

Joint Meeting on
4th International Conference on
CRYSTALLOGRAPHY & NOVEL MATERIALS
&
9th International Conference on
BIOPOLYMERS AND POLYMER SCIENCES
November 19-20, 2018 Bucharest, Romania



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Mechanical properties of heat treated 3D printed semi-crystalline PEEK material

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Relatively new manufacturing processes such as 3D printing or additive manufacturing impose a set of thermos-mechanical influences on materials. These influences have neither been extensively studied nor reported in the literature. For high temperature semi-crystalline thermoplastic materials like PEEK (poly-ether-ether-ketone) these influences can be quite pronounced. The 3D printing of PEEK requires a strict definition of the processing conditions and parameters. One of the challenging aspects of the processing is the control of the temperature profile dominant in and around the printed part. This is especially important because the development of the crystalline phase in 3D printed PEEK part depends on the cooling rate of the melt during the printing process. A typical attribute of 3D printed parts is the structural discontinuities observable on the surface and in the vicinity of the deposited layers. To improve on the structural integrity of the printed part, some heat treatment is conducted on the part. In the current presentation, results for tempered 3D printed PEEK parts are presented. The mechanical properties as well as the microstructural state of the PEEK parts are reported and explained within the context of the tempering process.

Biography

Uwe Popp has completed his Diploma in Material Science and Engineering from the University of Stuttgart in 2012 and worked for two years at the Karlsruhe Institute of Technology as a Research Assistant. He is currently the Head of Research and Development at Apium Additive Technologies GmbH as well as one of the Founders of the company. He has participated in publishing more than 5 papers in reputed journals.

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Enhanced T1 MRI contrast and fluorescence stability within a plasmonic core-shell nanoparticle

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Multifunctional plasmonic nanostructures have enormous potential in the treatment of solid tumors; however, tracking particles with drug cargo and triggering the release of the cargo in mapped tumors is still impossible. To overcome this challenge we have developed an MRI and fluorescent active nanostructure nanomatryoshka. This new nanostructure with IR plasmonic signatures is composed of a 50 nm Au core surrounded by dye molecules and Gd(III)-DOTA chelate doped SiO₂ inner-shell and an outer Au shell. The experimental results demonstrates an enhanced T1 relaxation ($r_1 \sim 24 \text{ mM}^{-1} \text{ s}^{-1}$ at 4.7 T) compared to the clinical Gd(III)-DOTA chelating agents ($r_1 \sim 4 \text{ mM}^{-1} \text{ s}^{-1}$). Further, this design preserves the fluorescence signal (65%) after 24 hours of exposure, leading to enhanced fluorescence photo-stability (23x). This dual-imaging functionality nano-system increases MRI sensitivity by concentrating Gd(III) ions into the Gd-NMs, reduces the potential toxicity of Gd(III) ions and dye molecules by preventing their release *in vivo* through the outer Au shell protection and the terminal gold layer surface can then be functionalized to increase cellular uptake, circulation time or thermal drug-release properties.

Biography

Oara Neumann has completed her PhD and Postdoctoral study in Applied Physics from Rice University and MS from Weizmann Institute of Science, Israel and Bucharest University, Romania. She is a Research Scientist in Naomi Halas group at Rice University. She holds 12 patents and she has published more than 25 papers in reputed journals.

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Synthesis of novel autoreactive and ecological monocomponent adhesives for the shoe industry

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Microencapsulation is a process in which active substances are enclosing inside an extremely small capsule. The wide applications of microcapsules in many fields have attracted increasing research on the synthesis as well as functionalization of different types of capsules. Besides the importance of microcapsules for controlled chemical release and uptake in many industrial applications, these are often difficult to produce with the desired combination of high mechanical strength and high shell permeability. We report on experimental studies for the synthesis of narrow size distribution polyurethane/polyurea shell microcapsules containing isocyanate, used as a crosslinker for adhesive formulations. The microcapsules were produced, in a continuous mode, by a system involving a microfluidic device, which originates a monodisperse oil-in-water emulsion, followed by interfacial polymerization at the emulsion droplets surface. The resulting microcapsules are intended to be added to an adhesive base (OH prepolymer), leading to an autoreactive and ecological monocomponent adhesive. The proposed technique has advantages of being readily controlled, cost-effective and easy to operate. In addition, microfluidics can control the process of encapsulation by varying flow parameters and/or using a proper geometry of microfluidic channels. By microencapsulating the reactive agent, the product is safer for handling by the industry operators, and the activation mechanism can be controlled more precisely (enabling higher flexibility of application /use case scenarios). The advances made of the current study can be an important contribution in the innovation and development of new sustainable/green methods and products that can, in the future, compete in the monocomponent adhesives market.

Biography

Mariana Costa has a Master's Degree in Chemical Engineering and she is currently working in Polytechnic Institute of Cavado and Ave. The project that she is involved is about the microencapsulation field where the goal is to produce a microfluidic device to encapsulate isocyanate.

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Microstructural evolution of nano-crystalline tungsten-25% rhenium-hafnium carbide composite synthesized by spark plasma sintering technique for FSW tool application

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Development of nano-crystalline tungsten-25% rhenium alloy reinforced with hafnium carbide is a challenging task as these alloys are difficult to synthesize by conventional methods. The problem of these difficult to alloy elements can be addressed by using a unique combination of mechanical alloying and Spark Plasma Sintering (SPS) techniques via powder metallurgy route. Rhenium was added to lower ductile-to-brittle transition temperature and to increase recrystallization temperature of tungsten. SPS is rapid consolidating technique which prevents grain growth. These tool materials can withstand high temperatures and harsh conditions in joining application such as Friction Stir Welding (FSW) of steel and titanium alloys. FSW is a green process which does not emit fume and toxic fumes during the process. Sintering was carried between 1500-1800 °C. Mechanically alloyed and SPS alloy and composite were characterized by optical microscopy, Field Emission Scanning Electron Microscopy (FESEM) and X-ray Diffraction. Microstructural investigations of consolidated specimens were initially carried out by conventional etching and metallography techniques. Optical micrographs showed no visible signs of grain boundary etching. SPS samples were further electrochemically etched in one molar concentrated solution of NaOH. The positive terminal of the low voltage direct current power supply was connected to the sample. The negative terminal was connected to a steel plate acting as cathode. Both electrodes were placed in the tank face to face with a gap of 6 to 10 centimeters between them. The voltage was kept constant as 5 volt during the etching process. Samples were etched for short time interval from 1 to 5 seconds and microstructural analysis was conducted after each etching step. The results of the FESEM images confirm microstructural revelation of these difficult to etch alloy and composites.

Biography

Zafar Iqbal has completed his PhD from King Fahd University of Petroleum and Minerals KFUPM, KSA. Currently, he is the Assistant Professor at Pakistan Institute of Engineering and Applied Sciences (PIEAS), Islamabad. He has published more than 6 papers in reputed journals.

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Composite nanostructures for VIS-active photocatalysts

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Transylvania University of Brasov, Romania

Photo-catalysis is a process that makes possible solving some critical environmental issues, as the pollutants removal at (very) low concentrations from waters or air. The first photo-catalyst and one of the most efficient is TiO_2 (the anatase polymorph) that is largely used and reported. However, anatase has one major drawback that limits its up-scaling which is activated only by UV radiation, thus photo-catalysis runs only under this type of radiation. Vis-active photo-catalysts are therefore very much searched and are developed based on several principles as, e.g. novel type of semiconductors, aqueous stable (which, so far, are not too many) or composite structures of TiO_2 with p-type semiconductors, resembling the structure of an inverted photovoltaic cell, as CuInS_2 (CIS) or $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) efficient in Vis radiation harvesting and stable in water. Composite structures are reported also considering the TiO_2 or ZnO matrix infiltrated with graphene, graphene oxide or reduced graphene oxide. The photo-catalytic material can be used as dispersed powder (in wastewater for advanced treatment) but this has the disadvantage of light scattering and the more complex treatment process involving the separation step of the (nanosized) powder, therefore, thin films of photo-catalytic materials are recommended. The properties of the thin photo-catalytic films obtained by Spray Pyrolysis Deposition (SPD) are presented and discussed in terms of process overall efficiency and efficiency of the key steps such as pollutants' adsorption and pollutants photo-degradation through oxidation up to mineralization with a focus on the influence of the crystallinity of the composite structure.

Biography

Anca DUTA has completed her PhD in Chemical Engineering in 1996 from the Polytechnica University of Bucharest, Romania. She is the Leader of the Advanced Materials for Energy and Environment group in the R&D Centre Renewable Energy Systems and Recycling in the Transylvania University of Brasov, Romania. She has published more than 150 papers out of which 122 papers in ISI journals and has been serving as an Editorial Board Member of repute.

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Synthesis and characterization of the complex nanostructured thin films based on titanium by Thermionic Vacuum Arc (TVA) method

Rodica VLADOIU

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Nowadays, a great interest is paid on the development of plasma technology applications with particular emphasis on the fabrication of nanostructured thin film, combined with the study of applications of plasmas in nanotechnology. For this reason, plasma/surface interactions and growth mechanisms have to be taken into account for the definition, evaluation and comparison of the different types of coating equipment and achievable coating results. Titanium based nanocomposites owing to their remarkable properties of the coating surfaces such as wear resistance, roughness, low friction coefficients have been synthesized and investigated in different combination and forms, such as multi-component composites. The aim of this work is to find the best combination for coating the mechanical parts of components by suitable complex nanocomposites and by using innovative technology. For instance, titanium nanocomposites are characterized by very high tensile strength even at high temperatures, light weight, high corrosion resistance, and as strong as steel, but 45% lighter. Binary, ternary thin films as well as single thin films were deposited using Thermionic Vacuum Arc (TVA) technology. The thermionic vacuum arc (TVA) is an original deposition method using a combination of anodic arc and powerful electron gun system (up to 600 W) for the growth of thin films from solid precursors under a vacuum of 10^{-6} Torr. For certain operating conditions the plasma source produce energetic ions without any additional ion acceleration means like acceleration grids or polarization systems. Results on the surface morphology and wettability of the obtained multifunctional thin films were reported by using: Transmission Electron Microscopy (TEM Phillips CM 120 ST, 100 kV), Scanning Electron Microscopy (SEM, Zeiss EVO 50 SEM) and Free Surface Energy (FSE) by See System. Nanostructured coatings with homogenous and dense surface without any faults (pinholes and cracks) were achieved at low temperatures to not affect the materials properties. Nanocomposite coatings of Ti based consisting of crystalline phase embedded into an amorphous matrix constitute a multifunctional coating architecture due to its combination of properties, suitable for emerging applications in metallurgical industry, yielding an enhanced corrosion resistance.

Biography

VLADOIU Rodica has completed his PhD at the age of 35 years from Bucharest University Romania. She was Head of the Physics Department between 2004-2006, Local Coordinator of the CEEPUS network from 2000, Member in the National University Research Council – CNCSIS in 2006, Member in the Scientific Committee in International conference II CESPC Central European Symposium on Plasma Chemistry 2008, Brno, Czech Republic. She is co-author in 78 papers published in reviews with ISI quotation (428 citations) and in 2 national patents. In the last ten years, she was involved with the research team in 11 National Research projects and 9 International projects.

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Conjoint AES-EELS analysis of the sub-nanometric coatings

Nikolay Plusnin

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The purpose of the work is to show possibilities of a joint electron spectroscopy of Auger Electrons (AES) and of energy losses on valence electrons (EEES) for analysis of the structural-chemical and phase state of 2D or sub-nanometric coatings. The composition, thickness, growth mechanism and electronic energy structure of coatings were determined according to the AES data. In addition, the structural-phase state and the local electronic spatial structure of the coating were determined according to the EELS data. The choice of the optimal probing depth (0.25 nm) has been ensured the mutual additivity of analysis by two methods and its adaptation to the sub-nanometric thickness of coatings. It is shown that EELS is very sensitive method for analysis of local valence electron density of atoms and that the variation of the energy of the primary beam and of parameters the coating (the thickness of the coating, the arrangement of adatoms-markers, the coating deposition regimes), as well as the subtraction of the contribution from the substrate, make possible to increase informativity of the AES-EELS analysis of sub-nanometric coatings and structural state of their interface.

Biography

Nikolay Plusnin is currently working as the Chief Researcher in the Institute of Automation and Control Processes of FEB of the RAS, Vladivostok, Russia. He has completed the studies as Doctor of Physical-Mathematical Sciences. His research interests are in nanomaterials for electronics and their structure-phase analysis. He was a Visiting Professor in Tohoku University, Sendai, Japan. He is also a Member of the Advisory Board of the International journal, *e-journal of Surface Science and Nanotechnology*. He has published more than 35 scientific articles. His research was supported by Russian Ministry of Education and Science, Academy of Sciences and Government.

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Effects of glycerol incorporation on Semi-Refined Carrageenan film properties

Bakti Berlyanto Sedayu

Victoria University, Australia

Derived from renewable, abundant seaweed, carrageenan-based films are becoming popular as food packaging material. In this work, semi-refined carrageenan (SRC) plasticized with glycerol were developed and characterised. The mechanical strength, moisture content, and optical properties of the films generally increased significantly with increasing glycerol concentration, however, the water vapor permeability decreased. In particular, the tensile strength and elongation at break increased at plasticizer additions of up to 40% and 50% (w/w) respectively. The addition of glycerol also improved the thermal stability and surface morphology of the films. The results show that the properties of the SRC films were comparable with refined carrageenan suggesting that SRC has potential to be furthered developed into less expensive food packaging materials.

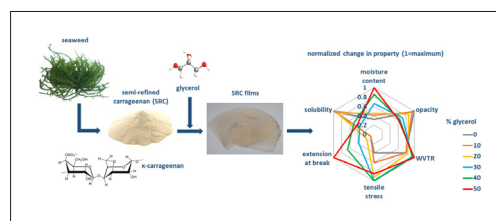


Figure 1. Experiment flowchart

Biography

Bakti B Sedayu is undertaking PhD research program in Victoria University, Australia. His project focuses on development of packaging material from seaweed.

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Structural properties and topological diversity of new ORGANOTIN(IV) coordination compounds

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Organotin(IV) coordination compounds have been the subject of interest for some time due to their properties, structural aspects and potential biomedical, environmental and commercial applications. A new series of coordination compounds with different organotin(IV) subunits as nodes and organic bridging ligands as spacers were prepared. The combination of organotin(IV) building blocks with O- and N-donor ligands resulted in the formation of new extended structures with 0D, 1D (an example is given in figure-1), 2D and 3D dimensionalities and interesting topologies. The influence of the nature of organotin(IV) nodes and the bridging ligands on the structural properties of the new systems obtained was investigated. All the synthesized compounds have been characterized by elemental analysis, standard spectroscopic techniques (FTIR, UV-Vis-NIR, NMR), thermal analysis, as well as by single crystal and powder X-ray diffraction. The ligands, metal precursors and their corresponding organotin(IV) complexes have also been screened for antimicrobial activities.

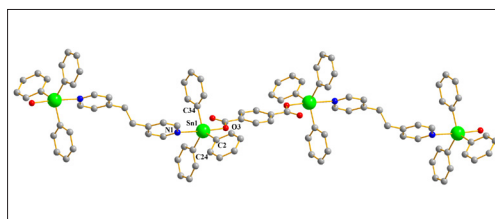


Figure-1: Structure of 1D coordination polymer $\{(\text{Ph}_3\text{Sn})(\mu\text{-bpa})(\text{Ph}_3\text{Sn})(\mu\text{-tpa})\}_n$. Hydrogen atoms were omitted for clarity.

Biography

Delia-Laura Popescu has completed her BS in Chemistry from Faculty of Chemistry, University of Bucharest. She has completed both MS and PhD degrees from the Carnegie Mellon University, Pittsburgh, USA, under the guidance of Professor Terrence J Collins having worked in green chemistry field. She was a Postdoctoral Researcher in Professor Nicolay Tsarevsky's group in the Department of Chemistry at Southern Methodist University, Dallas, USA. She is currently an Assistant Professor in the Department of Inorganic Chemistry at Faculty of Chemistry, University of Bucharest. Her research interests include porous materials (MOFs), supra-molecular hybrid metal-organic materials, poly-nuclear coordination systems with biological properties.

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Assessment of biodegradation and biological properties of modified biopolymers

Tasnim Kossentini Kallel

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There has been a growing interest over the past few years in the development of biopolymers partly because of their renewable, sustainable and biodegradable properties. They generally display interesting properties such as biodegradability, biocompatibility and their generated products are not toxic. Therefore, they possess various biological activities such as antibacterial, antioxidant and antifungal activities. These advantages, in parallel with the recent technological developments in biopolymer production, have rapidly expanded their applications as a competitive commodity polymer in a variety of processes. However, because of their inherent brittle nature, biopolymers generally need to be modified to be suitable for use in various applications where mechanical properties are important. So it is very interesting to toughen them with the goal of balancing and increasing tensile strength, impact strength and modulus while retaining the biocompatible and biodegradable nature of the polymer. The study concentrates on the biological activity and biodegradation capability of biopolymer blends in the solid state and in the liquid phase under aerobic and anaerobic conditions. To this end, blends were processed by casting method and on a twin-screw extruder with a film die and to determine the efficiency of the biodegradation of polymers, quantitative (mass variations, BOD) and qualitative (DSC and SEM) analyses were made. Otherwise, biopolymers were evaluated for their biological, structural and thermal properties.

Biography

Tasnim Kossentini Kallel is an associate professor in the Materials Engineering Department in the National School of Engineers of Sfax (Sfax University; Tunisia). In 1998-1999 she was Senior Safety Engineer at the Association of Health and Security at Work of Sfax "ASSETS" and in 2000-2003 she was a Researcher Member in the Laboratory of Macromolecular Materials INSA Lyon: Institute National des Sciences Appliqués de Lyon (France). In the Laboratory of Advanced Materials, she currently supervises a research team investigating the areas of advanced polymer blends and composite materials. She has been interested in various research areas including, polymer blends and composites designed for recycling, processing control of nano-composites and bio-composites via solvent casting method and reactive extrusion. She has planned, managed and completed projects under collaboration agreements with several foreign laboratories and industrial businesses. She has published a patent and 27 research articles.

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Synthesis, structural analysis and DNA interaction of bis[4'-(4-methylphenyl)-2,2':6',2''-terpyridine]Co(III)(NO₃)₃.2H₂O complex

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There has been extensive studies of binding of chiral Ru(II) complexes to DNA backbone structures. J K Barton has studied the cationic coordination of a variety of chiral poly-pyridine Ru(II) complexes to demonstrate chiral discrimination in binding to different forms of DNA. Many experimental techniques have been applied to study the interaction of tris(phenanthroline) ruthenium(II) ([Ru(phen)₃]₂⁺) with DNA, but despite this, its binding mode and its effect on the DNA structure are uncertain and have been the subject of much controversy. In this study, bis[4'-(4-methylphenyl)-2,2':6',2''-terpyridine]Co(III) tris(nitrate) complex was synthesized and characterized using conventional method such as ¹H NMR, ES-MS, UV-vis spectrophotometry. The crystal structure of the complex was also determined. The complex was crystallized in the triclinic space group, P₁ with two well separated complex molecules in the unit cell along with four hydrogen bounded water molecules and six nitrate groups. The Co ion was six coordinated, but the geometry was significantly distorted from that of an ideal octahedral. In this study, the terpyridine type ligand fragment appealed because the ligand structure ensures a meridional arrangement of the donor atoms, which reduces the number of possible isomers. Co(III) ion was attracted because of its higher positive charge compared to Ru(II) which will have more affinity towards the negatively charged DNA structure. Absorbance and fluorescence methods and circular dichroism were used to study the interaction of the Co(III) complex solution in water with DNA.

Biography

Ramin Zibaseresht is a Professor in Chemistry at Maritime University of Imam Khomeini in Noshahr and Adjunct Professor at Aja University of Medical Sciences in Tehran. He has completed his BSc in Chemistry from Shiraz University and his MSc in Inorganic Chemistry from Pune University. He has completed his PhD in Inorganic Chemistry from the University of Canterbury. He is currently the Head of Biomaterials and Medicinal Chemistry Research Centre in Tehran. He has published more than 50 papers in reputed journals and some international conferences and more than 10 books in the area of chemistry and 4 patents. He has been serving as an Editorial Board Member of some peer-reviewed journals, academic book publishers, member of more than 10 academic committees, organizing committees and academic boards of international conferences.

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Biopharmaceutical and functional activities improvement by drug-biopolymers association

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Federal University of Amapa School of Pharmacy, Brazil

Zein is a biodegradable protein found in the maize endosperm (*Zea mays*). In the pharmaceutical industry, it has been used as a coating agent in solid forms and in the composition of drug delivery systems, where it has shown the ability to entrap drugs, lipids and genetic material, promoting their controlled release. Its biological potential has gained attention lately. Thus, the antioxidant and antimicrobial activities of zein solely have been identified, but barely explored. The associations of biopolymers to drugs could result in synergistic or additive effects, depending on the structure, solubility, partition coefficient and chemical interactions to the other compounds, resulting in new outcomes. In view of the biological properties of zein, we assessed the improvement in the antimicrobial and antioxidant activities of this biopolymer when associated to some phenolic bioactive, such as Ellagic Acid (EA). Their chemical association was accessed by 1H saturation Transfer-Difference Nuclear Magnetic Resonance (STD-NMR) to explain these outcomes. The micro dilution method was used to assess the minimum inhibitory and bactericide concentrations. The antioxidant activity was determined using the 2, 2-diphenyl-1-picryl-hydrazila free radical scavenging method. EA has shown inhibitory activity against *Staphylococcus aureus* and *Pseudomonas aeruginosa* and an antioxidant IC₅₀ of 0.079 mg/mL. Zein has shown antimicrobial and antioxidant activities itself and enhanced synergically the antioxidant and the antimicrobial activity against *P. aeruginosa* when combined with EA. ¹H STD-NMR experiment confirmed the formation of a complex between EA and zein that could be related with the improvement on its biological performance over the individual compounds.

Biography

Francisco Fabio Oliveira de Sousa has completed his PhD from University of Santiago de Compostela, Spain and Postdoctoral studies from Federal University of Ceara School of Dentistry, Brazil. He is the Director of Experimental and Clinical Pharmacy research group with 9 PhD and undergraduate students, coordinating different projects in pharmaceutical technology and biomaterials. He has published more than 10 papers in reputed journals and has been serving as an Editorial Board Member for many journals. In 2018, he has been awarded the Scientific Yearly Prize by the Brazilian Council Research.

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