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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Organisations: Materials Science, B. N. Yeltsin Ural Federal University, Russian Academy of Sciences, Ural Branch of the Russian Academy of Sciences
Contributors: Yury, K., Filippov, M., Makarov, A., Malygina, I., Soboleva, N., Fantozzi, D., Andrea, M., Koivuluoto, H., Vuoristo, P.
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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.

General information

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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, 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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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.

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

Source ID: 84903466740
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.

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Contributors: Vuoristo, P., Varis, T., Meschini, D., Bolelli, G., Lusvarghi, L.
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Name: Proceedings of the International Thermal Spray Conference
ASJC Scopus subject areas: Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces
URLs:

http://www.scopus.com/inward/record.url?scp=85073880821&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 85073880821
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

Erosive-abrasive wear behavior of carbide-free bainitic and boron steels compared in simulated field conditions
The wear resistance of carbide-free bainitic microstructures have recently shown to be excellent in sliding, sliding-rolling, and erosive-abrasive wear. Boron steels are often an economically favorable alternative for similar applications. In this study, the erosive-abrasive wear performance of the carbide-free bainitic and boron steels with different heat treatments was studied in mining-related conditions. The aim was to compare these steels and to study the microstructural features affecting wear rates. The mining-related condition was simulated with an application oriented wear test method utilizing dry abrasive bed of 8–10 mm granite particles. Different wear mechanisms were found; in boron steels, micro-cutting and micro-ploughing were dominating mechanisms, while in the carbide-free bainitic steels, also impact craters with thin platelets were observed. Moreover, the carbide-free bainitic steels had better wear performance, which can be explained by the different microstructure. The carbide-free bainitic steels had fine ferritic-austenitic microstructure, whereas in boron steels microstructure was martensitic. The level of retained austenite was quite high in the carbide-free bainitic steels and that was one of the factors improving the wear performance of these steels. The hardness gradients with orientation of the deformation zone on the wear surfaces were one of the main affecting factors as well. Smoother work hardened hardness profiles were considered beneficial in these erosive-abrasive wear conditions.

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Organisations: Materials Science, Research group: Materials Characterization, Lulea University of Technology, Univ of Oulu
Contributors: Vuorinen, E., Heino, V., Ojala, N., Haiko, O., Hedayati, A.
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Source: Scopus
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Improved corrosion properties of Hot Dip Galvanized Steel by nanomolecular silane layers as hybrid interface between zinc and top coatings
Thin organic coatings (TOC) or paints on hot dip galvanized steel (HDGS) improve the corrosion properties and create visually pleasing surfaces. Delamination of these coatings lead to corrosion and peeling of the paints. Hence, a novel method for improved adhesion and corrosion properties for HDGS surfaces is introduced. It is shown how the fabrication of a nanomolecular silane film as an interfacial layer between the HDGS and TOC or paint improves the corrosion properties of HDGS in different pH regimes. Understanding the corrosion behavior of ultra-thin silane layers under differing pH is crucial as subsequent coatings have different pHs. By varying the silanization parameters two different nanomolecular surface structures of aminopropyl trimethoxysilane (APS) on HDGS were fabricated: well-ordered monolayers with approximately 1 nm thickness and highly clustered APS films with a thickness in the range of 5–8 nm. To verify the nanomolecular APS structures, photoelectron spectroscopy (PES) and contact angle (CA) measurements were employed. The corrosion properties of HDGS and silanized HDGS were studied with linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS). It is shown that at pH 5 and 7 passivation behavior is observed on silanized samples but the most significant improvement in corrosion resistance is found at pH 10 where the corrosion currents of silanized samples are up to two orders of magnitude lower than on uncoated metallic samples. Also, it is demonstrated that the corrosion inhibition of APS is not only dependent on the thickness of the silane film, but also the molecular ordering at the surface. The thin, well-ordered APS monolayer is more resistant towards corrosion in NaCl solution (pH 7) than thicker clustered APS layer. This indicates that the highly ordered nanomolecular surface structure protects the HDGS-silane interface
from the Cl- adsorption better than the thicker, but more randomly ordered APS layers. Nanomolecular interfacial silane films for enhanced corrosion and adhesion properties on HDGS are transferrable to industrial production lines providing a low cost and environmentally friendly method for improved HDGS products.

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MoE publication type: A1 Journal article-refereed
Organisations: Optoelectronics Research Centre, Research group: Surface Science, MAX IV Laboratory, Lund University
Contributors: Vuori, L., Ali-Löytty, H., Lahtonen, K., Hannula, M., Lehtonen, E., Niu, Y., Valden, M.
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Research output: Contribution to journal › Article › Scientific › peer-review

Photoinduced Electron Transfer in CdSe/ZnS Quantum Dot-Fullerene Hybrids

Photoinduced electron transfer (ET) in CdSe/ZnS core-shell quantum dot (QD) - fullerene (COOH-C<inf>60</inf>) hybrids was studied by the means of time-resolved emission and absorption spectroscopy techniques. A series of four QDs with emission in the range 540-630 nm was employed to investigate the dependence of the electron transfer rate on the QD size. Emission of the QDs is quenched upon hybrid formation, and the quenching mechanism is identified as photoinduced electron transfer from the QD to the fullerene moiety due to the fullerene anion signature observed in transient absorption. In order to obtain quantitative information on the ET reaction, several kinetic data analysis techniques were used, including a conventional multiexponential fitting and a maximum entropy method for emission decay analysis, as well as a distributed decay model based on the Poisson distribution of fullerenes in the hybrids. The latter gradually simplifies the interpretation of the transient absorption spectra and indicates that the spectra of QD cations are essentially similar to those of neutral QDs, differing only by a minor decrease in the intensity and broadening. Furthermore, only a minor decrease in the ET rate with the increasing QD size was observed, the time constants being in the range 100-200 ps for all studied QDs. The charge recombination is extended to 10 ns or longer for all hybrids.

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
Contributors: Virkki, K., Demir, S., Lemmetyinen, H., Tkachenko, N. V.
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Research output: Contribution to journal › Article › Scientific › peer-review

Photoinduced Electron Injection from Zinc Phthalocyanines into Zinc Oxide Nanorods: Aggregation Effects

Phthalocyanines (Pc) are well-known light-harvesting compounds. However, despite the tremendous efforts on phthalocyanine synthesis, the achieved energy conversion efficiencies for Pc-based dye-sensitized solar cells are moderate. To cast light on the factors reducing the conversion efficiency, we have undertaken a time-resolved spectroscopy study of the primary photoinduced reactions at a semiconductor-Pc interface. ZnO nanorods were chosen as a model semiconductor substrate with enhanced specific surface area. The use of a nanostructured oxide surface allows to extend the semiconductor-dye interface with a hole transporting layer (spiro-MeOTAD) in a controlled way, making the studied system closer to a solid-state dye-sensitized solar cell. Four zinc phthalocyanines are compared in this study. The compounds are equipped with bulky peripheral groups designed to reduce the self-aggregation of the Pcs. Almost no signs of aggregation can be observed from the absorption spectra of the Pcs assembled on a ZnO surface. Nevertheless, the time-resolved spectroscopy indicates that there are inter-Pc charge separation-recombination processes in the time frame of 1-100 ps. This may reduce the electron injection efficiency into the ZnO by more than 50%, pointing out to a remaining aggregation effect. Surprisingly, the electron injection time does not correlate with the length of the linker

connecting the Pc to ZnO. A correlation between the electron injection time and the "bulkiness" of the peripheral groups was observed. This correlation is further discussed with the use of computational modeling of the Pc arrangements on the ZnO surface. (Figure Presented).

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Instituto Madrileño de Estudios Avanzados (IMDEA)-Nanociencia, Universidad Autónoma de Madrid, Mersin University, South-Ukrainian National Pedagogical University
Contributors: Virkki, K., Hakola, H., Urbani, M., Tejerina, L., Ince, M., Martínez-Díaz, M. V., Torres, T., Golovanova, V., Golovanov, V., Tkachenko, N. V.
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Source ID: 85020915273
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.

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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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Source: Scopus
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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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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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Source ID: 84873899176
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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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Organisations: Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Center for Biomolecules and Complex Molecular Systems, Division of Organic Chemistry and Biochemistry, Rudjer Bošković Institute, J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, V.v.i.
Contributors: Vazdar, M., Jurkiewicz, P., Hof, M., Jungwirth, P., Cwiklik, L.
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Research output: Contribution to journal › 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

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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.
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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
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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).

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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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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:

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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.

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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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ISSN (Print): 1059-9630
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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
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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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MoE publication type: A1 Journal article-refereed
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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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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DOIs:
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Source: Scopus
Source ID: 85081673256
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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Organisations: Materials Science and Environmental Engineering, Research group: Surface Engineering, Research group: Applied Material Science, VTT Technical Research Centre of Finland
Contributors: Varis, T., Suhonen, T., Laakso, J., Jokipii, M., Vuoristo, P.
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ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
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Electronic versions:

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

Impact wear and mechanical behavior of steels at subzero temperatures
In this study, the deformation behavior of three steels was studied at Arctic temperatures by controlled single and multiple oblique angle impacts. The results were compared with the mechanical properties of the steels determined at the corresponding temperatures. At subzero temperatures, the hardness and strength of the studied steels increased and their ability to deform plastically steadily decreased. In the martensitic steels, adiabatic shear bands were observed to form during the impacts at subzero temperatures, indicating that the deformation ability of the steels was critically impaired. At −60 °C, the adiabatic shear bands commonly acted as initiation sites for subsurface cracks. Moreover, the surface characterization of the test samples revealed formation of cracks and wear particles, which was connected to the opening of grain boundaries and martensite laths at low temperatures. Finite Element Modeling was also used to obtain more information about the impact event.

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Materials Characterization, University of Nottingham
Contributors: Valtonen, K., Ratia, V., Ramakrishnan, K. R., Apostol, M., Terva, J., Kuokkala, V.
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Original language: English
ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Impact, Low temperature, Steel, Wear
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DOIs:

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Source: Scopus
Source ID: 85053014382
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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Organisations: Research group: Materials Characterization, Materials Science and Environmental Engineering, Robit Ltd, Univ of Oulu
Contributors: Valtonen, K., Ojala, N., Haiko, O., Kuokkala, V.
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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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http://urn.fi/URN:NBN:fi:tuni-202001271549. Embargo ends: 10/04/21
Source: Scopus
Source ID: 85058455176
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

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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.
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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: Cardiac cells, Enhanced optical read-out, Fluorimetric oxygen sensor, in vitro cell models, PtOEPK, Thin film fluorescence
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Source ID: 85019164799
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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.

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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.
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Original language: English
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Source: Scopus
Source ID: 85042152539
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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.

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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.
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Peer-reviewed: Yes

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Issue number: 7
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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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Source: Scopus
Source ID: 79960241231
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.

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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

Superamphiphobic overhang structured coating on a biobased material

A superamphiphobic coating on a biobased material shows extreme liquid repellency with static contact angles (CA) greater than 150° and roll-off angles less than 10° against water, ethylene glycol, diiodomethane and olive oil, and a CA for hexadecane greater than 130°. The coating consisting of titania nanoparticles deposited by liquid flame spray (LFS) and hydrophobized using plasma-polymerized perfluorohexane was applied to a birch hardwood. Scanning electron microscopy (SEM) imaging after sample preparation by UV laser ablation of coated areas revealed that capped structures were formed and this, together with the geometrically homogeneous wood structure, fulfilled the criteria for overhang structures to occur. The coating showed high hydrophobic durability by still being non-wetted after 500 000 water drop impacts, and this is discussed in relation to geometrical factors and wetting forces. The coating was semi-transparent with no significant coloration. A self-cleaning effect was demonstrated with both water and oil droplets. A self-cleanable, durable and highly transparent superamphiphobic coating based on a capped overhang structure has a great potential for commercial feasibility in a variety of applications, here exemplified for a biobased material.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Department of Physics, Research area: Aerosol Physics, Research group: Aerosol Synthesis, Research group: Materials Characterization, SP Technical Research Institute of Sweden, Paper Converting and Packaging Technology, Aerosol Physics Laboratory, Surface and Corrosion Science
Contributors: Tuominen, M., Teisala, H., Haapanen, J., Mäkelä, J. M., Honkanen, M., Vippola, M., Bardage, S., Wålinder, M. E. P., Swerin, A.
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Original language: English
ASJC Scopus subject areas: Surfaces, Coatings and Films
Keywords: Biobased material, Coating, Deposition, Nanoparticle, Oil repellency, Perfluorohexane, Plasma, Self-cleaning, Superamphiphobic, Superhydrophobic, Superoleophobic, Titania, Water repellency, Wetting, Wood
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Source ID: 84979009546
Research output: Contribution to journal › Article › Scientific › peer-review

Hematite Surface Modification toward Efficient Sunlight-Driven Water Splitting Activity: The Role of Gold Nanoparticle Addition

Localized surface plasmon resonance has been investigated to enhance light harvesting in hematite-based photoelectrodes modified with gold nanoparticles (AuNPs); meanwhile, an extensive understanding about the different processes involved in the hematite-AuNP system remains unclear. This work addresses a majority of effects associated with AuNP addition by comparing charge transfer, catalytic and light harvesting efficiencies. The obtained results revealed that the lower AuNP amount leads to a higher photocurrent response of 1.20 mA cm^{-2} at 1.23 V_{RHE} in comparison with all photoelectrodes designed here. X-ray photoelectron data revealed that hematite photoelectrodes loaded with higher concentrations of AuNPs immersed in an alkaline electrolyte showed hydrated/oxidized gold phase formation at the electrode/electrolyte interface. This change on the semiconductor-metal interface may affect the conductivity impairing the photocatalytic performance because of the passivation layer on the AuNP surface, decreasing the efficiency of charge transfer. Notoriously, increasing AuNP amount supported on the hematite surface clearly promoted higher light absorption, which was surprisingly not followed by photoelectrochemical efficiency. This result suggests here that the plasmon effect is not a dominant phenomenon that drives the photoelectrode performance. In fact, a deeper analysis showed that the loaded hematite photoelectrodes with low amounts of AuNPs provides a Schottky contact at the semiconductor-metal interface leading to Fermi level equilibration enhancing charge transport efficiency, which is classified as the predominant effect leading to higher photoresponse in the system.

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Organisations: Physics, Universidade Federal do ABC, Microscopy Centre
Contributors: Tofanello, A., Freitas, A. L., Carvalho, W. M., Salminen, T., Niemi, T., Souza, F. L.
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Peer-reviewed: Yes

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ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Energy(all), Physical and Theoretical Chemistry, Surfaces, Coatings and Films
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Source ID: 85082009064
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.
Number of pages: 12
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Publication date: 15 Sep 2017
Peer-reviewed: Yes

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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
DOIs:

10.1016/j.wear.2017.05.010
Source: Scopus
Source ID: 85020872795
Research output: Contribution to journal › 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.
Number of pages: 11
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Peer-reviewed: Yes
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Journal: Journal of Physical Chemistry Part B
Volume: 119
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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:

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http://www.scopus.com/inward/record.url?scp=84938277609&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note
EXT="Bondar, Alexey"
Source: Scopus
Source ID: 84938277609
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.
Number of pages: 9
Pages: 631-639
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:

10.1007/s11666-012-9880-9
URLs:

http://www.scopus.com/inward/record.url?scp=84878626773&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84878626773
Research output: Contribution to journal › Review Article › Scientific › peer-review

ESD qualification data used as the basis for building electrostatic discharge protected areas
ESD control programs that are based on the standards IEC61340-5-1 and ANSI/ESD S20.20 are targeted to provide safer handling of electronic parts now susceptible to damage by electrostatic discharge. However, ESD failures have occurred in EPA even when all standard control methods are met. To further improve EPAs, ESD control programs should be updated to cover all known common discharge scenarios, and multiple parallel ESD source parameters should be used to assess the level of ESD risks. In addition, a reliable ESD risk assessment should be based on discharge source circuit analysis and product sensitivity tests using the real discharge waveforms found in EPA.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Electronics and Communications Engineering, Research group: Wireless Identification and Sensing Systems Research Group, Sensing Systems for Wireless Medicine (MediSense), Cascade Metrology
Contributors: Tamminen, P., Viheriäkoski, T., Sydänheimo, L., Ukkonen, L.
Number of pages: 8

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Original language: English
ASJC Scopus subject areas: Electrical and Electronic Engineering, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Condensed Matter Physics, Biotechnology
Keywords: CDM, Control program, EPA, ESD, HBM, Standards
DOIs:

10.1016/j.elstat.2015.08.009
Source: Scopus
Source ID: 84940760492
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
Publication date: 28 Apr 2011
Peer-reviewed: Yes

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Journal: Journal of Physical Chemistry Part B
Volume: 115
Issue number: 16
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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
DOIs:

10.1021/jp2015676
URLs:

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

Switchable light reflectance in dilute magneto-optical colloids based on nickel ferrite nanowires

Optical properties of diluted narrow band gap magnetic semiconductor nanowire colloids are controlled by modest magnetic fields under 100 Oe. High aspect ratio NiFe2O4 nanowires are used to achieve responsiveness to magnetic field, light absorption and -scattering. Visible light reflectance of the diluted colloids can be either increased or decreased depending on the nanowire alignment relative to the direction of the light propagation. The prepared colloids can be applied as magneto-optical switches or as smart window devices.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Photonics, Institute of Physics, University of Tartu, Riga Technical University, CRPP, University of Latvia
Contributors: Sutka, A., Timusk, M., Joost, U., Ignatans, R., Maiorov, M.
Number of pages: 3
Pages: 119-121
Publication date: 2 May 2018
Peer-reviewed: Yes

Publication information

Journal: e-Journal of Surface Science and Nanotechnology
Volume: 16
ISSN (Print): 1348-0391
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Scopus rating (2018): CiteScore 0.9 SJR 0.216 SNIP 0.317
Original language: English
ASJC Scopus subject areas: Biotechnology, Bioengineering, Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Colloid, Ferrimagnetic, Magneto-optical, Nanowire, NiFe2O4
DOIs:

10.1380/ejssnt.2018.119

Bibliographical note

INT=fot,"Joost, Urmas"
Source: Scopus
Source ID: 85047369076
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

Host publication information

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Publisher: TAPPI Press
ISBN (Electronic): 9781510871885
ASJC Scopus subject areas: Media Technology, Materials Chemistry, Surfaces, Coatings and Films
URLs:

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Source: Scopus
Source ID: 85059262851
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › 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
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Publication date: 15 Jul 2016
Peer-reviewed: Yes

Publication information

Journal: Wear
Volume: 358-359
ISSN (Print): 0043-1648
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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

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
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Publication date: 28 Dec 2014
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Journal: Chemical Communications

Volume: 50
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ISSN (Print): 1359-7345
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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

Adjustable wetting properties of paperboard by liquid flame spray process
Liquid flame spray process (LFS) was used for depositing TiO_x and SiO_x nanoparticles on paperboard to control wetting properties of the surface. By the LFS process it is possible to create either superhydrophobic or superhydrophilic surfaces. Changes in the wettability are related to structural properties and chemical composition of the surface, which were characterized using scanning electron microscope (SEM), atomic force microscope (AFM) and X-ray photoelectron spectroscopy (XPS). The surface properties can be ascribed as a correlation between wetting properties of the paperboard and the surface texture created by nanoparticles. Surfaces can be produced inline in a one step roll-to-roll process without need for additional modifications. Furthermore, functional surfaces with adjustable hydrophilicity or hydrophobicity can be fabricated simply by choosing appropriate liquid precursors.

General information
Publication status: Published
MoE publication type: A4 Article in a conference publication
Organisations: Department of Materials Science, Department of Physics, Abo Akad Univ, Abo Akademi University, Dept Phys, Institute of Paper Converting, Aerosol Physics Laboratory
Contributors: Stepien, M., Saarinen, J. J., Teisala, H., Tuominen, M., Aromaa, M., Kuusipalo, J., Mäkelä, J., Toivakka, M.
Number of pages: 9
Pages: 80-88
Publication date: 2010

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ISBN (Print): 1595102035, 9781595102034
ASJC Scopus subject areas: Surfaces, Coatings and Films, Surfaces and Interfaces
URLs:

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Source: Scopus
Source ID: 79951939367
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › 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
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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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Source: Scopus
Source ID: 84878363659
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
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Issue number: 22
ISSN (Print): 0040-6090
Ratings:

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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: Germanium, Near infrared, Photodetectors, Raman characterization, Thermal evaporation
DOIs:

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Source: Scopus
Source ID: 80052110605
Research output: Contribution to journal › Article › Scientific › peer-review

Micro-Raman characterization of Germanium thin films evaporated on various substrates

We perform an extensive micro-Raman analysis of Germanium thin films physically evaporated on several substrates including silicon, silicon oxide and glass. We investigate the dependence of crystal quality on thin film deposition parameters such as substrate temperature and growth rate. We also study the continuous transitional change of the material structure from amorphous to crystalline phases. Ge films obtained by this simple and low cost technique are a viable solution towards the realization of virtual substrates and devices.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, University “Roma Tre”, Nonlinear Optics and OptoElectronics Lab, Universit Degli Studi dell'Aquila
Contributors: Sorianello, V., Colace, L., Assanto, G., Nardone, M.
Number of pages: 4
Pages: 492-495
Publication date: Apr 2011
Peer-reviewed: Yes

Publication information

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ISSN (Print): 0167-9317
Ratings:

Scopus rating (2011): CiteScore 2.8 SJR 0.813 SNIP 1.148
Original language: English
ASJC Scopus subject areas: Electrical and Electronic Engineering, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Atomic and Molecular Physics, and Optics, Condensed Matter Physics
Keywords: Germanium, Raman characterization, Thin films
DOIs:

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http://www.scopus.com/inward/record.url?scp=79751538206&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 79751538206
Research output: Contribution to journal › Article › Scientific › peer-review

Thermal evaporation of Ge on Si for near infrared detectors: Material and device characterization

Using a low-temperature process, we thermally evaporated Ge thin films on Si substrates and investigated both structural and electrical properties of samples grown at various temperatures. The characterization included X-ray diffraction, atomic force microscopy and Hall measurements and aimed at determining a suitable temperature range in terms of crystal quality and transport properties. Finally, we employed Ge films on Si to fabricate near infrared photodiodes and test them in terms of dark current and responsivity.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, University “Roma Tre”, Nonlinear Optics and OptoElectronics Lab, Centro S3, Institute IMEM-CNR
Contributors: Sorianello, V., Colace, L., Assanto, G., Notargiacomo, A., Armani, N., Rossi, F., Ferrari, C.
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Publication information

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Ratings:

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Original language: English
ASJC Scopus subject areas: Electrical and Electronic Engineering, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Atomic and Molecular Physics, and Optics, Condensed Matter Physics
Keywords: Germanium, Photodetectors, Thermal evaporation
DOIs:

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Source: Scopus
Source ID: 79751530052
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.
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Peer-reviewed: Yes

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ISSN (Print): 0257-8972
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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
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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
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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

Digital correction of frequency response mismatches in 2-channel time-interleaved ADCs using adaptive I/Q signal processing
A novel adaptive compensation architecture for the frequency response mismatch of 2-channel time-interleaved ADC (TI-ADC) is proposed for developing high-performance self-adaptive systems. The proposed approach overcomes the existing methods in the sense that the TI-ADC mismatch identification can be performed without allocating a region where only the TI-ADC mismatch spurs are present. This is accomplished via mapping the TI-ADC problem into an I/Q mismatch problem which allows deploying complex statistical signal processing. As proof of concept, the compensation architecture is demonstrated and tested on a 16-bit TI-ADC measured hardware data.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Wireless Communications and Positioning (WICO), Department of Electronics and Communications Engineering, Research group: Wireless Communications and Positioning, Airbus Defense and Space
Contributors: Singh, S., Valkama, M., Epp, M., Anttila, L., Schlecker, W., Ingber, E.
Number of pages: 13
Pages: 543-555
Publication date: 2015
Peer-reviewed: Yes

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Journal: Analog Integrated Circuits and Signal Processing
Volume: 82
Issue number: 3
ISSN (Print): 0925-1030
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Scopus rating (2015): CiteScore 1.2 SJR 0.197 SNIP 0.42
Original language: English
ASJC Scopus subject areas: Surfaces, Coatings and Films, Hardware and Architecture, Signal Processing
Keywords: Circularity, Complex I/Q signal processing, Digitally assisted analog (DASA), Frequency response mismatch identification, Time-interleaved ADC
DOIs:

10.1007/s10470-014-0476-9

Source: Scopus
Source ID: 84925535772
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.

General information

Publication status: E-pub ahead of print
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Plastics and Elastomer Technology
Contributors: Shakun, A., Sarlin, E., Vuorinen, J.
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Peer-reviewed: Yes

Publication information

Journal: Journal of Applied Polymer Science
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Original language: English
ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry
Keywords: dielectric properties, elastomers, mechanical properties, rubber
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Source: Scopus
Source ID: 85087303061
Research output: Contribution to journal › Article › Scientific › peer-review

Piezoresistive natural rubber-multiwall carbon nanotube nanocomposite for sensor applications

We explore, both experimentally and theoretically, the possibility to use a composite of natural rubber (NR) and multiwall carbon nanotubes (MWCNT) as a piezoresistive tensile sensor. As an essentially new feature relative to the previous work, we have performed a systematic study of the mechanism of the piezoresistance at large deformations in a wide range of MWCNT concentrations and crosslinking degrees of the host rubber material. In qualitative agreement with the previous work, the conductivity of the unstrained NR/MWCNT nanocomposite is shown to be adequately described by the percolation theory with the critical exponent evaluated to ~2.31. Varying tensile stress-induced strains in the composite has been shown to results in a non-linear electrical response that cannot be described by simple modifications of the percolation theory. In order to explain the observed non-linear dependence of the resistance R of the composite on the strain ε, we have developed a scaling theory that relates this resistance to the structural changes in the conducting MWCNT network caused by deforming the host NR. Based on the obtained results, we discuss the ways of using the highly stretchable conductive elastomer composites as an efficient piezoresistive tensile sensor.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Rubber Technology Centre, Indian Institute of Technology Kharagpur, Vodafone Department of Mobile Communications Systems, University of Münster, Leibniz-Institut für Polymerforschung Dresden E.V.
Contributors: Selvan, N. T., Eshwaran, S. B., Das, A., Stöckelhuber, K. W., Wießner, S., Pötschke, P., Nando, G. B., Chervanyov, A. I., Heinrich, G.
Number of pages: 12
Pages: 102-113
Publication date: 1 Mar 2016

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Journal: Sensors and Actuators, A: Physical
Volume: 239
ISSN (Print): 0924-4247
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Scopus rating (2016): CiteScore 4.8 SJR 0.787 SNIP 1.619
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Instrumentation, Condensed Matter Physics, Surfaces, Coatings and Films, Metals and Alloys, Electrical and Electronic Engineering
Keywords: Sensor rubber filler strain nano-composite conductivity
DOIs:

10.1016/j.sna.2016.01.004
Source: Scopus
Source ID: 84955467512
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.

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Publication status: Published
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.
Number of pages: 18
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Publication date: 25 Mar 2018
Peer-reviewed: Yes

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Journal: Surface and Coatings Technology
Volume: 338
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Scopus rating (2018): CiteScore 5.2 SJR 0.973 SNIP 1.494
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:

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Source: Scopus
Source ID: 85041473768
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.

General information

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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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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Erosion, FRP, Glass fibre, Mineral fillers, Vinylester
Electronic versions:

WEA_2017_668_Revised manuscript. Embargo ended: 21/07/19
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10.1016/j.wear.2017.07.011
URLs:

http://urn.fi/URN:NBN:fi:tty-201801311179. Embargo ended: 21/07/19

Bibliographical note

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

The effect of substrate pre-treatment on durability of rubber-stainless steel adhesion

In many applications, rubber linings protect metal surfaces from the environment and prolong the service life of the metal components significantly. The loss of adhesion and resulting premature failure at the rubber-metal interface may generate an un-planned shutdown and production losses. This work focuses on the effect of various sand blasting methods on the long-term adhesion between bromobutyl rubber and stainless steel in a hot and humid environment. Softer austenitic stainless steel and harder, chemically more resistant super duplex stainless steel grades were used as substrates. It was found, that the developed interfacial area ratio S_{dr}, which is the additional surface area contributed by the texture as compared to the planar definition area, had the best correlation with the sand blasting media characteristics, namely to the hardness. The proportionality between other sand blasting medium characteristics and the S_{dr} value was poor. The initial adhesion between the rubber and the substrates was defined by the cohesive strength of the rubber and unaffected by the substrate characteristics and the sand blasting medium contaminants on the substrates. After a 4–12-week exposure in hot and humid environment, the use of corrosive sand blasting medium (steel grit) resulted in significant adhesion loss whereas the use of inert sand blasting media (feldspar or corundum) maintained the adhesion better. However, the adhesion system at the interface degraded causing performance loss. Neither the better corrosion resistance of super duplex stainless steel nor increased surface roughness improved the reliability of rubber lining in extreme conditions.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Plastics and Elastomer Technology, Research group: Materials Characterization, Engineering materials science and solutions (EMASS), Outotec Research Center, Teknikum Oy
Contributors: Sarlin, E., Honkanen, M., Lindgren, M., Laihonen, P., Juutilainen, M., Vippola, M., Vuorinen, J.
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Publication date: 1 Dec 2020
Peer-reviewed: Yes

Publication information
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ISSN (Print): 2468-0230
Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Physics and Astronomy(all), Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Ageing, Sand blasting, Steel-rubber adhesion, Surface roughness
DOIs:
10.1016/j.surfin.2020.100646

Bibliographical note
EXT="Lindgren, M."
EXT="Laihonen, P."
EXT="Juutilainen, M."
Source: Scopus
Source ID: 85090330517
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
Publication status: Published
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

ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
Keywords: abrasive-erosive wear, CrC-based cermet, elevated temperature, mechanically activated thermal synthesis, room temperature, thermal spraying
DOIs:
10.1007/s11666-017-0638-2
Source: Scopus
Source ID: 85029407112
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.

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: Santangelo, P. E., Allesina, G., Bolelli, G., Lusvarghi, L., Matikainen, V., Vuoristo, P.
Number of pages: 12
Pages: 1982–1993
Publication date: Dec 2017
Peer-reviewed: Yes
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Original language: English
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:
10.1007/s11666-017-0642-6
Source: Scopus
Source ID: 85029487592
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.
Number of pages: 7
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Publication date: 8 Jun 2015
Peer-reviewed: Yes

Publication information
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Volume: 219
ISSN (Print): 0925-4005
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Scopus rating (2015): CiteScore 7.4 SJR 1.225 SNIP 1.486
Original language: English
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
Keywords: Complex permittivity, Inductive coupling, Passive resonance sensor, Slurry, Suspension
DOIs:

10.1016/j.snb.2015.04.121
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http://www.scopus.com/inward/record.url?scp=84930646590&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note
ORG=ase,0.5
ORG=mol,0.5
Source: Scopus
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
Publication status: Published
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
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Source: Scopus
Source ID: 85020132649
Research output: Contribution to journal › Article › Scientific › peer-review

Roll-to-roll application of photocatalytic TiO_2 nanoparticles for printed functionality

In this work ultraviolet A (UVA) light controlled photocatalytic activity of TiO_2 nanoparticles is utilized on paper, paperboard, and plastic films for controlled wetting and oxygen sensors for modified atmosphere packages (MAPs). A liquid flame spray (LFS) process is used for a large-area TiO_2 nanoparticle deposition on natural fibre based substrates such as paperboard that results in a superhydrophobic surface. Controlled wettability is achieved using an UVA light activation that converts the surface to hydrophilic whereas an oven heat treatment recovers the initial superhydrophobicity. On the other hand, a TiO_2 nanoparticles with methylene blue (MB) dye is used to detect the presence of oxygen in modified atmosphere packages. We believe that photocatalytically active surfaces with tailorable properties will find many applications in the near future, for example, with printed functional devices.

General information
Publication status: Published
MoE publication type: A4 Article in a conference publication
Organisations: Department of Physics, Research area: Aerosol Physics, Research group: Aerosol Synthesis, Center for Functional Materials at Biological Interfaces (FUNMAT), Abo Akad Univ, Abo Akademi University, Dept Phys, Omya International AG, AGH University of Science and Technology, Aerosol Physics Laboratory
Contributors: Saarinen, J. J., Valtakari, D., Bollström, R., Stepien, M., Haapanen, J., Mäkelä, J. M., Toivakka, M.
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Publication date: 2016

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Keywords: Controlled wetting, Nanoparticles, O sensor, Photocatalysis, TiO
URLs:
http://www.techconnect.org/proceedings/paper.html?volume=TCB2016v4&chapter=1&paper=785
URLs:
http://www.scopus.com/inward/record.url?scp=84988974879&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84988974879
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › 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.

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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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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
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10.1016/j.surfcoat.2017.10.047
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
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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
Publication date: 2018
Peer-reviewed: Yes
Early online date: 1 Jan 2018

Publication information
Journal: Surface and Interface Analysis
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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:
10.1002/sia.6429
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

Journal: Materials and Corrosion
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
DOIs:

10.1002/maco.202011653
Source: Scopus
Source ID: 85084611702
Research output: Contribution to journal › Article › Scientific › peer-review

Atomikerroskasvatusmenetelmällä kasvatetun titaanidioksidikalvon ominaisuudet valosähkökemiallisessa veden hajottamisessa

Photoelectrochemical water splitting is one of the potential ways of utilizing solar energy. A major issue for the method and for renewable energy production would be the development of an efficient and a cost-effective semiconductor photoanode. In this Master of Science Thesis properties of atomic layer deposited (ALD) titanium dioxide film (TiO_2), such as a chemical composition, a crystal structure and the ability to absorb sunlight, are studied in as-deposited conditions and after oxidative annealing. By understanding thoroughly the properties of atomic layer deposited titanium dioxide and the effects of post-annealing in air, titanium dioxide can be better utilized in semiconductor photoanodes used in photoelectrochemical water splitting.

Titanium dioxide films examined in this study were grown on n-type phosphorus-doped silicon (n-Si(100)(P)) and fused quartz used as substrates by atomic layer deposition at 200 °C using tetrakis(dimethylamido)titanium (TDMAT) and deionized water as precursors. The annealing of some of the samples at 500 °C in air was made in a tube furnace. The concentrations of the elements and chemical states of the atomic layer deposited titanium dioxide films were studied by X-ray photoelectron spectroscopy (XPS). The film thickness and refractive index were determined by ellipsometer and the absorption properties of the titanium dioxide film were measured by UV/Vis/NIR spectrophotometer. In addition, crystallographic results from X-ray diffraction (XRD) and Raman spectroscopy were also utilized, as well as the results of the photoelectrochemical cell and solar simulator on titanium dioxide photoanode performance.

Based on the results, at 200 °C atomic layer deposited titanium dioxide is amorphous and absorbs visible light as ”black” TiO_2. At the oxidative annealing at 500 °C titanium dioxide crystallizes into rutile and becomes ”white” TiO_2 that absorbs less visible light. Both titanium dioxide films contain the lower $Ti^{3+/2+}$ oxidation states of titanium that may indicate oxygen vacancies. Nitrogen is found only in as-deposited titanium dioxide. The annealed titanium dioxide is stable in electrolyte, achieving 0.20 % ABPE for water splitting reaction.

General information

Publication status: Published
MoE publication type: G2 Master's thesis, polytechnic Master's thesis
Organisations: Photonics, Research group: Surface Science
Contributors: Saari, J.
Number of pages: 74
Publication date: 4 Oct 2017

Publication information

Original language: Finnish
ASJC Scopus subject areas: Surfaces, Coatings and Films, Renewable Energy, Sustainability and the Environment
Keywords: Photoelectrochemical water splitting, Titanium dioxide, ALD, Atomic layer deposition, XPS, X-ray photoelectron spectroscopy, Ellipsometry, UV/Vis/NIR spectrophotometry
URLs:

http://URN.fi/URN:NBN:fi:tty-201709201911
Research output: Book/Report › Master's Thesis › Scientific

Role of Oxide Defects in ALD grown TiO_2 Coatings on Performance as Photoanode Protection Layer

Photoelectrochemical (PEC) water splitting is one of the potential methods of utilizing solar energy. A major issue for the method and for renewable energy production is the development of an efficient, chemically stable and cost-effective semiconductor photoanode. Recently, titanium dioxide (TiO_2) coatings grown by atomic layer deposition (ALD) have appeared to be a promising approach to stabilize semiconductor photoanodes under PEC conditions. In particular, amorphous ALD grown TiO_2 has shown exceptional charge transfer properties compared to its crystalline form that are not properly understood yet. Therefore, we target to gain better understanding on the defect structure of ALD grown TiO_2 and utilize the information in the development of optimal photoanode protection layer for efficient solar water splitting.

In this work, structural, optical and photoelectrochemical properties of the ALD grown TiO_2 films were studied in as-deposited condition and after annealing in air at 500 °C. TiO_2 films were grown on n-type phosphorus-doped silicon and fused quartz by ALD at 200 °C using tetrakis(dimethylamido)titanium (TDMAT) and deionized water as precursors. The properties of TiO_2 were investigated by X-ray photoelectron spectroscopy (XPS), ellipsometry and UV/Vis/NIR spectrophotometry. In addition, results from X-ray diffraction (XRD), Raman spectroscopy and photoelectrochemical (PEC) cell are discussed.

Based on the results, as-deposited TiO_2 is amorphous and absorbs visible light as "black" TiO_2. After annealing in air at 500 °C TiO_2 crystallizes as rutile and becomes "white" TiO_2 that absorbs light only in the UV region. As-deposited TiO_2 contains significant amount of $Ti^{3+/2+}$ oxygen vacancies that are oxidized as Ti^{4+} upon annealing in air. In addition, nitrogen is found only in as-deposited titanium dioxide. As-deposited TiO_2 is not chemically stable under PEC conditions. In contrast, the annealed TiO_2 is chemically stable and showed 0.20 % ABPE efficiency for water splitting reaction.

As a conclusion, Ti^{3+} defects induce photocorrosion of ALD TiO_2 under PEC conditions. After annealing in air at 500 °C ALD TiO_2 is chemically stable and it can be used as a photoanode protection layer. In the future, research will be focused on optimizing the properties of ALD TiO_2/Si interface and studying the structure of the surface after deposition of nickel electrocatalysts on TiO_2/Si photoanode.

General information

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Organisations: Photonics, Research group: Surface Science
Contributors: Saari, J., Ali-Löytty, H., Valden, M.
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Peer-reviewed: Unknown
Event: Paper presented at Optics & Photonics Days 2018, Jyväskylä, Finland.
ASJC Scopus subject areas: Renewable Energy, Sustainability and the Environment, Surfaces, Coatings and Films
Keywords: Atomic layer deposition, Titanium dioxide, Photoelectrochemical water splitting
Research output: Other conference contribution › Paper, poster or abstract › Scientific

CLC a Colored Liquid Crystal: Prototype Description and Design Opportunities

General information

Publication status: Published
MoE publication type: A4 Article in a conference publication
Organisations: University of Virginia
Contributors: Rubio Hernandez, R.
Publication date: 2009

Host publication information

Title of host publication: Proceedings of the 11th International Conference: Glass Performace Days
ASJC Scopus subject areas: Architecture , Surfaces, Coatings and Films
Keywords: Glass, Liquid crystal, Polarization, Light, Colour, Smart materials
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

Envolvente de Vidrio Electrocrómico

General information

Publication status: Published
MoE publication type: A4 Article in a conference publication
Organisations: Uppsala Univ, Uppsala University, Angstrom Lab, Dept Chem Angstrom, Universidad Politecnica de Madrid
Contributors: Rubio Hernandez, R., Marshall-Berenguer, R., De la Flor San Vicente, L.

Publication date: 2004

Host publication information
Title of host publication: Foro ARCA II. Arquitectura y Calidad de vida. : Edificación y sostenibilidad: un compromiso posible
ASJC Scopus subject areas: Architecture , Surfaces, Coatings and Films
Keywords: Glass, Smart Materials, Light, intelligent facade
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › 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.
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Volume: 120
Issue number: 35
ISSN (Print): 1520-6106
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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

Magnetic non-contact friction from domain wall dynamics actuated by oscillatory mechanical motion
Magnetic friction is a form of non-contact friction arising from the dissipation of energy in a magnet due to spin reorientation in a magnetic field. In this paper, we study magnetic friction in the context of micromagnetics, using our recent implementation of smooth spring-driven motion (Rissanen and Laurson 2018 Phys. Rev. E 97 053301) to simulate ring-down measurements in two setups where domain wall dynamics is induced by mechanical motion. These include a single thin film with a domain wall in an external field and a setup mimicking a magnetic cantilever tip and substrate, in which the two magnets interact through dipolar interactions. We investigate how various micromagnetic parameters

influence the domain wall dynamics actuated by the oscillatory spring-driven mechanical motion and the resulting damping coefficient. Our simulations show that the magnitude of magnetic friction can be comparable to other forms of non-contact friction. For oscillation frequencies lower than those inducing excitations of the internal structure of the domain walls, the damping coefficient is found to be independent of frequency. Hence, our results obtained in the frequency range from 8-112 MHz are expected to be relevant also for typical experimental setups operating in the 100 kHz range.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Physics, Research area: Computational Physics, Aalto University, COMP Centre of Excellence
Contributors: Rissanen, I., Laurson, L.
Publication date: 13 Aug 2019
Peer-reviewed: Yes

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Journal: Journal of Physics D: Applied Physics
Volume: 52
Issue number: 44
Article number: 445002
ISSN (Print): 0022-3727
Ratings:

Scopus rating (2019): CiteScore 5.3 SJR 0.899 SNIP 1.144
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Condensed Matter Physics, Acoustics and Ultrasonics, Surfaces, Coatings and Films
Keywords: magnetic friction, micromagnetics, thin films
DOIs:

10.1088/1361-6463/ab351f
Source: Scopus
Source ID: 85072336407
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of Multiple Impacts on the Deformation of Wear-Resistant Steels
More durable materials enable reducing the downtime and maintenance costs by decreasing the number of replaced core components in various industrial applications. In this study, the behavior of three wear-resistant quenched martensitic steel grades and the S355 structural steel was examined in controlled impact conditions. The materials' impact behavior was investigated by several methods including residual stress measurements and electron backscatter diffraction. For all studied materials, the size and depth of the impact marks correlate via a logarithmic function to the number of impacts mostly due to work hardening. The underlying deformation behavior of the material depends on the mechanical properties and microstructure of the material. At high impact counts, softer martensitic steel was found to behave differently when compared to the other tested materials as it underwent severe changes in its microstructure and exhibited marked hardening.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Materials Characterization, Engineering materials science and solutions (EMASS), AC2T Research GmbH
Contributors: Ratia, V., Rojacz, H., Terva, J., Valtonen, K., Badisch, E., Kuokkala, V. T.
Publication date: 21 Jan 2015
Peer-reviewed: Yes

Publication information
Journal: Tribology Letters
Volume: 57
Issue number: 2
Article number: 15
ISSN (Print): 1023-8883
Ratings:

Scopus rating (2015): CiteScore 3.7 SJR 1.013 SNIP 1.237
Original language: English
ASJC Scopus subject areas: Mechanical Engineering, Mechanics of Materials, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Deformation, EBSD, Impact, Martensite, Residual stresses, Steel
DOIs:

10.1007/s11249-014-0460-7
URLs:

http://www.scopus.com/inward/record.url?scp=84937924221&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84937924221
Research output: Contribution to journal › Article › Scientific › peer-review

The role of edge-concentrated wear in impact-abrasion testing

The role of edge wear was studied in impact-abrasion testing conditions with an impeller-tumbler type test device. Three steels with different mechanical properties were tested at 30° and 90° sample angles using natural granite stone as abrasive particles. The edge and planar (inner) areas were carefully exposed to the same conditions by using tightly fitted two-part samples to obtain relevant information about the differences in their wear behavior. The role of edge-concentrated wear was dominant in all materials, and the edge wear rate was several times higher than the wear rate of the inner parts of the specimens. The difference in wear rate was particularly large in short tests and with the 90° sample angle. However, the dominance of the edge-concentrated wear decreased as the test duration became longer. The wear mechanism was largely microfatigue in all materials, but the samples tested at the 30° sample angle showed more microcutting in comparison to the 90° samples. Moreover, the role of microcutting was higher in the wear of the edge parts than in the inner parts.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Materials Characterization, SSAB
Contributors: Ratia, V., Valtonen, K., Kemppainen, A., Kuokkala, V. T.
Number of pages: 7
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Publication date: 2016
Peer-reviewed: Yes

Publication information

Journal: Tribology Online
Volume: 11
Issue number: 2
ISSN (Print): 1881-218X
Ratings:

Scopus rating (2016): CiteScore 0.7 SJR 0.3 SNIP 0.644
Original language: English
ASJC Scopus subject areas: Surfaces, Coatings and Films
Keywords: Abrasion, Angle, Edge, Impact, Steel, Testing, Wear, Wear mechanism
DOIs:

10.2474/trol.11.410
Source: Scopus
Source ID: 84969135979
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
Journal: Colloids and Interface Science Communications
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
URLs:

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:

10.1016/j.tsf.2012.09.017
URLs:

http://www.scopus.com/inward/record.url?scp=84868593394&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84868593394
Research output: Contribution to journal › Article › Scientific › peer-review

Morphology evolution of PS-b-PDMS block copolymer and its hierarchical directed self-assembly on block copolymer templates
Cylinder-forming polystyrene-block-polydimethylsiloxane (PS-b-PDMS, 27.2k-b-11.7k, SD39) block copolymer having a total molecular weight of 39 kg mol^{-1} was exploited to achieve in-plane morphologies of lines, dots and antidots. Brush-

free self-assembly of the SD39 on silicon substrates was investigated using solvents that were PS or PDMS selective, neutral and non-solvents based on their Hansen solubility parameters. The different morphologies were achieved with annealing times ranging from 10 min to 1 h at room temperature. The SD39 patterns were used as an etch mask for transferring the pattern into the underlying substrate. Directed self-assembly and hierarchical directed self-assembly on block copolymer templates for confinement of dots was successfully demonstrated. The strategy for achieving multiple morphologies using one BCP by mere choice of the annealing solvents on unmodified substrates provides a simplified method for surface nanopatterning, templated growth of nanomaterials and nanofabrication.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Photonics, Danmarks Tekniske Universitet, DTU Informatik, Trinity College Dublin, Laboratory of Photonics
Contributors: Rasappa, S., Schulte, L., Borah, D., Hulkkonen, H., Ndoni, S., Salminen, T., Senthamaraikanan, R., Morris, M. A., Niemi, T.
Number of pages: 7
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Publication date: 15 May 2018
Peer-reviewed: Yes

Publication information
Journal: Microelectronic Engineering
Volume: 192
ISSN (Print): 0167-9317
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Scopus rating (2018): CiteScore 4.2 SJR 0.561 SNIP 0.958
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Atomic and Molecular Physics, and Optics, Condensed Matter Physics, Surfaces, Coatings and Films, Electrical and Electronic Engineering
Keywords: Block copolymer, Hansen solubility, Hierarchical self-assembly, Selective solvent
DOIs:

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Source: Scopus
Source ID: 85041706803
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
Publication status: Published
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
Pages: 173-181
Publication date: 1986
Peer-reviewed: Yes

Publication information
Journal: Studies in Surface Science and Catalysis
Volume: 26
Issue number: C
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

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.

General information

Publication status: Published
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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Publication information

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Volume: 135
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Article number: 46673
ISSN (Print): 0021-8995
Ratings:

Scopus rating (2018): CiteScore 4 SJR 0.554 SNIP 0.842
Original language: English
ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry
Keywords: cellulose and other wood products, functionalization of polymers, mechanical properties, thermal properties, thermosets
DOIs:

10.1002/app.46673

Bibliographical note

EXT="Skrifvars, Mikael"
Source: Scopus
Source ID: 85049105961
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).

General information

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MoE publication type: A1 Journal article-refereed

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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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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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
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Influence of As/group-III flux ratio on defects formation and photovoltaic performance of GaInNAs solar cells
The correlation between the As to group III flux ratio and photovoltaic performance of $GaIn_{0.1}N_{0.03}As$ solar cells fabricated by molecular beam epitaxy is systematically investigated. The results show that flux ratio has a remarkable influence on the formation of defect traps. Furthermore, the formation of defects at different flux ratios is correlating with the variation of the background doping level and the photovoltaic performance. In particular, this study reveals a linear dependency between current generation, dark saturation current, defect densities, photoluminescence peak intensity and

the flux ratio. A significant increase in solar cell performance, exhibiting maximum external quantum efficiency of 90%, is obtained when As/group-III ratio is decreased close to the stoichiometric limit. For optimized growth condition, the 1 eV $GaIn_{0.1}N_{0.03}As$ solar cell exhibits a short circuit current density as high as 17.9 mA/cm^2 calculated from the external quantum efficiency data (AM0 conditions) with 870 nm high-pass filter. This value reflects the potential of the GaInNAs cell for current matching and power generation in high efficiency solar cells incorporating three- or four- junctions.

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Organisations: Optoelectronics Research Centre, Research group: Semiconductor Technology and Applications
Contributors: Polojärvi, V., Aho, A., Tukiainen, A., Raappana, M., Aho, T., Schramm, A., Guina, M.
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ASJC Scopus subject areas: Renewable Energy, Sustainability and the Environment, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films
Keywords: Defects, Dilute nitrides, III-V semiconductors, Material characterization, Molecular beam epitaxy, Multijunction solar cells
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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.

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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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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.

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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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Bibliographical note

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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···Na^+ ion pair) has only a weak effect on the electron binding energy.

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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.
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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.

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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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Original language: English
ASJC Scopus subject areas: Surfaces, Coatings and Films, Physical and Theoretical Chemistry, Materials Chemistry
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Source: Scopus
Source ID: 79952844542
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

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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.
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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
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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

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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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Source ID: 84880155215
Research output: Contribution to journal › 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

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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.
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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

Microwave induced hierarchical nanostructures on aramid fibers and their influence on adhesion properties in a rubber matrix

Several commercial surface treatments are used to increase the adhesion between aramid fibers and the matrix material in composite structures but each of these has some limitations. The aim of this study is to address some of these limitations by developing a surface treatment method for aramid fibers that would not affect mechanical properties of the fibers negatively, could be used with any matrix material and that could withstand handling of the fibers and ageing. The method used is microwave assisted surface treatment that uses microwave radiation together with dry reactive chemicals to create hierarchical structures to the fiber surface and so makes it possible to control the adhesion properties of the fibers. SEM and AFM imaging, fiber tensile tests and modified bundle pull-out test were used to investigate the outcome of the surface treatment and measure adhesion between aramid fiber bundles and rubber. SEM and AFM imaging revealed that nanoscale deposits are formed on to the fiber surface which enable mechanical interlocking between the fiber and the matrix material. Fiber tensile tests showed that the surface treatment does not influence the tensile properties of the fiber negatively. Results from the bundle pull-out tests confirmed that this kind of method can lead up to 259% improvement in adhesion when compared to untreated aramid fibers in the rubber matrix.

General information

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Organisations: Materials Science, Research group: Plastics and Elastomer Technology, Institute for Materials and Processes, University of Edinburgh
Contributors: Palola, S., Sarlin, E., Kolahgar Azari, S., Koutsos, V., Vuorinen, J.
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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

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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.
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Source: Scopus
Source ID: 85087483658
Research output: Contribution to journal › Review Article › Scientific › peer-review

Modification of Surface States of Hematite-Based Photoanodes by Submonolayer of TiO_2 for Enhanced Solar Water Splitting

Surface states are inherently involved with photoelectrochemical (PEC) solar fuel production; some of them are beneficial and participate in the surface reactions, but some act as recombination centers and therefore limit the PEC efficiency. Surface treatments have been applied to modify the surface states, but interrelated effects of the treatments on both types of surface states have not been properly considered. This research examines the modification of the surface states on hematite-based photoanodes by atomic layer deposition of submonolayer amount of TiO2 and by postannealing treatments. Our results show that the postannealing causes diffusion of Ti deeper into the hematite surface layers, which leads to an increased saturation photocurrent and an anodic shift in the photocurrent onset potential. Without postannealing, the separate TiO2 phase on the hematite surface results in a second intermediate surface state and delayed charge carrier dynamics, i.e., passivation of the recombination surface states. It is evident by these results that the intermediate surface states observed with impedance spectroscopy in a PEC cell are directly involved in the surface reaction and not with the recombination surface states observed with ultrafast (picoseconds-nanoseconds) transient absorption spectroscopy in air. These results open new optimization strategies to control the beneficial and detrimental surface states independently.

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Contributors: Palmolahti, L., Ali-Löytty, H., Khan, R., Saari, J., Tkachenko, N. V., Valden, M.
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Source: Scopus
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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.

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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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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films, Medicine(all)
DOIs:
10.1021/jp5111086
URLs:
http://www.scopus.com/inward/record.url?scp=84915764488&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84915764488
Research output: Contribution to journal › Article › Scientific › peer-review

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
Publication date: 24 Sep 2015
Peer-reviewed: Yes
Early online date: 26 Aug 2015

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Volume: 119
Issue number: 38
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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.5b06457

Bibliographical note
AUX=fys,"Pöyry, Annika"
Source: Scopus
Source ID: 84942342622
Research output: Contribution to journal › 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
Pages: 73-81
Publication date: 15 Oct 2015
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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
URLs:

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

Publication information

Journal: Wear
Volume: 388-389
ISSN (Print): 0043-1648
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: Bearings, Bimetals, Lead substitution, Non-ferrous metals, Solid lubricants
Electronic versions:

Oksanen Wear paper. Embargo ended: 4/05/19
DOIs:

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
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.

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: Oksa, M., Varis, T., Ruusuvuori, K.
Number of pages: 10
Pages: 191-200

Publication date: 25 Jul 2014
Peer-reviewed: Yes

Publication information
Journal: Surface and Coatings Technology
Volume: 251
ISSN (Print): 0257-8972
Ratings:

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:

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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:

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URLs:

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Source: Scopus
Source ID: 84878627004
Research output: Contribution to journal › Review 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.
Pages: 11807-11811
Publication date: Jun 2018
Peer-reviewed: Yes
Early online date: 1 Jan 2018

Publication information
Journal: Ceramics International
Volume: 44
Issue number: 10
ISSN (Print): 0272-8842
Ratings:

Scopus rating (2018): CiteScore 5.2 SJR 0.888 SNIP 1.297
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:

10.1016/j.ceramint.2018.03.267
Source: Scopus
Source ID: 85044921933
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.
Number of pages: 8
Pages: 225-232
Publication date: 15 Sep 2014
Peer-reviewed: Yes

Publication information
Journal: Wear
Volume: 317
Issue number: 1-2
ISSN (Print): 0043-1648
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:

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DOIs:

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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
Source: researchoutputwizard
Source ID: 1185
Research output: Contribution to journal › Article › Scientific › peer-review

The formation and characterization of fretting-induced degradation layers using quenched and tempered steel
Fretting movement is dangerous for machines, because it can cause cracking and surface degradation. The aim of this work was to characterize fretting-induced material degradation in large flat-on-flat contacts without edge effects in a sliding direction using quenched and tempered steel 34CrNiMo6. The focus was on the adhesive contact spots, which were formed under a wide variety of operating conditions. Characterization methods were optical microscopy, Vickers hardness tests and scanning electron microscopy. Three different degradation areas were observed: a general deformation layer, a tribologically transformed structure and a third body layer. All the degradation phases have high hardness and low ductility compared to the base material. The formation and behavior of the degradation layers in different operating conditions were discussed.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Tribology and Machine Elements, Research group: Materials Characterization, Wärtsilä
Contributors: Nurmi, V., Hintikka, J., Juoksukangas, J., Honkanen, M., Vippola, M., Lehtovaara, A., Mäntylä, A., Vaara, J., Frondelius, T.
Number of pages: 10
Pages: 258-267
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Peer-reviewed: Yes
Early online date: 14 Sep 2018

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Journal: Tribology International
Volume: 131
ISSN (Print): 0301-679X
Ratings:

Scopus rating (2019): CiteScore 7.9 SJR 1.536 SNIP 2.373
Original language: English
ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Adhesion, Fretting, Friction, Microscopy
Electronic versions:

1-s2.0-S0301679X18304523-main
DOIs:

10.1016/j.triboint.2018.09.012
URLs:

http://urn.fi/URN:NBN:fi:tty-201812202882

Bibliographical note
INT=mol,"Nurmi, Verner"
EXT="Hintikka, Jouko"
Source: Scopus
Source ID: 85056207084
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).

General information

Publication status: Published
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
Publication date: 2015
Peer-reviewed: Yes

Publication information

Journal: Journal of Thermal Spray Technology
Volume: 24
Issue number: 3
ISSN (Print): 1059-9630
Ratings:

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

RF measurements to pinpoint defects in inkjet-printed, thermally and mechanically stressed coplanar waveguides

In this work 10-GHz-band RF measurement and microscopy characterizations were performed on thermally and mechanically long-term-stressed coplanar waveguides (CPW) to observe electrical and mechanical degradation in 1-mm-thick PPO/PPE polymer substrates with inkjet-printed Ag conductors. The structure contained two different CPW geometries in a total of 18 samples with 250/270 μm line widths/gaps and 670/180 μm line widths/gaps. A reliability test was carried out with three sets. In set #1 three 250 μm and three 670 μm lines were stored in room temperature conditions and used as a reference. In set #2 six samples were thermally cycled (TC) for 10,000 cycles, and in set #3 six samples were thermally cycled and bent with 6 mm and 8 mm bending diameters. Thermal stressing was done by cycling the samples in a thermal cycling test chamber operating at 0/100 °C with 15-minutes rise, fall, and dwell times, resulting in a one-hour cycle. The samples were analyzed during cycling breaks using a vector network analyzer (VNA). In addition to optical microscopy, field emission scanning electron microscopy (FESEM) and atomic force microscopy (AFM) imaging were used to mechanically characterize the structures. The results showed that the line width of 670 μm had better signal performance and better long-term reliability than the line width of 250 μm. In this study, the average limit for proper RF operation was 2500 thermal cycles with both line geometries. The wide CPW lines provided more stable characteristics than the narrow CPW lines for the whole 10,000-cycle duration of the test, combined with repeated bending with a maximum bending radius of 6 mm. A phenomenon of nanoparticle silver protruding from cracks in the print of the bent samples was observed, as well as fracturing of the silver print in the CPW lines.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Electronics and Communications Engineering, Microelectronics Research, University of Oulu, Tampere University of Applied Sciences
Contributors: Myllymäki, S., Putaala, J., Hannu, J., Kunnari, E., Mäntysalo, M.
Number of pages: 9
Pages: 142-150
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Journal: Microelectronics Reliability
Volume: 65
ISSN (Print): 0026-2714
Ratings:

Scopus rating (2016): CiteScore 2.6 SJR 0.447 SNIP 0.991
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Atomic and Molecular Physics, and Optics, Condensed Matter Physics, Safety, Risk, Reliability and Quality, Surfaces, Coatings and Films, Electrical and Electronic Engineering
DOIs:

10.1016/j.microrel.2016.08.021

Bibliographical note
EXT="Kunnari, Esa"
EXT="Myllymäki, Sami"
Source: Scopus
Source ID: 84992618636
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
Peer-reviewed: Yes

Publication information
Journal: Journal of Applied Polymer Science
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Article number: 42595
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
DOIs:

10.1002/app.42595
URLs:

http://www.scopus.com/inward/record.url?scp=84937636904&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note
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
Publication status: Published
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.
Number of pages: 6
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Journal: Journal of Applied Polymer Science
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Issue number: 28
Article number: 42246
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: aging, degradation, rheology, thermoplastics, PHOTOOXIDATION, FILMS, PHOTOLYSIS
Electronic versions:

comparison_of_rheology_and_ftir_post-print
DOIs:

10.1002/app.42246
URLs:

http://urn.fi/URN:NBN:fi:tty-201612024837
URLs:

http://www.scopus.com/inward/record.url?scp=84928363110&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note
ORG=mol,0.7
ORG=keb,0.2
ORG=mei,0.1
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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.

General information

Publication status: Published
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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ISSN (Print): 0021-8995
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: Ageing, Degradation, Polyolefins, Recycling
DOIs:

10.1002/app.43766
Source: Scopus
Source ID: 84992303578
Research output: Contribution to journal › Article › Scientific › peer-review

Morphological and structural changes in laser CVD of silicon: comparison of theoretical temperature calculations with experimental results

The paper considers to what extent theoretical calculation of the laser induced temperature profile in a substrate can be used to predict the morphology and structure of silicon tracks deposited by pyrolytic LCVD. The micron scale tracks are deposited from silane using a focussed argon ion laser onto a substrate consisting of 1000 Å SiO_2 upon a 300 μm thick, 100 mm diameter, [100] silicon wafer. The influence of various experimental parameters such as scan speed, laser power, gas pressure and gas composition on the temperature profile and on the deposited silicon track is investigated. Temperature profiles and their time evolution are simulated by numerically solving the heat diffusion equation using a finite difference approach. The track deposition is simulated using experimental temperature and pressure dependent growth rates. Gaussian shaped low laser power track profiles are well reproduced but the volcano like structures of high power deposition are not explained by the present model alone. The calculations are found to explain, at least qualitatively, the observed relationships between various experimental parameters.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Herriot-Watt University, Microelectronics and Materials Physics Laboratories, University of Oulu
Contributors: Milne, D., Wilson, J. I. B., Rantala, T. T., Lenkkeri, J.
Number of pages: 6
Pages: 81-86
Publication date: 2 Dec 1989
Peer-reviewed: Yes

Publication information

Journal: Applied Surface Science

Volume: 43
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ISSN (Print): 0169-4332
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Condensed Matter Physics
DOIs:
10.1016/0169-4332(89)90194-3
Source: Scopus
Source ID: 0024900802
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
Pages: 1312-1322
Publication date: 2015
Peer-reviewed: Yes

Publication information

Journal: Journal of Thermal Spray Technology
Volume: 24
Issue number: 7
ISSN (Print): 1059-9630
Ratings:
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: corrosion behavior, Fe-based coatings, HVAF, structure
DOIs:
10.1007/s11666-015-0298-z
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.
Number of pages: 10
Pages: 81-90
Publication date: 15 Sep 2015
Peer-reviewed: Yes

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Journal: Surface and Coatings Technology
Volume: 277
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, Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Corrosion behaviour, Fe-based coating, HVAF, Structure
DOIs:

10.1016/j.surfcoat.2015.07.018
URLs:

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

Publication status: Published
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.
Number of pages: 16
Pages: 1040–1055
Publication date: Jun 2016
Peer-reviewed: Yes
Early online date: 27 Apr 2016

Publication information

Journal: Journal of Thermal Spray Technology
Volume: 25
Issue number: 5
ISSN (Print): 1059-9630
Ratings:

Scopus rating (2016): CiteScore 3.1 SJR 0.659 SNIP 0.932

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:

10.1007/s11666-016-0410-z
Research output: Contribution to journal › Article › Scientific › peer-review

Evaluation of screen printed silver trace performance and long-term reliability against environmental stress on a low surface energy substrate

Otherwise attractive substrate materials for printed electronics may have such surface characteristics that make patterning challenging. This article focuses on the printability and performance characterization of conductive patterns on a low surface energy substrate. Surface characteristics of a hydrophobic polyphenylene ether (PPE) substrate and the effects of surface modification using chemical and physical pre-treatments were studied. In addition, silver ink performance and its reliability on this substrate were evaluated. The surface was characterized by surface energy measurements and surface profile analysis. Screen-printed test patterns were characterized to evaluate print quality and electrical and mechanical performance. A further inspection of substrate-ink interactions was conducted using environmental reliability tests. It was observed that ink adhesion could be significantly promoted by choosing a suitable surface pre-treatment method. Low sheet resistances were obtained, and thus, suitable inks for further characterization were found. In addition, it was observed that environmental stress has a significant impact on ink-substrate interactions.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Electronics and Communications Engineering, Nano Communication Centre
Contributors: Mikkonen, R., Mäntysalo, M.
Number of pages: 12
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Publication date: 1 Jul 2018
Peer-reviewed: Yes

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Journal: Microelectronics Reliability
Volume: 86
ISSN (Print): 0026-2714
Ratings:

Scopus rating (2018): CiteScore 2.6 SJR 0.376 SNIP 1.017
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Atomic and Molecular Physics, and Optics, Condensed Matter Physics, Safety, Risk, Reliability and Quality, Surfaces, Coatings and Films, Electrical and Electronic Engineering
Keywords: Adhesion, Environmental stress, PPE, Printed electronics, Reliability, Surface modification
Electronic versions:

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DOIs:

10.1016/j.microrel.2018.05.010
URLs:

http://urn.fi/URN:NBN:fi:tuni-201909273544. Embargo ended: 20/05/20
Source: Scopus
Source ID: 85047240351
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.
Number of pages: 12
Pages: 4546-4557
Publication date: 26 Apr 2018
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Publication information
Journal: Journal of Physical Chemistry B
Volume: 122
Issue number: 16
ISSN (Print): 1520-6106
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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:

10.1021/acs.jpcb.7b12510

Bibliographical note
EXT=”Martinez-Seara, Hector”
EXT="Ollila, O. H. Samuli"
Source: Scopus
Source ID: 85046019210
Research output: Contribution to journal › Article › Scientific › peer-review

Advanced coatings by novel high-kinetic thermal spray processes
Thermal spraying includes a group of coating processes in which metallic and non-metallic materials are spray deposited as fine particles in a molten or semi-molten condition, or even in fully solid state to form a coating. Thermal spraying allows deposition of relatively thick coatings, from some tens of micrometers up to several millimeters in thickness. Thermally sprayed coatings are used in different applications including protective and functional coatings in mechanical engineering, energy technology, biomedical, steel, automotive and aerospace technologies and in many other industrial sectors. Novel high-kinetic spray processes, e.g., the high velocity air-fuel (HVAF) technology are the latest developments in the area and therefore they are actively studied in the framework of the Hybrid Materials research program in collaboration with Finnish industrial and research partners. Novel multifunctional coatings are under development for specific industrial applications.

General information
Publication status: Published
MoE publication type: D1 Article in a trade journal
Organisations: Department of Materials Science, Research group: Surface Engineering
Contributors: Matikainen, V., Koivuluoto, H., Milanti, A., Vuoristo, P.
Number of pages: 5
Pages: 46-50
Publication date: 9 Feb 2015
Peer-reviewed: Unknown

Publication information
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Issue number: 1
ISSN (Print): 1459-9694
Original language: English
ASJC Scopus subject areas: Surfaces, Coatings and Films
Keywords: thermal spraying, HVOF, HVAF
Electronic versions:

M1-15 s 46-50 Matikainen, Koivuluoto, Milanti, Vuoristo
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http://www.vuorimiesyhdistys.fi/sites/default/files/materia/pdf/Materia%201-2015.pdf

Research output: Contribution to journal › Article › Professional

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

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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
Contributors: Matikainen, V., Bolelli, G., Koivuluoto, H., Sassatelli, P., Lusvarghi, L., Vuoristo, P.
Pages: 57-71
Publication date: 2017
Peer-reviewed: Yes
Early online date: 6 Apr 2017

Publication information

Journal: Wear
Volume: 388-389
ISSN (Print): 0043-1648
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
DOIs:

10.1016/j.wear.2017.04.001
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.

General information
Publication status: Published
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.
Number of pages: 18
Pages: 1-18
Publication date: Aug 2017
Peer-reviewed: Yes

Publication information
Journal: Journal of Thermal Spray Technology
Volume: 26
Issue number: 6
ISSN (Print): 1059-9630
Ratings:

Scopus rating (2017): CiteScore 3.3 SJR 0.688 SNIP 1.209
Original language: English
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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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
Publication status: Published
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
Number of pages: 15
Pages: 680-694
Publication date: 1 Apr 2018
Peer-reviewed: Yes

Publication information
Journal: Journal of Thermal Spray Technology
Volume: 27
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_3C_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_3C_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

Publication status: Published
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
Pages: 196-212
Publication date: 25 Jul 2019
Peer-reviewed: Yes

Publication information

Journal: Surface and Coatings Technology
Volume: 370
ISSN (Print): 0257-8972
Ratings:

Scopus rating (2019): CiteScore 5.8 SJR 0.938 SNIP 1.614
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

INT=msee,"Rubio Peregrina, S."
Source: Scopus
Source ID: 85065223119
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
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Research group: Surface Engineering, Materials Science and Environmental Engineering
Contributors: Matikainen, V., Koivuluoto, H., Vuoristo, P.
Number of pages: 11
Publication date: 15 Apr 2020
Peer-reviewed: Yes

Publication information
Journal: Wear
Volume: 446-447
Article number: 203188
ISSN (Print): 0043-1648
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
DOIs:
10.1016/j.wear.2020.203188
Source: Scopus
Source ID: 85077986604
Research output: Contribution to journal › Article › Scientific › peer-review

Slurry and dry particle erosion wear properties of WC-10Co4Cr and Cr_3C_2-25NiCr hardmetal coatings deposited by HVOF and HVAF spray processes

Thermally sprayed hardmetal coatings were produced to provide improved erosion wear compared to conventional cast GX4CrNi13-4 martensitic steel (CA6NM) used in hydro turbine components. Sprayed coatings and reference materials were tested with high-speed slurry pot tester using either fine or coarse quartz as the erosive media. Additional erosion tests were carried out with centrifugal dry erosion tester. Tungsten carbide based coatings provided the highest wear resistance due to the high hardness and even distribution of the fine carbide particles. The cast 13-4 steel samples experienced up to 180 times higher wear rates in fine quartz slurry and up to 36 times higher wear rates in coarse slurry compared to the sprayed coatings.

General information
Publication status: Published
MoE publication type: B1 Article in a scientific magazine
Organisations: Research group: Surface Engineering, Materials Science and Environmental Engineering, Research group: Materials Characterization, VZÚ Plzeò
Contributors: Matikainen, V., Rubio Peregrina, S., Ojala, N., Koivuluoto, H., Schubert, J., Houdková, Vuoristo, P.
Number of pages: 4
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Publication date: 2019
Peer-reviewed: No

Publication information
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Volume: 36
Issue number: 1-2
ISSN (Print): 0780-2285
Ratings:
Scopus rating (2019): SJR 0.146 SNIP 0.277
Original language: English
ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Coating, Erosion, Hardmetal, Slurry erosion, Thermal spray
DOIs:
10.30678/FJT.83590

Bibliographical note
INT=msee,"Rubio Peregrina, S."
Source: Scopus

Source ID: 85084464052
Research output: Contribution to journal › Article › Scientific

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

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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
Contributors: Mason, P. E., Wernersson, E., Jungwirth, P.
Number of pages: 9
Pages: 8145-8153
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Peer-reviewed: Yes

Publication information

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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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http://www.scopus.com/inward/record.url?scp=84863696122&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84863696122
Research output: Contribution to journal › Article › Scientific › peer-review

Tribocorrosion behaviour of two low-alloy steel grades in simulated waste solution

The tribocorrosion behaviour of two low-alloy steels not previously investigated, was examined in a Pin-on-Disc test device, both in the presence and absence of mechanical wear and/or corrosion in simulated waste solution. Volume losses through wear, corrosion and synergy processes were calculated and changes in the material surfaces investigated. The tribocorrosion behaviour and the volume losses caused by the synergy processes were found to be dependent on the steel grade, instead of applied potential. For both steel grades, material losses were caused by two main degradation mechanisms: wear and wear-induced corrosion. Total material losses and the percentage of wear-corrosion synergy were higher for the ferritic grade than for the martensitic grade. These results are presented and discussed in this paper.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Physics, VTT Technical Research Centre of Finland, Microscopy Center
Contributors: Mäntyranta, A., Heino, V., Isotahdon, E., Salminen, T., Huttunen-Saarivirta, E.
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Original language: English
ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Contact: sliding, Synergism: tribochemistry, Wear: corrosive
DOIs:

10.1016/j.triboint.2019.05.032

Bibliographical note
EXT="Heino, Vuokko"
EXT="Isotahdon, Elisa"
Source: Scopus
Source ID: 85066497579
Research output: Contribution to journal › Article › Scientific › peer-review

Prediction of contact condition and surface damage by simulating variable friction coefficient and wear
A simulation method to predict the reliability of clamped metal contacts under cyclic loading is presented. The main idea is to predict the development of contact condition of a joint by simulating a spatially variable coefficient of friction (COF) and wear. Frictional energy dissipation drives the COF evolution rule, and classic Archard's equation is employed as the evolution rule for wear depth. As both the COF and wear evolution are considered, the presented approach is capable of predicting changes in the contact condition over time. The approach is based on the Finite Element Method (FEM) and is generally applicable to industrial cases. The method is implemented as a subroutine to a FEM solver Abaqus to define a contact formulation in both normal and tangential directions. The subroutine allows full coupling between normal and tangential contact variables, which makes the approach robust also in complex industrial applications. As the effect of wear is described in the contact pressure calculation, there is no need for mesh modification. The presented approach was validated by simulating cylinder-on-plane configuration. The presented method provides similar results obtained with a simulation where geometry is updated due to wear. The results of the case study were qualitatively verified against a bolted joint type fretting experiment. The area of slip after stabilized COF distribution corresponds well with the experimental fretting scars. However, Archard's wear law seems to be limited, at least in partial slip cases, as it overestimates the amount of wear without considering entrapment of wear debris in the contact. A case study of medium speed combustion engine component is presented to show how the simulation method can be used in engine development to ensure reliable contact interfaces.

General information
Publication status: E-pub ahead of print
MoE publication type: A1 Journal article-refereed
Organisations: Research group: Tribology and Machine Elements, Materials Science and Environmental Engineering, University of Oulu, Research and Development, Wärtsilä Finland
Contributors: Mäntylä, A., Hintikka, J., Frondelius, T., Vaara, J., Lehtovaara, A., Juoksukangas, J.
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Article number: 106054
ISSN (Print): 0301-679X
Ratings:

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Original language: English
ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Contact, Fatigue, Finite element method, Fretting, Friction, Wear
DOIs:

10.1016/j.triboint.2019.106054
Source: Scopus
Source ID: 85075347573
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

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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

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Issue number: 2
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

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.
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Publication information

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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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10.1002/app.40341
URLs:

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Source: Scopus
Source ID: 84897664169
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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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

Catalytic Activity of AuCu Clusters on MgO(100): Effect of Alloy Composition for CO Oxidation
Density functional simulations have been performed for Au_7Cu_{23} and $Au_{23}Cu_7$ clusters on MgO(100) supports to probe their catalytic activity for CO oxidation. The adsorption of reactants, O_2 and CO, and potential O_2 dissociation have been investigated in detail by tuning the location of vacancies (F-center, V-center) in MgO(100). The total charge on Au_7Cu_{23} and $Au_{23}Cu_7$ is negative on all supports, regardless of the presence of vacancies, but the effect is significantly amplified on the F-center. Au_7Cu_{23}/MgO(100) and $Au_{23}Cu_7$/MgO(100) with an F-center are the only systems to bind O_2 more strongly than CO. In each case, O_2 can be effectively activated upon adsorption and dissociated to 2 × O atoms. The different reaction paths based on the Langmuir-Hinshelwood (LH) and Eley-Rideal (ER) mechanisms for CO oxidation have been explored on the Au_7Cu_{23} and $Au_{23}Cu_7$ clusters on F-centers, and the results are compared with the previous findings for $Au_{15}Cu_{15}$. Overall, the reaction barriers are small, but the changes in the Au:Cu ratio tune the reactant

adsorption energies and sites considerably, showing also varying selectivity for CO and O_2. The microkinetic model built on the basis of the above results shows a pronounced CO_2 production rate at low temperature for the clusters on F-centers.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Physics, Research group: Materials and Molecular Modeling, COMP Centre of Excellence, Department of Applied Physics, Aalto University, Aalto University, Norwegian Univ. of Sci. and Technol.
Contributors: Ma, L., Laasonen, K., Akola, J.
Number of pages: 11
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Volume: 121
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Energy(all), Surfaces, Coatings and Films, Physical and Theoretical Chemistry
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URLs:

http://urn.fi/URN:NBN:fi:tty-201905021452. Embargo ended: 17/02/18
Source: Scopus
Source ID: 85020757142
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.
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Peer-reviewed: Yes

Publication information

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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

Running-in effects on friction of journal bearings under slow sliding speeds

Hydrodynamic thrust and journal bearings are facing challenges in modern heavy-duty machinery where full film lubrication cannot always be achieved or sustained. This is due to reasons such as start–stop operation, increased power density and the use of thinner lubricants. Although this leads to increased overall efficiency, bearings are operating more often under mixed lubrication conditions. This is why the running-in behavior of the bearing material is important. In this study, running-in behavior of traditional leaded tin bronze and its environmentally sustainable alternative, bimetal bismuth, was studied. Experimental friction tests were performed with journal bearings under full film and mixed lubrication conditions in order to find the Stribeck curves. The results are analyzed using frictional energy, and friction coefficient values based on continuous friction monitoring. Remarkable reduction of friction was observed with both bearing materials due to running-in.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Research group: Tribology and Machine Elements, Materials Science and Environmental Engineering, Metso Minerals, Inc., Kugler Bimetal SA
Contributors: Linjamaa, A., Lehtovaara, A., Kallio, M., Léger, A.
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ASJC Scopus subject areas: Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
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Source ID: 85069872376
Research output: Contribution to journal › Article › Scientific › peer-review

The deformation, strain hardening, and wear behavior of chromium-alloyed hadfield steel in abrasive and impact conditions

The alloying of Hadfield steels aims at enhanced mechanical properties and improvements in the wear resistance. In this work, the impact and abrasive properties of a chromium-alloyed high-manganese Hadfield steel were experimentally studied using a wide variety of testing techniques and characterization methods. In addition, an in-service sample was characterized to identify the wear and hardening mechanisms in a real application (jaw crusher). The dynamic mechanical behavior of the steel was determined using the Hopkinson split bar technique. The abrasion properties were studied with three-body abrasion tests using several different natural abrasives. The effects of existing plastic strain and normal loading on the surface hardening and wear rate were further investigated with scratch testing. High-velocity impact testing was performed to evaluate the effect of pre-strain on the impact wear behavior of the material. It was shown that the dynamic loading affects both the yield behavior and the strain hardening rate of the studied steel. The connection between pre-strain, hardness, and wear rate in abrasion was established. In impact conditions, plastic straining of the surface layer first has a positive effect on the wear resistance, but when strain hardening reached the observed ductility limit, it showed an adverse effect on the material's performance. The addition of chromium and an increase in the manganese content from the nominal ASTM Hadfield composition provided some improvements in the strength, ductility, and surface hardening of the studied steel.

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), VTT Technical Research Centre of Finland
Contributors: Lindroos, M., Apostol, M., Heino, V., Valtonen, K., Laukkanen, A., Holmberg, K., Kuokkala, V. T.
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Original language: English
ASJC Scopus subject areas: Mechanical Engineering, Mechanics of Materials, Surfaces, Coatings and Films, Surfaces and Interfaces
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The deformation, strain hardening and wear behavior of chromium alloyed Hadfield steel in abrasive and impact conditions
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URLs:

http://urn.fi/URN:NBN:fi:tty-201603223737
Source: Scopus
Source ID: 84921751364
Research output: Contribution to journal › Article › Scientific › peer-review

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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Publication information
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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: 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

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
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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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Publication information
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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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Bibliographical note
EXT="Lindgren, M."
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
Publication status: Published
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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Peer-reviewed: Yes

Publication information
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Ratings:

Scopus rating (2016): CiteScore 5.3 SJR 1.588 SNIP 2.105
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
DOIs:

10.1016/j.wear.2016.06.007

Bibliographical note
EXT="Lindgren, M."
Source: Scopus
Source ID: 84975744612
Research output: Contribution to journal › Article › Scientific › peer-review

Numerical simulation of temperature distributions in layered structures during laser processing
A numerical simulation approach for the evaluation of temperature distribution in layer structured substrates during laser processing is introduced. The explicit finite-difference solution of the heat equation is used and the full non-linearity of the heat diffusion is taken into account by temperature dependent substrate parameters. The heat equations for layered structures are solved using both rectangular and cylindrical coordinate systems. The method is applied to CW Ar^+ laser-induced temperature distributions in some commonly used layer structures in microelectronics, such as silicon on sapphire (SOS) and SiO_2 coated silicon. Results are compared with experiments.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: University of Oulu, Microelectronics and Materials Physics Laboratories
Contributors: Levoska, J., Rantala, T. T., Lenkkeri, J.
Number of pages: 11
Pages: 12-22
Publication date: 1989
Peer-reviewed: Yes

Publication information
Journal: Applied Surface Science
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ISSN (Print): 0169-4332
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Condensed Matter Physics
DOIs:

10.1016/0169-4332(89)90895-7
Source: Scopus

Source ID: 0024301353
Research output: Contribution to journal › Article › Scientific › peer-review

Electrospun Black Titania Nanofibers: Influence of Hydrogen Plasma-Induced Disorder on the Electronic Structure and Photoelectrochemical Performance

This work encompasses a facile method for tailoring surface defects in electrospun TiO2 nanofibers by employing hydrogen plasma treatments. This amiable processing method was proven with SQUID, EPR, and XPS to be highly effective in generating oxygen vacancies, accompanied by the reduction of Ti4+ centers to Ti3+, resulting in the formation of black titania. The treatment temperature was found to affect the Ti3+/Ti4+ ratios and surface valence, while preserving the original 1D morphology of the titania fibers. Ab initio DFT calculations showed that a high concentration of oxygen vacancies is highly efficient in producing midgap states that enhance the system absorption over the whole visible range, as observed with UV/vis/NIR diffuse reflectance spectroscopy. Pristine TiO2 nanofibers produced a photocurrent density of similar to 0.02 mA/cm(2) at 1.23 V vs RHE, whereas the hydrogen plasma treatment resulted in up to a 10-fold increase in the photoelectrochemical performance.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Universita degli Studi di Padova, Italy, Univ Cologne, University of Cologne, Dept Chem, Chair Inorgan & Mat Chem, Padova University, INSTM, J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Institute of Inorganic Chemistry, Catalonia Institute for Energy Research (IREC), Multiscale Materials Modelling and Tribo Simulation, CNR-IENI
Contributors: Lepcha, A., Maccato, C., Mettenbörger, A., Andreu, T., Mayrhofer, L., Walter, M., Olthof, S., Ruoko, T. P., Klein, A., Moseler, M., Meerholz, K., Morante, J. R., Barreca, D., Mathur, S.
Number of pages: 8
Pages: 18835-18842
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Peer-reviewed: Yes

Publication information

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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)
Keywords: ROOM-TEMPERATURE, WATER, SURFACE, NANOSTRUCTURES, NANOPARTICLES, PHOTOCATALYSIS, INSULATORS, CONVERSION, DEFECTS, ARRAYS
Electronic versions:

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http://www.scopus.com/inward/record.url?scp=84939825598&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84939825598
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.
Number of pages: 12
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Publication information
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Article number: 53
ISSN (Print): 2079-6412
Original language: English
ASJC Scopus subject areas: Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Cold gas spraying, High-entropy alloy, Microstructure
Electronic versions:

Cold gas spraying of a high-entropy 2020
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Source: Scopus
Source ID: 85079063520
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
Publication status: E-pub ahead of print
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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Publication information
Journal: Materials and Corrosion
ISSN (Print): 0947-5117
Ratings:

Scopus rating (2019): CiteScore 2.4 SJR 0.433 SNIP 0.878
Original language: English
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
DOIs:

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Source: Scopus
Source ID: 85071360769
Research output: Contribution to journal › Article › Scientific › peer-review

Optimization of convectively cooled heat sinks

Many factors of heat sink, such as its size and mass, component locations, number of fins, and fan power affect heat transfer. Owing to the opposite effects of these factors on heat sink maximum temperature, we have now a multi-objective optimization problem. A typical optimization case consists of hundreds of heat sink temperature field evaluations, which would be impractical to do with CFD. Instead, we propose to combine analytical results of convection and numerical solution of conduction to address these so-called conjugated heat transfer problems. We solve heat conduction in a solid numerically using the finite volume method and tackle convection with the analytical equation of forced convection in a parallel plate channel.This model is suitable for forced and natural convection heat sinks, and we have verified its validity by comparing its results to measured data and CFD calculations. We use the model to improve two industrial examples, using a multi-objective version of the particle swarm optimization (PSO) algorithm. The first example is a forced convection heat sink composed of nine heat generating components at the base plate, and the other is a natural convection case with two components. In both cases, mass is minimized; the other criterion is maximum temperature for the forced convection case and heat sink outer volume for the natural convection case. Our method is many orders of magnitude faster than CFD. Additionally, we provide some LES results of pin fins with natural convection for further use in similar optimizations.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Mechanical Engineering and Industrial Systems
Contributors: Lampio, K., Karvinen, R.
Pages: 473-479
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Journal: Microelectronics Reliability
Volume: 79
ISSN (Print): 0026-2714
Ratings:

Scopus rating (2017): CiteScore 2.6 SJR 0.388 SNIP 0.907
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Atomic and Molecular Physics, and Optics, Condensed Matter Physics, Safety, Risk, Reliability and Quality, Surfaces, Coatings and Films, Electrical and Electronic Engineering
Keywords: Fin array, Forced convection, Heat sink, Multi-objective optimization, Natural convection, Pin fins
DOIs:

10.1016/j.microrel.2017.06.011
Source: Scopus
Source ID: 85020690970
Research output: Contribution to journal › Article › 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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Publication date: 2016

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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 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.
Number of pages: 10
Pages: 10042-10051
Publication date: 6 Aug 2015
Peer-reviewed: Yes

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Ratings:

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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.5b03604
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http://www.scopus.com/inward/record.url?scp=84938696964&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84938696964
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 ($\sim 10^2$-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.
Number of pages: 8
Pages: 4245-4252
Publication date: 17 Apr 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B
Volume: 118
Issue number: 15
ISSN (Print): 1520-6106
Ratings:

Scopus rating (2014): CiteScore 5.9 SJR 1.449 SNIP 1.13
Original language: English
ASJC Scopus subject areas: Surfaces, Coatings and Films, Physical and Theoretical Chemistry, Materials Chemistry
DOIs:

10.1021/jp500713q
URLs:

http://www.scopus.com/inward/record.url?scp=84899003075&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84899003075
Research output: Contribution to journal › Article › Scientific › peer-review

Fluid flow simulations meet high-speed video: Computer vision comparison of droplet dynamics
Hypothesis: While multiphase flows, particularly droplet dynamics, are ordinary in nature as well as in industrial processes, their mathematical and computational modelling continue to pose challenging research tasks - patent approaches for tackling them are yet to be found. The lack of analytical flow field solutions for non-trivial droplet dynamics hinders validation of computer simulations and, hence, their application in research problems. High-speed videos and computer vision algorithms can provide a viable approach to validate simulations directly against experiments. Experiments: Droplets of water (or glycerol-water mixtures) impacting on both hydrophobic and superhydrophobic surfaces were imaged with a high-speed camera. The corresponding configurations were simulated using a lattice-Boltzmann multiphase scheme. Video frames from experiments and simulations were compared, by means of computer vision, over entire droplet impact events. Findings: The proposed experimental validation procedure provides a detailed, dynamic one-on-one comparison of a droplet impact. The procedure relies on high-speed video recording of the experiments, computer vision, and on a software package for the analyzation routines. The procedure is able to quantitatively validate computer simulations against experiments and it is widely applicable to multiphase flow systems in general.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Physics, Natural Resources Institute Finland (Luke), BioFluidix GmbH, Faculty of Information Technology, Jyväskylän yliopisto
Contributors: Kulju, S., Riegger, L., Koltay, P., Mattila, K., Hyväluoma, J.
Number of pages: 9
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Journal: Journal of Colloid and Interface Science
Volume: 522
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Scopus rating (2018): CiteScore 9 SJR 1.29 SNIP 1.342
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Biomaterials, Surfaces, Coatings and Films, Colloid and Surface Chemistry
Keywords: Computer vision, Droplet, Experimental, High-speed video, Hydrophobic, Lattice Boltzmann, Simulation
DOIs:

10.1016/j.jcis.2018.03.053

Bibliographical note
EXT="Kulju, S."
Source: Scopus
Source ID: 85044153494
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.

General information
Publication status: Published
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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Publication date: 9 Jan 2014
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Ratings:

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
DOIs:

10.1021/jp410446d
URLs:

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Source: Scopus
Source ID: 84892594412
Research output: Contribution to journal › Article › Scientific › peer-review

Influence of temperature-induced copper diffusion on degradation of selective chromium oxy-nitride solar absorber coatings
Temperature-induced copper diffusion process and its influences on optical degradation and long-term stability of solar absorber coatings on copper substrates were investigated at intermediate temperatures of 248-500. °C. The studied absorbers were sputtered chromium oxy-nitride absorbers having tin oxide anti-reflection coatings. The absorbers were aged by means of thermal accelerated ageing studies and short-period heat treatments up to 500. °C for two hours.Ageing mechanisms and degradation of the absorbers were analysed before and after the ageing studies by optical measurements (solar absorptance with a UV/Vis/NIR spectrophotometer and thermal emittance by FTIR spectrophotometry), microstructural analysis using a field-emission scanning electron microscope (FESEM) equipped with an energy dispersive X-ray spectrometer (EDS) and a transmission electron microscope (TEM) with an EDS, composition by time-of-flight elastic recoil detection analysis (TOF-ERDA) and an X-ray photoelectron spectroscope (XPS), and adhesion by tensile test. The relation between optical degradation and diffusion mechanisms was studied using optical modelling and simulation. The results clearly revealed the mechanism of outward copper diffusion: diffusion of copper substrate atoms into the coating and through the coating to the surface, formation of copper oxide islands on the surface of the coating, and formation of voids in the substrate surface. The relation between the diffusion mechanisms and increase in thermal emittance of the absorber surface was demonstrated.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Surface Engineering, Research group: Materials Characterization, University of Helsinki
Contributors: Kotilainen, M., Honkanen, M., Mizohata, K., Vuoristo, P.
Number of pages: 10
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Publication date: 2016
Peer-reviewed: Yes

Publication information

Journal: Solar Energy Materials and Solar Cells
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Original language: English
ASJC Scopus subject areas: Renewable Energy, Sustainability and the Environment, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films
Keywords: Coating, Copper, Diffusion mechanisms, Solar absorber, Thermal diffusion, Void growth
DOIs:

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Source: Scopus
Source ID: 84949090386
Research output: Contribution to journal › Article › Scientific › peer-review

Hafnium oxide thin films as a barrier against copper diffusion in solar absorbers

The thermal stability of copper substrate material used in solar thermal collectors was investigated with and without atomic layer deposited (ALD) hafnium oxide barrier films at temperatures of 200–400 °C. HfO_2 films were studied as barriers against thermal diffusion of copper substrate atoms. The ALD HfO_2 thin films were deposited in a thermal process at 200 °C using Tetrakis(Dimethylamido)Hafnium($Hf(NMe_2)_4$) and H_2O precursors, with 200, 400, and 600 cycles. The Cu substrates with and without HfO_2 thin films were aged by means of heat treatment in air. The influence of the HfO_2 barriers was determined by optical, microstructural, and morphological analyses before and after the ageing procedures. The optical performance of the HfO_2 barriers as a part of solar absorber stack was modelled with CODE Coating Designer. The copper surface without a HfO_2 barrier thin film oxidized significantly, which increased thermal emittance and surface roughness. 200 cycles of HfO_2 deposition did not result in a completely continuous coating and only provided a little protection against oxidation. Films of 200 and 400 cycles gave continuous coverage and the thickest HfO_2 thin film studied, which was deposited from 600 ALD cycles and had a thickness ~50 nm, prevented Cu oxidation and diffusion processes after 2 h heat treatment in air at 300 °C, and retained low thermal emissivity. At 400 °C, diffusion and formation of copper oxide hillocks were observed but the HfO_2 thin film significantly retarded the degradation when compared to a Cu substrate without and with thinner barrier layers.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Surface Engineering, R&D Center for Low-Cost Plasma and Nanotechnology Surface Modifications (CEPLANT), Masaryk University
Contributors: Kotilainen, M., Krumpolec, R., Franta, D., Souček, P., Homola, T., Cameron, D. C., Vuoristo, P.
Number of pages: 7
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Publication date: 1 Jul 2017
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Volume: 166
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Renewable Energy, Sustainability and the Environment, Surfaces, Coatings and Films
Keywords: Copper diffusion, Diffusion barrier, HfO thin film, Solar absorber, Thermal ageing
DOIs:

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Source: Scopus
Source ID: 85016025672
Research output: Contribution to journal › Article › Scientific › peer-review

Surface-relief gratings and stable birefringence inscribed using light of broad spectral range in supramolecular polymer-bisazobenzene complexes

We report on phenol-pyridine hydrogen-bonded supramolecular polymer-azobenzene complexes made from a newly designed polar bisazobenzene chromophore. Because of the substitution with a polar nitro group, the chromophore possesses an extremely broad absorption band, spanning from near-UV up to 650 nm. Moreover, the inclusion of two methoxy groups to the central benzene ring prevents excessive chromophore-chromophore intermolecular interactions and provides advantageous size-related properties. Together, these features of the prepared photoresponsive polymer materials enable efficient inscription of (i) photoinduced birefringence with outstanding stability at various chromophore concentrations and (ii) surface-relief grating formation over a wide range of writing wavelengths from 405 to 633 nm. The photoresponsive behavior is compared to that of Disperse Yellow 7-based supramolecular complexes.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Department of Applied Physics, Aalto University, Tokyo Institute of Technology, University of Bristol
Contributors: Koskela, J. E., Vapaavuori, J., Hautala, J., Priimagi, A., Faul, C. F. J., Kaivola, M., Ras, R. H. A.
Number of pages: 8
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Publication date: 26 Jan 2012
Peer-reviewed: Yes

Publication information

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Volume: 116
Issue number: 3
ISSN (Print): 1932-7447
Ratings:

Scopus rating (2012): CiteScore 8 SJR 2.529 SNIP 1.461
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)
DOIs:

10.1021/jp210706n
URLs:

http://www.scopus.com/inward/record.url?scp=84856360260&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84856360260
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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MoE publication type: A1 Journal article-refereed
Organisations: University of Oulu, Department of Physical Sciences
Contributors: Koivusaari, K. J., Rantala, T. T., Leppävuori, S.
Number of pages: 5
Pages: 736-740

Publication date: Apr 2000
Peer-reviewed: Yes

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Volume: 9
Issue number: 3
ISSN (Print): 0925-9635
Ratings:

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:

10.1016/S0925-9635(99)00286-1
Source: Scopus
Source ID: 0033748066
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
Publication status: Published
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.
Number of pages: 10
Pages: 423–432
Publication date: 2018
Peer-reviewed: Yes
Early online date: 11 Jan 2018

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Volume: 27
Issue number: 3
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: cold spraying, diagnostics, in-flight properties, particle size, particle velocity
DOIs:

10.1007/s11666-018-0685-3
Source: Scopus
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
Publication status: Published
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.
Number of pages: 16
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Peer-reviewed: Yes

Publication information
Journal: Coatings
Volume: 10
Issue number: 4
Article number: 348
ISSN (Print): 2079-6412
Original language: English
ASJC Scopus subject areas: Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Al6061, Aluminum, Coatings, Cold spray, Diagnostics, Online monitoring, Process parameters
Electronic versions:

Cold-Sprayed Al6061 Coatings 2020
DOIs:

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URLs:

http://urn.fi/URN:NBN:fi:tuni-202008136463
Source: Scopus
Source ID: 85083845948
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.
Number of pages: 8
Pages: 7902-7909
Publication date: 17 Jul 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B
Volume: 118
Issue number: 28
ISSN (Print): 1520-6106
Ratings:

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)
DOIs:
10.1021/jp5005693
URLs:
http://www.scopus.com/inward/record.url?scp=84904581115&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84904581115
Research output: Contribution to journal › Article › Scientific › peer-review

Characterization Of High-Velocity Single Particle Impacts On Thermally Sprayed Ceramic Coatings

High-velocity impact wear may have a significant effect on the lifetime of thermally sprayed coatings in multiple applications, e.g. in process- and aero industries. An experimental impact study was performed on thermally sprayed coatings with a high velocity particle impactor (HVPI) in oblique angles to investigate the damage, failure and deformation of the coating. The impact site was characterized with a profilometer, optical microscopy and SEM. Furthermore, the connection between the microstructural details and impact behaviour were studied to reveal the damage and failure characteristics in a more comprehensive level. Additionally, traditional dry-erosion behaviour with small particles and different angles was compared with the high-velocity single particle impact phenomena. Differences in wear volume and deformation of the impact site and in absorbance of kinetic energy were also studied, focusing on the effect of material properties as well as the impact characteristics.

General information

Publication status: Unpublished
MoE publication type: A4 Article in a conference publication
Organisations: Department of Materials Science, Research group: Surface Engineering, Research group: Materials Characterization
Contributors: Kiilakoski, J., Lindroos, M., Matikainen, V., Apostol, N., Koivuluoto, H., Vuoristo, P.
Publication date: 13 May 2015

Host publication information

Title of host publication: International Thermal Spray Conference & Exposition 2015
ISBN (Print): 978-1-62708-093-4
ASJC Scopus subject areas: Surfaces, Coatings and Films
URLs:
https://asm.confex.com/asm/itsc15/webprogram/Paper38348.html

Bibliographical note

Conference presentation, unpublished in proceedings.
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

Wear Properties of Thermally Sprayed Tungsten-Carbide Coatings in Paper Machine Environments

Thermally sprayed tungsten-carbide (WC) coatings have proven to be one of the most wear resistant coatings available and a respectable replacement for hard-chromium coatings. They are used in paper machine parts such as calender rolls. However, improved lifetime and performance are continuing considerations, as well as finding more economical alternatives. This study researched the wear phenomena of tungsten-carbide coatings in a paper machine environment. To achieve this, five different feedstock materials and coatings manufactured from these were compared by electron microscopy as well as dry abrasion-, high-speed slurry abrasion- and cavitation erosion tests. Improvements in ductility by changing the matrix material were found, while changing the particle strength had no effect on the behavior of the coatings. The findings suggest further research on altering the matrix of the feedstock could lead to overall improvements in coating quality and component lifetime.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Surface Engineering, Valmet Technologies Oy
Contributors: Kiilakoski, J., Eronen, V., Vuoristo, P.
Number of pages: 35
Pages: 29
Publication date: 21 Sep 2015
Peer-reviewed: Yes

Publication information

Journal: Tribologia - Finnish Journal of Tribology

Volume: 33
Issue number: 2
ISSN (Print): 0780-2285
Ratings:

Scopus rating (2015): SJR 0.101 SNIP 0
Original language: English
ASJC Scopus subject areas: Surfaces, Coatings and Films, Materials Science (miscellaneous)
Electronic versions:

Tribologia_Kiilakoski_et.al_2015_Scanned
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Bibliographical note
xoa Tribologia_Kiilakoski_et.al_2015_Scanned ei tarkistettu, siirretty kohdasta additional files
Research output: Contribution to journal › Article › Scientific › peer-review

Fracture Characteristics of High-Velocity Suspension Flame-Sprayed Aluminum Oxide Coatings

General information
Publication status: Published
MoE publication type: B3 Non-refereed article in conference proceedings
Organisations: Department of Materials Science, Research group: Surface Engineering, Research group: Materials Characterization, University of Stuttgart
Contributors: Kiilakoski, J., Lutoschkin, A., Plachetta, M., Apostol, M., Koivuluoto, H., Killinger, A., Vuoristo, P.
Number of pages: 6
Pages: 466-471
Publication date: 2016

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Title of host publication: International Thermal Spray Conference & Exposition, ITSC 2016
Publisher: DVS Media GmbH
ISBN (Electronic): 978-3-87155-574-9
ASJC Scopus subject areas: Surfaces, Coatings and Films, Engineering (miscellaneous)
Keywords: ALUMINA COATINGS, HVOF spraying, Thermal spray coating, Bending test, Fracture
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific

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.
Number of pages: 11
Pages: 1127-1137
Publication date: 24 Jun 2016
Peer-reviewed: Yes

Publication information
Journal: Journal of Thermal Spray Technology
Volume: 25
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Ratings:

Scopus rating (2016): CiteScore 3.1 SJR 0.659 SNIP 0.932
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:

10.1007/s11666-016-0428-2
URLs:

http://urn.fi/URN:NBN:fi:tty-201801161083
Source: Scopus
Source ID: 84976320961
Research output: Contribution to journal › Article › Scientific › peer-review

Cavitation wear characteristics of Al2O3-ZrO2-ceramic coatings deposited by APS and HVOF -processes

Thermally sprayed ceramic coatings are used in environments requiring good wear- and corrosion resistance among others. However, a typical issue with ceramic coatings is their low impact resistance and tendency to fail catastrophically by cracking. In bulk ceramics, the Al2O3-ZrO2–composition has been of interest for long since already small additions of ZrO2 into Al2O3 have shown improvements in fracture toughness compared to pure Al2O3. Efforts are being made to induce this increased resistance to fracturing in thermally sprayed coatings as well, resulting in higher wear resistance due to a more predictable behavior and damage-tolerance. In this work, Al2O3-ZrO2-coatings have been deposited by atmospheric plasma spray (APS) and high-velocity oxy-fuel spray (HVOF) processes. The wear characteristics of the coatings were evaluated with cavitation erosion, delving into the mechanics of the erosion and the resulting microstructural changes in the coatings. Evidence of phase transformation of t-ZrO2 to m-ZrO2 was found during the erosion. The HVOF-sprayed coating exhibited greater wear resistance against the cavitating bubbles due to its finer microstructure.

General information

Publication status: Published
MoE publication type: B3 Non-refereed article in conference proceedings
Organisations: Materials Science, Research group: Surface Engineering, Institute of Plasma Physics, Academy of Sciences of the Czech Republic
Contributors: Kiilakoski, J., Lukac, F., Koivuluoto, H., Vuoristo, P.
Number of pages: 6
Pages: 928-933
Publication date: 9 Jun 2017

Host publication information

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Volume: 336
Place of publication: Düsseldorf
Publisher: DVS Media GmbH
ISBN (Electronic): 978-3-96144-000-9

Publication series

Name: DVS-Berichte / DVS - Deutscher Verband für Schweißen und Verwandte Verfahren e.V.
Publisher: DVS Media GmbH
ISSN (Electronic): 0418-9639
ASJC Scopus subject areas: Mechanics of Materials, Surfaces, Coatings and Films
Keywords: Thermal spray coating, HVOF spraying, Cavitation damage, alumina-yttria-stabilized zirconia, Erosion testing, PLASMA SPRAY
URLs:

https://www.dvs-ev.de/call4papers/index.cfm?vid=85&id=5
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific

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
Publication status: Published
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.
Pages: 245-254
Publication date: 15 Aug 2019
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Journal: Surface and Coatings Technology
Volume: 371
ISSN (Print): 0257-8972
Ratings:

Scopus rating (2019): CiteScore 5.8 SJR 0.938 SNIP 1.614
Original language: English
ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Ceramic coating, Characterization, Fracture, Impact test, Surface fatigue, Thermal spray
Electronic versions:

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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
Publication status: Published
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.
Pages: 98-107
Publication date: Jan 2019
Peer-reviewed: Yes
Early online date: 2018

Publication information
Journal: Journal of Thermal Spray Technology
Volume: 28
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ISSN (Print): 1059-9630
Ratings:

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
Keywords: AlO-ZrO, ceramic matrix composite, coating, HVOF, hybrid, solution-precursor spraying
Electronic versions:

Kiilakoski2018_Article_CharacterizationOfPowder-Precu

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.

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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.
Number of pages: 12
Publication date: 2019
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Journal: Journal of Thermal Spray Technology
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
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DOIs:
10.1007/s11666-019-00940-7
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http://urn.fi/URN:NBN:fi:tuni-201912026472
Source: Scopus
Source ID: 85074710199
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.

General information
Publication status: Published
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
Pages: 3724-3733
Publication date: 2020
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry B
Volume: 124
Issue number: 18
ISSN (Print): 1520-6106
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: 85084379376
Research output: Contribution to journal › Article › Scientific › peer-review

Fabrication of ssDNA/oligo(ethylene glycol) monolayers by promoted exchange reaction with thiol and disulfide substituents
Biorepulsive oligo(ethylene glycol)-substituted alkanethiolate (OEG-AT) monolayers on gold can serve as primary templates for promoted (by electron irradiation) exchange reaction with thiolated ssDNA species, resulting in the formation of mixed OEG-AT/ssDNA monolayers of desired composition. Here we test the ability of alternative, disulfide precursors to serve as substituents in such a reaction. Two representative molecules, based on adenine-based homo-oligonucleotide (25-mer), were used, viz., asymmetric disulfide with a short second chain (A25SSOH) and symmetric disulfide (A25SSA25). The results were compared to the reference system of thiolated ssDNA (A25SH). Both disulfide precursors were found to be suitable for the reaction, further extending the types of commercially available compounds which can be used for this approach. A25SSOH exhibited quite high efficiency, similar to A25SH, while the efficiency of A25SSA25 was noticeably lower, especially at low irradiation doses (2). Also, the single component, A25SSA25-based ssDNA monolayer, was of lower quality as compared to the films prepared from the A25SH and A25SSOH precursors. The above observations were explained by the bulky character and conformational flexibility of A25SSA25, which hinder the proper assembly and efficient exchange reaction.

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Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Universitat Heidelberg
Contributors: Khan, M. N., Zharnikov, M.
Number of pages: 9
Pages: 3093-3101
Publication date: 13 Feb 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 118
Issue number: 6
ISSN (Print): 1932-7447
Ratings:

Scopus rating (2014): CiteScore 8.4 SJR 2.032 SNIP 1.434
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)
DOIs:

10.1021/jp411353f
URLs:

http://www.scopus.com/inward/record.url?scp=84894037828&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84894037828
Research output: Contribution to journal › Article › Scientific › peer-review

Fabrication of ssDNA/Oligo(ethylene glycol) monolayers and patterns by exchange reaction promoted by ultraviolet light irradiation

Using a representative test system, we present here a versatile approach to prepare mixed monolayers of thiolated single-stranded DNA (ssDNA) and oligo(ethylene glycol) substituted alkanethiols (OEG-AT) in a broad range of compositions as well as ssDNA/OEG-AT patterns of desired shape imbedded into a biorepulsive background. The procedure involves two steps. First, a primary, well-defined OEG-AT monolayer on a solid support is exposed to UV light in either homogeneous or lithographic fashion. Second, the exchange reaction between the damaged OEG-AT species in the film and ssDNA substituents in solution occurs, resulting in formation of ssDNA/OEG-AT monolayer or pattern. The above procedure relies on commercially available compounds and does not require vacuum, which simplifies its application in research and industrial laboratories. The composition of the mixed films or ssDNA/OEG-AT spots (lithography) can be precisely adjusted by UV dose in an almost entire composition range. It was demonstrated that the procedure can be performed with UV light of different wavelengths (254 or 365 nm), which opens new possibilities for lithography. Using advanced spectroscopic tools, it was shown that ssDNA molecules imbedded into the OEG-AT matrix maintain their identity and intact character as well as exhibit predominant upright orientation typical of one-component films of thiolated ssDNA. The OEG-AT constituents of the mixed monolayers were found to be intact as well, with all UV damaged OEG-AT species being exchanged for ssDNA. Finally, a representative ssDNA/OEG-AT pattern was fabricated.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Universitat Heidelberg
Contributors: Khan, M. N., Zharnikov, M.
Number of pages: 11
Pages: 24883-24893
Publication date: 27 Nov 2013
Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C
Volume: 117
Issue number: 47
ISSN (Print): 1932-7447
Ratings:

Scopus rating (2013): CiteScore 8.3 SJR 2.143 SNIP 1.432
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)
DOIs:

10.1021/jp408819k
URLs:

http://www.scopus.com/inward/record.url?scp=84889582340&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84889582340
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.

General information

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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
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Source: Scopus
Source ID: 84883395998
Research output: Contribution to journal › Article › Scientific › peer-review

Irradiation promoted exchange reaction with disulfide substituents
Exchange reaction between the primary self-assembled monolayer (SAM) on gold and potential molecular substituents capable of forming a SAM on the same substrate can be promoted by electron irradiation. Here we demonstrate that such a promoted reaction can be performed not only with thiols but with disulfides as substituents as well. This extends significantly the assortments of the suitable compounds, resulting in a broader variety of mixed SAMs and chemical patterns which can be fabricated by this technique. The kinetics of the promoted exchange reaction was studied in detail. The feasibility and practical usefulness of the approach were demonstrated by the experiments with a disulfide substituent bearing a tail group which can serve as an initiator for surface-initiated polymerization. A variety of complex polymer brush patterns was prepared using several representative polymers, relevant for biomedical research and applications, as test systems.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Integrated Technologies for Tissue Engineering Research (ITTE), Universitat Heidelberg
Contributors: Khan, M. N., Zharnikov, M.
Number of pages: 10
Pages: 14534-14543
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Peer-reviewed: Yes

Publication information
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ISSN (Print): 1932-7447
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Scopus rating (2013): CiteScore 8.3 SJR 2.143 SNIP 1.432
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)
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Source: Scopus
Source ID: 84880559790
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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Peer-reviewed: Yes
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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
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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

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

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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.
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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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Source: Scopus
Source ID: 84961282502
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.
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Publication date: 2 Apr 2015
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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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Source: Scopus
Source ID: 84926433475
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.

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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.
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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: Mining tailings, Mullite, Reaction sintering, Refractory ceramics, Utilization
DOIs:

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Bibliographical note
EXT="Lagerbom, Juha"
Source: Scopus
Source ID: 85057276435
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
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Article number: 43717
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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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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.
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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:

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Source: Scopus
Source ID: 84900485659
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.

General information

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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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:

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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

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.
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Bibliographical note
EXT="Kalimeri, Maria"
Source: Scopus
Source ID: 84887752230
Research output: Contribution to journal › Article › Scientific › peer-review

A comparison of relative displacement fields between numerical predictions and experimental results in fretting contact
In this paper, a comparison is made between calculated and measured displacements from a complete contact fretting test device. An experimental technique based on digital image correlation was used to measure the local displacement field at the contact interface. The material of the fretting specimen and pads was quenched and tempered steel. The effect of test device compliances and rigid body movement was minimized by measuring displacements very close to the contact interface. The measured displacements were successfully compared to the computed displacements of a corresponding finite element model. The relative slip amplitude in partial slip conditions, slip distribution across the contact, length of the slip region, and accumulated slip distribution, were compared. Relative slip decreases markedly with increasing normal load and friction coefficient. The friction coefficient was calibrated and determined as a function of loading cycles of fretting fatigue tests with two normal loads. The friction coefficient was found to increase at the beginning of tests and stabilize after about 1000 cycles, which is in agreement with general observations.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Tribology and Machine Elements, Wärtsilä Finland Oy
Contributors: Juoksukangas, J., Lehtovaara, A., Mäntylä, A.
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Peer-reviewed: Yes

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Volume: 230
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ISSN (Print): 1350-6501
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Original language: English
ASJC Scopus subject areas: Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Digital image correlation, finite element method, friction coefficient, relative displacement, slip
DOIs:

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Source ID: 84987650902
Research output: Contribution to journal › Article › Scientific › peer-review

Experimental and numerical investigation of fretting fatigue behavior in bolted joints
Bolted joints may suffer from fretting damage which can significantly decrease fatigue life. A testing arrangement was developed to study the effect of different operating and design parameters of a single bolted joint on fretting fatigue life. Fretting fatigue stress-life (S-N) tests were conducted to investigate in particular the effect of bolt preload and cyclic bulk loading on fatigue life. Fretting fatigue life decreased when increasing the preload and also when increasing the bulk stress. The Digital Image Correlation method was applied to measure tangential displacements close to the contact. A corresponding finite element model of the test setup was used to analyze contact variables in greater detail. The numerical results corresponded well to the experimental results.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Research group: Tribology and Machine Elements, Department of Materials Science, Wärtsilä Finland Oy

Contributors: Juoksukangas, J., Lehtovaara, A., Mäntylä, A.
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Peer-reviewed: Yes

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Ratings:

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Original language: English
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Keywords: Contact, Fatigue, Finite-element method, Fretting
DOIs:

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Bibliographical note
INT=MOL, "Juoksukangas, Janne"
Source: Scopus
Source ID: 84981164556
Research output: Contribution to journal › Article › Scientific › peer-review

Characterization of cracks formed in large flat-on-flat fretting contact
Fretting fatigue may lead to severe damage in machines. Adhesive material transfer spots in millimeter scale have previously been observed on fretted surfaces, which have been related to cracking. In this study, fretting-induced cracks formed in a large annular flat-on-flat contact are characterized. Optical and scanning electron microscopy of the fretting scar cross-section samples of self-mated quenched and tempered steel specimens revealed severe cracking and deformed microstructure. Two major cracks typically formed around an adhesion spot, which propagated at an oblique angle, regardless of the test parameters used. Millimeter-scale cracks were observed already within a few thousand loading cycles.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Research group: Tribology and Machine Elements, Materials Science and Environmental Engineering, Research group: Materials Characterization, Wärtsilä, University of Oulu, Tampere University
Contributors: Juoksukangas, J., Nurmi, V., Hintikka, J., Vippola, M., Lehtovaara, A., Mäntylä, A., Vaara, J., Frondelius, T.
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Peer-reviewed: Yes

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Original language: English
ASJC Scopus subject areas: Materials Science(all), Mechanics of Materials, Mechanical Engineering, Surfaces, Coatings and Films, Surfaces and Interfaces
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Electronic versions:

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INT=msee,"Nurmi, Verner"
EXT="Hintikka, Jouko"
Source: Scopus
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Research output: Contribution to journal › Article › Scientific › peer-review

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.

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science and Environmental Engineering, Research group: Tribology and Machine Elements, Wärtsilä, University of Oulu
Contributors: Juoksukangas, J., Hintikka, J., Lehtovaara, A., Mäntylä, A., Vaara, J., Frondelius, T.
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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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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.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
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.
Number of pages: 8

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Peer-reviewed: Yes

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Original language: English
ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Polymers and Plastics, Materials Chemistry
Keywords: mechanical properties, recycling, rheology, thermal properties, thermoplastics
DOIs:

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Source ID: 85079375444
Research output: Contribution to journal › Article › Scientific › peer-review

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.

General information
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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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Source: Scopus
Source ID: 85021689400
Research output: Contribution to journal › Article › Scientific › peer-review

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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Organisations: Physics, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, University of Helsinki
Contributors: Javanainen, M., Ollila, O. H., Martinez-Seara, H.
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Bibliographical note
EXT="Martinez-Seara, Hector"
EXT="Ollila, O. H.Samuli"
Source: Scopus
Source ID: 85083545186
Research output: Contribution to journal › Article › Scientific › peer-review

Active packaging by paper coating

General information
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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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Publication date: 1 Jan 2016

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Source: Scopus
Source ID: 85062284627
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › 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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Publication status: Published
MoE publication type: A1 Journal article-refereed
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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Keywords: Abrasion, CrC, Heat treatment, HVOF, Mechanical properties
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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.

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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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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Surfaces, Coatings and Films, Materials Chemistry
Keywords: abrasion resistance, chromium carbide, feedstock powder, heat treatment, HVAF, HVOF
DOIs:

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Source: Scopus
Source ID: 85027972309

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.

General information

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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
Keywords: Abrasive wear, CrC-NiCr, Hardmetal, High temperature, Thermal spray, WC
DOIs:

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Source: Scopus
Source ID: 85041378943
Research output: Contribution to journal › Article › Scientific › peer-review

Photovoltaic properties of low-bandgap (0.7–0.9eV) lattice-matched GaInNAsSb solar junctions grown by molecular beam epitaxy on GaAs

We demonstrate single junction GaInNAsSb solar cells with high nitrogen content, i.e. in the range of 5–8%, and bandgap energies close to 0.7 eV grown by molecular beam epitaxy. A good crystalline quality is demonstrated for the entire range of N concentrations. An average external quantum efficiency of 0.45 is demonstrated for GaInNAsSb solar cell with 6.2% N exhibiting a bandgap of 0.78 eV (no antireflection coatings has been applied). The internal quantum efficiency for the cell is 0.65 at E_g + 0.2 eV. The solar cells exhibited bandgap-voltage offsets between 0.55 V (for N = 5.3%) and 0.66 V (for N = 7.9%). When used in a six-junction solar cell architecture under AM1.5D illumination, the estimated short-circuit current density corresponding to the 0.78 eV cell is 8.2 mA/cm^2. Furthermore, using the parameters obtained for the GaInNAsSb junction with 6.2% N, we have estimated that such six-junction solar cell architecture could realistically attain an efficiency of over 50% at 1000 suns concentration.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Physics, Research group: ORC, Research group: Nanophotonics, Microscopy Center
Contributors: Isoaho, R., Aho, A., Tukiainen, A., Aho, T., Raappana, M., Salminen, T., Reuna, J., Guina, M.
Number of pages: 6
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Journal: Solar Energy Materials and Solar Cells
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Renewable Energy, Sustainability and the Environment, Surfaces, Coatings and Films
Keywords: Dilute nitrides, GaInNAsSb, Molecular beam epitaxy, Multijunction solar cells
DOIs:

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Source: Scopus
Source ID: 85062810786
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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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Surface Engineering, Ernst-Mach-Institut
Contributors: Isakov, M., Matikainen, V., Koivuluoto, H., May, M.
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Original language: English
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URLs:

http://urn.fi/URN:NBN:fi:tty-201712202430. Embargo ended: 3/06/19
Source: Scopus
Source ID: 85019992522

Behaviour of leaded tin bronze in simulated seawater in the absence and presence of tribological contact with alumina counterbody: Corrosion, wear and tribocorrosion

Corrosion, wear and tribocorrosion behaviours of leaded tin bronze were examined in simulated seawater using alumina counterbody for tribological contact. Active dissolution of alloy and corrosion product development on surfaces were the dominant corrosion mechanisms. Tribological contact with counterbody removed majority of the products, thus contributing to active dissolution of freshly exposed surface. This wear-induced corrosion mechanism contributed to 45% and 60% of total material losses at the two highest potentials, 50 mV and 250 mV vs. Ag/AgCl. Pure wear of alloy occurred in the form of abrasive wear. At anodic potentials under tribological contact, corrosion raised the friction coefficient as compared to pure wear and increased wear of the alloy. These results are presented and discussed in this paper.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Photonics, VTT Technical Research Centre of Finland
Contributors: Huttunen-Saarivirta, E., Isotahdon, E., Metsäjoki, J., Salminen, T., Ronkainen, H., Carpén, L.
Number of pages: 15
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Early online date: 22 Aug 2018

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Original language: English
ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Contact: sliding, Surface: chemical analysis, Synergism: tribochemistry, Wear: corrosive
DOIs:
10.1016/j.triboint.2018.08.021

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EXT="Metsäjoki, J."
EXT="Isotahdon, E."
Source: Scopus
Source ID: 85052665246
Research output: Contribution to journal › Article › Scientific › peer-review

Tribocorrosion behaviour of tin bronze CuSn12 under a sliding motion in NaCl containing environment: Contact to inert vs. reactive counterbody

Tribocorrosion behaviour of tin bronze was examined in NaCl environments using two counterbodies: inert alumina and reactive bearing steel. The results with inert counterbody disclosed growing alloy losses with increasing potential, due to wear-influenced corrosion. Degradation progressed through the development, modification and removal of corrosion products, exposing fresh surface for the environment. With reactive counterbody, galvanic coupling between the two metals played an important role in the behaviour of the tribopair. At the lowest potential, where counterbody corrosion progressed slowly, the metals were in a direct mechanical contact, introducing wear in the ploughing mode in tin bronze. At anodic potentials, counterbody provided cathodic protection to tin bronze, with most material losses occurring in the counterbody by corrosion and wear-influenced corrosion.

General information

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Organisations: Physics, VTT Technical Research Centre of Finland, Microscopy Center
Contributors: Huttunen-Saarivirta, E., Kilpi, L., Pasanen, A. T., Salminen, T., Ronkainen, H.
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Keywords: Corrosion, Galvanic coupling, Tribocorrosion, Wear
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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.

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MoE publication type: A1 Journal article-refereed
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 ID: 85077933290
Research output: Contribution to journal › Article › Scientific › peer-review

Global energy consumption due to friction and wear in the mining industry

Calculations on the global energy consumption due to friction and wear in the mineral mining industry are presented. For the first time, the impact of wear is also included in more detailed calculations in order to show its enormous tribological and economic impacts on this industry. A large variety of mining equipment used for the extraction, haulage and beneficiation of underground mining, surface mining and mineral processing were analysed. Coefficients of friction and wear rates of moving mechanical assemblies were estimated based on available information in literature in four general cases: (1) a global average mine in use today, (2) a mine with today's best commercial technology, (3) a mine with today's most advanced technology based upon the adaptation of the latest R&D achievements, and (4) a mine with best futuristic technology forecasted in the next 10 years. The following conclusions were reached: • Total energy consumption of global mining activities, including both mineral and rock mining, is estimated to be 6.2% of the total global energy consumption. About 40% of the consumed energy in mineral mining (equalling to 4.6 EJ annually on global scale) is used for overcoming friction. In addition, 2 EJ is used to remanufacture and replace worn out parts and reserve and stock up spare parts and equipment needed due to wear failures. The largest energy consuming mining actions are grinding (32%), haulage (24%), ventilation (9%) and digging (8%). • Friction and wear is annually resulting in 970 million tonnes of CO_2 emissions worldwide in mineral mining (accounting for 2.7% of world CO_2 emissions). • The total estimated economic losses resulting from friction and wear in mineral mining are in total 210,000 million Euros annually distributed as 40% for overcoming friction, 27% for production of replacement parts and spare equipment, 26% for maintenance work, and 7% for lost production. • By taking advantage of new technology for friction reduction and wear protection in mineral mining

equipment, friction and wear losses could potentially be reduced by 15% in the short term (10 years) and by 30% in the long term (20 years). In the short term this would annually equal worldwide savings of 31,100 million euros, 280 TWh energy consumption and a CO_2 emission reduction of 145 million tonnes. In the long term, the annual benefit would be 62,200 million euros, 550 TWh less energy consumption, and a CO_2 emission reduction of 290 million tonnes. Potential new remedies to reduce friction and wear in mining include the development and uses of new materials, especially materials with improved strength and hardness properties, more effective surface treatments, high-performance surface coatings, new lubricants and lubricant additives, and new designs of moving parts and surfaces of e.g. liners, blades, plates, shields, shovels, jaws, chambers, tires, seals, bearings, gearboxes, engines, conveyor belts, pumps, fans, hoppers and feeders.

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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Research group: Materials Characterization, VTT Technical Research Centre of Finland , Argonne National Laboratory
Contributors: Holmberg, K., Kivikytö-Reponen, P., Härkisaari, P., Valtonen, K., Erdemir, A.
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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.
Number of pages: 9
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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: 84930682015
Research output: Contribution to journal › Article › Scientific › peer-review

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.

General information

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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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Pages: 14329-14335
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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films
DOIs:

10.1021/jp409040u
URLs:

http://www.scopus.com/inward/record.url?scp=84888618153&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84888618153
Research output: Contribution to journal › Article › Scientific › peer-review

Fretting-induced friction and wear in large flat-on-flat contact with quenched and tempered steel

Fretting may cause severe surface damage and lead to unexpected fatigue failure. Our test apparatus was designed based on reciprocating, large, annular flat-on-flat contact without any edge effects in the direction of the fretting movement. Fretting wear tests were run with quenched and tempered steel with different normal pressures and sliding amplitudes under gross sliding conditions. The development of the friction coefficient and total wear mass depended mostly on the accumulated sliding distance. Initially, friction and wear were highly adhesive but gradually changed to abrasive due to third body accumulation in the interface.

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Organisations: Department of Materials Science, Research group: Tribology and Machine Elements, Engineering materials science and solutions (EMASS), Research and Development, Wärtsilä Finland
Contributors: Hintikka, J., Lehtovaara, A., Mäntylä, A.
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ASJC Scopus subject areas: Mechanical Engineering, Mechanics of Materials, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Fretting, Friction, Steel, Wear
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Source ID: 84933509998
Research output: Contribution to journal › Article › Scientific › peer-review

Normal displacements in non-Coulomb friction conditions during fretting
Non-Coulomb friction may occur in gross sliding fretting conditions, in which the tangential force increases as the fretting movement approaches its extreme position and produces 'hooked' fretting loops. Uncertainties in frictional behaviour make the design of highly loaded contacts against fretting a challenging task. Experiments were made with quenched and tempered steel, and cyclic normal displacements were discovered during non-Coulomb friction conditions. Normal displacement and non-Coulomb friction were caused by tangential fretting scar interactions between protrusions and depressions formed by material transfer. Tangential interlocking leads to inclined sliding conditions, which produce loading components in both tangential and normal directions; this explains most non-Coulomb friction.

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Tribology and Machine Elements, Research and Development, Wärtsilä Finland
Contributors: Hintikka, J., Lehtovaara, A., Mäntylä, A.
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Publication date: 2016
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ASJC Scopus subject areas: Mechanical Engineering, Mechanics of Materials, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Fretting, Friction, Wear
DOIs:

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Source: Scopus
Source ID: 84946600355
Research output: Contribution to journal › Article › Scientific › peer-review

Third Particle Ejection Effects on Wear with Quenched and Tempered Steel Fretting Contact

The design and life prediction of fretting wear-sensitive mechanical components remain a challenge. In the present work, the role of wear particle movements under conditions of axisymmetric loading of an annular flat-on-flat contact were investigated using self-mated quenched and tempered steel specimens. Total fretting wear significantly increased when loose wear particles were periodically removed from the interface, and this effect increased as a function of the sliding amplitude. Additionally, increased wear was measured when grooves perpendicular to the sliding direction were added to the interface. Increasing the rate of wear debris ejection leads to increased wear rate because naturally occurring entrapped third-body particles significantly reduce the wear. The shape of fretting loops and values of the average and maximum coefficient of friction remained unaffected by the removal of entrapped wear debris and by the introduction of the grooves.

General information

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Organisations: Department of Materials Science, Research group: Tribology and Machine Elements, Research and Development
Contributors: Hintikka, J., Lehtovaara, A., Mäntylä, A.
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Original language: English
ASJC Scopus subject areas: Mechanical Engineering, Mechanics of Materials, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Fretting, third body, unlubricated friction, unlubricated wear, wear debris
Electronic versions:

Third Particle Ejection Effects on Wear with Quenched and Tempered Steel Fretting Contact - Latest own version
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URLs:

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Source: Scopus
Source ID: 84978160752
Research output: Contribution to journal › Article › Scientific › peer-review

Stable and unstable friction in fretting contacts

Designing contacts susceptible to fretting is a challenging task due to uncertainties related to friction. For example, coefficient of friction has shown to vary as a function of load cycles and so-called non-Coulomb friction can exist during individual load cycles. Concepts of stable and unstable friction are presented in this manuscript. Based on experiments, no fretting is to be expected if the utilization of friction is kept below unstable friction threshold. If contact is subjected to tangential load above this threshold, reciprocating slippage, fretting, is to be expected even if the contact was initially in stick. Experimental evidence for existence of such threshold is presented in form of friction data, slip data and fretting scars.

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Contributors: Hintikka, J., Mäntylä, A., Vaara, J., Frondelius, T., Lehtovaara, A.
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ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Fretting, Friction, Stick-slip, Wear
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http://urn.fi/URN:NBN:fi:tty-201908272031
Source: Scopus
Source ID: 85055737240
Research output: Contribution to journal › Article › Scientific › peer-review

Running-in in fretting, transition from near-stable friction regime to gross sliding
It has been shown that quenched and tempered steel in gross-sliding fretting conditions, with tens of microns of slip amplitude, leads to fretting induced cracking and high and non-Coulomb friction. At low tangential load levels, there was only insignificant cracking. However, the running condition tends to change from stick to gross-sliding with a slip amplitude of a few micrometres. In this study, novel two-phase fretting experiments were done where quenched and tempered steel contact is run first at low loads that are initially in stick (running-in phase), followed by a gross-sliding phase with a slip amplitude of 35μm. The results show that gross-sliding phase friction was reduced and the fretting induced cracks were shorter when the running-in phase was done at high enough load level and lasted more than 10^6 load cycles. At the highest running-in load levels, the resulting crack lengths were approximately halved in comparison to experiments without running-in, and it was possible to achieve nearly ideal Coulomb friction in the gross-sliding phase when the running-in duration was 10.2×10^6 load cycles. It is concluded that it is possible to control fretting-induced friction and cracking by carefully controlled running-in.

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Contributors: Hintikka, J., Mäntylä, A., Vaara, J., Frondelius, T., Juoksukangas, J., Lehtovaara, A.
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ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Fretting, Friction, Running-in, Wear
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Source: Scopus
Source ID: 85075897578
Research output: Contribution to journal › Article › Scientific › peer-review

Design aspects of all atomic layer deposited TiO2–Fe2O3 scaffold-absorber photoanodes for water splitting
Iron and titanium oxides have attracted substantial attention in photoelectrochemical water splitting applications. However, both materials suffer from intrinsic limitations that constrain the final device performance. In order to overcome the limitations of the two materials alone, their combination has been proposed as a solution to the problems. Here we report

on the fabrication of an atomic layer deposited (ALD) Fe2O3 coating on porous ALD-TiO2. Our results show that successful implementation requires complete mixing of the TiO2 and Fe2O3 layers via annealing resulting in the formation of a photoactive iron titanium oxide on the surface. Moreover, we found that incomplete mixing leads to crystallization of Fe2O3 to hematite that is detrimental to the photoelectrochemical performance. IPCE and transient photocurrent measurements performed using UV and visible light excitation confirmed that the iron titanium oxide extends the photocurrent generation to the visible range. These measurements were complemented by transient absorption spectroscopy (TAS), which revealed a new band absent in pristine hematite or anatase TiO2 that we assign to charge transfer within the structure. Taken together, these results provide design guidelines to be considered when aiming to combine TiO2 and Fe2O3 for photoelectrochemical applications.

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Organisations: Chemistry and Bioengineering, Research group: Chemistry & Advanced Materials, Research group: Surface Science, Photonics, Materials Science, Research group: Plastics and Elastomer Technology
Contributors: Hiltunen, A., Ruoko, T., Iivonen, T., Lahtonen, K., Ali-Löytty, H., Sarlin, E., Valden, M., Leskelä, M., Tkachenko, N.
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Original language: English
ASJC Scopus subject areas: Electrochemistry, Renewable Energy, Sustainability and the Environment, Surfaces, Coatings and Films
Keywords: Water splitting, Atomic layer deposition (ALD), Titanium dioxide, Hematite, Cellulose, Template
DOIs:

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

Wetting hysteresis induced by temperature changes: Supercooled water on hydrophobic surfaces
The state and stability of supercooled water on (super)hydrophobic surfaces is crucial for low temperature applications and it will affect anti-icing and de-icing properties. Surface characteristics such as topography and chemistry are expected to affect wetting hysteresis during temperature cycling experiments, and also the freezing delay of supercooled water. We utilized stochastically rough wood surfaces that were further modified to render them hydrophobic or superhydrophobic. Liquid flame spraying (LFS) was utilized to create a multi-scale roughness by depositing titanium dioxide nanoparticles. The coating was subsequently made non-polar by applying a thin plasma polymer layer. As flat reference samples modified silica surfaces with similar chemistries were utilized. With these substrates we test the hypothesis that superhydrophobic surfaces also should retard ice formation. Wetting hysteresis was evaluated using contact angle measurements during a freeze-thaw cycle from room temperature to freezing occurrence at -7 °C, and then back to room temperature. Further, the delay in freezing of supercooled water droplets was studied at temperatures of -4 °C and -7 °C. The hysteresis in contact angle observed during a cooling-heating cycle is found to be small on flat hydrophobic surfaces. However, significant changes in contact angles during a cooling-heating cycle are observed on the rough surfaces, with a higher contact angle observed on cooling compared to during the subsequent heating. Condensation and subsequent frost formation at sub-zero temperatures induce the hysteresis. The freezing delay data show that the flat surface is more efficient in enhancing the freezing delay than the rougher surfaces, which can be rationalized considering heterogeneous nucleation theory. Thus, our data suggests that molecular flat surfaces, rather than rough superhydrophobic surfaces, are beneficial for retarding ice formation under conditions that allow condensation and frost formation to occur.

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Organisations: Department of Physics, Research area: Aerosol Physics, Research group: Aerosol Synthesis, KTH Royal Institute of Technology, Surface and Corrosion Science, SP Technical Research Institute of Sweden, Department of Civil and Architectural Engineering, Nanostructure Physics
Contributors: Heydari, G., Sedighi Moghaddam, M., Tuominen, M., Fielden, M., Haapanen, J., Mäkelä, J. M., Claesson, P. M.
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Journal: Journal of Colloid and Interface Science
Volume: 468
ISSN (Print): 0021-9797
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Original language: English
ASJC Scopus subject areas: Surfaces, Coatings and Films, Electronic, Optical and Magnetic Materials, Biomaterials, Colloid and Surface Chemistry
Keywords: Contact angle, Hydrophobization, Liquid flame spray (LFS), Morphology, Multi-scale roughness, Plasma polymerization, Supercooled water, Superhydrophobicity, Wetting hysteresis, Wood
DOIs:

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Source: Scopus
Source ID: 84955276633
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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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.
Number of pages: 15
Pages: 8910-8924
Publication date: 21 Jul 2011
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Ratings:

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
DOIs:

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Source: Scopus
Source ID: 79960344032
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.

General information

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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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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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Bibliographical note

EXT="Heiskanen, J. P."
Source: Scopus
Source ID: 84921286591
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.

General information

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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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Original language: English
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
DOIs:

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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.
Number of pages: 10
Pages: 410-419
Publication date: 30 Sep 2017
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Volume: 638
ISSN (Print): 0040-6090
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Original language: English
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

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.

General information

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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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Pages: 1934-1937
Publication date: 1 Jan 2012
Peer-reviewed: Yes

Publication information

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Scopus rating (2012): CiteScore 3.3 SJR 0.897 SNIP 1.153
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry
Keywords: Flexible coatings, Phase separation, Porous films, Printable coatings, Protein immobilization, Sol-gel
DOIs:

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http://www.scopus.com/inward/record.url?scp=84855940396&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84855940396
Research output: Contribution to journal › Article › Scientific › peer-review

Characteristics of nFOG, an aerosol-based wet thin film coating technique

An atmospheric pressure aerosol-based wet thin film coating technique called the nFOG is characterized and applied in polymer film coatings. In the nFOG, a fog of droplets is formed by two air-assist atomizers oriented toward each other inside a deposition chamber. The droplets settle gravitationally and deposit on a substrate, forming a wet film. In this study, the continuous deposition mode of the nFOG is explored. We determined the size distribution of water droplets inside the chamber in a wide side range of 0.1–100 μm and on the substrate using aerosol measurement instruments and optical microscopy, respectively. The droplet size distribution was found to be bimodal with droplets of approximately 30–50 μm contributing the most to the mass of the formed wet film. The complementary measurement methods allow us to estimate the role of different droplet deposition mechanisms. The obtained results suggest that the deposition velocity of the droplets is lower than the calculated terminal settling velocity, likely due to the flow fields inside the chamber. Furthermore, the mass flux of the droplets onto the substrate is determined to be in the order of 1 $g/m^3 s$, corresponding to a wet film growth rate of 1 μm/s. Finally, the nFOG technique is demonstrated by preparing polymer films with thicknesses in the range of approximately 0.1–20 μm.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Physics, Materials Science, RISE Bioscience and Materials, Research Institutes of Sweden, Lund University
Contributors: Harra, J., Tuominen, M., Juuti, P., Rissler, J., Koivuluoto, H., Haapanen, J., Niemelä-Anttonen, H., Stenroos, C., Teisala, H., Lahti, J., Kuusipalo, J., Vuoristo, P., Mäkelä, J. M.
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Volume: 15
Issue number: 3
ISSN (Print): 1547-0091
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ASJC Scopus subject areas: Chemistry(all), Surfaces and Interfaces, Surfaces, Coatings and Films, Colloid and Surface Chemistry
Keywords: Aerosol measurement, Droplet size distribution, nFOG, Polymer film, Wet coating technique
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Research output: Contribution to journal › Article › Scientific › peer-review

Thermal Modification of ALD Grown Titanium Oxide Ultra Thin Film for Photoanode Applications

General information
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Organisations: Optoelectronics Research Centre, Research group: Surface Science
Contributors: Hannula, M. K., Lahtonen, K. T., Isotalo, T. J., Saari, J. S., Valden, M. O.
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ASJC Scopus subject areas: Renewable Energy, Sustainability and the Environment, Surfaces, Coatings and Films, Surfaces and Interfaces, Atomic and Molecular Physics, and Optics
Keywords: Titanium dioxide, titanium silicide, Atomic layer deposition (ALD), photoemission electron microscopy, PEEM, hydrogen energy
Research output: Other conference contribution › Paper, poster or abstract › Scientific

Effect of Hole Transporting Material on Charge Transfer Processes in Zinc Phthalocyanine Sensitized ZnO Nanorods
The photoinduced electron transfer processes were studied for hybrid systems consisting of self-assembled monolayer of zinc phthalocyanine (ZnPc) assembled on ZnO nanorods and a film of organic hole transporting material (HTM) atop. Polythiophene (P3HT) or Spiro-OMeTAD were used as HTM. The study was carried out by ultrafast transient absorption spectroscopy technique with selective excitation of ZnPc at 680 nm or P3HT at 500 nm. Data analysis revealed that photoexcitation of ZnPc in the structure ZnO|ZnPc|P3HT results in a fast (1.8 ps) electron transfer from ZnPc to ZnO, which is followed by a hole transfer from the ZnPc cation to P3HT roughly in 30 ps. However, in the case of ZnO|ZnPc|Spiro-OMeTAD structure, the primary reaction upon excitation of ZnPc is a fast (0.5 ps) hole transfer from ZnPc to Spiro-OMeTAD, and the second step is electron injection from the ZnPc anion to ZnO in roughly 120 ps. Thus, we demonstrate two structurally very similar hybrid architectures that implement two different mechanisms for photoinduced charge separation found in dye-sensitized or in organic solar cells.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry
Contributors: Hakola, H., Sariola-Leikas, E., Efimov, A., Tkachenko, N. V.
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DOIs:

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Source: Scopus
Source ID: 84964529902
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of finish rolling and quench stop temperatures on impact-abrasive wear resistance of 0.35 % carbon direct-quenched steel

Novel high-hardness medium-carbon martensitic laboratory steel has been produced and tested for abrasive wear resistance. Different finish rolling temperatures (FRT) combined with either direct quenching (DQ) or interrupted quenching to 250 °C was applied to vary the content of retained austenite and hardness. The steel carbon content was set to 0.35 % to obtain a surface hardness of approximately 600 HB. Lowering the finish rolling temperature in the range 920-780 °C, i.e. into the non-recrystallization regime resulted in a more elongated prior austenite grain structure, which increased the hardness of the DQ variants without any significant loss of Charpy-V impact toughness. Although increasing the degree of autotempering by raising the quench stop temperature reduces the hardness of the martensitic microstructure, it was found that proper quenching stop temperature could be utilized to achieve balanced toughness and hardness properties. Impact-abrasive wear resistance as measured in impeller-tumbler tests with natural granite as the abrasive demonstrated that wear resistance increased with increasing surface hardness.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Materials Science, Univ of Oulu, SSAB
Contributors: Haiko, O., Miettunen, I., Porter, D., Ojala, N., Ratia, V., Heino, V., Kemppainen, A.
Number of pages: 17
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Original language: English
ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Hardness, Impact abrasion, Steel, Wear
URLs:

https://journal.fi/tribologia/article/view/59344
Source: Scopus
Source ID: 85039708969
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.
Publication date: 15 Dec 2019
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Journal: Wear
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Original language: English
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Keywords: Abrasion, Impact-abrasion, Steel, Tempering, Wear testing
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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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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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Article number: 203336
ISSN (Print): 0043-1648
Original language: English
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
DOIs:

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Source: Scopus
Source ID: 85085742604
Research output: Contribution to journal › Article › Scientific › peer-review

Effect of microstructure on the abrasive wear resistance of steels with hardness 450 HV
Hardness has been considered the main factor controlling the abrasive wear of steels. However, microstructure also affects the wear behavior. Four steels with different microstructures were produced with a Gleeble 3800 thermomechanical simulator and tested for abrasive wear behavior. Different cooling rates and heat treatments were applied to obtain a surface hardness of approximately 450 HV. Mainly tempered martensite, pearlite and some bainite could be observed in the microstructures. Scratch testing with a CETR UMT-2 tribometer was conducted to produce wear tracks. The results revealed that each steel showed distinct wear behavior.

General information

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MoE publication type: B1 Article in a scientific magazine
Organisations: Research group: Materials Characterization, Materials Science and Environmental Engineering, University of Oulu
Contributors: Haiko, O., Heino, V., Porter, D. A., Uusitalo, J., Kömi, J.
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ASJC Scopus subject areas: Mechanics of Materials, Mechanical Engineering, Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Abrasion, Microstructure, Steel
DOIs:

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Source: Scopus
Source ID: 85084455366
Research output: Contribution to journal › Article › Scientific

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.

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
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Keywords: Abrasion, Bainite, Microstructure, Steel, Wear testing

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Source: Scopus

Source ID: 85087215937

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

On the limit of superhydrophobicity: Defining the minimum amount of TiO_2 nanoparticle coating

Fabrication of superhydrophobic surfaces in large scale has been in high interest for several years, also titanium oxide nanostructures having been applied for the purpose. Optimizing the amount and structure of the TiO_2 material in the coating will play a key role when considering upscaling. Here, we take a look at fabricating the superhydrophobic surface in a one-step roll-to-roll pilot scale process by depositing TiO_2 nanoparticles from a Liquid Flame Spray onto a moving paperboard substrate. In order to find the minimum amount of nanomaterial still sufficient for creating superhydrophobicity, we varied nanoparticle production rate, flame distance from the substrate and line speed. Since the deposited amount of material sideways from the flame path was seen to decrease gradually, spatial analysis enabled us to consistently determine the minimum amount of TiO_2 nanoparticles on the substrate needed to achieve superhydrophobicity. Amount as low as 20-30 mg m^{-2} of TiO_2 nanoparticles was observed to be sufficient. The scanning electron microscopy revealed that at this amount, the surface was covered with nanoparticles only partially, but still sufficiently to create a hierarchical structure to affect wetting significantly. Based on XPS analysis, it became apparent that TiO_2 gathers hydrocarbons on the surface to develop the surface chemistry towards hydrophobic, but below the critical amount of TiO_2 nanoparticles, the chemistry could not enable superhydrophobicity anymore. While varying the deposited amount of TiO_2, besides the local spatial variance of the coating amount, also the overall yield was studied. Within the text matrix, a yield up to 44% was achieved. In conclusion, superhydrophobicity was achieved at all tested line speeds (50 to 300 m min^{-1}), even if the amount of TiO_2 varied significantly (20 to 230 mg m^{-2}).

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MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research group: Aerosol Synthesis, Research area: Aerosol Physics, Materials Science, Packaging Technology Research Team, Physics at Interfaces, Max Planck Institute for Polymer Research, Bioscience and Materials/Surface, RISE Research Institutes of Sweden AB, Finnish Environment Institute, Abo Akad Univ, Abo Akademi University, Dept Phys, AGH University of Science and Technology, University of Eastern Finland

Contributors: Haapanen, J., Aromaa, M., Teisala, H., Juuti, P., Tuominen, M., Sillanpää, M., Stepien, M., Saarinen, J. J., Toivakka, M., Kuusipalo, J., Mäkelä, J. M.

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Journal: Materials Research Express

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Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Biomaterials, Surfaces, Coatings and Films, Polymers and Plastics, Metals and Alloys

Keywords: liquid flame spray, nanocoatings, nanoparticles, superhydrophobic, TiO, titanium dioxide, wetting

DOIs:

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Source: Scopus

Source ID: 85059238010

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

Interfacial design and structure of protein/polymer films on oxidized AlGaN surfaces

Protein detection using biologically or immunologically modified field-effect transistors (bio/immunoFETs) depends on the nanoscale structure of the polymer/protein film at sensor interfaces (Bhushan 2010 Springer Handbook of Nanotechnology 3rd edn (Heidelberg: Springer); Gupta et al 2010 The effect of interface modification on bioFET sensitivity, submitted). AlGaN-based HFETs (heterojunction FETs) are attractive platforms for many protein sensing applications due to their electrical stability in high osmolarity aqueous environments and favourable current drive capabilities. However, interfacial

polymer/protein films on AlGaN, though critical to HFET protein sensor function, have not yet been fully characterized. These interfacial films are typically comprised of protein-polymer films, in which analyte-specific receptors are tethered to the sensing surface with a heterobifunctional linker molecule (often a silane molecule). Here we provide insight into the structure and tribology of silane interfaces composed of one of two different silane monomers deposited on oxidized AlGaN, and other metal oxide surfaces. We demonstrate distinct morphologies and wear properties for the interfacial films, attributable to the specific chemistries of the silane monomers used in the films. For each specific silane monomer, film morphologies and wear are broadly consistent on multiple oxide surfaces. Differences in interfacial film morphology also drive improvements in sensitivity of the underlying HFET (coincident with, though not necessarily caused by, differences in interfacial film thickness). We present a testable model of the hypothetical differential interfacial depth distribution of protein analytes on FET sensor interfaces with distinct morphologies. Empirical validation of this model may rationalize the actual behaviour of planar immunoFETs, which has been shown to be contrary to expectations of bio/immunoFET behaviour prevalent in the literature for the last 20 years. Improved interfacial properties of bio/immunoHFETs have improved bio/immunoHFET performance: better understanding of interfaces may lead to mechanistic understanding of FET sensor properties and to clinical translation of the immunoFET platform.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Augmented Human Activities (AHA), Ohio State University, Department of Electrical and Computer Engineering
Contributors: Gupta, S. K., Wu, H. H., Kwak, K. J., Casal, P., Nicholson, T. R., Wen, X., Anisha, R., Bhushan, B., Berger, P. R., Lu, W., Brillson, L. J., Lee, S. C.
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Journal: Journal of Physics D: Applied Physics
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Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Electronic, Optical and Magnetic Materials, Acoustics and Ultrasonics, Surfaces, Coatings and Films
DOIs:

10.1088/0022-3727/44/3/034010
Source: Scopus
Source ID: 78650639127
Research output: Contribution to journal › Article › Scientific › peer-review

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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Keywords: Alumina, Cellular arrangement, Ceramic nanocomposite, Laser patterning, Osseous differentiation, Zirconia
DOIs:

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

Silver sulfide nanoclusters and the superatom model
The superatom model of electron-shell closings has been widely used to explain the stability of noble-metal nanoclusters of few nanometers, including thiolate-protected Au and Ag nanoclusters. The presence of core sulfur atoms in silver sulfide (Ag-S) nanoclusters renders them a class of clusters with distinctive properties as compared to typical noble-metal clusters. Here, it is natural to ask whether the superatom model is still applicable for the Ag-S nanoclusters with mixed metal and nonmetal core atoms. To address this question, we applied density functional simulations to analyze a series of Ag-S nanoclusters: $Ag_{14}S(SPh)_{12}(PPh_3)_8$, $Ag_{14}(SC_6H_3F_2)_{12}(PPh_3)_8$, $Ag_{70}S_{16}(SPh)_{34}(PhCO_2)_4$(triphos)$_4$, and $[Ag_{123}S_{35}(StBu)_{50}]^{3+}$. We observed that superatomic orbitals are still present in the conduction band of these Ag-S clusters where the cluster cores comprise mostly silver atoms. Our Bader charge analysis illustrates that thiolates play a significant role in withdrawing charge (electron density) from the core Ag atoms. The simulated optical absorption properties of the selected Ag-S clusters reflect the substantial band gaps associated with typical molecular orbitals on both sides. Apart from $Ag_{14}S(SPh)_{12}(PPh_3)_8$, which has a central sulfur atom in the cluster core, superatomic orbitals of the Ag-S clusters can have contributions for individual transitions in the conduction band.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research group: Materials and Molecular Modeling, Computational Science X (CompX), University of Jyväskylä, Departments of Physics and Chemistry
Contributors: Goh, J., Malola, S., Häkkinen, H., Akola, J.
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Peer-reviewed: Yes

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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)
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Source ID: 84921476515
Research output: Contribution to journal › Article › Scientific › peer-review

Superatom Model for Ag-S Nanocluster with Delocalized Electrons
Several Ag–S nanoclusters where the cluster core comprises mixed metal (main component) and sulfur atoms show superatomic orbitals in the conduction band edge. However, there are no superatomic states, i.e., delocalized electrons, in the valence band, and the clusters in question can be labeled as “zerovalent”. We show here an example of an Ag–S cluster which fulfills the superatom model and has delocalized electrons: The recently synthesized and characterized

[Ag62S12(StBu)32]2+ cluster has four delocalized valence electrons based on a simple counting rule, and we compare it to the zerovalent cluster [Ag62S13(StBu)32]4+. Our electronic structure analysis confirms the existence of superatomic states in the valence and conduction bands, but the locations of these states do not agree completely with the conventional prediction based on the spherical Jellium model. [Ag62S12(StBu)32]2+ displays the 1S2 electronic shell closure at the Fermi energy instead of the 1S21P2 configuration as suggested by its electron count. This shift of energy levels and electron shell closing has been introduced by the core–shell structure of the cluster. Our optical absorption simulation can reproduce the features observed in the experiments, and we assign these features to the transitions involving superatomic states within the conduction band.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research group: Materials and Molecular Modeling, Computational Science X (CompX), COMP Centre of Excellence, Department of Applied Physics, Aalto University
Contributors: Goh, J. Q., Akola, J.
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Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)
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Source ID: 84941254956
Research output: Contribution to journal › Article › Scientific › peer-review

Geometric Structure and Chemical Ordering of Large AuCu Clusters: A Computational Study

Understanding the structure and composition of nanosized gold-copper (AuCu) clusters is crucial for designing an effective AuCu catalyst. Global optimization of AuCu clusters using atomistic force fields is a viable solution for clusters with at least a few nm sizes, because of its fast computation. Here we develop an atomistic many-body potential for AuCu on the basis of the second-moment approximation to the tight-binding model. We show that our potential is in good agreement with density-functional theory calculations, and use it to study the structure and chemical ordering of clusters of sizes up to ~4 nm by means of global optimization searches. We show that the clusters present a surface enrichment in Au, while subsurface and central sites are enriched in Cu. Surface enrichment in Au and center enrichment in Cu are stronger in icosahedra. Surface Cu atoms prefer terrace sites on (111) facets. Both atomistic and DFT calculations show that $L1_0$ and $L1_2$ ordered phases are not favorable, even at their ideal compositions for these sizes, because of the tendency of Au to surface segregation. The stability range of icosahedral structures is wider in AuCu nanoalloys than in Au and Cu pure clusters.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Physics, COMP Centre of Excellence, Department of Applied Physics, Aalto University, Aalto University, Università di Genova
Contributors: Goh, J., Akola, J., Ferrando, R.
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Energy(all), Physical and Theoretical Chemistry, Surfaces, Coatings and Films
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Source: Scopus
Source ID: 85016919329
Research output: Contribution to journal › Article › 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.

General information

Publication status: Published
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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Peer-reviewed: Yes

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10.1039/c1cc12780b
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Source: Scopus
Source ID: 79961012632
Research output: Contribution to journal › Article › Scientific › peer-review

Luminescent $(Er,Ho)_2O_3$ thin films by ALD to enhance the performance of silicon solar cells

We have fabricated luminescent $(Er,Ho)_2O_3$ thin films by atomic layer deposition (ALD) and studied their capability to enhance the performance of state-of-the-art single-junction c-Si bifacial solar cells. The films convert IR photons (e.g. 1523 nm) by three- and two-photon upconversion process to emit visible-light in the 400–700 nm range. When the films were coupled with solar cells, ~3% improvement in the short-circuit current density (620 ± 5 to 638 ± 5 $mAcm^{-2}$) was recorded under a simulated solar excitation equivalent to 16 suns. These findings highlight a potential of ALD for the design and fabrication of luminescent coatings for practical solar cell devices.

General information

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MoE publication type: A1 Journal article-refereed
Organisations: Physics, Research group: ORC, Aalto University, University of Turku
Contributors: Ghazy, A., Safdar, M., Lastusaari, M., Aho, A., Tukiainen, A., Savin, H., Guina, M., Karppinen, M.
Number of pages: 5
Publication date: 2020

Peer-reviewed: Yes

Publication information
Journal: Solar Energy Materials and Solar Cells
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Article number: 110787
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Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Renewable Energy, Sustainability and the Environment, Surfaces, Coatings and Films
Keywords: Atomic layer deposition, c-Si solar cell, Luminescence, Photonics, Upconversion
DOIs:
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Source: Scopus
Source ID: 85090731507
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.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
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.
Number of pages: 9
Pages: 97-105
Publication date: 15 May 2014
Peer-reviewed: Yes

Publication information
Journal: Wear
Volume: 313
Issue number: 1-2
ISSN (Print): 0043-1648
Ratings:
Scopus rating (2014): CiteScore 4.1 SJR 1.711 SNIP 2.302
Original language: English
ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Damage mechanism, Scratch test, Sliding wear, Thermal spray coating
DOIs:
10.1016/j.wear.2014.02.017
URLs:
http://www.scopus.com/inward/record.url?scp=84896278052&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84896278052
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

Publication status: Published
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.
Number of pages: 7
Pages: 465-471
Publication date: 2012

Host publication information

Title of host publication: International Thermal Spray Conference and Exposition, ITSC 2012 - Air, Land, Water and the Human Body: Thermal Spray Science and Applications
Publisher: ASM International
ISBN (Print): 9781632666796
ASJC Scopus subject areas: Materials Chemistry, Surfaces, Coatings and Films, Surfaces and Interfaces
URLs:

http://www.scopus.com/inward/record.url?scp=84907084172&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84907084172
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

Surface reactivity and silanization ability of borosilicate and Mg-Sr-based bioactive glasses

Borosilicate bioactive glasses are attracting an increasing interest due to their good hot forming ability, low crystallization tendency and high bioactivity. Surface functionalization of bioactive glasses is a versatile tool for modulation of their properties and consequently of their biological response and it is still an unexplored topic in the case of borosilicate glasses. The possibility to graft 3-aminopropyltriethoxysilane (APTES) to various borosilicate bioactive glasses have been investigated in the present research work. Glasses were produced by melting and completely characterized (SEM-EDS, density, FTIR-ATR, Raman, NMR, zeta potential and reactivity in SBF and TRIS/HCl). Then, APTES was grafted to the surface of the glasses and its presence was verified by means of XPS, contact angle and zeta potential measurements. This study has shown the possibility to silanize borosilicate bioactive glasses for the first time, however, this silanization protocol does not induce the formation of a continuous coating on the glass surface.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Faculty of Biomedical Sciences and Engineering, Research group: Biomaterials and Tissue Engineering Group, Politecnico di Torino
Contributors: Ferraris, S., Nommeots-Nomm, A., Spriano, S., Vernè, E., Massera, J.
Number of pages: 13
Pages: 43-55
Publication date: 1 May 2019
Peer-reviewed: Yes
Early online date: 26 Dec 2018

Publication information

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Scopus rating (2019): CiteScore 8.7 SJR 1.23 SNIP 1.439
Original language: English
ASJC Scopus subject areas: Surfaces, Coatings and Films
Keywords: APTES, Borosilicate bioactive glasses, Silanization

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Source: Scopus
Source ID: 85059228057
Research output: Contribution to journal › Article › Scientific › peer-review

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.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science
Contributors: Fatarelle, E., Mylläri, V., Ruzzante, M., Pogni, R., Baratto, M. C., Skrifvars, M., Syrjälä, S., Järvelä, P.
Publication date: 1 Feb 2015
Peer-reviewed: Yes

Publication information
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Volume: 132
Issue number: 8
Article number: 41509
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, Photochemistry, Polyolefins
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10.1002/app.41509
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Contribution: organisation=mol,FACT1=1
Portfolio EDEND: 2014-12-30
Publisher name: JohnWiley & Sons, Inc.
Source: researchoutputwizard
Source ID: 296
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
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., 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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Journal: Journal of Applied Polymer Science
Volume: 132
Issue number: 9
Article number: 41539
ISSN (Print): 0021-8995
Ratings:

Scopus rating (2015): CiteScore 3.6 SJR 0.587 SNIP 0.846
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
DOIs:

10.1002/app.41539
URLs:

http://www.scopus.com/inward/record.url?scp=84913616731&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 84913616731
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.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
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.
Number of pages: 12
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Publication date: 4 Jun 2015
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B
Volume: 119
Issue number: 22
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.5b01351
URLs:

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Source: Scopus
Source ID: 84930960276
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
Publication status: Published
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
Pages: 14029-14032
Publication date: 2018
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Publication information
Journal: Chemical Communications
Volume: 54
Issue number: 99
ISSN (Print): 1359-7345
Ratings:

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
Keywords: triplet-triplet annihilation, triplet-triplet energy transfer, triplet state lifetime, upconversion, triplet fusion
Electronic versions:

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URLs:

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Source: Scopus
Source ID: 85058301188
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

Publication status: Published
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.
Number of pages: 13
Publication date: 15 Dec 2020
Peer-reviewed: Yes

Publication information
Journal: Surface and Coatings Technology
Volume: 403
Article number: 126396
ISSN (Print): 0257-8972
Original language: English
ASJC Scopus subject areas: Chemistry(all), Surfaces, Coatings and Films, Surfaces and Interfaces, Materials Chemistry, Condensed Matter Physics
Keywords: Ice adhesion, Icephobic coatings, Polymer coatings, Thermal degradation, Thermal spraying
Electronic versions:

Donadei et al. Lubricated icephobic coatings prepared by flame spraying with hybrid feedstock injection
DOIs:

10.1016/j.surfcoat.2020.126396
URLs:

http://urn.fi/URN:NBN:fi:tuni-202009217065
Source: Scopus
Source ID: 85090860951
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
Journal: Biomedical Glasses
Volume: 6
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
Keywords: Borosilicate glasses, Direct particle doping method, Dy microparticles, In-vitro testing, Persistent luminescence , Scaffold, SrAlO:Eu
Electronic versions:

Novel borosilicate bioactive scaffolds 2020
DOIs:

10.1515/bglass-2020-0001
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

Optical power monitors in Ge monolithically integrated on SOI chips

We report on the fabrication and operation of optical power monitors monolithically integrated on silicon-on-insulator optical chips. The devices consist of near-infrared waveguide pn heterojunction photodiodes in evaporated germanium. The low temperature growth of Ge is compatible with silicon waveguide technology. The photodetectors exhibit typical responsivities of 10-30 mA/W; the power monitors are used with front-end trans-impedance amplifiers based on commercially available operational amplifiers and can operate with optical signals as small as 10 nW, with errors below 0.2% and 2% at 1 and 0.1 μW, respectively.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, University “Roma Tre”, Nonlinear Optics and OptoElectronics Lab
Contributors: Colace, L., Sorianello, V., Romagnoli, M., Socci, L., Assanto, G.
Number of pages: 4
Pages: 514-517
Publication date: Apr 2011
Peer-reviewed: Yes

Publication information
Journal: Microelectronic Engineering
Volume: 88
Issue number: 4
ISSN (Print): 0167-9317
Ratings:

Scopus rating (2011): CiteScore 2.8 SJR 0.813 SNIP 1.148
Original language: English
ASJC Scopus subject areas: Electrical and Electronic Engineering, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Atomic and Molecular Physics, and Optics, Condensed Matter Physics
Keywords: Germanium, Integrated optoelectronics, Photodetectors, Powermonitor, Silicon-on-insulator
DOIs:

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Source: Scopus
Source ID: 79751538504
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
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Karlstad University
Contributors: Christophliemk, H., Ullsten, H., Johansson, C., Järnström, L.
Number of pages: 10
Pages: 13-22
Publication date: 1 Oct 2017
Peer-reviewed: Yes

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Volume: 111
ISSN (Print): 0300-9440
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
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Karlstad University
Contributors: Christophliemk, H., Johansson, C., Ullsten, H., Järnström, L.
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Publication date: 1 Dec 2017
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Volume: 113
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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, Drying, Oxygen transmission rate, Poly(vinyl alcohol), Starch, Water vapor transmission rate
DOIs:

10.1016/j.porgcoat.2017.04.019
Source: Scopus
Source ID: 85019946529
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
Publication status: Published
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.
Number of pages: 8
Pages: 430-437
Publication date: 15 Jun 2019
Peer-reviewed: Yes

Publication information
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Volume: 428-429
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, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry
Keywords: Abrasion, Fracture toughness, Impact-abrasion, Steel, Wear testing
Electronic versions:

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Source: Scopus
Source ID: 85064619336
Research output: Contribution to journal › Article › Scientific › peer-review

Light-trapping enhanced thin-film III-V quantum dot solar cells fabricated by epitaxial lift-off
We report thin-film InAs/GaAs quantum dot (QD) solar cells with n-i-p+ deep junction structure and planar back reflector fabricated by epitaxial lift-off (ELO) of full 3-in wafers. External quantum efficiency measurements demonstrate twofold enhancement of the QD photocurrent in the ELO QD cell compared to the wafer-based QD cell. In the GaAs wavelength range, the ELO QD cell perfectly preserves the current collection efficiency of the baseline single-junction ELO cell. We demonstrate by full-wave optical simulations that integrating a micro-patterned diffraction grating in the ELO cell rearside provides more than tenfold enhancement of the near-infrared light harvesting by QDs. Experimental results are thoroughly discussed with the help of physics-based simulations to single out the impact of QD dynamics and defects on the cell photovoltaic behavior. It is demonstrated that non radiative recombination in the QD stack is the bottleneck for the open circuit voltage (Voc) of the reported devices. More important, our theoretical calculations demonstrate that the Voc offset of 0.3. V from the QD ground state identified by Tanabe et al., 2012, from a collection of experimental data of high quality III-V QD solar cells is a reliable - albeit conservative - metric to gauge the attainable Voc and to quantify the scope for improvement by reducing non radiative recombination. Provided that material quality issues are solved, we demonstrate - by transport and rigorous electromagnetic simulations - that light-trapping enhanced thin-film cells with twenty InAs/GaAs QD layers reach efficiency higher than 28% under unconcentrated light, ambient temperature. If photon recycling can be fully exploited, 30% efficiency is deemed to be feasible.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Photonics, Research group: ORC, Research group: Nanophotonics, Politecnico di Torino, Department of Applied Health Research, Radboud University Nijmegen, tf2 devices B.V.
Contributors: Cappelluti, F., Kim, D., van Eerden, M., Cédola, A. P., Aho, T., Bissels, G., Elsehrawy, F., Wu, J., Liu, H., Mulder, P., Bauhuis, G., Schermer, J., Niemi, T., Guina, M.
Pages: 83-92
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: Solar Energy Materials and Solar Cells
Volume: 181
ISSN (Print): 0927-0248
Ratings:

Scopus rating (2018): CiteScore 10.2 SJR 1.62 SNIP 1.681

Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Renewable Energy, Sustainability and the Environment, Surfaces, Coatings and Films
Keywords: Epitaxial lift-off, Light-trapping, Quantum dot, Solar cell, Thin-film
DOIs:

10.1016/j.solmat.2017.12.014
Source: Scopus
Source ID: 85039853836
Research output: Contribution to journal › Article › Scientific › peer-review

Observation of off-axis directional beaming via subwavelength asymmetric metallic gratings

It is possible to obtain enhanced and directional beams using subwavelength metallic structures. However, the enhanced beams throughout such structures are only directed towards the propagation direction. In this study, we design the output surface gratings asymmetrically in order to steer the beaming angle. We use a metallic structure with a subwavelength slit (λ/10) and grating periods of 14 mm and 22 mm on different sides of the output surface. We demonstrate off-axis directional beaming in the microwave regime with an FWHM of 10° with a beaming angle of 15°. The beaming angle can be changed by arranging the grating periods of the output surface of the metallic structure.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Bilkent University, Harvard University
Contributors: Caglayan, H., Bulu, I., Ozbay, E.
Publication date: 2009
Peer-reviewed: Yes

Publication information

Journal: Journal of Physics D: Applied Physics
Volume: 42
Issue number: 4
Article number: 045105
ISSN (Print): 0022-3727
Ratings:

Scopus rating (2009): SJR 1.269 SNIP 1.326
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Acoustics and Ultrasonics, Condensed Matter Physics
DOIs:

10.1088/0022-3727/42/4/045105
URLs:

http://www.scopus.com/inward/record.url?scp=67650075571&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note

EXT="Caglayan, H."
Source: Scopus
Source ID: 67650075571
Research output: Contribution to journal › Article › Scientific › peer-review

One-step flame synthesis of silver nanoparticles for roll-to-roll production of antibacterial paper

Nanoparticles are used in several applications due to the unique properties they possess compared to bulk materials. Production techniques have continuously evolved over the years. Recently, there has been emphasis on environmentally friendly manufacturing processes. Substrate properties often limit the possible production techniques and, for example; until recently, it has been difficult to incorporate nanoparticles into paper. Chemical reduction of a precursor in the presence of paper changes the bulk properties of paper, which may limit intended end-use. In this study, we present a novel technique for incorporating silver nanoparticles into paper surface using a flame pyrolysis procedure known as Liquid Flame Spray. Papers precoated with mineral pigments and plastic are used as substrates. Silver nanoparticles were analyzed using SEM and XPS measurements. Results show a homogeneous monolayer of silver nanoparticles on the surface of paper, which demonstrated antibacterial properties against E. coli. Paper precoated with plastic showed more nanoparticles on the surface compared to pigment coated paper samples except for polyethylene-precoated paper. The results demonstrate a dry synthesis approach for depositing silver nanoparticles directly onto paper surface in a process which produces no effluents. The production technique used herein is up scalable for industrial production of antibacterial paper.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Physics, Abo Akad Univ, Abo Akademi University, Dept Phys, Turun Yliopisto/Turun Biomateriaalikeskus
Contributors: Brobbey, K. J., Haapanen, J., Gunell, M., Mäkelä, J. M., Eerola, E., Toivakka, M., Saarinen, J. J.
Number of pages: 8
Pages: 558-565
Publication date: 31 Oct 2017
Peer-reviewed: Yes

Publication information
Journal: Applied Surface Science
Volume: 420
ISSN (Print): 0169-4332
Ratings:

Scopus rating (2017): CiteScore 6.7 SJR 1.093 SNIP 1.328
Original language: English
ASJC Scopus subject areas: Surfaces, Coatings and Films
Keywords: Antibacterial paper, Liquid flame spray, Roll-to-roll processing, Silver nanoparticles
DOIs:

10.1016/j.apsusc.2017.05.143
Source: Scopus
Source ID: 85020047753
Research output: Contribution to journal › Article › Scientific › peer-review

The sensitivity of random polymer brush-lamellar polystyrene-b-polymethylmethacrylate block copolymer systems to process conditions

The use of random copolymer brushes (polystyrene- r-polymethylmethacrylate - PS- r-PMMA) to 'neutralise' substrate surfaces and ordain perpendicular orientation of the microphase separated lamellae in symmetric polystyrene- b-polymethylmethacrylate (PS- b-PMMA) block copolymers (BCPs) is well known. However, less well known is how the brushes interact with both the substrate and the BCP, and how this might change during thermal processing. A detailed study of changes in these films for different brush and diblock PS- b-PMMA molecular weights is reported here. In general, self-assembly and pattern formation is altered little, and a range of brush molecular weights are seen to be effective. However, on extended anneal times, the microphase separated films can undergo dimension changes and loss of order. This process is not related to any complex microphase separation dynamics but rather a degradation of methacrylate components in the film. The data suggest that care must be taken in interpretation of structural changes in these systems as being due to BCP only effects.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Tyndall National Institute at National University of Ireland, Cork, Materials Chemistry and Analysis Group, University College Cork, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Leixlip Co.
Contributors: Borah, D., Rasappa, S., Senthamaraikannan, R., Shaw, M. T., Holmes, J. D., Morris, M. A.
Number of pages: 11
Pages: 192-202
Publication date: 1 Mar 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Colloid and Interface Science
Volume: 393
Issue number: 1
ISSN (Print): 0021-9797
Ratings:

Scopus rating (2013): CiteScore 6.1 SJR 1.195 SNIP 1.437
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Biomaterials, Surfaces, Coatings and Films, Colloid and Surface Chemistry
Keywords: Microphase separation, Polymer brush, Polystyrene-b-polymethylmethacrylate, Polystyrene-r-polymethylmethacrylate, Surface morphology
DOIs:

10.1016/j.jcis.2012.10.070
URLs:

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Source: Scopus
Source ID: 84873060382
Research output: Contribution to journal › Article › Scientific › peer-review

Plasma etch technologies for the development of ultra-small feature size transistor devices

The advances in information and communication technologies have been largely predicated around the increases in computer processor power derived from the constant miniaturization (and consequent higher density) of individual transistors. Transistor design has been largely unchanged for many years and progress has been around scaling of the basic CMOS device. Scaling has been enabled by photolithography improvements (i.e. patterning) and secondary processing such as deposition, implantation, planarization, etc. Perhaps the most important of the secondary processes is the plasma etch methodology whereby the pattern created by lithography is 'transferred' to the surface via a selective etch to remove exposed material. However, plasma etch technologies face challenges as scaling continues. Maintaining absolute fidelity in pattern transfer at sub-16 nm dimensions will require advances in plasma technology (plasma sources, chamber design, etc) and chemistry (etch gases, flows, interactions with substrates, etc). In this paper, we illustrate some of these challenges by discussing the formation of ultra-small device structures from the directed self-assembly of block copolymers (BCPs) where nanopatterns are formed from the micro-phase separation of the system. The polymer pattern is transferred by a double etch procedure where one block is selectively removed and the remaining block acts as a resist pattern for silicon pattern transfer. Data are presented which shows that highly regular nanowire patterns of feature size below 20 nm can be created using etch optimization techniques and in this paper we demonstrate generation of crystalline silicon nanowire arrays with feature sizes below 8 nm. BCP techniques are demonstrated to be applicable from these ultra-small feature sizes to 40 nm dimensions. Etch profiles show rounding effects because etch selectivity in these nanoscale resist patterns is limited and the resist thickness rather low. The nanoscale nature of the topography generated also places high demands on developing new etch processes.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Frontier Photonics, Trinity College Dublin, University College Cork
Contributors: Borah, D., Shaw, M. T., Rasappa, S., Farrell, R. A., O'Mahony, C., Faulkner, C. M., Bosea, M., Gleeson, P., Holmes, J. D., Morris, M. A.
Publication date: 4 May 2011
Peer-reviewed: Yes

Publication information

Journal: Journal of Physics D: Applied Physics
Volume: 44
Issue number: 17
Article number: 174012
ISSN (Print): 0022-3727
Ratings:

Scopus rating (2011): CiteScore 4.4 SJR 1.266 SNIP 1.424
Original language: English
ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Condensed Matter Physics, Acoustics and Ultrasonics, Surfaces, Coatings and Films
DOIs:

10.1088/0022-3727/44/17/174012
URLs:

http://www.scopus.com/inward/record.url?scp=79954607730&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
Source ID: 79954607730
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
Pages: 125-144
Publication date: 15 Mar 2015
Peer-reviewed: Yes

Publication information

Journal: Surface and Coatings Technology
Volume: 265
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, 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

Wear and impact behaviour of High Velocity Air-Fuel sprayed Fe-Cr-Ni-B-C alloy coatings

The tribological properties of High Velocity Air-Fuel sprayed Fe-31Cr-12Ni-3.6B-0.6C (wt%) coatings are studied as a function of the deposition parameters. At room temperature, ball-on-disk sliding against Al_2O_3 is controlled by abrasive grooving and interlamellar cracking, with some tribo-oxidation. Interlamellar crack propagation also controls the coatings response to cavitation erosion and cyclic impact tests. Coatings deposited with higher powder feed rate exhibit poorer performance under all conditions, because of weaker interlamellar cohesion. At 700 °C, sliding wear rates are levelled out, and they are one order of magnitude higher than at room temperature, because of severe abrasive grooving.

General information

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Research group: Surface Engineering, University of Modena and Reggio Emilia
Contributors: Bolelli, G., Milanti, A., Lusvarghi, L., Trombi, L., Koivuluoto, H., Vuoristo, P.
Pages: 372-390
Publication date: 2016
Peer-reviewed: Yes
Early online date: 30 Nov 2015

Publication information

Journal: Tribology International
Volume: 95
ISSN (Print): 0301-679X
Ratings:

Scopus rating (2016): CiteScore 4.4 SJR 1.386 SNIP 2.125

Original language: English
ASJC Scopus subject areas: Mechanical Engineering, Mechanics of Materials, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Cavitation damage, Impact wear, Sliding contact, Thermally-sprayed coating
DOIs:
10.1016/j.triboint.2015.11.036
Source: Scopus
Source ID: 84949804098
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
Publication status: Published
MoE publication type: A1 Journal article-refereed
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.
Number of pages: 19
Pages: 32-50
Publication date: 15 Jul 2016
Peer-reviewed: Yes

Publication information
Journal: Wear
Volume: 358-359
ISSN (Print): 0043-1648
Ratings:
Scopus rating (2016): CiteScore 5.3 SJR 1.588 SNIP 2.105
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:
10.1016/j.wear.2016.03.034
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
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 , ECOR Research SpA
Contributors: Bolelli, G., Bursi, M., Lusvarghi, L., Manfredini, T., Matikainen, V., Rigon, R., Sassatelli, P., Vuoristo, P.
Number of pages: 21
Pages: 113-133
Publication date: 2018
Peer-reviewed: Yes
Early online date: 5 Nov 2017

Publication information
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:

10.1016/j.wear.2017.10.014
Source: Scopus
Source ID: 85032352458
Research output: Contribution to journal › Article › Scientific › peer-review

The correlation between gear contact friction and ball on disc friction measurements
Running experiments with full-size gearboxes from the actual application has the advantage of giving realistic results in terms of power losses. The drawback is extensive costs, lengthy testing, and the difficulty in differentiating between load dependent and load independent losses, and which losses are coming from the gears, seals, bearings or synchronizers. In this work, the correlation between friction measurements conducted in a ball-on-disc machine and friction measurements conducted in a back-to-back gear rig is investigated. The correlation between the gear tests and the ball-on-disc tests was reasonably good in terms of absolute values, and the shape of the friction curves was similar, indicating that the ball-on-disc measurements to a large extent are capturing the behavior of the gear contact.

General information
Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Department of Materials Science, Engineering materials science and solutions (EMASS), Luleå University of Technology, Department of Engineering Sciences and Mathematics, Division of Energy Science, Luleå University of Technology, Division of Machine Elements
Contributors: Björling, M., Miettinen, J., Marklund, P., Lehtovaara, A., Larsson, R.
Number of pages: 6
Pages: 114-119
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Tribology International
Volume: 83
ISSN (Print): 0301-679X
Ratings:

Scopus rating (2015): CiteScore 4.2 SJR 1.421 SNIP 2.104
Original language: English
ASJC Scopus subject areas: Mechanical Engineering, Mechanics of Materials, Surfaces, Coatings and Films, Surfaces and Interfaces
Keywords: Ball-on-disc, EHL, Friction, Gears
DOIs:

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URLs:

http://www.scopus.com/inward/record.url?scp=84912551787&partnerID=8YFLogxK (Link to publication in Scopus)

Bibliographical note

Available online 24 November 2014; (vol 83 (2015), s. 114-119
Contribution: organisation=mol,FACT1=1
Portfolio EDEND: 2015-01-13
Publisher name: Pergamon

Source: researchoutputwizard

Source ID: 171

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

Construction of an Interconnected Nanostructured Carbon Black Network: Development of Highly Stretchable and Robust Elastomeric Conductors

In the present work, a strong filler-filler network of conductive carbon black was strategically established in an elastomer matrix, which leads to a unique combination of electrical and mechanical properties. The novelty of our composites was the development of a strong percolated morphology of nanostructured conducting carbon black particles by the incorporation of relatively large nonreinforcing spherical silica particles, inside the soft elastomer matrix. This technique allowed us to fabricate solution styrene butadiene rubber (S-SBR) composites with outstanding electrical conductivity of 40 S/m, tensile strength ~10 MPa, and extensibility up to 200%. Furthermore, the electrical conductivity was strain-independent up to 50% elongation strain. The electrical conductivity was found to be unaltered after 2000 loading-unloading cycles. This is the first ever report of a robust elastomeric system with such high electrical conductivity where all the basic ingredients used were selected from well-known commercially available raw materials of rubber industry. This work directly manifests an industrially viable method for preparing high-performance elastic conductors that can be utilized in robust and flexible applications.

General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Engineering materials science and solutions (EMASS), Leibniz-Institut für Polymerforschung Dresden E.V., Technische Universität Dresden, Institut für Werkstoffwissenschaft, Institut für Polymerwerkstoffe E.V., Elkem AS, Silicon Materials

Contributors: Bhagavatheswaran, E. S., Parsekar, M., Das, A., Le, H. H., Wiessner, S., Stöckelhuber, K. W., Schmaucks, G., Heinrich, G.

Number of pages: 9

Pages: 21723-21731

Publication date: 17 Sep 2015

Peer-reviewed: Yes

Publication information

Journal: Journal of Physical Chemistry C

Volume: 119

Issue number: 37

ISSN (Print): 1932-7447

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Scopus rating (2015): CiteScore 7.9 SJR 1.886 SNIP 1.246

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

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http://www.scopus.com/inward/record.url?scp=84941928016&partnerID=8YFLogxK (Link to publication in Scopus)

Source: Scopus

Source ID: 84941928016

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
Publication status: Published
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
Pages: 140-147
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: Biomedical Glasses
Volume: 5
Issue number: 1
ISSN (Print): 2299-3932
Ratings:

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
Electronic versions:

[Biomedical Glasses] Mechanical characterization of pore-graded bioactive glass scaffolds produced by robocasting
DOIs:

10.1515/bglass-2019-0012
URLs:

http://urn.fi/URN:NBN:fi:tuni-202002031763

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

On the alignment of ZnO nanowires by Langmuir – Blodgett technique for sensing application
Nanowires are of interest for gas sensing application due to their one dimensional nature and size approaching quantum confinement limit, best studied in single nanowire devices. The reaction between gases and the semiconductor surface is better exploited when one, or few nanowires are involved. Yet, the widespread use of single nanowire devices is prevented by the need of expensive techniques to fabricate contacts. Here we applied the Langmuir-Blodgett technique to align ZnO nanowires between electrodes being two microns apart in a configuration that possess both the quality of single nanowire devices and the advantages of multiple nanowires. We achieved alignment without using lithography, so the procedure is inexpensive and scalable. As a proof of concept, we demonstrated that the obtained chips are suitable for sensing of NO_2, either at 200 °C or at room temperature with light activation. We discussed the obtained sensing parameters as a function of supra and sub-bandgap photoactivation.

General information
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MoE publication type: A1 Journal article-refereed
Organisations: Physics, Materials Science and Environmental Engineering, National Research Council -, Universita degli Studi di Brescia, South–Ukrainian National University
Contributors: Baratto, C., Golovanova, V., Faglia, G., Hakola, H., Niemi, T., Tkachenko, N., Nazarchurk, B., Golovanov, V.
Publication date: 30 Oct 2020
Peer-reviewed: Yes
Early online date: Jun 2020

Publication information
Journal: Applied Surface Science
Volume: 528
Article number: 146959
ISSN (Print): 0169-4332
Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Physics and Astronomy(all), Surfaces and Interfaces, Surfaces, Coatings and Films
Keywords: Aligned nanowires, Chemical sensor, Langmuir Blodgett, NO, Photoactivation, Surface reaction, ZnO
DOIs:

10.1016/j.apsusc.2020.146959
Source: Scopus
Source ID: 85086826170
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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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.
Number of pages: 8
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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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Long-Range Observation of Exciplex Formation and Decay Mediated by One-Dimensional Bridges

We report herein unprecedented long-range observation of both formation and decay of the exciplex state in donor (D)-bridge (B)-acceptor (A) linked systems. Zinc porphyrins (ZnP) as a donor were tethered to single-walled carbon nanotube (SWNT) as an acceptor through oligo(p-phenylene)s (ZnP-ph_n-SWNT) or oligo(p-xylene)s (ZnP-xy_{n-1}-ph_1-SWNT) with systematically varied lengths (n = 1-5) to address the issue. Exponential dependencies of rate constants for the exciplex formation (k_{FEX}) and decay (k_{DEX}) on the edge-to-edge separation distance between ZnP and SWNT through the bridges were unambiguously derived from time-resolved spectroscopies. Distance dependencies (i.e., attenuation factor, β) of k_{FEX} and k_{DEX} in ZnP-ph_n-SWNT were found to be considerably small (β = 0.10 for k_{FEX} and 0.12 $Å^{-1}$ for k_{DEX}) compared to those for charge separation and recombination (0.2-0.8 $Å^{-1}$) in D-B-A systems with the same oligo(p-phenylene) bridges. The small β values may be associated with the exciplex state with mixed characters of charge-transfer and excited states. In parallel, the substantially nonconjugated bridge of oligo(p-xylene)s exhibited larger attenuation values (β = 0.12 for k_{FEX} and 0.14 $Å^{-1}$ for k_{DEX}). These results provide deep insight into the unique photodynamics of electronically strongly coupled D-B-A systems involving exciplex.

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Contributors: Baek, J., Umeyama, T., Stranius, K., Yamada, H., Tkachenko, N. V., Imahori, H.
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Photophysical properties of porphyrin dimer-single-walled carbon nanotube linked systems

Porphyrin dimers were covalently grafted onto electron-accepting single-walled carbon nanotube (SWNT) sidewalls by direct aryl radical addition reaction with an m-or p-phenylene linker with the help of p-p interaction between the porphyrins. A splitting of the porphyrin Soret band and DFT calculations supported the selective formation of the porphyrin dimers on the sidewall of SWNTs. Photoexcitation of the porphyrin dimers on the SWNT resulted in the formation of the exciplex state, which directly decayed to the ground state without yielding the complete charge-separated state. Lifetimes of the porphyrin dimer-SWNT exciplex were longer than that of a porphyrin monomer-SWNT exciplex due to the stabilization by p-electron interaction over two porphyrin rings. In addition, the weaker electronic coupling through the meta-linkage than the para-one may be responsible for the exciplex lifetime of the porphyrin dimer-SWNT with the m-phenylene linker (49 ps) longer than that with the p-phenylene one (24 ps). The results obtained here provide the basic information on the effect of the donor dimerization on the photodynamic behavior of the exciplex state in donor-acceptor linked systems. [Figure presented]

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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

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Contributors: Auer, S., Koho, T., Uusi-Kerttula, H., Vesikari, T., Blazevic, V., Hytönen, V. P.
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Research output: Contribution to journal › Article › Scientific › peer-review

Static friction measurements on steel against uncoated and coated cast iron

Static friction is a phenomenon we may mainly consider as related to frictional joints within static mechanics. The step from static friction to tribological phenomena is, however, rather short, since at the onset of sliding in a mechanical contact, the static friction determines the initial resistance against motion. Static friction furthermore plays a role in contacts subjected to traction and fretting. Although being a phenomenon of short duration, the tribological phenomena during the transition from static friction to sliding friction may be of great importance for the operational life of the contact surfaces, particularly if the procedure is repeated for a sufficient number of times. The present paper describes the principles of static friction measurements, details of the employed static friction tribometer and the results of measurements with unlubricated and lubricated sliding couples consisting of steel against uncoated and coated cast iron.

General information

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Organisations: Research group: Tribology and Machine Elements, Department of Materials Science, VTT Technical Research Centre of Finland
Contributors: Andersson, P., Kilpi, L., Holmberg, K., Vaajoki, A., Oksanen, V.
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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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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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Original language: English
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Source: Scopus
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Research output: Contribution to journal › Article › Scientific › peer-review

Ambient-Pressure XPS Study of a Ni-Fe Electrocatalyst for the Oxygen Evolution Reaction
Chemical analysis of solid-liquid interfaces under electrochemical conditions has recently become feasible due to the development of new synchrotron radiation techniques. Here we report the use of "tender" X-ray ambient-pressure X-ray photoelectron spectroscopy (APXPS) to characterize a thin film of Ni-Fe oxyhydroxide electrodeposited on Au as the working electrode at different applied potentials in 0.1 M KOH as the electrolyte. Our results show that the as-prepared 7 nm thick Ni-Fe (50% Fe) film contains Fe and Ni in both their metallic as well as oxidized states, and undergoes further oxidation when the sample is subjected to electrochemical oxidation-reduction cycles. Metallic Fe is oxidized to Fe^{3+} and metallic Ni to $Ni^{2+/3+}$. This work shows that it is possible to monitor the chemical nature of the Ni-Fe catalyst as a function of potential when the corresponding current densities are small. This allows for operando measurements just above the onset of OER; however, current densities as they are desired in photoelectrochemical devices (~1-10 mA cm^{-2}) could not be achieved in this work, due to ohmic losses in the thin electrolyte film. We use a two-dimensional model to describe the spatial distribution of the electrochemical potential, current density, and pH as a function of the position above the electrolyte meniscus, to provide guidance toward enabling the acquisition of operando APXPS at high current density. The shifts in binding energy of water with applied potential predicted by the model are in good agreement with the experimental values.

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MoE publication type: A1 Journal article-refereed
Organisations: Optoelectronics Research Centre, Research group: Surface Science, SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Department of Chemical and Biomolecular Engineering, Berkeley, Materials Sciences Division, Lawrence Berkeley National Laboratory, Materials and Corrosion Engineering, Exponent, Inc., Polymer Science and Materials Chemistry
Contributors: Ali-Löytty, H., Louie, M. W., Singh, M. R., Li, L., Sanchez Casalongue, H. G., Ogasawara, H., Crumlin, E. J., Liu, Z., Bell, A. T., Nilsson, A., Friebel, D.
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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.

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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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Keywords: Langmuir monolayer, Langmuir-Schaefer film, Polydiacetylenes with urethane group, Solid topochemical photopolymerization
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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.

General information

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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
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Composition dependent growth dynamics in molecular beam epitaxy of GaInNAs solar cells

We have investigated the role of the nitrogen content, the growth parameters, and the annealing processes involved in molecular beam epitaxy of GaInNAs solar cells lattice-matched to GaAs. The nitrogen composition was varied between 1% and 5%. The influence of the growth temperature was assessed by performing photoluminescence, atomic force microscopy, X-ray diffraction, reflection high-energy electron diffraction, quantum efficiency and light-biased current-voltage measurements. The growth temperature ensuring the best cell parameters was found to be 440 C. At this temperature we were able to incorporate up to 4% of nitrogen and achieve a good material quality. Further increase of the N composition to 5% led to phase separation. For the lattice matched samples grown within the optimal temperature range, we have identified a clear (1×3) surface reconstruction. Using the optimized growth we have demonstrated a GaInNAs p-i-n solar cell structure containing 4% nitrogen, that exhibited a short-circuit current density as high as 33.8 mA/cm^2 in respect to effective area illuminated. These measurements have been performed under real sun AM1.5 (~1000 W/m^2) illumination. © 2014 Elsevier B.V.

General information

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Organisations: Optoelectronics Research Centre, Frontier Photonics, Department of Physics and Astronomy, University of Turku, Turun Yliopisto/Turun Biomateriaalikeskus
Contributors: Aho, A., Polojärvi, V., Korpijärvi, V. M., Salmi, J., Tukiainen, A., Laukkanen, P., Guina, M.
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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.

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