EuroSciCon

DAY 1

Scientific Tracks & Abstracts

JOINT EVENT

22nd International Conference on

Advanced Materials and Simulation

&

22nd Edition of International Conference on

Nano Engineering & Technology

December 10-12, 2018 | Rome, Italy

DAY 1

December 10, 2018

Sessions

Nano devices and structured materials | Polymer Science and Engineering | Nano Sensors and Biosensors Advancement in Nanomaterials and Nanotechnology | Nano engineering and Nano Technologies | Biomaterials | Nano Biotechnology Simulation of Materials Processing and Technology | Carbon based Nanomaterials Devices and Technologies | Failure Analysis and Preventions | Adhesives and Joining Technologies

Session Chair
Imran Rizvi
University of North Carolina, USA

Session Co-Chair
Woojin Lee
Nazarbayev University, Kazakhstan

Session Introduction

Title: Electrochromic and electrochemical sensors based on conjugated polymers doped Prussian blue
Arunas Ramanavicius, Vilnius University, Lithuania

Title: Physicochemical properties and antineoplastic effect of omega-3 PUFA loaded in resveratrol-based solid lipid nanoparticles in human colorectal cancer cells in vitro
Simona Serini, Universita Cattolica del S. Cuore, Italy

Title: Vacuum insulation glass finite element analysis of temperature induced stresses and displacements: The EEnsulate case study
Andrea Trevisi, RINA Consulting S P A , Italy

Title: The characteristics of Ni-Cr-Mn-Y-Cu thin film resistors
Ying Chieh Lee, National Pingtung University of Science & Technology, Taiwan

Title: Fluidic stress modulates biomarker expression and therapy response in 3d ovarian cancer nodules
Imran Rizvi, University of North Carolina, USA

Title: Silver Nanoparticles in water treatment: The heavy metals capture
Iole Venditti, University of Rome, Italy

Title: Nondestructive and stealth performance evaluations of composites
Jung-Ryul Lee, Korea Advanced Institute of Science and Technology, South Korea

Title: Application of quantum dots in solar cells and biomedical applications
Mannix P Balanay, Nazarbayev University, Kazakhstan

Title: Multi-scale modeling and performance driven virtual design of advanced steels and coatings for industrial use
Matti Lindroos, VTT Research Center, Finland

Title: Research on post-Si devices based on Ge and 2D channel materials and TCAD simulation
Kazuhiko Endo, National Institute of Advanced Industrial Science and Technology, Japan

Title: Titanium-based catalyst systems for photo-catalytic CO_2 reduction
Aigerim Baimyrza, School of Engineering, Nazarbayev University, Astana, Kazakhstan

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Arunas Ramanavicius et al., Nano Res Appl 2018, Volume 4
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Electrochromic and electrochemical sensors based on conjugated polymers doped Prussian blue

Arunas Ramanavicius, Mindaugas Gicevicius, Gintautas Bagdziunas, Benediktas Brasiunas *and* Almira Ramanaviciene

Vilnius University, Lithuania

Due to unique physical and chemical properties, conjugated polymers are applied in various areas of technology. Synthesis of π-conjugated polymers and modification of electrodes can be performed in several different ways, the most popular of which are chemical, biochemical and electrochemical methods. The electrochromic effects of electrodes modified with electrochromic materials can be evaluated in addition to electrochemical signals. More advanced overview of electrochromic materials and their application in sensor design can be found in our recent review and in our papers, which report the applicability of the electrochemically deposited conjugated polymers (such as polyaniline (PANI) and azo benzene with 3,4-ethylenedioxythiophene moieties) and even inorganic materials (such as Prussian blue). In this presentation, the performance of several electrochemical and electrochromic sensors based on electrochemically deposited π-π conjugated polymers (such as PANI, poly pyrrole and some others) towards the determination of some heavy metal ions, NH_3 and CO_2 will be reported. In present investigation, we have simultaneously studied the electrochemical and electrochromic performances of PANI film before and after the incubation of the PANI/ITO electrode in the solution containing analyte. Two potential steps based on pulse profile have been applied in order to generate chronoamperometric and electro chromic responses of the PANI/ITO electrodes in this investigation.

Recent Publications

1. **Celiesiute R, Ramanaviciene A, Gicevicius M and Ramanavicius A (2018) Electro chromic sensors based on conducting polymers, metal oxides and coordination complexes. Critical Reviews in Analytical Chemistry 1-14.**
2. **Gicevičius M, Bagdziunas G, Abduloglu Y, Gumusay O, Soganci T, Ramanaviciene A, Ak M and Ramanavicius A (2018) Experimental and theoretical investigations of the electrochromic azobenzene and 3, 4-ethylenedioxythiophene-based electrochemically formed polymeric semiconductor. ChemPhysChem 19(20):2735-2740.**
3. **Virbickas P, Valiūnienė A and Ramanavičius A (2018) Towards electrochromic ammonium ion sensors. Electrochemistry Communications 94:41-44.**
4. **Gicevicius M, Celiesiute R, Kucinski J, Ramanaviciene A, Bagdziunas G and Ramanavicius A (2018) Analytical evaluation of optical pH-sensitivity of polyaniline layer electrochemically deposited on ITO electrode. Journal of Electrochemical Society 165(14):H903-H907.**
5. **Deshmukh M A, Gicevicius M, Ramanaviciene A, Shirsat M D, Viter R and Ramanavicius A (2017) Hybrid electrochemical/ electrochromic Cu(II) ion sensor prototype based on PANI/ITO-electrode. Sensors and Actuators B Chemical 248:527-535.**

Biography

Arunas Ramanavicius is a Professor at Vilnius University, Lithuania. He is a Head of Department of Physical Chemistry at Vilnius University and Nanotechnas-Centre of Nanotechnology and Materials Science. He is also leading the Department of Nano Biotechnology at Research Center of Physical Sciences and Technologies. He is a Member of Lithuanian Academy of sciences. He has completed his PhD and Doctor Habilitus degree at Vilnius University in 1998 and 2002, respectively. He is serving as Expert-Evaluator in EU-FP7 program coordinated by European Commission and he is a Technical Advisor of many foundations located in European and Non-European countries. He has research interests in various aspects of nanotechnology, bio-nanotechnology, nanomaterials, biosensorics, bioelectronics, biofuel cells and MEMS based analytical devices. He is a National Coordinator of several nanotechnology related COST actions.

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S Serini et al., Nano Res Appl 2018, Volume 4
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Physicochemical properties and antineoplastic effect of omega-3 PUFA loaded in resveratrol-based solid lipid nanoparticles in human colorectal cancer cells *in vitro*

S Serini[1], R Cassano[2], P A Corsetto[3], A M Rizzo[3], G Calviello[1] and **S Trombino[2]**
[1]Universita Cattolica del Sacro Cuore Italy
[2]Università della Calabria, Italy
[3]Università degli Studi di Milano, Italy

A great effort is being expended during the last years in order to find new strategies able to increase the efficacy and to reduce the deleterious side effects of the drugs currently used for the therapy of cancer. It has been widely demonstrated that the antineoplastic therapies with either conventional or single-targeted drugs could take advantage from a combined treatment with omega-3 polyunsaturated fatty acids (omega-3 PUFA). These nutrients, normally present in our diet, especially in marine fish, have been demonstrated to be safe at the concentrations generally used in human trials, and to be able to modulate molecules involved in cancer cell growth, differentiation and survival. It is accepted that inflammation plays a key role in the development of cancer and, among the mechanisms most often invoked to explain the anti-neoplastic role of omega-3 PUFA, there is their ability to act as potent anti-inflammatory agents. In particular, colorectal cancer (CRC) has been extensively studied among the most common malignancies in the Western world. In the present study, solid lipid nanoparticles (SLN), characterized by a lipid matrix containing resveratrol esterified to stearic acid, have been synthesized and used to encapsulate docosahexaenoic acid (DHA) and α-linolenic acid (LNA). Our aim was to increase the efficiency of the incorporation of these fatty acids into the cells and to prevent their peroxidation and degradation. The resveratrol-based SLN were characterized for their physical-chemical properties, including their antioxidant and for their anti-neoplastic activity. It was observed that the encapsulation of omega-3 PUFA into the SLN enhanced significantly their incorporation in human HT-29 CRC cells in vitro, and their growth inhibitory effects in these cancer cells, mainly by reducing cell proliferation.

Recent Publications

1. Serini S and Calviello G (2018) Long-chain omega-3 fatty acids and cancer: any cause for concern? Current Opinion in Clinical Nutrition & Metabolic Care 21:83-89.
2. Serini S, Cassano R, Corsetto P A, Rizzo A M, Calviello G and Trombino S (2018) Omega-3 PUFA loaded in resveratrol-based solid lipid nanoparticles: physicochemical properties and antineoplastic activities in human colorectal cancer cells in vitro. International Journal of Molecular Sciences 19: pii: E586.
3. Serini S, Ottes Vasconcelos R, Fasano E and Calviello G (2016) How plausible is the use of dietary n-3 PUFA in the adjuvant therapy of cancer? Nutrition Research Reviews 29:102-125.
4. Serini S, Ottes Vasconcelos R, Fasano E, Calviello G (2016) Epigenetic regulation of gene expression and M2 macrophage polarization as new potential omega-3 polyunsaturated fatty acid targets in colon inflammation and cancer. Expert Opinion on Therapeutic Targets 20:843-858.
5. Serini S, Zinzi A, Ottes Vasconcelos R, Fasano E, Riillo MG, Celleno L, Trombino S, Cassano R, Calviello G (2016) Role of β-catenin signaling in the anti-invasive effect of the omega-3 fatty acid DHA in human melanoma cells. Journal of Dermatological Science 84:149-159.

Biography

S Serini is currently an Assistant Professor at the Catholic University of Sacred Heart, School of Medicine, Italy. She completed her MSc degree in Biological Sciences in 1999 at Tor Vergata University, Rome. She received a Post-graduate Diploma (Specialty) in Clinical Pathology in 2004, and a PhD degree in Integrated Oncology in 2009 at Catholic University. In addition to research, she teaches General Pathology and Physiopathology in different courses of the School of Medicine, Catholic University of Sacred Heart, Rome. Her professional interests are in the area of neoplastic and inflammatory disease research, with particular attention to the molecular bases of cancer and to the role of nutrition in the prevention/therapy of cancer. She has authored and co-authored over 50 publications in peer-reviewed journals.

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Andrea Trevisi et al., Nano Res Appl 2018, Volume 4
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Vacuum insulation glass finite element analysis of temperature induced stresses and displacements: the Eensulate case study

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[2]Ulster University, Ireland

Vacuum insulate glass (VIG) are often employed in buildings where exists the necessity of reducing the U-value of the walls, without compromising the amount of sunlight in the inner spaces. The system is mainly made of two glass panes spaced through the presence of several support pillars applied on their surfaces and the insulation performance of this kind of glazing unit are obtained by removing the filling gas between the glasses and by creating the vacuum between them. As consequence, the heat transport due to the presence of the interposed gas is removed but at the same time, the atmospheric pressure and the thermal deformations act on the glass panes by inducing a deflection of the system and stress on its components (pillars, panes and sealing). In Eensulate European Project (HORIZON 2020 research program), an innovative light weight VIG glazing unit has been developed, by employing a low temperature durable edge seal system based on polymeric seal materials instead of glass frit. The aim of this paper is to describe the finite element model of the innovative system, developed to evaluate its behavior during its operative condition, considering the thermal expansion and the effect of vacuum pressure, focusing specifically on the interaction between glass panes and sealant. In particular, the induced deflection, the stress on both components and the strain on the sealant were investigated. In addition, the effects of glass dimension, temperature difference, type of sealant and sealant thickness were analyzed, by evaluating the behavior of VIG as function of the mentioned parameters. Simulations results were useful to optimize the design of the glazing unit and to support the choice of the employed materials.

Recent Publications

1. **P Henshall, P Eames, F Arya, T Hyde, R Moss and S Shire (2016) Constant temperature induced stresses in evacuated enclosures for high performance flat plate solar thermal collectors. Solar Energy 127:250-261.**
2. **Y Fang, T Hyde, F Arya, N Hewitt, R Wang and Y Dai (2015) Enhancing the thermal performance of triple vacuum glazing with low emittance Coatings. Energy and Buildings 97: 186-195.**
3. **Y Fang, T Hyde, F Arya, N Hewitt, P C Eames, B Norton and S Miller (2014) Indium alloy-sealed vacuum glazing development and context. Renewable and Sustainable Energy Reviews 37:480-501.**
4. **Y Fang, T Hyde, F Arya and N Hewitt (2013) A novel building component hybrid vacuum glazing-a modeling and experimental validation. ASHRAE Transactions 119(2):430-442.**
5. **Cioffi M, Di Gennaro F, Zinetti S, Bax L, Boudjabeur S, Bourdeau L, Dankl C, Herrmann E, Jadwiga F, Oakey J, Scalia M and Elvnert J (2012) Cross-ETP research and innovation roadmap for the energy efficiency in building. Steinbeis-Edition ISBN 978-3-943356-37-3.**

Biography

Andrea Trevisi is a Researcher at RINA Consulting S P A where, he is working as a Finite Element Method Analyst since 2017. He has expertise in FEM simulation, dealing with several types of analyses (structural, thermal, vibration and dynamic). Through his Master's degree in Materials Engineering and Nanotechnology, he has in-depth knowledge in composites, metallic materials and polymeric materials, covering main related topics, manufacturing processes and degradation phenomena.

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Ying Chieh Lee et al., Nano Res Appl 2018, Volume 4
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The characteristics of Ni-Cr-Mn-Y-Cu thin film resistors

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Ni-Cr-Mn-Y-Cu resistive thin films were prepared on glass and Al_2O_3 substrates by DC magnetron co-sputtering from targets of Ni-Cr-Mn-Y casting alloy and Cu metals. Electrical properties and microstructures of Ni-Cr-Mn-Y-Cu films under different proportion of elements and annealing temperatures were investigated. The phase evolution, microstructural and composition of Ni-Cr-Mn-Y-Cu resistive films were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and Auger Electron Spectroscopy (AES). When the annealing temperature was set to 350°C, the Ni-Cr-Mn-Y-Cu films with an amorphous structure were observed. The Ni-Cr-Mn-Y films with 6.4% Cu addition annealed at 300°C which was exhibited the resistivity 770-cm with +15 ppm/°C of temperature coefficient of resistance (TCR).

Recent Publications

1. **Jie-Ting Shang, Chih-Ming Chen, Ta-Chih Cheng and Ying-Chieh Lee (2015) influences of annealing temperature on microstructure and properties for TiO2 films deposited by DC magnetron sputtering. Japan Journal of Applied Physics 54(12):5501-6.**
2. **Wei-Ju Chen, Tung-Yueh Liu, Ho-Yun Lee and Ying-Chieh Lee (2018) Ni-Cr-Mn-Y-Nb resistive thin film prepared by co-sputtering. Materials Chemistry and Physics 210:327-335.**
3. **Chein-Hui-Yang, Chih-Neng Yang and Ying-Chieh Lee (2017) Surface roughness improvement of alumina substrates coated using aluminum nitride sol gel. Journal of Ceramic Processing Research 18(9):628-633.**
4. **Cheng-Hsien-Lin, Ho-Yun Lee, Yaw-Teng Tseng and Ying-Chieh Lee (2018) A Study on the Ni-Cr-Mn-Zr thin film resistors prepared using the magnetron sputtering technique. Thin Solid Film DOI: 10.1016/j.tsf.2018.04.015.**
5. **Ming-Yuan-Yeh, Pin-Yung Lee, Jie-Ting Shang and Ying-Chieh Lee () The effect of thermal oxidation temperatures on the phase evolution and photocatalytic property of tungsten doped TiO2 thin film. Japan Journal of Applied Physics 57:125801.**

Biography

Ying Chieh Lee has completed his PhD from Department of Materials Science and Engineering, National Chung Hsing University. He is a Professor in Department of Materials Engineering, National Pingtung University of Science and Technology. He has published more than 70 papers in reputed journals and has been serving as coatings editorial board member of repute.

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Fluidic stress modulates biomarker expression and therapy response in 3D ovarian cancer nodules

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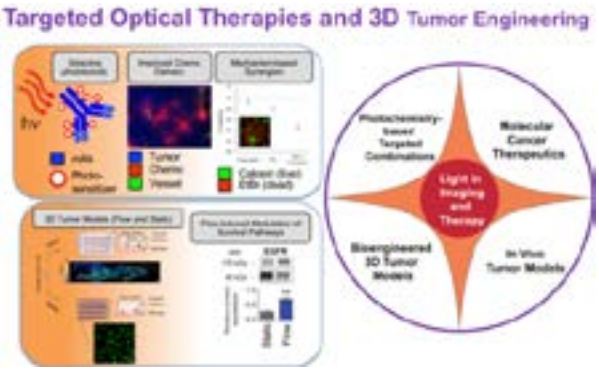
This presentation will focus on the mechanistic rationale for using lasers in medicine, biology and principles of tumor engineering to address chemoresistance in cancer. Physiological barriers to drug delivery and therapy induced molecular selection pressures preclude durable improvements in survival for many cancer patients. It is increasingly evident that the most effective treatments will involve cooperative regimens that target multiple non-overlapping pathways, while minimizing systemic toxicities. Photodynamic therapy (PDT) is a light based treatment that can improve the therapeutic index of traditional and emerging treatments. The photochemical cytotoxic mechanisms triggered by PDT induce damage to sub cellular organelles, prime tumor cells, disrupt stromal compartments and enhance drug delivery. This presentation will describe key factors that guide the development of PDT based therapeutic regimens. A specific focus is on enhancing the efficacy of camptothecin analogues and platinum based chemotherapies, which are commonly used to manage cancers, but suffer from significant toxicities, poor drug penetration and resistance. PDT overcomes these barriers of efficacy, due to its distinct mechanisms and non-overlapping toxicities. Capturing these attributes in rationally designed combinations leads to synergistic tumor reduction in 3D models and durable tumor control in orthotopic xenograft mouse models for ovarian and pancreatic cancer. The mechanistic basis of these improved outcomes will be presented by harnessing photo initiated sub cellular cytotoxic mechanisms (e.g. damage to mitochondria/ER and degradation of bcl-2) to prime tumor cells for subsequent mechanistically distinct chemotherapeutic insult, thereby lowering the threshold to tumor destruction; stromal and vasculature disruption to improve drug delivery, significantly enhancing the penetration of chemotherapeutics and increasing intratumoral accumulation by >10 fold and mitigation of chemotherapy induced enrichment of cellular stemness markers (e.g. CD44, CXCR4) to provide significant and sustained reductions in local and distant tumor burden and prolonged improvements in survival. Results will be discussed in the context of imaging and therapeutic applications of light, bioengineered 3D models and targeted drug delivery for inhibition of molecular survival pathways in tumors.



Biography

Imran Rizvi has completed his PhD in Engineering Sciences in the Thayer School of Engineering at Dartmouth College, an MS in Tumor Biology in the Lombardi Comprehensive Cancer Center at Georgetown University, and a BA at Johns Hopkins University. He was an Assistant Professor of Dermatology (tenure-track) at Harvard Medical School (HMS) and an Assistant Biomedical Engineer at the Wellman Center for Photomedicine (WCP), Massachusetts General Hospital (MGH), Boston. His expertise is in imaging and therapeutic applications of light, bioengineered 3D models and animal models for cancer and targeted drug delivery for inhibition of molecular survival pathways in tumors. His K99/R00 (NCI) develops photodynamic therapy (PDT) based combinations against molecular pathways that are altered by fluidic stress in ovarian cancer. He is also Co-PI on an Innovation Award with Bristol-Myers Squibb to develop optical techniques in immuno oncology for light-based modulation of immune response. He has co-authored 39 peer-reviewed publications and five book chapters with a focus on PDT, biomedical optics and molecular targeting in cancer. He is a Council Member of the of the American Society for Photobiology (ASP), Chair of the ASP Awards Committee and Secretary of the Executive Committee of the Pan American Photodynamic Association. He serves in several organizing committees and Scientific Advisory Boards including the Program Committee for SPIE Photonics West (BIOS Conference B0110) and the World Congress of the International Photodynamic Association.

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Silver nanoparticles in water treatment: the heavy metals capture

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[2]Tor Vergata University of Rome, Italy
[3]INAIL, Italy
[4]Sapienza University of Rome, Italy

Chemical sensors are generally based on the concomitant presence of two elements, a recognition element (active element) sensitive to stimuli produced by various chemical compounds (analytes) and a transduction element that produces a signal whose magnitude is related, through a known relationship, to the concentration of the analyte itself. The use of silver nanoparticles (AgNPs) as active element in sensors has a recent story and the first attempts date back to the early 2000s [1]. In particular the use foe water treatment becomes very significant in the last years. AgNPs, in comparison for example with metal oxides, present numerous advantages such as a high sensitivity, a short response time, room temperature operation, the possibility of tuning both chemical and physical properties by using different capping agent. In the present work, AgNPs were prepared and their interaction with heavy metal ions was studied using different techniques. Morphological and dimensional characterizations of the AgNPs-3MPS (average size and shape) before and after the interaction with heavy metals were obtained by Transmission Electron Microscopy (TEM) and Dynamic Light Scattering (DLS) studies. Moreover, the system was investigated by means of different techniques, such as Uv-vis, Fourier Transform Infrared Spectroscopy (FTIR) and High-Resolution X-ray photoelectron spectroscopy (HR-XPS), in order to understand the mechanism of Surface plasmon resonance (SPR) sensing.

Recent Publications

1. **F. Mochi, L. Burratti, I. Fratoddi, I. Venditti*, C. Battocchio, L. Carlini, G. Iucci, M. Casalboni, F. De Matteis, S. Casciardi, S. Nappini, I. Pis, P. Prosposito; Interaction of colloidal silver nanoparticles with Co2+ and Ni2+ in water for sensing application; Nanomaterials 8 (2018) 488; doi:10.3390/nano8070488**
2. **F. Porcaro, L. Carlini, A. Ugolini, D. Visaggio, I. Luisetto, P. Visca, I. Fratoddi, I. Venditti, L. Simonelli, C. Marini, W. Olszewski, N. Ramanan, C. Battocchio; Synthesis and Structural Characterization of Silver Nanoparticles Stabilized with 3-Mercapto-1-Propansulfonate and 1-Thioglucose Mixed Thiols for Antibacterial Applications; Materials 9 (2016) 1028 doi:10.3390/ma9121028**
3. **P. Prosposito, F. Mochi, E. Ciotta, M. Casalboni, I. Venditti*, L. Fontana, G. Testa, I. Fratoddi; Hydrophilic silver nanoparticles with tunable optical properties: application for the detection of heavy metals in water ; Beilstein J. Nanotechnol. 7 (2016) 1654-1661. doi:10.3762/bjnano.7.157**

Biography

Venditti I is a Researcher in Inorganic Chemistry in Department of Sciences at University of Rome Tre, Italy. Her scientific interests are focused in the field of micro and nanostructured materials for advanced technological applications. The preparation of such structures material used was noble metals (Au, Ag, Pt and Pd) and polymeric materials (organometallic polymers, polyenes and polyacrylates) obtained in nano micrometric dimensions and controlled shape through different approaches. These research activities have been reported in 70 papers in international peer-reviewed journals, two book chapters and two patents.

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Application of quantum dots in solar cells and biomedical applications

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[2]National Laboratory Astana - Nazarbayev University, Kazakhstan

There has been an increasing use of quantum dots for various applications in recent years. In this talk, author will be focusing on the use of quantum dots as counter electrodes in dye-sensitized solar cells (DSSCs) and as bioimaging and possible cancer treatment. In DSSCs, the use of Pt is still widely used as counter electrodes (CE) owing to its high catalytic efficiency and stability but the downside is its cost. In this regard, we synthesized a tri-doped natural carbon dots as an alternative CE in DSSCs. We assessed different metal ions with ethylenediamine and sulfur powder as additives. We also applied sulfur-limonene polysulfide as substrate for our quantum dots. All our results showed efficiency very close to the Pt electrodes which could be used as low-cost CE alternatives. Water-soluble fluorescent carbon-dots derived from natural sources having a particle size <2 nm were used as possible bioimaging agent and cancer treatment. Various characterization data and possible new approach in the stimulation of ARF-mediated signaling to inhibit nuclear YAP using nanomaterials will be discussed.

Recent Publications

1. **Estrella L L, Balanay M P and Kim D H (2018) Theoretical insights into D-D-A sensitizers employing N-annulated perylene for dye-sensitized solar cells. Journal of Physical Chemistry A DOI:10.1021/acs.jpca.8b03331.**
2. **Xie Y, Sun Q, Nurkesh AA, Lu J, Kauanova S, Feng J, Tursynkhan D, Yang Q, Kassymbek A, Karibayev M, Duisenova K, Fan H, Wang X, Manarbek L, Maipas A, Chen Z and Balanay M P (2017) Dysregulation of YAP by ARF stimulated with tea-derived carbon nanodots. Scientific Reports 7:16577.**
3. **Balanay M P and Kim D H (2017) Strategic design of bacteriochlorins as possible dyes for photovoltaic applications. Journal of Physical Chemistry A 121:6660-6669.**
4. **Balanay M P, Choi K S, Lee S H and Kim D H (2017) Experimental and theoretical analysis of organic dyes having double D- -A configurations for dye-sensitized solar cells. Spectrochimica Acta Part A 173:361-368.**

Biography

Mannix P Balanay has completed his PhD in Physical Chemistry from Kunsan National University, Republic of Korea and subsequently hired as a Research Professor in the same University. Before coming to Korea, he was an Instructor at Siquijor State College and Silliman University. Currently, he is an Assistant Professor in Chemistry at Nazarbayev University, Astana, Kazakhstan. His work applies both computational and experimental techniques to study various materials that are relevant to the current needs of the society, such as energy, environment and health.

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Multi-scale modeling and performance driven virtual design of advanced steels and coatings for industrial use

Lindroos M, Laukkanen A, Andersson T, T J Hakala and **Holmberg K**
VTT Research Center of Finland, Finland

The demand for more efficient and durable material solutions is continuously rising in industry. Longer material life spans combined with energy efficient solutions reduce environmental load and enhances business potential. The conventional research and development (R&D) routes in searching for new material solutions make use of extensive experimental programs and material characterization, which often results in a high cost trial and error scenario. Furthermore, it is quite difficult to ascertain prevailing stress/strain states and the dynamic nature of failure initiation and progression. It is therefore challenging to establish causalities and links between microstructure of a material and its performance. Optimization of the microstructure for a certain application requires a considerable joint effort of material processing and retesting of different solutions. Integrated computational materials engineering (ICME) offers one solution to cut down costs and reduce uncertainties of materials R&D process. Virtual modeling utilized together with advanced characterization and experimental work allows designing microstructures more effectively and understanding the prevailing phenomena more easily. Multi-scale modeling makes it possible to couple macroscopic application scale with a large amount of concurrent physical phenomena and fine scale microstructure level with detailed individual phenomena, which enables performance driven virtual design on material solutions. In the present work, we demonstrate ICME based approach on developing advanced steels and coatings for industrial applications. For example, tribological contacts are examined at different length and time scales. Microstructure based models are employed to reveal microscale deformation behavior and failure mechanisms. For advanced steels including martensitic and high manganese austenitic steels, high stress abrasive conditions are analyzed at macroscopic and microscopic scales. Crystal plasticity models are used to describe micromechanics and evaluate the performance of different virtually designed microstructure alternatives. Coatings are studied in terms of coating structures and topographical features to evaluate the damage mechanisms, tolerances and ultimately tendency to fatal cracking. The effect of coating microstructural features and properties are discussed from the wear resistance point of view.

Biography

Lindroos M is working at VTT Research Center of Finland in the Multiscale Materials Modeling Research Group. His current active research interests are related to multi scale modeling and integrated computational materials engineering with an application to a wide range of different materials and industrial/academic material challenges.

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Research on post-Si devices based on Ge and 2D channel materials and TCAD simulation

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The scaling limit of current CMOS technologies has been approaching rapidly. To further enhance performance of CMOS devices, advanced materials such as Ge and 2D materials are promising candidates. Advanced materials and devices integration group in AIST explore device integration technologies for going beyond the performance limit of Si CMOS. The research topics include Ge/III-V MOSFETs, 3D build-up integration, 2D channel materials and devices incorporating new materials and mechanisms such as spin FET and negative capacitance FET. We also focus on methodology and modeling of TCAD simulation and their application for various semiconductor devices. In this presentation, author will briefly introduce their current research activities. Recently, high-performance and low-power LSI is realized by miniaturization and scaling. However, as technology node approaches below 10 nm in 2020s, the end of the scaling is speculated. We are working on 3D build-up integration by vertical stacking of 2D circuits after the end of the scaling. For the stacking channel materials, we are focusing on both Ge and 2D-dichalcogenide materials. Ge substrate is one of the promising platforms for high-mobility channel transistors and photonic devices. We focus on high quality Ge platform by bonding epitaxially grown Ge layers to any substrates. Also, 2D-dichalcogenide materials attract much attention because of their unique characteristics. We focus on gas source Chemical Vapor Deposition of 2D-dichalcogenide and its 3D-stacked device application to realize beyond Si high-performance and low-power integrated circuits. In addition, the technology CAD (TCAD), a computer simulation for semiconductor manufacturing process and semiconductor device physics is very important for the post Si devices. We focus on methodology and modeling of TCAD simulation and their application for various semiconductor devices. We collaborate with other institutes in AIST to apply TCAD simulation for various devices and various projects and we also focus on industrial collaboration.

Biography

Kazuhiko Endo is a Group Leader in the Advanced Materials and Devices Integration Group, Nanoelectronics Research Institute and National Institute of Advanced Industrial Science and Technology, Japan. He has completed his PhD in Electrical Engineering at the Waseda University in 1999. His research interests include nanometer scale manufacturing for aggressively scaled multi gate devices in advanced CMOS technologies. Prior to joining AIST, he was with Silicon Systems Research Laboratories, NEC Corporation from 1993 to 2003 where, he worked on the research and development of multilevel interconnects and high-k gate-stack technologies for ULSI. He was a Visiting Scholar at the Stanford University in 1999 and at the University of California Santa Barbara in 2015.

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Aigerim Baimyrza et al., Nano Res Appl 2018, Volume 4
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Titanium-based catalyst systems for photo-catalytic CO_2 reduction

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The development of facile and robust photo-catalyst to establish the photo-catalytic CO_2 reduction in industrial scale would considerably reduce the amount of greenhouse gases in the atmosphere and as a renewable source of industrially valuable compounds like methanol, formic acid and other hydrocarbon compounds.

Ti-based compounds including TiO_2 remains to be the most robust photo-catalyst for CO_2 reduction with two main drawbacks: poor selectivity and high activation energy [1]. Incorporation of vanadium with titanium in ternary metal oxides considerably narrows the band gap energy from 3.2 eV for pure TiO_2 up to 1.7 eV for Ti-V-O ternary oxide with the increase of vanadium content, making the ternary oxide visible light active [2]. Ti-based MOFs are an ideal class of materials to apply as a catalyst for the range of photo-catalytic processes including the photo-reduction of CO_2 [3]. Introduction of Ti into MOF may allow to tune the photo-responsive properties and selectivity of titanium and enhance other properties of the catalyst as the porosity and stability by changing the organic counterpart. Herein we report on TixVyOz and new type Ti-MOF composites and their photo-catalytic properties. The obtained composites were characterized by XRD, TEM, SEM, BET and TGA. The CO_2 conversion rate was also studied by changing reaction parameters such as UV wavelengths, gas flow rate, etc.

Recent Publications

1. **S. Nahar, M. F. Zain, A. Kadhum, H. Hasan and M. Hasan. Materials 10 (2017) 629.**
2. **M. Park, Y. Lim, Y. Sung , D. Kwak and J.Lee. Acta Physica Polonica A, 129 (2016) 875.**
3. **J. Zhu, P-Z. Li, W. Guo, Y Zhao and R. Zou. Coordination Chemistry Reviews 359 (2018) 80.**

Biography

Aigerim Baimyrza hold a BTech degree in Chemical Engineering of Organic Substance from Al-Farabi Kazakh National University and MSc degree in Polymer Material Science and Engineering from University of Manchester. After the graduation she joined Nazarbayev University (Astana, Kazakhstan) as a Teaching Assistant and the Institute of Batteries (Astana, Kazakhstan) as a Junior Researcher. Currently she is a Research Assistant in Nazarbayeve University and a part of research team working on photo-catalytic conversion of CO_2 into hydrocarbon fuel.

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DAY 2

Scientific Tracks & Abstracts

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DAY 2

December 11, 2018

Sessions

Surface Coatings and Tribology | Nano Biotechnology Electrical, Optical and Magnetic Materials | Nano engineering and Nano Technologies | Additive Manufacturing | Polymer Science and Engineering | Construction Materials

Session Chair
Lev Rapoport
Holon Institute of Technology, Israel

Session Co-Chair
Ying Chieh Lee
National Pingtung University of Science & Technology, Taiwan

Session Introduction

Title: Development of nanocellulose for studies of iron speciation in aquatic systems

Danielle Goveia, Sao Paulo State University, Brazil

Title: Microstructure, nanohardness and chemical composition of thin layers after friction of four FCC metals in lubricated conditions

Lev Rapoport, Holon Institute of Technology, Israel

Title: Electronic state of sulfide-based solid-state electrolytes applied to all-solid-state lithium ion secondary batteries

Yoshiyuki Kowada, Hyogo University of Teacher Education, Japan

Title: Piezoelectric MEMS devices: From material aspects to low-power applications

Michael Schneider, Institute of Sensor and Actuator Systems, Austria

Title: Additive manufactured lightweight porous materials

Che-Nan Kuo, Asia University, Taiwan

Title: Energy input effects on microstructure evolution of Ti- 6Al-4V fabricated by electron beam additive manufacturing

Min-Tsang Tsai, Asia University, Taiwan

Title: Potential for using natural pozzolana for concrete in Kuwait

Saud Al-Otaibi, Kuwait Institute for Scientific Research, Kuwait

Title: Nanochip-induced epithelial to mesenchymal transition: Impact pf physical microenvironment on cancer metastasis

Udesh Dhawan, Academia Sinica, Taiwan

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Development of nanocellulose for studies of iron speciation in aquatic systems

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[2]UNESP, Araraquara, Brazil
[3]Federal University of ABC, Brazil

Cellulose is a natural abundant material advising of renewable and sustainable resources. This material and intense research subject but how will this material behave in aquatic systems? The synthesis route was development of cellulose in a reduced scale starting from the bleached pulp from the extraction of the wood by kraft process. A particulate concentration measured by analysis of zeta potential. The concentration of the particles was measured by Nanoparticles Tracking Analysis (NTA-Malvern®). The Figure 1 presented the relationship between concentration and particle size of sample for conditions using 3.0 g cellulose pulp, 20 minutes sonication and 450 nm membrane filtration.

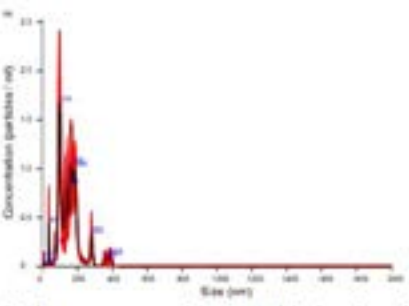

Figure 1 - Relationship between concentration and particle size of sample.

The particles were obtained on a nanoscale and can be applied in environmental studies. Nanocellulose were added in solution containing complexes of the iron and Aquatic Humic Substances (Fe-AHS). By ultrafiltration system and determination in atomic absorption spectrometry was made the speciation of metallic species in the presence of organic matter in the form of humic substances and subsequent addition of nanoparticles. The iron total concentration (Fetotal) in the solution 1.70 mg.L-1. After 24 hours 0.29 mg.L-1 of free iron in solution (Fefree) and 1.41 mg.L-1 of complexed iron with humic substances (Fe-SHA) were determined. After 24 hours of the addition of the nanoparticles to this solution the free metal concentration increased to 0.85 mg.L-1 (Fefree). Before addition of nanocellulose more than 80% of the ions are complexed to the AHS. The kinetics of the reaction were evaluated as a function of time. It also presents the concentration of iron complexed for a period of 24 hours in the presence of nanocellulose showing its influence on the SHA-Metal complexes. In the first minutes after the addition of nanocellulose, a concentration of iron complexed with SHA occurs the ions originally complexed to SHA may be available in solution. This result indicates that there is interaction between the nanoparticle and the humic substance.

Recent Publications

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2. Monteiro, Adnívia ; Goveia, Danielle ; Rotureau, Elise ; Rosa, André ; Masini, Jorge ; Pinheiro, José (2018). Especiação Dinâmica De Metais Traço Em Ambiente Aquático Usando Cronopotenciometria De Redissolução Anódica. Quimica Nova , V. 41, P. 796-809.
3. Cunha, Graziele Da Costa ; Goveia, Danielle ; Romão, Luciane Pimenta Cruz ; Oliveira, Luciana Camargo De (2015). Effect Of The Competition Of Cu(Ii) And Ni(Ii)

On The Kinetic And Thermodynamic Stabilities Of Cr(Iii)-Organic Ligand Complexes Using Competitive Ligand Exchange (Edta). Journal Of Environmental Management, V. 154, P. 259-265.

4. **Pinheiro, Jose Paulo ; Rocha, Luciana S. ; Goveia, Danielle ; Town, Raewyn M. (2014). Scanned Stripping Chronopotentiometry At Bismuth Film Rotating Disc Electrodes: A Method For Quantitative Dynamic Metal Speciation. Environmental Chemistry (Collingwood. Print), V. 11, P. 150.**
5. **Goveia, Danielle; Milkova, Viktoria ; van Leeuwen, Herman P. ; Rosa, Andreì Henrique ; Pinheiro, José Paulo (2011). Dynamics and Heterogeneity of Pb(II) Binding by SiO. Langmuir, v. 27, p. 7877-7883.**

Biography

Post-doctorate in Chemistry, PhD and Master in Analytical Chemistry by the Institute of Chemistry of the São Paulo State University - UNESP, graduated in Chemistry from the State University of Maringá. She is currently Assistant Professor of the Production Engineering Course at Campus Itapeva at the UNESP. Has experience abroad, through internships in the Netherlands (University of Wageningen) and in Portugal (University of Algarve) in collaboration with professors Herman H. P. van Leewen and José Paulo Pinheiro. Professor accredited in the Post-Graduate Program in Engineering of Biomaterials and Bioprocesses of the Faculty of Pharmaceutical Sciences of UNESP of Araraquara-SP. Since 2014 it is leader of the Research Group: Energy, Pulp and Environment. He works in Analytical Chemistry, with emphasis on Trace Analysis and Environmental Chemistry. She has published 28 articles in leading magazines.

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Microstructure, nano hardness and chemical composition of thin layers after friction of four FCC metals in lubricated conditions

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[2]Holon Institute of Technology, Israel
[3]The Weizmann Institute of Science, Israel

In the present work the evolution of deformation microstructure, nano hardness and chemical composition of four FCC metals (Ag, Cu, Ni, Al) after friction in the lubricated conditions are studied. Deformation hardening and grain size as well as friction and wear depend strongly on stacking fault energy (SFE). In light of the above, we evaluate here the effect of plastic deformation on microstructure evolution, chemical composition and hardness and their connection to the friction and wear properties of studied metals with different SFE. All friction lubricated tests were conducted using pure polycrystalline FCC metals with different SFE. The cross sectional transmission electron microscopy (TEM) lamellae were prepared from the pins using a focused ion beam (FIB). In TEM we analyzed regions of the pins after friction in steady state, where the friction coefficient ( ) and hardness (Hs) remained unchanged with deformation in boundary lubrication (BL). Thermally activated process of the rearrangement and annihilation of dislocations are accelerated during friction of Ni due to high SFE and contact temperature. Cross-sectional microstructures observed normal and parallel to the direction of friction are dissimilar. Steady state values of grain size, ds and hardness, Hs after friction in lubricated conditions are explained by a balance between hardening and dynamic recovery in surface layers strongly depending on the SFE and temperature. A correlation between the wear properties (wear coefficient) and total work of deformation during nano indentation shows a similarity in the nano and micro scales in lubricated friction.

Recent Publications

1. **A Moshkovich, I Lapsker, Y Feldman and L Rapoport (2017) Severe plastic deformation of four FCC metals during friction under lubricated conditions. Wear 386:49-57.**
2. **I Popov, A Moshkovich, S R Cohen, V Perfilyev, A Vakahy and L Rapoport (2018) Microstructure and nano hardness of Ag and Ni under friction in boundary lubrication. Wear 404:62-70.**
3. **I Popov, A Moshkovich, T Bendikov and L Rapoport (2018) Deformation Microstructure and Chemical Composition of Surface Layers of Cu and Al Under Friction in Lubricated Conditions. Tribology Letters 66(3):78.**

Biography

Lev Rapoport is the Head of the Center for Materials Engineering and the Laboratory of Tribology at the Holon Institute of Technology. Friction and wear properties of fullerene-like nanoparticles were studied at first in his laboratory. Last some years he studied the interaction between structure friction and wear. He is the Principal Investigator in several research grants sponsored by the Israel Ministry of Science, the Bi-national Israel-USA and Germany-Israel Funds. He is the author more than 100 publications. He is Vice-President of the Tribology Council in Israel.

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Yoshiyuki Kowada, Nano Res Appl 2018, Volume 4
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Electronic state of sulfide based solid state electrolytes applied to all solid state lithium ion secondary batteries

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All solid state batteries are expected as the next generation secondary batteries for their higher energy density, inflammable properties, and so on. In order to develop these batteries, there are several problems to improve. One of the important to improve is the ionic conductivities of the solid state electrolyte. In order to improve the ionic conductivity, electronic states of the sulfide based lithium ion conducting glasses were calculated by the DV-Xα cluster method, which is one of the first principle density functional methods. The cluster models were constructed by the coordination number reported by experimental methods and the bond length estimated from the ionic radii of each ion. The movement of the Li ion was simulated by several model clusters with different positions of the moving ion. The relationship between ionic conductivity and the differential total bond overlap population (DBOP) of the moving ion was discussed for the sulfide based glasses in the systems $Li_2S–SiS_2–Al_2S_3$ and $Li_2S–SiS_2–P2S_5$. In these glasses, the DBOP with the movement of the lithium ion had good negative correlations with the ionic conductivities and positive correlations with the activation energies obtained by the experimental measurements. In any cases, the smaller change of DBOP of the moving cations played an important role for the fast ion movement in the superionic conducting glasses. In order to search for additives with higher ionic conductivity, the composition dependence of differential total bond overlap population with addition of various fourth periodic elements to Li_2S-SiS_2 solid state electrolyte was estimated, as shown in the figure. As described above, the smaller change of the total bond overlap population with the moving Li ion makes lager ionic conductivities. The figure suggests that the addition of In, Sn and Sb to Li_2S-SiS_2 solid state electrolyte could show larger ionic conductivities. This bonding state of the moving cations is one of the characteristics of the electronic state in the sulfide based lithium ion conducting glasses.

Recent Publications

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2. Matsuyama T, Deguchi M, Mitsuhara K, Ohta T, Mori T, Orikasa Y, Uchimoto Y, Kowada Y, Hayashi A and Tatsumisago M (2016) Structure analyses using X-ray photoelectron spectroscopy and X-ray absorption near edge structure for amorphous MS3 (M: Ti, Mo) electrodes in all-solid-state lithium batteries. Journal of Power Sources 313:104-111.
3. Kowada Y, Hayashi A and Tatsumisago M (2010) Chemical bonding of li ions in li7p3s11 crystal. Journal of the Physical Society of Japan 79:65-68.
4. Kowada Y, Tatsumisago M and Minami T (2009) Chemical bonding and lithium ion conductions in Li3N. Solid State Ionics 180(6-8):462-466.
5. Kowada K, Nishitani W and Ogasawara K (2009) Total cluster energy calculation of lithium ion conductors by the dv-xα method. International Journal of Quantum Chemistry 109(12):2658-2663.

Biography

Yoshiyuki Kowada has his expertise in structural analysis, electronic state calculation and chemical bonding analysis of amorphous materials. He applied the DV-Xα cluster method, which is one of the first principle molecular orbital calculations to the solid-state electrolytes and phosphor materials with rare earth ions. Recently, he pays attention on the study about materials to all solid state Li ion batteries for electric vehicles. He is the President of the Society for Discrete Variational Xα.

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Piezoelectric MEMS devices from material aspects to low-power applications

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Electromechanical transducers based on the piezoelectric effect are continuously finding their way into micro-electromechanical systems (MEMS), typically in the form of thin films. Piezoelectric transducers feature a linear voltage response, no snap in behavior and can provide both attractive and repulsive forces. This removes inherent physical limitations present in the commonly used electrostatic transducer approach while maintaining beneficial properties such as low power operation. Furthermore, piezoelectric materials can serve for both actuation and sensing purposes, thus enabling pure electrical excitation and read out of the transducer element in combination with a compact design. Based on these outstanding features, piezoelectric transducers are operated most beneficially in a large variety of different application scenarios, ranging from resonators in liquid environment, advanced acoustic devices to sensors in harsh environments. In order to exploit the full potential of piezoelectric MEMS in the future, interdisciplinary research efforts are needed ranging from investigations of advanced piezoelectric materials over the design of novel piezoelectric MEMS sensor and actuator devices to the integration of Piezo MEMS devices into full low-power systems. In this presentation, we will highlight latest results on the electrical, mechanical and piezo electrical characterization of sputter-deposited aluminium nitride (AlN) including the impact of sputter parameters, film thickness and substrate pre-conditioning. We will present the impact of doping of AlN with scandium, which leads to an increase of the moderate piezoelectric coefficient of AlN upto a factor of four. We will also present first results on the piezoelectric co-polymer PVDF TrFE. In next step, these films are implemented into fabrication processes of cantilever type MEMS devices. In combination with a tailored electrode design resonators are realized featuring in liquid Q-factors upto about 300 in the frequency range of 12 MHz. This enables the precise determination of the viscosity and density of fluids upto dynamic viscosity values of almost 300 mPas. Besides this application, such as high Q factors are useful when targeting mass sensitive sensors, thus paving the way, for e.g., particle detection even in highly viscous media. Given the low increase in permittivity of ScAlN compared to AlN, another field of application for this functional material class is vibrational energy harvesters, where the benefit of ScAlN compared to pure AlN is demonstrated. Finally, we will present some selected results of ScAlN thin films within SAW devices ranging from high temperature applications to droplet manipulation in microfluidics.

Recent Publications

1. P M Mayrhofer, C Rehlendt, M Fischeneder, M Kucera, E Wistrela, A Bittner and U Schmid (2017) ScAlN MEMS cantilevers for vibrational energy harvesting purposes. Journal of Micro electromechanical Systems 26:102-112.
2. M Schneider, A Bittner and U Schmid (2015) Improved piezoelectric constants of sputtered aluminium nitride thin films by pre-conditioning of the silicon surface. Journal of Physics D: Applied Physics 48(40):405301.
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4. W Wang, P M Mayrhofer, X He, M Gillinger, Z Ye, X Wang, A Bittner, U Schmid and J K Luo (2014) High performance AlScN thin film based surface acoustic wave devices with large electromechanical coupling coefficient. Applied Physics Letters 105(3):133502.
5. M Schneider, A Bittner, F Patocka, M Stöger-Pollach, E Halwax and U Schmid (2012) Impact of the surface-near silicon substrate properties on the microstructure of sputter-deposited AlN thin films. Applied Physics Letters 101(22):221602.

Biography

Michael Schneider studied physics at the Karlsruhe Institute of Technology from 2003-2009. He performed his diploma work at the Forschungszentrum Karlsruhe on the measurement of Lorentz angles in highly irradiated silicon strip detectors for high energy collider applications, such as the large hadron collider at CERN. He finished his studies in 2009 and started his PhD thesis on the optimization of ultra-thin aluminum nitride films for actuation and sensing applications in micro electromechanical systems at the Department of Microsystems Technology at TU Vienna. He received his PhD in 2014 and is currently working as a postdoc on advanced materials such as silicon carbide and doped aluminum nitride, as well as MEMS devices based on piezoelectric thin films.

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Additive manufactured lightweight porous materials

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[3]3D Printing Medical Research Center-China Medical University Hospital, Republic of China

Now-a-days, light weighting is an important topic for global researchers since it is a significant and efficient way to save energy and reduce carbon emission. There are two major approaches to achieve the purpose of light weighting, one is to introduce the materials with high specific strength and the other one is to vary the design by introducing the topology or lightweight porous structure. Either, of these two approaches was very difficult to be achieved due to the limitation of traditional process. However, due to the maturation of additive manufacturing process, it is possible to realize these two approaches at the same time. In this study, a high specific strength Al alloys was introduced to fabricate samples by using selective laser melting (SLM) process. Meanwhile, a porous structure was introduced to develop the potentially lightweight materials. To further examine the potential of this high specific strength porous material as a lightweight material, the porous samples with different porosity were fabricated. In this research, all of the samples were analyzed and tested carefully, including XRD, SEM and compression test. The relationship between the materials, process, porous structure, microstructure and mechanical properties is explored and discussed in details.

Recent Publications

1. **Y C Wu, C N Kuo, M Y Shie, Y L Su, L J Wei, S Y Chen and J C Huang (2018) Structural design and mechanical response of gradient porous Ti-6Al-4V fabricated by electron beam additive manufacturing. Materials and Design 158:256-265.**
2. **Zhong Xun Khoo, Yong Liu, Jia An, Chee Kai Chua, Yu Fang Shen and Che Nan Kuo (2018) A review of selective laser melted NiTi shape memory alloy. Materials, 11(4):519.**
3. **S Y Chen, C N Kuo, Y L Su, J C Huang, Y C Wu, Y H Lin, Y C Chung and C H Ng (2018) Microstructure and fracture properties of open-cell porous Ti-6Al-4V with high porosity fabricated by electron beam melting. Materials Characterization 138:255-262.**

Biography

C N Kuo is an Assistant Professor in Department of Bioinformatics and Medical Engineering at Asia University, Taiwan. He dedicated himself in study the metal 3D printing for over four years. His research topics are focused on the 3D printed advanced materials and porous materials.

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Energy input effects on microstructure evolution of Ti- 6Al-4V fabricated by electron beam additive manufacturing

M T Tsai[1, 2], Y C Wu[3], Y L Su[2, 4] and C N Kuo[1, 2]

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[3]National Sun Yat-Sen University, Republic of China
[4]3D Printing Medical Research Cente-China Medical University Hospital, Republic of China

In recent years, additive manufacturing (AM) technology, especially powder bed fusion method has been well developed. One of the powder bed fusion technologies is called electron beam additive manufacturing (EBAM). The microstructure of EBAM parts of the Ti-6Al-4V alloy is usually characterized by the acicular martensitic alpha ( ) and fine lamellar Widmanstätten (+) structure inside the prior grain. However, there are challenges to control the volume fractions between different phases during this process. In this study, the effect of energy input on the microstructure of Ti-6Al-4V samples fabricated by EBAM is examined. The processing parameters of energy input are designed by the prediction of thermal field simulation. The relationship between the current input and the microstructure evolution is clarified by analyzing the volume fractions of different phases and the mechanical properties. The results show that the energy input would influence the microstructure of the samples made by EBAM and thus would differ in the mechanical properties accordingly.

Recent Publications

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2. **S L Sing, J An, W Y Yeong and F E Wiria (2016) Laser and electron-beam powder-bed additive manufacturing of metallic implants: a review on processes, materials and designs. Journal of Orthopaedic Research 34(3):369-385.**
3. **P Wang, X Tan, M L S Nai, S B Tor and J Wei (2016) Spatial and geometrical-based characterization of microstructure and microhardness for an electron beam melted Ti–6Al–4V component. Materials & Design 95:287-295.**
4. **X Zhao, S Li, M Zhang, Y Liu, T B Sercombe, S Wang, Y Hao, R Yang and L E Murr (2016) Comparison of the microstructures and mechanical properties of Ti–6Al–4V fabricated by selective laser melting and electron beam melting. Materials and Design 95:21-31.**

Biography

M T Tsai is a Postdoctoral fellow in the 3D Printing Medical Research Institute at Asia University in Taiwan. He has completed his PhD at National Sun Yat-sen University, Republic of China in 2018. His research fields include nano/micro scaled mechanical behavior and microstructure. Currently, his main research is focused on aluminum- scandium alloys by additive manufacturing.

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Potential for using Natural Pozzolana for Concrete in Kuwait

Saud Al- Otaibi

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The meaning of the word 'sustainability' is arbitrary and depends on many factors like availability of raw materials, construction safety, functionality, and energy. Concrete is the second largest manufactured product in volume on earth after processed water. Thus, any positive action toward the reduction of specific CO2 emission would significantly contribute globally to the reduction of overall greenhouse gas emissions. In an era of climate change and potentially depleting natural resources, countries need to introduce more sustainable construction. The use of pozzolanic materials as a replacement for cement in construction field has become an unavoidable practice nowadays because of its economic and environmental advantages and durability. Especially in countries like Kuwait, belonging to Gulf region, where there are severe climatic conditions along with chemical exposure due to the coastal area effects, use of pozzolanic materials has more relevance. This paper presents results of a study carried out on using a natural pozzolanic material obtained from Super Burkani Quarry in Saudi Arabia. This material is a natural volcanic ash processed and pulverized in different particle sizes. The research work included paste, and mortar mixes with different levels of OPC replacement. The experimental program covered microstructure, rheology, hydration process, and hardened mechanical and durability properties. The results were promising as to improvement of properties in most aspects.

Recent Publications

1. Suad Al-Bahar, Saud Al-Otaibi, Sharifa Al-Fadala, Ali Abduljaleel, Mahmoud Fawzy Taha, Fatma Al-Fahad, Amer Al-Arbeid, Tarun K. Mkherjee, (May 17 20160"Process Using Multiple Waste Streams to Manufacture Synthetic Lightweight Aggregate", US 9340456 B2.
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5. Al-Bahar S., Al-Otaibi S., Taha M., Al-Arbeed, S. Abduljaleel A., Al-Fahad F. and Al-Fadala S., (2013) "Heating Electron Microscope for Evaluation of Melting Behavior of Lightweight Aggregates Mixtures", International Journal of Civil Engineering and Building Materials, V. 3, No. 2, pp. 49-66.

Biography

Dr. Saud Fahhad Al-Otaibi hold Ph.D. Civil and Structural Engineering from University of Sheffiled , UK since 2002. He is working as a research scientist in Kuwait Institute for Scientific Research. He is currently the president of the ACI Kuwait Chapter. His field of interest and expertise is in construction materials in general with some focus on cement and concrete, also worked on building systems and construction management.

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Udesh Dhawan et al., Nano Res Appl 2018, Volume 4
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Nanochip-induced epithelial to mesenchymal transition: impact of physical microenvironment on cancer metastasis

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Epithelial-to-mesenchymal transition (EMT) is a highly orchestrated process motivated by the nature of physical and chemical compositions of the tumor microenvironment (TME). The role of the physical framework of the TME in guiding cells toward EMT is poorly understood. To investigate this, breast cancer MDA-MB-231 and MCF-7 cells were cultured on nanochips comprising tantalum oxide nanodots ranging in diameter from 10 to 200 nm, fabricated through electrochemical approach and collectively referred to as artificial microenvironments. The 100 and 200 nm nanochips induced the cells to adopt an elongated or spindle-shaped morphology. The key EMT genes, E-cadherin, N-cadherin, and vimentin, displayed the spatial control exhibited by the artificial microenvironments. The E-cadherin gene expression was attenuated, whereas those of N- cadherin and vimentin were amplified by 100 and 200 nm nanochips, indicating the induction of EMT. Transcription factors, snail and twist, were identified for modulating the EMT genes in the cells on these artificial microenvironments. Localization of EMT proteins observed through immunostaining indicated the loss of cell–cell junctions on 100 and 200 nm nanochips, confirming the EMT induction. Thus, by utilizing an in vitro approach, we demonstrate how the physical framework of the TME may possibly trigger or assist in inducing EMT in vivo. Applications in the fields of drug discovery, biomedical engineering, and cancer research are expected.

Recent Publications

1. **Dhawan U, Sue MW, Lan KC, Waradee B, Huang PH, Chen YC, Chen PC, Chen WL (2018) "Nanochip induced Epithelial to mesenchymal transition: Impact of Physical microenvironment on cancer metastasis". ACS Applied Materials and Interfaces.**
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Biography

Dr. Udesh earned his Ph.D. in Biomedical Engineering from the Department of Materials Science and Engineering at National Chiao Tung University, Taiwan. He is currently a postdoctoral fellow at the Institute of Chemistry, Academia Sinica, Taiwan. He has published several articles in the field of Biomaterials and cancer biology. He serves as an editorial board member for the journal SF journal of Materials and Chemical Engineering and is the managing editor for the journal Frontiers in Bioscience. His research interests include engineering nanostructured biomaterials for cancer therapy, drug discovery and drug development.

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Growth of graphene by plasma-assisted chemical vapor deposition synthesis, modeling and diagnostics

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In this work, we report on some of the fundamental chemical and physical processes responsible for the deposition of graphene by plasma enhanced chemical vapor deposition (PECVD). The graphene is grown by plasma decomposition of a methane and hydrogen mixture (CH_4/H_2) at moderate pressures over polycrystalline metal catalysts. In situ optical emission spectroscopy (OES) technique was used to measure the rotational temperature of the plasma and the H-atom relative concentration under different experimental conditions obtained by varying the plasma power (300-400 W), total pressure (10-25 mbar), substrate temperature (700-1000°C), methane flow rate (1-10 sccm) and catalyst nature (Co-Cu). Then, three complementary modeling approaches (0D, 1D and 2D) were developed to analyze the plasma environment during graphene growth. The transient zero-dimensional (0D) configuration was used for evaluation of the effects of reactor conditions and permits the identification of dominant reactions and key species during graphene growth. This approach is useful for identifying the relevant set of species and reactions to consider in a higher-dimensional model. The one-dimensional and two-dimensional models were developed to predict the gas temperature and the species concentrations for different process conditions by involving gas-phase and surface reaction mechanisms. The 0D, 1D and 2D models are validated by comparison with experimental data obtained from atomic and molecular emission spectra, providing insight into graphene growth under specific plasma conditions.

Recent Publications

1. **A Mehedi, B Baudrillart, D Alloyeau, O Mouhoub, C Ricolleau, V D Pham, C Chacon, A Gicquel, J Lagoute, and S Farhat (2016) Synthesis of graphene by cobalt-catalyzed decomposition of methane in plasma-enhanced CVD: Optimization of experimental parameters with Taguchi method. Journal of Applied Physics 120:065304.**
2. **G Shivkumar, S S Tholeti, M A Alrefae, T S Fisher, and A A Alexeenko (2016) Analysis of hydrogen plasma in a microwave plasma chemical vapor deposition reactor. Journal of Applied Physics 119:113301.**
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Biography

K Pashova studied Chemical Engineering at University of Chemical Technology and Metallurgy Sofia, Bulgaria, and obtained her MSc degree in Chemical and Process Engineering from University of Chemical Technology and Metallurgy, Sofia, Bulgaria. She is currently a PhD student in the group of Dr. Samir Farhat at Laboratoire des Sciences des Procédés et des Matériaux, CNRS, LSPM – UPR 3407, Université Paris 13, France. Her research interests include the synthesis of nanomaterials by Microwave plasma chemical vapor deposition and induction; plasma diagnostics and plasma modeling.

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Bhaskarchand Gautam et al., Nano Res Appl 2018, Volume 4
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Developing "SMART" Nano by Nano System for Efficient Liposome Delivery in vitro

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Nanotechnology-based cargo delivery to cells is a promising assay due to its efficiency and biocompatibility. Time-consuming and uncontrollable deliver amount are still thresholds in related research. In this study, we design a nanopillar-based platform for liposome delivery in vitro. Thermoreponsive copolymer (p(NIPAm-co-AEMA)) is grafted from silicon nanowire (SINW) as a polymer nano brush to equip temperature-controllable liposome conjugations of the SINW. A liposome is introduced onto the polymer nano brush to form a nano-by-nano interface and is released through thermal-stimuli to generate a high local concentration for cellular uptake. Cryo-TEM images show that liposomes can attach to the polymer nano brush to form liposome-tethered nanopillars. Fluorescence quantifications suggest that up to 90% of the attached liposomes can be released with intactness. Furthermore, HEK 293T cell and calcein-loaded liposome are employed to investigate the cellular uptake kinetics. We found that the cellular uptake kinetic of HEK 293T cell is highly correlated to temperature stimulus in the nano-by-nano system. Fluorescence intensity difference quantified by flow cytometry indicate elevated cellular uptake efficiency, which is more than 10-fold increments at 4-hour incubation. Confocal images show that the liposomes stay at cytoplasm instead of lipid membrane after cellular uptake. In conclusion, we could deliver liposome to cells efficiently with the designed system and we hope these efforts could open a new era in biological engineering and tissue engineering.

Biography

Mr. Gautam received his master degree in Chemical Science from Institute of chemical technology (ICT), Mumbai, India. After completing his master degree he worked 2 years as Research Assistance at Aditya Birla Science and Technology Company. He is currently a pursuing his Ph.D. study at Institute of Chemistry, Academia Sinica, Taiwan.

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Jayakrishnan A. J et al., Nano Res Appl 2018, Volume 4
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Design and Fabrication of Functionalized, Chiral Poly(3,4-ethylenedioxythiophene) (PEDOT) Nanostructures for Biosensing Applications

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Nanotopological cues can be exploited to investigate the molecular interactions between biomolecules and nanomaterials. However, studies highlighting the synergistic effect of nanostructure shape, size and geometry in modulating biosensing parameters are non-existent. To explore this, poly(3,4- ethylenedioxythiophene) bearing hydroxyl functional group in the side chain having R or S chirality with dot and tube morphology were synthesized and the synergistic effect of polymer chirality and nano-topography morphology in controlling the biomolecule-polymeric nano-surface binding affinity were studied. Accordingly, the design of a bio-sensing nanosurface for enhanced sensitivity and signal/ noise ratio is proposed. Chiral polymers were synthesized via electrochemical polymerization using cyclic voltammetry or chrono-amperometry techniques. The formation of polymers was confirmed through UV/ Visible spectrophotometry and Fourier Transform Infrared spectroscopy (FTIR) while the chirality was confirmed through circular dichroism (CD). Hydrophobicity or hydrophilicity of the polymeric nanostructures was analysed by measuring their respective water contact angles. Electrochemical polymerization temperature was varied to obtain either nanodot or nanotube morphology while the potential was changed to modulate the nano-topography size. The nanostructure morphology was confirmed using Scanning Electron Microscopy (SEM). Fetal Bovine Serum (FBS) was used as a model protein and Quartz crystal microbalance (QCM) was used to analyse the binding affinity of biomolecules to different chiral nanostructures. Water contact angle measurement confirmed that, nanotubes showed a greater hydrophilicity as compared to dots irrespective of the chirality. Finally, QCM data revealed a 15 and 20Hz difference in the binding affinities of R and S-PEDOT when the nanostructure morphologies were same and a 12 and 17Hz difference in the binding affinities when the polymer chirality were same, confirming that polymer chirality and nanostructure morphology play a crucial role in determining the binding affinity of biomolecules to nanostructures. These results collectively indicated the existence of a fine balance between nanostructure and analyte size, which has to be optimized to achieve maximal bio sensing response. Applications in the field of bio-materials and biomedical engineering are expected.

Biography

Jayakrishnan A.J is expertized in designing of organic molecules for various applications. He is currently working on the design, synthesis and electrochemical fabrication of conducting polymer nanostructures, especially functionalized poly (3,4- ethylenedioxythiophene) for various material as well as biological applications. He is pursuing his doctoral studies in Institute of Chemistry at Academia Sinica, Taiwan with the prestigious Taiwan International Graduate Program (TIGP) scholarship.

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Experimental analysis of environmental effects on polymer concrete

Pedram Ghasemi and Vahab Toufigh
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Developing high-performance engineering materials was one of the most important priority of civil engineering. Such materials perform high strength, durability, ductility, toughness and energy absorption. One of these materials is polymer concrete (PC) that has become well-known due to its application in repair and rehabilitation of structures, precast components as thin over lays and floors. Also, PC is used as a repair material for concrete infrastructure like sewer structure applications, drainage channels, swimming pools and other structures that comprise chemically corrosive aggregate. The purpose of this study is to assess the chemical resistance of polymer concrete when exposed to two environments including chemical solutions at two pH contents (2.5 and 12.5) which simulate acidic and alkali environment. In this research, PC samples with two different contents of epoxy resin (10% and 12% of the total weight of composition) have been studied. Five cylindrical and one cubic specimen were prepared for each of the epoxy resin content. A uniaxial compression test as destructive test and non-destructive method such as ultrasonic test was applied to determine the change of the features. Results show the loss of compression strength in the PC samples which were exposed to chemical solutions. The study showed that the amount of strength loss is related to the pores of PC specimens. Factors as type and content of resin and hardener, type and concentration of chemical solution and interaction between them considerably affected samples strength. This material could be a good candidate for repair and rehabilitation of structures.

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4. **Saadatmanesh H, Tavakkolizadeh M and Mostofinejad D (2010) Environmental effects on mechanical properties of wet lay-up fiber-reinforced polymer. ACI materials journal 107.**
5. **Gorninski J P, Dal Molin D C and Kazmierczak C S (2007) Strength degradation of polymer concrete in acidic environments. Cement and Concrete Composites 29(8):637-645.**

Biography

Pedram Ghasemi is a graduate student in civil engineering and his research interest is sustainable and high-performance materials which have less detrimental effects on environment and rehabilitation and repair of stuctures with proper techniques and materials. His research based on experimental and numerical evaluation to assess mechanical properties and chemical resistance. He has determined this evaluation after three months with making and testing specimens. This study will lead civil engineering to use this type of materials as a repair material or precast component properly and efficiently in each structure, situation and position.

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2D materials assisted membrane crystallization: A new combined theoretical and experimental approach

Maria Luisa Perrotta
Institute of Membrane Technology, Italy

In the field of nanotechnologies, nano-composite membranes [1-2] enriched with two-dimensional (2D) materials are attracting interest in various areas of the scientific research, due to their peculiar and exceptional electronic properties. Actually 2D materials are becoming promising in membrane technology dedicated to water treatment as well. Specifically, 2D materials confined in defined volumetric spaces can assist mass transfer through membranes under specific conditions. New mechanisms are envisaged to control water sequestration from ion solutions causing quicker ion aggregation processes during Membrane Crystallization (MCr). The latter is part of the membrane technology enabling recovery of valuable salts from seawater and brine. In the recent past [1,3-4], atomistic simulations have provided a detailed picture of the formation of the critical nucleus of salts in supersaturated solution. Herein, for the first time we explore the potential of 2D materials in MCr technology from experimental and computational points of view. A combined molecular approach has been employed to predict and validate the effects of 2D materials on salts nucleation and growth rate when NaCl solution comes in contact with membrane surfaces. Experimental tests and simulations have been performed using different concentrations of exfoliated 2D flakes, designing three different models: pristine PVDF, PVDF with Graphene at 5% wt and PVDF with Graphene at 10% wt. As a first outcome, MD simulation demonstrate how the chemical composition of the membrane surface, can affect the crystallization of salts, while experimental test yield clear the role of the filler in nucleation grow rate, crystal size and shape, but also in the energy of the system [5]. In the overall, the nanomaterials influence kinetics of crystal formation, reducing the nucleation times.

Recent Publications

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5. Espinosa JR, Vega C, Valeriani C, Sanz E (2015) The crystal – fluid interfacial energy and nucleation rate of NaCl from different simulation methods, J. Chem. Phys, 142 , 194709.

Biography

Maria Luisa Perrotta, Ph.D Student at Institute of Membrane Technology of National Research Council (CNR-ITM), has her experience in membrane technology. At first she focused the attention on preparation, characterization and testing of nano-composite membranes in membrane processes (MD and MCr). In the last year she extended her interest in Molecular Dynamics Simulation in order to study at molecular level the behavior of membranes prepared, and also to compare with experimental test. At the moment she is studying Membrane Crystallization process (MCr). The basic aim of this work is to evalue the possible contribute of 2d nanomaterial, used like filler in these polymeric membranes, in crystals growth .

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