



## **Emerging Trends in Materials Science and Nanotechnology**

January 28-29, 2019 | Barcelona, Spain

Nanomat 2019

## **DAY 1** January 28, 2019

#### Sessions

Advanced Nanomaterials | Nano Electronics Nanotechnology for clean Energy | Nano Applications | Nano Biotechnology | Nano Bio Medicine | Polymer Science Engineering | Advanced Materials Science Nano Tecnology in Material Science

**Session Chair Paolo Bondavalli** Thales Research and Technology, France Session Chair Xinhua Yang Huazhong University of Science and Technology, China

#### **Session Introduction**

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Title:	Atomic layer deposition growth of laminated oxides as dielectric thin films
	Raffaella Lo Nigro, Institute for Microelectronics and Microsystems - CNR, Italy



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## Emerging Trends in Materials Science and Nanotechnology

# 2D molybdenum disulfide and its polymer composites - characterization and thermal properties

#### Karolina Wenelska and Ewa Mijowska

West Pomeranian University of Technology, Poland

he discovery of graphene has aroused enormous scientific interests in fabrication and application of new two-dimensional (2D) materials in the past decade. As a typical layered graphene-like material, molybdenum disulfide (MoS2) shows the unique properties exhibiting great potential applications in the field of electronic and optoelectronic devices. Despite the enormous scientific interests aroused by MoS2, little attention has been focused on the progress in fabrication, properties, and applications of MoS2/polymer nanocomposites up to now. In this work, exfoliated molybdenum disulfide (MoS2) modified by a metal oxide (MoS2/MxOy) and carbon nanotubes (MoS2/CNT) was prepared and characterized by atomic force microscopy (AFM), Raman spectroscopy and transmission electron microscopy (TEM). The samples were used in polymer composite preparation by using an extruder blending method. Nanocomposites of polymer with nanofillers were obtained.

The morphology, thermal properties, fire resistant properties and thermal conductivity of the nanocomposites were studied. We observed good flame retardance for all composites. All composites with exfoliated MoS2 exhibit greater potential for preparation of smart and functional nanomaterials with good thermal and fire resistant properties.

#### Biography

Karolina Wenelska has completed her PhD from West Pomeranian University of Technology. She is a Professor Assistant in Nanomaterials Physicochemistry Department. She has published 15 papers in reputed journals and she is an Author of 3 patents. She works with functional nanomaterials that can be used in various fields such as flame retardancy, supercapacitors or Li-ion batteries.

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## Nanostructuration of biomaterials and materials by electrochemical methods

#### Lidia Benea

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Electrochemical methods for the preparation of high quality Enanostructured surfaces and functionalization through active biomolecules electrodeposition are highlighted in this work. There are two applied electrochemical methods in our laboratory in order to obtain hybrid and nanocomposite structured layers or advanced functionalization of material surfaces. They are direct electrochemical synthesis by electro codeposition process and anodization of materials to controlled growth of nanoporous oxide films and the second method could be followed by electrodeposition of hydroxyapatite or organic compounds into porous films to form more complex hybrid layers. The main goal of the present paper is to make a summary of results obtained from applying electrochemical surface modification techniques in obtaining advanced functional surfaces and their properties characterization in terms of surface morphology and structure (SEM-EDX, XRD), the roughness and thickness, corrosion, tribocorrosion as well as the mechanical properties as nano hardness or wear resistance. Electrodeposition of metals and alloys or electro-codeposition of nano and microdispersed particles with metallic matrix to obtain micro and nano structured films and layers or hybrid coatings are a bottom-up approach of nanotechnology methods. Electrochemical oxidation or anodization to obtain thin films, layers of nano porous oxides, templates for nanowires or active biomolecules electrodeposition is a top down approach of nanotechnology method. Electrodeposition and the combination of electrodeposition with other electrochemical processes as controlled oxide growth by anodization can lead to a large class of hybrid layers and composite coatings or nanostructured layers (films) on different support materials and structures necessary for a future based on nanotechnology and nanomaterials to improve the surface functionalization of materials and to face of aggressive environments and degradation processes. Improving surface properties for corrosion and tribocorrosion of materials in specific environments give more valuable industrial and biomedical applications by increasing their life cycle.

#### **Recent Publications**

- 1. Valentin Marian Dumitraşcu and Lidia Benea (2017) Improving the corrosion behavior of 6061 aluminum alloy by controlled anodic formed oxide layer. Revista de Chimie. 68:77-80.
- Lidia Benea and Eliza Danaila (2016) Nucleation and growth mechanism of Ni/TiO2 nanoparticles electrocodeposition. Journal of The Electrochemical Society 163(13):D655-D662.
- Benea L, Başa S B, Dănăilă E, Caron N, Raquet O, Ponthiaux P and Celis J P (2015) Fretting and wear behaviors of Ni/nano-WC composite coatings in dry and wet conditions. Materials and Design 65:550–558.
- Benea L, Dănăilă E and Ponthiaux P (2015) Effect of titania anodic formation and hydroxyapatite electrodeposition on electrochemical behaviour of Ti-6Al-4V alloy under fretting conditions for biomedical applications. Corrosion Science 91:262–271.
- 5. Benea L, Mardare-Danaila E and Celis J P (2014) Increasing the tribological performances of Ti–6Al–4V alloy by forming a thin nanoporous TiO2 layer and hydroxyapatite electro deposition under lubricated conditions. Tribology International 78:168–175.

#### Biography

Lidia Benea has completed her PhD (Doctor of Science in Chemistry) in 1996 from Dunarea de Jos University of Galati, Romania and Postdoctoral Studies from Ecole Centrale Paris - France and University Pierre et Marie Curie Paris - France. She is a University Professor, PhD Supervisor in Materials Engineering, Director of Doctoral School Fundamentals and Engineering Sciences and Director of Competences Research Center Interfaces - Tribocoorosion and Electrochemical Systems. She has published more than 300 papers in reputed journals and has been serving as an editorial board member and reviewer of reputed journals and also handled 65 externally funded project including international and national projects.

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## Emerging Trends in Materials Science and Nanotechnology

### Development and characterization of organoclay filled polyetherimide nanocomposites for anticorrosive coatings

#### Ajith James Jose

St.Berchmans College, India

**P**olyetherimide (PEI)/organically modified Fluorohectorite (OFH) clay nanocomposites were prepared by dispersing OFH clay in PEI matrix. The structural as well as morphological characteristics of the nanocomposites were investigated using X-ray diffraction (XRD), Atomic Force Microscopy (AFM) and Transmission Electron Microscopy (TEM). The thermal, mechanical properties of the PEI nanocomposites were found to be significantly improved by the incorporation of organically modified flurohectorite nano clay into the PEI matrix. The water uptake of the nanocomposites was investigated in detail as a function of clay content. The water uptake was minimum for composites with 3 wt % of filler. The anticorrosion properties of clay polymer nanocomposite (CPN) coatings were evaluated by means of various electrochemical methods which include Electrochemical Impedance Spectroscopy (EIS), Open Circuit

Potential Measurements (OCP) and water adsorption test. The topological changes on the PEI/OFH clay nanocomposite coated metallic surfaces during immersion test were evaluated by means of SEM and AFM analyses. The results obtained from various analyses showed that the PEI/OFH nanocomposites coatings possess better anticorrosion properties.

**Keywords:** Nanocomposite; Polyetherimide; Thermal properties, Mechanical properties; Anticorrosion

#### Biography

Ajith James Jose working on nanocomposites at st. Berchamans college(Autonomous), changanassery, Kerala, India

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## Emerging Trends in Materials Science and Nanotechnology

### Performance of Dye Sensitized Solar Cells (DSSCs) based on Cu-doped TiO<sub>2</sub> nanostructures photoanodes.

#### Sara Chahid, Desireé M. de los Santos, and Rodrigo Alcántara

Universidad de Cádiz, Spain

In this research study, Cu-doped TiO2 nanostructures with different doping contents from 0 to 10.0% (mole fraction) were synthesized through hydrolysis at low temperature. The as-prepared Cu-doped TiO2 nanostructures was characterized with several techniques, X-ray diffraction (XRD) and Raman spectroscopy were used to study the morphology and structure of the nanoparticles, which confirmed the crystalline anatase tetragonal structure. The UV-Vis Spectroscopy analysis was found that incorporation of Cu2+ into titanium affects the band gap of TiO2 and extending his activity towards visible sunlight region. Scanning Electron Microscopic (SEM) analysis confirming the Cu content is incorporated into TiO2 lattice affecting efficiency of doped samples. Further, the active specific surface area of the system was investigated employing Brunauer-Emmet-Teller (BET) measurement. Then the Dye-sensitized solar cells (DSSCs) based on Cu-doped TiO2 photoanaodes were fabricated and investigated with chemically absorbed Ruthenium N3 dye electrode under light illumination with standard solar simulator (AM 1.5G, 100mW/cm2). Results demonstrated that the 1.0% Cu-doped TiO2 sample annealed at 773K for 60 minutes exhibited the best photovoltaic performance of open circuit voltage (Voc = 957.5 mV), short circuit current density (Jsc = 0.795 mAcm-2), and the cell efficiency was reached  $(\eta = 4.524 \%)$ , which consists 50% higher than the un-doped cell. The BET analysis was supported the founding results, indicating that the 1.0% Cu-doped TiO2 nanoparticle presented the higher active specific surface area of 143.2 m2g-1. A highest active surface area is a key parameter for solar cells effectiveness, allowing more organic dye and electrolyte to be absorbed and stored into the semiconductor, that give photon from solar light energy more probability to be adsorbed which obviously led to improve global cell efficiency. This study may open up more investigated works applying Cu doped TiO2 in photovoltaic fields.

#### **Recent Publications**

- Desireé M. de los Santos, Sara Chahid, Rodrigo Alcántara, Javier Navas, Teresa Aguilar, Juan Jesús Gallardo, Roberto Gómez-Villarejo, Iván Carrillo-Berdugo and Concha Fernández-Lorenzo Mo/Cu/TiO2 nanoparticles: synthesis, characterization and effect on photocatalytic decomposition of methylene blue in water under visible light, DOI: 10.2166/wst.2018.101 (Publicado).
- Desireé M. de los Santos, Sara Chahid, Rodrigo Alcántara, Javier Navas, Teresa Aguilar, Juan Jesús Gallardo, Antonio Sánchez-Coronilla, and Concha Fernández-Lorenzo. Mo/TiO2 mixture: A modification strategy of TiO2 nanoparticles to improve photocatalytic activity under visible light. Beilstein journal of nanotechnology, 2017 (En revisión).
- Sara Chahid, Desireé M. de los Santos, Rodrigo Alcántara: The effect of Cu-doped TiO2 photoanode on photovoltaic performance of dye-sensitized solar cells. (Accepted in ACM digital library (ISBN: 978-1-4503-6562-8).
- Sara Chahid, Desireé M. de los Santos, Rodrigo Alcántara, Javier Navas: Isotherm, Kinetic, and thermodynamic analysis for removal of organic pollutants Using Synthesized Mo/Cu/ co-doped TiO2 Nanostructured (sent).

#### Biography

Sara Chahid has her expertise in synthesis and characterization of semiconductors, with photovoltaic and photocatalytic applications. Her open and contextual evaluation of new semiconductors based on TiO2 (Cu/ TiO2, MoS2/TiO2 and Cu-MoS2/TiO2) creates new pathways for improving renewable energy.

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## Emerging Trends in Materials Science and Nanotechnology

### Corrosion behavior of marine in steels black sea water protected with modified polymeric coating by addition of TiO<sub>2</sub> nanoparticles

#### Laurentiu Mardare and Lidia Benea

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Many engineered structures have a limited life span and are deteriorated because of the loss of material properties, exposure to severe environments or increases in service loads. Carbon steel is one of the most widely used materials in the ship and offshore structure industry. Corrosion and corrosionrelated problems are considered to be the most important factors leading to age-related structural degradation of ships and many other types of steel structures. Corrosion considered as the most important factor leads to the structural degradation of ships and other types of steel structures intended for work in the marine environment. Corrosion of carbon steel in marine environment becomes serious due to the highly corrosive nature of seawater with high salinity and microorganisms. Various organic and inorganic coatings are used to protect metallic materials particularly steel against corrosion occurrence. The most used are the polymeric protective coatings. The nanostructured TiO2 polymer coating is able to offer higher protection to steel against corrosion and performed relatively better than other polymer coatings. The aim of the paper is to show the role of TiO2 nanoparticles in the enhancement of protective coatings and the lifespan of marine structures. The novelty of this research consist of the comparative assessment of corrosion resistance of different types of surfaces: E32 low alloy steel without protective coating, E32 coated with polymeric primer and E32 steel coated with polymeric primer mixed with TiO, nanoparticles. All samples were subjected to corrosion in sea water collected from the Black Sea, Năvodari Oil Terminal. The corrosion properties have been

studied by electrochemical methods. The purpose is to improve the protection capabilities of polymeric coatings by adding dispersed inert ceramic nanoparticles as titanium oxide with an average diameter of 200 nanometers.

#### **Recent Publications**

- 1. Mardare L and Benea L (2017) Development of anticorrosive polymer nanocomposite coating for corrosion protection in marine environment. Materials Science and Engineering 209:012056.
- 2. Lidia Benea, Laurentiu Mardare and Nicoleta Simionescu (2018) Anticorrosion performances of modified polymeric coatings on E32 naval steel in sea water. Progress in Organic Coatings 123:120-127.
- Mardare L, Benea L, Danaila E and Dumitrascu V (2015) Polymeric coatings used against marine corrosion of naval steel en32. Key Engineering Materials 699:71-79.

#### Biography

Laurentiu Mardare has five years of working research experience within the Doctoral School, Fundamental and Engineering Sciences, Faculty of Engineering at Dunarea de Jos University of Galati. He is specialized in engineering of integrated manufacturing systems. He handled externally funded and institute projects and published more than 10 international and national research papers. He is now working as an engineer at Oriana Engineering Project Itd, Galati, Romania.

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## Corrosion and wear performances of Co/nano-CeO2 bio-coatings in biological solution

#### Nicoleta Lucica Simionescu and Lidia Benea

CC-ITES - Dunarea de Jos University of Galati, Romania

Metal matrix composite layers are widely used as advanced functional materials for different applications. The electrochemical deposition technique or anodization have been increasingly being established as efficient preparation route for obtaining nano and micro structured composites, cermets or hybrid coatings with specific properties to be used in industrial or biomedical applications. The process of electro-co-deposition essentially consist inclusion of solid particles suspended in an electrolytic bath into the electro crystallizing metal which is in fact the metal matrix. The particles co-deposited with a metallic matrix are generally considered insoluble. The development of modern technology requires metallic materials with better surface properties and better corrosion and wear resistance. Nanocomposites made up of highly fine particles (nanometer size) of pure metals, ceramics and polymers in a metallic matrix have been the object of investigation for some decades in science, industry and biomedical applications. Apart from the intrinsic advantages of in situ electrochemical synthesis, the route provides the opportunity of producing the coating with desired thickness and composition. Co/nano-CeO2 composite coatings were developed by electro deposition method from a cobalt plating solution containing dispersed CeO2 nanoparticles (25 nanometers size). The content of co-deposited CeO2 into nanocomposite coatings was controlled by the addition of different CeO2 particle concentrations into the electroplating solution. The corrosion and tribocorrosion performances of Co/nano-CeO2 nanocomposite coatings and pure Co coating were comparatively investigated in an electrochemical cell and unidirectional reciprocating of tribometer in lubricating conditions using simulated biological solution (Hank). During the tribocorrosion test, the normal force, tangential force, coefficient of friction, number of cycles as well as the electrochemical parameters (potential), were continuously monitored. Schematic representation of tribocorrosion tests are shown in fig. 1. The corrosion and wear performances of Co/nano-CeO2 bio-coatings are closely related with CeO2 content. The nanocomposite coating with all CeO2 content shows increased wear resistance when compared with pure Co coating.

#### **Recent Publications**

- 1. Lidia Benea (2012) Electrochemical impedance spectroscopy and corrosion behavior of Co/CeO2 nanocomposite coatings in simulating body fluid solution. Metallurgical and Materials Transactions A. 44A:1114-1122.
- Lidia Benea, Pierre Ponthiaux and Francois Wenger (2011) Co-ZrO2 electrodeposited composite coatings exhibiting improved micro hardness and corrosion behavior in simulating body fluid solution. Surface and Coatings Technology 205:5379-5386.
- 3. V M Dumitrascu, L Benea and N Simionescu (2018) Evaluation of sealing process on the surface properties of nano porous aluminium oxide layers electrochemically growth on 1050 aluminum alloy surface. Mater. Sci. Eng. DOI: 10.1088/1757-899X/374/1/012013.
- Lidia Benea, Laurentiu Mardare and Nicoleta Simionescu (2018) Anticorrosion performances of modified polymeric coatings on E32 naval steel in sea water. Progress in Organic Coatings 123:120-127.

#### Biography

Nicoleta Lucica Simionescu is a second year PhD student in Materials Science and Engineering at Dunarea de Jos, University of Galati, Romania. Her field of study is the degradation of metallic biomaterials by corrosion processes in bio-fluid environments. She received the Diploma of Second Award at the Conference of Doctoral Schools from Dunarea De Jos University of Galati, 2018.

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## Atomic layer deposition growth of laminated oxides as dielectric thin films

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Wide bandgap semiconductors (SiC or GaN) based devices have shown excellent progress in recent years for high frequency and high power electronics. Nevertheless, several issues still needed to be addressed such as finding of an appropriate gate insulator. Moreover, since device frequency performance is strongly dependent on maintaining a high geometric aspect ratio between the gate length and barrier thickness, precise control over the thickness of gate insulators is very important. In this context, atomic layer deposition (ALD) is considered as a key enabling technique because of its controlled layer-by-layer growth. Huge efforts are nowadays devoted to the fabrication of multicomponent gate insulators having high dielectric constants and good chemical stability. In particular, the growth of Al2O3-HfO2 laminated layers is among the most studied combination because of the possibility to combine the complimentary characteristics of the two materials. Plasma enhanced ALD growth of three different Al2O3/HfO2 combinations has been considered: a bilayer system of the two Al2O3 and HfO2 oxides each having a 15 nm thickness, a nanolaminated 10 stacked Al2O3HfO2 bilayers with each sub-layer thickness of about 3 nm and of a homogeneous HfAlO layer, have been fabricated. The dielectric properties and the structural evolution upon annealing treatment have been compared. On the basis of all the collected data, the 10AB laminated can be considered the most promising system. In fact, it showed an amorphous structure before and after annealing treatments and better dielectric behavior in terms of dielectric constant value and charge traps amounts.

#### Biography

Raffaella Lo Nigro received her BSc in Chemistry cum Laude in 1996 and in 2000 she received her PhD from Catania University. From 1996 to 2000 she acquired an advanced know-how in the field of MOCVD and in 2001 she joined the IMM-CNR as permanent researcher, where she is responsible of the research group "advanced materials for power devices and their nanocharaterization". Her current research interests include the synthesis of high k dielectric by atomic layer deposition. She is author of more than 120 papers and 4 book chapters.

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