EuroSciCon

DAY 1

Scientific Tracks & Abstracts

8th International Conference on

Smart Materials and Structures

August 01-02, 2019 | Dublin, Ireland

DAY 1

August 01, 2019

Sessions

Insight into Smart Materials and Technology | Headway of Smart Structures | Smart Control Systems in Industrial Applications Advances in Material Science & Engineering | Architecture & Civil Engineering | Nanomaterials | Biomaterials | Physics & Chemistry of Smart Materials | Optical & Electronic Smart Materials | Artificial Intelligence-Automation Revolution

Session Chair
Armin Mehrabi
Florida International University, USA

Session Co-Chair
Mineo Hiramatsu
Meijo University, Japan

Session Introduction

Title: **3D graphene network, synthesis, functionalization and applications**
Mineo Hiramatsu, Meijo University, Japan

Title: **Machine learning techniques to predict the characteristics of zeolite**
Aiman Darwiche, Nova Southeastern University, USA

Title: **Influence of chemical and electrochemical surface treatment of ECAP titanium on resulting corrosion properties and wettability**
Katerina Dedkova, VSB Technical University of Ostrava, Czech Republic

Title: **Microstructure simulator to predict grain formation during thermo-mechanical processing of long products**
Ahmad Fakih, Friedrich Kocks GmbH & Co KG, Germany

Title: **Results of using laser triangulation for measuring surface defects in long products**
Matthias Schuck, Friedrich Kocks GmbH & Co KG, Germany

Title: **Self-Healing in rapidly solidified aluminium alloys**
Alena Michalcová, University of Chemistry and Technology, Czech Republic

Title: **A DFT investigation on multiferroism and magnetic coupling in $NiBO_3$ materials**
Sergio Ricardo de Lazaro, State University of Ponta Grossa, Brazil

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Mineo Hiramatsu et al., Nano Res Appl 2019, Volume 05

3D graphene network, synthesis, functionalization and applications

Mineo Hiramatsu[1], **Keigo Takeda**[1], **Hiroki Kondo**[2] and **Masaru Hori**[2]

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[2]Nagoya University, Japan

3-dimensional (3D) graphene network with large surface area could be promising material as a platform for electrochemical and bio applications. This kind of carbon nanostructure is called as carbon nanowalls (CNWs), carbon nanoflakes, carbon nanosheets, graphene nanosheets, and graphene nanowalls. CNWs and similar materials are basically self-supported network of few-layer graphenes standing almost vertically on the substrate to form 3D structure. CNWs can be synthesized by plasma-enhanced chemical vapor deposition (PECVD) on heated substrates (600-800˚C) employing methane and hydrogen mixtures. The height of CNWs increases almost linearly with the growth period, while the thickness of each sheet and interspaces between adjacent sheets are almost constant. The maze-like architecture of CNWs with large-surface-area graphene planes would be useful as electrodes for energy storage devices and scaffold for cell culturing. Especially, combined with surface functionalization including surface termination and decoration with nanoparticles and biomolecules, CNWs can be suitable as platform in electrochemical and biosensing applications. We have carried out CNW growth using several PECVD techniques. Moreover, graphene surface was decorated with Pt nanoparticles by the reduction of chloroplatinic acid. We also report the performances of hydrogen peroxide sensor and fuel cell, where CNW electrode was used. Electrochemical experiments demonstrate that CNWs offer great promise for providing a new class of nanostructured electrodes for electrochemical sensing, biosensing and energy conversion applications.

Biography

Mineo Hiramatsu has completed his PhD from Nagoya University and is a Full Professor in the Department of Electrical and Electronic Engineering, Meijo University, Japan. He served as the Director of Research Institute, Meijo University in 2017-2018. His main fields of research are plasma diagnostics and plasma processing for the synthesis of thin films and nanostructured materials. Author of more than 150 scientific papers and patents on plasma processes for materials science. He served as a Chairman and Member of organizing and scientific committees of international conferences on plasma chemistry and plasma processing. He was awarded the Japan Society of Applied Physics Fellow in 2017.

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Aiman Darwiche, Nano Res Appl 2019, Volume 05

Machine learning techniques to predict the characteristics of zeolite

Aiman Darwiche
Nova Southeastern University, USA

Machine learning can predict characteristics of material with high accuracy rates. Using Random Forest, we built a prediction model that depends on the geometric features, such as local geometry, structure, and porosity of the material, to predict the bulk and shear moduli of material with a high accuracy. The prediction model will be used on zeolites to predict the elastic response but can be extended to other materials. The proposed model is evaluated by comparing its predictive accuracy to those of extant methods.

Biography

Aiman Darwiche has completed his PhD from Nova Southeastern University in 2018. He is the Co-founder and Chief Data Scientist at Compu-House, a startup that emphasizes on building prediction models for life threatening health conditions before their occurrences. Besides, he teaches undergraduate courses at Northern Kentucky University. He has several papers.

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Katerina Dedkova et al., Nano Res Appl 2019, Volume 05

Influence of chemical and electrochemical surface treatment of ECAP titanium on resulting corrosion properties and wettability

Katerina Dedkova[1], Josef Hlinka[1], Ludek Dluhos[2] and **Kristina Cabanova[1]**

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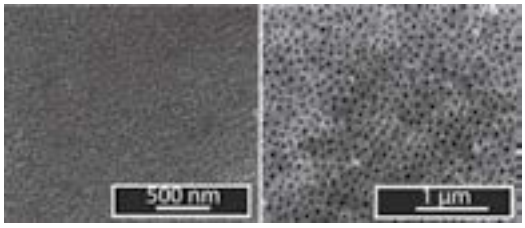
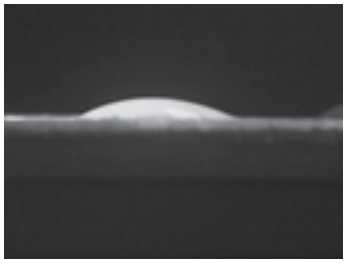
ECAP titanium of lower grades with extra fine grains may be used for manufacturing of highly loaded implant or their parts and presents excelent replacement of strandartly used Ti-6Al-4V alloy. This type of material aslo showes excelent corrosion properties ang high level of biocompatibility, which can be even impoved by different surface treatment. This paper deals with possibility oxidic anodization as a method of creation highly organised nanostructures on implant surface and further chemical treatment of anodized layer in acid/alkaline solutions. It was proved that chemical treatment increases content of specific ions in anodized structure, which will leads into more effective osteointegration process while not affecting its of corrosion properties, which was tested by potentiodynamic polarization methods in artificial isotonic physiological solution according ASTM standards for implants. On the other hand chemical treatment positively affects wettabilility resp. surface energy of studied samples. Many previous studies focused on osteointegration process confirmed that lower values of contact angle directly corelate with effectivity of ossteointegration process and a relation between preferred induced type of organic tissue and implants surface energy has been previously published. Presented procedures of surface treatments shows promising results and might find its use in commertial implants manufacturing.





Biography

Katerina Dedkova has completed her PhD from VSB-Technical University of Ostrava. She is the Researcher at Center of Advanced Innovative Technologies. She has published more than 14 papers in reputed journals and has been serving as a Rewiever of repute journals. Her research interest include biocompatible materials and nanocomposite materials.

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Ahmad Fakih, Nano Res Appl 2019, Volume 05

Microstructure simulator to predict grain formation during thermo-mechanical processing of long products

Ahmad Fakih

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Today, temperature-controlled rolling is a well-known application in rolling mills to improve the technological properties of the materials in accordance with the market requirements. In comparison to standard operation procedures, this processing especially requires a reliable and holistic concept in daily operation. It becomes even more important, when special demands need to be met especially with fast reaction times concerning first results. In order to fulfill such demands successfully without the necessity of extensive test trials, an overall integrated concept for thermo-mechanical rolling of long products has been developed. Special attention is placed on a recently developed microstructure simulator. It is a semi-empirical model for temperature and process calculation predicting the resulting grain sizes, microstructure distribution and mechanical properties. Especially with its customized, flexible database, which can be individually extended, the producers are enabled to react fast to market movements and specific requirements. The simulation software has its focus on the specific microstructure evolution of long products e.g. bar, wire rod and tubes. The simulation model features an analytic model to calculate strain distribution for different reduction configurations and varieties of technological parameters, e.g. temperature, speed, pass geometry for standard mill configurations as well as for the 3-roll technology. Based on the distribution of the strain modification and temperatures over the cross-section of the rolled product, the microstructure simulation is carried out to get a realistic image of the final obtained micro-structural formation.

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Matthias Schuck, Nano Res Appl 2019, Volume 05

Results of using laser triangulation for measuring surface defects in long products

Matthias Schuck

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Alongside profile measurement the technology of laser triangulation is increasingly used to detect surface defects. Such defects can either be of dimensional nature or result from the rolling or sometimes casting process. In the first part, the presentation describes the first-time installation of such a laser triangulation system in a combined long product rolling mill and then goes on to introduce the operative software as well as to give examples of applications. The second part of the presentation illustrates the idea of using the potential of artificial intelligence with regard to detection systems for material defects.

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Alena Michalcová, Nano Res Appl 2019, Volume 05

Self-Healing in rapidly solidified aluminium alloys

Alena Michalcová

University of Chemistry and Technology, Czech Republic

Rapid solidification of alloys can be preformed e.g. by melt spinning method. This process leads to several changes in the microstructure, the main are increase of solubility of allying elements, microstructure refinement and formation of metastable phases such as quasicrystals. These microstructural features have prommising potential for self-healing behaviour of the material. Decomposition of supersaturated solid solution can lead to precipitation healing mechanism that was already proven in underaged aluminium alloy. Decomposition of quasicrystals can also cause closing of the crack in the alloy. The self-healing behaviour in the Al-Cr-Fe alloy was observed in this work. The alloy was studied by LM, SEM and TEM. Correlative SEM/AFM microscopy was also performed.

Biography

Alena Michalcová has completed her PhD from University of Chemistry and Technology in Prague and Postdoc Fellowship in Max-Planck Institute für Eisenforschung in Düsseldorf, Germany. She has published morethan 58 papers in reputed journals.

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Sergio Ricardo de Lazaro et al., Nano Res Appl 2019, Volume 05

A DFT investigation on multiferroism and magnetic coupling in $NiBO_3$ materials

Sergio Ricardo de Lazaro, Luis Henrique da Silveira Lacerda, Renan Augusto Pontes Ribeiro and **Leonardo Konopaski Andreani**

State University of Ponta Grossa, Brazil

In technological field, the emergent materials are known as smart materials because present high sensibility and the ability to adapt to external stimuli. Among the smart materials stand out the multiferroic (MF) materials. The multiferroism effect is associated to the coexistence and coupling between magnetic ordering and ferroelectricity in the same crystalline phase. The most common form of multiferroism is called magnetoelectric (ME) coupling. Some example of MF materials are: $BiFeO_3$ (BFO) which shows a unique set of electronic, optical, magnetic and ferroelectric properties and that can be easily obtained through an epitaxial growing on $SrTiO_3$ substrates; the present abstract aim to show of new MF materials based on $PbNiO_3$ (PNO) materials with R3c structure considering an occupation in A and B sites. Therefore, the A sites were occupied by Ni atoms while the B sites were occupied by Ti, Ge, Zr, Sn and Hf atoms, respectively. The calculation level was choose as Density Functional Theory (DFT) at set B3LYP hybrid functional; employed in CRYSTAL09 software. For all materials investigated as ferromagnetic (FM) as antiferromagnetic (AFM) ordering were simulated. For NiTiO, the AFM ordering was calculated as more stable, in agreement to experimental and other theoretical results. Similar result was calculated for NiHfO, i.e., an AFM ordering. However, the FM ordering was found for NiGeO, NiZrO, NiSnO and NiPbO materials suggesting a relation between structural regularity and magnetic phase. Along the y axis was not observed the formation of charge path between the atomic layers due to proximity between atoms. In case of z direction, discreet charge paths and charge polarization were observed while the higher polarization was exhibited along x direction once superiors charge paths and high polarization are formed. Thus, the ferroelectric properties in R3c materials are preferentially oriented in x direction in crystalline structure as expected for an anisotropic ferroelectric. The multiferroic effect was determined by analysis of magnetic and ferroelectric properties along x, y and z direction of unit cell; it was noted that the magnetic property is oriented along z axis, while the ferroelectric property is oriented preferentially along x axis. Hence, the coupling between both properties evidences a multiferroism effect on $NiBO_3$ (B=Ti, Ge, Zr, Sn, Hf and Pb) materials.

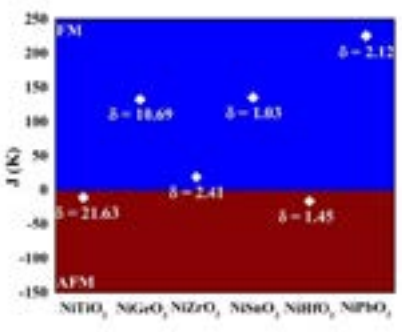

Figure 1: Magnetic coupling constant (J) for NiBO3 (B=Ti)

Figure 2: Electrons oriented in [111] direction within R3c primitive cell. Ge, Zr, Sn, Hf, Pb) investigated materials.

Recent Publications

1. H Tian, X-Y Kuang, A –J Mao, H –J Zhao, H Li and F-G Kuang (2015) Comparing hydrostatic-pressure- and epitaxial-strain-induced phase transitions in multiferroic PbNiO3 from first principles Solid State Communications 203:75-80.
2. L W Martin and R Ramesh (2012) Multiferroic and magnetoelectric heterostructures Acta Materialia 60(6-7): 2449-2470.
3. L W Martin, Y H Chu and R Ramesh (2010) Advances in the growth and characterization of magnetic, ferroelectric, and multiferroic oxide thin films Materials Science and Engineering: R: Reports, 68(2010):89-133.
4. S Picozzi and C Ederer (2009) First principles studies of multiferroic materials, Journal of Physics: Condensed Matter 21 (2009) 303201-303219.
5. S Picozzi, K Yamauchi, I A Sergienko, C Sen, B Sanyal and E Dagotto (2008) Microscopic mechanisms for improper ferroelectricity in multiferroic perovskites: a theoretical review, Journal of Physics: Condensed Matter 20(2008):434208-434218.

Biography

Sergio Ricardo de Lazaro has his expertise in silico experiments, more specifically in solid state chemistry, defects, electronic structure, optical property, magnetism and surface. The main tool used is Density Functional Theory from CRYSTAL code. He proposes a new approach for properties in multiferroic materials and morphology analyses. He is a full Professor at State University of Ponta Grossa acting as a Referee in PCCP *Physical Chemistry Chemical Physics, Journal of Alloys and Compounds, The Journal of Physical Chemistry* and others.

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