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Effect of Steel Fibers on Static and Blast Response of High Strength Concrete

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International Journal of Impact Engineering. Volume 107, September 2017, Pages 23-37

Abstract
The advantages of High Strength Fiber Reinforced Concrete (HSFRC) in static behavior highlighted by many researchers suggest it is a promising material to withstand dynamic loads. However, available experimental results regarding blast performance of HSFRC structural elements are still limited. The results of exploratory series of tests using a high strength concrete, over 100 MPa compressive strength, reinforced with long hooked-end steel fibers are presented in this paper. The results of static characterization tests performed on prisms and slabs and the results of blast tests on slabs are presented and analyzed. The improvements found in static flexure response with different fibers contents are compared with those found under blast loads. The effects of fibers controlling cracking, scabbing and spalling under close-in explosions are also addressed.

Microstructure of as-cast single and twin roller melt-spun Ni2MnGa ribbons

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Materials Characterization, 124 (2017) 171-181.

Abstract:
Stoichiometric Ni2MnGa alloys are processed by two rapid solidification techniques single-roller (SR) and twin-roller(TR) melt spinning and the resulting microstructures and magnetic properties determined. Samples processed at tangential wheel speeds of 10 m/s (V10) and 15 m/s (V15) are studied in the as-cast condition to analyze the influence of the production methods on the microstructure. Important aspects like the resulting phases, their crystallographic texture, magnetic properties, martensitic transformation temperatures and Curie temperatures are compared. In addition, the magnetization mechanism involving twin boundary motion is explored. Our results indicate that the TR method provides lower cooling rates, thicker samples, higher internal stresses and larger MnS precipitates. However, the quenching rate is mainly determined by the tangential wheel velocity. TR samples also exhibit [100] texture normal to the ribbon plane but in a lesser extent than SR ribbons. Martensitic transformation temperatures are higher in samples V15 (~150 K) than in V10 (~100 K), with no clear difference between the SR and TR modes. This behavior is explained by considering distinct degrees of disorder in the L2 austenite phase resulting from quenching. The hysteresis of the transformation, defined as the difference Af-MS, takes similar values in the four samples analyzed. Pre-martensitic transformation temperatures are also slightly higher in samples V15, (230± 3)K, than in samples V10, (222± 3)K, as the magnitude of the Hopkinson effect, in good agreement with a higher residual stress level in TR ribbons. In the martensitic state, all ribbons ex- hibit hysteresis loops characteristic of a magnetization mechanism involving twin boundary motion. The switching magnetic fields for the onset of Type I twin boundary motion result between 220 mT and 365 mT, values equivalent to twinning stresses of about 1 MPa. It is concluded that both procedures, SR and TR melt spinning, provide microstructures favoring magnetic field induced twin variant reorientation.

Supercritical CO_2-assisted impregnation of LDPE/sepiolite nanocomposite films with insecticidal terpene ketones: impregnation yield, crystallinity and mechanical properties assessment

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Journal of Supercritical Fluids. En prensa (2017) https://doi.org/10.1016/j.supflu.2017.06.013

Abstract:
In this contribution, supercritical CO_2-assisted impregnation of LDPE/sepiolite nanocomposite films with two insecticidal terpene ketones (thymoquinone and *R*-(+)-pulegone) is investigated, as a strategy to enhance the loading capacity compared to pure LDPE. A factorial experimental design was applied in order to evaluate the effect of five process variables at two levels (sepiolite content: 1–10% w/w; initial ketone mole fraction: 0.0017–0.0025; pressure: 9–13 MPa; depressurization rate: 0.5–2.0 MPa/min; time: 2–4 h) on impregnation yield, at 45°C. ANOVA test of the results indicated that pressure, time and ketone molar fraction significantly affect impregnation yield (ranging between 2.36±0.18 and 8.60±1.66% w/w). Thermal analysis (DSC) and X-ray diffraction (XRD)

allowed to investigate the nanocomposite morphology and the modifications induced by the impregnation. The mechanical properties of the films were assessed by stress-strain tests, showing that the impregnation process had a very low impact on the material ductility and strength.

Año 2016

Chemiresistor Arrays Prepared by Simple and Fast Vapor Phase Thiol Place-Exchange Functionalization of Gold Monolayer-Protected Cluster Films

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ChemelectroChem: Wiley. 2016, 3, 1230 - 1236.

Abstract
We describe a simple, versatile, and relatively fast method to alter the sensor selectivity of chemiresistors based on films of Au monolayer-protected clusters (MPCs) by varying their functionalization via vapor-phase thiol place-exchange reactions. Drop-cast deposited films of hexanethiolate (C6S)-coated Au MPCs are exposed to volatile thiol liquids, such as mercaptoethanol (HOC2S), mercaptopropionic acid (HOOCC2S), and mercaptopropyltrimethoxysilane (H3COSiC3S), which leads to thiol place-exchange and new functionalities in the film. Generally, the film is about 10–20 % exchanged during the first 4 to 5 h and 80–90 % exchanged after 24 h. The extent and the rate of exchange decreases as the thickness of the film of C6S Au MPCs increases, leading to irreproducibility issues if film thickness is not carefully controlled. Importantly, the chemiresistive sensing response ratio of 2-propanol relative to toluene vapor increased significantly from about 0.3 prior to exchange to 2.0 after 24 to 48 h of exchange with HOC2S, showing that the selectivity of the sensor could be significantly altered by this method, which is simpler, faster, and more amenable to a wide variety of ligands compared to solution-based functionalization methods. The chemiresistive response of an unexchanged C6S Au MPC films and those exchanged with HOC2S, HOOCC2S, and H3COSiC3S demonstrates potential electronic nose applications.

Dielectric and ultrasonic attenuation at low temperatures on BST ceramics with high strontium concentration.

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Integrated Ferroelectrics, 174:1 (2016) 111-120

Abstract
This work presents experimental investigation of the low temperature dielectric and ultrasonic responses of $(Ba_{1-x}Sr_x)TiO_3$ ceramics with high strontium concentration compositions, x > 0.825. Impedance spectroscopy measurements were performed at frequencies between 0.1 kHz and 100 kHz, and the results were correlated to those obtained with ultrasonic measurements. The anomalies observed in ultrasonic data were associated to ferroelastic and ferroelectric phase transitions. For x = 0.875 the "pinching" of ferroelectric phase transitions was observed. A brief discussion associates some peaks in the ultrasonic attenuation to anomalies in the dielectric response at temperatures below phase transition.

Chemical composition and electronic structure of anodic passive films on low-C 13CrNiMo stainless steel

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J Solid State Electrochem (2016) 20: 1065. doi:10.1007/s10008-015-2986-5

Abstract
Mott–Schottky analysis and electrochemical and X-ray photoelectron spectroscopy (XPS) measurements were performed on passive films formed on low-C13CrNiMo stainless steel with different applied heat treatments. Heat treatments render particular microstructural features of the alloy with a significant impact on the ability of the passive films to afford adequate protection against localized corrosion. A lower level of retained austenite in the substrate renders thinner passive films. Phosphates coexist with oxidized Fe(III) compounds as the prevailing species in the anodic layers. Mo was only detected in the oxide film formed on the sample with a higher retained austenite content.
Passive layers behave as *n*-type semiconductors with two types of donors, namely, shallow-level and deep-level states. The observed flat band potential $V_{FB} \cong$ -0.425 ± 0.005 V vs. standard calomel electrode (SCE) is independent of the thermal treatment of the alloy but under potential bias conditions at the corrosion potential the occurrence of the cathodic reaction on the oxide surface is hindered on the sample with higher retained austenite in its microstructure as compared to the sample with lower retained austenite content.

CVD Graphene Transferred with Au Nanoparticles: An Ideal Platform for TERS and SERS on a Single Triangular Nanoplate.

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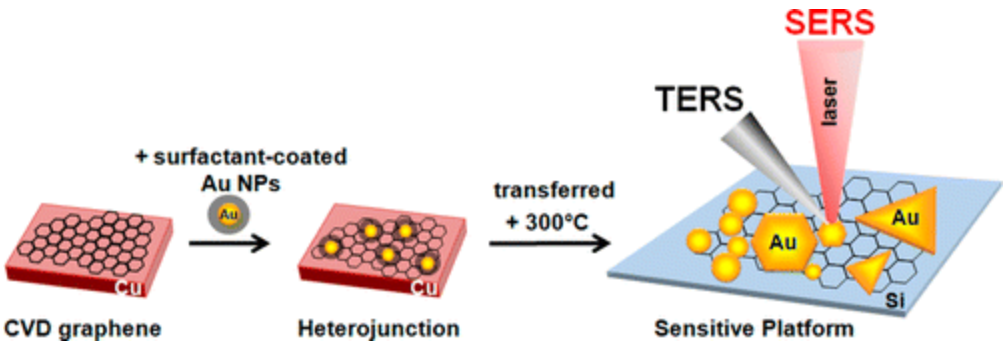
J. Phys. Chem. C, 2016 DOI: 10.1021/acs.jpcc.5b12372

Abstract



Transferring CVD graphene using surfactant-protected Au nanoparticles (Au NPs) avoids the use of PMMA and opens new ways of building heterojunctions for TERS and SERS applications. Thermal treatment removes organics from the Au NPs and leads to larger nanoparticles and the formation of networks, dimmers, and nanoplates of various shapes (circles, hexagons, and triangles). Raman and HRTEM revealed bilayer graphene and Moiré patterns as determined by the 2D band and dislocated atomic layers, respectively. TERS performed on the heterojunction exhibits a reversible increase in frequency and sharpening of the characteristic bands in graphene along with the exaltation of bands such as D + D′. A close examination into a single triangular-shape nanoplate reveals that the most irregular area of the nanoplate is consistent with the higher Raman enhancement of Rh6G when compared to other areas of the same feature. This work may shed light onto new ways of transferring graphene, fundamental aspects concerning local strains in the heterojunction, and SERS on a single Au nanostructure.

Spin reorientation, magnetization reversal, and negative thermal expansion observed in RFe0.5Cr0.5O3 perovskites (R = Lu, Yb, Tm)

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Physical Review B, 94 (1) (2016)

Abstract:
Three members of the perovskite family RFe0.5Cr0.5O3 (R = Lu, Yb, and Tm) have been synthesized and characterized. A systematic study of the crystal and magnetic structures was performed by neutron powder diffraction combined with magnetization measurements. All these compounds crystallize in a Pbnm orthorhombic unit cell and they are already antiferromagnetic at room temperature. The study of the magnetic structure vs temperature showed the occurrence of a progressive spin reorientation from Gamma(TM)(4) to Gamma(TM)(2) for the transition metal sublattice, and in the Tm-based sample, a long-range magnetic order of the Tm3+ sublattice was found (Gamma(R)(8)). These results are in excellent agreement with the magnetic susceptibility measurements. No spin reorientation is observed in the Lu-based sample for which a magnetization reversal at a compensation temperature T-comp = 225K was detected. A clear magnetostrictive effect was observed in the samples with R = Yb and Tm associated with a negative thermal expansion and was assigned to a magnetoelastic effect produced by repulsion between the magnetic moments of neighboring transition metal ions.

Synthesis In situ of gold nanoparticles by a dialkynyl Fischer carbene complex anchored to glass surfaces.

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Applied Surface Science, 383 (2016), 375–381

Abstract:
In this work we present a detailed study of classic reactions such as “click reaction” and nucleophilic substitution reaction but on glass solid surface (slides). We used different reactive center of a dialkynylalcoxy Fischer Carbene complex of Tungsten(0) to be anchored to modified glass surface with amine, to obtain aminocarbene, and azide terminal groups. These cycloaddition reaction showed regioselectivity to internal triple bond of dialkynyl Fischer carbene complex without Cu(I) as catalyst. Anyway the carbene anchored was able to act as a reducing agent to produce in situ very stable gold nanoparticles fixed on surface. We showed the characterization of modified glasses by contact angle measurements and XPS. Synthesized nanoparticles were characterized by SEM, XPS, EDS and UV-visible. The modified glasses showed an important enhancement Raman-SERS. This simple, fast and robust method to create a polifunctional and hybrid surfaces can be valuable in a wide range of applications such as Raman-SERS substrates and other optical fields.

Self dispersible nanocrystals of Albendazole produced by High Pressure Homogenization and Spray Drying

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Drug Development and Industrial Pharmacy, 42 (10) (2016) 1564-1570

Abstract:
Albendazole (ABZ) is a broad-spectrum antiparasitic drug used in the treatment of human or animal infections.
Although ABZ has shown a high efficacy for repeated doses in monogastric mammals, its low aqueous solubility leads to erratic bioavailability. The aim of this work was to optimize a procedure in order to obtain ABZ self-dispersible nanocrystals (SDNC) by combining high pressure homogenization (HPH) and spray-drying (SD). The material thus obtained was characterized and the variables affecting both the HPH and SD processes were studied. As expected, the homogenizing pressure and number of cycles influenced the final particle size, while the stabilizer concentration had a strong impact on SD output and redispersion of powders upon contact with water. ABZ SDNC was successfully obtained with high process yield and redispersibility. The characteristic peaks of ABZ were clearly identified in the X-ray patterns of the processed samples. A noticeable increase in the dissolution rate was observed in the aqueous environment.

Creep behaviour of cracked steel and macro-synthetic fibre reinforced concrete

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Materials and Structures (2016) 49 (8):3397–3410.

Abstract
The study of creep behaviour of fibre concrete in cracked conditions is nowadays one of the main subjects of interest; many research groups in the world are working on this matter and the development of test methods and the definition of parameters for its characterization becomes an urgent necessity. This paper explores the use of different types and levels of long term bending loads and compares the creep rates of fibre reinforced concretes (FRC) incorporating steel and two macro-synthetic fibres. Tests arrangements with three and four point loadings were used. An initial crack

width of 0.5 mm was adopted. It was verified that the creep rate clearly increases in macrosynthetic FRC and that the application of loading–unloading cycles does not imply significant changes in the creep rate when compared to permanent loads of similar magnitude. After creep tests the remaining residual bending capacity of FRC is considerable. Similar creep behaviour was observed by using three or four point loading configuration.

Efecto del tratamiento térmico post-alcalino sobre las propiedades de implantes dentales de titanio tratado superficialmente

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Acta Microscopica, Vol. 25 Supp. A., 2016

Abstract

El titanio es ampliamente utilizado como implante dental y ortopédico dado que es bioinerte y osteointegrable. No obstante, debido a la incapacidad de este material de inducir el crecimiento de hueso directamente desde su superficie, se llevan a cabo distintos tratamientos superficiales, dependiendo de la aplicación específica, para desarrollar un recubrimiento bioactivo que aumente tanto la velocidad inicial de desarrollo óseo como el anclaje biológico de fijación del implante al hueso, sobre todo en los críticos primeros estadíos post implantación. Teniendo en cuenta que la respuesta biológica se encuentra estrechamente relacionada con las propiedades superficiales, una de las actividades más importantes en el estudio de los implantes se encuentra enfocada al uso de modificaciones superficiales para mejorar mejorar la bioactividad y la triada osteogénesis-osteoinducción-osteoconducción. El tratamiento alcalino tiene por objetivo formar un gel de titanato de sodio, el cual se puede estabilizar, por medio de un tratamiento térmico, como una capa de titanato de sodio denso y amorfo [1] cuyo propósito es la mejora de la adhesión y bioactividad del recubrimiento en la superficie del implante. En el presente trabajo se analizó el efecto que produce un tratamiento térmico en implantes de titanio tratados químicamente en una solución de NaOH. Se utilizó como material de estudio titanio c.p. ASTM grado 4. Las condiciones de partida fueron: (a) blastinizado con partículas de fosfato de calcio y anodizado por plasma químico (APQ) [2] y (b) blastinizado con partículas de fosfato de calcio. Las muestras se sumergieron en un baño alcalino de NaOH 10M a 60°C durante 24h. Posteriormente, se les efectuó un tratamiento térmico a 400 ºC durante 1 hora y se dejaron enfriar en el horno. Por último, se enjuagaron con agua bidestilada y se sumergieron en una solución de SBF a 37 º C durante 7 días. La calidad y la resistencia adhesiva de la capa de titanato se evaluó mediante el ensayo de indentación Rockwell C. Para ello, se realizaron indentaciones con una carga de 150kg. Estas indentaciones se observaron mediante microscopía electrónica de barrido y la calidad de adhesión del recubrimiento se comparó con la clasificación especificada por la norma VDI 3198 [3]. El tratamiento térmico a 400 º C desarrolló una buena adhesión entre el sustrato y el metal, sin desprendimiento de la capa de APQ ni formación de fisuras

sobre la superficie (Figura 1). Por otro lado, se realizó el ensayo de determinación del ángulo de contacto inicial por goniometría. En la Figura 2 se observan imágenes representativas de la gota de agua depositada sobre las muestras, revelando estas gran hidrofilidad, ya que el proceso de mojado fue muy rápido y el ángulo de contacto de ambas muestras se redujo a 180º. Por último, se analizó la formación de la capa de apatita sobre la superficie de los implantes luego de la inmersión en el SBF mediante MEB-EDS. En la Figura 3 se presentan las imágenes y espectros de EDS correspondientes a cada muestra. En ambos casos se produjo el crecimiento de la apatita. Comparativamente, en la muestra (a) se detectó solo la presencia de Ca y P en la superficie. En la muestra (b) en cambio, a pesar de formar la capa de apatita y obtener una buena relación de Ca/P se observó el pico de titanio. Esto significaría que el espesor de la capa formada en la muestra blastinizado-APQ es mayor.

Stability of Furosemide Polymorphs and the effects of complex formation with β-Cyclodextrin and Maltodextrin

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Carbohydrate Polymers 152 (2016) 598-604

Abstract:

The effect of the formation of supramolecular binary complexes with β-cyclodextrin and maltodextrin on the chemical and physical stability of the polymorphs I and II of Furosemide was evaluated in solid state. The solid samples were placed under accelerated storage conditions and exposed to daylight into a stability chamber for a 6-month period. Chemical stability was monitored by high performance liquid chromatography, while the physical stability was studied by using the following techniques: solid state nuclear magnetic resonance, powder X-ray diffraction and scanning electron microscopy. Changes in the physical appearance of the samples were also evaluated. The first-order rate constants for the photodegradation reactions were determined. The data showed that the complexes obtained by the kneading method significantly reduced the photodegradation process of Furosemide polymorphs I and II. The physical studies performed and the appearance of the samples demonstrated that form II of Furosemide is susceptible to suffer phase transformation under stress conditions. Furthermore, the experiment conducted showed a significant stabilizing effect of βCD on form II of Furosemide. Our results suggest that the complex formation is a useful tool for improving the stability of FUR polymorphs. These new complexes are promising candidates that can be used in the pharmaceutical industry for the preparation of alternative matrices that improve physicochemical properties.

CVD Graphene transferred with Au Nanoparticles: an Ideal Platform for TERS and SERS on a Single Triangular Nanoplate

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Journal of Physical Chemistry C., 216 (2016)

Abstract:
Transferring CVD graphene using surfactantprotected Au nanoparticles (Au NPs) avoids the use of PMMA and opens new ways of building heterojunctions for TERS and SERS applications. Thermal treatment removes organics from the Au NPs and leads to larger nanoparticles and the formation of networks, dimmers, and nanoplates of various shapes (circles, hexagons, and triangles). Raman and HRTEM revealed bilayer graphene and Moirépatterns as determined by the 2D band and dislocated atomic layers, respectively. TERS performed on the heterojunction exhibits a reversible increase in frequency and sharpening of the characteristic bands in graphene along with the exaltation of bands such as D + D′. A close examination into a single triangular-shape nanoplate reveals that the most irregular area of the nanoplate is consistent with the higher Raman enhancement of Rh6G when compared to other areas of the same feature. This work may shed light onto new ways of transferring graphene, fundamental aspects concerning local strains in the heterojunction, and SERS on a single Au nanostructure.

Investigation by mechanical spectroscopy at different frequencies of the nucleation processes in amorphous Cu-Zr-Al alloys.

W.B. Marques[a], O. Florencio[a], P.S. Silva Jr[a], F.H. Santa Maria[b], J.M. Chave [b], A. Moreno-Gobbi[c], L.C.R. Aliaga[d], W.J. Botta[e]

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[e] Departamento de Engenharia de Materiais, Universidade Federal de São Carlos, CEP 13565-905, São Carlos, SP, Brazil.

Materials Science and Engineering A-Structural Materials Properties Microstructure and Processing, v.: 694, (2017) 66-71

Abstract
The anelastic spectra of Cu 39.5 Zr 51 Al 9.5, Cu 54 Zr 40 Al 6 and Cu 47.75 Zr 47.75 Al 4.5 bulk metallic glasses were obtained by Mechanical Spectroscopy Technique at different frequencies.

Studies below room temperature show two principal mechanisms: one broad peak, similar to β relaxation, and another sharp peak, similar to α relaxation. This observation suggests that the interaction between amorphous structure and mechanical waves demosntrates that β´ relaxation can be decomposed in two principal peaks, one due to the movement of flow units and another owing to the growth of molecular-like structures. The behaviour of hybridization among Al-Cu atoms tends to decrease the free space in the amorphous matrix, increasing internal friction. The mechanical excitation and interaction among nanostructures such as cluster type, supercluster and molecular-like structure, can lead to growth of microalloy which may give rise to the medium-range order structure as well as increasing the small nanocrystalline region scattered into the glassy structure. In addition, the effect of mechanical vibration and cryogenic temperature acting on the amorphous structure can promote interaction among nanostructures resulting in a barrier that tends to block the propagation of shear bands in the mettallic glasses.

Año 2015

Mechanical spectroscopy study on the Cu54Zr40Al6 amorphous matrix alloy at low temperature.

P.W.B. Marques[a], J.M. Chaves[a], P.S. Silva Jr.[a], O. Florêncio[a], A. Moreno-Gobbi[b], L.C.R. Aliaga[c], W.J. Botta[c]

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Journal of Alloys and Compounds 621 (2015) 319–323

Abstract
A mechanical spectroscopy study of $Cu_{54}Zr_{40}Al_6$ bulk metallic glasses composites was carried out in the kHz and MHz frequency ranges, by means of flexural and ultrasonic methods, respectively, in the temperature interval 150–300 K. In internal friction and attenuation curves at low temperature were observed peaks which were associated with distortions in the configuration of atomic clusters, which absorbed different quantities of energy due to short and medium order rearrangements. Changes within the clusters or atomic jumps between clusters occurring in the specimen induced the onset of polyamorphic peaks, since electronic interactions and bonding changed abruptly.

Removal and cementitious immobilization of heavy metals: chromium capture by zeolite-hybridized materials obtained from spent fluid cracking catalysts

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Journal of Cleaner Production 91 (2015), pp 187-190

Abstract
An alternative for the reutilization of spent catalyst industrial residue for removal and immobilization of heavy metals is presented. A solid containing about 80% (w/w) of NaA zeolite was hydrothermally synthesized by reconversion of a spent catalyst discarded from a fluidized-bed catalytic cracking unit (FCC). The obtained material (ZFCC) was afterwards used for Cr(III) removal from aqueous solutions. Chromium cation was incorporated in the zeolitized structure by ionic

exchange in liquid media, and the exchange level was determined by atomic absorption spectrometry. To analyze the viability of final disposal for the chromium sludge obtained using this methodology (Cr-ZFCC), cement mortars containing Cr-ZFCC in variable percentages were prepared and their mechanical and metal retention properties were evaluated. Mechanical strengths and drying shrinkage shown by mortars containing not more than Cr-ZFCC 5% (w/w) were similar to those corresponding to control mortars without zeolitic additions. Leaching tests indicated that mortars with Cr-ZFCC 5% (w/w) produce an effective immobilization of Cr(III) and should be considered as a viable alternative for safe chromium disposal.

Contribution of fiber reinforcement in concrete affected by alkali–silica reaction

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Cement and Concrete Research 67 (2015), pp 310-317

Abstract
Fiber reinforced concrete (FRC) is a high performance material that is frequently used for structures in contact with aggressive environments, because the fibers can control the propagation of cracks. This paper analyzes the residual properties of FRC after the alkali–silica reaction has taken place. The potential contribution of different types of fibers for mitigating the degradation process and their effects on the mechanical and transport residual properties are discussed. The expansions, presence of cracks, compressive strength and modulus of elasticity, and the behavior under flexural loads were evaluated. Steel fibers were the most efficient for reducing the crack density, followed by synthetic macrofibers. The coefficient of air permeability followed the same tendency, showing the positive effect of macrofibers in transport properties. Concretes incorporating steel or synthetic macrofibers conserve their original post-peak loading capacity when severe alkali–silica reaction damage has taken place.

Mechanical response of fiber reinforced concrete overlays over asphalt concrete substrate: experimental results and numerical simulation.

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Construction and Building Materials 93 (2015), pp 1022–1033

Abstract
Fiber reinforced concrete overlays are nowadays an alternative for repairing and reinforcing pavements. The contribution of concrete overlays strongly depends on the bond with the substrate. The fibers help sewing contraction joints and eventual cracks and, in this way prevent the propagation of cracks along the substrate–overlay interface. Therefore, the addition of fibers to the overlay allows reducing repair thickness, increasing service life and improving pavements general performance. Some experimental tests performed for the development of a method to assess different fibers efficiency in this type of applications are presented in this paper. Substrate–overlay composite beams are tested under flexure. The beams consist of overlays of plain and fiber reinforced concretes, containing steel and macro-synthetic fibers, applied over an asphalt concrete substrate. The numerical simulation of the beams is also included in the paper. Fiber reinforced concrete is considered as a composite material made of a concrete matrix and fibers and its mechanical behavior is modeled with a simple homogenization approach based on modified mixture theory. The numerical simulation can accurately reproduce material characterization tests and predict the bearing capacity of the composite beams. Furthermore, other substrate/overlay alternatives are numerically studied. The numerical results could be useful to improve the design of these intervention techniques.

Wheel tracking test (WTT) conducted under different standards. Study and correlation of test parameters and limits

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CONICET, LEMIT-CIC La Plata Argentina

Materials and Structures December 2015, Volume 48, Issue 12, pp 4019–4028

Abstract
The wheel tracking test (WTT) is an important tool to define asphalt mixture rutting performance. In this study, the rutting behaviour in the WTT was compared under two different standards, BS 598-110 and EN 12697-22 small size device procedures. A significant number of mixtures were studied considering different volumetric characteristics, binder types and test temperatures. The relationship between calculated test parameters in both standards is discussed. Similar deformation rate responses in mixtures using both test methods were observed. A correlation between the calculated parameters rutting rate of BS 598-110 and wheel tracking slope (WTS) of EN 12697-22 was obtained. Possible WTS limits are discussed, considering previous experience in the WTT according to BS 598-110 and the relations obtained with the low shear viscosity of the binders.

Blasting and Passivation Treatments for ASTM F139 Stainless Steel for Biomedical Applications: Effects on Surface Roughness, Hardening, and Localized Corrosion.

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J. of Materi Eng and Perform (2015) 24: 175. doi:10.1007/s11665-014-1300-5

Abstract

Due to the combination of good biofunctionality and biocompatibility at low cost, AISI 316 low carbon vacuum melting (LVM) stainless steel, as considered in ASTM F139 standard, is often the first choice for medical implants, particularly for use in orthopedic surgery. Proper surface finish must be provided to ensure adequate interactions of the alloy with human body tissues that in turn allows the material to deliver the desired performance. Preliminary studies performed in our laboratory on AISI 316LVM stainless steel surfaces modified by glass bead blasting (from industrial supplier) followed by different nitric acid passivation conditions disclosed the necessity to extend parameters of the surface treatments and to further consider roughness, pitting corrosion resistance, and surface and subsurface hardening measurements, all in one, as the most effective characterization strategy. This was the approach adopted in the present work. Roughness assessment was performed by means of amplitude parameters, functional parameters, and an estimator of the fractal dimension that characterizes surface topography. We clearly demonstrate that the blasting treatment should be carried out under controlled conditions in order to obtain similar surface and subsurface properties. Otherwise, a variation in one of the parameters could modify the surface properties, exerting a profound impact on its application as biomaterial. A passivation step is necessary to offset the detrimental effect of blasting on pitting corrosion resistance.

Real-time Monitoring Distance Changes in Surfactant-coated Au Nanoparticle Films upon Volatile Organic Compounds (VOCs).

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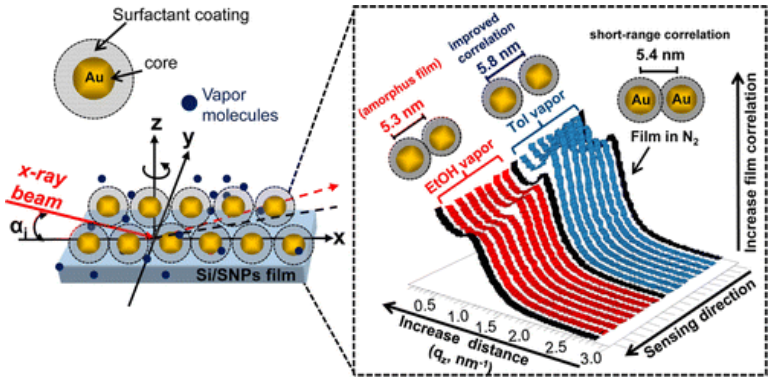
J. Phys. Chem. C 2015, 119, 5098−5106

Abstract



We explore into the role of the organic ligands composition surrounding Au nanoparticles (NPs) toward internanoparticles distance changes and film structure during vapor sensing by the use of *in situ* grazing-incidence small-angle X-ray scattering (GISAXS) and other relevant techniques. We observed distinct changes in *core-to-core* distance and film structure upon measured concentrations of polar ethanol (EtOH) and nonpolar toluene (Tol) vapors. As-formed tetraoctylammonium bromide (TOABr)-coated Au NPs (SNPs) film exhibited ~0.4 nm core-to-core increase in distance and improved SNPs correlation upon 80% Tol. In the presence of EtOH, SNPs distance seems not to change and correlation critically diminishes, leading to an amorphous film. As-formed films were exchanged with nonanedithiol (NDT) and exposed to 100% Tol vapor. Interestingly, the incorporation of NDT increased distance between NPs and rendered film flexibility. It is determine that just a small number of S, from NDT ligands, binds to Au NPs, and those exchanged alkanedithiol chains adopted a loop conformation around the Au NPs as evidenced by X-ray absorption near-edge structure (XANES) and kink defects by Fourier transformed infrared (FT-IR) experiments, respectively. These findings may solve some fundamental questions about internanoparticle distance-dependent phenomena such as electron transport in chemiresistors and coupling effects in localized surface plasmon resonance (LSPR) solid-state sensors.

Año 2014

Mechanical properties of polyvinylalcohol/hydroxyapatite cryogel as potential artificial cartilage

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Journal of the Mechanical Behavior of Biomedical Materials, 34 (2014) 47-56.

Abstract

The technological advances in material science are not enough to overcome the challenge of construct a material be able to replace the cartilage. The designed material has to meet the mechanical properties of cartilage and has to be also capable to be integrated with the articulation. Articular cartilage damage is a persistent and increasing problem which affects millions of people worldwide. Poly vinyl alcohol (PVA) hydrogels are promising implants, due to their similar properties as soft tissue; however their low mechanical resistance and durability together with its lack to integrate with the surrounding tissue restrict their application in this area. The poor adhesion can be solved by the development a composite hydrogel with bioactive and biocompatible filler, as hydroxyapatite (HA). The aim of this work was to obtain and characterize (physically, chemically and mechanically) PVA/HA composite hydrogels for potential application as articular replacement. Hence, composite hydrogels were prepared by adding of different amounts of HA in an aqueous solution of PVA and subsequent freezing-thawing cycles. It was observed that the addition of HA modified the physical and chemical features of the hydrogel and promoted the material crosslinking and stability. Moreover, it was found that the mechanical properties (compression, tension and nanoindentation) of the hydrogels were improved by the addition of HA. All these result indicate that these materials could be used as a potential cartilage replacement. However, further in vitro and in vivo studies are mandatory for future possible clinical applications and are actually being carried out.

Electrodeposited Cu2ZnSnS4 thin films

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Electrochimica Acta, 128 (2014) 393-399.

Abstract

Cu2ZnSnS4 (CZTS) thin films have been prepared using Electrochemical Atomic Layer Deposition (EC-ALD) and also by one-step conventional constant potential electrodeposition. Optimal deposition conditions were investigated using cyclic voltammetry (CV). Then, based on CVs results, CZTS films were grown employing EC-ALD deposition cycles using the sequence Au/S/Cu/S/Zn/S/Sn/S to form the desired quaternary compound. In parallel, conventional one-step electrodeposition was carried out at -0.85 V vs. Ag/AgCl over 1 hour. A thermal treatment in sulfur vapor was also investigated in an attempt to optimize the stoichiometry. The crystal structure of the films was characterized by XRD and micro Raman spectroscopy, while the morphology, thickness, topography and elemental composition were investigated using FIB-SEM and EDS.

Investigation of a relationship between dielectric peak diffuseness and elastic modulus variations in a ferroelectric relaxor

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Journal of Applied Physics 115 (2014) 114110

Abstract

The dependence with temperature of elastic modulus of relaxor ferroelectric ceramics is modeled with a Landau-Devonshire-type cluster theory. The effective elastic modulus obtained from experimental data of ultrasonic longitudinal velocity in PCT and PLZT ferroelectric ceramics are compared with the proposed model. This comparison shows that the model is able to reproduce the dependence with temperature of elastic modulus c very well. We obtained that as impurity concentration increases in both families, the diffuseness of the transition shows important variations, but the strengths of the couplings between the polarization and the strain remain almost unchanged. In contrast, other models assigned a change in the strengths of the couplings between the polarization and the strain to explain the diffuse transition in these compounds.

Interface evaluation of experimental dental adhesives with nanostructured hydroxyapatite incorporation

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Applied Adhesion Science, v. 2, p. 2, 2014

Abstract
The aim of this study was to evaluate the adhesive interface with dentin of an experimental adhesive resin with nanostructured hydroxyapatite addition. The organic phase of the adhesive resin was produced by mixing 50 wt.% Bis-GMA, 25 wt.% TEGDMA and 25 wt.% HEMA. CQ and EDAB were added at 1 mol% to all groups, according to the monomer moles. HA_{nano} was added at the following two concentrations: 0 and 2 wt%. One commercial adhesive system was used as control. Nine lower incisor bovine teeth were used to produce interfaces of adhesive resin and dentin. Tooth slices were analysed using the following micro-Raman parameters: a 100 mW diode laser with 785 nm wavelength and spectral resolution of ~ 3–5 cm^{-1}. One-dimensional mapping was performed over a 150 μm line across the adhesive-dentine interface at 1 μm intervals using a computerized XYZ stage. These areas covered the composite resin, adhesive layer, hybrid layer, partially demineralised and un-affected dentine and were visualised and focused at x500 magnification. Raman analysis showed the penetration of experimental and commercial adhesive systems into dentin. HA_{nano} was observed into the hybrid layer. Based on results of the present study, is possible to observe resin and nanostructured hydroxyapatite penetration at the hybrid layer.

Evaporation kinetics in swollen porous polymeric networks

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Langmuir 2014, 30, 4129−4136

Abstract
NMR is a fast, nondestructive, and noninvasive technique that can provide information about the pore structure of macroporous polymer beads and the dynamics of liquids confined in them. In this work, we describe the study of the pore structure of the macroporous polymer of ethylene glycol dimethacrylate and 2-hydroxyethyl methacrylate [poly(EGDMA-co- HEMA)] in the dry but also in the swollen state by measuring relaxation times of liquids contained in the polymer network. The results show that the pore architecture differs from the dry to the soaked state. The behavior of polar liquids during evaporation and deswelling dynamics is monitored and described. An internal migration of water from the swollen polymer mesh into expanding pores takes place. With this procedure it is possible to obtain information about the microscopic morphology behavior of the matrix during evaporation and deswelling. This information is of great interest with the aspect of possible and future applications for these types of materials.

Forming of thin porcelain tiles: A comparison between tape casting and dry pressing

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Ceramics International, 40, (2014) 3761-3767

Abstract
Thin porcelain tiles (down to 3 mm thickness) are currently made by dry pressing, while thin advanced ceramics (down to 0.1 mm thickness) use tape casting as forming step. This study proposes an alternative way of manufacturing thin porcelain tiles by tape casting. A systematic comparison between dry pressing and tape casting was made for a 2 mm thick tile fabrication. A current industrial formulation with the same particle size distribution and green density was employed, and the sintering temperature was varied in the range of 1180–1220 °C with heating rate of 40 °C/min. Firing shrinkage, loss on ignition, mechanical strength, and water absorption were measured and the microstructure after sintering was analyzed. The results showed that tape cast tiles are more homogenous and therefore presented higher values of mechanical properties.

Fast electrochromic response of ultraporous polyaniline nanofibers

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Polymer 55 (2014) 2440-2444

Abstract
Polyaniline (PAni) nanofibers were prepared by a one-step electrosynthetic method. A gold sputtered electrode was used as the substrate for the nanofiber growth at a constant current density value of 100 mA cm^{-2}. Substrate morphology induces fiber growing and allows having a remarkable quantity of fibers in a short period of time. Tandem chronoabsorptometric and chronocoulometric data of the electro-synthesis process were collected and analyzed. Several electrochromic parameters were characterized and a short response time (T90) of 20 ms was obtained for a contrast (DT %) of 10%. The main reason for this fast response is the ultraporous nature of the prepared nanofibers. This approach represents a straightforward, easy and low cost method to obtain a fast color switching film with potential application in the deployment of an electrochromic device.

Characterization and Corrosion Resistance of Galvanized Steel/Passivation Composite/ Polyurethane Paint Systems

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British Journal of Engineering and Technology, 4(6) (2014) 853-878.

Abstract
The corrosion performance of electrogalvanised steel sheets pre-treated with a Cr^{3+} or Cr^{+6}-based conversion layer and then covered with polyurethane-waterborne topcoat paint has been studied. The pre-treated metallic panels were coated with one of the three tested polyurethane (PU) topcoat paints, in which the dispersion type was the formulation variable. The pigment was TiO_2 (rutile) with a PVC value of 10. Before and after the immersion in 0.05 M NaCl (pH 5.70) or 0.1 M Na_2SO_4 (pH 6.36) solutions, replicates of the different samples were subjected to standardized tests (porosity, gloss and color, hardness, flexibility). During the immersion, blistering and rusting degrees were evaluated through periodical visual inspections, while the coated steel performance was monitored by Electrochemical Impedance Spectroscopy (EIS) measurements. Initial (dry) and final (wet) paint adhesion was also determined. EIS data were interpreted and discussed in terms of the time dependence of the electrical (paint coating) and electrochemical (steel substrate) parameters associated with interfacial processes describing the metal/paint system deterioration. According to the electrochemical properties, visual inspection and standardized tests results, it was concluded that the studied polyurethane-based polymeric films applied on pretreated electrogalvanised steel provided a very effective protection against corrosion as a result of their excellent barrier properties.

Corrosion behaviour of steel/55%Al–Zn alloy/paint systems exposed to natural and artificial environments

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The Canadian Journal of Chemical Engineering, 92 (4) (2014) 623–632

Abstract
The corrosion performance of steel/55%Al–Zn alloy sheets pre-treated with 5% Fe $(NO_3)_3$ + 15% H_3PO_4 solution, and then coated with acrylic (AC), alkyd (AQ), vinyl (VL), solvent-based epoxy (ES) or waterborne epoxy (EA) corrosion-inhibiting primers + a barrier topcoat alkyd paint was studied. Exposure conditions included weathering chambers and natural atmospheres (La Plata-Argentina and San Luis-Potosí, México). The panels' behaviour was evaluated through visual inspections and EIS measurements. Their results allowed inferring that: (1) most of the painting systems have a satisfactory performance during their exposure to the accelerated weathering chamber or the natural atmospheric stations and (2) the correlation between them allowed explaining some problems arising in service. This information will allow extending the useful life by adjusting the painting system formulation.

Effect of the in-air heat treatment in the phase formation and morphology of electrospun Cu_2ZnSnS_4 fibers

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Ceramics International. Available online 27 March 2014. In Press, Corrected Proof

Abstract
Cu_2ZnSnS_4 was successfully synthesized by the electrospinning process using thiourea as the sulfur source and heat treated in air without further sulfurization. The XRD and Raman spectroscopy investigation of heat treatments showed a good synthesis of Cu_2ZnSnS_4 film at a temperature of 400 °C. Scanning electron microscopy (SEM) revealed a homogeneous and compact film. The

optical band gap was around 2.2 eV and the main secondary products formed were binary sulfides and oxides.

Mechanical Behavior of Yttria-Stabilized Zirconia Aqueous Cast Tapes and Laminates

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Journal of Ceramics. Volume 2014 (2014) Article ID 713916, 5 pages

Abstract
Aqueous tape casting was used to produce yttria-stabilized zirconia films for electrolyte-supported solid oxide fuel cell (SOFC). Tape casting slurries were prepared varying the binder content between 20 and 25 wt%. A commercial acrylic emulsion served as binder. Rheological measurements of the two slurries were performed. Both slurries showed a shear-thinning behavior. Tapes with 25 wt% binder exhibited adequate flexibility and a smooth and homogeneous surface, free of cracks and other defects. Suitable conditions of lamination were found and a theoretical density of 54% in the laminates was achieved. Laminated tapes showed higher tensile strength compared to single sheets. Tape orientation has a significant influence on the mechanical properties. Tensile strength, elongation to strain, and Young's modulus measured in samples produced in the direction of casting showed higher property values.

Corrosion Performance of Steel Coated with Different Duplex Systems and Exposed to Salt Spray and Continuous Immersion Tests

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Advances in Research, 2(3) (2014) 153-178.

Abstract
55%Al-Zn alloy coated steel sheets pre-treated with 5% Fe $(NO_3)_3$ + 15% H_3PO_4 solution, coated with acrylic (AC), alkyd (AQ), vinyl (VL), solvent-based epoxy (ES) or waterborne epoxy (EA) corrosion-inhibiting primers + a barrier topcoat alkyd paint, and exposed to different media were studied. Exposure conditions included salt spray or continuous immersion in solutions containing chloride or sulphate ions. The state of the exposed samples was evaluated by visual inspections, standardized physicochemical tests and electrochemical impedance (EIS) measurements. Their results allowed inferring that: 1) under immersion conditions, the best performance was offered by the ES samples; 2) most of the painting systems performed satisfactorily during their exposure to the salt spray chamber; and 3) the correlation between them permitted to explain some problems arising in service and opened the door to extend the useful life by adjusting the painting system formulation.

Effect of oxidizing concentration on the corrosion resistance of the cerium conversion coating on galvanized steel.

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CTAIJ 9(3) 2014 [85-94]

Abstract
Ce-based conversion films have been assessed as alternatives for replacement of Cr^{6+}-based films, which have been forbidden for their toxicity and carcinogenic properties. However, corrosion protection associated with chromate films is difficult to achieve by other surface treatments. Experimental results have revealed that to obtain the highly satisfactory results provided by chromate-based conversion coatings, it is necessary to improve the anticorrosive properties of the new chromium-free coatings. The present work deals with the effect of the oxidant concentration in the cerium-based conversion baths on the corrosion resistance of the films deposited on galvanized steel. Electrogalvanized steel sheets were exposed to cerium chloride-based baths with different concentrations of oxidant for a minute. The surface of the treated samples was analyzed by XPS and SEM-EDXS, while its corrosion resistance was investigated using electrochemical tests (EIS) conducted in a 0.05 M NaCl solution and the impedance spectra evolution analyzed as a function of the exposure time. The results showed a direct relationship between oxidant concentration and corrosion resistance. When the oxidant concentration rose from 2mL.L^{-1} to 12 mL.L^{-1}, the corrosion

resistance increased about 5 times, and this was attributed to the decrease in the Ce^{3+}/Ce^{4+} relationship of the conversion film.

A conversion layer based on trivalent chromium and cobalt for the corrosion protection of electrogalvanized steel

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Surface & Coatings Technology 258 (2014) 426-436

Abstract
The corrosion resistance of pure zinc coatings can be improved through the application of suitable chemical passivation treatments. Hexavalent chromium (Cr^{6+}) compounds have widely been used to formulate conversion layers providing better anticorrosive protection as well as anchorage properties to painting systems. However, taking into account that they are produced using hazardous chemical compounds, the development of alternative and "green" technologies with equivalent protective performance is a paramount purpose of many R&D laboratories working around the world. In the present paper, the corrosion behavior of industrially electrogalvanized steel subjected to a Cr^{3+} + Co^{2+}-based passivation treatment was studied. The experimental work involved electrochemical impedance spectroscopy (EIS) measurements and polarization curves in a 0.1 mol/L Na_2SO_4 solution, surface microstructural and morphological characterization by electronic microscopy as well as chemical analysis by EDXS and XPS. The most commonly observed failures on the Cr6 + treated samples were attributed to microstructural features of the substrate that were not adequately healed by the Cr6 + passivation treatment.

Adjuvant activity of CPG-ODN formulated as a liquid crystal

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Biomaterials 35 (2014) 2529-2542

Abstract
The adjuvants approved in human vaccine with recombinant/purified antigens induce weak cellular immune response and so the development of new adjuvant strategies is critical. CpG-ODN has successfully been used as an adjuvant (phase IeIII clinical trials) but its bioavailability needs to be improved.
We investigated the adjuvant ability of CpG-ODN formulated with a liquid crystal nanostructure of 6-Oascorbyl palmitate (Coa-ASC16). Mice immunized with OVA/CpG-ODN/Coa-ASC16 elicited a potent specific IgG1, IgG2a, Th1 and Th17 cellular response without systemic adverse effects. These responses were superior to those induced by OVA/CpG-ODN (solution of OVA with CpG-ODN) and to those induced by the formulation OVA/CpG-ODN/$Al(OH)_3$. Immunization with OVA/CpG-ODN/Coa-ASC16 resulted in a long-lasting cell-mediated immune response (at least 6.5 months). Furthermore, Coa-ASC16 alone allows a controlled release of CpG-ODN in vitro and induces local inflammatory response, independent of TLR4 signaling, characterized by an influx of neutrophils and Ly6Chigh monocytes and pro-inflammatory cytokines.
Remarkably, the adjuvant capacity of CpG-ODN co-injected with Coa-ASC16 (OVA/CpG-ODN plus Coa-ASC16) was similar to the adjuvant activity of OVA/CpG-ODN, supporting the requirement for whole formulation to help CpG-ODN adjuvanticity. These results show the potential of this formulation, opening a new avenue for the development of better vaccines.

Influence of natural coarse aggregate type on the transport properties of recycled concrete

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Journal of Materials in Civil Engineering, V26 N6, 2014, pp 4014006-1 a 4014006-9

Abstract
The use of recycled concrete represents a friendly environmental solution for minimizing the impact of the construction and demolition wastes. In many countries, the incorporation of recycled coarse aggregates (RCA) is a common practice, being the maximum contents of RCA usually limited to around 25% of the total content of coarse aggregate. The incorporation of higher volumes of RCA represents a field of discussion mainly regarding to the concrete durable behaviour. This paper analyzes different transport properties of 20 to 50 MPa compressive strength concretes prepared with variable contents of RCA (0, 25, and 75%). Eight types of RCA were obtained from concretes incorporating four different natural coarse aggregates: granitic, basaltic, and quartzitic crushed stones and siliceous river gravel. Capillary absorption, water penetration and chloride diffusion tests were performed. The variation of transport properties with concrete compressive strength and the effect of

RCA content on the transport properties variability were analyzed. According to the results obtained, the durable behaviour of recycled concretes will be different according to the transport mechanisms at which are exposed and it can be as good as that of concretes made with natural coarse aggregates.

Synthesis, structural characterization and magnetic properties of the monoclinic ordered double perovskites $BaLaMSBO_6$, with M = Mn, Co and Ni

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Journal of Alloys and Compounds 606 (2014) 139–148

Abstract
Double perovskites $BaLaMnSbO_6$, $BaLaCoSbO_6$ and $BaLaNiSbO_6$, were synthesized by conventional ceramic method in air, as polycrystalline powders. The Mn and Ni compounds belong to the I 2/m monoclinic space group, while the Co perovskite belongs to the I 4/m tetragonal space group. Effective presence of Mn^{2+} has been well established by X-ray emission spectroscopy for $BaLaMnSbO_6$, and there is no evidence of Mn^{3+}. $BaLaCoSbO_6$ and $BaLaNiSbO_6$ only show the expected 3D-antiferromagnetic behavior typical of super-superexchange interactions, while $BaLaMnSbO_6$ displays signs of superparamagnetism in the 40– 160 K range, which arises from unbalanced antiferromagnetism inside nanoclusters formed by regions which are rich in Mn^{2+}–O^{2-}–Mn^{2+} paths. Neutron powder diffraction data for $BaLaMnSbO_6$ reveals that at 3 K, only long range order antiferromagnetic arrangement of Mn^{2+} spins on 2d octahedral sites is obtained.

Self-assembled Monolayers of Thiolates on Metals: a Review Article on Sulfur-metal Chemistry and Surface Structures

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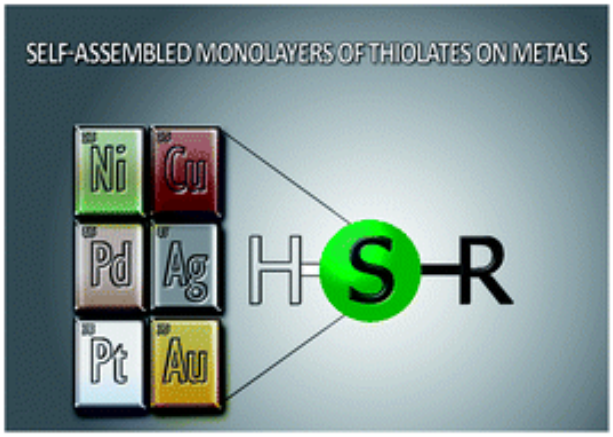
[RSC Adv., 2014, 4, 27730-27754]

Abstract
A review article on fundamental aspects of thiolate self-assembled monolayers (SAMs) on the (111) and (100) surfaces of the Cu and Ni groups is presented. In particular this work is focused on two important points that remain poorly understood in most of these metals: the chemistry of the S-metal interface, which strongly depends on the nature of the metallic surface, and the role of the interaction forces that not only guide the self-assembly process but also influence the surface structure of SAMs. In addition to recent experimental and theoretical data on these issues we present new density functional calculations including van der Waals forces for an important number of known thiolate surface structures as a function of the hydrocarbon chain length.



Synergy between Graphene and Au Nanoparticles (Heterojunction) towards Quenching, Improving Raman Signal, and UV Light Sensing

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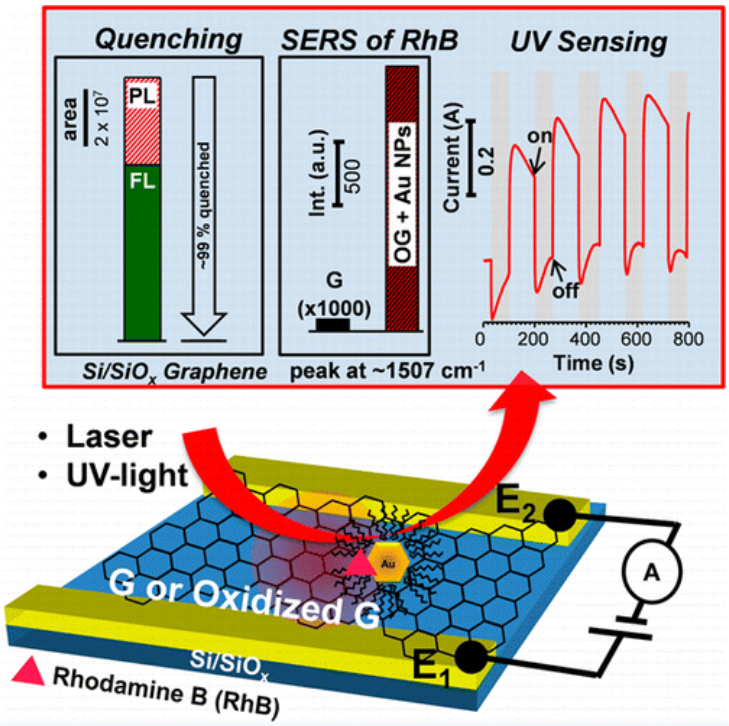
ACS Appl. Mater. Interfaces, 2014, 6 (9), pp 6384–6391

Abstract



Here, we developed a simple method for obtaining a heterojunction composed of graphene (G) and surfactant-coated Au nanoparticles (NPs) to measure film conductivity and surface enhanced Raman scattering (SERS). Monolayer G is obtained by chemical vapor deposition (CVD) and transferred via poly(methyl methacrylate) (PMMA) to microfabricated Au electrodes, glass, and silicon. Post-synthesis treatments of G with PMMA and ozone (O_3) showed 1 and 6 orders of magnitude decrease in film conductivity, respectively. The heterojunction formation with Au NPs had no major effect on G conductivity. In this work is demonstrated that G quenches more than 90% of the combined photoluminescence and fluorescence of Au NPs and Rhodamine B (RhB), respectively. Signal quenching permitted quantitative analysis of SERS of RhB on various substrates including as-transferred graphene, oxidized graphene (OG), and the heterojunction. While G is mainly responsible for quenching photoluminescence and fluorescence, ~3 orders of magnitude increase SERS activity for RhB was accomplished by the heterojunction. Finally, we wanted to correlate changes in film current during UV light sensing experiments. We found striking differences in the sensing profiles at different UV energies.

Evaluation of alkali-silica reaction in concretes with natural rice husk ash using optical microscopy

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Construction and Building Materials 44 (2014) 706–715

Abstract

The use of rice husk ash as a supplementary cementing material is of great interest to many developing countries where rice production is in abundance. A highly reactive pozzolan is obtained when rice husk ash is burnt under controlled conditions. Previous work showed that it is possible to use residual rice husk ash ‘‘as nature’’ (natural rice husk ash). Nevertheless, it was observed that the incorporation of natural rice husk ash implies risks of expansions and mechanical degradation due to the reactions with alkalis. Based on the performance of slab prototypes placed outdoors during more than 3 years, this work analyzes the causes and the damage processes involved in the development of expansions in presence of natural rice husk ash. Optical microscopy observations on thin sections; crack patterns of the slabs and the strength and surface strain evolution along the time were evaluated. Visual and microscope observations showed clear signs of damage due to expansive reactions in concretes incorporating natural rice husk ash when high alkalis contents are available; although not gel was found, numerous cracks and voids were observed close to unburned rice husk particles, as well as high expansions and significant decreases in strength and stiffness. In concretes with alkalis contents lower than 3 kg/m^3, even with the same percentages of natural rice husk ash, there were no significant decreases in the mechanical properties.

Wheel tracking rutting performance estimation based on bitumen Low Shear Viscosity (LSV), loading and temperature conditions

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Materials and Structures (2014) 47, april, pp 683–692

Abstract

The development of new technologies and road pavement materials require the evaluation of the asphalt mixture performance. Rutting is one of the main modes of failure of asphalt mixtures; it is typically studied at the laboratory through the wheel tracking test (WTT). Weather and traffic conditions (temperature, loads) significantly affect the pavement rutting performance. The bitumen rheological properties also have a main role in mixture rutting response; they can adequately characterized by the bitumen Low Shear Viscosity (LSV). The estimation of rutting performance appears as a useful decision tool to optimize pavement design process. This paper studies the rutting performance of asphalts mixtures utilizing the WTT. The specimens were tested at different temperatures and loading levels to simulate different climatic and traffic pavement conditions. A

performance estimator was developed including temperature and traffic load on the pavement, and LSV of the binder as input data.

Challenges and opportunities in polymer technology applied to veterinary medicine

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J Vet Pharmacol Ther. 2014 Apr;37(2):105-24. 2013.

Abstract
An important frontier in the administration of therapeutic drugs to veterinary species is the use of different polymers as drug delivery platforms. The usefulness of polymers as platforms for the administration of pharmaceutical and agricultural agents has been clearly recognized in the recent decades. The chemical versatility of polymers and the wide range of developed controlled release strategies enhance the possibilities for the formulation of active molecules.
In particular, the veterinary area offers opportunities for the development of novel controlled-release drug delivery technologies adapted to livestock or companion animal health needs. In some cases, it also allows to improve profitability in meat production or to meet the safety criteria related to drug residues. A number of factors affect the selection of polymers and subsequent properties of the controlled-release drug delivery system. However, their selection also dictates the release kinetics of the drug from the delivery system. Such choices are therefore crucial as they affect the success and potential of the delivery system for achieving the therapeutic goals of the veterinarian.
It is the intention of this review to give an overview of the most relevant polymers, which are used or have been tested as drug delivery release rate modifiers in the veterinary field. The article highlights some recent developments focusing on their advantages and applications and analyzes the future direction of the scientific and technological advancements in this area

Cationic cellulose and its interaction with chondroitin sulfate. rheological properties of the polyelectrolyte complex

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European Polymer Journal 50 (2014) 142–149

Abstract
This work describes the polyelectrolyte complexation between polyquaternium cellulose (PQ-10) and chondroitin 4-sulfate (C-4S), an important structural component of cartilages.
The complex shows different behaviors with increasing concentrations of the polyanion.
Initially, PQ-10/C-4S interaction forms a soluble, translucent hydrogel that reaches maximum viscosity at a sulfate carboxylate/quaternary ammonium molar ratio lower than 1.
After that, the complex begins to aggregate until complete precipitation, and finally, at higher concentrations of C-4S, the resuspension of the aggregate is observed. Further addition of PQ-10 initiates new cycles of precipitation/resuspension for at least seven times.
C-4S contains sulfates and carboxylates able to interact with quaternary ammonium of PQ-10. The results of a comparative study with polymers containing only carboxylate or sulfate to evaluate the influence of each group suggest that the phenomena observed involved, essentially, carboxylate groups

Año 2013

Synthesis, crystal structure and magnetic properties of the Re(II) complexes $NBu_4[Re(NO)Br_4(L)]$ (L = pyridine and diazine type ligands)

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Dalton Trans, 42 (2013) 15361

Abstract
Four novel Re(II) complexes of formula NBu4[Re(NO)Br4(L)] [NBu4+ = tetra-n-butylammonium cation and L = pyridine (1), pyrazine (2), pyrimidine (3), pyridazine (4)] have been prepared by a substitution reaction involving NBu4[Re(NO)Br4(EtOH)] and L. Their crystal structures have been determined by single crystal X-ray diffraction. They are all mononuclear complexes whose structure is made up of [Re(NO)Br4L]− anions and NBu4+ cations. Each Re(II) ion is six-coordinate with four bromide ligands, a linear nitrosyl group and one monodentate nitrogen donor L building a tetragonally distorted octahedral surrounding. The Re–Br bond distances cover a narrow range [2.5048(8)–2.5333(5) Å] and they are longer than the Re–NO [1.688(15)–1.736(3) Å] and Re–N bonds [2.219(4)–2.234(3) Å]. The magnetic properties of 1–4 have been investigated in the temperature range 1.9–295 K. They behave like quasi magnetically isolated spin doublets with very weak antiferromagnetic interactions through intermolecular Br···Br contacts. Their magnetic properties are discussed through a deep analysis of the influence of the ligand field, spin–orbit coupling, tetragonal distortion and covalence effects. The values of the temperature-independent paramagnetism for 1–4 are also substantiated and compared to those previously reported in related systems.

Backscattered electron images, X-ray maps and Monte Carlo simulations applied to the study of plagioclase composition in volcanic rocks

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Spectrochimica Acta Part B: Atomic Spectroscopy, **81**, 50 – 58 (2013)

Abstract
Zoning patterns in plagioclases are related to abrupt changes in the anorthite content along the crystal growing direction. Accurate characterization of these patterns by electron microprobe is useful to identify magma chamber processes such as recharge, mingling and whole-chamber overturn events.
In this work, a new procedure to obtain high resolution quantitative maps of anorthite concentration in single plagioclase crystals is developed. The methodology consists of performing a calibration of backscattered electron images using quantitative X-ray maps. The ultimate resolution of characteristic X-rays and backscattered electron signals is studied by Monte Carlo simulation. The method is applied to characterize the chemical composition of a volcanic plagioclase from the Cerro Vilama, Argentina. The results obtained are more precise than the values given by the methods commonly used in the study of plagioclase composition, i.e. the classical profiling by electron microprobe point analysis or the modern backscattered electron image calibration by means of quantitative energy or wavelength dispersive X-ray analysis at a few selected points.

Cation effect on the crystal structure of polynuclear complexes with 2,2'-oxydiacetate as bridging ligand

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Inorg. Chim. Acta, 394 (2013) 196.

Using the flexible ligand oxydiacetic acid (H2oda), nine heterodimetallic polymers [{Ca(H2O)6}{CaLn(oda)3}2]_xH2O (Ln = Y, Eu, Tb, Dy, Ho, Er, Tm, Yb, Lu) were synthesized and structurally characterized. The syntheses were performed in aqueous solution by reaction of the ligand and salts of the two ions. They are isostructural and possess a highly ordered 3D structure with [CaLn(oda)3]_ as building blocks. The charge is balanced with [Ca(H2O)6]2+ ions which occupy the holes of the anionic framework. The complexes are thermally stable up to 250 °C. Magnetic susceptibility measurements of Yb and Eu complexes show deviations from the Curie law mainly owing to the split of the ground term due to the ligand field and to the depopulating of paramagnetic excited states in the Yb and Eu compounds, respectively.

Towards decentralized analysis of mercury(II) in real samples. A critical review on nanotechnology-based methodologies

S. Botasini, G. Heijo, E. Méndez

Analytica Chimica Acta 800 (2013) 1-11

Laboratorio de Biomateriales, Instituto de Química Biológica, Facultad de Ciencias, Universidad de la República, Iguá 4225 casi Mataojo, 11400 Montevideo, Uruguay

Abstract

In recent years, it has increased the number of works focused on the development of novel nanoparticle-based sensors for mercury detection, mainly motivated by the need of low cost portable devices capable of giving fast and reliable analytical response, thus contributing to the analytical decentralization. Methodologies employing colorimetric, fluorometric, magnetic, and electrochemical output signals allowed reaching detection limits within the pM and nM ranges. Most of these developments proved their suitability in detecting and quantifying mercury (II) ions in synthetic solutions or spiked water samples. However, the state of art in these technologies is still behind the standard methods of mercury quantification, such as cold vapor atomic absorption spectrometry and inductively coupled plasma techniques, in terms of reliability and sensitivity. This is mainly because the response of nanoparticle-based sensors is highly affected by the sample matrix. The developed analytical nanosystems may fail in real samples because of the negative incidence of the ionic strength and the presence of exchangeable ligands. The aim of this review is to critically consider the recently published innovations in this area, and highlight the needs to include more realistic assays in future research in order to make these advances suitable for on-site analysis.

Silver nanoparticle aggregation not triggered by an ionic strength mechanism

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Journal of Nanoparticle Research 15 (2013) 1526-1532

Abstract
The synthesis of stable colloidal solutions of silver nanoparticles is a major goal in the industry to control their fate in aqueous solutions. The present work studies 10–20-nm silver nanoparticle aggregation triggered by the presence of chloride ions. The aggregation process was followed by UV–Vis–NIR spectroscopy and transmission electron microscopy. We found that the mechanism involved differs from the classic explanation of nanoparticle aggregation triggered by an increase in the ionic strength. Moreover, our results give evidence that even when nanoparticles are resistant to an increment of the total amount of ions, the formation of insoluble salts in the vicinity of the nanoparticle is enough to induce the aggregation. The presence of silver chloride around the silver nanoparticles was documented by an X-ray diffraction pattern and electrochemical methods because chloride anions are ubiquitous in real media; this alternative process jeopardized the development of many applications with silver nanoparticles that depend on the use of stable colloids.

Dielectric behavior of epoxy/BaTiO3 composites using nanostructured ceramic fibers obtained by electrospinning

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ACS Applied Materials and Interfaces, 5 (2013) 505-510.

Abstract
Composite materials made of epoxy resin and barium titanate (BT) electrospun nanostructured fibers were prepared. BT fibers were synthesized from a sol based on barium acetate, titanium isopropoxide, and poly(vinyl pyrrolidone). The fibers were heat-treated at different temperatures and characterized by X-ray diffraction, scanning electron microscopy (SEM), and Raman spectroscopy. Mats of BT fibers heat-treated at 800 C were embedded in epoxy resin into suitable molds. The composites were characterized by SEM, and dielectric measurements were performed by means of dielectric spectroscopy. The dielectric permittivity and dielectric modulus of epoxy resin/BT-fiber composites were measured for two types of samples: with the electrodes parallel and perpendicular to the BT fiber layers. Interestingly, composite samples with electrodes perpendicular to the fiber

layers and a BT content as low as 2 vol % led to dielectric permittivities three times higher than that of pure epoxy resin.

Lead nitroprusside: A new precursor for the synthesis of the multiferroic $Pb_2Fe_2O_5$, an anion-deficient perovskite

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Materials Chemistry and Physics 141 (2013) 355-361

Abstract
In order to investigate the formation of multiferroic oxide $Pb_2Fe_2O_5$, the thermal decomposition of Pb $[Fe(CN)_5NO]$ has been studied. The complex precursor and the thermal decomposition products were characterized by IR and Raman spectroscopy, thermal analysis, powder X-ray diffraction (PXRD), scanning electron microscopy and magnetic measurements. The crystal structure of $Pb[Fe(CN)_5NO]$ was refined by Rietveld analysis. It crystallizes in the orthorhombic system, space group Pnma. The thermal decomposition in air produces highly pure $Pb_2Fe_2O_5$ as final product. This oxide is an anion deficient perovskite with an incommensurate superstructure. The magnetic measurements confirm that $Pb_2Fe_2O_5$ shows a weak ferromagnetic signal probably due to disorder in the perfect antiferromagnetic structure or spin canting. The estimated ordering temperature from the fit of a phenomenological model was 520 K. The SEM images reveal that the thermal decomposition of $Pb[Fe(CN)_5NO]$ produces $Pb_2Fe_2O_5$ with small particle size.

Feasibility of non-invasive temperature estimation by the assessment of the average gray-level content of B-mode images

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Ultrasonics 54 (2014) 1692–1702

Abstrct
This paper assesses the potential of the average gray-level (AVGL) from ultrasonographic (B-mode) images to estimate temperature changes in time and space in a non-invasive way. Experiments were conducted involving a homogeneous bovine muscle sample, and temperature variations were induced by an automatic temperature regulated water bath, and by therapeutic ultrasound. B-mode images and temperatures were recorded simultaneously. After data collection, regions of interest (ROIs) were defined, and the average gray-level variation computed. For the selected ROIs, the AVGL–Temperature relation were determined and studied. Based on uniformly distributed image partitions, two-dimensional temperature maps were developed for homogeneous regions. The color-coded temperature estimates were first obtained from an AVGL–Temperature relation extracted from a specific partition (where temperature was independently measured by a thermocouple), and then extended to the other partitions. This procedure aimed to analyze the AVGL sensitivity to changes not only in time but also in space. Linear and quadratic relations were obtained depending on the heating modality. We found that the AVGL–Temperature relation is reproducible over successive heating and cooling cycles. One important result was that the AVGL–Temperature relations extracted from one region might be used to estímate temperature in other regions (errors inferior to 0.5 ºC) when therapeutic ultrasound was applied as a heating source. Based on this result, two-dimensional temperature maps were developed when the samples were heated in the water bath and also by therapeutic ultrasound. The maps were obtained based on a linear relation for the water bath heating, and based on a quadratic model for the therapeutic ultrasound heating. The maps for the water bath experiment reproduce an acceptable heating/cooling pattern, and for the therapeutic ultrasound heating experiment, the maps seem to reproduce temperature profiles consistent with the pressure field of the transducer, and in agreement with temperature maps developed by COMSOL MultiPhysics simulations.

Catalytic EC` reaction at a thin film modified electrode

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Electrochimica Acta 88 (2013) 66–73

Abstract
Numerical simulations of cyclic voltammograms corresponding to a catalytic EC´ reaction taking place at a thin film modified electrode are performed by way of finite difference method. Besides considering the

chemical kinetic occurring inside the thin film, the model takes into account the different diffusion coefficients for each species at each of the involved phases, i.e. the thin film layer and bulk solution. The theoretical formulation is given in terms of dimensionless model parameters but a brief discussion of each of these parameters and their relationship to experimental variables is presented.
Special emphasis is given to the use of working curve characteristics to quantify diffusion coefficient, homogeneous kinetic constant and thickness of the thin layer in a real system.
Validation of the model is made by comparison of experimental results corresponding to the electron charge transfer of $Ru(NH_3)_6^{3+}/Ru(NH_3)_6^{2+}$ hemi-couple at a thin film of a cross-linked chitosan film containing an immobilized redox dye.

Influence of Natural Coarse Aggregate Type on the Transport Properties of Recycled Concrete

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Journal of Materials in Civil Engineering, 26, 6 (2013) 706–715.

Abstract
The use of recycled concrete represents an environmentally friendly solution for minimizing the impact of construction and demolition wastes. In many countries, the incorporation of recycled coarse aggregate (RCA) is a common practice because the maximum contents of RCA are usually limited to approximately 25% of the total coarse aggregate content. The incorporation of higher volumes of RCA is a field of discussion, primarily regarding the durable behavior of concrete. This study analyzes different transport properties of concretes with compressive strength of 20–50 MPa prepared with variable contents of RCA (0, 25, and 75%). Eight types of RCA were obtained from concretes incorporating four different natural coarse aggregates: granitic, basaltic, quartzitic crushed stones, and siliceous river gravel. Capillary absorption, water penetration, and chloride diffusion tests were conducted. The variation of transport properties with concrete compressive strength and the effect of RCA content on the variability of transport properties were analyzed. According to the results, the durable behavior of recycled concretes is different according to the transport mechanisms to which they are exposed and this behavior can match that of concretes made with natural coarse aggregates.

Real-time study of protein adsorption kinetics in porous silicon

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Colloids and Surfaces B: Biointerfaces 111, 1 (2013), 354–359

Abstract
This paper presents an optical method for real-time monitoring of protein adsorption using porous silicon self-supported microcavities as a label-free detection platform. The study combines an experimental approach with a physical model for the adsorption process. The proposed model agrees well with experimental observations, and provides information about the kinetics of diffusion and adsorption of proteins within the pores, which will be useful for future experimental designs.

Biodegradation study by *Pseudomonas* sp. of flexible polyurethane foams derived from castor oil.

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Icnternational Biodeterioration & Biodegradation, 85 (2013) 85-94

Abstract
The synthesis and biodegradation of polyurethane foams obtained from environmentally benign processes were studied. Flexible polyurethane foams based on castor oil modified with maleic anhydride (MACO) were synthesized. The synthesis involved a single-stage process by mixing castor oil/MACO (weight ratios 75:25 and 25:75) and 2-4 toluene diisocyanate (TDI) in stoichiometric amount of OH:NCO. The biodegradability studies with cultures of a *Pseudomonas* sp. strain (DBFIQ-P36) involved incubation periods of 2 months at 37°C. Polymers were characterized before and after biodegradation by Fourier Transform Infrared Spectroscopy (FT-IR), INSTRON mechanical tester, and Scanning Electron Microscopy (SEM). The results showed that the addition of MACO produces a considerable increase in the rate of degradation and an important change in the chemical and morphological structures. This is due to the presence of ester groups that are vulnerable to chemical hydrolysis and enzymatic attack. The eco-toxicity after the biodegradation was evaluated. Toxic compounds such as primary amines were identified by Gas Chromatography-Mass

Spectrometry (GC-MS) in combination with Nuclear Magnetic Resonance (NMR) as degradation products.

Failure-Oriented Multi-scale Variational Formulation: Micro-structures with nucleation and evolution of softening bands

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Computer Methods in Applied Mechanics and Engineering, 257, 15 (2013) 221–247

Abstract
This contribution presents the theoretical foundations of a *Failure-Oriented Multi-scale variational Formulation* (*FOMF*) for modeling heterogeneous *softening-based* materials undergoing strain localization phenomena. The multi-scale model considers two coupled mechanical problems at different physical length scales, denoted as *macro* and *micro* scales, respectively. Every point, at the macro scale, is linked to a *Representative Volume Element* (*RVE*), and its constitutive response emerges from a consistent homogenization of the micro-mechanical problem.
At the macroscopic level, the initially continuum medium admits the nucleation and evolution of cohesive cracks due to progressive strain localization phenomena taking place at the microscopic level and caused by shear bands, damage or any other possible failure mechanism. A cohesive crack is introduced in the macro model once a specific macroscopic failure criterion is fulfilled.
The novelty of the present *Failure-Oriented Multi-scale Formulation* is based on a proper kinematical information transference from the *macro-to-micro* scales during the complete loading history, even in those points where macro cracks evolve. In fact, the proposed *FOMF* includes two multi-scale sub-models consistently coupled:
(i) a *Classical Multi-scale Model* (*ClaMM*) valid for the stable macro-scale constitutive response.
(ii) A novel *Cohesive Multi-scale Model* (*CohMM*) valid, once a macro-discontinuity surface is nucleated, for modeling the macro-crack evolution.
When a macro-crack is activated, two important kinematical assumptions are introduced: (i) a change in the rule that defines how the increments of generalized macro-strains are inserted into the micro-scale and (ii) the *Kinematical Admissibility* concept, from where proper *Strain Homogenization Procedures* are obtained. Then, as a consequence of the Hill–Mandel Variational Principle and the proposed kinematical assumptions, the *FOMF* provides an adequate homogenization formula for the

stresses in the continuum part of the body, as well as, for the traction acting on the macro-discontinuity surface.
The assumed *macro-to-micro* mechanism of kinematical coupling defines a specific admissible *RVE*-displacement space, which is obtained by incorporating additional boundary conditions, *Non-Standard Boundary Conditions* (*NSBC*), in the new model. A consequence of introducing these *Non-Standard Boundary Conditions* is that they guarantee the existence of a physically admissible *RVE*-size, a concept that we call through the paper "*objectivity*" of the homogenized constitutive response. Several numerical examples are presented showing the *objectivity* of the formulation, as well as, the capabilities of the new multi-scale approach to model material failure problems.

Photocatalytic activity of nanoneedles, nanospheres, and polyhedral shaped ZnO powders in organic dye degradation processes

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Journal of Alloys and Compounds, 572 (2013) 68-73

Abstract
In this work acicular ZnO nanostructures were successfully produced by an adapted thermal evaporation method. The obtained material was compared with a commercial ZnO nanopowder of similar size and surface area but different morphology, and a commercial micro-powder of different morphology, size and surface area, in the degradation of Methyl Orange (MO) and Safranin O (SAF). Photoluminescence spectroscopy was used to evaluate the native point defects in the samples. It was observed that the nanostructured ZnO powder synthesized by the thermal evaporation process presented the highest amount of native point defects of all samples analyzed, which could be related with the better photocatalytic performance in despite of the specific surface area and crystallite size of the evaluated powders.

Characterization, dissolution and in vivo evaluation of solid acetazolamide complexes

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Carbohydrate Polymers 98 (2013) 380–390

Abstract
The effects of binary and ternary systems of acetazolamide (ACZ) with hydroxypropyl-cyclodextrin (HP-β-CD) alone or with triethanolamine (TEA) on the crystalline properties, dissolution and intraocular pressure (IOP)-lowering effect were investigated.
It was found that the crystal structure of ACZ powder could be modified by the processing conditions.
Freeze-drying ACZ powder affected not only the particle morphology but also its polymorphic form and the starting ACZ was converted to pure form A upon freeze-drying treatment. Results provided by DSC/TGA, XRPD, SEM and FT-IR suggested the formation of inclusion complexes between ACZ with HP- β -CD alone or with TEA, obtained by the freeze-drying method and the conversion of the drug into the amorphous state. Binary and ternary systems of ACZ obtained by freeze-drying exhibited significantly enhanced ACZ dissolution rates. The IOP-lowering effects of ACZ and its complexes with HP- β -CD alone or with TEA were studied in normotensive rabbits. Whereas the maximum IOP-lowering effect (~4 mmHg, ~33%), obtained with these binary and ternary lyophilized ACZ systems occurred at around 90 min, the ternary system exhibited a longer maximum IOP-lowering effect peak compared with that of the binary system. These results are in line with those obtained from the dissolution studies, where the ternary system exhibited longer dissolution times compared to the lyophilized binary one.
Results obtained from the dissolution studies, also showed that freeze-drying the native crystalline form of ACZ significantly increased the dissolution rate of ACZ, thus improving the IOP-lowering effect of this drug.

Valve based on novel hydrogels: from synthesis to application

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Sensors and Actuators B 188 (2013) 176–184

Abstract
New hydrogels as materials with potential application in the area of actuators have been developed. Hydrogel synthesis was performed using tris[(hydroxymethyl) methyl]acrylamide (NAT) and itaconic acid (ITA) as monomers and (+)N,N`-diallyltartradiamide (DAT) as crosslinker. The hydrogels NAT–ITA were prepared using different molar fraction of monomers and characterized by FTIR-ATR, rheology, swelling properties and mechanical force. The hydrogel prepared with 80% and 20% of NAT and ITA, respectively, has the lowest equilibrium swelling ratio (ESR = 16) in water but the highest elastic modulus(10 ± 1 kPa) and strength (2.2 ± 0.1 N h−1). The gel strength increased 0.5 N in a half hour, while the volume increased 4 times when passed from an acid medium to a basic medium. This hydrogel was chosen toprepare a pH-sensitive valve to control the

flux in a capillary tube. The valve was tested using a system to control the formation of Fe^{3+}–EDTA complex. The response time was 3 and 15 min to open and close the valve, respectively. The flow of the solution through the valve was 11 _L min−1. The pressure of the solution during the closing of the valve was 10 kPa. The continuous opening and closing of the valve involves repetitive expansion and collapse of the network that could damage the structure of the network. However, the valve produced a reproducible and stable response. The dynamic hydrogen bonding existing in the polymeric chains of NAT–ITA products could assist in the reversible process when the hydrogels were subjected to repetitive work. The mechanical properties of the gels and self-healing capacity of the networks indicated that the products could be applicable in the development of systems for controlled drug release.

A comparative study of the effect of different rigid fillers on the fracture and failure behavior of polypropylene based composites

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Composites Part B: Engineering, 52 (2013) 72-83

Abstract
Polypropylene (PP) composites with 5 wt% of different rigid particles (Al2O3 nanoparticles, SiO2 nanoparticles, Clay (Cloisite 20A) nanoparticles or CaCO3 microparticles) were obtained by melt mixing. Composites with different CaCO3 content were also prepared. The effect of fillers, filler content and addition of maleic anhydride grafted PP (MAPP) on the composites fracture and failure behavior was investigated. For PP/CaCO3 composites, an increasing trend of stiffness with filler loading was found while a decreasing trend of strength, ductility and fracture toughness was observed. The addition of MAPP was beneficial and detrimental to strength and ductility, respectively mainly as a result of improved interfacial adhesion. For the composites with 5 wt% of CaCO3 or Al2O3, no significant changes in tensile properties were found due to the presence of agglomerated particles. However, the PP/CaCO3 composite exhibited the best tensile behavior: the highest ductility while keeping the strength and stiffness of neat PP. In general, the composites with SiO2 or Clay, on the other hand, displayed worse tensile strength and ductility. These behaviors could be probably related to the filler ability as nucleating agent. In addition, although the incorporation of MAPP led to improved filler dispersion, it was damaging to the material fracture

behavior for the composites with CaCO 3, Al2O3 or Clay, as a result of a higher interfacial adhesion, the retardant effect of MAPP on PP nucleation and the lower molecular weight of the PP/MAPP blend. The PP/MAPP/SiO2 composite, on the other hand, showed slightly increased toughness respect to the composite without MAPP due to the beneficial concomitant effects of the presence of some amount of the β crystalline phase of PP and the better filler dispersion promoted by the coupling agent which favor multiple crazing. From modeling of strength, the effect of MAPP on filler dispersion and interfacial adhesion in the PP/CaCO3 composites was confirmed.

Photocatalytic degradation of methyl orange dye in water solutions in the presence of MWCNT/TiO2 composites.

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Materials Research Bulletin, v. 48, p. 1845-1850, 2013.

Abstract

The textile and dyestuff industries are the primary sources of the release of synthetic dyes into the environment and usually there are major pollutants in dye wastewaters. Because of their toxicity and slow degradation, these dyes are categorized as environmentally hazardous materials. In this context, carbon nanotubes/TiO_2 (CNTs/TiO_2) composites were prepared using multi-walled CNTs (MWCNTs), titanium (IV) propoxide and commercial TiO_2 (P25®) as titanium oxide sources, to degrade the methyl orange dye in solution through photocatalyst activity using UV irradiation. The composites were prepared by solution processing followed by thermal treatment at 400, 500 and 600 °C. The heterojunction between nanotubes and TiO_2 was confirmed by XRD, specific surface area. The coating morphology was observed with SEM and TEM.

Preparation of ceramic nanoparticles *via* cellulose-assisted glycine nitrate process: a review

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RSC Adv., 2013, 3, 2873–2884

Abstract
Ceramics exhibit several interesting properties, which make them the material of choice for a broad range of applications. Their physical and chemical properties are significantly improved by sub-micrometer ceramic powders with narrow particle size distribution, high chemical purity and crystallinity and no/weak agglomeration. However, powders with such superior characteristics are mostly synthesized by complex and costly processes, which are usually not ideal for production at an industrial scale. Therefore, developing simple, efficient, inexpensive and environmentally-benign processes for the preparation of high quality ceramic powders is of great interest both for the research community and industry. In this regard, this article reviews the research efforts in the preparation of ceramic nanopowders from cotton-cellulose, which is used as a sacrificial bio-template, in a glycine–nitrate process. Low processing temperatures, self-propagating nature of the reactions, high reaction rates, no necessity for extra energy and special apparatus are the characteristics of this process yielding extremely fine, homogenous and non-agglomerated powders.

Formulation of mortars with nano-SiO_2 and nano-TiO_2 for degradation of pollutants in buildings

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Composites. Part B, Engineering, v. 44, p. 40-47, 2013.

Abstract
This paper reports on the design of cement mortars that use nano-SiO_2 (nS) and nano-TiO_2 (nT) particles, aiming to improve the durability of traditional building materials while giving new functionalities (aerial decontamination of pollutants). Samples with 0–2 wt.% nS, 0–20 wt.% nT, 0.45–7 wt.% superplasticizer (SP) and 0.45–0.58 water/binder weight ratio were prepared. The formulations of mortars were defined according to rheology and flow table measurements, then showing suitable workability. The temperature of hydration, compressive strength, water absorption, and photocatalytic degradation of pollutants (NO_x and Orange II dye) were also evaluated. In general, the rheological behavior and the temperature of hydration changed in distinct levels, depending on the dosage and type of nanoadditives, but nT influenced more significantly the results.

However, such differences were not identified on the compressive strength and water absorption. In addition, NO_x photocatalytic degradation up to 1 h under solar light ranged from 65% to 80%, while Orange II degradation after 9 h under visible light changed from 18% to 50%.

Near-field effects in Green's function retrieval from cross-correlation of elastic fields: Experimental study with application to elastography

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J. Acoust. Soc. Am., 133 (5) (2013) 2755-2767

Abstract
In a lossless system, the causal and acausal Green's function for elastic waves can be retrieved by cross-correlating the elastic field at two positions. This field, composed of converging and diverging waves, is interpreted in the frame of a time-reversal process. In this work, the near-field effects on the spatio-temporal focusing of elastic waves are analyzed through the elastodynamic Green's function. Contrary to the scalar field case, the spatial focusing is not symmetric preserving the directivity pattern of a simple source. One important feature of the spatial asymmetry is its dependency on the Poisson ratio of the solid. Additionally, it is shown that the retrieval of the bulk wave speed values is affected by diffraction. The correction factor depends on the relative direction between the source and the observed field. Experimental verification of the analysis is carried out on the volume of a soft-solid. A low-frequency diffuse-like field is generated by random impacts at the sample's free surface. The displacement field is imaged using ultrasound by a standard speckle tracking technique. One important application of this work is in the estimation of the shear elastic modulus in soft biological tissues, whose quantification can be useful in non-invasive diagnosis of various diseases.

Años 2012 - 2010

Effect of nano-SiO_2 and nano-TiO_2 addition on the rheological behavior and the hardened properties of cement mortars

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Materials Science and Engineering: A. Volume 532, 15 January 2012, Pages 354–361

Abstract
This paper reports on the use of nano-SiO_2 (nS) and nano-TiO_2 (nT) in cement pastes and mortars. Samples with 0–3 wt.% nS, 0–12 wt.% nT and 0.5 water/binder weight ratio were prepared. Rheological and flow table measurements were carried out. In addition, the design of experiments was applied to validate the results found. The temperature of hydration and compressive strength with 28 days was also determined. In general, mortars exhibited noticeable differences in the rheological behavior, but less evident in temperature of hydration and compressive strength. The values of torque, yield stress and plastic viscosity of mortars with nanoadditives increased significantly, reducing the open testing time in rheology tests. Meanwhile, the flow table values reduced. In addition, spread on table and initial yield stress exhibited a power correlation, while the spread on table and plastic viscosity did not show any special relationship. The results of kinetics of hydration followed the same tendency found by rheology, in which samples with higher amounts of nS and nT showed remarkable changes in relation to the samples without nanoadditives. Mechanical properties were not significantly affected by nanoparticles in the range considered in this work.Ultrasonic investigation of the relaxor behaviour of ferroelectric ceramics $(Pb_{1-x}Ca_x)TiO_3$ for x = 0.475, 0.50 and 0.5

X-ray evaluation of dislocation density in ODS-Eurofer steel

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Materials Science and Engineering: A. Volume 534, 1 February 2012, Pages 142–146

Abstract
The dislocation density of ferritic–martensitic oxide dispersion strengthened ODS-Eurofer steel was evaluated by using the modified Williamson–Hall method (peak broadening analysis). Measurements were performed in several metallurgical conditions (ferritic and martensitic structures). The monochromatic X-ray radiation was provided by a synchrotron source. The results match qualitatively with those provided by Vickers microhardness measurements and metallographic inspection using transmission electron microscopy.

Ultrasonic investigation of the relaxor behaviour of ferroelectric ceramics $(Pb_{1-x}Ca_x)TiO_3$ for $x = 0.475$, 0.50 and 0.55

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Materials Research Bulletin. Volume 47, Issue 2, February 2012, Pages 486–490

Abstract
Three samples of calcium modified lead titanate $(Pb_{1-x}Ca_x)TiO_3$ with $x = 0.475$, 0.50 and 0.55 were studied in terms of their ultrasonic properties. The samples were prepared using the solid state reaction technique. Ultrasonic attenuation and velocity were measured as a function of the temperature at 5 MHz and 10 MHz with X-cut quartz transducers, using the ultrasonic pulse-echo technique and Papadakis method for accuracy determination of the transit time of ultrasonic RF pulses. An equation regarding elastic–electric coupling between strain and spontaneous polarization was used in order to fit the elastic modulus. The nature of the phase transition was characterized through the diffusivity exponent obtained from this fit. Our results show that, as calcium concentration increases from 0.475 to 0.55, the behaviour of ferroelectric phase transition changes

from normal to relaxor. This process is accompanied by a systematic decrease of the critical temperature.

Shape memory properties of highly textured Cu–Al–Ni–(Ti) alloys

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Materials Science and Engineering: A. Volume 536, 28 February 2012, Pages 207–215

Abstract
A strong α-fiber I texture with components from {0 0 1}$\langle 1\,1\,0\rangle_{\beta_1}$ to {1 1 2} $\langle 1\,1\,0\rangle_{\beta_1}$ was developed in a polycrystalline Cu–13Al–5.5Ni–1Ti (wt%) shape memory alloy by hot extrusion at 800 °C (followed by recrystallization). Nearly fully recoverable strains up to the order of 6%, associated with cubic to monoclinic martensitic transformation $\beta_1 \rightarrow \beta_1'$, have been measured by thermal cycling under constant load experiments. Such a degree of strain recovery is typical of single crystals or polycrystalline arrays with a low degree of grain constraint, such as highly textured, “bamboo” like, extruded materials. The reversible transformation strains reached about 68% of the upper bound predicted by a Sachs-type model which averages the most favorable martensite variants in each grain, taking into account their orientation and disregarding interactions between them. Due to the strong texture introduced in the material, such high values of recoverable transformation strains are obtained even for specimens having a grain size/thickness ratio of ∼0.05, producing relatively high grain constraint.

Fluorescent nanohybrids: quantum dots coupled to polymer recombinant protein conjugates for the recognition of biological hazards

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J. Mater. Chem., 2012, 22, 9006–9018

Abstract
The present research introduces the concept of developing a novel nanohybrid system based on fluorescent quantum dots coupled to polymer–protein bioconjugates for the detection of potential

biological hazards. The organic–inorganic hybrids were constructed by the chemical conjugation of carboxylic functionalized poly(vinyl alcohol) with the designed synthetic recombinant protein specific to bovine herpesvirus (rHBoV5), followed by coupling to II–VI semiconductor quantum dots (QDs). These nanostructures were characterized by UV-visible spectroscopy, Fourier transform infrared (FTIR) spectroscopy, photoluminescence (PL) spectroscopy, and transmission electron microscopy (TEM). The results clearly showed that the polymer–protein bioconjugates (PVA–COOH/rHBoV5) were synthesized *via* the proposed zero-length linker route. Moreover, these bioconjugates proved to be successful capping agents for producing CdS and CdSe quantum dots using aqueous colloidal chemistry. The TEM images associated with the optical absorption results indicated the formation of nanocrystals with estimated diameters in the range of 4.0–5.0 nm. The "blue-shift", in the visible absorption spectra, and the PL values present strong evidence that the CdS and CdSe QDs behaved as fluorophores in the quantum-size confinement regime. Finally, the hybrid system was validated by immunochemical assay of bovine herpesvirus utilized as the model for detecting biological hazards. This research opens a window of opportunity of using a new class of hybrid nanomaterials for the rapid detection of potentially threatening biological species.

ZnO/Cu_2O heterostructure nanopillar arrays: synthesis, structural and optical properties

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Journal of Physics D: Applied Physics 45 (24), art. no. 245301 (10pp) (2012)

Abstract
Vertically aligned ZnO/Cu_2O heterostructure nanopillar arrays consisting of a ZnO core and a Cu_2O shell were fabricated by a two-step electrochemical deposition method. Morphological, structural and optical properties of the nanopillar heterojunctions were investigated. The surface of the single-crystalline ZnO nanopillars was coated uniformly, conformally and densely over the entire nanopillar length by numerous Cu_2O nanocrystals (25–35 nm mean diameter), constituting a conformal shell layer 90 nm thick, integrating these two materials into an electronically intimate composite. The optical properties can be interpreted, by appropriate fittings of each feature, as being due to the properties of the bare ZnO nanopillar array plus the increased absorption of Cu_2O. This study demonstrates that electrodeposition is a suitable and accessible technique for large-scale fabrication of nanopillar heterostructures and to achieve conformal coverage of nanostructured samples.

Crystallographic relationships in the crossed lamellar microstructure of the shell of the gastropod *Conus marmoreus*

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Acta Biomaterialia. Volume 8, Issue 2, February 2012, Pages 830–835

Abstract

The crossed lamellar microstructure of mollusk shells shows a very complex hierarchical architecture constituted of long rod-shaped aragonite crystals stacked parallel to each other inside each first order lamella, which are almost perpendicular to the ones contained in parallel neighboring lamellae. To better understand the construction and properties of the crossed lamellar microstructure we have performed a detailed study to determine the crystallographic characteristics and their evolution during shell growth using scanning electron microscopy, transmission electron microscopy and X-ray diffraction texture analysis. The arrangement of crystals is rationalized by a set of twin law relationships between aragonite crystals. Specifically, the aragonite rods, or third order lamellae within each first order lamella, internally consist of polysynthetic twins bounded by {1 1 0} mirror planes. In turn, the polysynthetically twinned aragonite crystals also show a constant crystallographic orientation with respect to aragonite crystals in adjacent first order lamellae. It can be seen as another twin law in which crystals from adjacent lamellae are bounded by (1 1 0) planes but with their *c*-axes rotated within this plane by 30°. Thus there are two sets of twin laws that relate crystal units at lower (third order lamellae) and higher (first order lamellae) length scales. These hierarchical relationships play a crucial role in the construction, organization and properties of this complex microstructure. The later orientational relationships have never been described in geological aragonite and are only found in biogenic materials with a crossed lamellar microstructure. Their occurrence is probably determined by the presence of shell organic components which regulate crystal growth and may favor unusual crystallographic relationships.

Bioconjugation of quantum-dots with chitosan and *N*,*N*,*N*-trimethyl chitosan

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Carbohydrate Polymers. Volume 90, Issue 1, 1 September 2012, Pages 189–196

Abstract
Novel carbohydrate-based hybrids combining chitosan and chemically modified chitosan with CdS inorganic nanoparticles were designed and prepared via aqueous route at room temperature. *N*,*N*,*N*-trimethylchitosan (TM-chitosan) was synthesized aiming at substantially improving the water solubility of chitosan for producing stable colloidal systems. UV–vis spectroscopy, photoluminescence spectroscopy, Nuclear magnetic resonance spectroscopy, Raman spectroscopy, and Fourier transform infrared spectroscopy were used to characterize the synthesis and the relative stability of biopolymer-capped CdS nanocrystals. The results have clearly indicated that chitosan and chitosan-derivative (TM-chitosan) were remarkably effective on nucleating and stabilizing CdS nanoparticles in aqueous suspensions. In addition, the CdS nanocrystals were produced in the so-called "quantum-size confinement regime", with the calculated average size below 3.5 nm and fluorescent activity in the visible range of the spectra. Therefore, a new single-step process was developed for the bioconjugation of quantum dots with water soluble chemically functionalized carbohydrates at room temperature for potential biomedical applications.

Application of 1-D transient elastography for the shear modulus assessment of thin-layered soft tissue: comparison with supersonic shear imaging technique.

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IEEE Trans Ultrason Ferroelectr Freq Control. 2012 Apr;59(4):703-14

Abstract
Elasticity estimation of thin-layered soft tissues has gained increasing interest propelled by medical applications like skin, corneal, or arterial wall shear modulus assessment. In this work, the authors

propose one-dimensional transient elastography (1DTE) for the shear modulus assessment of thin-layered soft tissue. Experiments on three phantoms with different elasticities and plate thicknesses were performed. First, using 1DTE, the shear wave speed dispersion curve inside the plate was obtained and validated with finite difference simulation. No dispersive effects were observed and the shear wave speed was directly retrieved from time-of-flight measurements. Second, the supersonic shear imaging (SSI) technique (considered to be a gold standard) was performed. For the SSI technique, the propagating wave inside the plate is guided as a Lamb wave. Experimental SSI dispersion curves were compared with finite difference simulation and fitted using a generalized Lamb model to retrieve the plate bulk shear wave speed. Although they are based on totally different mechanical sources and induce completely different diffraction patterns for the shear wave propagation, the 1DTE and SSI techniques resulted in similar shear wave speed estimations. The main advantage of the 1DTE technique is that bulk shear wave speed can be directly retrieved without requiring a dispersion model.

Study of the Anelastic Behavior of PZT and PLZT Ferroelectric Ceramics

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Defect and Diffusion Forum Vols. 326-328 (2012) pp 719-724

Abstract

The anelastic behavior of the ferroelectric ceramics (Pb)(Zr/Ti)O 3 (PZT) and (Pb/La)(Zr/Ti)O 3 (PLZT), with Zr/Ti = 65/35, La = 5 at.% and 8 at.%, was investigated in the region of the ferroelectric phase transitions. Anelastic spectroscopy experiments were performed in an acoustic elastometer system, operating in a kilohertz bandwidth, at temperatures rising from 300 K to 770 K, at a heating rate of 1 K/min, under pressure of 10 -5 mbar. Anelastic measurements on PZT showed only one anomaly, associated with the occurrence of a ferroelectric-paraelectric phase transition, while the PLZT data showed two anomalies, which were associated with the following transitions: the ferroelectric-paraelectric phase transition and a ferro-ferroelectric phase transition between distinct rhombohedral ferroelectric phases. The behavior of the relative variation of the elastic moduli with temperature, near the phase transitions, which describes the change in the type of coupling between strain and the order parameter in ferroelectric-paraelectric phase transition, with the increase of lanthanum amount and, linear coupling in the strain and order parameter type to PZT ceramic and linear coupling in the strain but quadratic in order parameter type for PLZT ceramics.

Dynamical Elastic Moduli of the Ti-13Nb-13Zr Biomaterial Alloy by Mechanical Spectroscopy

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Materials Research. 2012; 15(6): 1-4

Abstract
Dynamical Elastic Moduli of the Ti-13Nb-13Zr biomaterial alloy were obtained using the mechanical spectroscopy technique. The sample with heat treatment at 1170K for 30 minutes and water quenched with subsequent aging treatment at 670 K for 3 hours (TNZ + WQ + 670 K/3 h), was characterized through decay of free oscillations of the sample in the flexural vibration mode. The spectra of anelastic relaxation (internal friction and frequency) in the temperature range from 300 K to 625 K not revealed the presence of relaxation process. As shown in the literature, the hcp structure usually does not exhibit any relaxation due to the symmetry of the sites in the crystalline lattice, but if there is some relaxation, this only occurs in special cases such as low concentration of zirconium or saturation of the stoichiometric ratio of oxygen for zirconium. Dynamical elastic modulus obtained for TNZ + WQ + 670 K/3 h alloy was 87 GPa at room temperature, which is higher than the value for Ti-13Nb-13Zr alloy (64 GPa) of the literature. This increment may be related to the change of the proportion of α and β phases. Besides that, the presence of precipitates in the alloy after aging treatment hardens the material and reduces its ductility.

Experimental and numerical study of the role of crystallographic texture on the formability of an electro-galvanized steel sheet

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Journal of Materials Processing Technology. Volume 212, Issue 6, June 2012, Pages 1367–1376

Abstract
In this work, the influence of plastic anisotropy on forming-limit strains for a drawing-quality steel sheet was investigated. For this purpose, hourglass-type samples, taken at 0°, 45° and 90° with respect to the sheet rolling direction were tested with a typical punch and die fixturing. Numerical simulations were carried out in order to validate two viscoplastic (VP) polycrystalline models, self-consistent (SC) and full-constraint Taylor-type (FC), in conjunction with the Marciniak and Kuczynski (MK) localization approach. The observed shift to the right in the minimum of the forming limit diagram (FLD), inherent to Nakazima test, was taken into account in the simulations. Keeping the set of adjustable parameters to a minimum in the calibration of the viscoplastic polycrystal model, only the material's initial texture and a power law fit to the tensile data needed to be measured. Without other adjustments to either model, MK-VPSC gives realistic predictions over the entire FLD, while the MK-FC predictions only follow the measured limit curve on the tensile side of plane strain. In the positive biaxial quadrant of the FLD, MK-FC predicts unrealistic high limit values. It was found that, despite these extremely high limit values, the similarity in the measured limit strains for the three sample orientations is captured by both models. However, a consistency in the MK-VPSC predictions indicates that this model seems to be a more suitable tool for describing the role of crystallographic texture on the sheet metal forming processes.

Ultrasonic investigation of the interaction of hydrogen-dislocations in copper crystals

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Materials Science and Engineering: A. Volume 528, Issue 12, 15 May 2011, Pages 4255–4258

Abstract
In this paper we present experimental data of ultrasonic velocity and attenuation obtained in a high purity crystalline sample of copper hydrogenated by gaseous charge. The sample is oriented in the 〈1 1 1〉 crystallographic direction and aged for this work in three stages between 64 and 97 days. The results indicate that the hydrogen is mainly segregated at the dislocation core, inhibiting the hydrogen Snoek–Köster relaxations verified at earlier ageing stages. Despite this, a contribution to viscosity in the kink-chain resonance is provided by the mobile hydrogen in the dislocation core by its side movement along the dislocation line. At temperatures at which the hydrogen begins to freeze in the lattice the geometrical kinks find a gradual increase on the hindering of their movements along

dislocation lines, becoming immobile when the hydrogen is completely frozen in the crystal, anchoring the dislocations in short loops. Although the viscosity associated with the mobile hydrogen is removed, the resonance associated with geometrical kinks is not completely cancelled. The interaction of hydrogen-dislocation can be fully described in terms of kinks in dislocations.

The Evolution of Texture in AA 1050 Alloy Deformed by Equal-Channel Angular Pressing

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Materials Science Forum, Volumes 667 – 669, (2011), pp. 557-582

Abstract
The aim of the present work is to analyze the evolution of texture after ECAP and post deformation heat treatment of an AA1050 alloy produced by roll casting. The initial plate exhibited a weak cube texture at the surface, decreasing in its intensity toward the sheet center, where the deformation texture consisted of Brass and Copper components. ECAP-deformation employed one to four passes at room temperature, following route A in a $\Phi = 120^{o}$ die. Texture evaluation was performed by x-ray analysis and by EBSD, using transverse cross section scans. Only the central part of the plate was studied. Results were analyzed by regular texture and orientation distribution function calculations. After 1, 2 and 4 passes the texture changed to a strong {111}// TD and after recrystallization at 350oC for 1 h this main orientation was maintained.

Anelastic relaxation due to hydrogen in Ti–35Nb–7Zr–5Ta alloy

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Materials Science and Engineering A 528 (2011) 3326–3329

Abstract
Titanium and its alloys are frequently used in the production of prostheses and dental implants due to their properties, such as high corrosion resistance, low elasticity modulus, and high mechanical strength/density relation. Among the Ti-based alloys, Ti–35Nb–7Zr–5Ta (TNZT) is one that presents the smallest elasticity modulus (around 45GPa), making it an excellent alternative to be used as a biomaterial. In this paper, mechanical spectroscopy measurements were made of TNZT alloys containing several quantities of hydrogen in solid solution. Mechanical spectroscopy measurements were made by using a torsion pendulum, operating at an oscillation frequency in the interval 2–20Hz, temperature in the range 100–300K, heating rate of about 1K/min, and vacuum lower than 10^{-5}Torr. A relaxation structure and a reduction in the elasticity modulus were observed for the heat-treated and doped samples. The observed peak was associated with the interaction of hydrogen trapped by oxygen atoms around the titanium atom of the metallic matrix.

Mechanical Spectroscopy Study on Cu53.5Zr42Al4.5 Alloy

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Defect and Diffusion Forum Vols. 312-315 (2011) pp 1233-1237

Abstract
This study consists of the characterization of the anelastic properties of a Bulk Metallic Glasses (BMG) by mechanical spectroscopy, which can be defined as an energy absorption technique. The equipment used was the acoustic elastometer system, the anelastic relaxation spectra were carried out with a heating rate of 1 K/min and vacuum better than 10 -5 torr, in the temperature range of 300 K to 640 K. The amorphous sample studied, with nominal composition of Cu 53.5 Zr 42 Al 4.5 , was processed by skull push-pull casting technique in a rectangular cavity cooper mould. Differential scanning calorimeter (DSC) curves have evidenced the amorphous structure although the X-ray diffraction (XDR) pattern has indicated a heterogeneous microstructure with amorphous matrix and some metaestable nanocrystalline phases which have not been identified yet. The dynamical elastic modulus of this alloy (between 54 GPa and 58 GPa at room temperature) and internal friction patterns as temperature function implied an increase of the crystalline phase during the measurements. This effect was confirmed with new X-ray diffraction measurements after the internal friction experiments.

Origin of solar thermal selectivity and interference effects in nickel–alumina nanostructured films

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Surface and Coatings Technology. Volume 204, Issue 14, 15 April 2010, Pages 2197–2201

Abstract
Selective surfaces for solar to thermal conversion were studied for understanding the main parameters affecting selectivity. For this purpose samples of Ni inclusions into nanoporous anodized aluminum were electrochemically prepared. Their optical reflectance from 200 nm to 17 μm was measured showing a step-like behavior and several interference fringes. Different models were used to interpret this behavior varying several of the involved parameters. The composition of Ni/alumina film is the first cause for selectivity. Interference effects occurring in this film strengthen the step-like behavior of the reflectance spectra and therefore, the selectivity.

Study of limitstrains for FCC and BCC sheetmetal using polycrystalplasticity

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International Journal of Solids and Structures. Volume 48, Issues 7–8, April 2011, Pages 1109–1119

Abstract
In this research, we analyze forming-limitstrains of FCC and BCC materials using a viscoplastic self-consistent polycrystal model (VPSC) in conjunction with the Marciniak–Kuczynski (MK) approach. In particular, our work is focused on the theoretical analysis and comparison between FCC and BCC

crystal structures made by Inal et al. [Inal, K., Neale, K.W., Aboutajeddine, A., 2005. Forming limit comparison for FCC and BCCsheets, International Journal of Plasticity, 21, 1255–1266]. These authors performed their simulations based on a generalized Taylor-type polycrystal model (MK-FC), finding a remarkably low forming-limit curve for the FCC material and an extremely high forming-limit curve for the BCC material, in the biaxial stretching range. We verified that our predictions are similar to Inal's results for both FCC and BCC materials when the MK-FC model is used. However, MK-VPSC calculations do not give such extreme values, and we believe that this theory predicts much more reliable results for both FCC and BCC crystallographic assumptions. We also found that localized necking depends on texture evolution in the vicinity of equi-biaxial stretching, through the sharpness of the predicted yield surface. Finally, it is shown that the MK-VPSC's predictions are in good agreement with experimental data for AA5182-O and a DQ-type steel-sheetmetal.

Temperature-induced changes in soft tissues analyzed by spectral methods and transient elastography: A comparative study

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AIP Conference Proceedings / Volume 1433 / BIOMEDICAL ULTRASOUND/2011

Abstract
Some biological tissues, such as skeletal muscle, have regular or quasi-periodic structures. Periodicity of these structures can be investigated by spectral methods based on ultrasonic backscattered signals. These methods estimate the Mean Scatterer Spacing (MSS). In this work we analyzed the MSS dependence with temperature in bovine skeletal muscle tissue samples. Through spectral analysis we found that the relative variation of the MSS, in the temperature range 20 - 48°C was of ~ 2% /°C. For the same sample and under the same experimental conditions, we analyzed the propagation velocity of shear waves by transient elastography. It was determined that the relative variation of shear elastic modulus was ~ 3% /°C in the same temperature range. The repeatability of the results was tested in three tissue samples, with a set of 6 measurements on each. The relative variation is therefore similar for both parameters. Thus, this study shows that both techniques can be used as a method of noninvasive thermometry for small temperature range. In addition we emphasize the conceptual differences between both methods. As temperature changes, MSS estimation varies due to two physical phenomena. An apparent variation in mean spacing is produced because the sound speed is temperature-dependent, while tissue expansion produces a real change. In practice it is difficult to discriminate the weight of each component in the MSS variation. On the other side, transient elastography is less sensitive to thermal expansion. Thus it measures the actual shear wave

speed change with temperature. This differentiation between both methods could be used to construct useful thermoelastic models for soft tissues in the future.

Texture vs morphology in ZnO nano-rods: On the x-ray diffraction characterization of electrochemically grown samples

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J. Appl. Phys. 110 (2011) 124901 (9 pages)

Abstract
Texture characterization in thin films from standard powder x-ray diffraction (XRD) rely on the comparison between observed peak relative intensities with those of powder diffraction standards of the same compound, trough the so-called texture coefficient (TC). While these methods apply for polycrystalline materials with isotropic grains, they are less accurate—and even wrong—for anisotropic materials like ZnO oriented single-crystal nano-rods, which would require the use of dedicated XRD texture setups. By using simple geometrical considerations, we succeed in discriminating between texture and morphology contributions to the observed intensity ratios in powder diffraction patterns. On this basis, we developed a method that provides a quantitative determination of both texture (polar distribution) and morphology (aspect ratio of nano-rods), using simple x-ray powder diffraction. The method is illustrated on a typical sample from a series of Zinc oxide (ZnO) nano-rod arrays grown onto a gold thin film sputtered onto a F:SnO_2-coated glass substrate (FTO) by using cathodic electro-deposition. In order to check the consistency of our method, we confronted our findings with scanning electron microscope (SEM) images, grazing incidence diffraction (GID), and XRD pole-figures of the same sample. Nevertheless, the proposed method is self-consistent and only requires the use of a standard powder diffractometer, nowadays available in most solid-state laboratories.

Monitoring heat induced changes in soft tissues by 1D transient elastography

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Phys. Med & Biol., 55, 1753-1765, (2010)
Abstract

In this paper 1D transient elastography was employed in fresh bovine skeletal muscle samples to assess the shear elastic modulus μ while the tissue was locally heated by means of an electrical resistance. The investigation is based on the study of the time shift of the shear wave propagation produced by the local temperature variation. The experiments show that the thermal expansion contribution to the time shift is negligible when compared with the shear wave speed variation. In such a case, the quantification of μ as a function of temperature becomes possible. Repeated experiments in different samples lead to a reproducible behavior of μ as a function of temperature. Irreversible elasticity changes are produced when the temperature exceeds a certain critical value T_c. The proposed method allows estimating this value as well as the spatial extension of the resulting thermal lesion. This point is important when considering applications in monitoring focused ultrasound surgery (FUS) because the surrounding normal tissue should remain unaffected.

Electronic and Structural Distortions in Graphene Induced by Carbon Vacancies and Boron Doping

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J. Phys. Chem. C, 2010, 114 (44), pp 18961–18971

Abstract
We present an ab initio study on the structural and electronic distortions of modified graphene by creation of vacancies, inclusion of boron atoms, and the coexistence of both, by means of thermodynamics and band structure calculations. In the case of coexistence of boron atoms and vacancy, the modified graphene presents spin polarization only when B atoms locate far from vacancy. Thus, when a boron atom fills single- and di-vacancies, it suppresses the spin polarization of the charge density. In particular when B atoms fill a di-vacancy a new type of rearrangement occurs, where a stable BC4 unit is formed inducing important out of plane distortions to graphene. All these findings suggest that new chemical modifications to graphene and new type of vacancies can be used for interesting applications such as sensor and chemical labeling.

Preparation, characterization and dissolution studies of fast release diclofenac sodium tablets from PVP solid dispersions

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Pharmaceutical Development and Technology, 15 (2), pp. 162-168.

Abstract
Diclofenac sodium is a non-steroidal anti-inflammatory drug widely used in the treatment of ankylosing spondylitis, rheumatoid arthritis and osteoarthritis. In this context, a rapid onset of action is required. Thus, the aim of this study was to formulate diclofenac sodium-PVP K-30 fast release tablets from solid dispersions. The physical state and drug:carrier interactions were analyzed by X-ray diffraction and scanning electron microscopy and stability upon storage was also studied. Dissolution rate of diclofenac sodium from solid dispersions was markedly enhanced by increasing the polymer concentration.

Mechanical properties of graphene nanoribbons

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Journal of Physics Condensed Matter, v.: 21, p.: 285304, 2009

Abstract
Herein, we investigate the structural, electronic and mechanical properties of zigzag graphene nanoribbons in the presence of stress by applying density functional theory within the GGA-PBE

(generalized gradient approximation-Perdew–Burke–Ernzerhof) approximation. The uniaxial stress is applied along the periodic direction, allowing a unitary deformation in the range of ± 0.02%. The mechanical properties show a linear response within that range while a nonlinear dependence is found for higher strain. The most relevant results indicate that Young's modulus is considerable higher than those determined for graphene and carbon nanotubes. The geometrical reconstruction of the C–C bonds at the edges hardens the nanostructure. The features of the electronic structure are not sensitive to strain in this linear elastic regime, suggesting the potential for using carbon nanostructures in nano-electronic devices in the near future.

Effect of quartz particle size on the mechanical behaviour of porcelain tile subjected to different cooling rates

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Journal of the European Ceramic Society. Volume 29, Issue 6, April 2009, Pages 1039–1046

Abstract
Porcelain tile is a high-performance ceramic tile, in which quartz is a major compositional component. After the firing cycle, macroscopic residual stresses develop in the product as a result of rapid cooling. Further, during cooling, the presence of quartz particles also increases natural flaw size. Both phenomena significantly affect the product's mechanical behaviour. This study examines the effect of quartz particle size on the mechanical behaviour of porcelain tile subjected to two very different cooling rates: a rapid or a slow cooling rate. A series of porcelain tile compositions were designed for this purpose, in which quartz particle size was varied. The mechanical behaviour of the sintered pieces was evaluated on the basis of linear elastic fracture mechanics. It was verified that, in the slowly cooled material, the modulus of elasticity and fracture energy increased, and natural flaw size decreased as quartz particle size decreased. However, fracture energy also diminished in pieces that contained excessively small particles, with an advanced state of dissolution. For the rapidly cooled material, though the larger sized quartz particles debonded at higher temperatures owing to thermal stress, their presence, even in small quantities, contributed to natural flaw growth. The lower fracture energy associated with this last type of piece also favours this phenomenon.

Synthesis and structural characterization of $La_xSr_{1-x}MnO_{2.6+\delta}$ ($0.1<x<0.4$) compounds displaying compressed octahedral coordination of $Mn^{(4-5x)+}$

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Journal of Solid State Chemistry. Volume 182, Issue 1, January 2009, Pages 187–195

Abstract

$La_xSr_{1-x}MnO_{2.6+\delta}$ (x=0.1–0.4) compounds have been obtained by low-temperature annealing of stoichiometric materials in hydrogen. $La_{0.1}Sr_{0.9}MnO_{2.6+\delta}$ (δ=0.15) and $La_{0.3}Sr_{0.7}MnO_{2.6}$, tetragonal ($P4/m$), and $La_{0.2}Sr_{0.8}MnO_{2.6,}$ pseudo-tetragonal monoclinic ($P2/m$), structures are isostructural with oxygen-vacancy-ordered $Sr_5Mn_5O_{13}$ ($a = b \approx \sqrt{5}a_P$, $c \approx a_P$). $La_{0.4}Sr_{0.6}MnO_{2.6}$ shows cubic perovskite structure with disordered oxygen vacancies. In the vacancy-ordered $(La_xSr_{1-x})_5Mn_5O_{13}$ phases four out of five Mn cations are Mn^{3+} and show a typical Jahn-Teller elongated pyramidal coordination while the fifth one $Mn^{(4-5x)+}$, in octahedral environment, shows decreasing formal charge from Mn^{4+} (x=0) to $Mn^{2.5+}$$x$=0.3. This unusual selective doping of the octahedral site produces structural strain due to increasing size of the $Mn^{(4-5x)+}$ and, in the case of $(La_{0.2}Sr_{0.8})_5Mn_5O_{13}$, the unusual compressed octahedral arrangement of oxygen atoms around it. The coordination geometry implies that either the $d_{x^2-y^2}$ orbital is occupied, which would be a rare example of inverted occupancy of e_g orbitals in manganites, or that disordered Mn^{3+} apically elongated MnO_6 octahedra are present with normal electronic configuration $d^3_{t_{2g}} d^0_{x^2-y^2} d^1_{z^2}$, and the observed bond distances are the average of the long and intermediate in-plane Mn–O bonds. Several structural features favor the second case.

Magnetic transitions in a double exchange-Holstein model with electron-phonon interactions coupled to magnetism

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Phys. Rev. B 79, 064408 (2009) [7 pages]

Abstract

In this work we study the double exchange-Holstein model with an electron-phonon interaction γ coupled to magnetism. The analysis is performed combining a mean-field approximation for the double exchange interaction and the Lang-Firsov transformation for the electron-phonon interaction. Discontinuous magnetic transitions appear when the dependence of g with m is sufficiently large, resembling those experimentally observed in manganites. We observe that the characteristic

resistivity peak that arises near the critical temperature appears for broad ranges of the system parameter values, unlike what occurs in a constant-γ model.

Uncertainty studies of topographical measurements on steel surface corrosion by 3D scanning electron microscopy

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Micron, **43,** (2-3) (2012) 387 – 395

Abstract
Pitting corrosion is a damage mechanism quite serious and dangerous in both carbon steel boiler tubes for power plants which are vital to most industries and stainless steels for orthopedic human implants whose demand, due to the increase of life expectation and rate of traffic accidents, has sharply increased. Reliable methods to characterize this kind of damage are becoming increasingly necessary, when trying to evaluate the advance of damage and to establish the best procedures for component inspection in order to determine remaining lives and failure mitigation.
A study about the uncertainties on the topographies of corrosion pits from 3D SEM images, obtained at low magnifications (where errors are greater) and different stage tilt angles were carried out using an in-house software previously developed. Additionally, measurements of pit depths on biomaterial surfaces, subjected to two different surface treatments on stainless steels, were carried out. The different depth distributions observed were in agreement with electrochemical measurements.

Hydrophilic and hydrophobic interactions in cross-linked chitosan membranes

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European Polymer Journal. 49, 9 (2013) 2635–2644

Abstract
Chitosan membranes with different cross-linking density were prepared by modifying cross-linking time. Sodium tripolyphosphate was the cross-linking agent. A pulsed nuclear magnetic resonance study was performed on uncross-linked and cross-linked membranes. Different fraction of water molecules were identified in different zones within the membranes. The ratio of water molecules per chitosan repeating unit were calculated. A maximum of twelve water molecules were tightly coordinated to the chitosan repeating unit. Also, a very small water molecule fraction was identified but it was mobile enough as not to contribute to the dipolar interactions. The cross-linking reaction could lead to the formation of hydrophilic and hydrophobic interactions. These two types of interactions could result in the coexistence of a network formed by hydrophilic and hydrophobic micropores. This knowledge could be useful for the interpretation of results of hydrophobic drugs permeation across hydrophilic membranes. For example, the increment of estradiol fluxes across chitosan membranes with an increase in cross-linking density.

A simple approach to model SFRC

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Construction and Building Materials, 37 (2012) 111–124

Abstract
Experimental research that shows the improvement in structural behavior of concrete with the addition of fibers has been developed in the last years. Fibers control cracking and thus increase concrete toughness and ductility. Much effort has been devoted in the last decade to model this material.
A simple homogenization approach based on a modified mixture theory is proposed in this paper to model Steel Fiber Reinforced Concrete (SFRC). The proposed and calibrated model takes information from the micro-scale to model the macro-scale. SFRC is considered as a composite material composed by concrete matrix and fibers. Concrete is modeled with an elastoplastic model

and steel fibers are considered as orthotropic elastoplastic inclusions that can debond and slip from the matrix. In order to include this inelastic phenomenon without explicitly modeling interface, constitutive equations of fibers are modified including information from the debonding–slipping phenomena. The model requires concrete properties, fibers material, geometry, distribution and orientation as input data. The fibers bond–slip behavior is automatically derived from concrete properties and fibers geometry or it can be alternatively obtained from pull out tests.
As illustration, the tension response of SFRC with different fiber contents is numerically simulated. The model is verified with the results of bending tests of beams extracted from a SFRC slab that present different fibers distribution due to the slab casting process. Comparisons with other numerical approaches modeling SFRC as an equivalent homogeneous material are also included in the paper.

Incorporation of polybutadiene into waterborne polystyrene nanoparticles via miniemulsion polymerization

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European Polymer Journal, 49, 9, (2013), 2635–2644

Abstract
The incorporation of polybutadiene in waterborne polystyrene nanoparticles by miniemulsion polymerization is expected to positively combine the properties of both materials, improving the impact resistance and toughness. The kinetics of the miniemulsion polymerization used to synthesize these hybrid nanomaterials and the effect of the reaction variables on the polymer microstructure and particle morphology were investigated. Both molecular microstructure and final particle morphology (core–shell, ‘‘salami’’ or three phase type) depended on the nature of the employed polybutadiene based rubbers and initiators. The mechanisms responsible for these effects were discussed.