

# ARTICULOS SELECCIONADOS DEL NUDCIMAT

PERIODO 2017-2019

**Año 2019**

**Development and evaluation of novel nanophotosensitizers as photoantimicrobial agents against *Staphylococcus aureus*.**

M. S. Gualdesi<sup>a</sup>, V. Aiassa<sup>a</sup>, J. Vara<sup>a</sup>, C. I. Alvarez Igarzabal<sup>b</sup>, C. S. Ortiz<sup>a</sup>

<sup>a</sup>Departamento de Ciencias Farmacéuticas, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, Argentina

<sup>b</sup>Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, IPQA-CONICET, Argentina

[Materials Science & Engineering C \(2019\) 94: 303–309](#)

## **Abstract**

The main aim of the present study was to synthesize polyacrylamide nanoparticles and to use them as photosensitizer carriers. The new monobrominated derivatives (monobrominated neutral red and monobrominated azure B) were the photosensitizers used for antimicrobial photodynamic therapy. They were loaded into the nanocarriers and their antibacterial and oxidative activities were evaluated. The polyacrylamide nanoparticles were evaluated and prepared by inverse microemulsion polymerization. The nanoparticles obtained were characterized by size, polydispersity index, and zeta potential analysis. The Dynamic Light Scattering indicated that the diameter of the particle (z-average) was optimal, with an acceptable polydispersity index. The antibacterial activity of the polyacrylamide nanoparticles loaded with photosensitizers was evaluated against *Staphylococcus aureus*. Both photosensitizers loaded into the nanoparticles showed great potential as antibacterial agents since they suppressed the bacterial growth. The maximum percentage of growth reduction was 35.5% (> 2 Log CFU/mL), with the monobrominated

azure B loaded into the nanocarrier with 2 hydroxyethyl methacrylate against methicillin resistant *S. aureus*. The improved physicochemical and photophysical properties of these photosensitizers were accompanied by a significant increase in the photoantimicrobial action, in conventional-sensitive and-methicillin resistant *S. aureus*. The results obtained clearly suggest that polyacrylamide nanoparticles loaded with photosensitizers have great potential for further application in antimicrobial photodynamic therapy.

## **The influence of solvent composition in the sol-gel synthesis of cobalt ferrite (CoFe<sub>2</sub>O<sub>4</sub>): A route to tuning its magnetic and mechanical properties**

**Janio Venturini<sup>a,b</sup>, Tiago Bender Wermuth<sup>a</sup>, Márcia Corrêa Machado<sup>a</sup>, Sabrina Arcaro<sup>a</sup>, Annelise Kopp Alves<sup>a</sup>, Alexandrea Cas Viegas<sup>c</sup>, Carlos PérezBergmann<sup>a,b</sup>**

<sup>a</sup>Graduate Program in Mining, Metallurgical and Materials Engineering, Federal University of Rio Grande do Sul, Osvaldo Aranha 99, Porto Alegre, 90035-190, Brazil

<sup>b</sup>Department of Industrial Engineering, Federal University of Rio Grande do Sul, Osvaldo Aranha 99, Porto Alegre, 90035-190, Brazil

<sup>c</sup>Institute of Physics, Federal University of Rio Grande do Sul, Bento Gonçalves 9500, Porto Alegre, 91501-970, Brazil

[Journal of the European Ceramic Society. In Press. Available online 22 January 2019.](#)

### **Abstract**

This work presents a successful, environmentally-friendly route for tuning the magnetic and mechanical properties of CoFe<sub>2</sub>O<sub>4</sub> sintered ceramics. The precursor powders were prepared from mixtures containing 100, 50 and 20% water, with the remaining volume composed of isopropanol. The synthesised powders were pressed into pellets and sintered at 1150 and 1200 °C. SEM micrographs indicate that the solvent exerts a major influence over the morphology of the ferrite grains. Vickers hardness shows a maximum for products from a medium containing 50% water, which could be directly related to the smaller average size of the CoFe<sub>2</sub>O<sub>4</sub> grains. The coercivity of the pellets is strongly influenced by the reactional medium, with a maximum of 501.7 Oe (sample prepared at 20% water and fired at 1150 °C). This work opens up possibilities for fine tuning of the final properties of CoFe<sub>2</sub>O<sub>4</sub> sintered ceramics, further enabling the utilisation of this material in advanced applications.

## **Flexible TiO<sub>2</sub>-coated nanocellulose membranes incorporated with CdTe as electrodes in photoelectrochemical cells.**

**Geneviève K. Pinheiro<sup>1</sup>, Daliana Muller<sup>2</sup>, Rafael B. Serpa<sup>2</sup>, Françoise T. Reis<sup>3</sup>, Maria L. Sartorelli<sup>3</sup>, Marco A. Schiavon<sup>4</sup>, Carlos R. Rambo<sup>1</sup>**

1. Department of Electrical and Electronic Engineering Federal University of Santa Catarina Florianópolis Brazil
2. Department of Mechanical Engineering Federal University of Santa Catarina Florianópolis Brazil
3. Department of Physics Federal University of Santa Catarina Florianópolis Brazil
4. Department of Chemistry Federal University of São João del-Rei São João del-Rei Brazil

[Journal of Materials Science-Materials in Electronics, 30 \(2019\) pp. 1891–1895](#)

### **Abstract**

Incorporation of quantum dots (QDs) into porous matrices has triggered the development of novel optical devices. In this work, TiO<sub>2</sub> sensitized by CdTe incorporated into bacterial nanocellulose (BNC) membranes were tested as photoelectrodes in a photoelectrochemical cell directed to the water splitting for hydrogen generation. The flexible membranes were produced by immersing BNC membranes in an aqueous solution of CdTe capped with glutathione (CdTe–GSH) and further deposited over a thin layer of TiO<sub>2</sub>. Incorporation of CdTe–GSH into BNC membranes was confirmed by infrared spectroscopy. Fluorescence spectroscopy revealed that the luminescence intensity increased with the immersion time in the CdTe–GSH solution. Field-emission gun scanning electron microscopy (FEG-SEM) images revealed that the CdTe/QDs (5 nm) were homogeneously dispersed on the cellulose nanofibers. BNC/CdTe–GSH membranes was tested as photoelectrodes. Photoelectrochemical cells exhibited a significant photocurrent in wavelengths ranging from 400 to 800 nm, which indicates their potential for applications as flexible electrodes, sensors and photovoltaic systems.

## **Nanopartículas de plata biogénicas a partir del hongo *Punctularia atropurpurascens* para el control de microorganismos**

**Paula Sanguineto, María Belén Estevez, Ricardo Faccio, Silvana Alborés**

Universidad de la República, Facultad de Química, Montevideo, Uruguay.

[Revista Interdisciplinaria en Nanociencias y Nanotecnología. Vol 12, No 22 \(2019\)](#)

### **Resumen**

Las nanopartículas de plata poseen propiedades particulares que le atribuyen sus muy prometedoras aplicaciones, novedosas en diversos campos de la ciencia. Una de las principales aplicaciones de las nanopartículas de plata es su actividad antimicrobiana. Las enfermedades infecciosas son aún una de las principales causas de muerte en el mundo. El desarrollo de resistencia a drogas, así como los efectos adversos que ocasionan hacen necesaria la búsqueda de estrategias alternativas para el tratamiento de dichas enfermedades. En el área agrícola, a pesar de las mejoras en la capacidad de diagnóstico y disponibilidad de tecnologías para el control de enfermedades, ellas aún son capaces de causar enormes pérdidas de cosechas. En este sentido, el potencial antimicrobiano de las nanopartículas de plata es muy prometedor.

La síntesis biológica de nanopartículas es de gran interés sobre otros métodos (físicos y químicos) porque se evita el uso de químicos tóxicos y condiciones drásticas de reacción. En el caso de la utilización de microorganismos la síntesis extracelular es ventajosa para la separación y purificación de las nanopartículas. Asimismo es importante el análisis de las condiciones de reacción que permitan una mayor producción de nanopartículas, así como el control del tamaño y la forma.

En el presente trabajo se realizó la síntesis de nanopartículas de plata por extractos provenientes del hongo *Punctularia atropurpurascens*. Se estudiaron diferentes condiciones de reacción de síntesis y se evaluó el potencial antimicrobiano de las nanopartículas biogénicas frente a microorganismos de interés en las áreas de salud y agroalimentaria.

## **Electrodeposition of Single Phase SnS Thin Films: Effect of Electrolytic Bath Temperature on the Final Film Properties**

**G. Riveros<sup>1,z</sup>, D. Ramírez<sup>1,\*</sup>, Daniel L. Gau<sup>2</sup>, L. Hernández<sup>1</sup>, P. Häberle<sup>3</sup>, Ricardo E. Marotti<sup>2</sup>, R. Romero<sup>4</sup>, A. Cuevas<sup>4</sup>, F. Martín<sup>5</sup> and Enrique A. Dalchiele<sup>2,\*\*</sup>**

<sup>1</sup>Instituto de Química y Bioquímica, Facultad de Ciencias, Universidad de Valparaíso, Playa Ancha, Valparaíso, Chile

<sup>2</sup>Instituto de Física, Facultad de Ingeniería, Julio Herrera y Reissig 565, C.C. 30, 11000 Montevideo, Uruguay

<sup>3</sup>Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso 2390123, Chile

<sup>4</sup>Nanotechnology Unit, Edificio de Bioinnovación, Universidad de Málaga, Málaga, Spain

<sup>5</sup>Laboratorio de Materiales y Superficies (Unidad Asociada al CSIC), Departamentos de Física Aplicada & Ing. Química, Universidad de Málaga, E29071 Málaga, Spain

[J. Electrochem. Soc. 2019 volume 166, issue 2, D44-D51](#)

### **Abstract**

In this article, the electrodeposition of single-phase tin monosulfide (SnS) films at different electrolytic bath temperatures is studied. The electrodeposition was carried out potentiostatically onto transparent conductive substrates (fluorine-doped tin oxide, and indium tin oxide on a glass substrate) from an acidic solution of SnSO<sub>4</sub> and Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> as tin and sulfur precursors, respectively. The films were characterized through different techniques: field-emission scanning electron microscopy, energy dispersive X-ray analyses, X-ray diffraction measurements, profilometry, Raman spectra, UV-vis measurements, electrochemical impedance spectroscopy and linear sweep photovoltammetry. The films obtained were stoichiometric and no other phases different from SnS were evidenced. A change in the morphology from cubic-like to sheet-like was observed with an increase of bath temperature, which was reflected in the texture coefficient obtained from X-ray diffraction analyses. The bandgap of the films was obtained using a direct absorption edge in the Tauc plots. A decreasing bandgap with electrodeposition temperature was observed,

which is attributed to an improvement in the crystallinity of the films. Mott-Schottky plots and linear sweep photovoltammetry measurements confirmed that the films are p-type semiconductors. An increase in the photocurrent of the photoelectrodes was observed with the electrolytic bath temperature, which is attributed to the change of SnS morphology with the electrodeposition temperature.

## **Slow and rapid cooling of Al–Cu–Si ultrafine eutectic composites: Interplay of cooling rate and microstructure in mechanical properties**

**Guilherme Lisboa de Gouveia<sup>1</sup>, Rafael Kakitani<sup>2</sup>, Leonardo Fernandes Gomes<sup>1</sup>,  
Conrado Ramos Moreira Afonso<sup>1</sup>, Noé Cheung<sup>2</sup>, José Eduardo Spinelli<sup>1</sup>**

1 Department of Materials Engineering, Federal University of São Carlos, São Carlos, SP 13565-905, Brazil

2 Department of Manufacturing and Materials Engineering, University of Campinas UNICAMP, Campinas, SP 13083-860, Brazil)

[Journal of Materials Research 2019](#)

### **Abstract**

Ternary Al–15 wt% Cu–7 wt% Si and Al–22 wt% Cu–7 wt% Si alloy specimens were generated by transient directional solidification (DS) and rapid solidification (RS) techniques. The microstructures are constituted by an  $\alpha$ -Al dendritic matrix surrounded by two eutectic, that is, a binary eutectic (Si +  $\alpha$ -Al) and a bimodal eutectic, consisting of cellular-type binary eutectic colonies ( $\alpha$ -Al + Al<sub>2</sub>Cu) in a ternary eutectic matrix consisting of  $\alpha$ -Al + Al<sub>2</sub>Cu + Si. The bimodal eutectic exists at cooling rates from 0.5 to 250 K/s. The secondary dendritic spacing,  $\lambda_2$ , of the DS samples varied from 5 to 20  $\mu\text{m}$  and from 10 to 18  $\mu\text{m}$  for both examined alloys. The  $\lambda_2$  from 2.7 to 4.0  $\mu\text{m}$  characterized the RS samples. Mechanical properties have been determined for various samples related to different dendritic spacing values. Based on the evaluation of the rapidly solidified microstructures, it was possible to assess the cooling rates.

## **Highly efficient hybrid Ni/nitrogenated-graphene electrocatalysts for hydrogen evolution reaction**

**M.J. Gómez, A. Loiácono, L. Pérez, E. Franceschini, G. Lacconi**

INFIQC, Dpto. de Físicoquímica, Facultad de Ciencias Químicas, UNC

[ACS Omega \(2019\) 4 \(1\) 2206-2216](#)

### **Abstract**

Two nickel/nitrogenated graphene hybrid electrodes (Ni-NrGONH<sub>3</sub> and Ni-NrGOAPTES) were synthesized, and their catalytic activity with respect to the hydrogen evolution reaction (HER) in alkaline media was analyzed. Incorporation of nitrogen to the carbon structure in graphene oxide (GO) or reduced GO (rGO) flakes in aqueous solutions was carried out based on two different configurations. NrGONH<sub>3</sub> particles were obtained by a hydrothermal method using ammonium hydroxide as the precursor, and NGOAPTES particles were obtained by silanization (APTES functionalization) of GO sheets. Aqueous dispersions containing NrGONH<sub>3</sub> and NGOAPTES particles were added to the traditional nickel Watts plating bath in order to prepare the Ni-NrGONH<sub>3</sub> and Ni-NrGOAPTES catalysts, respectively. Nickel substrates were coated with the hybrid nickel electrodeposits and used as electrodes for hydrogen production. The Ni-NrGO catalysts show a higher activity than the conventional nickel electrodeposited electrodes, particularly the ones containing APTES molecules because they allow obtaining a hydrogen current density 130% higher than conventional Ni-plated electrodes with a Watts bath in the absence of additives. In addition, both catalysts show a low deactivation rate during the ageing treatment, which is a sign of a longer midlife for the catalyst. Cyclic voltammetry and electrochemical impedance spectroscopy measurements were used for examination of the catalytic efficiency of hybrid Ni-NrGO electrodes for HER in KOH solution. High values of exchange current densities,  $8.53 \times 10^{-4}$  and  $2.53 \times 10^{-5}$  mA cm<sup>-2</sup> for HER in alkaline solutions on Ni-NrGONH<sub>3</sub> and Ni-NrGOAPTES electrodes, respectively, were obtained.

## **Superhydrophobic Polypropylene Surfaces Prepared with TiO<sub>2</sub> Nanoparticles Functionalized by Dendritic Polymers**

**Cintia Contreras,1,2; Francisco Figueroa,1,2; Daniel Weibel,3; Miriam Strumia 1,2**

1: Facultad de Ciencias Químicas, Departamento de Química Orgánica, Laboratorio de Materiales Poliméricos (LAMAP), Universidad Nacional de Córdoba, Córdoba, Argentina; 2: CONICET, IPQA, Córdoba, Argentina; 3: Laboratorio de Fotoquímica e Superficies, Departamento de Físico-Química, Instituto de Química, UFRGS, Porto Alegre, RS, Brasil

[J. Polym. Sci., Part A: Polym. Chem. 2018, 56, 2019–202](#)

### **Abstract**

Hybrid inorganic–organic nanomaterials have received increasing interest due to the possibility of implementing different functions and characteristics within a single material. Their functionalities are a consequence of the synergy of the properties of distinct building blocks and are related to their varied natures and spatial locations. In this work, we present the development of superhydrophobic properties on polypropylene (PP) surfaces using hybrid nanomaterials from TiO<sub>2</sub> nanoparticles (NPs) and dendronized polymers. The dendron acryl Behera's amine was successfully grafted on the TiO<sub>2</sub> NP surfaces by Surface-Initiated Atom Transfer Radical Polymerization (SI-ATRP) and a core-brush material was obtained. Finally, PP substrates were coated with NP hybrids to produce superhydrophobic surfaces with water contact angles of over 158 degrees. Controlling the

organic silane concentration on the TiO<sub>2</sub> NPs allowed the dendronized process to be driven and thereby permitted the selection of specific wettability properties on PP substrate surfaces with high water adhesion or self-cleaning conditions. This dendronized effect with consequent steric congestion of the polymeric brushes on the NPs changed their behaviors from Wenzel to the Cassie Baxter state.

## **Preparation and characterization of soy protein films reinforced with cellulose nanofibers obtained from soybean by-products**

**Agustín González, a,b; Gabriela Gastelú, a,c; Gabriela N. Barrera, d,e; Pablo D. Ribotta, d,e; Cecilia I. Álvarez Igarzabal a,b**

<sup>a</sup>Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Departamento de Química Orgánica, Córdoba, Argentina

<sup>b</sup>Instituto de Investigación y Desarrollo en Ingeniería de Procesos y Química Aplicada (IPQA-CONICET), Córdoba, Argentina

<sup>c</sup>Instituto de Investigaciones en Físico-química de Córdoba (INFIQC-CONICET), Córdoba, Argentina

<sup>d</sup>Universidad Nacional de Córdoba, Facultad de Ciencias Exactas, Físicas y Naturales, Córdoba, Argentina

<sup>e</sup>Instituto de Ciencia y Tecnología de Los Alimentos Córdoba (ICYTAC-CONICET), Córdoba, Argentina

[Food Hydrocolloids, 89 \(2019\) 758–764](#)

### **Abstract**

In this paper, we report the preparation of nanofibers obtained from low-cost agro-industrial by-products (soybean hulls and pods) and their use as nano reinforcers of soy protein films. From hulls, we obtained white and stable in-time aqueous dispersions of cellulose nanofibers of about 20 nm wide and 500 nm long and a hydrodynamic diameter of 269 nm, with a marked increase in the crystalline index as compared to raw material.

Filmogenic solutions of soy proteins were prepared using glycerol as a plasticizer and different amounts of cellulose nanofibers (0; 10; 20 and 40% in relation to the amount of soy protein). The rheological behavior of filmogenic solutions containing nanofibers suggests an interaction between matrix and reinforcements. Films were prepared by casting of filmogenic solutions. As a result, we obtained films with a homogeneous surface having a large number of nanofibers, showing increasing opacity in samples with larger amounts of cellulose nanofibers. The addition of nanofibers decreases the film's susceptibility to water, by which a significant decrease in the total soluble matter and swelling in water was observed with an increase in contact angle. In addition, mechanical properties were also improved, obtaining more rigid films as the number of nanofibers

increased.

## **Dye sensitized solar cells based on Antarctic *Hymenobacter* sp. UV11 dyes**

**Tatiana Montagni 1, Paula Enciso 1, Juan José Marizcurrena 2, Susana Castro-Sowinski 2, Carolina Fontana 3, Danilo Davyt 4, María Fernanda Cerdá 1**

1 Laboratorio de Biomateriales, Facultad de Ciencias Universidad de la República (UdelaR) Montevideo Uruguay

2 Sección Bioquímica y Biología Molecular, Facultad de Ciencias UdelaR Montevideo Uruguay

3 Laboratorio de Espectroscopía y Fisicoquímica Orgánica, Departamento de Química del Litoral, Facultad de Química & CENUR Litoral Norte UdelaR Paysandú Uruguay

4 Departamento de Química Orgánica, Facultad de Química UdelaR Montevideo Uruguay

[Environmental Sustainability. March 2018, Volume 1, Issue 1, pp 89–97 | Cite as](#)

### **Abstract**

Xanthophylls pigments extracted from *Hymenobacter* sp. UV11 (a bacterium that produces reddish colonies on agar) collected at Fildes Peninsula, King George Island, Antarctica, were tested as sensitizers in dye sensitized solar cells (DSSC). Experiments were performed in the presence and in the absence of a co-adsorbent, a slimy substance produced by UV11 and identified as a polysaccharide during this work. Results suggest that the highest conversion efficiency (0.03%) was obtained when using the orange-xanthophylls pigment in the presence of the  $\alpha$ -1,4-glucan both co-extracted from UV11. This work highlights the importance of using co-adsorbents as co-adjuvants in the production of more efficient DSSC manufactured with bacterial dyes. These results may contribute to the development of an exploration program of Antarctic resources, and offer the possibility to start the change in the energetic matrix in that remote area of the Planet, decreasing the environmental impact associated with the use of fossil fuels.

## **Characterization of chemically treated Ti-Zr system alloys for dental implant application**

**Jairo M. Cordeiro<sup>a,b</sup>, Leonardo P. Faverani<sup>c</sup>, Carlos R. Grandini<sup>b,d</sup>, Elidiane C. Rangel<sup>e</sup>, Nilson C. da Cruz<sup>e</sup>, Francisco H. Nociti Junior<sup>a</sup>, Amanda B. Almeida<sup>a</sup>, Fabio B. Vicente<sup>b,f</sup>, Bruna R. G. Morais<sup>c</sup>, Valentim A. R. Barão<sup>a,b</sup>, Wirley G. Assunção<sup>g</sup>**

a University of Campinas (UNICAMP), Piracicaba Dental School, Department of Prosthodontics and Periodontology, Av Limeira, 901, Piracicaba, São Paulo 13414-903, Brazil

b Institute of Biomaterials, Tribocorrosion and Nanomedicine (IBTN), Brazil

c Univ Estadual Paulista (UNESP), Aracatuba Dental School, Department of Surgery and Integrated Clinic, R. José Bonifácio, 1193, Aracatuba, São Paulo 16015-050, Brazil



<sup>d</sup> Univ Estadual Paulista (UNESP), Laboratório de Anelasticidade e Biomateriais, Av. Eng. Luiz Edmundo Carrijo Coube, Bauru, São Paulo 17033-360, Brazil

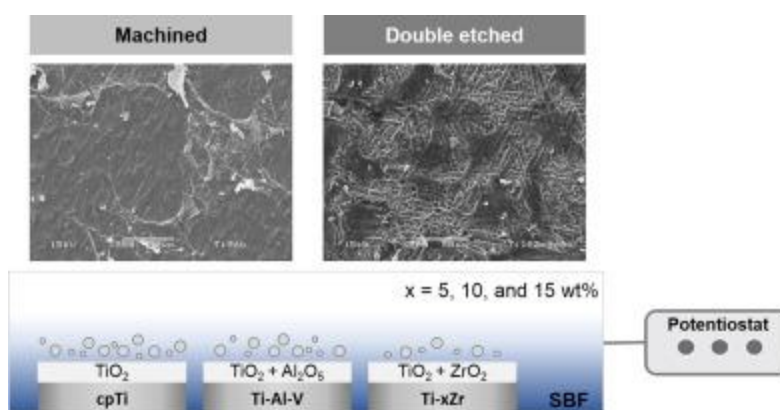
<sup>e</sup> Univ Estadual Paulista (UNESP), ICTS, Laboratory of Technological Plasmas, Av Três de Março, 511, Sorocaba, São Paulo 18087-180, Brazil

<sup>f</sup> Universidade Paulista (UNIP), Av. Luís Levorato, 1-40, Bauru, São Paulo 17048-290, Brazil

<sup>g</sup> Univ Estadual Paulista (UNESP), Aracatuba Dental School, Department of Dental Materials and Prosthodontics, R. José Bonifácio, 1193, Aracatuba, São Paulo 16015-050, Brazil

[Materials Science and Engineering: C. Volume 92, 1 November 2018, Pages 849-861](#)

## Abstract



Materials and surfaces developed for dental implants need to withstand degradation processes that take place in the oral cavity. Therefore, the aim of the study was to develop and evaluate the topographical, mechanical, chemical, electrochemical and biological properties of Ti-xZr alloys ( $x = 5, 10, \text{ and } 15 \text{ wt}\%$ ) with two surface features (machined and double acid etched). Commercially pure titanium (cpTi) and Ti-6Al-4V alloy were used as controls. Surface characterization was performed using dispersive energy spectroscopy, X-ray diffraction, scanning electron microscopy, atomic force microscopy, profilometry and surface energy. The mechanical properties were assessed using Vickers microhardness, elastic modulus and stiffness. The electrochemical behavior analysis was conducted in a body fluid solution (pH 7.4). In addition, MC3T3-E1 cells were used to determine the impact of material and surface treatment on cell morphology by SEM analysis. Data were analyzed by two-way ANOVA and Bonferroni test ( $\alpha = 0.05$ ). Ti-Zr alloys showed lower surface roughness, elastic modulus and stiffness, as well as higher hardness and surface energy when compared to cpTi. Ti-Zr system increased the polarization resistance values and significantly decreased the capacitance, corrosion current density ( $i_{\text{corr}}$ ), and passivation current density ( $i_{\text{pass}}$ ) values. The acid treatment increased the resistance and corrosion potential of the oxide layer. SEM data analysis demonstrated that Ti-Zr alloys displayed normal cell attachment/spreading and slightly changed cell morphology in the double etched surface. In conclusion, Zr addition and surface treatment altered surface, mechanical, biological and electrochemical properties of Ti material.

## Integration of graphene onto silicon through electrochemical reduction of graphene oxide layers in non-aqueous medium

Andrea Giacomo Marrani<sup>a</sup>, Anna Chiara Coico<sup>a</sup>, Daniela Giacco<sup>a</sup>, Robertino Zanoni<sup>a</sup>, Francesca Anna Scaramuzzo<sup>b</sup>, Ricardo Schrebler<sup>c</sup>, Danilo Dini<sup>a</sup>, Matteo Bonomo<sup>a</sup>, Enrique A. Dalchiele<sup>d</sup>

<sup>a</sup> Dipartimento di Chimica, Università di Roma La Sapienza, p.le A. Moro 5, I-00185 Rome, Italy

<sup>b</sup> Dipartimento di Scienze di Base e Applicate per l'Ingegneria (S.B.A.I.), Università di Roma La Sapienza, Via del Castro Laurenziano 7, I-00161 Rome, Italy

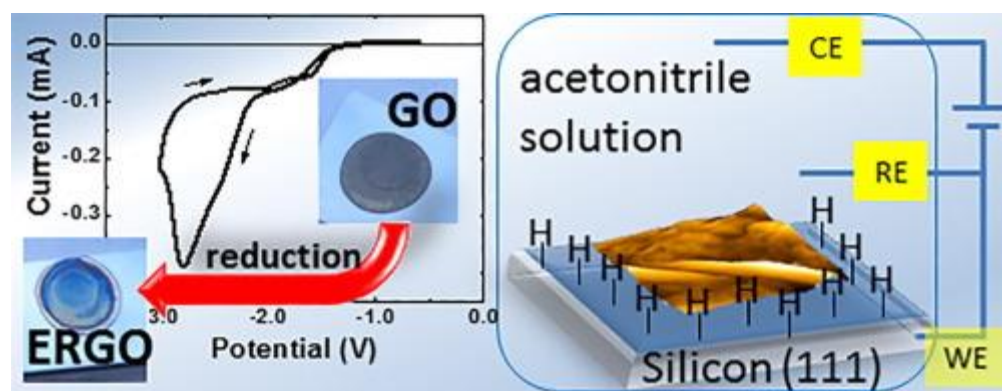
<sup>c</sup> Instituto de Química, Facultad de Ciencias, Pontificia Universidad Católica de Valparaíso, Av. Brasil, 2950 Valparaíso, Chile

<sup>d</sup> Instituto de Física & CINQUIFIMA, Facultad de Ingeniería, Julio Herrera y Reissig 565, C.C. 30, 11000 Montevideo, Uruguay

Received 16 January 2018, Revised 2 March 2018, Accepted 20 March 2018, Available online 23 March 2018.

[Applied Surface Science. Volume 445, 1 July 2018, Pages 404-414](#)

### Abstract



Wafer-scale integration of reduced graphene oxide with H-terminated Si(1 1 1) surfaces has been accomplished by electrochemical reduction of a thin film of graphene oxide deposited onto Si by drop casting. Two reduction methods have been assayed and carried out in an acetonitrile solution. The initial deposit was subjected either to potential cycling in a 0.1 M TBAPF<sub>6</sub>/CH<sub>3</sub>CN solution at scan rates values of 20 mV s<sup>-1</sup> and 50 mV s<sup>-1</sup>, or to a potentiostatic polarization at  $E_{\lambda,c} = -3$  V for 450 s. The resulting interface has been characterized in its surface composition, morphology and electrochemical behavior by X-ray photoelectron spectroscopy, Raman spectroscopy, atomic force microscopy and electrochemical measurements. The results evidence that few-layer graphene deposits on H-Si(1 1 1) were obtained after reduction, and use of organic instead of aqueous medium led to a very limited surface oxidation of the Si substrate and a very low oxygen-to-carbon

ratio. The described approach is fast, simple, economic, scalable and straightforward, as one reduction cycle is already effective in promoting the establishment of a graphene-Si interface. It avoids thermal treatments at high temperatures, use of aggressive chemicals and the presence of metal contaminants, and enables preservation of Si(1 1 1) surface from oxidation.

## **Coupled High Spin CoII Ions Linked by Symmetrical Double Hydrogen Bonds: Role of a Slowly Relaxing CuII Impurity in Interrupting the CoII–CoII Exchange Interaction.**

**Ana L. Pérez, [a] Axel Kemmerer, [a] Marilin A. Rey, [a] Sergio D. Dalosto, [b] Carlos A. Ramos, [c] Mario C. G. Passeggi, [a,b] Alberto C. Rizzi, [a] and Carlos D. Brondino [a]**

[a] Departamento de Física, Facultad de Bioquímica y Ciencias Biológicas, Universidad Nacional del Litoral - CONICET, Ciudad Universitaria, S3000ZAA Santa Fe, Argentina

[b] Instituto de Física del Litoral, Universidad Nacional del Litoral - CONICET, Güemes 3450, 3000 Santa Fe, Argentina

[c] Centro Atómico Bariloche, Comisión Nacional de Energía Atómica, Av. Bustillo 9500, 8400 Bariloche, Río Negro, Argentina

[European Journal of Inorganic Chemistry, año: 2018, Volume: 2018, Pages 4604-4613](#)

### **Abstract**

CoII and CuII ions are two paramagnetic transition metal ions showing different relaxation rates ( $\nu$ ), with  $\nu_{\text{Co II}} \gg \nu_{\text{Cu II}}$ . To measure the isotropic exchange constant ( $J$ ) between high spin CoII ions and between CuII ions and high spin CoII ions, we performed magnetic and EPR measurements complemented with computational calculations on pure trans-diaqua-bis(picolinato-N,O)-cobalt(II) dihydrate (1), on the CuII ion doped compound of 1 (2), and on the CuII ion doped compound in a ZnII matrix isomorphous to 1. The temperature dependence of the CuII EPR resonance lines of 2 induced by the fast relaxing CoII ion host as well as the evaluation of the temperature-independent CoII–CoII and CuII–CoII isotropic exchange interaction are analyzed. We determined an antiferromagnetic interaction [ $J_{\text{Co–Co}} = -1.07(1) \text{ cm}^{-1}$ ] associated with a double symmetrical hydrogen bond bridge and another one [ $J_{\text{Co–Cu}} = 0.0015(2) \text{ cm}^{-1}$ ] associated with a double but asymmetrical hydrogen bond bridge, which are in line with the values obtained from computational calculations. This work shows that EPR spectroscopy can advantageously be used to evaluate weak exchange interactions between distinct metal ions with different relaxation rates by using the fact that those metal–metal interactions that broaden the EPR resonance line, which are described by matrices with a trace of zero, are averaged out at high temperatures

## **Nanocellulose biosynthesis by *Komagataeibacter hansenii* in a defined minimal culture medium**

**Samara S. de Souza<sup>1</sup>, Fernanda V. Berti<sup>1</sup>, Karla P. V. de Oliveira<sup>1</sup>, Camila Q. P. Pittella<sup>1</sup>, Julia V. de Castro<sup>1</sup>, Catiane Pelissari<sup>2</sup>, Carlos R. Rambo<sup>3</sup>, Luismar M. Porto<sup>1</sup>**

1 Genomic and Tissue Engineering Group, InteLab – Integrated Technologies Laboratory, Department of Chemical and Food Engineering Federal University of Santa Catarina Florianópolis Brazil

2 GESAD - Decentralized Sanitation Research Group, Department of Sanitary and Environmental Engineering Federal University of Santa Catarina - UFSC Florianópolis Brazil

3 Department of Electrical and Electronic Engineering Federal University of Santa Catarina Florianópolis Brazil

[Cellulose \(2019\) 26: 1641](#)

### **Abstract**

This study evaluates the capability of *Komagataeibacter hansenii* ATCC 23769 to synthesize bacterial nanocellulose (BNC) under strict limitation of nutrients with different carbon and nitrogen sources in a defined minimal culture medium in static culture. Five carbon sources were prepared based on the C-molar basis concentration: glycerol, glucose, fructose, mannitol and saccharose, combined with three different nitrogen sources: NH<sub>4</sub>Cl, NH<sub>4</sub>NO<sub>3</sub> and (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>. BNC production yields were determined based on the dry weight of the produced BNC-Minimal membranes and the carbon consumption for each condition. The combination of 25 mM of glucose and 10 mM of NH<sub>4</sub>Cl showed the best concentration of C and N sources regarding BNC yield and membrane stability. This is a new proposal of defined minimal culture medium that supports growth of BNC membranes production, without the addition of complex elements such as yeast extract and peptone. BNC membranes produced under these conditions exhibited great optical transparency compared to the membranes produced in complex media (Mannitol and Hestrin–Schramm), therefore increasing a wide range of technological applications. Graphical abstract Open image in new window

## **FeCrAlloy Monoliths Coated with Ni/Al<sub>2</sub>O<sub>3</sub> Applied to the Low-Temperature Production of Ethylene.**

**Paula Brussino<sup>1</sup>, Juan Pablo Bortolozzi<sup>1</sup>, Oihane Sanz<sup>2</sup>, Mario Montes<sup>2</sup>, María Alicia Ulla<sup>1</sup> and Ezequiel David Banús<sup>1,\*</sup>**

<sup>1</sup>Instituto de Investigaciones en Catálisis y Petroquímica, INCAPE (UNL-CONICET), Santiago del Estero 2829, 3000 Santa Fe, Argentina

<sup>2</sup>Departamento de Química Aplicada, Universidad del País Vasco (UPV/EHU), 20018 San Sebastián, Spain

[Catalysts 2018, 8, 291.](#)

## Abstract

This paper investigates the oxidative dehydrogenation of ethane to produce ethylene at low temperatures (500 C) in metallic structured substrates. To check this point, the FeCrAlloy® monoliths with different channel sizes (289–2360 cpsi) were prepared. The monoliths were coated with a Ni/Al<sub>2</sub>O<sub>3</sub> catalyst (by washcoating of alumina and the latter nickel impregnation) and characterized by Scanning Electron Microscopy and Energy-Dispersive X-ray analysis (SEM-EDX), Temperature-Programmed Reduction (TPR), X-ray Diffraction (XRD) and X-ray Photoelectron Spectroscopy (XPS). The catalytic results showed that all monoliths coated with ~300 mg of catalyst presented similar ethane conversion (15%) at 450 C. However, the lowest selectivity to ethylene was found for the monolith with the lower channel size and the higher geometric surface area, where a heterogeneous catalyst layer with Ni enriched islands was generated. Therefore, it can be said that the selectivity to ethylene is linked to the distribution of Ni species on the support (alumina). Nevertheless, in all cases the selectivity was high (above 70%). On the other hand, the stability in reaction tests of one of the coated monoliths was done. This structured catalyst proved to be more stable under reaction conditions than the powder catalyst, with an initial slight drop in the first 8 h but after that, constant activity for the 152 h left.

## Band Structure Effects on the Charge Exchange Processes in H<sup>+</sup> Colliding with a Cu(111) Surface.

V. Quintero Riascos<sup>†</sup>, M. Tacca<sup>†</sup>, R. Vidal<sup>†‡</sup>, C. Gonzalez<sup>§</sup>, E. C. Goldberg<sup>†‡</sup>, and F. Bonetto<sup>\*†‡</sup>

<sup>†</sup> Instituto de Física del Litoral (CONICET-UNL), Güemes 3450, S3000GLN Santa Fe, Argentina

<sup>‡</sup> Departamento de Física, Facultad de Ing. Química, Universidad Nacional del Litoral, Santiago del Estero 2829, S3000AOM Santa Fe, Argentina

<sup>§</sup> Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Facultad de Ciencias, Universidad Autónoma de Madrid, 28049 Madrid, Spain

[The Journal of Physical Chemistry C, 2018, vol. 122, pag: 28192-28203](#)

## Abstract

The low energy ion scattering (LEIS) technique was used to experimentally determine the formation of positive and negative ions in the scattering of protons by a Cu(111) surface for a large scattering angle in the backscattering configuration and a wide range of incoming energies (2 to 8keV). Two different collisional geometries were analyzed for a 135° fixed scattering angle: 45°/90° and 67.5°/67.5° incoming/exit angles measured with respect to the target surface. The total fraction of backscattered ions ranges from 10% to 25% and a peculiarly high yield of negative ions, which always exceeds that of positive ions, was detected for the whole energy range analyzed. A strong dependence of the measured ion fractions with the geometrical conditions was experimentally found. On the theoretical side, a first principles quantum-mechanical formalism that takes into account the three possible final charge states of the H<sup>+</sup> in a correlated way and the fine details of the band structure of Cu(111) surface, was applied to describe the charge transfer processes involved in the experimental situation. The theoretical calculation leads to a non-monotonous dependence

with the incoming energy that properly describes the experimental results, especially the negative ion fraction in the specular collisional geometry. The oscillatory behavior predicted by the theory in the range of low energies is a clear evidence of the charge exchange between localized states, that is the situation related with the presence of the surface state immersed in the L-gap present in Cu(111) surface. The positive ion fraction is discussed for the first time for this collisional system. The differences found between the measurements and the theory seem to indicate that the neutralization to excited states, and also the formation of excited negative hydrogen ions, are possible charge exchange channels in the dynamic process analyzed.

## **Linear segmented polyurethanes. II. A mathematical model for the prepolymerization stage**

M. L. Polo,<sup>1</sup> J. I. Pesoa,<sup>1</sup> V. V. Nicolau,<sup>2</sup> M. E. Spontón,<sup>1</sup> D. A. Estenoz,<sup>1</sup> G. R. Meira<sup>1</sup>

<sup>1</sup> INTEC, Universidad Nacional del Litoral and CONICET, 3000 Santa Fe, Argentina

<sup>2</sup> GPol, Universidad Tecnológica Nacional, Regional San Francisco, 2400 Córdoba, Argentina

[Journal of Applied Polymer Science, 2018, 136\(3\), 46946](#)

### **Abstract**

In the first part of this sequel, an experimental investigation on the synthesis of linear segmented polyurethanes was presented, that included estimation of the kinetic constants at 60°C for the prepolymerization and finishing stages. This work presents two comprehensive mathematical models that simulate the mentioned prepolymerizations, in reactions between two poly(tetramethylene oxide) PTMO macrodiols and an excess of methylene diphenyl diisocyanate. The models require to input the molar mass distribution (MMD) of the initial macrodiol. The single-phase (or homogeneous) model calculates a final MMD of approximately 40,000 different molecular species, and somewhat underestimates the observed molar mass dispersities. The double-phases (or heterogeneous) model produces a better fit of the observed MMDs by simulating two independent polymerizations carried out in parallel. The double-phases model contains three adjustable parameters: the reaction imbalances into both phases, and an “effective” rate constant. In part III of this sequel, the presented models will be extended to simulate the finishing stages.

## **High Solid Acrylic–Melamine Latexes with Tunable Crosslinking Capability.**

**Carlos A. Córdoba Ludmila I. Ronco Celina E. Barrios Luis M. Gugliotta Roque J. Minari**

Grupo de Polímeros y Reactores de Polimerización, INTEC (UNL – CONICET).  
Argentina.

**Abstract**

Miniemulsion polymerization is employed to produce high solid content (50%) acrylic/melamine latexes with varied crosslinking capability, for their potential application as waterborne crosslinkable coatings. This synthesis strategy allows the efficient incorporation of a hydrophobic crosslinker, iso-butylated melamine (iBMF), into polymer particles, and to obtain latexes with different iBMF concentrations and acrylic polymer with varied content of hydroxylic groups (OH<sup>-</sup>). The involved crosslinking mechanisms and the physical transformations during film thermosetting of acrylic/iBMF nanocomposite are exhaustively investigated by combining thermal, spectroscopic, and thermo-mechanical analyses. The influence of reactive groups concentration (iBMF and OH<sup>-</sup> content in the acrylic polymer) on the rate of curing, the crosslinking degree, and consequently onto the sensitive properties of cured films are discussed here.

**MÉTODO PARA LA PREDICCIÓN DE LA ENERGÍA ANUAL GENERADA POR UNA INSTALACIÓN FOTOVOLTAICA CONECTADA A LA RED**

**Gustavo Risso, Mario Battioni, Javier Schmidt**

Instituto de Física del Litoral, CONICET-UNL. Güemes 3450, 3000 Santa Fe, Argentina

[Avances en Energías Renovables y Medio Ambiente, 2018, Vol. 6, pp. 03.107-03.113.](#)

**Abstract**

Se calcularon las energías generadas por plantas fotovoltaicas de diversas potencias distribuidas por todo el mundo, a partir de datos de irradiación en el plano horizontal y datos climáticos. Posteriormente se compararon con las energías efectivamente inyectadas a la red eléctrica por estas plantas, verificando que los valores calculados presentan muy poca diferencia con las reales. Esto nos permite concluir que el método resulta de utilidad para estimar con buena precisión la energía que una planta fotovoltaica puede producir en distintas ubicaciones, a partir de datos disponibles públicamente.

**Polyelectrolyte complexes for assisting the application of lignocellulosic micro/nanofibers in papermaking.**

**Carla N. Schnell 1, Quim Tarrés 2, María V. Galván 1, Paulina Mocchiutti 1, Marc Delgado-Aguilar 2, Miguel A. Zanuttini 1, Pere Mutjé 2.**

1. Instituto de Tecnología Celulósica. Facultad de Ingeniería Química, Universidad Nacional del Litoral, Santa Fe, Argentina
2. LEPAMAP Research Group University of Girona, Girona, Spain

[Cellulose \(2018\) 25: 6083.](#)

### **Abstract**

A novel procedure based on the addition of polyelectrolyte complexes (PECs) onto the pulp containing lignocellulosic micro/nanofibers (LCMNF) is presented. This procedure allows increasing paper strength avoiding an excessive loss in drainability. LCMNF were obtained from partially delignified kraft pine sawdust using a high-pressure homogenizer. Cationic complexes (CatPECs) were prepared by adding the anionic polyelectrolyte solution (polyacrylic acid) on the cationic polyelectrolyte solution (poly(allylamine hydrochloride)). According to turbidity and surface morphology changes, an interaction between CatPECs and LCMNF could be established. Different CatPEC dosages (from 0.3 to 1.0% on pulp) were added on a recycled unbleached softwood kraft pulp containing 3% of LCMNF. For a PEC dosage of 0.75% on pulp, an optimum balances between negatively and positively charged materials [near to zero value of the logarithm of the colloidal titration ratio (logCTR)] was found. Britt Dynamic Drainage Jar test showed a high retention of fines and LCMNF for all PEC dosages. A maximum in retention value was obtained for the addition of 0.75% of PECs on pulp, dosage that was suggested as optimum by the logCTR. In addition, the best drainability value (18\_SR) was obtained for this PEC addition level. Papermaking properties were clearly improved for all dosage of PECs. Particularly for a dosage of 0.75% of PECs on pulp, tensile strength was noticeably increased (+48%) and both compressive resistance Concora Medium Test (CMT) and Short-span Compressive Test (SCT) were markedly increased (+64% and +39%, respectively). These results suggest that PECs are a possible alternative to assist the application of LCMNF in papermaking.

## **Raman Microscopy Insights on the Out-of-Plane Electrical Transport of Carbon Nanotube-Doped PEDOT:PSS Electrodes for Solar Cell Applications**

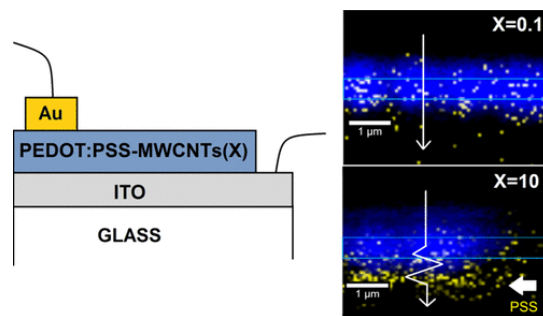
**Dominique Mombrú, Mariano Romero , Ricardo Faccio , and Alvaro W. Mombrú**

Centro NanoMat/CryssMat/Física, DETEMA Facultad de Química, Universidad de la República (UdelaR), Montevideo C.P. 11800, Uruguay

[J. Phys. Chem. B, 2018, 122 \(9\), pp 2694–2701](#)



## Abstract



In the present report, we focused on the study of the out-of-plane electrical transport of multiwalled carbon nanotube (MWCNT)-doped poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) composites (PEDOT:PSS-MWCNTs) as electrodes for solar cell applications. The out-of-plane direct current and alternating current electrical transport, rarely studied but not less relevant, was additionally supported with in-plane and out-of-plane confocal Raman microscopy and grazing incidence small-angle X-ray scattering characterizations. The main relevance of our study is the monitoring of the polymer structure all across the polymeric film by using confocal Raman spectroscopy and its correlation with electrical transport. Modifications in the PEDOT benzenoid and quinoid conformations were observed in the vicinities of MWCNTs, and the enrichment of PSS at the indium tin oxide electrode interface was also evidenced. In consequence, the low MWCNT loadings into PEDOT:PSS lead to an increase of the out-of-plane conductivity, but the heavier MWCNT loadings lead to a drastic decrease. The tuning of the doping level of these polymer composites and the understanding of the interface structure are crucial to fabricate electrodes with higher out-of-plane conductivities for organic solar cell applications.

## Hydrogen titanate nanotubes for dye sensitized solar cells applications: Experimental and theoretical study

Fernando Pignanelli<sup>a</sup>, Luciana Fernández-Werner<sup>a</sup>, Mariano Romero<sup>a</sup>, Dominique Mombrú<sup>a</sup>, Milton A. Tumelero<sup>b,c</sup>, André A. Pasa<sup>c</sup>, Estefanía Germán<sup>ad</sup>, Ricardo Faccio<sup>a</sup>, Álvaro W. Mombrú<sup>a</sup>

<sup>a</sup>Centro NanoMat, DETEMA, Facultad de Química, Universidad de la República, Montevideo, Uruguay

<sup>b</sup>Instituto de Física – Universidade Federal do Rio Grande do Sul (UFRGS), Porto Alegre C.P. 91501-970, Brazil

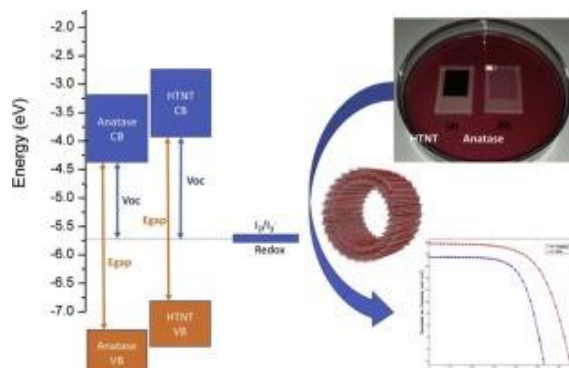
<sup>c</sup>Laboratório de Filmes Finos e Superfícies – Departamento de Física–Universidade Federal de Santa Catarina (UFSC), Florianópolis C.P. 88040-900, Brazil

<sup>d</sup>Departamento de Física, Universidad Nacional del Sur & IFISUR (UNS-CONICET), Av. Alem 1253, 8000, Bahía Blanca, Argentina

Received 11 March 2018, Revised 16 May 2018, Accepted 25 May 2018, Available online 26 May 2018.

[Materials Research Bulletin. Volume 106, October 2018, Pages 40-48](#)

## Abstract



The existent research literature of Dye Sensitized Solar Cells (DSSC) is mainly focused on the dye but there are very few studies focused in the semiconductor. Here, we present the performance of hydrogen titanate nanotubes (HTNT), showing an enhancement of the solar cell efficiency from 5.95% to 7.63%, respect to anatase as photoelectrode. This enhancement could be explained in terms of open-circuit voltage, directly associated to the value of the HTNT band gap ( $E_g = 3.3$  eV), the relative position of the edge conduction band; and the increase of the short-circuit current, directly associated to the enhancement of the specific area of the photoelectrode. All these characteristics are in very good concordance with our theoretical modelling of the system, based on First Principles calculations. We expect that this system could be further characterized, utilizing different dyes or absorbers, in order to evaluate the potential use of hydrogen titanate nanotubes for solar cell applications.

## Comparison of standard DFT and Hubbard-DFT methods in structural and electronic properties of $\text{TiO}_2$ polymorphs and H-titanate ultrathin sheets for DSSC application

Estefania German<sup>ab</sup>, Ricardo Faccio<sup>b</sup>, Alvaro W. Mombrú<sup>b</sup>,

a Instituto de Física del Sur (IFISUR), Departamento de Física, Universidad Nacional del Sur (UNS), CONICET, Av. L. N. Alem 1253, B8000CPB, Bahía Blanca, Argentina

<sup>b</sup> Centro NanoMat-DETEMA, Facultad de Química, Universidad de la República, Uruguay

[Applied Surface Science. Volume 428, 15 January 2018, Pages 118-123](#)

The structural and electronic properties of several  $\text{TiO}_2$  polymorphs and hydrogen titanate surfaces are modeled and studied by density functional theory (DFT). By implementing the Hubbard parameter “U” in our calculations more realistic results of electronic properties are

obtained, paying with a small deviation in geometric optimization. Lattice parameters difference is found to be less than 6.2%, as well as some changes in surface energy are found, but the reactivity tendency of surfaces is maintained. Calculated work function is less energetic for faces (001) for anatase, (101) for rutile and (001) for TiO<sub>2</sub>-B.

## **Optimization and characterization of nisin-loaded alginate-chitosan nanoparticles with antimicrobial activity in lean beef**

**Patricia Zimet<sup>a</sup>, Álvaro W. Mombrú<sup>a,b</sup>, Ricardo Faccio<sup>a,b</sup>, Giannina Brugnini<sup>c</sup>, Iris Miraballes<sup>d</sup>, Caterina Rufo<sup>c</sup>, Helena Pardo<sup>a,b</sup>.02**

<sup>a</sup> Centro NanoMat, Instituto Polo Tecnológico de Pando, Facultad de Química, UdelaR, Camino Aparicio Saravia s/n, 91000 Pando, Canelones, Uruguay

<sup>b</sup> Cátedra de Física, Facultad de Química, DETEMA, UdelaR, General Flores 2124, 11800 Montevideo, Uruguay

<sup>c</sup> Alimentos y Nutrición, Instituto Polo Tecnológico de Pando, Facultad de Química, UdelaR, Camino Aparicio Saravia s/n, 91000 Pando, Canelones, Uruguay

<sup>d</sup> Laboratorio de Biotecnología, Instituto Polo Tecnológico de Pando, Facultad de Química, UdelaR, Camino Aparicio Saravia s/n, 91000 Pando, Canelones, Uruguay

[LWT. Volume 91, May 2018, Pages 107-116](#)

### **Abstract**

Nanoencapsulation may improve antimicrobial activity of nisin when applied on food systems such as lean beef. Nisin-loaded nanoparticles were prepared by alginate ionic gelation and further complexation with chitosan. A 3-factor, 3-level Box-Behnken experimental design and response surface methodology were used to optimize the formulation. Nanoparticles had an encapsulation efficiency of  $36.1 \pm 0.6\%$ , a z-average of  $66.4 \pm 8.9$  nm and a zeta potential of  $-31.7 \pm 2.6$  mV. Transmission electron microscopy and atomic force microscopy observations confirmed particle size found by dynamic light scattering. Also, Raman spectroscopy analyses and zeta potential measurements showed ionic interactions between nisin and alginate. *In vitro* assessment of inhibition of *Listeria monocytogenes* growth at 4 °C indicated sustained antimicrobial activity of nisin-loaded nanoparticles for 21 days. Furthermore, encapsulated nisin was able to inhibit *L. monocytogenes* growth in vacuum-sealed, refrigerated beef samples for 10 days when applied at 400 IU/g and for 24 days when applied at 800 IU/g, while free nisin controlled microbial growth for only 4 and 17 days respectively. In sum, we describe the application of experimental design tools to produce nisin-loaded nanoparticles that may be used in the food industry to control microbial growth and hence extend the shelf-life of lean beef.

# Modeling of Interface and Internal Disorder Applied to XRD Analysis of Ag-Based Nano-Multilayers

Daniel Ariosa<sup>†</sup>, Claudia Cancellieri<sup>\*‡</sup>, Vicente Araullo-Peters<sup>‡</sup>, Mirco Chiodi<sup>‡</sup>, Elizaveta Klyatskina<sup>‡§</sup>, Jolanta Janczak-Rusch<sup>‡</sup>, and Lars P. H. Jeurgens<sup>‡</sup>

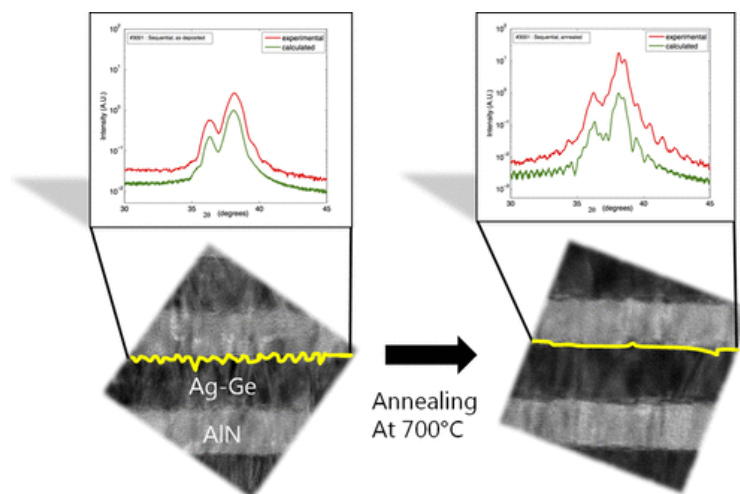
<sup>†</sup> Instituto de Física, Facultad de Ingeniería, Universidad de la República, Herrera y Reissig 565, C.C. 30, 11000 Montevideo, Uruguay

<sup>‡</sup> Swiss Federal Laboratories for Materials Science and Technology (Empa), Überlandstrasse 129, 8600 Dübendorf, Switzerland

<sup>§</sup> Institute of Solid State Physics of the Russian Academy of Sciences, 142432 Chernogolovka, Russian Federation

[ACS Appl. Mater. Interfaces, 2018, 10 \(24\), pp 20938–20949](#)

## Abstract



Multilayered structures are a promising route to tailor electronic, magnetic, optical, and/or mechanical properties and durability of functional materials. Sputter deposition at room temperature, being an out-of-equilibrium process, introduces structural defects and confers to these nanosystems an intrinsic thermodynamical instability. As-deposited materials exhibit a large amount of internal atomic displacements within each constituent block as well as severe interface roughness between different layers. To access and characterize the internal multilayer disorder and its thermal evolution, X-ray diffraction investigation and analysis are performed systematically at differently grown Ag–Ge/aluminum nitride (AlN) multilayers (co-deposited, sequentially deposited with and without radio frequency (RF) bias) samples and after high-temperature annealing treatment. We report here on model calculations based on a kinematic formalism describing the displacement disorder both within the multilayer blocks and at the interfaces to reproduce the experimental X-ray diffraction intensities. Mixing and displacements at the interface are found to be

considerably reduced after thermal treatment for co- and sequentially deposited Ag–Ge/AlN samples. The application of a RF bias during the deposition causes the highest interface mixing and introduces random intercalates in the AlN layers. X-ray analysis is contrasted to transmission electron microscopy pictures to validate the approach.

## **Catalytic properties of Fe-Pd ferromagnetic nanowires at liquid/liquid interfaces**

**Julieta S. Riva (1,2), Andrea V. Juárez (3,4), Silvia E. Urreta (1), Lidia M. Yudi (3,4)**

1-UNC, Facultad de Matemática, Astronomía, Física y Computación, Córdoba, Argentina

2- Consejo Nacional de Investigaciones Científicas y Técnicas, CONICET, Instituto de Física Enrique Gaviola, IFEG. Córdoba, Argentina

3- UNC, Facultad de Ciencias Químicas, Departamento de Fisicoquímica, Haya de la Torre y Medina Allende, Ciudad Universitaria, Córdoba, Argentina

4- Consejo Nacional de Investigaciones Científicas y Técnicas, CONICET, Instituto de Investigaciones en Fisicoquímica de Córdoba, INFIQC, Córdoba, Argentina

[Electrochimica Acta 298 \(2019\) 379-388](#)

### **Abstract**

Fe-Pd binary alloy nanowires (NWs) were synthesized by electrodeposition method with the assistance of nanoporous anodic alumina (AAO). We focus on the synthesis conditions of Fe-Pd nanowires and the characterization of the resulting composition, size and morphology, and their magnetic and catalytic properties at liquid/liquid interfaces. A number of factors may affect the formation and properties of nanoparticles during the synthesis. Here, we focused on finding the effect of the applied potential on the resulting NWs. Moreover, it is shown that Fe-Pd NWs catalyse ion transfer across a soft water/1,2-dichloroethane interface, with a lower overpotential to that reported at bare soft interfaces. Furthermore, the NWs' motion at a liquid/liquid interface is monitored by optical microscopy which allows demonstrating that the magnetic field generated by the ionic current makes the NWs to act as nano-stirrers, improving the local flow of material towards the active sites of the catalyst. During cyclic voltammetry experiments magnetic nanowires move back and forth in a given direction at the liquid/liquid interface according to the direction of polarization.

## **Micropatterning of fluorescent silver nanoclusters in polymer films by Laser Interference**

**Lucinda E. Mulko, Maximiliano Rossa, Juan P. Aranguren-Abrate, Gustavo A. Pino**

INFIQC (CONICET-UNC) - Dpto. de Fisicoquímica - Fac. de Ciencias Químicas - Centro Láser de Ciencias Moleculares - UNC

[Applied Surface Science](#), en Prensa (2019)

### **Abstract**

Hybrid films of poly (methacrylic acid) (PMAA) and silver fluorescent nanocluster were structured by the Direct Laser Interference Patterning technique (DLIP) using few nanosecond laser pulses (355 nm) to obtain an arranged and well-defined periodic surface pattern. It is shown that the films of neat PMAA are not structured by irradiation at 355 nm due to its low absorbance at this wavelength. However, the silver nanoclusters act as chromophores increasing the absorbance of the film and allowing the surface patterning. Also, the interaction of the laser beam with a film of PMAA doped with Ag<sup>+</sup> induces the formation of fluorescent silver nanoclusters and the subsequent surface patterning. The patterned films maintain the luminescent properties of the PMAA/Ag nanoclusters in solution. The structured and unstructured films were characterized by optical, atomic force and spectral laser confocal scanning microscopy showing highly oriented lines patterning already after just one laser pulse.

## **Monitoring of engine oil aging by diffusion and low-field nuclear magnetic resonance relaxation**

**E. Förstera, C. C. Fraenzab, J. Küstnera, E. Anardob, H. Nirschla, G. Guthausenac**

a Institute of Mechanical Process Engineering and Mechanics, Karlsruhe Institute of Technology, Karlsruhe, Germany

b Facultad de Matemática, Astronomía, Física y Computación, Universidad Nacional de Córdoba and IFEG – CONICET, Ciudad Universitaria X5000HUA, Córdoba, Argentina

c Engler-Bunte-Institute, Water Chemistry and Water Technology, Karlsruhe Institute of Technology, Karlsruhe, Germany

[Measurement \(2019\) 137, 673-682](#)

### **Abstract**

Time domain, also named low-field nuclear magnetic resonance is used to monitor oil degradation by measuring relaxation and diffusion. As quality control of oils is indispensable to optimize oil change intervals while simultaneously preventing machinery damage, the technique was applied to detect the degradation state of engine oils as time domain nuclear magnetic resonance is known as a well suited tool to measure quality

control parameters for example in food industry. Correlations with commonly applied oil analytics like viscosity measurements and inductively coupled plasma optical emission spectrometry allow to interpret relaxation and diffusion data in detail and finally to deepen the understanding of oil aging processes. Additionally, the measurement temperature was varied to achieve the maximum sensitivity towards oil aging. Low-field NMR is not only realized in form of table top instruments, but also in form of field cycling and single sided NMR devices. Fast field cycling as well as single-sided NMR were also explored to study oil aging and to provide valuable insight. The latter device was used to obtain information about translational diffusion and transverse relaxation of oils simultaneously.

## **Percolation of hydrogen atoms adsorbed on Cu(100) surfaces: DFT, Monte Carlo and finite size scaling techniques.**

**Elizabeth del V. Gómez, Lucía B. Avalle y M. Cecilia Gimenez**

FaMAF (Facultad de Matemática, Astronomía, Física y Computación), UNC, Córdoba, Argentina

[International Journal of Hydrogen Energy, 44, 7083-7094 \(2019\)](#)

### **Abstract**

Hydrogen adsorption on Cu (100) surfaces was studied taking into account percolation problem. In order to represent the real system, DFT calculations were performed to calculate adsorption energies of a hydrogen atom in different environments, according to the number of first neighbours present at each adsorption site. This information was employed in canonical and grand canonical Monte Carlo simulations and the percolation threshold was calculated for different temperatures. A phase diagram which separates percolating and non percolating regions was obtained. Critical exponents were also calculated in order to study the universality of the system. At temperatures below 200K, a particular and interesting behavior was observed, which is evidenced by the results obtained for the isotherms, phase diagram and critical exponents. At higher temperatures, the behavior observed for percolating properties is that expected for repulsive interactions between neighboring adsorbed hydrogen atoms.

## **Alkali-silica reaction in plain and fibre concretes in field conditions**

**Graciela Giaccio<sup>1,4</sup>, María Celeste Torrijos<sup>2,4</sup>, Carlos Milanese<sup>3</sup>, Raúl Zerbino<sup>2,4</sup>**

1 CIC, Commission of Scientific Research, Department of Civil EngineeringLa Plata National UniversityLa PlataArgentina

2 CONICET, National Council of Scientific and Technological Research, Department of Civil EngineeringLa Plata National UniversityLa PlataArgentina

3 Cementos Avellaneda S.A.CABAArgentina

[Mater Struct \(2019\) 52:31](#)

**Abstract**

This paper presents an experimental study on the effects of alkali–silica reaction (ASR) in concrete blocks placed outdoors, exposed to weather conditions. To promote different reaction kinetics and damage levels, the size of the reactive aggregates, the alkali content and incorporation of different fibre types (steel, polymer) were the variables considered. Expansions, crack patterns and air permeability were monitored for more than 3 years. In addition, standard expansion, compression and flexion tests were performed. The volume of concrete involved in ASR enhances the development of expansions and cracking; in the blocks different expansions were measured in vertical or horizontal directions and important cracks were observed. While the prisms expansions were attenuated after the first 12 months, in the blocks the damage by ASR continues growing for more than 3 years. Although the incorporation of macrofibers does not inhibit the development of ASR, it led to benefits such as reduction in cracking and deformations.



## Año 2018

### Selective contrast agents with potential to the earlier detection of tumors: Insights on synthetic pathways, physicochemical properties and performance in MRI assays

María Gabriela Montiel Schneider<sup>a</sup>, María Julia Martín<sup>b</sup>, Diego Fernando Coral<sup>cd</sup>, Diego Muraca<sup>e</sup>, Claudia Gentili<sup>b</sup>, Marcela Fernández van Raap<sup>c</sup>, Verónica Leticia Lassalle<sup>a</sup>

<sup>a</sup>INQUISUR, Departamento de Química, Universidad Nacional del Sur (UNS)-CONICET, Av. Alem 1253, Bahía Blanca, 8000, Argentina

<sup>b</sup>INBIOSUR, Departamento de Biología, Bioquímica y Farmacia, Universidad Nacional del Sur (UNS)-CONICET, San Juan 671, Bahía Blanca, 8000, Argentina

<sup>c</sup>Instituto de Física La Plata IFLP-CONICET, Departamento de Física, Universidad Nacional de La Plata, La Plata, Buenos Aires, Argentina

<sup>d</sup>Institución Universitaria CESMAG, Pasto, Colombia

<sup>e</sup>Laboratório de Materiais e Dispositivos, Instituto de Física 'Gleb Wataghin', Universidade Estadual de Campinas, Campinas, Brazil

[Biointerfaces, 170, 470-478 \(2018\).](#)

#### Abstract

Magnetic iron oxide nanoparticles (MNPs) have been prepared and stabilized with three organic acids (tartaric, malic and ascorbic) in order to obtain biocompatible and water dispersible MNPs with potential to bind specifically to tumoral cancer cells. An in deep characterization was performed aiming to verify the presence and effect of the coating and stabilizer on MNPs surface. Besides the mechanisms followed by the different acids to bind MNPs were elucidated and used to justify the differences in the physicochemical properties of each formulation. Data related to characterization revealed that MNPs coated with ascorbic acid (MNPs-AA) resulted the most suitable in terms of their size, surface charge and stability along the time. Besides, ascorbic acid may be recognized by GLUTs receptors that are overexpressed in several kinds of tumoral cells. Therefore, MNPs-AA was selected to explore its performance in both MRI and in vitro assays using human colon cancer cells HCT 116. MRI experiments were performed in clinical equipment using a series of aqueous dispersions of MNPs-AA that were evaluated as  $T_2$  contrast agent. The  $T_2$ - weighted images obtained as well as the calculated  $r_2$ , indicated that MNPs-AA could act as efficient  $T_2$  contrast agent for MRI.

Regarding in vitro assays, MNPs-AA did not alter the cellular function neither exert cytotoxicity using the three explored doses. The internalization of the nanoparticles on the cellular structure was confirmed quanti and qualitatively using atomic absorption spectroscopy and Prussian blue techniques respectively.

From these results, it emerges that ascorbic acid coated-magnetite nanoparticles may be used as alternative contrast agent to avoid or minimize some toxicological issues related to the widely used gadolinium.

## **Sol-gel synthesis of substoichiometric cobalt ferrite (CoFe<sub>2</sub>O<sub>4</sub>) spinels: Influence of additives on their stoichiometry and magnetic properties**

**Janio Venturini, Rubia Young, Sun Zampiva, Sabrina Arcaro, Carlos Pérez Bergmann**

Department of Materials Engineering, Federal University of Rio Grande do Sul, Osvaldo Aranha 99, Porto Alegre 90035-190, Brazil

[Ceramics International. Volume 44, Issue 11, 1 August 2018, Pages 12381-12388ç](#)

### **Abstract**

Spinel cobalt ferrites (CoFe<sub>2</sub>O<sub>4</sub>) with varying levels of substoichiometry were prepared via sol-gel synthesis with different combinations of citric acid, dextrose and PVP (polyvinylpyrrolidone). The gels, prepared from the metal nitrates, were dried at 110 °C, further treated at 850 °C and finally subjected to thorough structural and magnetic characterization in order to correlate the composition of the gel to the structural and magnetic properties displayed by the ferrites. The materials synthesized in the present work have shown to be rather iron-depleted, reaching over 50% deficiency of the metal, which leaves the spinel lattice and forms Fe<sub>2</sub>O<sub>3</sub> instead. The fuel/oxidant ratio and the thermal behavior of the xerogels exert a direct influence on the compositional variation of the prepared spinels, which could in turn be correlated to the magnetic properties displayed by the particles. A maximum in coercivity of 2154.4 Oe was achieved without the application of any additive to the nitrate precursors. On the other hand, the magnetic remanence displayed by the ferrites shows a linear relationship to the iron content in their chemical formula. The results open up the possibility of fine-tuning the structural and magnetic properties displayed by the spinel product via careful control of the composition of the reaction medium.

## **Activated nanocarbons produced by microwave-assisted hydrothermal carbonization of Amazonian fruit waste for methane storage.**

**Orlando F. Cruz Jr.<sup>1,2</sup>, Joaquín Silvestre-Albero<sup>2</sup>, Mirian E. Casco<sup>2</sup>, Dachamir Hotza<sup>3</sup>, Carlos R. Rambo<sup>4</sup>**

<sup>1</sup> Instituto Nacional de Pesquisas da Amazônia (INPA), 69011-970 Manaus, AM, Brazil

<sup>2</sup> Departamento de Química Inorgánica, Universidad de Alicante, E-03080 Alicante, Spain

<sup>3</sup> Department of Chemical and Food Engineering (EQA)

<sup>4</sup> Department of Electrical and Electronic Engineering (EEL), Federal University of Santa Catarina (UFSC), 88040-900 Florianópolis, SC, Brazil

### **Abstract**

This work reports the preparation and characterization of biomass-derived renewable microporous carbon nanoparticles obtained by microwave-assisted hydrothermal carbonization (MAHC), following by physical activation, of assai stone waste. Conventional routes (i.e. carbonization in furnace and chemical activation) was also investigated. The highest yield provided by MAHC combined with CO<sub>2</sub> as activating agent resulted in nanocarbons with surface area of 1100 m<sup>2</sup>/g and a very narrow pore size distribution with a micropore volume of 0.45 cm<sup>3</sup>/g. Owing to the excellent combination of microporosity and high bulk density (0.89 g/cm<sup>3</sup>). The biomass-derived carbon shows great potential to be used as adsorbent for natural gas storage. Indeed, high pressure methane adsorption isotherm in volumetric basis revealed an uptake value of 140 V(STP)/V at 25 °C and 4 MPa.

## **Casein films crosslinked by tannic acid for food packaging applications**

**Matías L. Picchio<sup>a,b</sup>, Yamila Garro Linck<sup>c,d</sup>, Gustavo A. Monti<sup>c,d</sup>, Luis M. Gugliotta<sup>e,f</sup>, Roque J. Minari<sup>f,g</sup>, y Cecilia I. Alvarez Igarzabal<sup>a</sup>**

<sup>a</sup>Facultad de Ciencias Químicas (UNC), IPQA-CONICET; <sup>b</sup>Facultad Regional Villa María (UTN); <sup>c</sup>FAMAF, UNC; <sup>d</sup>IFEG, CONICET; <sup>e</sup>INTEC, CONICET; <sup>f</sup>Facultad de Ingeniería Química (UNL)

[Food Hydrocolloids, 84 \(2018\) 424-434](#)

### **Abstract**

Natural proteins are good candidates for producing food packaging films due to their excellent functional properties. However, some deficiencies as their poor water resistance need to be addressed before films can be used in daily applications. This article explores the use of a low-cost plant-derived phenolic compound, tannic acid, as crosslinking agent for producing plasticized casein films. FTIR, high-resolution NMR, and rheological measurements confirmed the crosslinking reaction between casein amine groups and tannic acid. The influence of crosslinking agent concentration on the mechanical and viscoelastic properties, thermal stability, swelling behavior, water vapor permeability, cytotoxicity and degradation in composting conditions were investigated. The obtained results showed that tannic acid was an effective crosslinking agent for casein protein, so the yielded films which exhibit improved physicochemical properties, can be employed for food packaging applications.

## **Temperature dependence of the effective anisotropy in Ni nanowire arrays**

**Fernando Meneses<sup>a</sup>, Silvia E. Urreta<sup>a</sup>, Juan Escrig<sup>b</sup>, Paula G. Bercoff<sup>a</sup>**

<sup>a</sup>Facultad de Matemática, Astronomía, Física y Computación, Universidad Nacional de Córdoba. Instituto de Física Enrique Gaviola, CONICET. Ciudad Universitaria, Córdoba, Argentina

<sup>b</sup>Departamento de Física, Universidad de Santiago de Chile, USACH. Center for the Development of Nanoscience and Nanotechnology, CEDENNA. 917-0124, Santiago, Chile  
Grupo Ciencia de Materiales, FAMAF, UNC

[Current Applied Physics 18 \(2018\) 1240–1247](#)

### **Abstract**

Magnetic hysteresis in Ni nanowire arrays grown by electrodeposition inside the pores of anodic alumina templates is studied as a function of temperature in the range between 5 K and 300 K. Nanowires with different diameters, aspect ratios, inter-wire distance in the array and surface condition (smooth and rough) are synthesized. These microstructure parameters are linked to the different free magnetic energy contributions determining coercivity and the controlling magnetization reversal mechanisms. Coercivity increases with temperature in arrays of nanowires with rough surfaces and small diameters —33 nm and 65 nm — when measured without removing the alumina template and/or the Al substrate. For thicker wires — 200 nm in diameter and relatively smooth surfaces— measured without the Al substrate, coercivity decreases as temperature rises. These temperature dependences of magnetic hysteresis are described in terms of an effective magnetic anisotropy  $K_a$ , resulting from the interplay of magnetocrystalline, magnetoelastic and shape anisotropies, together with the magnetostatic interaction energy density between nanowires in the array. The experimentally determined coercive fields are compared with results of micromagnetic calculations, performed considering the magnetization reversal mode acting in each studied array and microstructure parameters. A method is proposed to roughly estimate the value of  $K_a$  experimentally, from the hysteresis loops measured at different temperatures. These measured values are in agreement with theoretical calculations. The observed temperature dependence of coercivity does not arise from an intrinsic property of pure Ni but from the nanowires surface roughness and the way the array is measured, with or without the alumina template and/or the aluminum support.

### **Heterogeneity of strain path, texture and microstructure evolution of AA6063-T6 processed by Equal Channel Angular Sheet Extrusion (ECASE)**

**Jairo Alberto Muñoz, Martina Avalos, Raúl E. Bolmaro**

Instituto de Física Rosario, Consejo Nacional de Investigaciones Científicas y Técnicas-CONICET, Universidad Nacional de Rosario, Ocampo y Esmeralda, 2000 Rosario, Argentina

[J. of Alloys and Comp. 768 \(2018\) 349-357. DOI: 10.1016/j.jallcom.2018.07.216](#)

## Abstract

An Aluminum alloy 6063T6 was processed at room temperature by Equal Channel Angular Sheet Extrusion (ECASE). Microstructure evolution was investigated by Electron Back Scattering Diffraction (EBSD), and X-ray diffraction analysis. The texture evolution was heterogeneous and represented by a mix of rolling and shearing components through the sheet thickness. Ncorr<sup>TM</sup> calculations showed higher shear strains close to the edges than in the sheet core, in agreement with the through thickness expected variation. The Geometrically Necessary Dislocation (GND) calculations corroborated the existence of a heterogeneous microstructure through the sheet thickness.

## Tunable green/red luminescence by infrared upconversion in biocompatible forsterite nanoparticles with high erbium doping uptake

Rúbia Young Sun Zampiva<sup>a</sup> Luiz Henrique Acauan<sup>b</sup> Janio Venturini<sup>a</sup> Jose Augusto Martins Garcia<sup>c,d</sup> Diego Silverio da Silva<sup>e</sup> Zhaohong Han<sup>f</sup> Luciana Reyes Pires Kassab<sup>f</sup> Niklaus Ursus Wetter<sup>e</sup> Anuradha Agarwal<sup>f</sup> Annelise KoppAlves<sup>a</sup> Carlos Pérez Bergmann<sup>a</sup>

<sup>a</sup>Department of Materials Engineering, Federal University of Rio Grande do Sul- UFRGS. Osvaldo Aranha 99, Porto Alegre, RS, 90035- 190, Brazil

<sup>b</sup>Department of Aeronautics and Astronautics, Massachusetts Institute of Technology-MIT, Cambridge, MA, 02139, United States

<sup>c</sup>Laboratório de Tecnologia em Materiais Fotônicos e Optoeletrônicos, Faculdade de Tecnologia de São Paulo, Praça Coronel Fernando Prestes, 30 - Bom Retiro, São Paulo, SP, 01124-060, Brazil

<sup>d</sup>Laboratório de Sistemas Integráveis, Escola Politécnica da Universidade de São Paulo, Av. Prof. Luciano Gualberto, 158, Travessa 3, 05508-900, São Paulo, SP, Brazil

<sup>e</sup>Centro de Lasers e Aplicações, Instituto de Pesquisas Energéticas e Nucleares-IPEN/SP, Prof. Lineu Prestes 2242, São Paulo, SP, 05508-000, Brazil

<sup>f</sup>Microphotonics Center, Massachusetts Institute of Technology-MIT, Cambridge, MA, 02139, United States

[Optical Materials. Volume 76, February 2018, Pages 407-415](#)

## Abstract

Nanoparticles represent a promising platform for diagnostics and therapy of human diseases. For biomedical applications, these nanoparticles are usually coated with photosensitizers regularly activated in a spectral window of 530–700 nm. The emissions at 530 nm (green) and 660 nm (red) are of particular interest for imaging and photodynamic therapy, respectively. This work presents the Mg<sub>2</sub>SiO<sub>4</sub>:Er<sup>3+</sup> system, produced by reverse strike co-precipitation, with up to 10% dopant and no secondary phase formation. These nanoparticles when excited at 985 nm show upconversion emission with peaks around 530 and 660 nm, although excitation at 808 nm leads to only a single emission peak at around 530 nm. The direct upconversion of this biomaterial without a co-dopant, and its tunability

by the excitation source, renders  $\text{Mg}_2\text{SiO}_4:\text{Er}^{3+}$  nanoparticles a promising system for biomedical applications.

## **Magnetic nanotechnological devices as efficient tools to improve the quality of water: analysis on a real case.**

**Maria Fernanda Horst<sup>1</sup>, Aldana Pizzano<sup>1</sup>, Carla Spetter<sup>2,3</sup>, Verónica Lassalle<sup>1</sup>**

1 Departamento de Química, INQUISUR Universidad Nacional del Sur (UNS)-  
CONICET Bahía Blanca Argentina

2 Instituto Argentino de Oceanografía (IADO) Universidad Nacional del Sur (UNS)-  
CONICET Bahía Blanca Argentina

3 Departamento de Química Universidad Nacional del Sur (UNS) Bahía Blanca Argentina

[Environ Sci Pollut Res, 25, 28, 28185–28194 \(2018\).](#)

### **Abstract**

Magnetic nanoparticles (MNPs), based on iron oxide (magnetite) and ferrogel of gelatin and MNPs, were employed as efficient tools for the removal of heavy metals and nutrients from water samples from Bahía Blanca estuarine (BBE). An exhaustive adsorption performance of Cu,  $\text{NO}_3^-$ , and  $\text{NO}_2^-$  was conducted in batch using model solutions aiming to adjust the adsorption conditions. Adsorption studies using water simulating the real samples were also performed. Both kinds of nanomaterials demonstrated an efficiency between 60 and 80%, and 85% for the removal of heavy metals and  $\text{NO}_3^-$  and  $\text{NO}_2^-$ , respectively. Similar adsorption assays were performed using BBE water samples, employing the experimental conditions explored with model and simulated water. The reached efficiency was 30 and 45% for heavy metal and nutrient removal, respectively, using nanoparticles; meanwhile, ferrogels displayed a removal capacity around 50–60%. The nanoparticles showed structural instability by the leaching of iron to the medium after the adsorption processes. Ferrogels remained almost inalterable in terms of their integrity during the adsorption time. These materials showed satisfactory perspectives regarding their reuse possibilities. They were used for almost five repeated cycles of adsorption without losing efficiency on the adsorption. The results of this study suggest that MNPs and FGs appear as versatile and promising materials that may be considered as valid alternatives to the actual tools for the remediation of real water samples.

## **Surface speciation of phosphate on goethite as seen by InfraRed Surface Titrations (IRST)**

**Arroyave J.M., Puccia V., Zanini G.P., Avena M.J.**

INQUISUR, Departamento de Química, Universidad Nacional del Sur (UNS)-CONICET,  
Av. Alem 1253, 8000 Bahía Blanca, Argentina

### **Abstract**

Phosphate adsorption at the metal oxide-water interface has been intensely studied, and the system phosphate-goethite in aqueous media is normally used as a model system with abundant information regarding adsorption-desorption under very different conditions. In spite of this, there is still discussion on whether the main inner-sphere surface complexes that phosphate forms on goethite are monodentate or bidentate. A new spectroscopic technique, InfraRed Surface Titration (IRST), is presented here and used to systematically explore the surface speciation of phosphate on goethite in the pH range 4.5–9.5 at different surface coverages. IRST enabled to construct distribution curves of surface species and distribution curves of dissolved phosphate species. In combination with the CD-MUSIC surface complexation model it was possible to conclude that surface complexes are monodentate. Very accurate distribution curves were obtained, showing a crossing point at pH 5.5 at a surface coverage of  $2.0 \mu\text{mol m}^{-2}$ , with a mononuclear monoprotonated species predominating at  $\text{pH} > 5.5$  and a mononuclear diprotonated species prevailing at  $\text{pH} < 5.5$ . On the contrary, at the low surface coverage of  $0.7 \mu\text{mol m}^{-2}$  there is no crossing point, with the mononuclear monoprotonated species prevailing at all pH. IRST can become a powerful technique to investigate structure, properties and reactions of any IR-active surface complex at the solid-water interface.

### **The shape recovery conditions for Fe–Mn–Si alloys: An interplay between martensitic transformation and plasticity.**

**A. Druker<sup>a,c</sup>, P. Vermaut<sup>b</sup>, J. Malarría<sup>a,c</sup>**

<sup>a</sup>Facultad de Cs. Ex., Ingeniería y Agrimensura (UNR), Av Pellegrini 250, Rosario, Argentina

<sup>b</sup>Groupe de Métallurgie Structurale, UMR CNRS 70 45, ENSCP, 75231 Paris, France

<sup>c</sup>Instituto de Física Rosario (CONICET-UNR), Bv. 27 de Febrero 210 bis, Rosario, Argentina

[Malarría Materials Characterization, 2018, 139, 319-327.](#)

### **Abstract**

This work analyses the improvement of the shape memory properties of Fe-Mn-Si based alloys, and expands upon and deepens recently published developments concerning this topic. We prepared TEM specimens from a Fe-15Mn-5Si-9Cr-5Ni sheet rolled at 800 °C and annealed at 650 °C–92% shape recovery – and from another sheet annealed at 1000 °C–45% shape recovery. Here, we analyse the development of microstructure during the  $\gamma \leftrightarrow \epsilon$  martensitic transformation and correlate it with the shape memory behaviour. Among the observed microstructural features, the introduction of complex dislocation arrays due to plastic deformation appears to be critical for shape memory development, since they can arrest the backward movement of Shockley partial dislocations over the original path. Tailoring the microstructure in order to introduce a high stacking-fault

density accompanied by an appropriate dislocation density remains a key issue in the design of these kinds of functional materials.

## **Mechanical and thermal properties of friction-stir welded joints of high density polyethylene using a non-rotational shoulder tool**

**Mirley Moreno-Moreno<sup>1</sup>, Yorledis Macea Romero<sup>1</sup>, Habib Rodríguez Zambrano<sup>2</sup>, Nora Catalina Restrepo-Zapata<sup>3</sup>, Conrado Ramos Moreira Afonso<sup>4</sup>, Jimy Unfried-Silgado<sup>5</sup>**

1 Facultad de ingeniería, Programa de ingeniería mecánica, Grupo IMTEF Universidad Autónoma del Caribe Barranquilla Colombia

2 División de Ingeniería, Grupo GIMYP Universidad del Norte Barranquilla Colombia

3 Núcleo de Matemáticas, Física y Estadística, Facultad de Ciencias Universidad Mayor Santiago Chile

4 Departamento de Engenharia de Materiais – DEMA Universidade Federal de São Carlos São Carlos Brazil

5 Departamento de Ingeniería mecánica, Grupo ICT Universidad de Córdoba Montería Colombia

[The International Journal of Advanced Manufacturing Technology. July 2018, Volume 97, Issue 5–8, pp 2489–2499](#)

### **Abstract**

The effects of rotational and welding speed on the mechanical properties and thermal behavior in friction stir welded joints of high-density polyethylene using a non-rotational shoulder have been investigated experimentally. Tensile properties and hardness were measured to determine the mechanical properties, and the effect of the welding parameters. Heating and cooling cycles of differential scanning calorimetry were used to establish thermal properties. Microstructure observations complemented experimental observations. Results showed that tensile strength, hardness, and crystallinity decreased when rotational speed was increased, while the welding speed effect was weak. Deleterious phenomena on molecular structure of the stir region were explained by means combination of selected welding parameters and the material flow during the process.

## **Minimization of polymerization shrinkage effects on composite resins by the control of irradiance during the photoactivation process**

**Gabriel Felipe GUIMARÃES<sup>1</sup>, Edilmar MARCELINO<sup>2</sup>, Ivana CESARINO<sup>1</sup>, Fábio Bossoi VICENTE<sup>3</sup>, Carlos Roberto GRANDINI<sup>3 4</sup>, Rafael Plana SIMÕES<sup>1</sup>**

<sup>1</sup> Univ. Estadual Paulista, Faculdade de Ciências Agrônômicas, Departamento de Bioprocessos e Biotecnologia, Botucatu, SP, Brasil.

<sup>2</sup> Univ. Estadual Paulista, Instituto de Biociências, Botucatu, SP, Brasil.



<sup>3</sup> Univ. Estadual Paulista, Faculdade de Ciências, Laboratório de Relaxações Anelásticas e Biomateriais, Bauru, SP, Brasil.

<sup>4</sup> Instituto de Biomateriais, Tribocorrosão e Nanomedicina - Ramo Brasileiro, Bauru, SP, Brasil.

[J. Appl. Oral Sci. vol.26 Bauru 2018 Epub June 18, 2018](#)

#### **Abstract**

High levels of shrinkage stress caused by volumetric variations during the activation process are one of the main problems in the practical application of composite resins.

### **Effect of crystal size on the tribological behavior of manganese phosphate coatings under lubricated sliding**

**Nicolás S Fochesatto<sup>1</sup>, Camila Müller<sup>2</sup>, Nicolás A Zabala<sup>1</sup>, Pablo A Castro<sup>3</sup>, Walter R Tuckart<sup>1</sup>**

<sup>1</sup>Departamento de Ingeniería, Universidad Nacional del Sur, Bahía Blanca, Argentina

<sup>2</sup>PLAPIQUI, Universidad Nacional del Sur – CONICET, Bahía Blanca, Argentina

<sup>3</sup>Department of Surface Chemistry and Coatings, TENARIS, Research and Development Centre, Campana, Argentina

[Journal of Engineering Tribology Part J., 232\(10\), 1285–1292 \(2018\).](#)

#### **Abstract**

In this study, the wear and friction behavior of manganese phosphate coatings with different crystal sizes were investigated. Crystal size was controlled modifying the chemical composition of the phosphating bath, particularly the concentration of the activator which modifies the number of nuclei for crystal growth. Activator concentration range used for this work varied from 0 to 0.7 g/L, and crystal size was measured using image analysis software on scanning electron microscopy photographs. Available volume for lubricant retention was determined measuring the phosphated surface with a 3D optical profilometer. At the same time, lubricated wear tests were carried out using a ring-on-block configuration at low speeds (23 mm/s) and high loads (14,500 N). Wear behavior was determined as the sliding distance to failure, which was noticed through signs of removal of the phosphate along with the increase of coefficient of friction. It was found that there is a competition between the availability of volume to hold the lubricant, which increases with the crystal size, and the surface coverage, which diminishes as the crystal size grows. Optimal results were obtained for an activator concentration of 0.3 g/L, which meant an average crystal size of 16 µm.

## **Electromechanical Anisotropy at the Ferroelectric to Relaxor Transition of (Bi<sub>0.5</sub>Na<sub>0.5</sub>)<sub>0.94</sub>Ba<sub>0.06</sub>TiO<sub>3</sub> Ceramics from the Thermal Evolution of Resonance Curves Applied**

**Nicolás Pérez<sup>1</sup>, Alvaro García<sup>2</sup>, Enrique Riera<sup>3</sup> and Lorena Pardo<sup>2</sup>,**

<sup>1</sup> Instituto de Ingeniería Eléctrica, Facultad de Ingeniería, Universidad de la República, Julio Herrera y Reissig 565, 11300 Montevideo, Uruguay.

<sup>2</sup> Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), c/Sor Juana Inés de la Cruz, 3. Cantoblanco, 28049 Madrid, Spain.

<sup>3</sup> Instituto de Tecnologías Físicas y de la Información (ITEFI-CSIC), c/Serrano 144, 28006 Madrid, Spain.

[Sciences-Basel, p.:1 - 6, 2018](#)

### **Abstract**

(Bi<sub>0.5</sub>Na<sub>0.5</sub>)<sub>0.94</sub>Ba<sub>0.06</sub>TiO<sub>3</sub> dense ceramics were obtained from autocombustion sol-gel synthesized nanopowders and sintered at 1050 °C for 1–2 h for the study of the electromechanical anisotropy. Measurement of the complex impedance spectrum was carried out on thin ceramic disks, thickness-poled, as a function of the temperature from 16 °C up to the vanishing of the electromechanical resonances at the ferroelectric to relaxor transition near 100 °C. The spectrum comprises the fundamental radial extensional mode and three overtones of this, together with the fundamental thickness extensional mode, coupled with other complex modes. Thermal evolution of the spectrum shows anisotropic behavior. Piezoelectric, elastic, and dielectric material coefficients, including all losses, were determined from iterative analysis of the complex impedance curves at the planar, thickness, and shear virtually monomodal resonances of disks and shear plates, thickness-poled. *d*<sub>33</sub> was measured quasi-statically at 100 Hz. This set of data was used as the initial condition for the optimization of the numerical calculation by finite elements of the full spectrum of the disk, from 100 kHz to 1.9 MHz, to determine the thermal evolution of the material coefficients. An appropriate measurement strategy to study electromechanical anisotropy of piezoelectric ceramics has been developed

## **Bismuth (III) sulfide as additive: towards better lubricity without toxicity**

**Camila Müller<sup>1</sup>, Franco Leonardo Redondo<sup>1</sup>, Mariana Dennehy<sup>2</sup>, Andrés Eduardo Ciolino<sup>1,3</sup>, Walter Roberto Tuckart<sup>3,4</sup>.**

<sup>1</sup> Planta Piloto de Ingeniería Química, Universidad Nacional del Sur, Consejo Nacional de Investigaciones Científicas y Técnicas, Bahía Blanca, Argentina, and Departamento de Ingeniería Química, Universidad Nacional del Sur, Bahía Blanca, Argentina

<sup>2</sup> Instituto de Química del Sur, Departamento de Química, Universidad Nacional del Sur, Bahía Blanca, Argentina.

<sup>3</sup> Departamento de Ingeniería Química, Universidad Nacional del Sur, Bahía Blanca, Argentina.

### **Abstract**

**Purpose:** The purpose of this study is to design a fluid formulation with good lubricant properties by using an environmentally friendly additive for: high and low contact pressure conditions and steel/steel and polymer/steel systems.

**Design/methodology/approach:** Bismuth (III) sulfide ( $\text{Bi}_2\text{S}_3$ , “green chemistry” synthesis) is added to a commercial vinyl-terminated silicone fluid (PDMS-Vi) to obtain different weight-per cent mixtures. Tribological performance of formulations is studied from Reichert’s tests (steel/steel system) and block on ring tests (polymer/steel). The results are compared with formulations prepared with commercial bismuth (III) sulfide ( $\text{Bi}_2\text{S}_3$ ), molybdenum (IV) sulfide ( $\text{MoS}_2$ ) and graphite.

**Findings:** An orthorhombic crystal lattice (XRD ) and a high-purity product (XRF) are evidenced for synthesized  $\text{Bi}_2\text{S}_3$ . Lubricant properties increase when the weight-per cent of the synthesized  $\text{Bi}_2\text{S}_3$  increases in formulations. The wear area decreases up to 90 per cent according to Reichert’s tests. The synthesized  $\text{Bi}_2\text{S}_3$  shows a better tribological behavior when compared to commercial  $\text{Bi}_2\text{S}_3$ ,  $\text{MoS}_2$  and graphite.

**Originality/value:** Replacement of lead derivatives by an environmentally friendly lubricant in extreme pressure (EP) formulations and excellent performance compared to commercially used additives are achieved.

## **Ultrasound-Assisted Deposition of Co–CeO<sub>2</sub> onto Ceramic Microfibers to Conform Catalytic Papers: Their Application in Engine Exhaust Treatment.**

**N. A. Sacco, E. D. Banús, J. P. Bortolozzi, V. G. Milt, E. E. Miró**

INCAPE (UNL-CONICET)

[ACS Omega 2018, 3, 18334–18342.](#)

### **Abstract**

The combination of the selective catalytic reduction technology with catalytic filters constitutes one of the most efficient ways for diesel engine exhaust treatment. In this paper, the development of catalytic ceramic papers as structured systems for the abatement of diesel soot particles is addressed. Ceramic papers were prepared by the dualpolyelectrolyte papermaking method, which is based on the conventional papermaking technique used for cellulosic papers, in which a portion of cellulosic fibers is replaced by ceramic ones. The deposition of Co and Ce as catalytic materials by the wet spray method on ceramic papers was studied for the development of structured catalysts using an ultrasonic nebulizer and different solvents. The use of alcohol–water solutions for the impregnation of cobalt generated smaller particles and a high dispersion of them on the ceramic fibers, greater than that obtained when pure water was employed. Temperature programmed oxidation (TPO)

assays showed that the best catalytic performance was acquired with the catalysts generated with alcohol solvents, showing a maximum rate for soot combustion at a temperature close to 400°C. The adequate soot combustion performance and the high thermal and catalytic stability make catalytic ceramic papers impregnated by the wet spray method, promising systems for their application as diesel particulate filters.

## **FeCr Alloy Monoliths Coated with Ni/Al<sub>2</sub>O<sub>3</sub> Applied to the Low-Temperature Production of Ethylene.**

**Paula Brussino<sup>1</sup>, Juan Pablo Bortolozzi<sup>1</sup>, Oihane Sanz<sup>2</sup>, Mario Montes<sup>2</sup>, María Alicia Ulla<sup>1</sup> and Ezequiel David Banús<sup>1</sup>**

<sup>1</sup>Instituto de Investigaciones en Catálisis y Petroquímica, INCAPE (UNL-CONICET), Santiago del Estero 2829, 3000 Santa Fe, Argentina

<sup>2</sup>Departamento de Química Aplicada, Universidad del País Vasco (UPV/EHU), 20018 San Sebastián, Spain

[Catalysts 2018, 8, 291.](#)

### **Abstract**

This paper investigates the oxidative dehydrogenation of ethane to produce ethylene at low temperatures (500 C) in metallic structured substrates. To check this point, the FeCrAlloy® monoliths with different channel sizes (289–2360 cpsi) were prepared. The monoliths were coated with a Ni/Al<sub>2</sub>O<sub>3</sub> catalyst (by washcoating of alumina and the latter nickel impregnation) and characterized by Scanning Electron Microscopy and Energy-Dispersive X-ray analysis (SEM-EDX), Temperature-Programmed Reduction (TPR), X-ray Diffraction (XRD) and X-ray Photoelectron Spectroscopy (XPS). The catalytic results showed that all monoliths coated with ~300 mg of catalyst presented similar ethane conversion (15%) at 450 C. However, the lowest selectivity to ethylene was found for the monolith with the lower channel size and the higher geometric surface area, where a heterogeneous catalyst layer with Ni enriched islands was generated. Therefore, it can be said that the selectivity to ethylene is linked to the distribution of Ni species on the support (alumina). Nevertheless, in all cases the selectivity was high (above 70%). On the other hand, the stability in reaction tests of one of the coated monoliths was done. This structured catalyst proved to be more stable under reaction conditions than the powder catalyst, with an initial slight drop in the first 8 h but after that, constant activity for the 152 h left.

## **Band Structure Effects on the Charge Exchange Processes in H<sup>+</sup> Colliding with a Cu(111) Surface.**

**Quintero Riascos, Marcos Tacca, Ricardo Vidal, Cesar Gonzalez, Edith C Goldberg and Fernando Bonetto.**

Instituto de Física del Litoral (CONICET-UNL), Santa Fe, Argentina.

### **Abstract**

The low energy ion scattering (LEIS) technique was used to experimentally determine the formation of positive and negative ions in the scattering of protons by a Cu(111) surface for a large scattering angle in the backscattering configuration and a wide range of incoming energies (2 to 8keV). Two different collisional geometries were analyzed for a 135° fixed scattering angle: 45°/90° and 67.5°/67.5° incoming/exit angles measured with respect to the target surface. The total fraction of backscattered ions ranges from 10% to 25% and a peculiarly high yield of negative ions, which always exceeds that of positive ions, was detected for the whole energy range analyzed. A strong dependence of the measured ion fractions with the geometrical conditions was experimentally found. On the theoretical side, a first principles quantum-mechanical formalism that takes into account the three possible final charge states of the H<sup>+</sup> in a correlated way and the fine details of the band structure of Cu(111) surface, was applied to describe the charge transfer processes involved in the experimental situation. The theoretical calculation leads to a non-monotonous dependence with the incoming energy that properly describes the experimental results, especially the negative ion fraction in the specular collisional geometry. The oscillatory behavior predicted by the theory in the range of low energies is a clear evidence of the charge exchange between localized states, that is the situation related with the presence of the surface state immersed in the L-gap present in Cu(111) surface. The positive ion fraction is discussed for the first time for this collisional system. The differences found between the measurements and the theory seem to indicate that the neutralization to excited states, and also the formation of excited negative hydrogen ions, are possible charge exchange channels in the dynamic process analyzed.

## **Linear segmented polyurethanes. II. A mathematical model for the prepolymerization stage**

**Polo, Mara Lis, Pesoa, Juan Ignacio, Nicolau, Verónica Viviana, Spontón, Marisa Elisabet, Estenoz, Diana Alejandra, Meira, Gregorio Raúl**

INTEC (UNL-CONICET)

[Journal of Applied Polymer Science, 2018, 136\(3\), 46946](#)

### **Abstract**

In the first part of this sequel, an experimental investigation on the synthesis of linear segmented polyurethanes was presented, that included estimation of the kinetic constants at 60°C for the prepolymerization and finishing stages. This work presents two comprehensive mathematical models that simulate the mentioned prepolymerizations, in reactions between two poly(tetramethylene oxide) PTMO macrodiols and an excess of methylene diphenyl diisocyanate. The models require to input the molar mass distribution (MMD) of the initial macrodiol. The single-phase (or homogeneous) model calculates a final MMD

of approximately 40,000 different molecular species, and somewhat underestimates the observed molar mass dispersities. The double-phases (or heterogeneous) model produces a better fit of the observed MMDs by simulating two independent polymerizations carried out in parallel. The double-phases model contains three adjustable parameters: the reaction imbalances into both phases, and an “effective” rate constant. In part III of this sequel, the presented models will be extended to simulate the finishing stages.

## **Steel fibers pull-out after exposure to high temperatures and its contribution to the residual mechanical behavior of high strength concrete**

**Gonzalo Ruano<sup>a</sup>, Facundo Isla<sup>a</sup>, Bibiana Luccioni<sup>a</sup>, Raúl Zerbino<sup>b</sup>, Graciela Giaccio<sup>c</sup>**

a CONICET, Structures Institute, National University of Tucumán, Av. Independencia 1800, S.M. de Tucumán, Argentina

b CONICET, LEMIT, Engineering Faculty, National University of La Plata, Argentina

c CIC, LEMIT, Engineering Faculty, National University of La Plata, Argentina

[Construction and Building Materials 163 \(2018\) 571-585](#)

### **Abstract**

Many concrete structures are exposed to high temperatures that produce material deterioration involving stiffness and strength loss. Although residual mechanical behavior of steel fiber reinforced concrete subjected to high temperatures has been studied in the last decades, the effect of the deterioration of each component of the composite behavior has not been assessed. This information together with a meso-mechanical model can be very useful for the design of steel fiber reinforced concrete to be used in structures that are expected to be exposed to high temperatures.

This paper analyzes the effect of temperature on steel fibers pull-out mechanism from a high strength concrete matrix and its contribution to the residual mechanical behavior of Steel Fiber Reinforced High Strength Concrete (SFRHSC). Pull-out tests of straight and hooked end fibers and uniaxial tension tests on the fiber filaments exposed to room and high temperature (300 °C, 375 °C and 475 °C) were performed. Additionally, two SFRHSC incorporating 30 kg/m<sup>3</sup> and 60 kg/m<sup>3</sup> of hooked end steel fibers and a plain High Strength Concrete (HSC) exposed to the same temperatures were studied. Uniaxial compression tests and bending tests on notched prisms were used to characterize the composite material. The experimental results were analyzed with the aid of a pull-out model and a meso-model for SFRHSC, both developed by the authors. It is shown that hooked end fibers pull-out strength was reduced after the exposure to high temperatures. Since concrete strength only contributes in a small region surrounding the hooks, the pull-out strength reduction can be mainly attributed to the reduction of steel strength and frictional effects due to high temperature exposition. HSC tension strength reduction begins earlier and it is proportionally greater than pull-out strength reduction. As a consequence, HSC bending strength decreases faster than SFRHSC strength.

## **Nanoparticles Reinforcement for the Improved Strength and High-Temperature Wear Resistance of Mn-Cr Steel**

**A. Kračun<sup>1</sup>, D. Jenko<sup>1</sup>, M. Godec<sup>1</sup>, S. V. Savirov<sup>2</sup>, G. Prieto<sup>3</sup>, W. Tuckart<sup>3</sup>, B. Podgornik<sup>1</sup>,**

1 Institute of Metals and Technology Ljubljana Slovenia

2 M.V. Lomonosov Moscow State University Moscow Russia

3 Universidad Nacional del Sur Bahía Blanca Argentina

[Metallurgical and Materials Transactions A. November 2018, Volume 49, Issue 11, pp 5683–5694 |](#)

### **Abstract**

Nanotechnologies offer tremendous potential when it comes to modifying the microstructure of steel through the incorporation of nanoparticles. While typical production methods for metal-matrix composites are difficult and expensive, conventional casting routes suffer from inhomogeneity and agglomeration of the added nanoparticles. The aim of this study was to investigate the feasibility and possibilities of introducing nanosized particles into a steel matrix through a conventional casting process and to determine the effect of different nanoparticles and methods of incorporation on the strength, toughness, and high-temperature wear resistance of martensitic steel. The results show that also in the case of a conventional casting process, it is possible to obtain a homogeneous distribution of nanoparticles in the metal matrix, resulting in improved strength, maintained toughness, and up to five times better high-temperature wear resistance of the Mn-Cr steel. However, the rate of improvement greatly depends on the method and type of nanoparticles incorporation. The most promising results were observed for the combination of carbon nanotubes, oxide nanoparticles, and dispersant, sealed in a steel tube, with the dispersant providing the uniform distribution, the carbon nanotubes delivering the good toughness and the adhesive wear properties, and the oxide nanoparticles ensuring oxidation and abrasive wear resistance.

## **Microparticles based on ionic and organosolv lignins for the controlled release of atrazine**

**María Eugenia Taverna<sup>ab</sup>, Carlos Alberto Busatto<sup>a</sup>, Maia Raquel Lescano<sup>a</sup>, Verónica Viviana Nicolau<sup>b</sup>, Cristina Susana Zalazar<sup>a</sup>, Gregorio Raúl Meira<sup>a</sup>, Diana Alejandra Estenoz<sup>a</sup>**

<sup>a</sup>INTEC (UNL-CONICET), Güemes 3450, (3000) Santa Fe, Argentina

<sup>b</sup>UTN Regional San Francisco, Av. de la Universidad 501, (2400) San Francisco, Córdoba, Argentina

### **Abstract**

Lignins are natural polymers of the lignocellulosic biomass. Nowadays, there is a growing interest in developing value-added products based on lignins due to their renewability, low cost and abundance. In this work, lignin microspheres from organosolv and ionic isolation processes were prepared for the controlled release of atrazine. Microspheres were prepared by the solvent extraction/evaporation technique. The controlled release of atrazine from organosolv and ionic lignins microparticles was studied in water. Mobility experiments were performed in an agricultural soil from Argentina. The results showed that microparticles prepared using dichloromethane as the dispersed phase were spherical, while lignins dispersed in ethyl acetate produce irregular microparticles. Organosolv lignin microparticles presented higher encapsulation efficiency for all herbicide loads. About 98% and 95% of atrazine was released in 24 and 48 h approximately from organosolv and ionic lignin microparticles, respectively. The release profiles of atrazine from both lignin microparticles were not affected by the herbicide load. Atrazine mobility experiments in soil showed that about 80% of free atrazine was leached in 37 days, while 65.0% and 59.7% of the herbicide was leached from ionic and organosolv lignin microparticles, respectively. Thus, atrazine-loaded microparticles could reduce leaching compared to a commercial formulation of free atrazine.

### **Effects of heat treatment on surface properties of different coatings with alkali treatment on titanium for dental implants.**

**Tatiana Ekkert<sup>1</sup>, Adriana Lemos<sup>1</sup>, Kyung Won Kang<sup>1</sup>, Florencia Gatti<sup>1</sup>, Carlos Llorente<sup>1,2</sup>, Pablo Bilmes<sup>1</sup>**

1 Laboratorio de Investigaciones de Metalurgia Física (LIMF), Facultad de Ingeniería, Universidad Nacional de La Plata, La Plata CP: 1900, Argentina.

2 Comisión de Investigaciones Científicas de la Provincia de Buenos Aires – CICPBA.

[Matéria, 2018, Vol. 23, N 2.](#)

### **Abstract**

Titanium is widely used as dental implant since it is bio-inert and osseointegratable. However, provided that this material cannot induce bone growth from its surface, it is usual to carry out different surface treatments in order to develop bioactive coatings that increase both the initial rate of bone development and the biological anchorage of implant attachment to the host bone. The aim of the alkaline treatment is to form an amorphous gel of sodium titanate, which can be stabilized by means of a subsequent thermal treatment. During this, the hydro gel is dehydrated and thickened to form a layer of stable and partially crystallized sodium titanate. In the present work it was analyzed the effects produced by different thermal treatments after the alkaline one, on surfaces of cp titanium with surface treatment of blasting and MAO (micro-arc oxidation process). For each case the surface was characterized in order to enhance the application condition. The



temperatura of the thermal treatments was 400, 600 and 800 °C, since titanate varies its ratio of amorphous and crystalline phase in this range and therefore its properties. The assessment of results was carried out by means of Rockwell-C adhesion standard test, measurement of the initial contact angle by goniometry, X-ray diffraction and analytic scanning electronic microscopy.

Characterized post thermal treatment samples, it was observed that the samples treated to 800 °C presented a crystalline superficial structure, bad adherence and did not develop apatite growth on its surface. Nevertheless, they presented sufficiently surface hydrophilic. On the contrary, the samples treated at 400 and 600 °C presented superficially a partially crystallized phase, with good adhesion and good hydrophilicity. Through SEM-EDS, the formation of a homogeneous apatite layer was observed on their surfaces.

## **Tratamiento Superficial de Ti6Al4V ELI mediante anodizado por plasma químico en electrolito de fosfato de sodio y acetato de calcio**

**E. F. Cardozo, K. W. Kang, A. L. Lemos, C. L. Llorente, P. D. Bilmes**

Laboratorio de Investigaciones de Metalurgia Física (LIMF), Comisión de Investigaciones Científicas de la Provincia de Buenos Aires (CICPBA), Facultad de Ingeniería, UNLP, La Plata, Argentina

[Acta Microscopica Vol. 27, No. 3, 2018, pp.175-181.](#)

### **Abstract**

Con el propósito de aumentar la velocidad inicial de desarrollo óseo, como así también, el anclaje biológico de fijación del implante al hueso, se realizan distintos tratamientos superficiales en el titanio (ampliamente utilizado como material para implantes dentales) entre los cuales se encuentran el anodizado por plasma químico (APQ) y el tratamiento alcalino. El tratamiento APQ produce un recubrimiento de tipo cerámico que posee una elevada microdureza, adhesión al metal base y resistencia al desgaste. El tratamiento alcalino es un proceso termoquímico que induce la formación de un hidrogel de titanato de sodio amorfo que generalmente favorece el crecimiento de apatita sobre la superficie del implante. Con el objetivo de determinar los parámetros de proceso del APQ en Ti6Al4V ELI, se efectuaron varios tratamientos en muestras mecanizadas bajo diferentes condiciones de densidad de corriente y tiempo de exposición en un electrolito de fosfato de sodio y acetato de calcio. A continuación, se efectuó un tratamiento alcalino para evaluar su influencia sobre la bioactividad del recubrimiento. Para caracterizar las superficies se realizaron análisis de rugosidad, ensayos de adhesión, medición del espesor del recubrimiento, evaluación de la bioactividad mediante el ensayo de simulación en fluidos corporales (SBF) y evaluación de la mojabilidad de la superficie a través del ensayo de ángulo de contacto. Los mejores resultados, en cuanto a rugosidad, espesor y adhesión del recubrimiento, bioactividad y mojabilidad, se obtuvieron en las muestras sin tratamiento alcalino en la condición de mayor densidad de corriente y tiempo utilizados en el tratamiento de APQ.

## Relevance of protein-protein interactions on the biological identity of nanoparticles

Cecilia Vasti<sup>a,b</sup>, Laura V. Bonnet<sup>c,d</sup>, Mauricio R. Galiano<sup>c,d</sup>, Ricardo Rojas<sup>a,b</sup>, Carla E. Giacomelli<sup>a,b</sup>

<sup>a</sup>INFIQC-CONICET, Ciudad Universitaria, X5000HUA Córdoba, Argentina

<sup>b</sup>Departamento de Fisicoquímica, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, Ciudad Universitaria, X5000HUA Córdoba, Argentina

<sup>c</sup>CIQUIBIC-CONICET, Ciudad Universitaria, X5000HUA Córdoba, Argentina

<sup>d</sup>Departamento de Química Biológica “Ranwell Caputto”, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, Ciudad Universitaria, X5000HUA Córdoba, Argentina

[Colloids and Surfaces B 166 \(2018\) 330-338](#)

### Abstract

Considering that the use of nanoparticles (NPs) as carriers of therapeutic or theranostic agents has increased in the last years, it is mandatory to understand the interaction between NPs and living systems. In contact with biological fluids, the NPs (synthetic identity) are covered with biomolecules that form a protein corona, which defines the biological identity. It is well known that the protein corona formation is mediated by non-specific physical interactions, but protein-protein interactions (PPI), involving specific recognition sites of the polypeptides, are also involved. This work explores the relationship between the synthetic and biological identities of layered double hydroxides nanoparticles (LDH-NPs) and the effect of the protein corona on the cellular response. With such a purpose, the synthetic identity was modified by coating LDH-NPs with either a single protein or a complex mixture of them, followed by the characterization of the protein corona formed in a commonly used cell culture medium. A proteomic approach was used to identify the protein corona molecules and the PPI network was constructed with a novel bioinformatic tool. The coating on LDH-NPs defines the biological identity in such a way that the composition of the protein corona as well as PPI are changed. Electrostatic interactions appear not to be the only driving force regulating the interactions between NPs, proteins and cells since the specific recognition also play a fundamental role. However, the biological identity of LDH-NPs does not affect the interactions with cells that shows negligible cytotoxicity and high internalization levels.

## UV sensor based on polyurethane foam

María Fernanda Stragliotto<sup>a,b</sup>, Giuliana Mosconi<sup>a,b</sup>, Miriam C. Strumia<sup>a,b</sup>, Marcelo R. Romero<sup>a,b</sup>, Cesar G. Gomez<sup>a,b</sup>

<sup>a</sup>Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Departamento de Química Orgánica, Córdoba, Argentina

<sup>b</sup>Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Instituto de Investigación y Desarrollo en Ingeniería de Procesos y Química Aplicada (IPQA), Córdoba, Argentina

[Sensors & Actuators: B. Chemical 277 \(2018\) 78–85](#)

### **Abstract**

Ultraviolet light (UV) present in solar radiation has an important effect on the health of human skin. For that reason, we developed a disposable and easy-to-manufacture UV light sensor based on surface color change of a polyurethane (PU) film and examined its performance against radiation received from a lamp or from the sun. The chemical modification after UV exposition and the consequent color variation from light yellow to brown in PU sensor were studied by using RGB image analysis and a reflectance prototype containing an Arduino board. It was found that the photochemical modification of PU films increases absorption of visible radiation in the blue spectrum range. Furthermore, PU surface was more sensitive to UV (<390) than that found in visible light when exposed to sunlight, which was associated with the presence of a chromophore in the material modified. In addition, it was found that the extract obtained from irradiated PU showed its maximum absorption at 309 nm. Hence, the use of this economical light radiation sensor seems to be a very promising tool to determine exposure to UV light from the solar spectrum.

## **Root Cause Analysis of Cracking in Shaft End and Coupling of a High-Power Generator.**

**Pablo Bilmes, Carlos Llorente, Juan Manuel Echarri, Tomás Echarri, Angel Martínez, José Zuzulich.**

Pablo Bilmes<sup>1</sup>, Carlos Llorente<sup>1,2</sup>, Juan Manuel Echarri<sup>1</sup>, Tomás Echarri<sup>3</sup>, Angel Martínez<sup>1</sup>, José Zuzulich<sup>1</sup>

1 Laboratorio de Investigaciones de Metalurgia Física (LIMF)Facultad de Ingeniería UNLPLa PlataArgentina

2 CICPBA-Comisión de Investigaciones Científicas de la Prov. Bs. AsLa PlataArgentina

3 UIDET Ingeniería Aplicada en Mecánica y Electromecánica (IAME)La PlataArgentina

[J. Fail. Anal. and Preven. \(2018\) 18: 727.](#)

### **Abstract**

Failure analyses and root cause determination were carried out on the rotor of a high-power generator of gas–diesel dual fuel which presented cracking due to torsional fatigue in its end (region of section change and coupling), after 30,000 h of service. The generator of 307 MW–3000 rpm has a rotor (shaft of 400 mm Ø) manufactured in a proprietary steel grade equivalent to ASTM A470 type, Class 7 of high hardenability. It was reported that the equipment control system showed, in service, a high level of vibrations, not admissible for

continuing the operation. First, and during the equipment shutdown for inspection, the presence of cracks, slant to the rotor shaft, was detected by means of visual inspection and dye penetrant test. The failure region corresponds to the zone of coupling–shaft joint, linked by means of fixation by interference, whereas the cracking spread on two fracture planes at 45° with respect to the rotor shaft. On this zone, where cracking started, a severe fretting corrosion damage was evidenced. The characterization and identification of present damage mechanisms were conducted through macrographic, fractographic, SEM, EDS, chemical analyses, and mechanical tests. It was recognized that from the damage by fretting corrosion, fatigue micro-cracks were produced that spread due to service tensions by a mechanism of fretting fatigue. The fatigue fracture propagation was developed into two orthogonal planes at 45° from the longitudinal shaft, which reveals an inversion in the loading condition, only justifiable by torsional vibrations that were assigned to a torsional resonance typical of the system dynamics. It was considered that the torsional vibrations cause micro-movements between components, promoting fretting corrosion and the subsequent fretting fatigue that finally induced the failure by high-cycle torsional fatigue with low-stress amplitude.

### **Severe Plastic Deformation by Equal Channel Angular Pressing and Rolling: The Influence of the Deformation Path on Strain Distribution.**

**Andrea M. Kliauga, Vitor L. Sordi, Natalia S. De Vincentis, Raúl E. Bolmaro, Norbert Schell, and Heinz-Günter Brokmeier.**

Prof. Dr. A.M. Kliauga Materials Engineering Department, São Carlos Federal University, Rodovia Washington Luiz km235, 13565-905 São Carlos, Brazil

Prof. Dr. V. L. Sordi Materials Engineering Department, São Carlos Federal University, São Carlos, Brazil

Dr. N. S. De Vincentis,

Prof. Dr. R.E. Bolmaro Instituto de Física Rosario FCEIA-UNR-CONICET, Rosario, Argentina

Dr. N. Schell, Prof. Dr. H.-G. Brokmeier Institut für Werkstoffkunde und Werkstofftechnik, TU Clausthal, Clausthal, Germany

Dr. N. Schell, Prof. Dr. H.-G. Brokmeier Helmholtz-Zentrum Geesthacht, GEMSO Outstation, Hamburg, Germany

[Advanced Engineering Materials. 2018.](#)

#### **Abstract**

The present work compares two deformation techniques, rolling and Equal Channel Angular pressing (ECAP), and the response offered by three different materials that differ in Stacking Fault Energy (SFE): AA1010 Al, commercially pure Cu, and an austenitic stainless steel. The objective of this investigation is to study the effect of each deformation mode on tensile behavior, deformation mechanism, texture, and microstructure and to establish the influence of the stacking fault energy on said effects. The results show that the different strain paths of ECAP and rolling do not affect the strength, but rolling leads to an

accentuated texture and thus to elastic and plastic anisotropy. This finding has practical relevance for micro manufacturing techniques. Furthermore, it is observed that lower SFE results in smaller domain size and higher dislocation density, which are microstructural details related to strength and to the work hardening capacity. Finally, both techniques are able to produce a high amount of high angle grain boundaries, a feature that characterizes refined microstructures. These processes operate at different strain rates; thus, in low SFE materials, a more effective grain fragmentation by deformation-induced twins is observed after the ECAP process.

## **Characterization of systems with amino-acids and oligosaccharides as modifiers of biopharmaceutical properties of furosemide**

**Julieta Abraham Miranda<sup>a</sup>, Claudia Garnero<sup>a</sup>, Ariana Zoppi<sup>a</sup>, Vanesa Sterren<sup>a</sup>, Alejandro P. Ayala<sup>b</sup>, Marcela R. Longhi<sup>a</sup>**

<sup>a</sup>Unidad de Investigación y Desarrollo en Tecnología Farmacéutica (UNITEFA), CONICET and Departamento de Ciencias Farmacéuticas, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, Ciudad Universitaria, 5000 Córdoba, Argentina

<sup>b</sup>Department of Physics, Federal University of Ceará, Fortaleza, Ceará, Brazil

[Journal of Pharmaceutical and Biomedical Analysis \(2018\) Volume 149, Pages 143-150](#)

### **Abstract**

Furosemide is the most commonly prescribed diuretic drug in spite of its suboptimal biopharmaceutical properties. In this work, the addition of different amino-acids was studied with the aim of selecting an enhancer of the furosemide solubility. The best results were obtained with arginine. Also, binary (furosemide:arginine) and ternary (furosemide:arginine:β-cyclodextrin and furosemide:arginine:maltodextrin) systems were prepared by the kneading method and they were compared with their corresponding physical mixtures. These new systems were characterized by Fourier transform infrared and Raman spectroscopy, X-ray powder diffractometry, scanning electron microscopy, thermogravimetric analysis, and differential scanning calorimetry. In addition, dissolution studies were performed in simulated gastric fluid. The best results in relation to improving biopharmaceutical properties were obtained with a binary combination of furosemide and arginine, demonstrating that this system could result in a suitable candidate for the development of a promising pharmaceutical formulation of the drug.

## **Cyclodextrin modified niosomes to encapsulate hydrophilic compounds**

**Noelia D. Machado, O. Fernando Silva, Rita H. de Rossi, Mariana A. Fernández**

INFIQC - Dpto. Química Orgánica, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba

**Abstract**

Niosomes were prepared from equimolar mixtures of two non-ionic surfactants, Span 80 and Tween 80. The capability of the vesicular systems was studied through the encapsulation of two azo dyes as molecular probes of different hydrophobicity (methyl orange (MO) and methyl yellow (MY)). To improve the efficiency of the niosomes to encapsulate the dyes, we employed an additional modification of the vesicular system, adding  $\beta$ -cyclodextrin ( $\beta$ -CD) or a modified amphiphilic  $\beta$ -CD (Mod- $\beta$ -CD) to the niosomes. Neither the inclusion of dyes nor the incorporation of  $\beta$ -CD to the niosomes produces considerable modifications in size and morphology of the vesicles. However, in the presence of Mod- $\beta$ -CD the niosomes became smaller, probably due to the anchoring of the cyclodextrin at the surface of vesicles through the hydrophobic chain, altering the curvature of the outer monolayer and reducing the surface charge of the interphase. The entrapment efficiency (EE) for MY was higher than that for MO in niosomes without cyclodextrin, however, the content of MO in the presence of  $\beta$ -CD increased considerably. Besides, the release of this dye under the same conditions was faster and reached 70% in 24 hours whereas in the absence of the macrocycle, the release was 15%, in the same time. UV-visible spectrophotometry and induced circular dichroism analysis allowed it to be established that MO is complexed with cyclodextrins inside vesicles, whereas MY interacts mainly with the niosome bilayer instead of with CD. Besides, the cavity of cyclodextrins is probably located in the interphase and preferably in the polar region of niosomes.

**Año 2017**

## **Enhancement of mechanical and optical performance of commercial polystyrenes by blending with siloxane-based copolymers**

**Ninago M., Hanzumi V., Passaretti Ma. G., Vega D., Ciolino A. Villar M.**

Departamento de Ingeniería Química, PlantaPiloto de Ingeniería Química, PLAPIQUI (UNS-CONICET), Universidad Nacional del Sur (UNS), Camino “La Carrindanga” Km 7, Bahía Blanca, 8000 Argentina

[Journal of Applied Polymer Science, 134, 1-9 \(2017\).](#)

### **Abstract**

Well-defined poly(styrene/*block*/dimethylsiloxane) copolymers (PS-*b*-PDMS) with low polydispersity index ( $M_w/M_n$ ) and different compositions were synthesized by sequential anionic polymerization of styrene (S) and hexamethyl(ciclotrisiloxane) (D<sub>3</sub>) monomers. Synthesized PS-*b*-PDMS copolymers were characterized by <sup>1</sup>H-nuclear magnetic resonance, size exclusion chromatography, Fourier transform infrared spectroscopy, and transmission electron microscopy. The physicochemical characterization determined that block copolymers have molar mass values close to  $\sim 135,000 \text{ g mol}^{-1}$ , narrow  $M_w/M_n < 1.3$ , and chemical composition ranging from low to intermediate PDMS content. Blends of these copolymers with a commercial polystyrene (PS) were obtained by melt mixing and subsequently injection. Films obtained were flexible, and showed lower transparency than the original PS matrix. On the other hand, a 10 wt % incorporation of PS-*b*-PDMS copolymers leads to better mechanical performance by enhancing elongation at break ( $\sim 8.8$  times higher) and opacity values ( $\sim 18$  times higher). In addition, UV-Vis barrier capacity of the resulting blends is also increased (up to 400% higher). © 2017 Wiley Periodicals, Inc.

## **Hybrid nanomaterials based on gum Arabic and magnetite for hyperthermia treatments**

**M. Fernanda Horst<sup>a</sup>, Diego F. Coral<sup>b</sup>, Marcela B. Fernández van Raap<sup>b</sup>, Mariana Alvarez<sup>a</sup>, Verónica Lassalle<sup>a</sup>**

<sup>a</sup>INQUISUR-CONICET, Dto. Química, Universidad Nacional del Sur, Bahía Blanca, Buenos Aires, Argentina

<sup>b</sup>Instituto de Física La Plata IFLP-CONICET, Departamento de Física, Universidad Nacional de La Plata, La Plata, Buenos Aires, Argentina

[Materials Science & Engineering C, 74, 1, 443-450 \(2017\).](#)

### **Abstract**

In this study, one-step co-precipitation method was conveniently adapted to obtain novel nanomaterials based on Gum Arabic and magnetite. Two synthesis procedures were evaluated: one employing the solid biopolymer in the co-precipitation media; a second using an aqueous solution of the polysaccharide. An exhaustive characterization of both formulations was performed using several specific techniques. The obtained data confirmed the successful incorporation of the gum Arabic on the magnetic core. Values of hydrodynamic diameters, measured by dynamic light scattering, in aqueous dispersions were about 70–80 nm, while sizes lower than 20 nm were registered by TEM microscopy. Surface charge of gum Arabic coated magnetic nanoparticles was significantly different from the corresponding to raw materials (magnetite and GA). This fact confirmed the formation of hybrid nanosystems with novel and specific properties.

The potential utility of these materials was tested regarding to magnetic hyperthermia therapy under radiofrequency fields. Magnetocalorimetric measurements were performed in a wide range of field amplitude and frequency. Specific absorption rate of 218 W/gFe was determined at field frequency of 260 kHz and amplitude of 52 kA/m. These results demonstrate their viability to be applied in tumor ablation treatments. Using the linear response theory and restricting field parameters to the accepted biomedical window, maximum useful value of 74 w/gFe is predicted at 417 kHz and 12 kA/m.

### **Magnetic nanoparticles for drug targeting: from design to insights into their systematic toxicity. Preclinical evaluation of hematological, vascular and neurobehavioral toxicology**

**Mariela A. Agotegaray,<sup>a</sup> Adrián E. Campelo,<sup>b</sup> Roberto D. Zysler,<sup>c</sup> Fernanda Gumilar,<sup>b</sup> Cristina Bras,<sup>b</sup> Ariel Gandini,<sup>d</sup> Alejandra Minetti,<sup>b</sup> Virginia L. Massheimer<sup>b</sup> and Verónica L. Lassalle<sup>a</sup>**

<sup>a</sup> INQUISUR, Departamento de Química, Universidad Nacional del Sur (UNS)-CONICET, Bahía Blanca, Argentina

<sup>b</sup> Instituto de Investigaciones Biológicas y Biomédicas del Sur (INBIOSUR-CONICET)-UNS Dpto. de Biología, Bioquímica y Farmacia, Universidad Nacional del Sur, Bahía Blanca, Argentina

<sup>c</sup> CONICET – Centro Atómico Bariloche, Instituto Balseiro, S.C. de Bariloche, Argentina

<sup>d</sup> Instituto de Investigaciones Bioquímicas de Bahía Blanca (INIBIBB-CONICET)-UNS Dpto. de Biología, Bioquímica y Farmacia, Universidad Nacional del Sur, Bahía Blanca, Argentina

[Biomaterials Science, 5, 772-783 \(2017\).](#)



## **Abstract**

A simple two-step drug encapsulation method was developed to obtain biocompatible magnetic nanocarriers for the potential targeted treatment of diverse diseases. The nanodevice consists of a magnetite core coated with chitosan (Chit@MNPs) as a platform for diclofenac (Dic) loading as a model drug (Dic-Chit@MNPs). Mechanistic and experimental conditions related to drug incorporation and quantification are further addressed. This multi-disciplinary study aims to elucidate the toxicological impact of the MNPs at hematological, vascular, neurological and behavioral levels. Blood compatibility assays revealed that MNPs did not affect either erythro sedimentation rates or erythrocyte integrity at the evaluated doses (1, 10 and 100  $\mu\text{g mL}^{-1}$ ). A microscopic evaluation of blood smears indicated that MNPs did not induce morphological changes in blood cells. Platelet aggregation was not affected by MNPs either and just a slight diminution was observed with Dic-Chit@MNPs, an effect possibly due to diclofenac. The examined formulations did not exert cytotoxicity on rat aortic endothelial cells and no changes in cell viability or their capacity to synthesize NO were observed. Behavioral and functional nervous system parameters in a functional observational battery were assessed after a subacute treatment of mice with Chit@MNPs. The urine pools of the exposed group were decreased. Nephritis and an increased number of megakaryocytes in the spleen were observed in the histopathological studies. Sub-acute exposure to Chit@MNPs did not produce significant changes in the parameters used to evaluate neurobehavioral toxicity. The aspects focused on within this manuscript are relevant at the pre-clinical level providing new and novel knowledge concerning the biocompatibility of magnetic nanodevices for biomedical applications.

## **Increasing incident photon to current efficiency of perovskite solar cells through TiO<sub>2</sub> aerogel-based nanostructured layers**

**Geneviève K. Pinheiro<sup>1</sup>, Rafael B. Serpa<sup>2</sup>, Luciana V. de Souza<sup>1</sup>, Maria L. Sartorelli<sup>2</sup>, Françoise T. Reis<sup>2</sup>, Carlos R. Rambo<sup>1</sup>**

<sup>1</sup>Department of Electrical and Electronic Engineering

<sup>2</sup>Department of Physics, Federal University of Santa Catarina, 88040-900, Florianópolis, Brazil

[Colloids and Surfaces A-Physicochemical and Engineering Aspects, 527 \(2017\) pp. 89-94](#)

## **Abstract**

In this work we report the use of a nanoporous layer of TiO<sub>2</sub> aerogel as an electron-transport layer in CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>-based solar cells. Due to its high surface area, the modified TiO<sub>2</sub> aerogel increases the contact surface, enabling the deposition of a higher concentration of perovskite, and enhances the layer interpenetration process. In order to avoid short circuit by the presence of pinholes in the aerogel layer, a thin film of TiO<sub>2</sub> paste was also deposited. The TiO<sub>2</sub> aerogel layer promoted an incident photon to current efficiency (IPCE) twice as large when compared to the IPCE in solar cells without the

aerogel layer. This result shows that aerogel based inks are quite promising for use in high-performance perovskite solar cells (PSCs).

## **Biodiesel production using coal fly ash-derived sodalite as a heterogeneous catalyst**

**Márcia Cardoso Manique, Luciane Venturini Lacerda, Annelise Kopp Alves, Carlos PérezBergmann**

Laboratory of Ceramic Materials, UFRGS, Porto Alegre, Brazil

[Fuel Volume 190, 15 February 2017, Pages 268-273](#)

### **Abstract**

This study aimed to synthesized zeolites via a hydrothermal process in an alkaline medium using coal fly ashes as an alternative source of silicon. The zeolites were evaluated for their crystallinity, morphology, and surface area. The characterization of the sample revealed that the zeolite type sodalite was synthesized, and quartz and mullite were identified as by-products. The microstructure of the powders showed clusters with specific surface areas of approximately 10 m<sup>2</sup>/g. The synthesized sodalite was used as a catalyst for transesterification of soy oil to obtain a maximum conversion of 95.5 wt% at 65 °C with a 4 wt% catalyst concentration, a 12:1 methanol-to-oil molar ratio, and a reaction time of 2 h. The mechanistic pathway for sodalite catalyzed transesterification and the possible formation of active sites was proposed.

## **Bimetallic Cu-Pd Nanoparticles Supported on Bio-silica as Efficient Catalyst for Selective Benzylic Alcohols Aerobic Oxidation**

**Buxaderas E.<sup>a</sup>, Graziano Mayer M.<sup>a</sup>, Volpe M.A.<sup>b</sup>, Radivoy G.<sup>a</sup>**

<sup>a</sup> Instituto de Química del Sur (INQUISUR-CONICET), Departamento de Química, Universidad Nacional del Sur, Avda. Alem 1253, 8000 Bahía Blanca, Argentina

<sup>a</sup> Instituto de Química del Sur (INQUISUR-CONICET), Departamento de Química, Universidad Nacional del Sur, Avda. Alem 1253, 8000 Bahía Blanca, Argentina

<sup>b</sup> Planta Piloto de Ingeniería Química, PLAPIQUI (CONICET-UNS), Camino La Carrindanga Km 7, CC 717, 8000 Bahía Blanca, Argentina

<sup>a</sup> Instituto de Química del Sur (INQUISUR-CONICET), Departamento de Química, Universidad Nacional del Sur, Avda. Alem 1253, 8000 Bahía Blanca, Argentina

[Synthesis, 49, 1387-1393 \(2017\).](#)

### **Abstract**

A new bimetallic heterogeneous catalyst consisting of copper and palladium nanoparticles supported on bio-silica is presented. The use of TEMPO as co-catalyst allowed the aerobic

oxidation of primary benzylic alcohols into the corresponding aldehydes with excellent selectivity and good activity. The methodology could be applied to the oxidation of allylic and heterobenzylic alcohols. The catalyst is easy to prepare from commercial starting materials and can be recovered and reused without apparent loss of activity.

## **Synthesis of high-density polyethylene/rGO-CNT-Fe nanocomposites with outstanding magnetic and electrical properties**

**Muhammad Nisar**<sup>1</sup>, **Carlos Pérez Bergmann**<sup>2</sup>, **Julian Geshev**<sup>3</sup>, **Raúl Quijada**<sup>4</sup>, **Thuany Maraschin**<sup>5</sup>, **Nara R. de Souza Basso**<sup>5</sup>, **Eliana G. Barrera**<sup>1</sup>, **Griselda Barrera Galland**<sup>1</sup>

1 Instituto de Química, Universidade Federal do Rio Grande do Sul, Porto Alegre, 91501-970 Brazil

2 Laboratório de Materiais Cerâmicos, Departamento de Materiais, Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil

3 Instituto de Física, Universidade Federal do Rio Grande do Sul, Porto Alegre, 91501-970 Brazil

4 Departamento de Ingeniería Química y Biotecnología, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Santiago, Chile

5 Faculdade de Química, Pontifícia Universidade Católica do Rio Grande do Sul, Porto Alegre, 90619-900 Brazil

[Applied Polymers. Volume134, Issue40, 2017, 45382](#)

### **Abstract**

Semi-conducting polyethylene (PE) nanocomposites with outstanding magnetic properties at room temperature were synthesized. These exceptional properties, for a diamagnetic and insulating matrix as PE, were obtained by polymerizing ethylene in the presence of a catalytic system formed by a metallocene catalyst supported on a mixture of reduced graphene oxide (rGO) and carbon nanotubes with encapsulated iron (CNT-Fe). It was used a constant and very low amount of CNT-Fe, obtained by vapor chemical deposition using ferrocene. The percolation threshold, to achieve conductivity, was obtained using a variable amount of rGO. The nanocomposites were semiconductors with the addition of 2.8 wt % and 6.0 wt % of the filler, with electrical conductivities of  $4.99 \times 10^{-6} \text{ S cm}^{-1}$  and  $7.29 \times 10^{-4} \text{ S cm}^{-1}$ , respectively. Very high coercivity values of 890–980 Oe at room temperature were achieved by the presence of only 0.04–0.06 wt % of iron in the nanocomposites. The novelty of this work is the production of a thermoplastic with both, magnetic and electric properties at room temperature, by the use of two fillers, that is rGO and CNT-Fe. The use of a small amount of CNT-Fe to produce the magnetic properties and variable amount of rGO to introduce the electrical conductivity in PE matrix let to balance both properties. The encapsulation strategy used to obtain Fe in CNT, protect Fe from easy oxidation and aggregation.

## **Corrosion in Concrete Structures with Permanent Deformation in Marine Environment.**

**N.F. Ortega<sup>1,2</sup>, J.M. Moro<sup>1</sup>, R. Meneses<sup>1</sup>**

<sup>1</sup> Engineering Department, Universidad Nacional del Sur, Av. Alem 1253, 8000 - Bahía Blanca, Argentina

<sup>2</sup> Comisión de Investigaciones Científicas de la Prov. de Buenos Aires, Argentina

[The Open Construction and Building Technology Journal, 2017, 11, 14-24](#)

### **Abstract**

Concrete is usually highly alkaline (pH around 12), thus protecting reinforcement against corrosion. The occurrence of oxides is favored when the medium pH surrounding the bar is in values near to 9 or lower. Aggressive substances for reinforcements generally enter concrete through its pore structure, and cracks tend to decrease pH, stimulating corrosion process. There are several causes for cracks, including structure bending caused by loads. This research established the influence of concrete coating cracks, caused by permanent deflection, on the durability of reinforced concrete beams in contact with chloride-containing water (at a similar ratio as seawater), over a five-year period. It analyzes the influence of deflections suffered by the specimens on corrosion potentials and concrete coating cracking. It was established that, from the durability point of view and for structures exposed to marine environment, it would be advisable to set stricter admissible deflection and/or concrete cracking limits than those set by the analyzed standards.

## **Physic-mechanical behavior of concretes exposed to high temperatures and different cooling systems.**

**Ercolani G., Ortega N.F., Priano C., Señas L.;**

[Structural Concrete, 18, 3, 487-495 \(2017\).](#)

### **Abstract**

Over their lifetime, concrete structures can suffer from different pathologies, one of them is exposure to high temperatures, which diminishes their load-bearing capacity. This study describes how different concrete types were exposed to high temperatures. To simulate fire extinction, where the temperature of the overheated concrete descends suddenly, different cooling systems were applied: slowly cooling in the open air and fast cooling by spraying different water volumes. Several physical–mechanical characteristics were analyzed such as compressive strength, splitting tensile strength, porosity, capillary suction, and carbonation depth. Ultrasound nondestructive tests were conducted to quantify deterioration. A petrographic study using a stereomicroscope and microscopy of polarization was performed on thin sections to evaluate aggregate composition and concrete characteristics, focusing on interface areas. Physical and mechanical properties were affected by the increase in

temperature, with damage worsening through the appearance of cracks and microcracks when water is used as a cooling system.

## **Ensayos de Creep por Torsión y Tracción**

**Daniela Alessio<sup>1</sup>, Sandra Robles<sup>1</sup>, Lilian Moro<sup>2</sup>, René Molina<sup>2</sup>,**

<sup>1</sup> Universidad Nacional del Sur, Departamento de Ingeniería, Av. Alem 1253, Bahía Blanca - Argentina

<sup>2</sup> Universidad Tecnológica Nacional, Facultad Regional Bahía Blanca, Departamento de Mecánica, Montevideo 340, Bahía Blanca – Argentina

[Avances en Ciencias e Ingeniería, 8, 4, octubre-diciembre, 39-45 \(2017\).](#)

### **Abstract**

In this study the analysis of two test methodologies is carried out to evaluate the creep behavior of a material or creep by thermal activation. Two tests types, torsion and tensile, of an austenitic steel commonly used in petrochemical equipment in the region, under comparable temperature and stress conditions were carried out in the laboratory. With the acquired records, deformation-time curves of the material were plotted. The steady-state analysis of creep through the Norton power law is presented. It is observed that, although the torsion tests have a deformation rate greater than the tensile tests, the characteristic parameters of creep, the tension factor  $n$  and the thermal activation energy  $Q$  are not affected, being independent of the test type

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

**B.Luccioni<sup>a</sup>, F.Isla<sup>b</sup>, R.Codina<sup>c</sup>, D.Ambrosini<sup>d</sup>, R.Zerbino<sup>e</sup>, G.Giaccio<sup>f</sup>. M.C.Torrijos<sup>e</sup>**

<sup>a</sup> Researcher CONICET, Structures Institute, National University of Tucumán, Av. Independencia 1800, 4000 S.M. de Tucumán, Argentina

<sup>b</sup> Post Doctoral CONICET fellow. Structures Institute, National University of Tucumán, Argentina

<sup>c</sup> Post Doctoral CONICET fellow, Engineering Faculty, National University of Cuyo, Argentina

<sup>d</sup> Researcher CONICET, Engineering Faculty, National University of Cuyo, Argentina

<sup>e</sup> Researcher CONICET, LEMIT, Engineering Faculty, National University of La Plata, Argentina

<sup>f</sup> Researcher CIC, LEMIT, Engineering Faculty, National University of La Plata, Argentina

[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.

## Low temperature heat treatments on Ti-15Zr-xMo alloys

Caio CastanhoXavier<sup>a,b</sup>, Diego Rafael Nespeque Correa<sup>a,b</sup>, Carlos Roberto Grandini<sup>a,b</sup>, Luís Augusto Rocha<sup>a,b,c</sup>

<sup>a</sup> UNESP - Univ Estadual Paulista, Faculdade de Ciências de Bauru, Bauru, SP, Brazil

<sup>b</sup> IBTN/Br, Brazilian Branch of the Institute of Biomaterials, Tribocorrosion and Nanomedicine, Bauru, SP, Brazil

<sup>c</sup> MEMS-UMinho, Center MicroElectroMechanical Systems, Universidade do Minho, Campus de Azurém, Guimarães, Portugal

[Journal of Alloys and Compounds Volume 727, 15 December 2017, Pages 246-253](#)

### Abstract

This paper regards the study of the effect of heat treatments on the microstructure and microhardness of Ti-15Zr-xMo alloys aimed to biomedical applications. The alloys were melted in an arc-furnace, with four different compositions in order to obtain samples with  $\alpha'$ ,  $\alpha'+\beta$  and  $\beta$  phase microstructures. The as-cast alloys exhibited a full lamellar structure for the Ti-15Zr, a bimodal structure composed by  $\beta$  phase grains along with an  $\alpha$  phase acicular structure at the grain boundaries for the Ti-15Zr-5Mo, predominant  $\beta$  phase for the Ti-15Zr-10Mo and only  $\beta$  phase for the Ti-15Zr-15Mo. Results showed that both microstructure and mechanical properties of the studied alloys can be tailored by relatively low temperature heat treatments, as they resulted in the growth of the  $\alpha'$  phase in all alloys. The formation of  $\alpha'$  phase resulted in a decrease in the microhardness of the alloys.

## Microstructure of as-cast single and twin roller melt-spun Ni<sub>2</sub>MnGa ribbons

G. Pozo-López, A.M. Condó, L.M. Fabietti, E. Winkler, N. Haberkorn, S.E. Urreta

Facultad de Matemática, Astronomía y Física, Universidad Nacional de Córdoba, Ciudad Universitaria, 5000 Córdoba, Argentina, Instituto de Física Enrique Gaviola, CONICET,

Argentina; Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina; Centro Atómico Bariloche, Comisión Nacional de Energía Atómica, Av. Bustillo 9500, 8400 San Carlos de Bariloche, Argentina; Instituto Balseiro, Universidad Nacional de Cuyo, Av. Bustillo 9500, 8400 San Carlos de Bariloche, Argentina

[Materials Characterization, 124 \(2017\) 171-181.](#)

**Abstract:**

Stoichiometric Ni<sub>2</sub>MnGa 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 exhibit 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<sub>2</sub>-assisted impregnation of LDPE/sepiolite nanocomposite films with insecticidal terpene ketones: impregnation yield, crystallinity and mechanical properties assessment**

**M. L. Goñi, N.A. Gañán, S.E. Barbosa, M.C. Strumia, R.E. Martini**

Instituto de Investigación y Desarrollo en Ingeniería de Procesos y Química Aplicada (IPQA, UNC, CONICET). Córdoba, Argentina.

[Journal of Supercritical Fluids. En prensa \(2017\)](#)

**Abstract:**

In this contribution, supercritical CO<sub>2</sub>-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.

## **Strain Path Dependence of Anisotropic Microstructure Evolution on Low Stacking Fault Energy F138 Steel.**

**N.S.De Vincentis<sup>a</sup>M.C.Avalos<sup>a</sup>A.Kliauga<sup>b</sup>H-G.Brokmeier<sup>cd</sup>R.E.Bolmaro<sup>a</sup>**

a Instituto de Física Rosario, FCEIA-UNR-CONICET, Bv. 27 de Febrero 210 bis, S2000EZP Rosario, Argentina

b Departamento de Engenharia de Materiais - Universidade Federal de São Carlos, Rodovia Washington Luís, km 235 - SP-310, São Carlos, SP 13565-905, Brazil

c Institut für Werkstoffkunde und Werkstofftechnik, TU Clausthal, Agricolastr. 6, 38678, Germany

d Helmholtz-Zentrum Geesthacht, GEMS Outstation, Notkestr. 85, 22607 Hamburg, Germany

[Materials Science and Engineering A 698, 1-11.](#)

### **Abstract**

Severe Plastic Deformation (SPD) techniques are widely used nowadays because of the mechanical properties improvements caused by grain refinement and development of dislocation arrays. Diffraction techniques can be used to assess the changes registered in the microstructure through these methods. Two sets of samples of F138 austenitic stainless steel were analyzed in this paper: one set was deformed by ECAE up to two pressings at room temperature, and the other set was cold rolled to 70% reduction and annealed at 600, 700, 800 and 900 °C for 1 hour. The microstructural changes were determined using X-Ray diffraction and EBSD, combining both, global and local information and characterizing domain sizes, dislocation and stacking fault densities and misorientation degree and distribution caused by the different thermomechanical processing. It was observed that, despite cold rolling and 2 ECAE passes rendered rather similar von Mises deformations, the microstructure through each deformation method was different: 2 ECAE passes seem to be more effective for grain refinement and generation of equiaxed domains than cold rolling. The more significant twin activation observed in the former sample, because of continuous



strain path change, may explain the difference, although dislocation densities and mechanical properties did not differ substantially for both deformation methods.

## **Experimental and Theoretical Study of Ionic Pair Dissociation in Lithium-Ion-Linear Polyethyleneimine-Polyacrylonitrile Blend for Solid Polymer Electrolytes.**

**Fernando Pignanelli; Mariano Romero; Ricardo Faccio; Álvaro W. Mombrú<sup>[1]</sup>**

Centro NanoMat/CryssMat/Física, DETEMA, Facultad de Química, Universidad de la República, C.P. 11800 Montevideo, Uruguay

[Journal of Physical Chemistry B, v.: 121 27, p.: 6759 - 6765, 2017](#)

### **Abstract**

Herein, we report the preparation and characterization of a novel polymeric blend between linear polyethylene imine (PEI) and polyacrylonitrile (PAN), with the purpose of facilitating the dissociation of lithium perchlorate salt (LiClO<sub>4</sub>) and thus to enhance Li ion transport. It is a joint theoretical and experimental procedure for evaluating and thus demonstrating the lithium salt dissociation. The procedure implies the correlation between the theoretical pair distribution function (PDF) and conventional X-ray diffraction (XRD) by means of a molecular dynamics (MD) approach. Additionally, we correlated the experimental and theoretical Raman and infrared spectroscopy for vibrational characterization of the lithium salt after dissociation in the polymeric blend. We also performed confocal Raman microscopy analysis to evidence the homogeneity on the distribution of all components and the LiClO<sub>4</sub> dissociation in the polymer blend. The electrochemical impedance analysis confirmed that the Li-PAN-PEI blend presents a slightly better lithium conductivity of  $\sim 8 \times 10^{-7} \text{ S cm}^{-1}$ . These results suggest that this polymer blend material is promising for the development of novel fluorine-free solid polymer lithium ion electrolytes, and the methodology is suitable for characterizing similar polymeric systems.

## **Analysis of the transient wave propagation in soft-solid elastic plates**

**Benech N<sup>1</sup>, Brum J<sup>1</sup>, Grinspan G<sup>1</sup>, Aguiar S<sup>2</sup>, Negreira CA<sup>1</sup>.**

1 Laboratorio de Acústica Ultrasonora, Instituto de Física, Facultad de Ciencias, Igua 4225, 11400, Montevideo, Uruguay.

2 Instituto de Ensayo de Materiales, Facultad de Ingeniería, J. Herrera y Reisig 565, 11300, Montevideo, Uruguay.

[J. Acoust. Soc. Am., 142, 2919-2932, 2017](#)

## Abstract

In dynamic elastography, the goal is to estimate the Young's modulus from audio-frequency wave propagation in soft-tissues. Within this frequency range, the shear wavelength is centimeter-sized while the compressional wavelength is meter-sized. Thus, the experimental data are usually collected in the near-field of the source. Near-field effects have been widely studied for bulk wave propagation. However, the near- and transient-fields of surface and guided waves have received less attention. In this work, the transient surface displacement field in soft-solid elastic plates in vacuum is analyzed. Due to the high Poisson's ratio, mode conversion has special characteristics in soft-solids. They are analyzed through this work where it is shown that the transient-field over the surface can be interpreted by tracing a few reflections. The authors show the existence of a critical distance needed for the formation of Rayleigh-Lamb modes. Below this distance, only direct surface waves propagate without contribution from reflected waves. Thus, the dispersion curve differs from that predicted by Rayleigh-Lamb modes. Instead, the authors propose a model based on the interference of surface waves, which agree with the experimental data. In addition, the conditions needed in order to retrieve the shear wave phase velocity from the surface field are given.

## Characterization of titanate nanotubes for energy applications.

**Luciana Fernández-Werner, Fernando Pignanelli, Benjamín Montenegro, Mariano Romero, Helena Pardo Ricardo Faccio , Álvaro W. Mombrú**

Centro NanoMat/CryssMat-Lab, DETEMA, Facultad de Química, Universidad de la República, Uruguay

[Journal of Energy Storage, v.: 12, p.: 66 - 77, 2017](#)

## Abstract

In this work we present the synthesis and full structural characterization of hydrothermally synthesized titanate nanotubes (TNTs) for energy applications. It is of interest to characterize the building block of certain nanomaterials and their surface termination. This task is particularly difficult for nanotubes, where the exhibited surface curvature is a limitation for its study. We present the synthesis and thorough structural characterization through several experimental techniques for morphology and compositional characterization. Simulated X-rays powder diffraction patterns (XRPD) of real size nanotubes models are refined with experimental data. The building blocks for the TNT models were obtained from computational simulations by means of Density Functional Theory for  $\text{H}_2\text{Ti}_2\text{O}_5 \cdot 0.5\text{H}_2\text{O}$ ,  $\text{H}_2\text{Ti}_2\text{O}_5 \cdot \text{H}_2\text{O}$ ,  $\text{H}_2\text{Ti}_3\text{O}_7$  and  $\text{H}_2\text{Ti}_3\text{O}_7 \cdot 0.67\text{H}_2\text{O}$ . Our procedure confirms that open-ended TNTs are obtained, with  $\sim 100$  nm of length and  $6(1)$  nm of inner diameter. By interpreting the XRPD data, the TNT building block was obtained and found to derive from  $\text{H}_2\text{Ti}_3\text{O}_7$ , where the distance between  $[\text{TiO}_6]$  octahedral layers is increased in

accordance with  $\text{H}_2\text{Ti}_3\text{O}_7 \cdot 0.67\text{H}_2\text{O}$ . This model fully agrees with all the structural characterizations, validating this methodology and suggesting its potential use to study other nanomaterials.

## **Texture, Microstructure, and Surface Mechanical Properties of AZ31 Magnesium Alloys Processed by ECASD.**

**Emigdio Mendoza Fandiño, Raúl E. Bolmaro, Pablo Risso, Vanina Tartalini, Patricia Fernández Morales and Martina Ávalos. Advanced Engineering**

Dr. R. E. Bolmaro, P. Risso, V. Tartalini, Dr. M. Avalos, Instituto de Física Rosario-CONICET-UNR. Bv. 27 de Febrero 210 bis, (S2000EZP), Rosario, Argentina

E. Mendoza Fandiño, Facultad de Ingeniería Mecánica. Universidad Pontificia Bolivariana, Medellín, Colombia

Dr. P. Fernández Morales, Facultad de Ingeniería Industrial. Universidad Pontificia Bolivariana, Medellín, Colombia

[Adv. Eng. Mater. 2017, 00, 1700228](#)

### **Abstract**

The current work presents the results on Mg AZ31B alloy sheets subject to four passes using Equal Channel Angular Sheet Drawing (ECASD) at various temperatures (25, 100, and 200 °C). Textures are determined by laboratory X-ray diffraction and EBSD. EBSD allows the evaluation of the evolution of crystal sizes in function of the distance to the surface and the presence of twinning. Twinning is evident by the analysis of the textures, which show mainly two components, one due to the spin induced by the shearing of ECASD and the other one as a direct product of twinning. Micro-hardness, by Knoop tests on the lateral face of the sheets, are performed, allowing the determination of the influence of SPD on the hardness from surface to surface, going through the center of the sheet. Almost 50% increase on hardening, with respect to the non-processed material, is obtained near to the surface after four and six passes. The effectiveness as a hardening technique declined after the first four passes.

## **Influence of organic additives on the behaviour of zinc electroplating from alkaline cyanide-free electrolyte**

**P. Pary<sup>1,3</sup>, J. F. Bengoa<sup>2,5</sup>, M. S. Conconi<sup>1,3</sup>, S. Bruno<sup>4</sup>, M. Zapponi<sup>4</sup> & W. A. Egli<sup>1</sup>**

1 CIDEPINT: Centro de Investigación y Desarrollo en Tecnología de Pinturas. (UNLP-CIC-CONICET). Av. 52 s/n, entre 121 y 122. La Plata, Argentina.

2 CINDECA: Centro de Investigación y Desarrollo en Ciencias Aplicadas. (UNLP-CIC-CONICET). 47 N° 257. La Plata, Argentina.

3 Facultad de Ingeniería - Universidad Nacional de La Plata. Av.1 y 47. La Plata, Argentina.

4 REDE-AR Siderca. Simini 250. Campana, Argentina

5 CETMIC: Centro de Tecnología de Recursos Minerales y Cerámica. (UNLP-CIC-CONICET). Camino Centenario y 506. M. B. Gonnet, La Plata, Argentina.

[Transactions of the IMF, 95:2,83-89](#)

### **Abstract**

Two similar polymeric organic compounds from the polyquaternium family were studied as levelling additives in an alkaline cyanide-free zinc plating electrolyte. One additive (LA) has amide bonds between its monomers and the other (LU) has urea unions in its chemical structure. Copper cementation on zinc and gas evolution during aging of the zinc coatings were used to evaluate the effect of the chemical structure of the organic additives on the characteristic deleterious aging process of the coatings when electrodeposited with LA. Scanning electron microscopy and X-ray diffraction were used to follow surface morphology and crystallographic modifications of the coatings during aging. Faster copper cementation kinetics, zinc whiskers growth, blistering of the coating and N<sub>2</sub>, CH<sub>4</sub>, CO<sub>2</sub> and H<sub>2</sub> evolution were observed during accelerated aging of the coatings when LA was used. The coatings produced with LU did not show any aging effect. These studies show the strong influence that subtle changes in the chemical structure of the organic additive may have on the performance of zinc coating during storage.

### **Ceramic behavior of ball clay with gadolinium oxide (Gd<sub>2</sub>O<sub>3</sub>) addition. Applied clay science.**

**M. F. Hernández<sup>a,b</sup>. M. S. Conconi<sup>a</sup> . M. Cipollone<sup>b,c</sup>. M. S. Herrera<sup>a</sup>. N. M. Rendtorff<sup>a,b</sup>**

a Centro de Tecnología de Recursos Minerales y Cerámica (CETMIC): (CIC-CONICET-CCT La Plata), Camino Centenario y 506 s/n, C.C.49 (B1897ZCA), M.B. Gonnet, Argentina

b Dpto. De Química, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, UNLP, 47 y 115 s/n, La Plata, Argentina

c Química Analítica, Y-TEC SA. Av. del Petróleo Argentino 900, Berisso, Buenos Aires, Argentina

[ELSEVIER SCIENCE BV, 2017. vol. 146, p. 380-387. ISSN 0169-1317](#)

### **Abstract**

The effect of the addition of gadolinium oxide (Gd<sub>2</sub>O<sub>3</sub>) in the thermal behavior of a (66%) kaolinitic ball clay was studied and compared with the pure clay.

The incorporation of Gd<sub>2</sub>O<sub>3</sub> is of technological interest for the design of smart ceramic proppants used for unconventional gas and oil well stimulation. This proppant material is used to obtain important information, such as the location and height of the created hydraulic fractures.

The studied comprised a set of thermal analysis up to 1400 °C and the sintering behavior of the clay, up to 5% addition. The developed texture and microstructure was also assessed.

No important effects in kaolinite dehydration temperature and mullites (primary and secondary) formation were observed (500–600 and 990 °C). The sintering range of the studied clay is 1080–1360 °C; the 5% wt. addition resulted in 80 °C decrease of the final sintering temperature.

Mixtures fired at 1250 and 1400 °C resulted in dense ceramic materials with mullite as principal crystalline phase accompanied by quartz and cristobalite; imbibed in a viscous glassy phase which was proportionally increased by the added oxide. The mullite content and cell parameters were not affected. No gadolinium containing binary or ternary crystalline phases were detected, inferring that the rare earth is dissolved by the active viscous glassy phase thermally formed from the clay crystalline phases.

Low concentration addition of the oxide did not affect the porosity or water absorption of the developed ceramics. Only the 5% wt. addition resulted in a slightly higher desinterization with the appearance of macro-porosity if fired at 1400 °C.

### **Development of oxyfluoroborate glass ceramics doped with Er<sup>3+</sup> and Yb<sup>3+</sup> (Completo, 2018)**

M. RODRIGUEZ , Keuchkerián, R , Maia, LJQ , Carvalho J.F , SUESCUN, L , FACCIO, R. , Fornaro L

Journal of Materials Science: Materials in Electronics (E), v.: 29 7 , p.:5472 - 5479, 2018

### **Synthesis, structural characterization and scalable preparation of new amino-zinc borates as potential additives for wood preservation. (Completo, 2017)**

IMER, MR , GONZÁLEZ, M , VEIGA, N , KREMER, C , SUESCUN, L , ARIZAGA,L

Dalton Transactions, v.: 46 p.:15736 - 15745, 2017

Palabras clave: Crystal Structure tetraborate wood preservative

### **Bimetallic Trifluoroacetates as Single-Source Precursors for Alkali–Manganese Fluoroperovskites**

DULANI, BB , MUNASHIGHE, H , SUESCUN, L , RABUFFETTI, FA

Inorganic Chemistry, v.: 56 21 , p.:13311 - 13320, 2017

### **Possible causes for rippling in a multivacancy graphene system**

**Dominique Mombrú , Ricardo Faccio , Alvaro W. Mombrú**

Centro NanoMat, Cryssmat-Lab, DETEMA, Facultad de Química, Universidad de la República, Montevideo, Uruguay

**Abstract**

The occurrence of ripples in an eight-atom vacancy graphene system was analyzed through first principles calculations based on density functional theory. The study focuses on the conditions that should be considered in order that ripples could occur in the single layer defected graphene. The vacancies concentration, especially the pentagonal figures formed after relaxation of the vacant system, and the distances between neighbor pentagons, are found to be key aspects for rippling occurrence, with no charge distribution consequence. Two different configurations of rippling have been found where the position of the pentagonal figures is discussed as the driving force for any of them to occur.

**Total Synthesis of Gabosine H and Two Non-natural Gabosines**

**Gaurao D. Tibhe<sup>a</sup>, Mario A. Macias<sup>b,c</sup>, Enrique Pandolfi<sup>a</sup>, Leopoldo Suescun<sup>b</sup>, Valeria Schapiro<sup>a</sup>**

<sup>a</sup> Departamento de Química Orgánica, Facultad de Química, Universidad de la República, C.C. 1157, Montevideo, Uruguay

<sup>b</sup> Cryssmat-Lab/Cátedra de Física/DETEMA, Facultad de Química, Universidad de la República, Montevideo, Uruguay

<sup>c</sup> Departamento de Química, Universidad de los Andes, Carrera 1 No 18A-12, Bogotá, Colombia,

<sup>a</sup> Departamento de Química Orgánica, Facultad de Química, Universidad de la República, C.C. 1157, Montevideo, Uruguay

<sup>b</sup> Cryssmat-Lab/Cátedra de Física/DETEMA, Facultad de Química, Universidad de la República, Montevideo, Uruguay

<sup>a</sup> Departamento de Química Orgánica, Facultad de Química, Universidad de la República, C.C. 1157, Montevideo, Uruguay

[Synthesis 2017; 49\(03\): 565-570](#)

**Abstract**

Gabosines constitute a group of naturally occurring compounds with unique structures that exhibit very interesting biological activities. Synthetic efforts have been continuously reported since 1985. In this work, multistep total syntheses of natural gabosine H and non-natural gabosines have been accomplished by using a chemoenzymatic approach. Chirality

was transferred from the starting material 3-methyl-cis-1,2-cyclohexadienediol, which was obtained by biotransformation of toluene. Protection of the diol followed by iodohydroxylation or dihydroxylation of the less hindered double bond and further functional group transformations, permitted us to build up the synthetic sequences to the final products. The chemical structures and the absolute configurations of two key intermediates and two final products were confirmed by X-ray diffraction.

## **Electrochemical synthesis of CuSCN nanostructures, tuning the morphological and structural characteristics: From nanorods to nanostructured layers**

**Daniel Ramírez<sup>a</sup>, Gonzalo Riveros<sup>a</sup>, Katherine Álvarez<sup>a</sup>, Bárbara González<sup>a</sup>, Carlos J. Pereyra<sup>b</sup>, Enrique A. Dalchiele<sup>b</sup>, Ricardo E. Marotti<sup>b</sup>, Daniel Ariosa<sup>b</sup>, Francisco Martín<sup>c</sup>, José R. Ramos-Barrado<sup>c</sup>**

<sup>a</sup> Instituto de Química y Bioquímica, Facultad de Ciencias, Universidad de Valparaíso, Avda. Gran Bretaña 1111, Playa Ancha, Valparaíso, Chile

<sup>b</sup> Instituto de Física & CINQUIFIMA, Facultad de Ingeniería, Universidad de la República, Herrera y Reissig 565, C.C. 30, Montevideo 11000, Uruguay

<sup>c</sup> Laboratorio de Materiales y Superficies. Departamentos de Física Aplicada & Ing. Química, Universidad de Málaga, E29071 Málaga, Spain

[Materials Science in Semiconductor Processing. Volume 68, September 2017, Pages 226-237](#)

### **Abstract**

P-type CuSCN nanorods (NRs) grown on CuSCN seed layers were obtained with modulated diameters through an electrochemical procedure. Their morphological, structural, optical, electrochemical and photoelectrochemical features were studied in depth. Morphology of samples can be tuned from a near vertically and dense 1D nanostructure to a quasi 2D film according the value of the  $\text{SCN}^-/\text{Cu}^{2+}$  molar ratio ( $r$ ) present in the electrochemical bath. Raman studies confirmed the nature of CuSCN in its beta phase. For low  $r$  values CuSCN NRs presented high preferential orientation along the c-axis and high optical scattering at low wavelengths which lead to both low haze and high integrated diffuse reflectance. Band gap values were also affected by the  $r$  value thus experiencing a redshift, probably related to both quantum confinement and light dispersion. Electrochemical and photoelectrochemical measurements confirmed the p-type behavior of samples together with the enhancement of their surface at low  $r$  values. This knowledge opens new and more objective perspectives in the real use of CuSCN nanostructures in photovoltaics.

## **Development of binary and ternary titanium alloys for dental implants**

**Jairo M. Cordeiro<sup>ab</sup>, Thamara Beline<sup>ab</sup>, Ana Lúcia R. Ribeiro<sup>cd</sup>, Elidiane C. Rangel<sup>e</sup>, Nilson C.da Cruz<sup>e</sup>, Richard Landers<sup>f</sup>, Leonardo P. Faverani<sup>g</sup>, Luís Geraldo Vaz<sup>h</sup>, Laiza M.,G.Fais<sup>h</sup>, Fabio B. Vicente<sup>bi</sup>, Carlos R. Grandini<sup>bj</sup>, Mathew T. Mathew<sup>bkl</sup>, Cortino Sukotjo<sup>bl</sup>, Valentim A. R. Barão<sup>ab</sup>**

<sup>a</sup>University of Campinas (UNICAMP), Piracicaba Dental School, Department of Prosthodontics and Periodontology, Av. Limeira, 901, Piracicaba, São Paulo 13414-903, Brazil

<sup>b</sup>Institute of Biomaterials, Tribocorrosion and Nanomedicine (IBTN), Brazil and USA

<sup>c</sup>Faculdade de Ciências do Tocantins (FACIT), Rua D 25, Qd 11, Lt 10, Setor George Yunes, Araguaína, Tocantins 77818-650, Brazil

<sup>d</sup>Faculdade de Ciências Humanas, Econômicas e da Saúde de Araguaína/Instituto Tocantinense Presidente Antônio Carlos (FAHESA/ITPAC), Av. Filadélfia, 568, Araguaína, Tocantins 77816-540, Brazil

<sup>e</sup>Univ Estadual Paulista (UNESP), Engineering College, Laboratory of Technological Plasmas, Av. Três de Março, 511, Sorocaba, São Paulo 18087-180, Brazil

<sup>f</sup>University of Campinas (UNICAMP), Institute of Physics Gleb Wataghin, Cidade Universitária Zeferino Vaz—Barão Geraldo, Campinas, São Paulo 13083-859, Brazil

<sup>g</sup>Univ Estadual Paulista (UNESP), Aracatuba Dental School, Department of Surgery and Integrated Clinic, R. José Bonifácio, 1193, Aracatuba, São Paulo 16015-050, Brazil

<sup>h</sup>Univ Estadual Paulista (UNESP), Araraquara Dental School, Department of Dental Materials and Prosthodontics, R. Humaitá, 1680, Araraquara, São Paulo 14801-903, Brazil

<sup>i</sup>Universidade Paulista (UNIP), Av. Nossa Sra. de Fátima, 9-50, Bauru, São Paulo 17017-337, Brazil

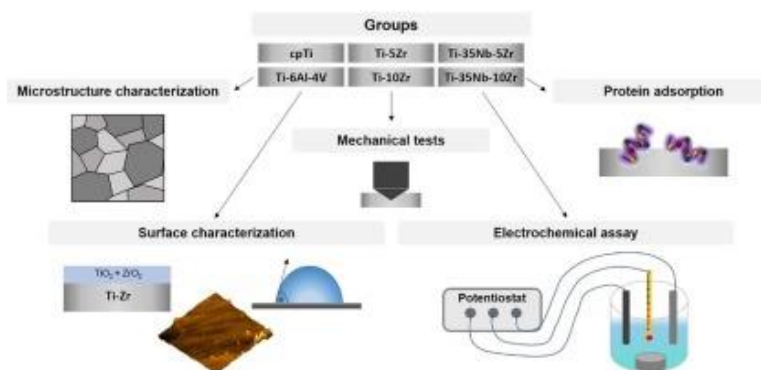
<sup>j</sup>Univ Estadual Paulista (UNESP), Laboratório de Anelasticidade e Biomateriais, Av. Eng. Luiz Edmundo Carrijo Coube, Bauru, São Paulo 17033-360, Brazil

<sup>k</sup>University of Illinois College of Medicine at Rockford, Department of Biomedical Sciences, 1601 Parkview Avenue, Rockford, IL 61107, USA

<sup>l</sup>University of Illinois at Chicago, College of Dentistry, Department of Restorative Dentistry, 801 S Paulina, Chicago, IL 60612, USA

[Dental Materials. Volume 33, Issue 11, November 2017, Pages 1244-1257](#)

## Abstract





## **Objective**

The aim of this study was to develop binary and ternary titanium (Ti) alloys containing zirconium (Zr) and niobium (Nb) and to characterize them in terms of microstructural, mechanical, chemical, electrochemical, and biological properties.

## **Methods**

The experimental alloys — (in wt%) Ti–5Zr, Ti–10Zr, Ti–35Nb–5Zr, and Ti–35Nb–10Zr — were fabricated from pure metals. Commercially pure titanium (cpTi) and Ti–6Al–4V were used as controls. Microstructural analysis was performed by means of X-ray diffraction and scanning electron microscopy. Vickers microhardness, elastic modulus, dispersive energy spectroscopy, X-ray excited photoelectron spectroscopy, atomic force microscopy, surface roughness, and surface free energy were evaluated. The electrochemical behavior analysis was conducted in a body fluid solution (pH 7.4). The albumin adsorption was measured by the bicinchoninic acid method. Data were evaluated through one-way ANOVA and the Tukey test ( $\alpha = 0.05$ ).

## **Results**

The alloying elements proved to modify the alloy microstructure and to enhance the mechanical properties, improving the hardness and decreasing the elastic modulus of the binary and ternary alloys, respectively. Ti–Zr alloys displayed greater electrochemical stability relative to that of controls, presenting higher polarization resistance and lower capacitance. The experimental alloys were not detrimental to albumin adsorption.

## **Significance**

The experimental alloys are suitable options for dental implant manufacturing, particularly the binary system, which showed a better combination of mechanical and electrochemical properties without the presence of toxic elements.