemistry, Polymers and Plastics, Materials Chemistry
Keywords: curing kinetics, exfoliation, Mooney-Rivlin equation, nanocomposites, propping-open approach
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http://www.scopus.com/inward/record.url?scp=84859811037&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
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Research output: Contribution to journal › Article › Scientific › peer-review

Preintercalation of an organic accelerator into nanogalleries and preparation of ethylene propylene diene terpolymer rubber-clay nanocomposites

A multifunctional additive, bis(diisopropyl) thiophosphoryl diisopropyl disulfide (DIPDIS), was melted in the presence of quaternary ammonium-modified montmorillonite clay and incorporated into an ethylene propylene diene terpolymer (EPDM) rubber matrix as a nanofiller to prepare EPDM rubber nanocomposites. The finer dispersion of the organoclay (OC) in the rubber matrix was observed when the OC was preintercalated by DIPDIS using the propping-open procedure. X-ray diffraction (XRD) results showed that the silicate layers of the OC were successfully preintercalated by the DIPDIS; that is, the basal spacing of clay galleries was expanded from 2.98 to 3.76 nm. Because of the larger interlayer distance, as evidenced by XRD studies, the delamination process was facilitated through the easy intercalation of macromolecular rubber chains, which was reflected in various properties, such as the stress-strain behavior, thermal stability, dynamic mechanical properties and swelling properties. XRD studies and transmission electron microscopy directly supported the effective filler dispersion in the non-polar EPDM rubber matrix.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V. , Vodafone Department of Mobile Communications Systems
Contributors: Rooj, S., Das, A., Heinrich, G.
Number of pages: 8
Pages: 285-292
Publication date: Mar 2011
Peer-reviewed: Yes

Publication information
Journal: POLYMER JOURNAL
Volume: 43
Issue number: 3
ISSN (Print): 0032-3896
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Scopus rating (2011): CiteScore 2.2 SJR 0.52 SNIP 0.598
Original language: English
ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry
Keywords: DIPDIS, montmorillonite, multifunctional additive, propping-open procedure
DOIs:
10.1038/pj.2010.132
URLs:
http://www.scopus.com/inward/record.url?scp=79952375182&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 79952375182
Research output: Contribution to journal › Article › Scientific › peer-review

Electromagnetic nonlinearities in a Roebel-cable-based accelerator magnet prototype: Variational approach

Superconducting magnets are the most expensive series of components produced in the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN). When developing such magnets beyond state-of-the-art technology, one possible option is to use high-temperature superconductors (HTS) that are capable of tolerating much higher magnetic fields than low-temperature superconductors (LTS), carrying simultaneously high current densities. Significant cost reductions due to decreased prototype construction needs can be achieved by careful modelling of the magnets. Simulations are used, e.g. for designing magnets fulfilling the field quality requirements of the beampipe, and adequate protection by studying the losses occurring during charging and discharging. We model the hysteresis losses

and the magnetic field nonlinearity in the beampipe as a function of the magnet's current. These simulations rely on the minimum magnetic energy variation principle, with optimization algorithms provided by the open-source optimization library interior point optimizer. We utilize this methodology to investigate a research and development accelerator magnet prototype made of REBCO Roebel cable. The applicability of this approach, when the magnetic field dependence of the superconductor's critical current density is considered, is discussed. We also scrutinize the influence of the necessary modelling decisions one needs to make with this approach. The results show that different decisions can lead to notably different results, and experiments are required to study the electromagnetic behaviour of such magnets further.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Electrical Energy Engineering, Research area: Electromagnetics, Institute of Electrical Engineering Slovak Academy of Sciences
Contributors: Ruuskanen, J., Stenvall, A., Lahtinen, V., Pardo, E.
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Article number: 024008
ISSN (Print): 0953-2048
Ratings:

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Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Condensed Matter Physics, Metals and Alloys, Materials Chemistry, Electrical and Electronic Engineering
Keywords: AC loss, accelerator magnets, high-temperature superconductors, interior point optimizer, magnetization, minimum magnetic energy variation, nonlinear optimization
DOIs:

10.1088/1361-6668/30/2/024008
Source: Scopus
Source ID: 85009227976
Research output: Contribution to journal › Article › Scientific › peer-review

Modelling thermodynamics in a high erature superconducting dipole magnet: An inverse problem based approach
The use of practical high temperature superconductors (HTS), REBCO tapes especially, in magnet applications has become possible thanks to the increasing interest of manufacturers. One difficulty has been the nonlinear material properties that are challenging to measure and model. To advance in such, demo systems are needed and they must be thoroughly analyzed. Recently, one of the first HTS dipole magnets was built to study the usability of REBCO Roebel cables in particle accelerator magnets. The prototype magnet Feather-M2 was designed, constructed and tested within EUCARD2 collaboration project at CERN in 2017. In the measurements, the magnet behaved in an unexpected way: the magnet was able to be operated at operation currents above the maximum current that was predicted based on short-sample measurements. Additionally, unexpectedly gradual dependency between magnet's resistive voltage and operation current was observed. In this work, a thermodynamical model is formulated in order to study the behavior of Feather-M2. The model was parametrized and the parameters were solved via inverse problem by finding the best match to experimental results. Thereby insight was gained on the prospects of the utilized thermodynamical model and also on the behavior and operation conditions of the magnet via the inverse problem solutions. To summarize, this paper presents a new methodology for analyzing magnets in operation and applies it to a state-of-the-art magnet.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Electrical Engineering, Research area: Power engineering, Research group: Modelling and superconductivity, European Organization for Nuclear Research
Contributors: Ruuskanen, J., Stenvall, A., Lahtinen, V., Nugteren, J. V., Kirby, G., Murtomäki, J.
Publication date: 2 Aug 2019
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Ratings:
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Original language: English
ASJC Scopus subject areas: Ceramics and Composites, Condensed Matter Physics, Metals and Alloys, Electrical and Electronic Engineering, Materials Chemistry
Keywords: HTS magnets, modelling, optimization, thermal stability
DOIs:
10.1088/1361-6668/ab2bc9
Source: Scopus
Source ID: 85072121234
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of rheological properties of dissolved cellulose/microfibrillated cellulose blend suspensions on film forming

Enzymatically treated cellulose was dissolved in a NaOH/ZnO solvent system and mixed together with microfibrillated cellulose (MFC) in order to find the threshold in which MFC fibers form a percolation network within the dissolved cellulose solution and in order to improve the properties of regenerated cellulose films. In the aqueous state, correlations between the rheological properties of dissolved cellulose/MFC blend suspensions and MFC fiber concentrations were investigated and rationalized. In addition, rheological properties of diluted MFC suspensions were characterized and a correlation with NaOH concentration was found, thus partly explaining the flow properties of dissolved cellulose/MFC blend suspensions. Finally, based on results from Dynamic Mechanical Analysis (DMA), MFC addition had strengthening/plasticizing effect on regenerated cellulose films if low concentrations of MFC, below the percolation threshold (5.5-6 wt%, corresponding to 0.16-0.18 wt% of MFC in the blend suspensions), were used.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Fibre Materials, PolymerTechnology, Department of Biotechnology and Chemical Technology, Aalto University
Contributors: Saarikoski, E., Rissanen, M., Seppälä, J.
Number of pages: 9
Pages: 62-70
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Peer-reviewed: Yes

Publication information
Journal: Carbohydrate Polymers
Volume: 119
ISSN (Print): 0144-8617
Ratings:
Scopus rating (2015): CiteScore 7.8 SJR 1.44 SNIP 1.82
Original language: English
ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics
Keywords: Blend, Dissolved cellulose, Microfibrillated cellulose, Rheology, Suspension
DOIs:
10.1016/j.carbpol.2014.11.033
URLs:
http://www.scopus.com/inward/record.url?scp=84916613635&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84916613635
Research output: Contribution to journal › Article › Scientific › peer-review

Supercritical carbon dioxide treatment of hot dip galvanized steel as a surface treatment before coating

Supercritical carbon dioxide ($scCO_2$) treatment was employed for rapid formation of a zinc patina layer on hot dip galvanized (HDG) steel. In the presence of H_2O and a Cu precursor, an artificial patina consisting of two distinctive phases was formed: a dense ~ 1 μm layer of anhydrous $ZnCO_3$ adjacent to native zinc coating, and a needle-like porous structure showing resemblance to hydrozincite ($Zn_5(CO_3)_2(OH)_6$). The artificial patina layer significantly decreased the surface free energy of HDG, which was evidenced also by good wettability by a polyester melamine coating. Furthermore, the needle-like patina surface structure stayed intact through the coating process, indicating improved coating adhesion. $ScCO_2$ treatment facilitates rapid and impurity-free surface treatment of hot dip galvanized steel, and could be used to tailor novel adhesion and corrosion promoting surface morphologies.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Ceramic materials, Top Analytica Oy, SSAB
Contributors: Saarimaa, V., Kaleva, A., Nikkanen, J., Heinonen, S., Levänen, E., Väisänen, P., Markkula, A., Juhanoja, J.
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Journal: Surface and Coatings Technology
Volume: 331
ISSN (Print): 0257-8972
Ratings:

Scopus rating (2017): CiteScore 4.5 SJR 0.928 SNIP 1.576
Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Basic zinc carbonate, Coatings, Corrosion resistance, Hot dip galvanized steel, Patina, Supercritical carbon dioxide, Zinc
DOIs:

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Source: Scopus
Source ID: 85032293898
Research output: Contribution to journal › Article › Scientific › peer-review

Convenient extraction method for quantification of thin zinc patina layers
Synthetic zinc patina was grown on galvanized steel sheets in supercritical carbon dioxide atmosphere. Different patina compounds were dissolved and quantified using a stepwise immersion and dissolution procedure. The distinct patina components, namely anhydrous zinc carbonate (a dense layer adjacent to metallic zinc) and zinc hydroxy carbonate (nanowires on the surface), were dissolved in glycine solutions, followed by quantification of Zn^{2+} in the solutes by X-ray fluorescence. The zinc hydroxy carbonate nanowires were readily glycine soluble, and the anhydrous zinc carbonate showed scarce glycine solubility, which enabled their selective quantification. The amount of the remaining (anhydrous) zinc carbonate after glycine extraction was determined from the glycine-soluble zinc oxide after calcination (heat treatment for 10 minutes at 350°C). The results were verified by scanning electron microscopy imaging and Fourier transform infrared spectroscopy measurements.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science
Contributors: Saarimaa, V., Kaleva, A., Paunikallio, T., Nikkanen, J., Heinonen, S., Levänen, E., Väisänen, P., Markkula, A.
Pages: 564-570
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Peer-reviewed: Yes
Early online date: 1 Jan 2018

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Volume: 50
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ISSN (Print): 0142-2421
Ratings:

Scopus rating (2018): CiteScore 2.4 SJR 0.451 SNIP 0.648
Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Galvanized steel, Glycine, Supercritical carbon dioxide, Zinc carbonate, Zinc nanowires, Zinc oxide
DOIs:

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Source: Scopus
Source ID: 85044219012
Research output: Contribution to journal › Article › Scientific › peer-review

Assessment of pitting corrosion in bare and passivated (wet $scCO_2$-induced patination and chemical passivation) hot-dip galvanized steel samples with SVET, FTIR, and SEM (EDS)

In this study, the local electrochemical activity of untreated and passivated (natural or chemical passivation) zinc specimens was observed during immersion in a 0.1-M NaCl solution. The localized anodic activity during the exposure, measured with the scanning vibrating electrode technique, was linked to zinc dissolution by the pitting corrosion mechanism. It was correlated to specific corrosion products characterized by Fourier transmission infrared (FTIR) microscopy. FTIR molecule maps were produced from individual pitting corrosion sites (100–200 µm in width). With argon ion beam milling and latest energy-dispersive X-ray spectroscopy (EDS) technology, element maps with a high spatial resolution (≪100 nm) were recorded from abrasion- and beam-sensitive corrosion products, showing a residual layer structure. This study demonstrates the capability of FTIR mapping, cross-section polishing, and state-of-the-art scanning electron microscopy imaging, and EDS element mapping to produce high-resolution elemental, molecular, and visual information about pitting corrosion mechanisms on a hot-dip galvanized steel sample.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Ceramic materials, Top Analytica Oy, Swerim AB, RISE, SSAB
Contributors: Saarimaa, V., Fuertes, N., Persson, D., Zavalis, T., Kaleva, A., Nikkanen, J., Levänen, E., Heydari, G.
Number of pages: 10
Publication date: 2020
Peer-reviewed: Yes

Publication information

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ISSN (Print): 0947-5117
Original language: English
ASJC Scopus subject areas: Environmental Chemistry, Mechanics of Materials, Mechanical Engineering, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
Keywords: anodic dissolution, FTIR microscopy, passivation, pitting corrosion, scanning electron microscopy, zinc
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Source: Scopus
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Research output: Contribution to journal › Article › Scientific › peer-review

Persistent luminescent particles containing bioactive glasses: Prospect toward tracking in-vivo implant mineralization using biophotonic ceramics

In this paper, we demonstrate that persistent luminescent bodies can be obtained by carefully choosing the sintering temperatures and duration. A borosilicate and a phosphate glasses were sintered into bodies with persistent luminescent (PeL) $SrAl_2O_4:Eu^{2+},Dy^{3+}$ microparticles which have a green emission up to tens of hours after ceasing irradiation. When sintered at high temperature for a short time or at lower temperature for a longer time, a decrease in the PeL from the bodies was observed and was related to the glasses crystallization. A decrease in the PeL from the bodies was also observed after immersion in simulated body fluid and was related to the mineralization of the sintered bodies. Therefore, we clearly show that by tracking the changes in the PeL overtime, these PeL bodies have a real potential application as biophotonic sensors to track dissolution and mineralization of the implant in the body.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Photonics, Faculty of Biomedical Sciences and Engineering, Research group: Biomaterials and Tissue Engineering Group, Materials Science, Turun Yliopisto/Turun Biomateriaalikeskus
Contributors: Saarinen, M., Nommeots-Nomm, A., Hokka, M., Laurila, J., Norrbo, I., Lastusaari, M., Massera, J., Petit, L.
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Publication information

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ASJC Scopus subject areas: Ceramics and Composites, Materials Chemistry
Keywords: Bioactivity, Biophotonic, Conventional luminescence, Microparticles containing glasses, Persistent luminescence, Sintering process
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Source: Scopus
Source ID: 85028445336
Research output: Contribution to journal › Article › Scientific › peer-review

Supramolecular hierarchy among halogen and hydrogen bond donors in light-induced surface patterning

Halogen bonding, a noncovalent interaction possessing several unique features compared to the more familiar hydrogen bonding, is emerging as a powerful tool in functional materials design. Herein, we unambiguously show that one of these characteristic features, namely high directionality, renders halogen bonding the interaction of choice when developing azobenzene-containing supramolecular polymers for light-induced surface patterning. The study is conducted by using an extensive library of azobenzene molecules that differ only in terms of the bond-donor unit. We introduce a new tetrafluorophenol-containing azobenzene photoswitch capable of forming strong hydrogen bonds, and show that an iodoethynyl-containing azobenzene comes out on top of the supramolecular hierarchy to provide unprecedented photoinduced surface patterning efficiency. Specifically, the iodoethynyl motif seems highly promising in future development of polymeric optical and photoactive materials driven by halogen bonding.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Aalto University, VTT Technical Research Centre of Finland, Politecn Milan, Polytechnic University of Milan, NFMLab, DCMIC Giulio Natta, ISTM-CNR, Institute of Molecular Sciences and Technologies of CNR, Università Degli Studi di Milano, McGill University, Politecnico di Milano
Contributors: Saccone, M., Dichiarante, V., Forni, A., Goulet-Hanssens, A., Cavallo, G., Vapaavuori, J., Terraneo, G., Barrett, C. J., Resnati, G., Metrangolo, P., Priimägi, A.
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Scopus rating (2015): CiteScore 5.6 SJR 1.713 SNIP 1.488
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Supramolecular hierarchy among halogen 2015
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http://www.scopus.com/inward/record.url?scp=84925407935&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note

EXT="Saccone, Marco"
EXT="Vapaavuori, Jaana"
Source: Scopus
Source ID: 84925407935
Research output: Contribution to journal › Article › Scientific › peer-review

Halogen bonding stabilizes a cis-azobenzene derivative in the solid state: A crystallographic study

Crystals of trans- and cis-isomers of a fluorinated azobenzene derivative have been prepared and characterized by single-crystal X-ray diffraction. The presence of F atoms on the aromatic core of the azobenzene increases the lifetime of the metastable cis-isomer, allowing single crystals of the cis-azobenzene to be grown. Structural analysis on the cis-

azobenzene, complemented with density functional theory calculations, highlights the active role of the halogen-bond contact (N...I synthon) in promoting the stabilization of the cis-isomer. The presence of a long aliphatic chain on the azobenzene unit induces a phase segregation that stabilizes the molecular arrangement for both the trans- and cis-isomers. Due to the rarity of cis-azobenzene crystal structures in the literature, our paper makes a step towards understanding the role of non-covalent interactions in driving the packing of metastable azobenzene isomers. This is expected to be important in the future rational design of solid-state, photoresponsive materials based on halogen bonding. We show by single-crystal X-ray diffraction studies and computational analysis that halogen bonding can stabilize a metastable cis-azobenzene derivative in the solid state.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials, Politecnico di Milano, Aalto University
Contributors: Saccone, M., Siiskonen, A., Fernandez-Palacio, F., Priimägi, A., Terraneo, G., Resnati, G., Metrangolo, P.
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Journal: ACTA CRYSTALLOGRAPHICA SECTION B : STRUCTURAL SCIENCE, CRYSTAL ENGINEERING AND MATERIALS
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Atomic and Molecular Physics, and Optics, Metals and Alloys, Materials Chemistry
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Halogen bonding stabilizes a cis-azobenzene derivative 2017
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URLs:

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Source: Scopus
Source ID: 85017113549
Research output: Contribution to journal › Article › Scientific › peer-review

Ortho-Fluorination of azophenols increases the mesophase stability of photoresponsive hydrogen-bonded liquid crystals

Photoresponsive liquid crystals (LCs) whose alignment can be controlled with UV-Visible light are appealing for a range of photonic applications. From the perspective of exploring the interplay between the light response and the self-assembly of the molecular components, supramolecular liquid crystals are of particular interest. They allow elaborating the structure-property relationships that govern the optical performance of LC materials by subtle variation of the chemical structures of the building blocks. Herein we present a supramolecular system comprising azophenols and stilbazoles as hydrogen-bond donors and acceptors, respectively, and show that ortho-fluorination of the azophenol dramatically increases the thermal stability of the LC phases, an important characteristics in their further utilization in photonics. The systems exhibit fast photoinduced order-disorder transitions, and rapid recovery of the liquid-crystalline state once the light irradiation is ceased, due to the photochemical properties of azophenols.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, University of Duisburg-Essen
Contributors: Saccone, M., Kuntze, K., Ahmed, Z., Siiskonen, A., Giese, M., Priimagi, A.
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Publication date: 1 Jan 2018
Peer-reviewed: Yes

Publication information

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Original language: English
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http://urn.fi/URN:NBN:fi:tty-201901111059. Embargo ended: 30/08/19
Source: Scopus
Source ID: 85054152271
Research output: Contribution to journal › Article › Scientific › peer-review

Passive resonance sensor based method for monitoring particle suspensions

Control of particle suspensions is needed in several modern industrial processes. A reason for the difficulty in this task has been the lack of a fast and reliable measurement. In this study, we tested the measurement of particle suspension by using a method based on a passive resonance sensor. The relative amounts of dispersing agent and aluminium oxide in the suspension were varied. The studied method yielded signals which depended on the complex permittivity of the suspension. The results indicated that we were able to measure information that can be used as feedback for the suspension preparation process. In addition, the tested instrumentation was simple and robust and thus this method may allow online measurements directly from the industrial processes.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Automation Science and Engineering, Research area: Microsystems, Research area: Measurement Technology and Process Control, Department of Materials Science, Research group: Ceramic materials, Engineering materials science and solutions (EMASS), Integrated Technologies for Tissue Engineering Research (ITTE), Smart Energy Systems (SES)
Contributors: Salpavaara, T., Järveläinen, M., Seppälä, S., Yli-Hallila, T., Verho, J., Vilkko, M., Lekkala, J., Levänen, E.
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ASJC Scopus subject areas: Electrical and Electronic Engineering, Condensed Matter Physics, Electronic, Optical and Magnetic Materials, Metals and Alloys, Surfaces, Coatings and Films, Materials Chemistry, Instrumentation
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Bibliographical note

ORG=ase,0.5
ORG=mol,0.5
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Source ID: 84930646590
Research output: Contribution to journal › Article › Scientific › peer-review

Non-destructive and wireless monitoring of biodegradable polymers

A method for monitoring changes in biodegradable polymers during hydrolysis is proposed. This wireless and non-destructive method is based on inductively coupled passive resonance sensors embedded in the polymer shell. In this study, we prepared specimens using two poly(lactide-co-glycolide) copolymers possessing different degradation profiles. The copolymer embedded sensors were immersed in buffer solution and their resonance features were compared with periodically performed conventional polymer characterization methods. A clear difference was noticed in the wirelessly measured signals between the two tested copolymer materials. Also the reference methods showed clear differences between the degradation profiles of the copolymers. The wirelessly measured signals are likely to correlate to the structural changes in the materials during the hydrolysis. In the future, this technique could be used in the laboratory to provide easy-to-access in situ information about the polymers. Even the state of biodegradable polymer implants could be wirelessly monitored.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Faculty of Biomedical Sciences and Engineering, Research area: Microsystems, Research group: Sensor Technology and Biomeasurements (STB), Research group: Biomaterials and Tissue Engineering Group, BioMediTech
Contributors: Salpavaara, T., Hänninen, A., Antniemi, A., Lekkala, J., Kellomäki, M.
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ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Instrumentation, Condensed Matter Physics, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry, Electrical and Electronic Engineering
Keywords: Biodegradable polymers, Passive resonance sensor, Poly(lactide-co-glycolide), Telemetry, Wireless monitoring
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non_destructive_and_wireless_2018. Embargo ended: 25/07/19
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http://urn.fi/URN:NBN:fi:tuni-201910234047
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Source ID: 85020132649
Research output: Contribution to journal › Article › Scientific › peer-review

Phenothiazine and carbazole substituted pyrene based electroluminescent organic semiconductors for OLED devices

Due to their easy availability, low cost and opportunities for exploiting reactions of bromo substituents, 1,3,6,8-tetrabromopyrene has attracted major attention in the organic electronics community for designing and constructing novel classes of pyrene based organic semiconducting functional materials. In the present work, 1,3,6,8-tetrabromo pyrene was transformed into the corresponding tetrasubstituted carbazole and phenothiazine derivatives using the classical Suzuki coupling reaction. These newly synthesized materials with a carbazole substituent (PY-CA) and a phenothiazine substituent (PY-PH) were characterised thoroughly and were successfully used as an active light-emitting layer in organic light emitting diodes which resulted in blue and green emission with promising device performance. PY-CA exhibited the maximum brightness at around 2500 cd m^{-2} and the power efficiency of 1.5 lm W^{-1} while that of PY-PH exhibited 2116 cd m^{-2} and 0.45 lm W^{-1} respectively.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Polymer Science and Engineering Division, Council of Scientific and Industrial Research India, University of Hong Kong, CSIRO Energy Centre, National University of Singapore , Queensland University of Technology QUT
Contributors: Salunke, J. K., Wong, F. L., Feron, K., Manzhos, S., Lo, M. F., Shinde, D., Patil, A., Lee, C. S., Roy, V. A. L., Sonar, P., Wadgaonkar, P. P.
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Materials Chemistry
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Source ID: 84957013671
Research output: Contribution to journal › Article › Scientific › peer-review

Infrared Thermography as a Non-destructive Testing Solution for Thermal Spray Metal Coatings
In this work, an infrared (IR) thermographic procedure was evaluated as a non-destructive testing tool to detect damage in thermal spray metallic coatings. As model systems, polished HVOF- and HVAF-sprayed Fe-based layers deposited onto steel plates were employed. Damage by external-object impingement was simulated through a cyclic impact-test apparatus, which induced circumferential and radial cracks across all model systems, and interface cracks of different sizes in distinct samples. Damaged and undamaged plates were bulk-heated to above 100 °C using an IR lamp; their free-convection cooling was then recorded by an IR thermocamera. The intentionally induced defects were hardly detectable in IR thermograms, due to IR reflection and artificial “hot” spots induced by residuals of transfer material from the impacting counterbody. As a micrometer-thin layer of black paint was applied, surface emissivity got homogenized and any artifacts were effectively suppressed, so that failed coating areas clearly showed up as “cold spots.” This effect was more apparent when large interface cracks occurred. Finite-element modeling proved the physical significance of the IR-thermography approach, showing that failed coating areas are cooled by surrounding air faster than they are heated by conduction from the hot substrate, which is due to the insulating effect of cracks.

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Organisations: Materials Science, Research group: Surface Engineering, Universita degli Studi di Modena e Reggio Emilia
Contributors: Santangelo, P. E., Allesina, G., Bolelli, G., Lusvarghi, L., Matikainen, V., Vuoristo, P.
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ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
Keywords: finite element modeling, high-velocity air fuel (HVAF), high-velocity oxy fuel (HVOF), impact testing, non-destructive inspection
DOIs:

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Source: Scopus
Source ID: 85029487592
Research output: Contribution to journal › Article › Scientific › peer-review

A study of electric transport in n- and p-type modulation-doped GaInNAs/GaAs quantum well structures under a high electric field
We present the results of longitudinal carrier transport under a high electrical field in n- and p-type modulation-doped $Ga_{0.68}In_{0.32}N_yAs_{1-y}$/GaAs (y = 0.009, 0.017) quantum well (QW) structures. Nitrogen composition-dependent drift velocities of electrons are observed to be saturated at and at 77 K for the samples with y = 0.009 and y = 0.017, respectively, while the drift velocities of holes do not saturate but slightly increase at the applied electric field in the range of interest. The hole drift velocity is observed to be higher than the electron drift velocity. The electron mobility exhibits an almost temperature-independent characteristic. On the other hand, the hole mobility exhibits a conventional temperature

dependence of modulation-doped QW structures. As the temperature increases, the drift velocity of the electrons exhibits an almost an temperature-insensitive characteristic, but, on the other hand, for holes, drift velocity decreases approximately from 10^{7}-10^{6} cm s^{-1}. It is observed that the drift velocities of electrons and holes are N-dependent and suppressed at higher electric fields. Furthermore, experimental results show that there is no evidence of negative differential velocity (NDV) behaviour for both n- and p-type samples. To explore the observed electron and hole drift velocity characteristic at high electric fields, we use a simple theoretical model for carrier transport, which takes into account the effect of non-drifting hot phonons. The mobility mapping technique (comparison method) is used to extract hot hole temperature in order to employ it in the non-drifted phonon distribution and to obtain the drift velocity-electric field curves. Then hot electron temperatures are obtained from the drift velocity-electric field curves as a fit parameter using non-drifted hot phonon dynamics. The analytical model is well-matched to the experimental -E curves, indicating that carrier-hot phonon scattering is the main reason for suppressing the NDV mechanism in GaInNAs/GaAs QW structures with a carrier density higher than 10^{17} cm^{-3}.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Photonics, Research group: ORC, Istanbul University
Contributors: Sarcan, F., Mutlu, S., Cokduygulular, E., Donmez, O., Erol, A., Puustinen, J., Guina, M.
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Ratings:
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Condensed Matter Physics, Electrical and Electronic Engineering, Materials Chemistry
Keywords: dilute nitride, GaInNAs, hot phonons, hot-electron and hole temperature, modulation-doped GaInNAs/GaAs quantum well
DOIs:
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Source: Scopus
Source ID: 85048073763
Research output: Contribution to journal › Article › Scientific › peer-review

Abrasive-Erosive Wear of Thermally Sprayed Coatings from Experimental and Commercial Cr_3C_2-Based Powders

In this paper, high-velocity oxy-fuel sprayed coatings from experimental Cr_3C_2-Ni powder produced by mechanically activated thermal synthesis and disintegrator milling are compared with coatings from commercial Cr_3C_2-NiCr powder under room- and elevated-temperature abrasive-erosive wear (AEW) conditions. In a room-temperature AEW test, the coating made from the experimental powder had wear rates that were 1.1-5.3 times higher than the coating from the commercial powder; this difference was the lowest at the highest impact velocity (80 m s^{-1}). Under AEW tests at elevated temperature (300 and 550 °C), the coating made from the experimental powder exhibited wear rates that were 1.2-2.8 times higher in comparison with that made from the commercial powder, but this difference was smaller under an oblique impact angle (30°) and higher temperature conditions. The reasons for the lower resistance against AEW of the coating made from the experimental powder were found to be its lower ability to resist plastic indentation and deformation as well as lower indentation fracture toughness at room temperature, weaker bonding between the matrix and reinforcement and probably lower mechanical properties as well as unfavourable residual stresses at elevated temperatures.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Surface Engineering, Ensto Ensek AS, Tallinn University of Technology
Contributors: Sarjas, H., Surzhenkov, A., Juhani, K., Antonov, M., Adoberg, E., Kulu, P., Viljus, M., Traksmaa, R., Matikainen, V., Vuoristo, P.
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Original language: English
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Keywords: abrasive-erosive wear, CrC-based cermet, elevated temperature, mechanically activated thermal synthesis, room temperature, thermal spraying
DOIs:

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Source ID: 85029407112
Research output: Contribution to journal › Article › Scientific › peer-review

Erosive wear of filled vinylester composites in water and acidic media at elevated temperature
Due to their good corrosion properties, fibre reinforced polymer composites are often used instead of metals for example in hydrometallurgical processes. However, the erosion performance of polymer composites is rather poor when compared to metals. This study focused on the effect of mineral fillers on the erosion performance of vinylester composites. The erosion rates were tested both in water and in acidic environments at high temperature. To improve the erosion performance of the filled composites in these environments, to increase the filler particle hardness was an effective method. Within similar filler materials, better adhesion to the matrix improved the erosion performance, regardless if it was achieved by adhesion promoters or better mechanical interlocking. The hardness of the matrix was found to be disadvantageous for filled composites, although for pure vinylesters higher hardness decreased erosion rate. At the high service temperature, softer matrix accommodated more deformations and better absorption of energy of the impacting erosive particles. Consequently, improved adherence of the filler particles into the matrix and slower erosion rate was observed.

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Plastics and Elastomer Technology, Outotec Research Center
Contributors: Sarlin, E., Saarimäki, M., Sironen, R., Lindgren, M., Siljander, S., Kanerva, M., Vuorinen, J.
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ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
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10.1016/j.wear.2017.07.011
URLs:

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Bibliographical note
INT=mol,"Sironen, Reija"
EXT="Lindgren, Mari"
Source: Scopus
Source ID: 85024891666
Research output: Contribution to journal › Article › Scientific › peer-review

Properties of HVOF-sprayed Stellite-6 coatings

Stellite-6 coatings were deposited onto AISI 304 stainless steel substrate by gas-fueled HVOF spraying, systematically varying the process parameter settings. By operating the HVOF torch with a fuel-rich mixture, dense coatings (<1% porosity) are produced, containing up to ≈3 vol% oxide inclusions. A substantial amount of a Cr-rich f.c.c. phase is found, mainly produced by quenching of molten lamellae, and distinct from the equilibrium, Co-based f.c.c. solid solution retained in unmelted particles. These coatings exhibit pseudo-passive behavior and survive 5 cycles (100 h) of the Corrodkote test (ASTM B380-97) with no substrate corrosion. Coatings obtained from oxygen-rich mixtures, on the other hand, contain fewer oxide inclusions but also greater porosity, and do not protect the substrate against corrosion. The wear behavior of the coatings is less influenced by deposition conditions. In ball-on-disk dry sliding tests, all coatings exhibit wear rates of 2–3 × 10^{-5} mm^3/(N·m), higher than those reported for bulk or clad Stellite, because of interlamellar delamination. Strain-induced, “martensitic” phase transformation from the f.c.c. structure to a h.c.p. one is observed over a 1–2 μm depth below the contact surface. Additional tribo-oxidation is onset when frictional heat dissipation has heated the wear debris enough to trigger its reaction with the environment. Correspondingly, a transition to a regime of higher friction occurs (from ≈0.6 to ≈0.8). At 400 °C, lamellar delamination is suppressed but wear rates rise to 5–8 × 10^{-5} mm^3/(N·m) because of abrasive and adhesive wear. At 800 °C, a dense “glaze” tribofilm is formed by sintered debris particles, firmly bonded to a thermally grown oxide scale on the underlying metal surface. The “glaze” protects the coating, lowering the wear rate to ≈1 × 10^{-5} mm^3/(N·m) and the friction coefficient to <0.45. Under high-stress particle abrasion conditions, wear rates of ≈1 × 10^{-3} mm^3/(N·m) are found.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Materials Characterization, Universita degli Studi di Modena e Reggio Emilia, Il Sentiero International Campus S.r.l., Univ of Oulu, ECOR Research SpA
Contributors: Sassatelli, P., Bolelli, G., Lassinantti Gualtieri, M., Heinonen, E., Honkanen, M., Lusvarghi, L., Manfredini, T. , Rigon, R., Vippola, M.
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Dry particles abrasion, Electrochemical corrosion test, High velocity oxygen-fuel (HVOF), High-temperature tribology, Sliding wear, Stellite coating
DOIs:

10.1016/j.surfcoat.2018.01.078
Source: Scopus
Source ID: 85041473768
Research output: Contribution to journal › Article › Scientific › peer-review

Improved electromechanical response in acrylic rubber by different carbon-based fillers

Dielectric elastomers are materials often utilized for the fabrication of electroactive actuators. Acrylic rubber (ACM) is very widely used in dielectric elastomer actuators (DEAs). However, its overall good performance is limited by the high operating electric field required. In the present work, we compare the effect of different types of conventionally used carbon black (CB) as well as other carbon-based fillers on the dielectric and actuation properties of ACM in order to show that performance of DEAs can be improved by the development of ACM composites. Indeed, addition of CB, carbon nanotubes (CNTs), and synthetic graphite leads to an increase in the relative dielectric permittivity of elastomeric material. Moreover, incorporation of nanodiamonds results in reduction of dielectric losses. Finally, actuation stress is remarkably improved by CNTs and different grades of CB.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Plastics and Elastomer Technology, Leibniz Institute of Polymer ResearchDresdenD

Contributors: Shakun, A., Poikelispää, M., Das, A., Vuorinen, J.
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Peer-reviewed: Yes

Publication information
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ASJC Scopus subject areas: Chemistry(all), Polymers and Plastics, Materials Chemistry
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URLs:

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Source: Scopus
Source ID: 85017528518
Research output: Contribution to journal › Article › Scientific › peer-review

Energy dissipation in natural rubber latex films: The effect of stabilizers, leaching and acetone-treatment
Natural rubber (NR) is a versatile material possessing outstanding mechanical properties, which can be used in multiple applications including the rapidly developing dielectric elastomer generators (DEGs). One of the drawbacks of the existing DEGs is their low efficiency, which can be improved by lowering the dielectric and mechanical losses originating from the material. Therefore, the present research was focusing on assessing the ways to minimize the dielectric and mechanical losses of NR films rather than developing a DEG. In this article, the effect of natural proteins and the rubber stabilizers on energy dissipation of NR films was evaluated. Moreover, the effect of sample posttreatment (with water and acetone), curing and time after cure was discussed. As a result, deproteinized NR stabilized by ammonium caseinate outperformed unmodified NR due to reduced dielectric losses, mechanical hysteresis and stress relaxation. Moreover, the posttreatment methods were found to moderately reduce the material-relates losses.

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Contributors: Shakun, A., Sarlin, E., Vuorinen, J.
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry
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Source: Scopus
Source ID: 85087303061
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of incorporation of CdS NPs on performance of PTB7: PCBM organic solar cells
It has been well known that incorporation of nano-heterostructures of various metals, semiconductors and dielectric materials in the active layer of organic solar cells (OSCs) helps in improving power conversion efficiency (PCE). In the present study, we demonstrated microwave synthesis of CdS nanoparticles (NPs) for their application in one of most

efficient OSCs consisting of poly[[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b′]dithiophene-2,6-diyl] [3-fluoro-2-[(2-ethylhexyl)carbonyl] thieno[3,4-b]thiophenediyl]] (PTB7): [6,6]-phenyl C_{71}-butyric acid methyl ester (PCBM) photoactive blend. This is crucial to fully explore the promising features of low cost and scalability in organic-inorganic hybrid solar cells. Synthesized CdS NPs are slightly elongated and highly crystalline with their absorption lies in the visible region as confirmed by High resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), UV-Vis absorption spectroscopy studies. Our experimental results for the devices in an inverted geometry having a structure ITO/ZnO/PTB7: CdS: PCBM/MoO_3/Ag has shown increase in Jsc and PCE by nearly 10%. However, it was observed that this increase is only when NPs were added in the low concentration in active layer. UV-Vis absorption spectroscopy, Photoluminescence (PL) and atomic force microscopy (AFM) studies were carried out in order understand the device performance.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Electronics and Communications Engineering, Indian Institute of Technology Bombay, Organic and Nano-electronics Group
Contributors: Sharma, R., Bhalerao, S., Gupta, D.
Number of pages: 7
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Publication date: 1 Jun 2016
Peer-reviewed: Yes

Publication information
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Biomaterials, Chemistry(all), Condensed Matter Physics, Materials Chemistry, Electrical and Electronic Engineering
Keywords: CdS nanoparticles, Microwave synthesis, Organic solar cells, PCBM, PL quenching, PTB7
DOIs:

10.1016/j.orgel.2016.03.030
Source: Scopus
Source ID: 84962355464
Research output: Contribution to journal › Article › Scientific › peer-review

Polymer looping is controlled by macromolecular crowding, spatial confinement, and chain stiffness
We study by extensive computer simulations the looping characteristics of linear polymers with varying persistence length inside a spherical cavity in the presence of macromolecular crowding. For stiff chains, the looping probability and looping time reveal wildly oscillating patterns as functions of the chain length. The effects of crowding differ dramatically for flexible versus stiff polymers. While for flexible chains the looping kinetics is slowed down by the crowders, for stiffer chains the kinetics turns out to be either decreased or facilitated, depending on the polymer length. For severe confinement, the looping kinetics may become strongly facilitated by crowding. Our findings are of broad impact for DNA looping in the crowded and compartmentalized interior of living biological cells.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, Max-Planck Institute for the Physics of Complex Systems
Contributors: Shin, J., Cherstvy, A. G., Metzler, R.
Number of pages: 5
Pages: 202-206
Publication date: 17 Feb 2015
Peer-reviewed: Yes

Publication information
Journal: ACS Macro Letters
Volume: 4
Issue number: 2
ISSN (Print): 2161-1653
Ratings:

Scopus rating (2015): CiteScore 10.1 SJR 2.392 SNIP 1.403
Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Inorganic Chemistry
DOIs:
10.1021/mz500709w
URLs:
http://www.scopus.com/inward/record.url?scp=84923204435&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84923204435
Research output: Contribution to journal › Article › Scientific › peer-review

Low-dimensional formamidinium lead perovskite architectures via controllable solvent intercalation

We report the formation of a new class of solvent-intercalated two-dimensional (SI-2D) formamidinium lead halide perovskites. They can be mixed with three-dimensional (3D) stoichiometric perovskites by controlling the ratio of the precursor solutions. The composite leads to greatly improved photoluminescence quantum yield (PLQY) over the 3D compound. The enhanced PLQY is attributed to a type-I band alignment between the 3D and SI-2D, as revealed by first-principles calculations, which results in confined excitons with enhanced radiative recombination. The films exhibited excellent thermal and air stability retaining PLQY > 20% over 2 months in ambient conditions. Assemblies of halide perovskites with mixed dimensionality offer a pathway to enhance optoelectronic performance and device lifetimes.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Korea Advanced Institute of Science and Technology (KAIST), Yonsei University
Contributors: Shin, M., Kim, J., Jung, Y. K., Ruoko, T., Priimagi, A., Walsh, A., Shin, B.
Number of pages: 7
Pages: 3945-3951
Publication date: 2019
Peer-reviewed: Yes

Publication information

Journal: Journal of Materials Chemistry C
Volume: 7
Issue number: 13
ISSN (Print): 2050-7534
Ratings:
Scopus rating (2019): CiteScore 10.9 SJR 1.934 SNIP 1.407
Original language: English
ASJC Scopus subject areas: Chemistry(all), Materials Chemistry
DOIs:
10.1039/c9tc00379g
Source: Scopus
Source ID: 85064717293
Research output: Contribution to journal › Article › Scientific › peer-review

Thermal, structural and optical properties of Er^{3+} doped phosphate glasses containing silver nanoparticles

The melt-quenching method is employed to prepare the amorphous phosphate glasses containing silver nanoparticles (Ag NPs). The structural characteristics of phosphate glasses were investigated by X-ray diffraction, thermal analysis, transmission electron microscopy, UV-Vis spectroscopy, Raman, and infrared spectroscopy. The transmission electron microscopic images confirm the presence of spherical silver NPs having an average diameter in the range of 20-40 nm. The EDX analysis spectrum shows the presence of Ag element. Important structural changes induced by the Ag_2CO_3 addition to the phosphate glass, Raman- and IR-spectroscopic studies were carried out in order to correlate the variations in the glass properties with variations of the glass structure. The surface plasmon resonance (SPR) peak of silver nanoparticles embedded in Er^{3+} doped phosphate glass is evidenced at ~403 nm. From the absorption spectra, the optical band gap is found to decrease with the increase of Ag NPs' concentration. All the obtained results in the present study were reported and discussed in detail.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Electronics and Communications Engineering, Research group: Biomaterials and Tissue Engineering Group, Physical Chemistry Laboratory of Mineral Materials and Their Applications, National Center of Research in Materials Science, Åbo Akademi
Contributors: Soltani, I., Hraiech, S., Horchani-Naifer, K., Massera, J., Petit, L., Férid, M.
Number of pages: 7

Pages: 67-73
Publication date: 15 Apr 2016
Peer-reviewed: Yes

Publication information
Journal: Journal of Non-Crystalline Solids
Volume: 438
ISSN (Print): 0022-3093
Ratings:

Scopus rating (2016): CiteScore 3.5 SJR 0.685 SNIP 1.154
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Ceramics and Composites, Electronic, Optical and Magnetic Materials, Materials Chemistry
Keywords: FTIR and Raman spectra, Phosphate glasses, Silver nanoparticles (Ag NPs), Thermal stability
DOIs:

10.1016/j.jnoncrysol.2015.12.022

Bibliographical note
EXT="Petit, L."
Source: Scopus
Source ID: 84960866255
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of melting state on the thermal shock resistance and thermal conductivity of APS ZrO_2-7.5wt.% Y_2O_3 coatings

The microstructures of two types of ZrO_2-7.5wt.% Y_2O_3 (YSZ) coatings fabricated by air plasma spraying (APS) but containing different amounts of columnar grains were investigated through scanning electron microscopy and electron backscatter diffraction analysis. Differences in the formation mechanisms of columnar and equiaxed grains were characterized using particles collected in a water container, from which it was found that these mechanisms are closely related to the melted state of the in-flight particles. Furthermore, it was found that the higher the columnar grain concentration of an as-sprayed coating, the higher its thermal shock resistance. This means that it is possible to improve the thermal shock resistance of APS YSZ coatings simply by introducing more columnar grains, as this increases their thermal conductivity. Using this knowledge, YSZ coatings with good thermal shock resistance and a thermal conductivity of 0.81$W\cdot(m\cdot K)^{-1}$ at 1100°C were successfully prepared.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Shanghai Institute of Ceramics Chinese Academy of Sciences, VTT Technical Research Centre of Finland
Contributors: Song, X., Liu, Z., Suhonen, T., Varis, T., Huang, L., Zheng, X., Zeng, Y.
Number of pages: 7
Pages: 132-138
Publication date: 25 May 2015
Peer-reviewed: Yes

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Journal: Surface and Coatings Technology
Volume: 270
ISSN (Print): 0257-8972
Ratings:

Scopus rating (2015): CiteScore 3.9 SJR 0.852 SNIP 1.376
Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Air plasma spraying, Columnar grains, Thermal conductivity, Thermal shock resistance, YSZ coatings
DOIs:

10.1016/j.surfcoat.2015.03.011
URLs:

http://www.scopus.com/inward/record.url?scp=84927174189&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84927174189
Research output: Contribution to journal › Article › Scientific › peer-review

Fabrication and Characterization of Amorphous Alumina-Yttria-Stabilized Zirconia Coatings by Air Plasma Spraying

Almost fully amorphous coatings of near-eutectic alumina-yttria-stabilized zirconia (Al_2O_3-YSZ) were prepared by air plasma spraying using $Al_2O_3$and 8 mol.% YSZ crystalline-mixed powders. The coatings consist of mostly an amorphous phase with a small amount of nanocrystals. Various characterization techniques were used to understand coating formation and the origins of the different phases within the coatings. The formation of the mostly amorphous structure is attributed to the high glass-forming ability of Al_2O_3-YSZ and the appropriate plasma spraying conditions. A small number of nanocrystals are produced during crystallization of the incoming molten droplets or by recrystallization of the solidified splats by accumulated heat. Scanning electron microscopy shows that the coatings have a dense, layered structure with low porosity, and bright-field transmission electron microscopy images indicate sharp interface rather than grit-blasted wavy surface between splats and substrates in the coatings. The as-sprayed amorphous coatings crystallized at around 920 °C and micro-hardness of the as-sprayed amorphous coatings was 8.12 GPa.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Shanghai Institute of Ceramics Chinese Academy of Sciences, VTT Technical Research Centre of Finland
Contributors: Song, X., Suhonen, T., Varis, T., Huang, L., Zheng, X., Zeng, Y.
Number of pages: 10
Pages: 1302-1311
Publication date: 25 Nov 2014
Peer-reviewed: Yes

Publication information

Journal: Journal of Thermal Spray Technology
Volume: 23
Issue number: 8
ISSN (Print): 1059-9630
Ratings:

Scopus rating (2014): CiteScore 3.1 SJR 0.837 SNIP 1.681
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films
Keywords: alumina-yttria-stabilized zirconia, amorphous phases, atmospheric plasma spraying, micro-hardness, nanocrystals, thermal stability
DOIs:

10.1007/s11666-014-0124-z
URLs:

http://www.scopus.com/inward/record.url?scp=84919593683&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84919593683
Research output: Contribution to journal › Article › Scientific › peer-review

Thermally evaporated single-crystal Germanium on Silicon

Using conventional and polarization-dependent Raman spectroscopy we investigate the structural properties of Germanium films thermally evaporated on Silicon under various conditions. The analysis suggests that the Ge films can be crystalline, amorphous and poly-oriented, depending on the substrate temperature. We use both comparison with Raman spectra of Ge films grown on amorphous substrates and polarization-dependent Raman measurements to demonstrate that in the 250-450 °C interval, crystalline Ge films are epitaxial. This result is validated by means of large angle X-ray diffraction measurements. We employ these films to fabricate and characterize near infrared heterojunction photodiodes that exhibit high responsivities and low dark current densities.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, University “Roma Tre”, Università dell'Aquila, Nonlinear Optics and OptoElectronics Lab
Contributors: Sorianello, V., Colace, L., Nardone, M., Assanto, G.
Number of pages: 4
Pages: 8037-8040
Publication date: 1 Sep 2011
Peer-reviewed: Yes

Publication information

Journal: Thin Solid Films
Volume: 519

Issue number: 22
ISSN (Print): 0040-6090
Ratings:

Scopus rating (2011): CiteScore 3.4 SJR 0.995 SNIP 1.323
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Materials Chemistry, Metals and Alloys, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Germanium, Near infrared, Photodetectors, Raman characterization, Thermal evaporation
DOIs:

10.1016/j.tsf.2011.06.023
URLs:

http://www.scopus.com/inward/record.url?scp=80052110605&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 80052110605
Research output: Contribution to journal › Article › Scientific › peer-review

Influence of ionic liquids on the dielectric relaxation behavior of CNT based elastomer nanocomposites

The influence of an imidazolium type ionic liquid (IL) on the relaxation behavior of carbon-nanotube (CNT) based polychloroprene nanocomposites prepared by melt mixing has been investigated by broadband dielectric spectroscopy. It is demonstrated that the presence of the ionic liquid modifies the relaxation behavior of the pure rubber matrix and leads to a significant increase of the conductivity for the CNT/rubber composites. For the unfilled rubber, a distinct glass transition of the IL is observed for high concentrations demonstrating that the IL forms a separate phase. The increased conductivity of the CNT-filled rubber composites is related to a physical coupling between CNTs and rubber matrix mediated by IL leading to a better dispersion of the CNTs.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Deutsches Institut für Kautschuktechnologie e.V., Leibniz-Institut für Polymerforschung Dresden E.V., Technische Universität Dresden, Vodafone Department of Mobile Communications Systems
Contributors: Steinhauser, D., Subramaniam, K., Das, A., Heinrich, G., Klüppel, M.
Number of pages: 10
Pages: 927-936
Publication date: Nov 2012
Peer-reviewed: Yes

Publication information

Journal: Express Polymer Letters
Volume: 6
Issue number: 11
ISSN (Print): 1788-618X
Ratings:

Scopus rating (2012): CiteScore 3.2 SJR 0.915 SNIP 1.605
Original language: English
ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry, Chemical Engineering(all), Organic Chemistry, Physical and Theoretical Chemistry
Keywords: Dielectric spectroscopy, Ionic liquid, Nanocomposites, Relaxation dynamics, Rubber
DOIs:

10.3144/expresspolymlett.2012.98
URLs:

http://www.scopus.com/inward/record.url?scp=84866131281&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84866131281
Research output: Contribution to journal › Article › Scientific › peer-review

Cation-specific effects on enzymatic catalysis driven by interactions at the tunnel mouth

Cationic specificity which follows the Hofmeister series has been established for the catalytic efficiency of haloalkane dehalogenase LinB by a combination of molecular dynamics simulations and enzyme kinetic experiments. Simulations provided a detailed molecular picture of cation interactions with negatively charged residues on the protein surface, particularly at the tunnel mouth leading to the enzyme active site. On the basis of the binding affinities, cations were ordered as $Na^+ > K^+ > Rb^+ > Cs^+$. In agreement with this result, a steady-state kinetic analysis disclosed that the smaller alkali cations influence formation and productivity of enzyme-substrate complexes more efficiently than the larger ones. A subsequent systematic investigation of two LinB mutants with engineered charge in the cation-binding site revealed that

the observed cation affinities are enhanced by increasing the number of negatively charged residues at the tunnel mouth, and vice versa, reduced by decreasing this number. However, the cation-specific effects are overwhelmed by strong electrostatic interactions in the former case. Interestingly, the substrate inhibition of the mutant LinB L177D in the presence of chloride salts was 7 times lower than that of LinB wild type in glycine buffer. Our work provides new insight into the mechanisms of specific cation effects on enzyme activity and suggests a potential strategy for suppression of substrate inhibition by the combination of protein and medium engineering.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), International Clinical Research Center, St. Anne's University Hospital Brno, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Department of Experimental Biology, Research Centre for Toxic Compounds in the Environment, Masaryk University
Contributors: Štěpánková, V., Paterová, J., Damborský, J., Jungwirth, P., Chaloupková, R., Heyda, J.
Number of pages: 9
Pages: 6394-6402
Publication date: 30 May 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B
Volume: 117
Issue number: 21
ISSN (Print): 1520-6106
Ratings:

Scopus rating (2013): CiteScore 6.3 SJR 1.504 SNIP 1.195
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
DOIs:

10.1021/jp401506v
URLs:

http://www.scopus.com/inward/record.url?scp=84878363659&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84878363659
Research output: Contribution to journal › Article › Scientific › peer-review

Abrasion and compression resistance of liquid-flame-spray-deposited functional nanoparticle coatings on paper

General information
Publication status: Published
MoE publication type: A4 Article in a conference publication
Organisations: Department of Materials Science, Research group: Paper Converting and Packaging, Department of Physics, Research area: Aerosol Physics, Research group: Aerosol Synthesis, Engineering materials science and solutions (EMASS), Abo Akad Univ, Abo Akademi University, Dept Phys, Paper and Fibre Research Institute (PFI), SP Technical Research Institute of Sweden
Contributors: Stepien, M., Chinga-Carrasco, G., Saarinen, J. J., Teisala, H., Tuominen, M., Haapanen, J., Kuusipalo, J., Mäkelä, J. M., Toivakka, M.
Number of pages: 15
Pages: 68-82
Publication date: 2014

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Publisher: TAPPI Press
ISBN (Print): 9781510801295
ASJC Scopus subject areas: Materials Chemistry, Electrical and Electronic Engineering
URLs:

http://www.scopus.com/inward/record.url?scp=84942588921&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note
ORG=mol,0.5
ORG=fys,0.5
EXT="Tuominen, Mikko"
Source: Scopus

Source ID: 84942588921
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

Stimuli-responsive photonic polymer coatings

This feature article focuses on the highlights in the development of photonic polymer coatings that can change their volume or surface topology in a reversible, dynamic fashion when exposed to an external stimulus. Topographic response is established using hydrogels or liquid crystal polymer networks. By changing the surface corrugation in response to light various functional coating properties can be modulated, for instance wettability and/or mechanical friction. The same volume changes in photonic coatings caused by different stimuli lead to changes in light reflection.

General information

Publication status: Published
MoE publication type: A2 Review article in a scientific journal
Organisations: Eindhoven University of Technology
Contributors: Stumpel, J. E., Broer, D. J., Schenning, A. P. H. J.
Number of pages: 10
Pages: 15839-15848
Publication date: 28 Dec 2014
Peer-reviewed: Yes

Publication information

Journal: Chemical Communications
Volume: 50
Issue number: 100
ISSN (Print): 1359-7345
Ratings:

Scopus rating (2014): CiteScore 11.6 SJR 2.692 SNIP 1.427
Original language: English
ASJC Scopus subject areas: Chemistry(all), Catalysis, Ceramics and Composites, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Materials Chemistry, Metals and Alloys
DOIs:

10.1039/c4cc05072j
URLs:

http://www.scopus.com/inward/record.url?scp=84911908006&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note

EXT="Stumpel, Jelle"
Source: Scopus
Source ID: 84911908006
Research output: Contribution to journal › Review Article › Scientific › peer-review

Elastomer composites based on carbon nanotubes and ionic liquid

Carbon nanotubes (CNTs) are known for excellent electrical conductivity and high elastic modulus. But difficulties arise in realizing their potential in matrices due to their existence in the form of aggregates or agglomerates. A simplified mixing technique using ionic liquid (IL) was developed to improve the dispersion of CNTs in elastomers. At first, CNTswere modified using an IL, 1-butyl-3-methyl-imidazolium-bis-(trifluoromethylsulfonyl)-imide in a mortar and pestle, and later, the modified tubes were incorporated into elastomers using a two-roll mill. The effect of modified tubes and IL on polar polychloroprene and nonpolar solution styrene butadiene rubber is studied. Enhanced dispersion and networking of CNTs can be achieved using this technique, based on which highly conducting composites were developed. Moreover, the composites with modified CNTs exhibited higher mechanical properties (tensile modulus, hardness) and thermal stability than the composites with unmodified CNTs. ILs are also found to have multifunctional roles (as antioxidants, as coupling agents) in the composites. The applications of composites with a particular focus on actuators and sensors are also discussed.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Vodafone Department of Mobile Communications Systems, Leibniz-Institut für Polymerforschung Dresden E.V.
Contributors: Subramaniam, K., Das, A., Stöckelhuber, K. W., Heinrich, G.
Number of pages: 34
Pages: 367-400
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Rubber Chemistry and Technology
Volume: 86
Issue number: 3
ISSN (Print): 0035-9475
Ratings:

Scopus rating (2013): CiteScore 1.6 SJR 0.442 SNIP 1.266
Original language: English
ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry
DOIs:

10.5254/rct.13.86984
URLs:

http://www.scopus.com/inward/record.url?scp=84904014953&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84904014953
Research output: Contribution to journal › Article › Scientific › peer-review

Highly conducting polychloroprene composites based on multi-walled carbon nanotubes and 1-butyl 3-methyl imidazolium bis(trifluoromethylsulphonyl)imide
Highly conducting flexible polychloroprene composites are prepared based on a novel mixing technique using ionic liquid (IL) modified multi-walled carbon nanotubes (MWCNTs). A conductivity of 0.1 S/cm is achieved for composites even at a low concentration of the tubes (5 phr). Extremely fine dispersion and a strong tube-tube networking of modified carbon nanotubes (M-CNTs), which are responsible for such high conductivity of the composites, are understood from transmission electron microscopy and amplitude sweep measurements. Several interesting applications can be visualised using these conducting composites: as a substrate for electronic circuits, and as an excellent construction material.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V.
Contributors: Subramaniam, K., Das, A., Heinrich, G.
Number of pages: 3
Pages: 44-46
Publication date: Jul 2012
Peer-reviewed: Yes

Publication information
Journal: KGK: KAUTSCHUK GUMMI KUNSTSTOFFE
Volume: 65
Issue number: 7-8
ISSN (Print): 0948-3276
Ratings:

Scopus rating (2012): CiteScore 0.7 SJR 0.235 SNIP 0.559
Original language: English
ASJC Scopus subject areas: Mechanical Engineering, Polymers and Plastics, Industrial and Manufacturing Engineering, Materials Chemistry
URLs:

http://www.scopus.com/inward/record.url?scp=84865498333&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84865498333
Research output: Contribution to journal › Article › Scientific › peer-review

Enhanced thermal stability of polychloroprene rubber composites with ionic liquid modified MWCNTs
Thermal degradation of polychloroprene rubber (CR) composites based on unmodified and ionic liquid modified multi-walled carbon nanotubes (MWCNTs) is studied using thermogravimetric analysis (TGA) in aerobic and anaerobic (nitrogen) conditions. The CR and its composites exhibit three stage and four stage degradation in nitrogen and air respectively. The presence of unmodified CNTs alone does not improve the thermal stability of composites to a great extent whereas a reasonable enhancement is observed in case of modified CNTs/CR composites which can be attributed to the interfacial interactions of ionic liquid/modified tubes with CR and to the fine dispersion of modified tubes in CR. The degradation products of CR and its composites were analysed using pyrolysis-gas chromatography-mass spectrometry (Py-GC-MS) and the mechanism of degradation is discussed. Non-isothermal degradation kinetics were studied using Kissinger and Flynn-Wall-Ozawa methods and the activation energy of thermal decomposition is found to be high for modified CNTs/CR composites. Isothermal degradation of modified CNTs/CR composites at 290°C for 30 min in nitrogen reveals decreased weight loss (14%) as opposed to CR (31%) and unmodified CNTs/CR composites (30%). The combustion behaviour of the composites was dealt using microscale combustion calorimeter (MCC) and the flame

retardancy of the composites is discussed.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V. , Vodafone Department of Mobile Communications Systems
Contributors: Subramaniam, K., Das, A., Häußler, L., Harnisch, C., Stöckelhuber, K. W., Heinrich, G.
Number of pages: 10
Pages: 776-785
Publication date: May 2012
Peer-reviewed: Yes

Publication information
Journal: Polymer Degradation and Stability
Volume: 97
Issue number: 5
ISSN (Print): 0141-3910
Ratings:

Scopus rating (2012): CiteScore 5 SJR 1.411 SNIP 2.079
Original language: English
ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry, Mechanics of Materials, Condensed Matter Physics
Keywords: Carbon nanotubes, Elastomeric composites, Ionic liquids, Polychloroprene rubber, Thermal degradation, Thermal stability
DOIs:

10.1016/j.polymdegradstab.2012.02.001
URLs:

http://www.scopus.com/inward/record.url?scp=84859216596&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84859216596
Research output: Contribution to journal › Article › Scientific › peer-review

Erosion wear of vinylester matrix composites in aqueous and acidic environments at elevated temperatures
Slurry erosion wear performance of glass fibre reinforced vinylester composite (FRP) has been studied using a pilot-scale erosion test apparatus. Tests were conducted at elevated temperatures in aqueous and acidic environments. When using fine quartz as an abrasive material, FRP showed higher mass losses in the aqueous environment than in the acidic conditions, especially at higher temperatures. In this case, the FRP degradation was governed by the penetration of the used medium into the FRP structure. According to the absorption studies, the weight gain of the laminate was more pronounced in the water immersion compared to the acidic solution, which can be a prediction of an increased degradation rate and explain the higher wear in the aqueous medium. When the abrasive material was changed from fine to coarse quartz, the removal of the shielding matrix phase was extensive and a direct route for the acidic solution to the fibres was created causing more severe damage. This was also shown in scanning electron microscopy (SEM) studies, where the samples tested in the acidic solution showed extensive fibre flattening along the erosion flux. By increasing the test temperature close to the boiling point of the medium, an increase in the FRP wear could be seen. The increase in the rotation speed, on the other hand, did not automatically mean higher mass losses. This shows that the wear environment in the present test device is highly complicated with several interrelated parameters affecting the results.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Outotec Research Center
Contributors: Suihkonen, R., Lindgren, M., Siljander, S., Sarlin, E., Vuorinen, J.
Number of pages: 10
Pages: 7-16
Publication date: 15 Jul 2016
Peer-reviewed: Yes

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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces and Interfaces, Materials Chemistry, Surfaces, Coatings and Films, Mechanics of Materials
Keywords: Erosion testing, Erosion-corrosion, Polymer-matrix composite, Slurry erosion
DOIs:
10.1016/j.wear.2016.03.026

Bibliographical note
EXT="Lindgren, Mari"
Source: Scopus
Source ID: 84962767507
Research output: Contribution to journal › Article › Scientific › peer-review

Simultaneous removal of tetrathionate and copper from simulated acidic mining water in bioelectrochemical and electrochemical systems
This study demonstrates (bio)electrochemical tetrathionate ($S_4O_6^{2-}$) degradation with simultaneous elemental copper recovery from simulated acidic mining water. The effect of applied external voltage on anodic tetrathionate removal, cathodic copper removal and current density was studied using two-chamber flow-through bioelectrochemical (MEC) and abiotic electrochemical (EC) systems. At low applied cell voltages (≤ 0.5 V), the highest tetrathionate removal rate (150–170 mg L^{-1} d^{-1}) and average current density (15–30 mA m^{-2}) was obtained with MEC. At applied external voltages above 0.75 V, abiotic EC provided the highest average current density (410–3600 mA m^{-2}). In bioelectrochemical systems, the current generation likely proceeds via intermediary reaction products (sulfide and/or thiosulfate), while in electrochemical system tetrathionate is oxidized directly on the electrode. The copper removal rates remained low (< 10 mg L^{-1} d^{-1}) in all systems at applied cell voltages below 0.5 V, but increased up to a maximum of 440 mg L^{-1} d^{-1} in MEC and to 450 mg L^{-1} d^{-1} in EC at applied cell voltage of 1.5 V. After seven days of operation at applied cell voltage of 1.5 V, copper removal efficiency was 99.9% in both MEC and EC and the average tetrathionate removal rates were 160 mg L^{-1} d^{-1} and 190 mg L^{-1} d^{-1}, respectively. This study shows that by applying external voltage, tetrathionate and copper can be efficiently removed from acidic waters with bioelectrochemical and electrochemical systems.

General information
Publication status: Unpublished
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy
Contributors: Sulonen, M. L., Kokko, M. E., Lakaniemi, A., Puhakka, J. A.
Number of pages: 10
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Publication date: 2018
Peer-reviewed: Yes
Early online date: Feb 2018

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Journal: Hydrometallurgy
Volume: 176
ISSN (Print): 0304-386X
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Scopus rating (2018): CiteScore 5.7 SJR 1.014 SNIP 1.852
Original language: English
ASJC Scopus subject areas: Industrial and Manufacturing Engineering, Metals and Alloys, Materials Chemistry
Keywords: Bioelectrochemical system, Copper removal, Electrochemical system, Reduced inorganic sulfur compound, Tetrathionate
DOIs:
10.1016/j.hydromet.2018.01.023
Source: Scopus
Source ID: 85041488580
Research output: Contribution to journal › Article › Scientific › peer-review

Process time importance in the product properties evolvement during extrusion coating of different LDPE grades
Process time in air gap region is one of the most important variables in the coating property development, when the molten polymer is moving from the die exit into the nip region in extrusion coating. Coating property evolvement of different LDPE grades are presented in the paper. The importance of the throughput rate and line speed to the process times is discussed by considering the effect of molecular structure of different polyolefins. The draw down ratio based on the grammage measurements is proposed to use in the practical situations.

General information
Publication status: Published
MoE publication type: A4 Article in a conference publication
Organisations: Materials Science, Research group: Paper Converting and Packaging
Contributors: Suokas, E., Kuusipalo, J.
Number of pages: 9
Pages: 151-159
Publication date: 1 Jan 2018

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Publisher: TAPPI Press
ISBN (Electronic): 9781510871885
ASJC Scopus subject areas: Media Technology, Materials Chemistry, Surfaces, Coatings and Films
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Source: Scopus
Source ID: 85059262851
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

Solvothermal synthesis derived Co-Ga codoped ZnO diluted magnetic degenerated semiconductor nanocrystals
Here we are reporting solvothermal synthesis derived diluted magnetic and plasmonic Co-Ga co-doped ZnO nanocrystals with high magnetization values (from 1.02 to 4.88 emu/g) at room temperature. Co-Ga co-doped ZnO nanocrystals show up to 2 fold increase in saturation magnetization compared to Co doped ZnO nanocrystals at the same Co concentration, with the observed room temperature magnetization higher than previously reported values for multifunctional magnetic and plasmonic nanocrystals, and the effect of Ga suggesting some role of the correspondingly introduced itinerant charge. While at the lowest Ga content the nanoparticles appear homogeneously doped, we note that already a moderate Ga content of several percent triggers a fraction of Co to segregate in metallic form in the bulk of the nanoparticles. However, the amount of segregated Co is not sufficient to account for the total effect, whereas a dominating contribution to the observed magnetism has to be related to itinerant charge mediated exchange interactions.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Photonics, Institute of Physics, University of Tartu, Riga Technical University, University of Turku, Helmholtz Centre Berlin for Materials and Energy, University of Latvia, RMS Foundation, Institute of Solid State Physics University of Latvia
Contributors: Šutka, A., Käämbre, T., Joost, U., Kooser, K., Kook, M., Duarte, R. F., Kisand, V., Maiorov, M., Döbelin, N., Smits, K.
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Original language: English
ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Metals and Alloys, Materials Chemistry
Keywords: Degenerated semiconductors, Diluted magnetic semiconductors, Doping, Plasmonic nanocrystals, Solvothermal synthesis, ZnO
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Bibliographical note
int=fot,"Joost, Urmas"
Source: Scopus
Source ID: 85048730804
Research output: Contribution to journal › Article › Scientific › peer-review

Fluorine losses in Er^{3+} oxyfluoride phosphate glasses and glass-ceramics

Er^{3+} doped phosphate glasses with the composition $75NaPO_3$-$25CaF_2$ (mol%) were prepared at different melting temperatures to demonstrate the importance to quantify the fluorine content when preparing oxyfluoride glasses. Indeed, increasing the melting temperature from 900 to 1000 °C leads to a small reduction in the fluorine content from 9.4 at % to 8.8 at % as quantified using EPMA. Whereas this loss of fluorine can be suspected from small changes in the thermal properties of the glass, it increases significantly the glass crystallization tendency in this glass system. This means that a heat treatment of the as-prepared glass should be performed when evaporation of fluorine during the glass melting is suspected. Sample preparation for the characterization of the spectroscopic properties of the glasses is discussed here as well; bulk glasses should be used when measuring the spectroscopic properties of oxyfluoride glasses, which are known to be hygroscopic. It is shown, in this work, that a heat treatment of the glass within the investigated glass system leads to transparent glass-ceramics with volume precipitation of Er^{3+} doped CaF_2 crystals with strong upconversion.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Research group: Materials Characterization, Materials Science and Environmental Engineering, Physics, Tampere University of Applied Sciences, Fondazione LINKS – Leading Innovation & Knowledge for Society
Contributors: Szczodra, A., Mardoukhi, A., Hokka, M., Boetti, N. G., Petit, L.
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Publication date: 15 Aug 2019
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Original language: English
ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Metals and Alloys, Materials Chemistry
Keywords: Crystal, Erbium, Fluorine, Glass, Glass-ceramic, Luminescence
DOIs:
10.1016/j.jallcom.2019.05.151
Source: Scopus
Source ID: 85065824926
Research output: Contribution to journal › Article › Scientific › peer-review

Structure and in vitro dissolution of Mg and Sr containing borosilicate bioactive glasses for bone tissue engineering

Borosilicate bioactive glasses are promising for bone tissue engineering. The objective was to assess the impact of magnesium and/or strontium, when substituted for calcium on the glasses' thermal and dissolution properties. Both Mg and Sr substitution appeared to enhance the hot forming domain, i.e. the ability to hot process (sinter, draw fibres) without adverse crystallization. Structural analysis indicated that substitution of MgO and/or SrO for CaO results in changes in the BO_3/BO_4 ratio as well as in the ratio between bridging and non-bridging oxygen atoms in the silicate structure. Additionally, a de-shielding effect was noticed when Ca, Mg and Sr are present together in the glass network, possibly owing to PO_4^{3-} charge-balanced preferentially by Na^+. The Mg and/or Sr substitution resulted in a lower ion release in simulated body fluid and delayed formation of hydroxyapatite. However, once this layer formed it consisted of a Mg/Sr-substituted apatite. This work highlights the effect of combined ionic substitutions on bioactive glass structure and properties.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: BioMediTech, Research group: Biomaterials and Tissue Engineering Group, Friedrich-Schiller-University Jena, Universite de Rennes
Contributors: Tainio, J. M., Salazar, D. A. A., Nommeots-Nomm, A., Roiland, C., Bureau, B., Neuville, D. R., Brauer, D. S., Massera, J.
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Publication information

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ISSN (Print): 0022-3093
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ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Ceramics and Composites, Condensed Matter Physics, Materials Chemistry
Keywords: Bioactive glasses, Borosilicate glasses, In vitro dissolution, Structural properties, Tissue engineering
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Source ID: 85078095947
Research output: Contribution to journal › Article › Scientific › peer-review

Energetic origin of proton affinity to the air/water interface

Recent experimental and theoretical studies showed the preference of the hydronium ion for the vapor/water interface. To investigate the mechanism responsible for the surface propensity of this ion, we performed a series of novel quantum chemical simulations combined with the theory of solutions. The solvation free energy of the H_3O^+ solute placed at the interface was obtained as -97.9 kcal/mol, being more stable by 3.6 kcal/mol than that of the solute embedded in the bulk. Further, we decomposed the solvation free energies into contributions from the water molecules residing in the oxygen and the hydrogen sides of the solute to clarify the origin of the surface preference. When the solute was displaced from the bulk to the interface, it was shown that the free energy contribution from the oxygen side is destabilized by ~10 kcal/mol because of a reduction of the number of surrounding solvent water molecules. It was observed, however, that the free energy contribution due to the hydrogen side of the solute is unexpectedly stabilizing and surpasses the destabilization in the opposite side. We found that the stabilization in the hydrogen side originates from the solute-solvent interaction in the medium range beyond the nearest neighbor. It was also revealed that the free energy contribution due to the solute's electronic polarization amounts to about the half of the total free energy change associated with the solute displacement from the bulk to the interface.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Tohoku University, Osaka University, Kyoto Women's University, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Japan Science and Technology Agency
Contributors: Takahashi, H., Maruyama, K., Karino, Y., Morita, A., Nakano, M., Jungwirth, P., Matubayasi, N.
Number of pages: 7
Pages: 4745-4751
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Journal: Journal of Physical Chemistry Part B
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Scopus rating (2011): CiteScore 6.3 SJR 1.801 SNIP 1.213
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
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http://www.scopus.com/inward/record.url?scp=79955461660&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 79955461660
Research output: Contribution to journal › Article › Scientific › peer-review

Immobilized bioactive agents onto polyurethane surface with heparin and phosphorylcholine group

Heparin (HEP) and phosphorylcholine groups (PC) were grafted onto the polyurethane (PU) surface in order to improve biocompatibility and anticoagulant activity. After the surface grafting sites of PU were amplified with the primary amine groups of polyethylenimine (PEI), heparin was covalently linked onto the surface by the reaction between the amino group and the carboxyl group. PC groups were covalently immobilized on the PU-PEI surface through the reaction between the amino group and the aldehyde group of phosphorylcholine glyceraldehyde (PCGA). The surface density of primary amine groups was determined by a ninhydrin assay. The amino group density reached a maximum of 0.88 μmol/cm^2 upon incorporation of 10 wt% PEI. The amount of heparin covalently immobilized on the PU-PEI surface was determined by the toluidine blue method. The grafting chemistry resulted in the comparatively dense immobilization of HEP (2.6 μg/cm^2) and PC to the PU-PEI surfaces. The HEP and PC modified surfaces were characterized by water uptake (PU 0.15 mg/cm^2,

PU-PEI 3.54 mg/cm^2, PU-HEP 2.04 mg/cm^2, PU-PC 2.38 mg/cm^2), water contact angle (PU 95.3, PU-PEI 34.0, PU-HEP 39.5, PU-PC 37.2), attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR), X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and scanning electron microscope (SEM). The results demonstrated that the PUPEI surface was successfully grafted with HEP and PC. The hydrophilicity and hemocompatibility of these grafted surfaces were significantly improved. These results suggested that the PU-HEP and PU-PC composite films are promising candidates for blood contacting tissue engineering.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Tianjin University, Shihezi University, School of Chemical Engineering and Technology, Tianjin Chest Hospital
Contributors: Tan, M., Feng, Y., Wang, H., Zhang, L., Khan, M., Guo, J., Chen, Q., Liu, J.
Number of pages: 9
Pages: 541-549
Publication date: May 2013
Peer-reviewed: Yes

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Journal: Macromolecular Research
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Issue number: 5
ISSN (Print): 1598-5032
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Original language: English
ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Chemical Engineering(all)
Keywords: hemocompatibility, heparin, phosphorylcholine group, polyethylenimine, polyurethane
DOIs:

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http://www.scopus.com/inward/record.url?scp=84877763417&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84877763417
Research output: Contribution to journal › Article › Scientific › peer-review

Processable aromatic polyesters based on bisphenol derived from cashew nut shell liquid: synthesis and characterization
A new bisphenol viz., 4-(4-hydroxyphenoxy)-3-pentadecylphenol (HPPDP) was synthesized starting from cashew nut shell liquid (CNSL). Aromatic (co)polyesters containing ether linkages in the main chain and pendent pentadecyl chains were synthesized by the interfacial polycondensation of HPPDP with terephthalic acid chloride (TPC), isophthalic acid chloride (IPC) and a mixture of TPC and IPC (50:50 mol %) and by polycondenation of varying composition of HPPDP and bisphenol-A (BPA) with TPC. The resultant (co)polyesters exhibited inherent viscosities in the range 0.70–1.21 dL g^{-1} and number-average molecular weights in the range 16,000–48,200 (GPC, polystyrene standard). Polyesters were soluble in common organic solvents such as chloroform and dichloromethane and could be cast into films from chloroform solution. Polyesters exhibited T_{10} values in the range 430–455 °C and Tg values were in the range 29–202 °C. Dynamic mechanical storage modulus and maximum on transition of tan δ curve decreased with increased content of HPPDP in copolyesters. Importantly, the large difference between Tg and T_{10} values offers the possibility to process these polyesters in the melt.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: CSIR-National Chemical Laboratory, Polymer Science and Engineering Division
Contributors: Tawade, B. V., Salunke, J. K., Sane, P. S., Wadgaonkar, P. P.
Publication date: 18 Nov 2014
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Publication information
Journal: JOURNAL OF POLYMER RESEARCH
Volume: 21
Issue number: 12
ISSN (Print): 1022-9760
Ratings:

Scopus rating (2014): CiteScore 3.3 SJR 0.666 SNIP 0.917

Original language: English
ASJC Scopus subject areas: Materials Chemistry, Polymers and Plastics, Organic Chemistry
Keywords: Aromatic polyesters, Cashew nut shell liquid, Pentadecyl, Polycondensation, Processability, Thermal properties
DOIs:

10.1007/s10965-014-0617-y
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Bibliographical note
EXT="Salunke, Jagadish"
Research output: Contribution to journal › Article › Scientific › peer-review

Molecular Design of Light-Responsive Hydrogels, for in Situ Generation of Fast and Reversible Valves for Microfluidic Applications
Reversible light-responsive hydrogel valves with response characteristics compatible for microfluidics have been obtained by optimization of molecular design of spiropyran photoswitches and gel composition. Self-protonating gel formulations were exploited, wherein acrylic acid was copolymerized in the hydrogel network as an internal proton donor, to achieve a swollen state of the hydrogel in water at neutral pH. Light-responsive properties were endowed upon the hydrogels by copolymerization of spiropyran chromophores, using electron withdrawing and donating groups to tune the gel-swelling and shrinkage behavior. In all cases, the shrinkage was determined by the water diffusion rate, while for the swelling the isomerization kinetics is the rate-determining step. For one hydrogel, reversible and reproducible volume changes were observed. Finally, gel-valves integrated within microfluidic channels were fabricated, allowing reversible and repeatable operation, with opening and closing of the valve in minutes.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Eindhoven University of Technology, Dublin City University
Contributors: Ter Schiphorst, J., Coleman, S., Stumpel, J. E., Ben Azouz, A., Diamond, D., Schenning, A. P. H. J.
Number of pages: 7
Pages: 5925-5931
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Peer-reviewed: Yes

Publication information
Journal: Chemistry of Materials
Volume: 27
Issue number: 17
ISSN (Print): 0897-4756
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Scopus rating (2015): CiteScore 12.8 SJR 3.958 SNIP 2.038
Original language: English
ASJC Scopus subject areas: Materials Chemistry, Chemical Engineering(all), Chemistry(all)
DOIs:

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URLs:

http://www.scopus.com/inward/record.url?scp=84941088068&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84941088068
Research output: Contribution to journal › Article › Scientific › peer-review

Development and application of HVOF sprayed spinel protective coating for SOFC interconnects
Protective coatings are needed for metallic interconnects used in solid oxide fuel cell (SOFC) stacks to prevent excessive high-temperature oxidation and evaporation of chromium species. These phenomena affect the lifetime of the stacks by increasing the area-specific resistance (ASR) and poisoning of the cathode. Protective $MnCo_2O_4$ and $MnCo_{1.8}Fe_{0.2}O_4$ coatings were applied on ferritic steel interconnect material (Crofer 22 APU) by high velocity oxy fuel spraying. The substrate-coating systems were tested in long-term exposure tests to investigate their high-temperature oxidation behavior. Additionally, the ASRs were measured at 700 C for 1000 h. Finally, a real coated interconnect was used in a SOFC single-cell stack for 6000 h. Post-mortem analysis was carried out with scanning electron microscopy. The deposited coatings reduced significantly the oxidation of the metal, exhibited low and stable ASR and reduced effectively the migration of chromium.

General information
Publication status: Published

MoE publication type: A2 Review article in a scientific journal
Organisations: Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland
Contributors: Thomann, O., Pihlatie, M., Rautanen, M., Himanen, O., Lagerbom, J., Mäkinen, M., Varis, T., Suhonen, T., Kiviaho, J.
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Publication date: Jun 2013
Peer-reviewed: Yes

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Journal: Journal of Thermal Spray Technology
Volume: 22
Issue number: 5
ISSN (Print): 1059-9630
Ratings:

Scopus rating (2013): CiteScore 3 SJR 0.933 SNIP 1.366
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films
Keywords: ASR, HVOF spraying, interconnect, protective coating, SOFC, spinel, stack testing
DOIs:

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URLs:

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Source: Scopus
Source ID: 84878626773
Research output: Contribution to journal › Review Article › Scientific › peer-review

Nonlinear Optical Properties of Fluorescent Dyes Allow for Accurate Determination of Their Molecular Orientations in Phospholipid Membranes
Several methods based on single- and two-photon fluorescence detected linear dichroism have recently been used to determine the orientational distributions of fluorescent dyes in lipid membranes. However, these determinations relied on simplified descriptions of nonlinear anisotropic properties of the dye molecules, using a transition dipole-moment-like vector instead of an absorptivity tensor. To investigate the validity of the vector approximation, we have now carried out a combination of computer simulations and polarization microscopy experiments on two representative fluorescent dyes (DiI and F2N12S) embedded in aqueous phosphatidylcholine bilayers. Our results indicate that a simplified vector-like treatment of the two-photon transition tensor is applicable for molecular geometries sampled in the membrane at ambient conditions. Furthermore, our results allow evaluation of several distinct polarization microscopy techniques. In combination, our results point to a robust and accurate experimental and computational treatment of orientational distributions of DiI, F2N12S, and related dyes (including Cy3, Cy5, and others), with implications to monitoring physiologically relevant processes in cellular membranes in a novel way.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Lawrence Berkeley National Laboratory, Department of Cybernetics, Faculty of Applied Sciences, University of West Bohemia, Institute of Nanobiology and Structural Biology GCRC, V.v.i., Academy of Sciences of the Czech Republic, University of South Bohemia
Contributors: Timr, Š., Brabec, J., Bondar, A., Ryba, T., Železný, M., Lazar, J., Jungwirth, P.
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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
DOIs:

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Bibliographical note
EXT="Bondar, Alexey"
Source: Scopus
Source ID: 84938277609
Research output: Contribution to journal › Article › Scientific › peer-review

Wear of cemented tungsten carbide percussive drill–bit inserts: Laboratory and field study
Design of the drill–bit and selection of the Cemented Tungsten Carbide (CC) grade for drill–bit inserts are crucial for efficient percussive drilling. This study presents the results of an experimental campaign executed with the aim to identify the distinctive wear mechanisms and behaviour of different CC grades. Three laboratory and one full–scale drilling tests were performed using nine CC grades with different binder contents, binder chemical compositions, mean tungsten carbide (WC) grain sizes, and grain size distributions. Wear traces found on the drill–bit inserts after the full–scale drilling test show noticeable differences depending on their position on the drill–bit. Tensile forces present on the leading edge of the inserts due to the sliding contact with rock are suspected to play a significant role. Laboratory tests performed include: (i) single impact tests using a modified Split Hopkinson Pressure Bar (SHPB) apparatus, (ii) Abrasion Value (AV) rotating disk tests, and (iii) impact abrasion (LCPC) tests. Volume loss and shape change were used as macroscopic measures of wear. Greater volume losses were found for the grades with nickel–based binders compared to those with pure cobalt binder. The use of a narrower WC grain size distribution leads to lesser volume loss in drilling and AV tests. Surface analysis of the damaged microstructure was performed using scanning electron microscope. Distinct meso–scale (few dozens of WC grain sizes) patterns of damaged microstructure zones surrounded by the intact surface were found on the surfaces of specimens after single impact test. The pattern indicates the potential influence of a non–uniform contact due to the rock roughness and internal rock heterogeneities, which is supported by the study of the rock crater roughness. Size of such zones could be seen as a certain length–scale, which determines the insert–rock contact behaviour. A specific “peeling” mechanism of material removal was observed in the full–scale drilling test, where portion of the CC microstructure fused with the rock tribofilm gets removed when that tribofilm peels off.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Materials Characterization, Norwegian Univ. of Sci. and Technol., Materials and Nanotechnology, CNRS UMR 7633, Im Schleeke, Rock Tools
Contributors: Tkalich, D., Li, C. C., Kane, A., Saai, A., Tkalich, D., Yastrebov, V. A., Hokka, M., Kuokkala, V., Bengtsson, M., From, A.
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Cemented tungsten carbide, Contact area, Impact abrasion, Rotary–percussive drilling, Roughness, SEM, Sliding abrasion, Split Hopkinson pressure bar, Surface deterioration mechanisms, Volume loss, Wear
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Source: Scopus
Source ID: 85020872795
Research output: Contribution to journal › Article › Scientific › peer-review

Unintentional boron contamination of MBE-grown GaInP/AlGaInP quantum wells
The effects of unintentional boron contamination on optical properties of GaInP/AlGaInP quantum well structures grown by molecular beam epitaxy (MBE) are reported. Photoluminescence and secondary-ion mass spectrometry (SIMS) measurements revealed that the optical activity of boron-contaminated quantum wells is heavily affected by the amount of boron in GaInP/AlGaInP heterostructures. The boron concentration was found to increase when cracking temperature of the phosphorus source was increased. Boron incorporation was enhanced also when aluminum was present in the

material.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Optoelectronics Research Centre, Research group: Semiconductor Technology and Applications, Frontier Photonics, VTT Technical Research Centre of Finland
Contributors: Tukiainen, A., Likonen, J., Toikkanen, L., Leinonen, T.
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Peer-reviewed: Yes

Publication information
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Volume: 425
ISSN (Print): 0022-0248
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Scopus rating (2015): CiteScore 3.3 SJR 0.686 SNIP 1.066
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Materials Chemistry, Inorganic Chemistry
Keywords: A1. Defects, A1. Impurities, A3. Molecular beam epitaxy, B1. Phosphides, B2. Semiconducting III-V materials
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URLs:

http://www.sciencedirect.com/science/article/pii/S0022024815001384 (Link to paper in Sciencedirect)
Source: Scopus
Source ID: 84951561374
Research output: Contribution to journal › Article › Scientific › peer-review

Microstructural and abrasion wear characteristics of laser-clad tool steel coatings
Several different tool steel grades were deposited on mild steel by the laser-cladding process with coaxial powder feeding. With bidirectional scanning pattern, most of the grades were deposited crack-free with hardness up to 1000 HV without additional preheating. In a 3-body abrasion wear study, the laser clad Ralloy® WR6 with significant portion of retained austenite exhibited superior abrasive wear resistance compared with the predominantly martensitic tool steel coatings (M2, M4, H13, HS-23, HS-30) and the reference material, Raex® Ar500 wear resistant steel. The abrasion wear resistance of austenitic–martensitic WR6 tool steel was further enhanced by the external addition of 20% volume percentage of relatively large (45–106 μm) vanadium carbides. In single point scratch tests, predominantly martensitic tool steels outperformed austenitic–martensitic tool steels and wear resistant steel. The differences in wear performances were explained by different wear mechanisms and types of contact between the abrasive and the surface.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Surface Engineering, Technology Centre Ketek Ltd.
Contributors: Tuominen, J., Näkki, J., Pajukoski, H., Hyvärinen, L., Vuoristo, P.
Number of pages: 11
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Publication date: 2016
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Scopus rating (2016): CiteScore 2.1 SJR 0.424 SNIP 0.754
Original language: English
ASJC Scopus subject areas: Surfaces and Interfaces, Condensed Matter Physics, Materials Chemistry, Surfaces, Coatings and Films, Conservation
Keywords: 3-Body abrasion wear, Laser cladding, Metal matrix composite, Scratch test, Tool steel, Wear resistant steel
DOIs:

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Bibliographical note

EXT="Näkki, J."
INT=mol,"Pajukoski, H."
Source: Scopus
Source ID: 84978499771
Research output: Contribution to journal › Article › Scientific › peer-review

Optimised selection of new protective coatings for biofuel boiler applications

Using biofuels in power and CHP boilers can pose a challenge for materials performance. Formation of deposits containing e.g. potassium, sulphur, calcium, sodium, and chlorine can result in severe corrosion of conventional steels and alloys at relatively modest temperatures. Given suitable component design and fabrication facilities, coatings may be considered to protect the fireside surfaces. This paper aims to present a systematic approach to the design and selection criteria for protective coatings of boilers. The approach includes modelling of the process and surface conditions, optimisation of the coating process and structure, and performance validation in the laboratory and plant scales. The applied examples have included iron and nickel based HVOF and arc sprayed coatings subjected to verification field testing in boiler testing under aggressive biofuel conditions. The coatings have shown good corrosion resistance in both laboratory tests and long-term harsh field tests. The paper discusses the used approach for finding a suitable and cost effective coating for biofuel boiler applications. The paper gives test results from microstructural, corrosion resistance and field testing experience for the selected coatings.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland
Contributors: Tuurna, S., Varis, T., Penttilä, K., Ruusuvuori, K., Holmström, S., Yli-Olli, S.
Number of pages: 8
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Publication date: Jul 2011
Peer-reviewed: Yes

Publication information

Journal: Materials and Corrosion-Werkstoffe und Korrosion
Volume: 62
Issue number: 7
ISSN (Print): 0947-5117
Ratings:

Scopus rating (2011): CiteScore 1.7 SJR 0.603 SNIP 1.109
Original language: English
ASJC Scopus subject areas: Environmental Chemistry, Mechanics of Materials, Mechanical Engineering, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
Keywords: biofuel boiler, coating performance, life extension, protection
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URLs:

http://www.scopus.com/inward/record.url?scp=79960241231&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 79960241231
Research output: Contribution to journal › Article › Scientific › peer-review

Entrapped Styrene Butadiene Polymer Chains by Sol-Gel-Derived Silica Nanoparticles with Hierarchical Raspberry Structures

A sol-gel transformation of liquid silica precursor to solid silica particles was carried out in a one-pot synthesis way, where a solution of styrene butadiene elastomer was present. The composites, thus produced, offered remarkable improvements of mechanical and dynamic mechanical performances compared to precipitated silica. The morphological analysis reveals that the alkoxy-based silica particles resemble a raspberry structure when the synthesis of the silica was carried out in the presence of polymer molecules and represent a much more open silica-network structure. However, in the absence of the polymer, the morphology of the silica particles is found to be different. It is envisaged that the special morphology of the in situ synthesized silica particles contributes to the superior reinforcement effects, which are associated with a strong silica-rubber interaction by rubber chains trapped inside the raspberry-like silica aggregates. Therefore, the interfaces are characterized in detail by low-field solid-state ^{1}H NMR spectroscopy, ^{29}Si solid-state NMR spectroscopy, and energy-dispersive X-ray spectroscopy. Low-field ^{1}H NMR-based double-quantum experiments provide a quantitative information about the cross-link density of the silica-filled rubber composites and about the influence of silane coupling agent on the chemical cross-link density of the network and correlates well with equilibrium swelling measurements. The special microstructure of the alkoxy-based silica was found to be associated with the interaction between alkoxy-based silica and rubber chains as a consequence of particle growth in the presence of rubber chains.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Leibniz-Institut für Polymerforschung Dresden E.V., Vodafone Department of Mobile Communications Systems, Martin-Luther-Universität Halle-Wittenberg
Contributors: Vaikuntam, S. R., Stöckelhuber, K. W., Subramani Bhagavatheswaran, E., Wießner, S., Scheler, U., Saalwächter, K., Formanek, P., Heinrich, G., Das, A.
Number of pages: 13
Pages: 2010-2022
Publication date: 15 Feb 2018
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Publication information
Journal: Journal of Physical Chemistry B
Volume: 122
Issue number: 6
ISSN (Print): 1520-6106
Ratings:

Scopus rating (2018): CiteScore 5.8 SJR 1.109 SNIP 0.979
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry
DOIs:

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Source: Scopus
Source ID: 85042152539
Research output: Contribution to journal › Article › Scientific › peer-review

Fluorimetric oxygen sensor with an efficient optical read-out for in vitro cell models
This paper presents a phase fluorimetric sensor for the monitoring of the oxygen concentration in in vitro cell models. The sensing surface of the sensor consists of oxygen sensitive fluorescent dyes (platinum(II) octaethylporphyrinketone) embedded in a thin polystyrene film. In order to optimize the optical read-out scheme of the sensor, we carried out electromagnetic simulations of a fluorescently doped polystyrene film deposited on a glass-water interface. The simulation results showed highly anisotropic angular emission distribution with the maximum irradiance being at super critical angles, which attracts tailored optical designs to maximize the fluorescence collection efficiency. For this purpose, we applied an efficient optical read-out scheme based on an in-contact parabolic lens. The use of parabolic lens also facilitates confocal total internal reflection excitation from the substrate side. This makes the excitation effective and insensitive to biofouling or other optical changes in the sensing surface and, more importantly, greatly reduces the amount of excitation power radiated into the cell culture chamber. Experimental results show that when applied together with phase fluorimetric lifetime sensing, this optical scheme allows one to use thin films (

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: BioMediTech, Faculty of Biomedical Sciences and Engineering, Research group: Micro and Nanosystems Research Group, Research area: Microsystems, Research group: Sensor Technology and Biomeasurements (STB), VTT Technical Research Centre of Finland, BioMediTech Institute and Faculty of Biomedical Sciences and Engineering
Contributors: Välimäki, H., Verho, J., Kreutzer, J., Kattipparambil Rajan, D., Ryynänen, T., Pekkanen-Mattila, M., Ahola, A. , Tappura, K., Kallio, P., Lekkala, J.
Number of pages: 9
Pages: 738-746
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Publication information
Journal: Sensors and Actuators B: Chemical
Volume: 249
ISSN (Print): 0925-4005
Ratings:

Scopus rating (2017): CiteScore 9.3 SJR 1.406 SNIP 1.453
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Instrumentation, Condensed Matter Physics, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry, Electrical and Electronic Engineering
Keywords: Cardiac cells, Enhanced optical read-out, Fluorimetric oxygen sensor, in vitro cell models, PtOEPK, Thin film fluorescence
DOIs:

10.1016/j.snb.2017.04.182
Source: Scopus
Source ID: 85019164799
Research output: Contribution to journal › Article › Scientific › peer-review

Comparison of various high-stress wear conditions and wear performance of martensitic steels

The demanding environments typically encountered by the wear resistant steels create challenges for the materials selection, because the hardness grades of the steels alone do not reveal the true nature of their wear behavior. In this study, five commercial wear resistant steels were tested using three application oriented test methods with five different test variables for abrasion, impact-abrasion, and slurry erosion. All the used test methods produced high-stress conditions that crushed the used mineral abrasive, plastically deformed the sample surfaces, and led to the formation of adiabatic shear bands. When the results produced by the chosen methods were compared, the normalization of the wear losses by the wear area and test time revealed well the differences between the methods. The test methods ranked the steels similarly, but there were clear differences in the wear rates and wear mechanisms between the tests. In addition, the abrasive methods produced surface adiabatic shear bands, while subsurface shear bands were initiated by the more impacting methods. In the studied conditions, the work hardening ability of the steel had a clear influence on its wear resistance, which largely explains the marked differences in the wear rates of the studied commercial 500HB grade steels.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Research group: Materials Characterization, Materials Science and Environmental Engineering, Robit Ltd, Univ of Oulu
Contributors: Valtonen, K., Ojala, N., Haiko, O., Kuokkala, V.
Number of pages: 11
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Publication information

Journal: Wear
Volume: 426-427
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ISSN (Print): 0043-1648
Ratings:

Scopus rating (2019): CiteScore 5.8 SJR 1.335 SNIP 2.458
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Abrasion, Impact wear, Steel, Wear testing, ABRASIVE WEAR, BEHAVIOR, FIELD, RESISTANT STEELS, COMPRESSION, MICROSTRUCTURE
DOIs:

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Source: Scopus
Source ID: 85058455176
Research output: Contribution to journal › Article › Scientific › peer-review

Photomechanical Energy Transfer to Photopassive Polymers through Hydrogen and Halogen Bonds

The supramolecular assembly of photoactive azobenzenes with passive polymers via halogen or hydrogen bonding is a cost-effective way to design materials for various photomechanical applications that convert light energy directly into macroscopic motion, for instance, in all-optical surface patterning and photochemical imaging of plasmonic structures. To elucidate the molecular-level origins of this motion, we show, by coupling dynamic infrared spectroscopy to a photo-orientation setup, that supramolecular bonds above a certain interaction strength threshold are photostable under vigorous photoisomerization cycling and capable of translating the photo-orientation of azobenzenes into the orientation of nonabsorbing host polymer side chains. A correlation is found between azobenzene photoinduced molecular orientation and macroscopic all-optical surface patterning efficiency. The improved performance of halogen-bonded systems in photopatterning applications can be related to the absence of a plasticizing effect on the polymer matrix, which may enable the material to retain an optimal glass transition temperature, in contrast to hydrogen-bonded and nonbonded references. Thus, our results provide design guidelines in terms of the nature and strength of the supramolecular interaction and of the degree of azo functionalization needed to optimize the motion transfer to passive polymers.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Département de Chimie, Succ. Centre-Ville, Aalto University, Politecnico di Milano, Royal Military College of Canada
Contributors: Vapaavuori, J., Heikkinen, I. T. S., Dichiarante, V., Resnati, G., Metrangolo, P., Sabat, R. G., Bazuin, C. G., Priimagi, A., Pellerin, C.
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Issue number: 20
ISSN (Print): 0024-9297
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Scopus rating (2015): CiteScore 10.1 SJR 2.357 SNIP 1.58
Original language: English
ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Inorganic Chemistry
Electronic versions:

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Bibliographical note
EXT="Vapaavuori, Jaana"
Source: Scopus
Source ID: 84945400553
Research output: Contribution to journal › Article › Scientific › peer-review

In Situ Photocontrol of Block Copolymer Morphology during Dip-Coating of Thin Films
We demonstrate a unique combination of simultaneous top-down and bottom-up control of the morphology of block copolymer films by application of in situ optical irradiation during dip-coating. A light-addressable and block-selective small molecule, 4-butyl-4′-hydroxyazobenzene (BHAB), is introduced into a diblock copolymer of polystyrene and poly(4-vinylpyridine) (PS-P4VP) of 28.4 wt % P4VP via supramolecular chemistry, notably by hydrogen bonding to P4VP. We show that the spherical morphology of thin films dip-coated from a THF solution at slow withdrawal rates in the dark convert to cylindrical morphology when dip-coated under illumination. This is attributed to volume expansion of the P4VP/BHAB phase due to trans-cis photoisomerization combined with a light-induced increase in BHAB uptake in the film. The demonstrated photocontrol highlights the potential of dip-coating as a scalable film preparation method that can be easily coupled with external stimuli to direct nanostructured self-assembly in the films as solvent evaporates.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Département de Chimie, Succ. Centre-Ville
Contributors: Vapaavuori, J., Grosrenaud, J., Pellerin, C., Bazuin, C. G.
Number of pages: 5
Pages: 1158-1162
Publication date: 20 Oct 2015
Peer-reviewed: Yes

Publication information
Journal: ACS Macro Letters
Volume: 4
Issue number: 10
ISSN (Print): 2161-1653
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Scopus rating (2015): CiteScore 10.1 SJR 2.392 SNIP 1.403

Original language: English
ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics, Inorganic Chemistry
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Source: Scopus
Source ID: 84946032702
Research output: Contribution to journal › Article › Scientific › peer-review

Nanoindentation study of light-induced softening of supramolecular and covalently functionalized azo polymers
Nanoindentation studies on thin films of the widely used azo polymer pDR1A and a supramolecular polymer-azobenzene complex p4VP(DY7)$_{0.5}$ demonstrate significant light-induced softening upon visible-light irradiation due to trans-cis-trans photoisomerization of the azobenzene units. More specifically, the strain-rate sensitivities of pDR1A and p4VP(DY7)$_{0.5}$ upon 532 nm irradiation increase by 80% and 120%, respectively. These results imply a photosoftening contribution to the mechanisms of light-induced surface patterning of azo polymers and the photomechanical effect. The finding that under the experimental conditions used photosoftening is more significant in the supramolecular complex than in the covalently functionalized polymer highlights the potential of noncovalent functionalization strategies in designing materials with efficient photomechanical response, and nanoindentation provides a powerful technique to quantify the connection between the photoinduced changes in mechanical properties and photoinduced macroscopic movement of azo polymer films.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Department of Applied Physics, Aalto University, McGill University
Contributors: Vapaavuori, J., Mahimwalla, Z., Chromik, R. R., Kaivola, M., Priimagi, A., Barrett, C. J.
Number of pages: 5
Pages: 2806-2810
Publication date: 28 Apr 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Materials Chemistry C
Volume: 1
Issue number: 16
ISSN (Print): 2050-7534
Ratings:
Scopus rating (2013): CiteScore 1.1
Original language: English
ASJC Scopus subject areas: Chemistry(all), Materials Chemistry
DOIs:
10.1039/c3tc30246f
URLs:
http://www.scopus.com/inward/record.url?scp=84879524974&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84879524974
Research output: Contribution to journal › Article › Scientific › peer-review

Efficient surface structuring and photoalignment of supramolecular polymer-azobenzene complexes through rational chromophore design
Rational selection of the para-substituent of azobenzene chromophores in supramolecular polymeric complexes is exploited to control the chromophore-chromophore intermolecular interactions occurring in the material system. This allows optimizing the material system for either efficient surface-relief formation or for high and stable photoalignment. The surface-relief gratings can be subsequently coated with amorphous TiO_2 using atomic layer deposition, resulting in high-quality and high-index organic-inorganic gratings with vastly improved thermal stability compared to all-polymeric gratings.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Frontier Photonics, Department of Applied Physics, Aalto University, Tokyo Institute of Technology
Contributors: Vapaavuori, J., Valtavirta, V., Alasaarela, T., Mamiya, J. I., Priimagi, A., Shishido, A., Kaivola, M.
Number of pages: 5

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Peer-reviewed: Yes

Publication information
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Issue number: 39
ISSN (Print): 0959-9428
Ratings:

Scopus rating (2011): SJR 2.614 SNIP 1.539
Original language: English
ASJC Scopus subject areas: Materials Chemistry, Chemistry(all)
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10.1039/c1jm12642c
URLs:

http://www.scopus.com/inward/record.url?scp=80053301644&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 80053301644
Research output: Contribution to journal › Article › Scientific › peer-review

Supramolecular design principles for efficient photoresponsive polymer-azobenzene complexes
Noncovalent binding of azobenzenes to polymers allows harnessing light-induced molecular-level motions (photoisomerization) for inducing macroscopic effects, including photocontrol over molecular alignment and self-assembly of block copolymer nanostructures, and photoinduced surface patterning of polymeric thin films. In the last 10 years, a growing body of literature has proven the utility of supramolecular materials design for establishing structure-property-function guidelines for photoresponsive azobenzene-based polymeric materials. In general, the bond type and strength, engineered by the choice of the polymer and the azobenzene, influence the photophysical properties and the optical response of the material system. Herein, we review this progress, and critically assess the advantages and disadvantages of the three most commonly used supramolecular design strategies: hydrogen, halogen and ionic bonding. The ease and versatility of the design of these photoresponsive materials makes a compelling case for a paradigm shift from covalently-functionalized side-chain polymers to supramolecular polymer-azobenzene complexes.

General information
Publication status: Published
MoE publication type: A2 Review article in a scientific journal
Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Département de Chimie , Succ. Centre-Ville
Contributors: Vapaavuori, J., Bazuin, C. G., Priimagi, A.
Number of pages: 21
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ISSN (Print): 2050-7534
Ratings:

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ASJC Scopus subject areas: Chemistry(all), Materials Chemistry
Electronic versions:

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http://urn.fi/URN:NBN:fi:tty-201803211417
Source: Scopus
Source ID: 85042792061
Research output: Contribution to journal › Review Article › Scientific › peer-review

Optimization of HVOF Cr3C2-NiCr coating for increased fatigue performance

Thermally sprayed coatings are strong candidates to be used for replacement of hard chromium – process which is regarded as an environmental risk – in many sliding surfaces for engineering applications such as hydraulic cylinders and aircraft landing gears. Recent advance in thermal spraying technology, based on the increase of the spray particle velocity, has led to improved coating quality. This study focuses on the fatigue performance of structural steel coated with Cr_3C_2[Formula presented] coating. Coating has been produced by using high kinetic HVOF thermal spray process. First, the coating was optimized for fatigue purposes by studying the residual stress generation. The optimized coating was selected for deposition of axial fatigue tests specimens, whose fatigue performance was compared to the uncoated steel specimens having different surface treatments (turning, polishing, and shot blasting) relevant for the target applications. The results showed that by using a high kinetic energy coating, the fatigue performance of Cr_3C_2[Formula presented] coated structural steel was clearly improved compared to uncoated steel of similar surface quality. Increased fatigue resistance of the coated material was attributed to the substantial compressive residual stresses that hindered crack initiation and that was caused by the high velocity spray particles during the coating process.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Surface Engineering, VTT Technical Research Centre of Finland, Aalto University, Technical University of Liberec
Contributors: Varis, T., Suhonen, T., Calonius, O., Čuban, J., Pietola, M.
Number of pages: 9
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Publication date: 15 Nov 2016
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Publication information

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Volume: 305
ISSN (Print): 0257-8972
Ratings:

Scopus rating (2016): CiteScore 4.4 SJR 0.882 SNIP 1.385
Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: CrC[Formula presented] coating, Fatigue performance, HVOF thermal spray, Residual stress, S-N curve, Wear resistance
DOIs:

10.1016/j.surfcoat.2016.08.012
Source: Scopus
Source ID: 84981273135
Research output: Contribution to journal › Article › Scientific › peer-review

High temperature corrosion of thermally sprayed NiCr and FeCr coatings covered with a KCl-K_2SO_4 salt mixture

Current boiler tube materials and designs are sensitive to changes in process conditions. The desire to increase efficiency through the increase in process temperature and the use of high-chlorine and alkali containing fuels such as biomass is challenging. The alloying of steel to increase the corrosion resistance leads to a significant increase in cost. Thermally sprayed coatings offer promising, effective, flexible and cost efficient solution to fulfil the material needs for the future. However, some heat exchanger design alterations have to be overcome before global commercialization. High temperature corrosion in combustion plants can occur by a variety of mechanisms, including passive scale degradation with subsequent rapid scaling, loss of adhesion and scale detachment, attack by molten or partly molten deposits via fluxing reactions and intergranular/interlamellar corrosion. The activated chlorine corrosion mechanism plays a key role in the thermally sprayed coatings due to their unique lamellar structure.In this study, the corrosion behaviour of NiCr and FeCr (HVOF and wire arc) thermally sprayed coatings was tested under simplified biomass combustion conditions. The tests were carried out by using a KCl-K_2SO_4 salt mixture as a synthetic biomass ash, which was placed on the coated materials and then heat treated for one week (168h) at two different temperatures (550°C and 600°C) and in two different gas atmospheres (air and air+30% H_2O). After exposure, the metallographic cross sections of the coatings were studied with SEM/EDX. The results showed that the coatings behaved relatively well at the lower test temperature while critical interlamellar corrosion was observed in some cases at the higher test temperature. A few coatings (HVOF Ni49Cr, HVOF Ni21Cr, and wire arc sprayed Fe30Cr) showed promising performance even at 600°C in both atmospheres (dry and wet).

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland, Abo Akad Univ, Abo Akademi University, Dept Phys

Contributors: Varis, T., Bankiewicz, D., Yrjas, P., Oksa, M., Suhonen, T., Tuurna, S., Ruusuvuori, K., Holmström, S.
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Volume: 265
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Ratings:

Scopus rating (2015): CiteScore 3.9 SJR 0.852 SNIP 1.376
Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Biomass, Corrosion protection, High temperature corrosion, HVOF, Thermal spray coating, Wire arc
DOIs:

10.1016/j.surfcoat.2014.11.012
URLs:

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Source: Scopus
Source ID: 84925343339
Research output: Contribution to journal › Article › Scientific › peer-review

Formation mechanisms, structure, and properties of HVOF-sprayed WC-CoCr coatings: An approach toward process maps

Our study focuses on understanding the damage tolerance and performance reliability of WC-CoCr coatings. In this paper, the formation of HVOF-sprayed tungsten carbide-based cermet coatings is studied through an integrated strategy: First-order process maps are created by using online-diagnostics to assess particle states in relation to process conditions. Coating properties such as hardness, wear resistance, elastic modulus, residual stress, and fracture toughness are discussed with a goal to establish a linkage between properties and particle characteristics via second-order process maps. A strong influence of particle state on the mechanical properties, wear resistance, and residual stress stage of the coating was observed. Within the used processing window (particle temperature ranged from 1687 to 1831 °C and particle velocity from 577 to 621 m/s), the coating hardness varied from 1021 to 1507 HV and modulus from 257 to 322 GPa. The variation in coating mechanical state is suggested to relate to the microstructural changes arising from carbide dissolution, which affects the properties of the matrix and, on the other hand, cohesive properties of the lamella. The complete tracking of the coating particle state and its linking to mechanical properties and residual stresses enables coating design with desired properties.

General information
Publication status: Published
MoE publication type: A2 Review article in a scientific journal
Organisations: Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland, Thermal Spray Advance Research Team, Universidad San Francisco de Quito, Stony Brook University State University of New York, Aalto University
Contributors: Varis, T., Suhonen, T., Ghabchi, A., Valarezo, A., Sampath, S., Liu, X., Hannula, S. P.
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Publication information
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Volume: 23
Issue number: 6
ISSN (Print): 1059-9630
Ratings:

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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
Keywords: fracture toughness, HVOF, process map, residual stress, WC-CoCr
DOIs:

10.1007/s11666-014-0110-5
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Source: Scopus
Source ID: 84906056443
Research output: Contribution to journal › Review Article › Scientific › peer-review

Influence of powder properties on residual stresses formed in high-pressure liquid fuel HVOF sprayed WC-CoCr coatings

This paper presents a systematic study of the effect of various WC-CoCr powders on the residual stresses of the high pressure HVOF sprayed coating. As the residual stresses are recognized to play a significant role in the mechanical and fatigue resistance of the coating, it is understandable that their management is important for damage tolerant coating design. Several studies have recently shown that processes, which produce high particle kinetic energy and lower particle temperature, such as Warm spray, HVAF and high-pressure HVOF processes, generate higher peening stresses and therefore final residual stresses is more compressive compared to lower kinetic energy HVOF systems. In addition to the spraying process, powder properties are known to be one of the most important variables in thermal spraying. Nevertheless, only few studies can be found on the effect of powder properties on residual stresses. The aim of this study was to understand the effect of different powder properties on the formation of residual stress. In situ monitoring was utilized to record curvature and temperature during spraying and to calculate coating residual stresses. This approach is a useful tool for understanding of residual stresses during the thermal spraying process enabling their manipulation. It was found that the powders, with only minor differences in density and particle size, produced a significant difference of about 350 MPa in the stress states of the coatings. The combined effect of spray powder properties and spray parameters on residual stress was almost 560 MPa.

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Organisations: Materials Science and Environmental Engineering, Research group: Surface Engineering, VTT Technical Research Centre of Finland
Contributors: Varis, T., Suhonen, T., Jokipii, M., Vuoristo, P.
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DOIs:
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Research output: Contribution to journal › Article › Scientific › peer-review

Evaluation of Residual Stresses and Their Influence on Cavitation Erosion Resistance of High Kinetic HVOF and HVAF-Sprayed WC-CoCr Coatings

Thermal spray processes have been developing toward lower particle temperature and higher velocity. Latest generation high-velocity oxygen-fuel (HVOF) and high-velocity air-fuel (HVAF) can produce very dense coating structures due to the higher kinetic energy typical for these thermal spray processes. Thermally sprayed coatings usually contain residual stresses, which are formed by a superposition of thermal mismatch, quenching and, in case of high kinetic energy technologies, peening stresses. These stresses may have a significant role on the mechanical response and fatigue behavior of the coating. Understanding these effects is mandatory for damage tolerant coating design and wear performance. For instance, wear-resistant WC-CoCr coatings having high compressive stresses show improved cavitation erosion performance. In this study, comparison of residual stresses in coatings sprayed by various thermal spray systems HVOF (Thermico CJS and Oerlikon Metco DJ Hybrid) and HVAF (Kermetico AcuKote) was made. Residual stresses were determined through thickness by utilizing Tsui and Clyne analytical model. The real temperature and deposition stress data were collected in the coating process by in situ technique. That data were used for the model to represent realistic residual stress state of the coating. The cavitation erosion and abrasion wear resistance of the coatings were tested, and relationships between residual stresses and wear resistance were discussed.

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Contributors: Varis, T., Suhonen, T., Laakso, J., Jokipii, M., Vuoristo, P.
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Research output: Contribution to journal › Article › Scientific › peer-review

Aqueous guanidinium-carbonate interactions by molecular dynamics and neutron scattering: Relevance to ion-protein interactions
Guanidinium carbonate was used in this study as a simple proxy for the biologically relevant arginine-carbonate interactions in water. Molecular dynamics (MD) simulations of guanidinium carbonate were performed with nonpolarizible water using two implementations of the ion force fields. In the first, the ions had full charges, while in the second, the ions had reduced charges in order to effectively account for electronic polarization effects of water. The results from the simulations were then compared to data from previous neutron scattering experiments. It was found that there were significant discrepancies between the full charge force field MD simulations and the experimental results due to excessive ion pairing and clustering in the former. In contrast, reducing the ionic charges yields a more regular solution with a simulated structure, which fits well the experimental data.

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Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Division of Organic Chemistry and Biochemistry, Bijenička Cesta 54
Contributors: Vazdar, M., Jungwirth, P., Mason, P. E.
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ASJC Scopus subject areas: Surfaces, Coatings and Films, Physical and Theoretical Chemistry, Materials Chemistry
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Research output: Contribution to journal › Article › Scientific › peer-review

Behavior of 4-hydroxynonenal in phospholipid membranes

Under conditions of oxidative stress, 4-hydroxy-2-nonenal (4-HNE) is commonly present in vivo. This highly reactive and cytotoxic compound is generated by oxidation of lipids in membranes and can be easily transferred from a membrane to both cytosol and the extracellular space. Employing time-dependent fluorescence shift (TDFS) method and molecular dynamics simulations, we found that 4-HNE is stabilized in the carbonyl region of a 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) bilayer. 4-HNE is thus able to react with cell membrane proteins and lipids. Stabilization in the membrane is, however, moderate and a transfer of 4-HNE to either extra- or intracellular space occurs on a microsecond time scale. These molecular-level details of 4-HNE behavior in the lipid membrane rationalize the experimentally observed reactivity of 4-HNE with proteins inside and outside the cell. Furthermore, these results support the view that 4-HNE may play an active role in cell signaling pathways.

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Contributors: Vazdar, M., Jurkiewicz, P., Hof, M., Jungwirth, P., Cwiklik, L.
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Original language: English
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Source: Scopus
Source ID: 84861861948
Research output: Contribution to journal › Article › Scientific › peer-review

Cysteine-tagged chimeric avidin forms high binding capacity layers directly on gold

Cysteine-tagged, genetically engineered avidin named ChiAvd-Cys and wild-type avidin form monolayers or bilayer structures when immobilised directly on gold. Non-specific binding can be reduced by a post-treatment of the avidin layers with a N-[tris(hydroxymethyl)methyl]-acrylamide (pTHMMAA) polymer. ChiAvd-Cys showed excellent activity when immobilised on gold. About 70% of the ChiAvd-Cys molecules were able to bind two biotinylated green fluorescent proteins (per avidin tetramer). Amino-biotinylated antibody $F(ab')_2$ fragments could be bound to every 4th and 8th ChiAvd-Cys and wild-type avidin molecule, respectively, whereas on average one thiol-biotinylated antibody Fab′-fragment was bound to every ChiAvd-Cys. Antigen binding to the thiol-biotinylated Fab′-fragment bound to the ChiAvd-Cys/pTHMMAA layer was almost twice compared to that of the amino-biotinylated $F(ab')_2$-fragments. The high antigen binding was due to a site-directed orientation of the thiol-biotinylated fragments. The ChiAvd-Cys/pTHMMAA layers offer high capacity that may be used to couple biotinylated compounds on biosensor surfaces.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Multi-scaled biodata analysis and modelling (MultiBAM), VTT Technical Research Centre of Finland, School of Management (JKK), Adult Stem Cells, Tampere University Hospital
Contributors: Vikholm-Lundin, I., Auer, S., Paakkunainen, M., Määttä, J. A. E., Munter, T., Leppiniemi, J., Hytönen, V. P., Tappura, K.
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ASJC Scopus subject areas: Instrumentation, Materials Chemistry, Surfaces, Coatings and Films, Metals and Alloys, Electronic, Optical and Magnetic Materials, Condensed Matter Physics, Electrical and Electronic Engineering
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Source: Scopus
Source ID: 84864284365
Research output: Contribution to journal › Article › Scientific › peer-review

Detection of 3,4-methylenedioxymethamphetamine (MDMA, ecstasy) by displacement of antibodies

A molecular layer with low non-specific binding enabling determination of low concentrations of 3,4-methylenedioxymethamphetamine (MDMA) by the displacement of antibodies has been developed. Antibody Fab′-fragments at various concentrations have been site-directly immobilised on gold and intercalated with a hydrophilic non-ionic polymer that reduces non-specific binding. Bovine serum albumin conjugated with MDMA and various concentrations of anti-MDMA antibodies were bound to the layer. The amount of conjugates and antibodies bound was dependent on the amount of Fab′-fragments in the layer. Antibodies were also bound to the conjugates physisorbed directly onto the gold surface and in mixtures with the polymer or with a lipoamide. A high displacement of antibodies was observed by surface plasmon resonance (SPR) on interaction of MDMA with the different layers in buffer solution. No displacement could, however, be observed in saliva with the pure conjugate layer because of a high non-specific binding of proteins. When the conjugates were coupled to the surface through the antibody Fab-fragment/polymer layer, MDMA concentrations as low as 0.02 ng mL^{-1} (0.14 nM) could easily be detected in buffer. In diluted saliva the lowest limit of detection was 0.4 ng mL^{-1} enabling determination of drugs from saliva with a cut-off concentration of 2 ng mL^{-1}. The molecular layer of antibody Fab′-fragments and polymer thus shows great potential for binding conjugates and antibodies that can be displaced on the interaction with very low concentrations of small-sized molecules. A low non-specific binding is guaranteed by the presence of the hydrophilic polymer.

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Contributors: Vikholm-Lundin, I., Auer, S., Hellgren, A. C.
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Instrumentation, Condensed Matter Physics, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry, Electrical and Electronic Engineering
Keywords: Antibody displacement, Drugs of abuse, Ecstasy, Immobilisation, MDMA, Surface plasmon resonance
DOIs:

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Source: Scopus
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Research output: Contribution to journal › Article › Scientific › peer-review

Corrosion properties of thermally sprayed bond coatings under plasma sprayed chromia coating in sulfuric acid solutions

Plasma sprayed chromia coatings are known to have excellent corrosion and wear properties in highly acidic conditions at ambient and elevated temperatures. In applications requiring extremely good corrosion resistance, the whole components are usually made of a corrosion resistant alloy. For increased adhesion of the ceramic coating to the corrosion resistant substrate material, thermally sprayed metallic bond coatings are used. It is well known that the corrosion environment in such bond coatings between the ceramic top coating and the substrate can be extremely difficult due to the absence of dissolved oxygen, increased concentration of the corrosive electrolytes under the top coating, and galvanic and crevice corrosion mechanisms inside the coating structure. When bond coatings are used, it is of high importance to select the bond layer chemistry and method of production so that the bond coating can survive in such harsh conditions. In the present study, four different bond coatings were studied to evaluate their performance in corrosive acidic electrolytes. The coatings studied were HVOF sprayed Ni-20Cr, Hastelloy C-276 and Ultimet alloy coatings, and plasma sprayed tantalum coating. The substrate material was a solid Hastelloy C-276 metal alloy. The top coating used was plasma sprayed Cr_2O_3. Corrosion properties of various coating types were studied by electrochemical measurements in sulfuric acid solutions with various concentrations at RT, and by immersion tests at RT and at the temperature of 60°C. The coating microstructures were studied before and after the corrosion tests. The results showed that HVOF sprayed Ni-20Cr and Ultimet alloy coatings were significantly attacked by the sulfuric acid electrolyte, whereas HVOF sprayed Hastelloy C-276 and plasma sprayed Ta coatings performed significantly better.

General information

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MoE publication type: A4 Article in a conference publication
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Contributors: Vuoristo, P., Varis, T., Meschini, D., Bolelli, G., Lusvarghi, L.
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Source: Scopus
Source ID: 85073880821
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

A supramolecular approach to photoresponsive thermo/solvoplastic block copolymer elastomers

With the aim of preparing supramolecular photoresponsive block copolymer elastomers, a series of ABA triblock copolymers with a poly(n-butyl acrylate) (PnBA) middle block and poly(dimethylaminoethyl methacrylate) (PDMAEMA or PDM) outer blocks were synthesized by atom transfer radical polymerization (ATRP), followed by PDM quaternization (giving PDMQ-PnBA-PDMQ) and then by ionic complexation with methyl orange (MO), an azo-containing and sulfonate-functionalized commercially available compound (giving PDMQ/MO-PnBA-PDMQ/MO). The PnBA block, which has a subambient glass transition, and the quaternized and complexed blocks, which have high glass transitions, form phase-separated soft and hard blocks, respectively. Simple elasticity tests of solvent-cast films show that the PDMQ/MO-PnBA-PDMQ/MO with hard block content between 18 and 29 wt % (as well as PDMQ-PnBA-PDMQ with 18 wt % hard block content) have significant elastomeric character. AFM and TEM (atomic force and transmission electron microscopies) of spin-coated films show a correlation between the elastomeric character and morphologies where the hard block forms a dispersed minority phase (spherical and/or short cylindrical domains). A continuous hard phase is observed for a hard block content of around 37 wt %; these materials show no significant elasticity. Reversible photoisomerization, with relatively high cis isomer content in the photostationary state, was also demonstrated.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Computer Systems, Frontier Photonics, Département de Chimie, Succ. Centre-Ville, Université de Sherbrooke

Contributors: Wang, X., Vapaavuori, J., Zhao, Y., Bazuin, C. G.
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Source: Scopus
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Research output: Contribution to journal › Article › Scientific › peer-review

A bifacial colour-tunable system via combination of a cholesteric liquid crystal network and hydrogel
We present a colour tunable system obtained by combining a humidity-responsive cholesteric liquid crystal network and hydrogel coatings, in a diligently designed cell-geometry. The design enables sensitive colour tuning via temperature-induced changes in humidity inside the cell. Uniquely, the system exhibits a bifacial response, causing either a blue- or red-shift in the reflected color when heated from opposite sides.

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials, Aalto University, Eindhoven University of Technology
Contributors: Wani, O. M., Schenning, A. P. H. J., Priimagi, A.
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Source: Scopus
Source ID: 85089309785
Research output: Contribution to journal › Article › Scientific › peer-review

Surface behavior of hydrated guanidinium and ammonium ions: A comparative study by photoelectron spectroscopy and molecular dynamics
Through the combination of surface sensitive photoelectron spectroscopy and molecular dynamics simulation, the relative surface propensities of guanidinium and ammonium ions in aqueous solution are characterized. The fact that the N 1s binding energies differ between these two species was exploited to monitor their relative surface concentration through their respective photoemission intensities. Aqueous solutions of ammonium and guanidinium chloride, and mixtures of these salts, have been studied in a wide concentration range, and it is found that the guanidinium ion has a greater

propensity to reside at the aqueous surface than the ammonium ion. A large portion of the relative excess of guanidinium ions in the surface region of the mixed solutions can be explained by replacement of ammonium ions by guanidinium ions in the surface region in combination with a strong salting-out effect of guanidinium by ammonium ions at increased concentrations. This interpretation is supported by molecular dynamics simulations, which reproduce the experimental trends very well. The simulations suggest that the relatively higher surface propensity of guanidinium compared with ammonium ions is due to the ease of dehydration of the faces of the almost planar guanidinium ion, which allows it to approach the water-vapor interface oriented parallel to it.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Swedish University of Agricultural Sciences, Lund University, Uppsala University, FOM-Institute AMOLF, Science Park 102, Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
Contributors: Werner, J., Wernersson, E., Ekholm, V., Ottosson, N., Öhrwall, G., Heyda, J., Persson, I., Söderström, J., Jungwirth, P., Björneholm, O.
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ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry
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Research output: Contribution to journal › Article › Scientific › peer-review

Orientational dependence of the affinity of guanidinium ions to the water surface

The behavior of guanidinium chloride at the surface of aqueous solutions is investigated using classical molecular dynamics (MD) simulations. It is found that the population of guanidinium ions oriented parallel to the interface is greater in the surface region than in bulk. The opposite is true for ions in other orientations. Overall, guanidinium chloride is depleted in the surface region, in agreement with the fact that the addition of guanidinium chloride increases the surface tension of water. The orientational dependence of the surface affinity of the guanidinium cation is related to its anisotropic hydration. To bring the ion to the surface in the parallel orientation does not require hydrogen bonds to be broken, in contrast to other orientations. The surface enrichment of parallel-oriented guanidinium indicates that its solvation is more favorable near the surface than in bulk solution for this orientation. The dependence of the bulk and surface properties of guanidinium on the force field parameters is also investigated. Despite significant quantitative differences between the force fields, the surface behavior is qualitatively robust. The implications for the orientations of the guanidinium groups of arginine side chains on protein surfaces are also outlined.

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Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Division of Organic Chemistry and Biochemistry, Bijenička Cesta 54, Lund University, Crop and Soil Sciences, Cornell Univ.
Contributors: Wernersson, E., Heyda, J., Vazdar, M., Lund, M., Mason, P. E., Jungwirth, P.
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Source ID: 80054988916
Research output: Contribution to journal › Article › Scientific › peer-review

Perfluoro-1,1′-biphenyl and perfluoronaphthalene and their derivatives as π-acceptors for anions

Addition of anions to perfluorinated 1,1′-biphenyl 1 or naphthalene 2 results in a shift of the ^{19}F NMR signals. However, any specific interaction cannot be assigned to this effect. In order to study the interaction in more detail, the salt derivatives 3 and 4 were prepared and studied by single crystal X-ray diffraction revealing weak anion-π interactions in the solid state.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, University of Jyväskylä, Institut für Organische Chemie, RWTH Aachen
Contributors: Yi, H., Albrecht, M., Valkonen, A., Rissanen, K.
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Catalysis, Materials Chemistry
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Source: Scopus
Source ID: 84919782132
Research output: Contribution to journal › Article › Scientific › peer-review

Photostable orange-red fluorescent unsymmetrical diketopyrrolopyrrole-BF_2hybrids

The straightforward synthesis of structurally unique DPP-BODIPY hybrids has been developed using unsymmetrical, imidazopyridine substituted DPPs. These hybrids exhibit a superb combination of photophysical properties including high photostability, good fluorescence quantum yield as well as markedly bathochromically shifted absorption and emission compared to conventional diketopyrrolopyrroles. Increasing the size of the imidazopyridine substituent and/or the electron donating power of the other aryl substituent can further redshift both absorption and emission to reach ~650 nm for the free-base and ca. 700 nm for boron-chelates. A strong intramolecular hydrogen bond is responsible for the small change in geometry between the ground and excited states and hence relatively small differences in photophysical properties upon formation of boron-chelates are observed. The solvent dependence of the photophysical properties for the free base and DPP-BF2 complexes were investigated and show strong fluorescence with long lifetimes in both non-polar and polar aprotic environments.

General information

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Organisations: Materials Science and Environmental Engineering, Polish Academy of Sciences, Umr 6230, University of Warsaw
Contributors: Young, D. C., Tasior, M., Laurent, A. D., Dobrzycki, Ł., Cyrański, M. K., Tkachenko, N., Jacquemin, D., Gryko, D. T.
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Research output: Contribution to journal › Article › Scientific › peer-review

Arc-sprayed Fe-based coatings from coredwires for wear and corrosion protection in power engineering
High wear and corrosion of parts lead to an increase in operating costs at thermal power plants. The present paper shows a possible solution to this problem through the arc spraying of protective coatings. Cored wires of the base alloying system Fe-Cr-C were used as a feedstock. Rise of wear- and heat-resistance of the coatings was achieved by additional alloying with Al, B, Ti, and Y. The wear and heat resistance of the coatings were tested via a two-body wear test accompanied by microhardness measurement and the gravimetric method, respectively. A high-temperature corrosion test was performed at 550 °C under KCl salt deposition. The porosity and adhesion strengths of the coatings were also evaluated. The microstructure was investigated with a scanning electron microscope (SEM) unit equipped with an energy dispersive X-ray (EDX) microanalyzer, and the phase composition was assessed by X-ray diffractometry. The test results showed the positive influence of additional alloying with Y on the coating properties. A comparison with commercial boiler materials showed that the coatings have the same level of heat resistance as austenite steels and are an order of magnitude higher than that of pearlite and martensite-ferrite steels. The coatings can be applied to wear- and heat-resistant applications at 20-700 °C.

General information
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Hybrid nanoparticle design based on cationized gelatin and the polyanions dextran sulfate and chondroitin sulfate for ocular gene therapy

We describe the development of hybrid nanoparticles composed of cationized gelatin and the polyanions CS and DS for gene therapy in the ocular surface. The physicochemical properties of the nanoparticles that impact their bioperformance, such as average size and zeta potential, can be conveniently modulated by changing the ratio of polymers and the crosslinker. These systems associate plasmid DNA and are able to protect it from DNase I degradation. We corroborate that the introduction of CS or DS in the formulation decreases the in vitro toxicity of the nanoparticles to human corneal cells without compromising the transfection efficiency. These nanoparticles are potential candidates for the development of safer and more effective nanomedicines for ocular therapy. New hybrid nanoparticles composed of cationized gelatin and natural polyanions are developed and characterized. The incorporation of chondroitin sulfate or dextran sulfate in cationized gelatin nanoparticles decreases their toxicity while preserving their transfection efficiency in human corneal cells. These nanoparticles are potential candidates for the development of safer and more effective nanomedicines for ocular therapy.

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