CMSE 2020

The 9th Global Conference on Materials Science and Engineering

CONFERENCE PROGRAM

November 20-23, 2020

Eastern European Time (EET)- UTC +2

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09:40-10:15	**Keynote Speech 2:** Smart Behavior of Spider Silks, Their Directional Water Collection and An Artificial Substitute ***Prof. Jinlian Hu**, Director of Laboratory of Wearable Materials for Healthcare, Joint Professor of Materials Science and Engineering, Department of Biomedical Engineering, City University of Hong Kong, HKSAR, China*
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Part II Keynote Speeches

Keynote Speech 1: Mixed-Anion Glass and Ceramics for High-Efficiency Luminescence in Rare-Earths

Prof. Setsuhisa Tanabe

Graduate School of Human and Environmental Studies
Kyoto University, Japan

Biography: Professor Setsuhisa Tanabe received Dr. Eng. at Department of Industrial Chemistry, Kyoto University (KU) in 1993. After working as an assistant professor, he was promoted to an associate professor in 2001 and to a full Professor in 2008 all in KU. He is the author of 250 original papers, 27 book chapters, and 51 review papers on rare-earth doped luminescent materials for upconversion lasers, optical amplifier for telecommunication, LED phosphors, quantum-cutters and persistent phosphors. He has served as a plenary, keynote or invited speaker at 150 international conferences.

He was the Chair of TC20 (Optoelectronic Glasses) of International Commission on Glass (ICG) during 2003-2011 and is now a member of Steering Committee of ICG since 2013. He is Associate Editor of Journal of Luminescence and Fellow of SPIE. He got various awards from The American Ceramic Society (2018), The Ceramic Society of Japan (2009), The Chemical Society of Japan (1998), The Rare-Earth Society of Japan (2002), and ICG (2012). His publications receive 8638 citations (h-index: 47) according to Scopus.

Abstract. While many of natural minerals, functional ceramic and glass materials are either oxides, chalcogenides or halides, the mixed-anion compounds, which contain several different anions, have now drawn attention as new types of inorganic material. Because of unique coordination, crystal structures and tunability of valence band in such mixed-anion compounds, it is possible that fundamentally different, innovative functions may be created. Materials with such innovative functions are expected to be created by using several different anions with differing electronegativity and polarizability and exploiting the exceptional ability of such anions to control chemical bonding and electronic structures. In addition, many elements that become anions have a high Clarke number, and mixed-anion compounds have the possibility of becoming materials that act as a driving force for element strategies.

In this talk, some examples of development of new luminescent materials will be introduced by giving asymmetric ligand field to the active center and achieving lower excitation energy of charge transfer band by the valence band engineering in oxynitride and oxyhydride systems. Also examples of oxyfluoride glass ceramics will be presented, which have both formability of silicate glasses and high luminescent efficiency because of low phonon energy environment around the active ions.

Keywords: Luminescence, Rare-earth, Ligand field, Mixed-anion, Oxynitride, Oxyhidride

Keynote Speech 2: Smart Behavior of Spider Silks, Their Directional Water Collection and An Artificial Substitute

Prof. Jinlian Hu

Director of Laboratory of Wearable Materials for Healthcare, Joint Professor of Materials Science and Engineering, Department of Biomedical Engineering, City University of Hong Kong, HKSAR, China

Biography: Prof. Jinlian HU is a smart polymer and textile materials scientist. Graduated from Donghua University in textile materials and received a PhD from Manchester University, she recently joined the Department of Biomedical engineering, City University of Hong Kong where she established a Laboratory of Wearable Materials for Healthcare. The laboratory focuses on unearthing scientific principles and providing solutions to key problems in Healthcare of Wearable Materials in three major areas: Traditional Chinese medical therapies and their materials, energy materials and healthcare as well as spider silks and their relatives as biomaterials as well as personal protective integration. As such, we apply advanced methods including custom-made wearable electronics as basic tools to examine materials, their application methods, and particularly their interactions with human body in terms of physical, chemical, biological, philological and informational relations. From the discoveries and models of basic research, applied investigation, product developments and standardization are envisaged, which can produce societal as well economic impact in addition to scientific advances. Before City University of Hong Kong, Professor Hu worked at Hong Kong Polytechnic University for more than 20 years. Professor Jinlian HU is a Fellow of the Royal Society of Chemistry, Hong Kong Institution of Textile and Apparel and the British Textile Institute. She is the founding chairman of the Hong Kong Health Science and Technology Park, the executive vice chairman of the Hong Kong Invention and Innovation Federation and a Council member of the Hong Kong Far Infrared Association.

Abstract. Spider silks are one of the extensively studied natural protein materials due to their outstanding mechanical and smart behavior. A spider web collects water by its capture-silk for recovering the daytime-distorted shape during night through water-sensitive shape memory effect. This unique smart function and geometrical structure of spider-silk has inspired the development of artificial fibers with periodic knots for directional-water-collection with vast potential applications in water scarce regions. Existing such fibers were mainly based on nylon filaments coated with petroleum-originated synthetic polymer solutions, which proves to have limited capability in water collection. Different from using synthetic materials, an all silk-protein fiber (ASPF) with periodic knots to endow extremely high volume-to-mass water collection capability. This fiber has a main body of B. mori degummed silk coated with recombinant eMaSp2 of spider dragline silk. It is 252 times lighter than synthetic polymer coated nylon fibers that once was reported to have the highest water collection performance. The ASPF collected a volume of 6.6 μL of water and has 100 times higher water collection efficiency compared to existing best water collection artificial fibers in terms of volume-to-mass index (VTMI) at the shortest length (0.8 mm) of three phase contact line (TCL). Since silkworm silks are available abundantly, effective use of recombinant spidroins tandemly shows great potential for scalability.

Keynote Speech 3: Low Temperature Growth of Gallium Oxide Based Ultrawide Bandgap Semiconductors

Prof. Qixin Guo

Department of Electrical and Electronic Engineering, Director of Synchrotron Light Application Center, Saga University, Japan

Biography: Prof. Dr. Guo received B. E., M.E., and Dr. E degrees in electronic engineering from Toyohashi University of Technology in 1990, 1992, and 1996, respectively. He is currently a Professor of Department of Electrical and Electronic Engineering, Saga University as well as Director of Saga University Synchrotron Light Application Center. His research interests include epitaxial growth and characterization of semiconductor materials. Prof. Guo has published more than 300 papers in scientific journals including Nature Communications, Advanced Materials, Physical Review B, and Applied Physics Letters with more than 6800 citations (h-index: 43).

Abstract. Ultrawide bandgap semiconductor $(AlGa)_2O_3$, which has a tunable bandgap between 4.9 (Ga_2O_3) and 8.7 eV (Al_2O_3), has recently emerged as a promising material for optoelectronic applications. The $(AlGa)_2O_3$ based solid state devices are almost based on material structures created by thin film deposition. Thus, the deposition technology can be regarded as one of the keys to the fabrication of $(AlGa)_2O_3$ based devices. Various growth techniques have been explored to deposit $(AlGa)_2O_3$ films, including sputtering, molecular beam epitaxy, mist chemical vapor deposition, metal organic chemical vapor deposition, and pulsed laser deposition (PLD). Among these deposition methods, PLD is a good candidate technology for low temperature growth because the ablated species generated in the PLD process have relatively high kinetic energies. In another aspect, the oxygen plasma has been found to be an effective assistant species for decreasing the growth temperature of thin films. Thus, the combination of PLD and oxygen plasma assistance should be a very effective method for low temperature film growth. In this talk, we report on the low temperature growth of $(AlGa)_2O_3$ films by oxygen plasma assisted PLD. The prepared films show a good (−201) orientation perpendicular to (0001) sapphire substrates even at a deposition temperature as low as 200 °C. The influences of the substrate temperature on the structural and optical properties of the films have been systematically investigated. Recent progress on the growth of these ultrawide oxide semiconductors will also been presented.

Keynote Speech 4: 2-D Nanostructures of Regularly Arranged Nanoparticles for Sensor Applications

Prof. Sigitas Tamulevičius
Member of the European Materials Research Society, Professor of the Physics Department, Kaunas University of Technology (KTU), Republic of Lithuania

Biography: Prof. Dr. Habil. Sigitas Tamulevičius (M) obtained the Physics Engineer degree from the Moscow Engineering Institute in Physics (Moscow, former USSR) in 1979, a Ph.D. degree from the University of Vilnius in 1984, Doctor Habilitus degree from Kaunas University of Technology (1994). From 1990 to 1991, he was postdoc at Royal Institute of Technology (Stockholm, Sweden). In 1994 he was Research Scholar, Fulbright Scholarship, Department of Physics, Massachusetts Institute of Technology (USA). Since 1996 he is full professor at the Physics Department and Research director of the Institute of Materials Science of Kaunas University of Technology. He has co-founded spin-off company, co-authored approx. 240 peer reviewed publications in the field of vacuum and plasma technologies and optical technologies and spectroscopy with more than 2200 citations (h-index: 24), and is (co-) author of 15 textbooks on different aspects of Materials Science. From 2002 he was Member expert and from 2010 he is full Member of Lithuanian Academy of Sciences. Prof. Sigitas Tamulevičius has received series of awards including Soros Foundation Research Grant, (1993) (Awarded by American Physical Society), Fulbright certificate (1997), National Award for Science (2000 and 2019), Recognition letter by the President of EMRS (2010), Honorary Professor of Southern Denmark University (2016), Laureate of Kaunas City Scientist Award (2017). He is Editor in Chief of Scientific Journal *Materials Science (Medžiagotyra)*, Member of Editorial Board of *Materials Research express* (IOPScience), *American Journal of Nanomaterials* (Science and Education Publishing), *Coatings* (MDPI), member of steering committee of European doctoral network Physics and Chemistry of Advanced materials. He was a national representative in FP7 programme "Nanosciences, nanotechnologies, materials and new production technologies". He headed multiple research projects funded by FP, Horizon 2020, COST, Eureka, NordForsk, Lithuanian State Foundation for Research and Studies, the Research Council, as well as Science and Innovation Agency of Lithuania. 15 PhD theses were defended under his guidance; he has supervised five postdoctoral researchers.

Abstract. Nanoparticles of group 11 metals like Cu, Ag and Au during the last decade attract attention of many researchers because of the localized surface plasmon resonance (LSPR) effect. This effect is important for many of the applications that employ localized surface plasmons and is described as collective charge oscillations confined to metallic nanoparticles. As one of the important emerging applications of such an effect, biomedical applications could be mentioned, where gold nanoparticles are used for plasmon-enhanced photothermal cancer therapy. Metallic nanoparticles of group 11 can act as well as a base of nanoscale devices and sensors with high selectivity and sensitivity. The resonances strongly depend on the local environment, allowing them to be used as ultrasensitive chemical and biological sensors. In addition, the strong electromagnetic field generated in the vicinity of the scatterer can greatly enhance the magnitude of the Raman scattering signal. This enhanced scattering process is known as surface-enhanced Raman scattering (SERS) - a term that emphasizes the key role of the noble metal substrate in this phenomenon. Finally, plasmonic field enhancement

has also enabled applications of nanoparticles for improved solar light harvesting and photocatalysis. In the current lecture the recent research results on the optical studies of colloidal solutions of silver nanoparticles, production of regular two dimensional nanostructures employing capillarity assisted particle assembly as well as studies of surface lattice resonance (mixed mode of LSPR and light diffraction in a regular structure) will be presented and discussed. The steady state light absorption measurements performed together with ultrafast transient pump-probe spectroscopy enabled to define spectral response as well as kinetics of the processes on the picosecond time scale. These issues are important in the mentioned fields of applications including development of smart sensors exhibiting high sensitivity.

Part III Online Oral Presentations

Online Oral Presentation Guidelines

- Online Oral Presentation will be conducted via Microsoft Teams Meeting (Click to see how to join CMSE 2020 via MS Teams).
- All presenters are requested to reach the Online Session Room prior to the scheduled time and deliver their presentations on time.
- The presentation timetable is shown in **Eastern European Time (EET)- UTC+2**.
- If a presenter is not able to show up via MS Teams, the session chair/conference secretary will download and play the pre-recorded video presentation during his/her scheduled presentation time; if listeners have questions about the presentation, please contact the conference secretary to forward the questions.
- If a presenter cannot show up on time or have problems with Internet connection, the session chair has the right to rearrange the presentation order and let the next presenter start.
- Signed and stamped electronic presentation certificate would be issued and delivered via e-mail after presentation.

Best Oral Presentations Selection

The session chair will select one best oral presentation from his/her session based on the following criteria and the "votes" on the conference website:

- ✓ Research Quality
- ✓ Presentation Performance
- ✓ Presentation Language
- ✓ PowerPoint Design

Best Oral Presentations Award

Best Presenters will receive an official certificate and free registration to the CMSE 2021.

Oral Session 1: Materials for Energy Applications and Catalysis

Time: 13:30-17:05, Nov. 21, 2020. Eastern European Time (EET)- UTC +2
Session Chair: Dr. Jianqiao Liu, Dalian Maritime University, China
Please Click Paper ID to Access the Video Presentation.
Session Room Link: http://www.academicconf.com/teamslink?confname=CMSE2020

13:30-14:00	**CMSE4251**	Strategies to Improve the Optical Properties and Sustainability of Solar Energy-Harvesting Photovoltaic Windows *Dr. Varun Vohra, Department of Engineering Science, the University of Electro-Communications, Japan*
14:00-14:15	**CMSE4370**	Anatase/Bronze-Type-TiO_2/Carbon Dot Multi-Junction Photocatalyst for H2 Generation *Dr. Sovann Khan, Photocatalysis International Research Center, Tokyo University of Science, Japan*
14:15-14:30	**CMSE4451**	Exfoliation Mechanism of Graphene-like MoS_2 Prepared by Intercalation-Detonation Method and Promising Exfoliation for 2D Materials *Mr. Fan Yang, Xi'an University of Architecture and Technology, China*
14:30-14:50	**CMSE4397**	Effect of Zn atom in Fe-N-C Catalysts for Electro-Catalytic Reactions: Theoretical Considerations *Dr. Li Yongcheng, School of Materials Science and Engineering, Beihang University, China*
14:50-15:05	**CMSE4411**	Structure Property Relation among Morphology of Electrode & Fuel Uptake in High Temperature SOFC: A Case Study using Ni/NiO@SZ *Dr. Madhumita Mukhopadhyay, Amity University, India*
15:05-15:20	**CMSE4416**	Phthalocyanine Based Materials for Chemiresistive Gas Sensing Applications *Dr. Aman Mahajan, Department of Physics, Guru Nanak Dev University, India*
15:20-15:45		**BREAK**
15:45-16:00	**CMSE4409**	Individual and Simultaneous Reduction of Azo Dyes in Presence of Core@shell Hybrid Microgel Catalyst *Dr. Khalida Naseem, Faculty of Sciences, University of Central Punjab, Pakistan*
16:00-16:25	**CMSE4243**	Evolution of Fuel Cell Cathode Catalyst under Simulated Operational Conditions *Dr. Ivan Khalakhan, Charles University, Czech Republic*
16:25-16:40	**CMSE4393**	Monte Carlo Study of Thin Magnetic Ashkin Teller Films at the Special Point *Dr. Amel Benmansour, Faculty of Sciences, University of Tlemcen, Algeria*
16:40-17:05	**CMSE4282**	Giant Dielectric Permittivity in Doped Strontium Titanate Ceramics *Dr. Oleksandr Tkach, University of Aveiro, Portugal*

Abstracts of Session 1

CMSE4251

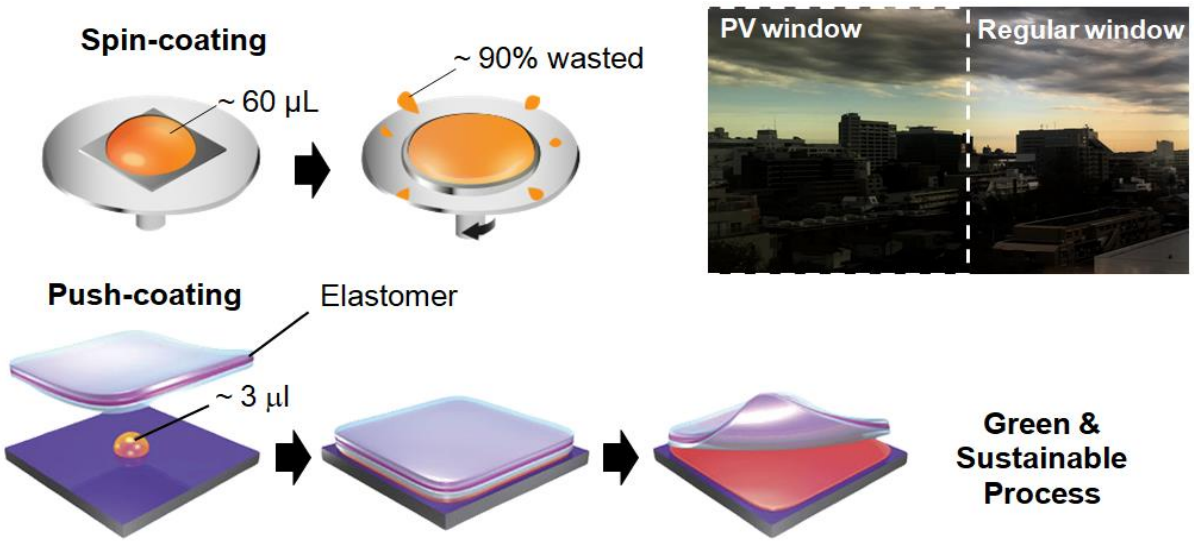
Strategies to Improve the Optical Properties and Sustainability of Solar Energy-Harvesting Photovoltaic Windows

Varun Vohra*, Takashi Sano, Tomoaki Takada and Shusei Inaba
Department of Engineering Science, the University of Electro-Communications, Tokyo, Japan

Abstract. Organic solar cells (OSCs) employ semi-transparent active layers deposited through solution processes. Combining these low-cost active layers with transparent electrodes, one can produce smart windows that harvest energy from the sun. To fulfill their role as energy source for sustainable urban designs, OSC-based photovoltaic windows have to overcome major drawbacks such as reducing materials and hazardous solvent wastes generated during active layer fabrication. Additionally, to replace conventional windows, the photovoltaic windows should transmit enough visible light and avoid having a colored-glass aspect which would change the spectrum of the transmitted light.

Here, we demonstrate that employing ternary active layers (three active materials) can simultaneously increase the photovoltaic performances and optical properties of light-harvesting windows. Following this strategy, we fabricated efficient neutral color photovoltaic windows with a color rendering index and an average visible transparency over 95 and 40%, respectively. Furthermore, to increase the sustainability and environment-friendliness of their production, we developed a new thin film fabrication process called push-coating. Using push-coating, uniform thin films that generate similar photovoltaic performances to spin-coated ones can be fabricated with no material waste and 20 times less hazardous solvents than with spin-coating.

Our results thus open the path to extremely low-cost and eco-friendly fabrication of innovative photovoltaic technologies which could strongly impact the global energy roadmap.



Keywords: Organic solar cells, Green & sustainable fabrication, Emerging photovoltaic technology

CMSE4370

Anatase/Bronze-Type-Tio_2/Carbon Dot Multi-Junction Photocatalyst for H_2 Generation

Sovann Khan[1], Yuta Kubota[2], Wenwei Lei[1], Norihiro Suzuki[1,3], Kazuya Nakata[1,3,4], Chiaki Terashima[1,3], Nobuhiro Matsushita[2], Akira Fujishima[1] and Ken-ichi Katsumata[1,3,5*]

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Abstract. We report the one-pot synthesis of anatase/bronze-type ((A/B)-TiO_2) and carbon dots (CDs) via a simple solvothermal method using only $TiCl_4$ and ethylene glycol. Control of the reaction temperature and duration enabled the compositions of pure (B) phase, (A/B)-TiO_2/CDs, and (A)-TiO_2/CDs to be tuned. A series of experiments on the synthesis conditions was carefully conducted at various temperatures (150–200 °C) for various reaction times (5–36 h). Pure phase (B)-TiO_2 was obtained at 150 °C for all reaction times (5 to 36 h). The (B)-phase was transformed to anatase at temperatures from 170 °C for reaction times longer than 12 h. At the same time, CDs were formed from the decomposition of ethylene glycol at temperatures greater than 160 °C and long reaction times (>12 h). The photocatalytic activities of the composite catalysts were evaluated by H_2 generation from a water-ethylene glycol mixed solution under UV–visible light. H_2 generation rates were observed in this order: (A/B)-TiO_2/CDs > (A)-TiO_2/CDs > (B)-TiO_2 > (A)-TiO_2. This high photocatalytic activity for (A/B)-TiO_2/CDs is attributed to effective charge-separation and broad-light absorption. The developed method will be important for the facile synthesis of (A/B)-TiO_2/CD materials and has more potential than conventional multi-step methods.

Keywords: Bronze-type-TiO_2, Carbon dots, Heterostructure, Hydrogen evolution

Acknowledgements: This research was financially supported by a Grant-in-Aid for JSPS Fellows (18F18337) from the Japan Society for the Promotion of Science (JSPS). S. Khan would like to thank JSPS for supporting his postdoctoral research (standard-P18337).

CMSE4451

Exfoliation Mechanism of Graphene-like MoS_2 Prepared by Intercalation-Detonation Method and Promising Exfoliation for 2D Materials

Fan Yang[1,2], Ping Hu[1,2] and Kuaishe Wang[1,2,*]
[1] *School of Metallurgical Engineering, Xi'an University of Architecture and Technology, Xi'an 710055, China*
[2]*State Local Joint Engineering Research Center for Functional Materials Processing, Xi'an University of Architecture and Technology, Xi'an 710055, China*

Abstract. Graphene-like MoS_2 has attracted significant interest because of its unique electronic, optical, and catalytic properties with two-dimensional lamellar structure. In this work, a novel intercalation-detonation method was used to prepare monolayer and multilayer graphene-like MoS_2. MoS_2 was first completely intercalated by abundant oxygen-containing functional groups bonded to the sulfur atom layer in basal planes of the MoS_2 structure, increasing the layer spacing and decreasing the Van-der-Waals' force between the layers. Then, the intercalated MoS_2 was rapid exfoliated by high energy of detonation. In addition, bulk WS_2 and h-BN powders were also exfoliated to single and few layers nanosheets successfully by detonation method, showing the promising wide range of application of exfoliation in two-dimensional materials. The further research on magnetic and electrocatalytic hydrogen evolution properties show that the exfoliated MoS_2 has excellent magnetic response and electrocatalytic efficiency, demonstrating promising potential for applications on diluted magnetic semiconductor and energy conversion.

Keywords: Graphene-like MoS_2, Intercalation-detonation method, Exfoliation mechanism, 2D materials, Magnetic property, Electrocatalytic hydrogen evolution

Acknowledgements: This work was supported by the Youth Innovation Team of Shaanxi Universities (2019-2022), Outstanding Doctorate Dissertation Cultivation Fund of Xi'an University of Architecture and Technology (6040317013), Fok Ying Tung Education Foundation (171101) and top young talents project of "Special Support Program for High Level Talents" in Shaanxi Province (2018-2023).

CMSE4397

Effect of Zn Atom in Fe-N-C Catalysts for Electro-Catalytic Reactions: Theoretical Considerations

Yongcheng Li[1], Riming Hu[1], Zhibin Chen[1], Xin Wan[1], Jia-Xiang Shang[1*], Fu-He Wang[2] and Jianglan Shui[1*]
[1]*School of Materials Science and Engineering, Beihang University, Beijing, 100191, China*
[2]*Department of Physics, Capital Normal University, Beijing 100048, China*

Abstract. Due to the high specific surface area, abundant nitrogen and micropores, ZIF-8 is a commonly used precursor for preparing high performance Fe-N-C catalysts. However, the Zn element is inevitably remained in the prepared Fe-N-C catalyst. Whether the residual Zn element affects the catalytic activity and active site center of the Fe-N-C catalyst caused widespread curiosity but has not been studied yet. Herein, we built several Fe, Zn and N co-doped graphene models to investigate the effect of Zn atoms on the electrocatalytic performance of Fe-N-C catalysts. by using density functional theory method. The calculation results show that all of the calculated Fe-Zn-N_x structures are

thermodynamically stable due to the negative formation energies and relative stabilities. The active sites around Fe and Zn atoms in the structure of Fe-Zn-N_6 (III) show the lowest ORR and OER overpotentials of 0.38 and 0.43 V, respectively. The bridge site of Fe-Zn in Fe-Zn-N_5 shows the lowest η^{HER} of -0.26 V. A few structures with a better activity than that of FeN_4 or ZnN_4 are attributed to the synergistic effects between Fe and Zn atoms. The calculated ORR reaction pathways on Fe-Zn-N_6 (III) show that H_2O is the final product and the ORR mechanism on the catalyst would be a four-electron process, and the existence of Zn element in the Fe-N-C catalysts plays a key role in reducing the ORR activation energy barrier. The results are helpful for the deep understand of high-performance Fe-N-C catalysts.

Keywords: Fe-N-C, Zn-N-C, Oxygen reduction reaction, Oxygen evolution reaction, Hydrogen evolution reaction, Density functional theory

CMSE4416

Phthalocyanine Based Materials for Chemiresistive Gas Sensing Applications

Aman Mahajan
Material Science Laboratory, Department of Physics, Guru Nanak Dev University, Amritsar-143005, India

Abstract. Phthalocyanine based organic semiconducting materials are promising candidates for room temperature chemiresistive sensors as their electrical conductivity changes on interaction with oxidizing/reducing gases at room temperature. Sometimes small response characteristics of these sensors at room temperature become a limitation, which can be overcome by exploring long range molecular nanostructures with high surface/volume ratio.

With this aim in view, our research group is engaged in the development of cost-effective, highly sensitive and reproducible phthalocyanine based room temperature chemiresistive sensors capable of detecting toxic gases at the parts-per-billion level. We have synthesized phthalocyanine based nanowires, nanoflowers, nanobelts and their nanocomposites with carbon nanotubes/graphene by using a simple and low-cost self-assembly technique. Recently we have reported for the first time phthalocyanine nanowires as highly selective and sensitive room temperature Cl_2 sensor with response as high as 715% and detection limit as low as 5 ppb. In this talk, we will discuss the room temperature gas sensing characteristics of phthalocyanine nanostructures and nanocomposites along with their formation, sensing mechanism and adsorption kinetics.

Keywords: Phthalocyanine, Gas sensors, Chlorine, Nanostructures

CMSE4411

Structure Property relation among Morphology of Electrode & Fuel Uptake in High Temperature SOFC: A Case Study using Ni/NiO@SZ

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[2]*Fuel Cell and Battery Division, CSIR-Central Glass and Ceramic Research Institute, Kolkata – 700 032, India*

Abstract. The functionality of a composite depends on the optimization of processing technique. Fuel cell being a solid-state device is primarily dependent on the compatibility among two electrode and the electrolyte. High temperature operation (800 to 1000ºC) demands stability of and cyclability of the compositions of electrode and electrolyte for a significant period of application. The present study focuses on the efficacy of core-shell nickel (Ni) @ stabilized zirconia (SZ) functional anode towards the oxidation of both hydrogen and reformed methane as fuel in presence of steam as one of the important components. The redox reaction is processed by adsorption on anode catalyst followed by decomposition and charge transfer reaction. This is further accelerated by the extension of triple phase boundary (TPB) regions (Ni/SZ/gas) within (intra-) and inter-anode involving electrolyte. Core-shell Ni@SZ cermet enables the extension of TPB regions in contrast to conventional matrix. Authors have reported four configurations for anode support, wherein the layered structure involving conventional Ni-SZ is placed at the fuel side and layers of Ni@SZ on the top. The thin anode layer in vicinity to the electrolyte with optimized Ni content of 28/32 vol % acts as the primary electrocatalytic layer and shows a maximum current density of ~4 $A.cm^{-2}$@0.7 V, 800ºC with moist hydrogen as fuel. Multifuel capability in the cell with similar functional anode is demonstrated using 20 % reformed methane with optimum steam/carbon ratio (2:1) having current density of ~ 1.13 $A.cm^{-2}$ under similar condition. The endurance analysis of such cermet shows more efficient usage in hydrogen as fuel and reasonable functionality in presence of reformed methane. This functionality is further correlated with extension of intra anode triple phase boundary regions within the core shell anode along with the co-existence of inter-anode triple phase boundary regions. This has been mathematically established by the author.

CMSE4409

Individual and Simultaneous Reduction of Azo Dyes in Presence of Core@Shell Hybrid Microgel Catalyst

Khalida Naseem
Department of Chemistry, Faculty of Sciences, University of Central Punjab, Lahore, Pakistan

Abstract. Industrial wastewater consists of various toxic dyes and nitro-aromatic compounds that are harmful to human as well as aquatic life. Therefore, removal/degradation of these toxic pollutants from wastewater sources is need of time. Here, polystyrene-poly (N-isopropyl methacrylamide-acrylic acid) [PSt-P(NIPMAM-Aac)] core@shell gel particles were prepared by adopting the precipitation polymerization method. Silver nanoparticles (AgNPs) were incorporated in P(NIPMAM-Aac) shell of core@shell particles using $AgNO_3$ as precursor of silver ions.

Ag@PSt-P(NIPMAM-Aac) core@shell hybrid particles were used as catalyst to enhance the rate of individual as well as simultaneous reduction of toxic pollutants (dyes and nitro-aromatic compounds) in presence of sodium borohydride ($NaBH_4$) reductant. Controlled reactions were also carried out to

prove the high catalytic activity of core@shell hybrid gel particles. Pseudo first order was adopted to study the kinetics of reduction of toxic pollutants. It was concluded that prepared Ag@PSt-P(NIPMAM-Aac) composite catalyst enhanced the rate of reduction reactions and made the reaction kinetically feasible. Catalyst also maintained it activity even in case of simultaneous degradation of toxic dyes and nitro aromatic compounds

Reduction of pollutants was evaluated on the basis of Langmuir Hinshelwood (L-H) mechanism. Pollutants degradation was also performed under varying reaction conditions such as catalyst dose, $NaBH_4$ and amount of pollutant. Percentage activity of hybrid catalyst was maintained up to fourth reusability cycle for reduction reactions.

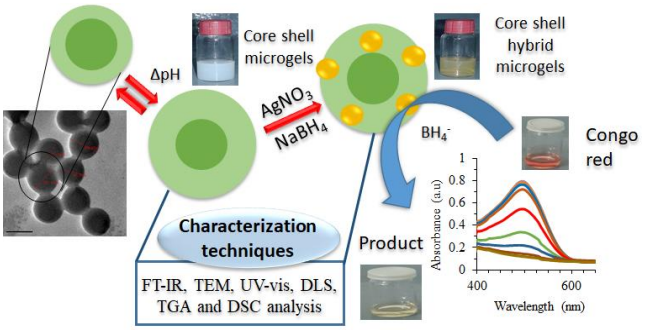

Figure 1. Diagrammatic representation of Ag@PSt-P(NIPMAM-Aac) hybrid particles catalyst for reduction of dye.

CMSE4243
Evolution of Fuel Cell Cathode Catalyst Under Simulated Operational Conditions

Ivan Khalakhan
Department of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Abstract. Platinum-transition metal bimetallic alloys have attracted enormous attention in the field of proton-exchange membrane fuel cells (PEMFC). It was suggested to replace seemingly indispensable platinum cathode catalyst. Along with reducing the cost, addition of transition metal to Pt induces its electronic and/or structural modifications so that it improves a sluggish kinetics of the oxygen reduction reaction (ORR). However, other than activity and cost, durability is another key issue that certainly deserves an attention as it is a prerequisite for of PEMFCs commercialization. The cathode catalyst in fuel cell needs to withstand corrosive conditions under high potentials and low pH which lead to its degradation. The corrosive degradation of fuel cell catalysts during its operation is a complex phenomenon involving an interplay between multiple mechanisms such as dissolution of both platinum and transition metal, Ostwald ripening, coalescence and carbon support corrosion. As a result, the PEMFC undergoes performance deterioration. Despite numerous works, a clear link between specific operating conditions of a fuel cell and above listed phenomena remains superficial. This is mainly because a vast majority of studies were limited by *ex situ* characterization techniques investigating catalyst only before and after reaction and lack true information about catalyst operando behavior. With the rising of the state-of-the-art *in situ* techniques, the behavior of fuel cell catalysts directly under reaction conditions is becoming a growing focus of researchers. Herein, I will present our recent results on the lifetime degradation of bimetallic fuel cell catalysts obtained using novel *in situ* techniques.

Keywords: Fuel cells, Cathode catalyst, Bimetallic alloy, Degradation

CMSE4393

Monte Carlo Study of Thin Magnetic Ashkin Teller Films at the Special Point

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Abstract. The magnetic properties and critical behaviours of an Ashkin Teller spin-1/2 model magnetic thin-film systems are studied as part of the Monte Carlo simulation method, based on the Metropolis algorithm, in a simple cubic lattice. The effect of the interaction with the exchange coupling J_4 (surface and bulk) is studied. Therefore, the phase diagrams present different ratios of the surface exchange interaction at the special point $(R_s = J_{2s}/J_{2b})_{sp}$, at which all the films thickness have the same critical temperature, these temperatures can be below, above or equal to the critical system bulk temperature. In addition, second order transition appears in the system. Moreover, to the special point descriptions, we found another partially ordered phase at high temperature for certain values of the parameter's interaction. Finally, the effective surface exponents and the critical exponents of the surface magnetization are computed.

Keywords: Thin film, Ashkin Teller model, Monte Carlo method, Special point, Effective exponents

CMSE4282

Giant Dielectric Permittivity in Doped Strontium Titanate Ceramics

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Abstract. Development of giant-permittivity and high-tunability dielectric materials has attracted great interest because of growing demand for smaller and faster energy-storage and electronic devices. Materials such as $CaCu_3Ti_4O_{12}$, displaying the giant dielectric permittivity due to extrinsic Maxwell-Wagner interfacial polarization effect, have previously been reported. Ferroelectric materials possessing intrinsic ionic polarization due to a phase transition to the polar state have also been indicated to possess high dielectric permittivity. Here, a class of the giant-permittivity materials based on $SrTiO_3$ ceramics doped with about 1% of trivalent ions like yttrium, dysprosium and gadolinium as well as their processing concept, which yields the dielectric permittivity up to ~209 000 at 10 kHz, is reported. The giant permittivity is explained by a coupling of the polar clusters relaxation mode with the donor substitution induced electrons at low temperatures and by the Maxwell-Wagner relaxation around room temperature. Besides the fundamental understanding, this discovery opens a new

development window for high-frequency and low-temperature electronic and energy-storage applications.

Keywords: Electroceramics, Doping, Sintering atmosphere, Polar order, Maxwell-Wagner polarisation

Oral Session 2: Nanostructured Materials, Sensors and Actuators, Microdevices, Testing of Materials

Time: 08:30-12:55, Nov. 22, 2020. Eastern European Time (EET)- UTC +2

Session Chairs: Dr. Ji Wang, Ningbo University, China

Dr. Evgeny Grigoryev, Russian Academy of Sciences, Russia

Please Click Paper ID to Access the Video Presentation.

Session Room Link: http://www.academicconf.com/teamslink?confname=CMSE2020

08:30-08:45	**CMSE4255**	Deformation and Fracture During Solidification and Adhesion Process of Paraffin Droplet Modelling Thermal Spray *Mr. Chao Kang, Tokyo Institute of Technology, Japan*
08:45-09:00	**CMSE4254**	Creation and Utilization of Straightness Standard due to Reciprocal Measurement of Linear Stage *Dr. Ryoshu Furutani, Tokyo Denki University, Japan*
09:00-09:15	**CMSE4381**	Continuous Segmented Flow Synthesis of Silver Nanowires *Dr. Chin-Hua Chia, Universiti Kebangsaan Malaysia, Malaysia*
09:15-09:40	**CMSE4399**	An Analysis of Propagation and Properties of Axisymmetric Waves in Elastic Solids *Dr. Ji Wang, Ningbo University, China*
09:40-09:55	**CMSE4435**	Preparation of the Nanostructure Manganese Oxide Modified Electrode by Chemical and Electrochemical Procedures and Comparison of Their Efficiency for Electrochemical Reduction of Niclosamide *Masoumeh Ghalkhani, Shahid Rajaee Teacher Training University, Iran*
09:55-10:20	**CMSE4260**	Aspects Regarding the Increase of the Protection Level of the Falling-Object Protective Structures (FOPS) by Using the Post-critical Behavior of the Support Elements *Dr. Petru Dumitrache, "Dunarea de Jos" University of Galati, Romania*
10:20-10:50	**CMSE4373**	New Trends in Fundamental Research Due to the Spontaneous Flexoelectric Effect in Nanosized and Bulk Ferroelectrics *Dr. Maya Glinchuk, National Academy of Sciences of Ukraine, Ukraine*
10:50-11:00		**BREAK**
11:00-11:20	**CMSE4402**	Very Thin Silver Films on PET and Optical Glass; Obtaining and Properties *Dr. Bogdan Alexandru Sava, National Institute for Laser, Plasma and Radiation Physics, Romania*
11:20-11:45	**CMSE4266**	Advantages High Voltage Consolidation of Powders Refractory Materials *Dr. Evgeny Grigoryev, Russian Academy of Sciences, Russia*

11:45-12:10 **CMSE4384**	Standardization of the Method of Magnetostriction Measurement of Grain-oriented Electrical Steel Strip and Sheet *Mr. Stefan Siebert, Brockhaus Measurements, Germany*
12:10-12:25 **CMSE4367**	Micro-Acoustic-Trap (μAT) for Microparticle Assembly in 3D *Dr. Varun Vyas, University of Connecticut, USA*
12:25-12:40 **CMSE4362**	Zn-Fe Bimetallic Nanostructured Films for Packaging Materials *Dr. Sebastian Calderon, University of Minho, Portugal*
12:40-12:55 **CMSE4300**	Nanomaterials Fe, Al and Ti, in the Mitigation of Potentially Reactive Basalt Aggregate in Portland Cement Dosages: Deposition of Thin Films by Pulsed Dc Plasma *Dr. Emerson Alberti, Centrais Elétricas do Rio Jordão, Brazil*

Abstracts of Session 2

CMSE4255

Deformation and Fracture During Solidification and Adhesion Process of Paraffin Droplet Modelling Thermal Spray

Motoki Sakaguchi*, Chao Kang, Hirotsugu Inoue

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Abstract. Stress evolution and fracture behaviours in paraffin droplet were experimentally and numerically studied, modelling thermal spray of thermal barrier coatings. Two series of experiments were conducted: drop test and cooling test. In the drop test, a molten paraffin droplet was dropped and impacted onto a stainless steel substrate to simulate solidification and rapid cooling of air-plasma-sprayed particle. During the impact, solidification and adhesion process, quenching strain was generated due to a contraction of droplet associating with its rapid cooling. The evolution of quenching strain was measured by a strain gauge attached on the substrate back surface, considering the effects of several experimental variables: drop height, substrate pre-set temperature, droplet initial temperature, and paraffin materials. Cooling test was conducted to simulate the cooling process of sprayed coating and substrate after deposited. Here, solidified paraffin splat and substrate were cooled down simultaneously and quenching strain variation was measured during the experiment. In the drop test and cooling test, fracture behaviours such as cracking and delamination were observed in splat. Two types of finite element analyses were performed to calculate the stress-strain variation and evaluate the fracture behaviours. At first, elastic analysis was performed to calculate quenching stress and interfacial stresses, which are driving forces for cracking and delamination in the experiment. On the basis of the numerical results, cracking and delamination behaviors were numerically discussed. And then a coupled thermo-mechanical analysis was carried out to calculate the quenching strain variation during drop test. Creep deformation of paraffin splat was considered using strain hardening creep law in which creep parameters were measured by a four-point bending method. Calculation

results revealed that creep deformation of splat and adhesion at interface were two main reasons for the relaxation of quenching stress and quenching strain. A series of findings showed some similarities to actual phenomena in air plasma spraying and provided meaningful guidance for optimizing air plasma spraying process.

Keywords: Thermal barrier coating, Model experiment, Fractures, Finite element method, Coupled thermo-mechanical analysis, Creep deformation

CMSE4254 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

CMSE4381
Continuous Segmented Flow Synthesis of Silver Nanowires

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Materials Science Program, Department of Applied Physics, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia

Abstract. One dimensional (1D) silver nanowires (AgNWs) with high aspect ratios and crystallinity have been receiving wide attention owing to their excellent plasmonic, optical and chemical properties, as well as high electric and thermal conductivities. These properties make AgNWs a suitable candidate in various applications, such as catalysis, transparent conductive films, sterilization, and surface enhanced Raman spectroscopy. Polyol method is among the most widely used processes in synthesizing AgNWs. However, most of the synthesis of AgNWs was performed using batch reactor system. Continuous flow chemistry has received increased interest in the synthetic organic chemistry community over the past decades due to many advantages derived from its small size and flow nature. In this study, AgNWs were produced using polyol method with the aid of a flow chemistry reactor (Figure 1). Biphasic segmented flow was created throughout the reaction using two immiscible liquids to create high internal mixing and minimize diffusion (Figure 2). Reaction parameters studied, including temperature of reactor heater, flow rate, NaCl and molecular weight of PVP.

Figure 1. Segmented flow of reaction for the continuous synthesis of AgNWs.

Figure 2. AgNWs collected from the outlet of the flow reaction system.

Keywords: Continuous, Flow chemistry, Silver

CMSE4399

An Analysis of Propagation and Properties of Axisymmetric Waves in Elastic Solids

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Abstract. The wave propagation in elastic solids is widely treated as plane waves with Cartesian coordinates for known modes such as Rayleigh and Love waves in broad engineering applications. Such distinct wave phenomena also exist in other coordinate systems but the essential property such as the velocity should be the same as known ones while many other special features related to coordinate systems are not presented in details in earlier literature. In a series of recent research, it confirmed that typical wave modes can be found in cylindrical coordinate system with axisymmetric feature and wave velocities are independent from coordinate systems of elastic solids. In general, the deformation solution is given in Bessel functions with a decaying feature along the radius that is different from the constant amplitude in Cartesian coordinates. Such feature is consistent with the energy decaying along the wavefront away from the origin. Consequently, there is a distinct feature of enhancement or reduction of signal strength and amplitudes related to the direction of wave propagation. Clearly, this feature can be exploited further through the consideration of wave modes and direction of propagation in relation with the source in measurement and detection by sensors utilizing the axisymmetric waves. Furthermore, it also showed through the properties of Bessel functions that wave modes are consistent with Cartesian coordinates from the asymptotic expansions, confirming the plane wave characteristics we are familiar with. However, in the vicinity of origin, wave properties can be better represented with cylindrical coordinates and solutions. These results, similar with major wave modes in cylindrical coordinates including Rayleigh, Love, Sezawa, and others, are analyzed in details for better understanding of their special properties to aid future applications involving elastic solids with axisymmetric configurations and required interests near the origin of typical wave propagation problems in engineering applications. These analyses are essential in future study of axisymmetric waves in finite elastic solids with practical engineering applications.

CMSE4435

Preparation of the Nano Manganese Oxide Based Modified Electrode and Evaluation of Its Efficiency for Electrochemical Reduction of Niclosamide

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Abstract. Recently, the synthesis and application of the nanostructured nonprecious metal oxides has received particular importance in different disciplines regarding their outstanding physicochemical properties. Here, we describe fabrication of the modified electrodes utilizing chemically synthesized manganese oxide nanostructures (nano-MnO_2). At first, the synthesized nano-MnO_2 was characterized by scanning electron microscopy (SEM), powder X-ray diffraction (XRD), and energy dispersive X-ray (EDX) analysis. Then, the effective surface area, electro-catalytic activity and electro-conductivity

of the nano-MnO_2 based modified electrodes were evaluated by cyclic voltammetry and electrochemical impedance spectroscopy (EIS). Finally, the most sensitive and efficient modified electrode was employed for study of the electrocatalytic reduction of niclosamide (NA). The impact of nano-MnO_2 loading, scan rate, pH and accumulation condition for the quantification of NA were evaluated and discussed. The oxidation peak currents of the reduction product of NA showed a linear relationship with its concentration in a wide range of 50 nM to 50 μM for which high sensitivity and low detection limit were obtained, respectively. The practical application of the nano-MnO_2 modified electrode demonstrated satisfactory outputs for analysis of NA in its dosage forms and in biological fluids.

Keywords: Nano-MnO_2, Niclosamide, Voltammetric, Catalytic, Electrochemical

CMSE4260 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

CMSE4373

New Trends in Fundamental Research Due to the Spontaneous Flexoelectric Effect in Nanosized and Bulk Ferroelectrics

Maya D. Glinchuk[1,*], Eugene A. Eliseev[1], and Anna N. Morozovska[2]
[1]*Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Kyiv, Ukraine*
[2]*Institute of Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine*

Abstract. Investigations of flexoelectric effect is a hot topic. Since the flexoeffect is defined by gradients of polarization and elastic strains, which obligatory exist in nanos, where all the properties change strongly from the surface to the bulk, we introduced the spontaneous flexoeffect, and establish its key role for explanation of mysterious experimental results. The strong influence of spontaneous flexoeffect explains unexpected phenomenon in nanos – the critical size disappearance at size-induced phase transition and reentrant ferroelectric phase appearance. This phenomenon was observed in $BaTiO_3$ nanospheres of radii 5–50 nm and was a puzzle up to our paper, where we explained it by the spontaneous flexoeffect and Vegard strains, created by oxygen vacancies. The developed mechanism opens the ways for miniaturization of electronic devices up to a few nm sizes. More than 15 years ago the appearance of ferroelectricity was observed in bulk PZN-PLZT relaxor sintered in nitrogen atmosphere, which induce high concentration of oxygen vacancies. This phenomenon stayed unexplained, until we have shown that the transition from relaxor to ferroelectric state is possible at high concentration of the vacancies, which are elastic dipoles, due to electrostriction, flexoelectric and Vegard effects. The flexoelectric origin of morphotropic region with high electromechanical properties in relaxors is very important for high-sensitive ultrasound devices. Recently we study the polar phenomenon in low-dimensional transition metals dichalcogenides and have shown that spontaneous out-of-plane polarization arises from the flexoeffect due to spontaneous bending and inversion symmetry breaking in the vicinity of surface/substrate.

Keywords: Spontaneous flexoelectric effect, Nanomaterials, Vacancies, Ferroelectricity

CMSE4402

Very Thin Silver Films on PET and Optical Glass; Obtaining and Properties

Bogdan Alexandru Sava[1,*], Rares Victor Medianu[1], Lucica Boroica[1], Marius Catalin Dinca[1], Ana Violeta Filip[1], Rovena Pascu[1], Antoniu Moldovan[1], Marius Dumitru[1], Mihai Oane[1] and Mihai Eftimie[2]

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[2]*Department Science and Engineering of Oxide Materials and Nanomaterials, University "Politehnica" Bucharest, Romania*

Abstract. Thin metal films have recently attracted scientific and practical interest due to their practical applications as transparent conductive coatings for UV spectrum, transparent electrodes for "smart windows" and solar cells, catalytic coatings, active component of surface plasmon resonance (SPR) based biosensors, etc. Thin films, especially of metals such as Au, Ag, and Cu, are of particular interest because of their stability and reproducibility. Silver as thin films has unique optical properties, best performance in optical applications, and present a significant difference from bulk material (they are partially transparent and conductive at the same time), being the most common plasmonic material. However, there are few reports focused on depositing very thin Ag layers directly onto a glass or PET substrate. In this work, we studied the changes in the optical properties of ultrathin Ag films deposited by RF Magnetron Sputtering onto glass and PET substrates. Samples were morphologically analysed by atomic force microscopy (AFM) showing roughness of up to 3 nm. The films' refractive index was obtained by means of spectroscopic ellipsometry data using a model-based technique by minimizing the difference between the measured spectrum of the ellipsometric parameters and the values calculated from the model. The refractive index n present very low values in the 345-1200 nm region. The transmittance and reflection of the samples, investigated using UV-Vis-NIR spectroscopy, show a transmission maximum specific to Ag and a transmittance minimum, which depends on the thickness of the deposited film, showing the appearance of surface plasmon resonance at low thickness of films.

Keywords: Very thin films, PET, Optical glass, Ellipsometry, AFM, Optical properties, Magnetron sputtering

Acknowledgements: This work was supported in the frame of PULSE-COM, H2020-FETOPEN-2018-2020, 863227 project. Authors thank to prof. Nicolae Țigău for the transmission/reflexion measurements and all his help.

CMSE4266

Advantages High Voltage Consolidation of Powders Refractory Materials

E.G. Grigoryev[1,*], V.Yu. Goltsev[2], A.V. Osintsev[2], A.S. Plotnikov[1,2], E.L. Strizhakov[3], S.V. Nescoromniy[3], V.G. Vinogradov[1,3] and S.O. Ageev[1,3]

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Abstract. The main features of high-voltage electropulse consolidation (H-VEC) of powder refractory materials and the unique possibilities of the method caused by them are considered. The electro-thermal processes in the H-VEC at the contacts between the powder particles and in the macroscale of the whole consolidated sample are analyzed. The results of calculations of the dynamics of closure (collapse) of interparticle pores in the consolidated material are presented.

The experimental results of high voltage consolidation W-based heavy alloys are discussed and a theoretical analysis of the kinetics of compaction of powder materials is made. The results of investigation of the macro- and microstructure of consolidated materials and the stress - strain testing are presented. Compression testing showed that all tested alloys bear compressive stress at room temperature without failure. The plasticity of the heavy tungsten alloy is one of the objectives of the current research. The high-voltage consolidation contributes to maintaining a initial fine-grained structure, more uniform distribution of iron-nickel binder and almost total absence of porosity. The optimal modes of high voltage consolidation W-based heavy alloys on the results of tests of short cylinders according to the “Brazilian test” scheme were obtained.

The process of high-voltage electropulse consolidation of hafnium carbide powder was experimentally studied. A criterion is established that defines the range of technological parameters for creating dense consolidated materials. The results of an experimental study of the microstructure of the obtained hafnium carbide are presented.

Examples of the use of high-voltage electropulse consolidation of powder materials and the direction of further research are considered.

Keywords: High-voltage electropulse consolidation, W-based heavy alloys, Hafnium carbide, Stress - strain testing, “Brazilian test”

CMSE4384

Standardization of the Method of Magnetostriction Measurement of Grain-oriented Electrical Steel Strip and Sheet

Stefan Siebert[1], Jumpei Kobori[2], Koji Fujiwara[2] and Piotr Klimczyk[1]
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Abstract. Standardization of the method of measurement of AC magnetostriction characteristics of grain-oriented electrical steel strip and sheet by means of a single sheet tester and an optical sensor, i.e. IEC 60404-17 Ed.1 [1], has been promoted in the IEC/TC68/WG2 to meet the demand of transformer industry. The relationship between the magnetostriction characteristics of grain-oriented electrical steel and transformer noise is complicated and yet not fully understood. One of basic problems has been the lack of a standard for the magnetostriction measurements. The measurement requires detection of slight vibration of the test specimen at a resolution of 0.01 μm/m or better. In order to ensure this resolution, not only magnetic aspects but also mechanical aspects of the test apparatus, e.g. the influence of friction and external vibrations, have to be specified. The size of test specimen is restricted to 100 mm × 500 mm. The flux closer is a vertical single yoke or a horizontal

double yoke. In order to avoid the influence of friction and vibration, no weight is put on the test specimen except an optical target and a clamp to fix the test specimen to the test apparatus. Also, no weight is connected to the end of test specimen to prevent additional vibration modes. The optical target is low mass and made of non-magnetic and non-conductive materials. The optical target and the clamp are placed between opposite pole faces of the yoke. In order to realize a low and constant friction coefficient, an insertion sheet with a thin fluorine resin-impregnated glass cloth adhesive film on its upper surface is placed under the test specimen. A round robin comparison using different test setups in accordance with the draft of standard was carried out.

CMSE4367
Micro-Acoustic-Trap (μAT) for Microparticle Assembly in 3D

Varun Vyas
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Abstract. Acoustic tweezers facilitate the manipulation of objects using sound waves. With the current state of the technology one can only control mobility for a single or few microparticles. This article presents a state of the art system where an Acoustic Lens was used for developing a Micro-Acoustic Trap for microparticle assembly in 3D. The model particles, 2 μm diameter polystyrene beads in suspension, were driven via acoustic pressure to form a monolayer at wavelength-defined distances above the substrate defined by the focal point of an Acoustic Lens The transducer was driven at 89 MHz, mixed with 100 ms pulses at a repetition rate of 2 Hz. Beyond a threshold drive amplitude sufficient to overcome Brownian motion, this led to 2D assembly of the microparticles into close-packed rafts>80 μm across (∼5 wavelengths of the carrier wave and >40 particles across). This methodology was further extended to manipulation of live Dictyostelium discoideum amoebae. This approach therefore offers maneuverability in controlling or assembling micrometer-scale objects using continuous or pulsed focused acoustic radiation pressure.

Keywords: Acoustic Tweezers, 2D microparticle Array, Acoustic Trap, Acoustic Lens, Acoustofluidics, Dictyostelium discoideum (Amoebae)

CMSE4362
Zn-Fe Bimetallic Nanostructured Films for Packaging Materials

H. Lamsaf[1,3] , Lina F. Ballesteros[2], J.A. Teixeira[2], L. Rebouta[1], S. Carvalho[1,2] and S. Calderon V.[1,3*]
[1]*University of Minho, Department of Physics, Campus of Azurém, 4800-058 Guimarães, Portugal*
[2]*CEB – Centre of Biological Engineering, University of Minho, 4710-057 Braga, Portugal*
[3]*INL - International Iberian Nanotechnology Laboratory, Av. Mestre José Veiga s/n, 4715-330 Braga, Portugal*

Abstract. Bimetallic nanostructured films have gained a lot of attention during the last decade due to their unusual characteristics when compared to monometallic counterparts. Such heterostructures demonstrated enhanced characteristics for catalysis, antibacterial, optical and magnetic properties among others. In this work, we produced ZnFe bimetallic nanostructures Polylactic acid (PLA) substrates to create materials with tunable antibacterial activity, by controlling the morphology and

composition of the coatings. However, in order to properly control their morphology and composition, the production process and growth mechanisms of these heterostructures must be well understood. Hence, this report focuses on studying the growth mechanisms taking place during the simultaneous production of Zn-Fe by magnetron sputtering and its effect on the nanostructured coatings composition. Zn and Zn-Fe nanostructures were produced using two different methodologies, (i) a classical magnetron sputtering, and (ii) a hybrid system composed by a cluster gun and a magnetron sputtering. All depositions were performed in Ar atmosphere varying the current density, from 0.1 to 0.5 A, and deposition time. The morphology and elemental analysis were characterized by scanning (transmission) electron microscopy (SEM and STEM), energy dispersive spectroscopy (EDS) and Inductively Coupled Plasma (ICP). Colour measurements were carried out in a CM-2600d/MINOLTA spectrometer and the antibacterial tests were assessed by the zone of inhibition (ZOI) assay.

The results demonstrated various nanostructures distributions, sizes and Zn/Fe fractions, along with a significant change of colour during the oxidation when the samples were exposed to high humidity environments. In addition, the samples exhibited a relevant antibacterial activity, being correlated in term of the thickness, concentration of Zn/Fe, and morphologies of the samples.

Acknowledgements: The authors thank the financial support by the Portuguese Foundation for Science and Technology (FCT) in the framework of the project NANOXYPACK co-financed via FEDER (PT2020) POCI-01-0145-FEDER-030789.

CMSE4300 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

Oral Session 3: Metals, Ceramics, Composites

Time: 13:30-18:25, Nov. 22, 2020. Eastern European Time (EET)- UTC +2
Session Chair: Dr. Zakaria Boumerzoug, University of Biskra, Algeria
Please Click Paper ID to Access the Video Presentation.
Session Room Link: http://www.academicconf.com/teamslink?confname=CMSE2020

13:30-13:55	**CMSE4414**	How Well Can Impacted Composite Laminates Take Up Load in the Presence of Drilling-Induced Damage for Resin-Injection Repair? *Dr. Kheng Lim Goh, Newcastle Research & Innovation Institute (NewRIIS), Singapore*
13:55-14:10	**CMSE4428**	Advanced Materials Processing Techniques to Produce Ultrafine-Grained Aluminum Alloys *Dr. Kandarp Changela, G H Raisoni College of Engineering and Management, India*
14:10-14:35	**CMSE4357**	A Study on the Effect of Free Acidity and Entrained TBP in UNPS on the Quality of ADU Powder *Dr. D. Mandal, Bhabha Atomic Research Centre, India*
14:35-15:00	**CMSE4297**	First Principles Calculations of Bulk and (001) Surface F-centers in ABO_3 Perovskites as well as ABO_3 Perovskite and ReO_3 Surfaces *Dr. Roberts Eglitis, University of Latvia, Latvia*
15:00-15:25	**CMSE4360**	Heat Affected Zone in Welded Metallic Materials *Dr. Zakaria Boumerzoug, University of Biskra, Algeria*
15:25-15:40	**CMSE4281**	Application of the Hereditary Creep Theory in Assessing the Effect of Temperature Influence on the Strength of Carbon Fiber Plastics *Dr. Irina Gadolina, Russian Academy of Sciences, Russia*
15:40-15:55	**CMSE4407**	Determination of the Yield Stress in a Square Al Thin Film Using the Bulge Test *Dr. Hector Andres Tinoco, Institute of Physics of Materials Science Academy of Czech Republic, Czech Republic*
15:55-16:05		**BREAK**
16:05-16:25	**CMSE4405**	Analytical Evaluation of Transformation Matrix between Functional Spaces and Its Application in Obtaining Exact Solutions of Thermo-Mechanical Stresses in Disks *Mr. Levan Antashvili, Fedinand Tavadze Metallurgy and Materials Science Institute, Georgia*
16:25-16:50	**CMSE4387**	Nanocellulose Fibers from Banana Waste as Carbon Nanotube Dispersing Agent *Dr. Alice G. Osorio, Universidade Federal de Pelotas, Brazil*
16:50-17:20	**CMSE4379**	Effects of Irradiation and Annealing on the Microstructure and Mechanical Properties of Bulk Metallic Glass Alloys *Dr. Jamieson Brechtl, Oak Ridge National Laboratory, USA*
17:20-17:45	**CMSE4316**	A New Percolation Threshold Model that Addresses both Filler Particle Shape and the Interfacial Surface Energy for Polymer Composite Electrical Conductivity Measurements *Dr. Richard Sudduth, Materials Research & Processing, LLC, USA*

17:45-18:00 **CMSE4449**	Functional Modification of Hexagonal Boron Nitride and Its Effect on Flame Retardancy of Polyvinyl Alcohol *Dr. Xiaodong Wang, University of Science and Technology of China, China*
18:00-18:25 **CMSE4450**	Solidification, Microstructure, and Mechanical Properties of the As-Cast ZRE1 Magnesium Alloy with Different Rare Earth Contents *Dr. Rosli B. Ahmad, Department of Materials and Design Engineering, Universiti Tun Hussein Onn Malaysia, Malaysia*

Abstracts of Session 3

CMSE4414

How Well Can Impacted Composite Laminates Take Up Load in the Presence of Drilling-Induced Damage for Resin-Injection Repair?

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Abstract. A study of drilling-induced damage in barely visible impact damaged (BVID) carbon fibre reinforced polymer (CFRP) laminates where small circular holes were intentionally drilled into the impacted zone as an intermediate step of the resin-injection repair process was reported. The pristine CFRP laminates were quasi-statically indented to yield damage that were barely visible. Following the drilling of open/blind, single and binary holes in the impacted laminates at selective locations within the BVID zone, the holed laminates were subjected to in-plane compression test until they broke apart. Binary-hole specimens at fixed distance apart were tested in parallel/normal to the external load. Statistical analysis was used to assess for diminution of laminate mechanical properties contributed by hole-hole interaction and hole-hole orientation effects. BVID specimens showed significant diminution of property value (compared to pristine ones). No dependence of mechanical properties on hole-hole orientation was observed. Owing to the large hole-hole separation, this significantly mitigated the hole-hole interactions. Finally, single/binary-hole BVID laminates revealed laminate stiffening effects: the stiffness was significantly higher than that of undrilled BVID specimens.

Keywords: Quasi-static indentation, In-plane compression testing, Infrared thermography, Elasticity, Fracture

CMSE4428

Advanced Materials Processing Techniques to Produce Nanostructured Aluminum Alloys

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Abstract. Cryorolling (CYR) and constrained groove pressing (CGP) are potential SPD techniques to produce nanostructured materials in the form of thin sheets. In this work, the influence of cryorolling on the microstructure and mechanical properties of the two aluminum alloys (AA 5083 and AA 6061) has been investigated. The as-received Al alloys sheets are solutionized and then cryorolled to reduce the thickness in multiple passes from 6.5 mm to 1 mm. Effect of post annealing treatment of cryorolled samples on microstructure, mechanical properties, and formability has been systemically studied. The results showed grain refinement after cryorolling with higher dislocation density when compared to solutionized condition, and their effect is reflected in mechanical properties. Limiting Dome Height test is used in the present work to compare the formability of the two alloys in cryorolled and annealed condition. In addition to that, a new SPD route is proposed by combining constrained groove pressing (CGP) and cold rolling (CR). Solutionized Al alloys with 3 mm thickness are subjected to CGP with an equivalent plastic strain of 1.16, and then, they are cold rolled at room temperature. This new processing route (CGP+CR) has the potential to overcome the disadvantages of CGP which have non uniform thickness in the transverse direction. The subsequent cold rolling improves the surface flatness that can alleviate the geometric inhomogeneity as a result of the CGP process. The new SPD route is evaluated using solutionized AA 5083 and AA 6061 alloys. The mechanical properties and microstructure from the proposed route (CGP+CR) are compared with cryorolling for similar sample thickness.

Keywords: Aluminum alloys, Cryorolling, Constrained groove pressing, Microstructure, Mechanical properties, Formability

CMSE4357

A Study on the Effect of Free Acidity and Entrained TBP in UNPS on the Quality of ADU Powder

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Abstract. Ammonium Di-Uranate (ADU) is precipitated from Uranyl Nitrate Pure Solution (UNPS) when ammonia gas is passed through it according to the Reactions 1 and 2.

$$NH_3 + H_2O \rightarrow NH_4OH \quad (1)$$

$$2UO_2(NO_3)_2 + 6NH_4OH \rightarrow (NH_4)_2U_2O_7 + 4NH_4NO_3 + 3H_2O \quad (2)$$

The mean particle size and size distribution of ADU particles, precipitated play an important role on the sintered density of UO_2 pellets. The quality of precipitated ADU depends on number of process parameters *viz*., pH of UNPS, concentration of uranium in UNPS, flow rate of ammonium-hydroxide, temperature etc. However, the effects of the presence of free acid and entrained Tri-Butyl-Phosphate (TBP) in UNPS on the quality of ADU powder were not studied till date. Experiments were conducted

to study the effect of free acidity and the presence of entrained TBP on the quality of precipitated ADU particles. It was found that as the concentration of free acid as well as the concentration of entrained TBP in UNPS increases, the particle size of precipitated ADU decreases. Based on the experimental results two correlations were developed to determine the mean particle size of ADU; one is based on the free acid content of UNPS and the other is based on the content of entrained TBP in UNPS, which is used for the precipitation. It was found that the correlated values are well fitted with the experimental data within ±3% errors for both the cases.

Both these correlations are applicable when other process parameters remain constant. The experimental details and results are discussed in this paper.
Keywords: Uranium, Ammonium di-uranate, Uranyl nitrate pure solution

Acknowledgements: The author would like to thank Shri P.V.S.N. Prudhvi Raju, Nuclear Fuel Complex, Hyderabad, India to carry out the experimental works.

CMSE4297

First Principles Calculations of Bulk and (001) Surface *F*-centers in ABO_3 Perovskites as well as ABO_3 Perovskite and ReO_3 Surfaces

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Abstract. We analyze the systematic trends in $BaTiO_3$, $SrTiO_3$, $SrZrO_3$ and $PbZrO_3$ bulk as well as very rarely performed (001) surface *F*-center *ab initio* calculations. The nearest neighbour atomic displacements around the bulk *F*-center in the ABO_3 perovskites are considerably smaller than the relevant neighbour atomic displacements around the (001) surface *F*-centers. The *F*-center electrons are more delocalized for the ABO_3 perovskite (001) surface *F*-center than for the bulk *F*-center. The calculated formation energy difference between the $BaTiO_3$, $SrTiO_3$, $SrZrO_3$ and $PbZrO_3$ bulk and (001) surface *F*-centers triggers the *F*-center segregation from the bulk towards the (001) surface.

We performed *ab initio* calculations for $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $SrZrO_3$, $BaZrO_3$, $PbZrO_3$ and $CaZrO_3$ neutral (001) as well as polar (011) and (111) surfaces. For ABO_3 perovskite (001) surfaces, with a few exceptions, all atoms of the upper surface layer relax inward, all atoms of the second surface layer relax outward, and all third layer atoms, again, inward. The ABO_3 perovskite (001) surface energies always are smaller than the (011) and especially (111) surface energies. The B-O chemical bond population in the ABO_3 perovskite bulk always are smaller than near the (001) and especially (011) surfaces.

Keywords: *Ab initio* calculations, ABO_3 perovskites, Surfaces, *F*-centers

CMSE4360
Heat Affected Zone in Welded Metallic Materials

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Abstract. Welding is a process of joining materials into one piece. Welding is used extensively for pipe welding, aerospace, aviation, biomedical implants, fabrication of race cars, choppers, etc. Welding processes include thermal fusion joining processes and solid-state joining processes. Arc welding process belongs to thermal fusion joining process. Generally, the metallurgy of the welded joint can be categorised into two major regions, the fusion zone (FZ) and the heat-affected zone (HAZ). The heat-affected zone (HAZ) is a region that is thermally affected by the welding treatment. The heat-affected zone (HAZ)is a transition zone because it is composed with the microstructure of the BM and the HAZ. The changes of microstructures in the HAZ depend on the level of thermal exposure and are varying with distance from the weld metal zone. The main difficulty associated with welding is the prevention of unexpected deterioration of properties as a result of the microstructure evolutions which reduce the resistance to brittle fracture in the heat-affected zone (HAZ). Properties of the HAZ are different from those of the base material. According to the literature, the HAZ is the most problematic area in the high strength steels weld. For this reason, many research works investigated this critical zone in welded joint. The main research questions and results related to the HAZ will be presented.

CMSE4281 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

CMSE4407 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

CMSE4405 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

CMSE4387
Nanocellulose Fibers from Banana Waste as Carbon Nanotube Dispersing Agent

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Abstract. Banana is the most consumed fruit in Brazil, mainly due to their all-year harvesting, ease of handling, and rapidity of ripening. The large volume of consumption generates a large amount of waste, as barks and stalks, which, in turn, have great potential for scientific technical exploitation. These stalks and banana peels are rich in polysaccharides with potential applications as raw material for the production of nanocellulose fibers (NCF). Carbon nanotubes (CNTs) are very promising materials for many distinct applications. Nonetheless, most of the known applications of CNTs require a well

dispersed solution of nanotubes, hence the best way to disperse these nanotubes is the use of highly concentrated acid functionalization. In this work, we produced NCF from banana peel stalks to use as a replacement for surfactants and acid functionalization in the dispersion of CNTs. The usage of NCF as a surfactant can be useful when seeking waterbased, efficient, and green pathways for their preparation, making the process less hazardous to the environment and keeping the structure of CNTs intact. Among possible applications, well dispersed CNT/NCF solution can be used to obtain conductive papers and additive 3D manufacture. Alkaline treatment followed by bleaching were carried out at the banana peel pulp to obtain the cellulose. Later, the pulp was exposed to acid hydrolysis in order to obtain the NCF. The nanofibers were confirmed by characterization methods as x-ray diffraction, Fourier-transform infrared spectroscopy and scanning electron microscopy. Aqueous suspension of CNT/NCF were analysed for up to 10 days and remained dispersed, indicating that the NCF may be a good dispersing agent for CNTs.

Keywords: Nanocellulose fibers, Carbon nanotubes, Dispersing agent

CMSE4379

Effects of Irradiation and Annealing on the Microstructure and Mechanical Properties of Bulk Metallic Glass Alloys

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Abstract. Bulk metallic glasses (BMGs) are composed of a topologically disordered structure which prohibits the creation of Frenkel pair defects during irradiation. However, there are still many unanswered questions as to how irradiation displacement damage affects their mechanical and microstructural properties. For this study, microstructural analysis and mechanical tests were performed on as-cast, annealed, and irradiated Zr52.5Cu17.9Ni14.6Al10Ti5 (BAM-11) and Cu60Zr20Hf10Ti10 BMGs. Samples were irradiated by both ion (midrange doses of 0.5 and 10 dpa) and neutrons (0.1 dpa) at temperatures ranging from ambient to ~360 ºC. Nanoindentation and in situ compression tests found that heat treatment and primary knock-on damage led to significant changes in short-range ordering and mechanical properties. Furthermore, neutron diffraction experiments revealed that neutron irradiation led to disordering while annealing led to structural relaxation in BAM-11.

Keywords: Bulk metallic glasses, Irradiation effects, Annealing effects, Mechanical testing

CMSE4316

A New Percolation Threshold Model that Addresses both Filler Particle Shape and the Interfacial Surface Energy for Polymer Composite Electrical Conductivity Measurements

Richard D Sudduth
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Abstract. The new Percolation Threshold model developed by this author gave excellent fits of Clingerman's electrical conduction data for three different carbon fillers in both Nylon 6,6 and Lexan over the whole concentration range. Three different Interfacial Surface Energy models were evaluated. The Fowkes Interfacial Surface Energy, γ_{fp}, was found to give the most consistent linear correlation with the Surface Interaction Magnitude constant, β, from the new percolation threshold model for all the carbon Fillers evaluated in both Nylon 6,6 and Lexan.

In general, it was also found that S-Shaped curves normally found in electrical conduction measurements have three extremely important conditions that occur at the same concentration. These three conditions are: the inflection point concentration, φ_{ip}; the concentration yielding the maximum slope; and the concentration at maximum slope that can be extrapolated back to yield the percolation threshold, φ_c.

This study also established that the concentration, φ_{max}, at maximum electrical conductivity for the S-shaped percolation threshold curve is most likely associated with the maximum random packing fraction associated with the shape of the conductive filler particle in the formulation.
One additional extraordinary characteristic of this new model is that it is also possible to separate this model into two different equations describing separately the conducting filler component and the insulating matrix component.

Keywords: Electrical conductivity, Carbon black, Nylon 6,6, Lexan, Carbon filled composite, Percolation threshold

CMSE4449

Functional Modification of Hexagonal Boron Nitride and Its Effect on Flame Retardancy of Polyvinyl Alcohol

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[2]*School of Chemistry and Material Engineering, Chaohu University, Chaohu 238000, P. R. China*

Abstract. In this study, h-BN nanosheets were obtained by aqueous phase ultrasonic stripping, and zinc molybdate ($ZnMoO_4$) was in situ grown on the surface of h-BN nanosheets to prepare hybrid materials (h-BN@$ZnMoO_4$). polyvinyl alcohol (PVA) composites were prepared by using hybrid materials as functional fillers and the effects of hybrid materials on the flame retardancy of PVA were studied. The results showed hybrid particles have an obvious improvement effect on the thermal stability and flame retardant performance of PVA composites, and effectively inhibited the release of

gases such as combustible pyrolysis products and CO, thus enhancing the fire safety of PVA composites. The main reasons for this are the physical barrier effect of h-BN and catalytic carbonization effect of zinc molybdate.

CMSE4450

Solidification, Microstructure, and Mechanical Properties of the As-Cast ZRE1 Magnesium Alloy with Different Rare Earth Contents

Rosli B. Ahmad

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Abstract. The influence of praseodymium (Pr) content on the solidification characteristics, microstructure, and mechanical properties of ZRE1 magnesium (Mg) cast alloy was investigated. The obtained solidification parameters showed that Pr strongly affected the solidification time, leading to refinement of the microstructure of the alloys. When the freezing time was reduced to approximately 52 s, the grain size decreased by 12%. Mg12Zn (Ce,Pr) was formed as a new phase upon the addition of Pr and was detected via X-ray diffraction analysis. The addition of Pr led to a substantial improvement in mechanical properties, which was attributed to the formation of intermetallic compounds; the ultimate tensile strength and yield strength increased by approximately 10% and 13%, respectively. Pr addition also refined the microstructure, and the hardness was recovered. The results herein demonstrate that the mechanical properties of Mg alloys are strongly influenced by their microstructure characteristics, including the grain size, volume fraction, and distribution of intermetallic phases.

Keywords: Mechanical, Microstructure, Rare earth elements

Oral Session 4: Materials for Electronics and Optoelectronics, Magnetic Materials

Time: 08:30-11:35, Nov. 23, 2020. Eastern European Time (EET)- UTC +2
Session Chair: Dr. Yaovi Gagou, LPMC, Université de Picardie Jules Verne, France
Please Click Paper ID to Access the Video Presentation.
Session Room Link: http://www.academicconf.com/teamslink?confname=CMSE2020

08:30-08:55	**CMSE4293**	Filterless Vacuum Ultraviolet Photoconductive Detector Based on Compound Fluoride with Controllable Band Gap *Dr. Marilou Cadatal-Raduban, Massey University, New Zealand*
08:55-09:10	**CMSE4438**	Magnetic Frustration in $YMn_{1-x}Ga_xO_3$ *Dr. A.K. Rajarajan, Homi Bhabha National Institute, India*
09:10-09:25	**CMSE4382**	Functionalization of Monolayer-CdS by Metal and Non-metal Elemental Substitution: First Principle Understanding *Dr. Altaf Ur Rahman, Riphah International University, Pakistan*
09:25-09:50	**CMSE4240**	A Comprehensive Technical Analysis and Overview of the Recent Theoretical and Experimental Advances in Metamaterials for Novel Opto-Electronic Devices *Dr. Kamal Chopra, Guru Gobind Singh Indraprastha University, India*
09:50-10:15	**CMSE4222**	3D and 4D Computer Models of T-x-y and T-x-y-z Diagrams on the Boundaries of Fe-Ni-Co-Cu-FeS-NiS-CoS-Cu_2S Subsystem *Dr. Vasily Lutsyk, Institute of the Physical Materials Science of the Siberian Branch of the Russian Academy of Sciences, Russia*
10:15-10:25		**BREAK**
10:25-10:50	**CMSE4228**	Lead Free Electrocaloric Materials for Ecological Cooling Devices *Dr. Yaovi Gagou, LPMC, Université de Picardie Jules Verne, France*
10:50-11:05	**CMSE4442**	New Design of a Dye Sensitized Solar Cell for Building Integrated Photovoltaics (BIPV) Applications *Dr. Marek Szindler, Silesian University of Technology, Poland*
11:05-11:20	**CMSE4352**	Effect of Inversion Asymmetry on Quantum Confinement of Dirac Semimetal Cd_3As_2 *Dr. Christopher Chou, Washington High School, USA*
11:20-11:35	**CMSE4303**	Heat Transfer Characteristics of Graphite Welding Pool in Penetration Brazing of Cu/Ni Dissimilar Metal Wires *Mr. Xiao Zeng, Guizhou University, China*

Abstracts of Session 4

CMSE4293

Filterless Vacuum Ultraviolet Photoconductive Detector Based on Compound Fluoride with Controllable Band Gap

Marilou Cadatal-Raduban[1,2,*], Seiya Kato[3], Xi Yu[3] and Shingo Ono[3]
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Abstract. Vacuum ultraviolet (VUV) lights are important for various applications such as surface treatment, optical cleaning of semi-conductor substrates and sterilization. Constant monitoring of high intensity VUV radiation is required to maintain the high standard of manufactured products in many industrial applications. Currently, VUV detectors based on oxide, nitride and diamond have been developed. However, these detectors require filters to block out deep-UV, leading to the reduction of the sensing area. The band gap of the photodetector material is an important consideration when developing the next generation of VUV detectors as the band gap determines the spectral response of the detector. Here, a filterless VUV detector using mixed crystals of calcium fluoride and strontium fluoride ($CaF_2 – SrF_2$, $CaxSr_{1-x}F_2$) will be presented. Generally, fluoride compounds have significantly wider band gaps that allow them to be highly transparent in the deep UV region. Unwanted low energy photons are therefore intrinsically blocked out without having to use filters. We experimentally demonstrate that the band gap of these mixed crystals can be engineered by modulating the composition ratio of CaF_2 and SrF_2. By increasing the CaF_2 content, the band gap increases, and the absorption edge is blue shifted. A range of band gap energies can be obtained between 9.73 eV for pure SrF_2 and 10.24 eV for pure CaF_2. The ability to manipulate the band gap is maintained even at very low temperatures. VUV photoconductive detectors were fabricated to explore the effect of varying composition ratios on spectral sensitivity. The spectral response of the photodetectors shifts to shorter wavelengths as the band gap increases. This allows the spectral response to be controlled by appropriately choosing the $CaF_2 – SrF_2$ ratio. Using $CaxSr_{1-x}F_2$ sensors also eliminate the need for extra filters to cut off unwanted longer wavelengths as the onset of their absorption occur in the VUV region. The controllable spectral response and the filterless feature of $CaxSr_{1-x}F_2$ photodetectors provide an advantage over currently available oxide-, nitride-, and diamond-based ones.

Keywords: Photoconductive detector, Vacuum ultraviolet, Fluoride crystal, Band gap control

CMSE4438
Magnetic Frustration in $YMn_{1-x}Ga_xO_3$

A.K. Rajarajan
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Abstract. $YMnO_3$ is a well-studied compound and known to have geometric frustration due to arrangement of Mn atoms in a triangular lattice. We studied the effect of Ga substitution on the magnetic frustration and valence fluctuation in $YMnO_3$. Studies of magnetization as a function of temperature and XPS at room temperature shows that the Mn atoms have fluctuating valency and magnetic frustration could also originate from the oxygen stoichiometry in these compounds.

Keywords: Magnetization, Valence fluctuation, Magnetic frustration

CMSE4382
Functionalization of Monolayer-CdS by Metal and Non-metal Elemental Substitution: First Principle Understanding

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Abstract. Herein, monolayer-CdS substitutional elemental doping with metal (X; Fe) and non-metal (X; H, N, F) atoms at possible site (see Figure 1) has been investigated by the first-principle calculations. In nonmagnetic monolayer-CdS, magnetism can be induced by metal and non-metal atom substitution at possible dopant sites except for F_S (F doped at the chalcogen site). In particular, Fe doping at Cd-Site (Fe_{Cd}) results in a maximum magnetic moment of 4.0 μ B, and half-metallic character with a small dispersion at point. Among all the substitutional dopants at the hole-site, F_h is ferromagnetic, being most energetically favorable under both atomic and molecular phases. The H_h in monolayer-CdS retained the semiconducting nature with reduced band gaps for spin-up and spin-down channels. N_h exhibits half-metallic character with a small dispersion of 0.13 eV at K- point. The F_h and Fe_h show metallic behavior. To determine the exchange-field strength ferromagnetic (FM) and anti-ferromagnetic (AFM) coupling between the two dopants at far positions (1, 3) and near positions (1, 2) have been considered. The effect of dopants concentration on FM and AFM coupling were also investigated. It was found NS (= 4 %) at near positions (1, 2) shows FM state with Curie temperature (T_c) of 106 K. As the biaxial strain of −5 % is applied the maximum FM state was achieved with T_c of 164 K. The functionalization of monolayer-CdS with the proposed elements provided in this work can help tailoring two-dimensional (2D) materials applied in spintronics and electronics devices.

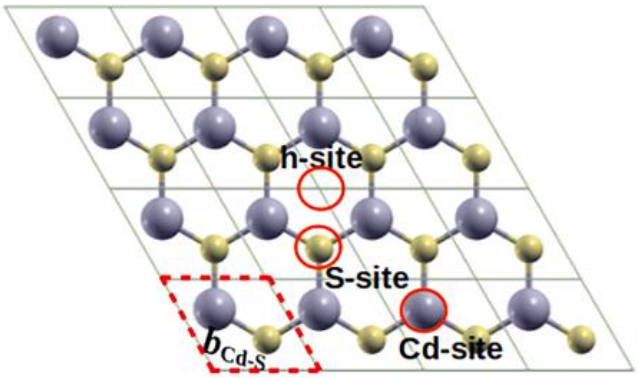

Figure 1. Schematic view of the crystal structure (4 × 4 × 1 -super-cell) for the planar monolayer-CdS indicating the possible doping sites labeled as S-site (doping at the S-site; denoted as X_S), Cd-site (doping at the Cd-site; denoted as X_{Cd}) and h-site (doping at the hole-site; denoted as X_h). The chalcogen (S) and metal (Cd) atoms are presented by yellow and light blue spheres. The primitive unit cell is presented by red dashed lines.

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CMSE4222

3D and 4D Computer Models of T-x-y and T-x-y-z Diagrams on the Boundaries of Fe-Ni-Co-Cu-FeS-NiS-CoS-Cu_2S Subsystem

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[2]*Banzarov Buryat State University, Ulan-Ude, Russia*

Abstract. Design of 3D computer model has been started with a scheme of uni- and invariant states in both tabular and 3D forms. Firstly the analysis of the geometric structure of T-x-y diagram is depicted in the form of template (prototype). Then experimental data are introduced, and the prototype is converted into the model of real diagram. It is convenient to use the Reference of 3D computer models of T-x-y diagrams of basic topological types, which contains the computer models of nearly 300 phase diagrams of ternary and quaternary systems and include the commentaries in the case of questionable (or incorrectly depicted in the literature source) geometric elements. Since the combined diagrams include the majority of real systems, then, composing the combinations of the known topology diagrams from the Reference, it is possible to obtain the computer models of necessary configuration. Based on the example of complex combined diagrams it is more easily to understand as with the aid of the scheme of uni- and invariant states to decode the geometric structure, given by liquidus and several isothermal sections and isopleths in the sub-solidus. E.g. the high-temperature part (above 914ºC) of the T-x-y diagram of the subsystem Fe-FeS-Cu_2S-Cu contains 68 surfaces, including the liquid immiscibility surface, and 32 phase regions. The analysis of geometric structure is carried out with the aid of the computer models of phase diagrams with the liquid immiscibility, which are formed by binary systems with monotectics, either with monotectic transformations in the ternary system without the immiscibility in binary systems, with immiscibility of three and even four liquid phases in the ternary system, and also diagrams with the syntectic uni- and invariant transformations have been designed. The coordinates of the prototype invariant points are given taking into account a temperature row, so as to most clearly show the diagram geometric structure.

Keywords: Phase diagram, Space computer model, Quaternary system

CMSE4228

Lead Free Electrocaloric Materials for Ecological Cooling Devices

Yaovi Gagou[1*], Soukaina Merselmiz[2], Hajar Zitouni[2], Meriem Chettab[3], Daoud Mezzane[2] and Mimoun El Marssi[1]

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[3]*GREMAN, IUT de Blois, 15 rue de la Chocolaterie, 41000 Blois, France*

Abstract. Cold production goes through refrigerant gases (coolants) describing a classic Carnot cycle. These gases are unfortunately harmful and cause the "greenhouse effect" as soon as they escape from their containers during production or in the various heat exchange devices already manufactured. It is therefore urgent to find alternatives; less energy consuming and environmentally friendly solutions. Ferroelectric materials constitute a solution due to their electrocaloric property in solid phase, described by the presence of permanent dipole moments. The ferroelectric-paraelectric phase transition takes place by a crystal symmetry break and a heat exchange takes place in the material, in a reversible process which can be exploited for cooling applications. To the latent heat at phase transition is added the temperature variation due to the change of entropy, compensated by the creation of phonons entropy in the material in a reversible transformation with a constant internal energy.

In order to have amplification of the electrocaloric effect, several avenues are currently being explored, in particular; studies on composites and multiferroics and heterostructures.

In this presentation we will show the recent results obtained on ceramics manufactured from a powder mixture of nanometric grain size that were ferroelectric oxides well chosen (for example, BCT and BCZT) for optimal dielectric and electro-caloric performances. We will also show the perspectives of this study.

Keywords: Cooling, Electrocaloric, Nanomaterial, Multiferroic, Heterostructure

CMSE4442

New Design of a Dye Sensitized Solar Cell for Building Integrated Photovoltaics (BIPV) Applications

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Abstract. One of the important research directions in the field of photovoltaics is its integration with construction (BIPV). The integration of solar cells system with a building enable to reduce installation costs and help to optimize the used space. One of the interesting type of cell is dye sensitized solar cells. In addition to interesting properties, they also bring aesthetic values. In the classic arrangement, the basis for their construction is glass with a transparent conductive layer (TCL). The article presents the possibility of replacing a classic glass counter electrode with an electrode based on a ceramic tile and nickel foil. This solution makes it possible to expand their application in construction. The advantage of this solution is full integration with construction with the simultaneous generation of

electricity. A dye sensitized solar cell was built layer by layer on the tile and nickel foil. A method of atomization was used to deposit fluorine doped tin oxide. Then the screen printing method was used to deposit platinum layer. Electrical parameters of manufactured DSSCs with and without counter electrode tile were characterized by measurements of current-voltage characteristics under standard AM 1.5 radiation. A dye sensitized solar cell integrated with ceramic tiles was produced successfully, which efficiency was over 3%.

Acknowledgements: This publication was supported under the own scholarship fund of the Silesian University of Technology in the field of scientific research and development works, Year 2020.

Keywords: Renewable energy, Nanotechnology, Building integrated photovoltaics (BIV), Thin films, Dye sensitized solar cells

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CMSE4303 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

Oral Session 5: Structural Materials

Time: 13:30-15:40, Nov. 23, 2020. Eastern European Time (EET)- UTC +2
Session Chair: Dr. Mohamed Ali, King Saud University, Saudi Arabia
Please Click Paper ID to Access the Video Presentation.
Session Room Link: http://www.academicconf.com/teamslink?confname=CMSE2020

13:30-13:45	**CMSE4447**	Deterioration in Cement-Based Composite Materials under Freeze-Thaw Cycles and Chloride Attack: A Numerical Study *Ms. Lin-jie Li, Shanghai Jiao Tong University, China*
13:45-14:00	**CMSE4448**	Numerical Investigation on Cement-based Composite Materials under Combined Actions of External Load and Chloride Erosion *Dr. Zhe Hu, Shanghai Jiao Tong University, China*
14:00-14:20	**CMSE4400**	Reforming Mushroom Wastes as Concrete Material Substitutions *Dr. Yap Soon Poh, University of Malaya, Malaysia*
14:20-14:35	**CMSE4421**	Advanced Characterizations of Sri Lankan Roof Tile Clays for more over Industrial Uses *Mr. Suresh Aluvihara, University of Peradeniya, Sri Lanka*
14:35-15:00	**CMSE4408**	Thermal and Acoustic Characteristics of New Materials extracted from Agro Wasted Materials as New Thermal Insulation Materials for Buildings *Dr. Mohamed Ali, King Saud University, Saudi Arabia*
15:00-15:25	**CMSE4347**	Mechanical Properties of a Wide Range of Pipe Steels under Influence of Hydrogen Pure or Blended with Natural Gas *Dr. Pluvinage Guy, FM.C Silly sur Nied, France*
15:25-15:40	**CMSE4359**	Iron and Steel in the Roman World *Dr. Janet Lang, Department of Scientific Research, British Museum, UK*

Abstracts of Session 5

CMSE4447

Deterioration in Cement-Based Composite Materials under Freeze-Thaw Cycles and Chloride Attack: A Numerical Study

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Abstract. Cement-based composite materials, e.g. reinforced concrete, would suffer serious deterioration when attacked by freeze-thaw cycles (FTCs) and chloride penetration in cold region and marine environments. Existing studies lack of models considering the development of pore structure, as well as crack propagation caused by FTCs. In this study, a multi-phase numerical model is proposed for studying chloride transport in concrete under the influence of FTCs, in which the concrete is treated as a composite material, that consist of mortar, aggregate, ITZ and crack. The crack is time-dependent and propagates in the mortar phase and the diffusion coefficient of the mortar is associated with pore structure and temperature. The validity of the presented model is verified against a third-part experiment. Some important factors, including FTCs, crack length and parameters of pore structure are elaborated to illustrate how these factors affect chloride transport. These findings can bring insights to the durability design of reinforced concrete structures locating in cold or marine regions.

Keywords: Cement-based composite materials, Freeze-thaw cycles, Chloride penetration, Pore structure, Multi-phase, Crack length

CMSE4448

Numerical Investigation on Cement-based Composite Materials under Combined Actions of External Load and Chloride Erosion

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Abstract. The durability problem of concrete with cracks has gradually received wide-spread attention. For reinforced concrete structures in coastal areas, chloride erosion is an important factor affecting the durability of concrete, which will have a strong corrosive effect on steel bars. This paper considers concrete under loading conditions combine chloride ingression. In contrast to previous work, a more ac-curate time scale is used to simulate the synergistic effects of load action and chloride ion diffusion. At the same time, we compare the numerical simulation results with the experimental results of rilem246. This paper also discusses the possible effects of crack diffusion coefficient, length, and width on the overall chloride ion transport. The diffusion effect of cracks on chloride ions can significantly affect the concentration distribution of chloride-ions. The width and length have the most significant effect on chloride ion transport, while the water-cement ratio and the volume fraction of aggregate all

have an effect on the chloride-ion transport. The number of small cracks had less influence on the concrete, and their transport effect mainly depended on the crack geometry.

Keywords: Cement-based composite materials, Load effect, Multi-phase, Damage evolution, Chloride ingression

CMSE4400
Reforming Mushroom Wastes as Concrete Material Substitutions

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Abstract. Spent Mushroom Substrate (SMS) is an agricultural by-product generated from mushroom farming. SMS has long been an environmental nuisance in the mushroom plantation industry without proper disposal methodology, for years. The goal of this study is to find alternative outlets for SMS while simultaneously investigating the effectiveness of recycling and reforming it into concrete. SMS is generally thermostable, hydrophobic, and capable of hardening when heated, in which these properties are highly desirable in structures. Hence, this study proposes to substitute SMS as (i) cement and (ii) fine aggregates in controlled low-strength composites (CLSC) for potential applications such as bricks and furniture. This research will investigate the characterizations of SMS. Then, performance assessments such as physical properties, workability and strengths will be conducted on CLSC containing recycled SMS.

Keywords: Cement replacement, Green concrete, Sand replacement, Spent mushroom substrate, Waste recycling

CMSE4421
Advanced Characterizations of Sri Lankan Roof Tile Clays for more over Industrial Uses

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Abstract. Roof tile industry is an abundant industry in different areas of Sri Lanka because of the availability of different clay verities at large number of specific locations in Sri Lanka. In the comparison of the modern uses of such clays, it is highly limited the advanced applications of such clays for advanced science and technological uses other than the primary uses such as the pottery industry, brick industry or roof tile industry. The advanced chemical analysis and identifications of the important chemical characters of a selected roof tile clay type were the aims and objectives of the existing research. The representative clay samples were collected from Dankotuwa area which is recognized as an abundant area of finer grained clays that much suitable for roof tile industry. The collected clay samples were chemically analysed using X-ray diffraction (XRD) spectrometer, X-ray fluorescence (XRF) spectrometer and Fourier transform infrared (FT-IR) spectrometer. The obtained

results showed the presence of Fe, Zr, Ba, Ti and K as the major elements, kaolinite, quartz, glauconite, muscovite and marcasite as the minerals. In the considerations of advanced characteristics of such minerals, kaolinite, glauconite and marcasite have been identified as strong adsorbents for some specific compounds such as some heavy metals, radioactive elements and pathogens and some of ferrous minerals may have the supporting capacities in the catalytic activities for some chemical reactions that combining with some specific solid compounds such as activated carbon. Therefore, as the suggestions, it is possible to recommend the developments and enhancements for such clays for the uses in the waste water treatment applications and catalytic activities as a supporting material in various forms such as the bulks, composite materials or nano-materials.

Keywords: Roof tile clay, X-ray diffraction (XRD) characterization, X-ray fluorescence (XRF) characterization, Fourier transform infrared (FT-IR) characterization, Advanced industrial uses

CMSE4408

Thermal and Acoustic Characteristics of New Materials extracted from Agro Wasted Materials as New Thermal Insulation Materials for Buildings

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Abstract. The international trend nowadays is to use natural insulating materials in buildings to be safe for human beings and to lower the environmental impact. Fibers extracted from the pods of the Apple of Sodom (AOS) plant are confirmed to have lower thermal conductivity compared to those extracted from synthetic fibers and close to the ASME standard. The fibers extracted from its seed pods can be used as a thermal insulating and absorbing sound materials in building. Palm tree surface fibers (PTSF), Agave fibers, wheat straw fibers, and palm tree leaves are all considered as agro wasted materials. These agro-wasted materials are tested for their promising side to be thermal insulating and sound absorbing materials. Hybrid samples are made of these agro materials on the lab scale. Thermal analysis, acoustic characteristics and the microstructure of these wasted materials are made. Sample specimens are made using different binders such as cornstarch, wood adhesive and others to determine their thermal conductivity and their applicability to be used as insulating material for buildings. Thermogravimetric analysis (TGA and DTGA) are obtained showing the stability of all agro fibers. The differential scanning calorimetry (DSC) analysis is also reported for all fibers and shows a broad endothermic transition indicating the melting point of the fibers. Sound absorption coefficients are obtained for the hybrid samples and indicate the potential of using these samples for sound absorption. Results also show that the average thermal conductivity at temperature range 10^{o}C to 60^{o}C of the developed specimens has average values of 0.0418 - 0.0568 W/m K. Figure 1 below shows some of the lab produced hybrid samples.

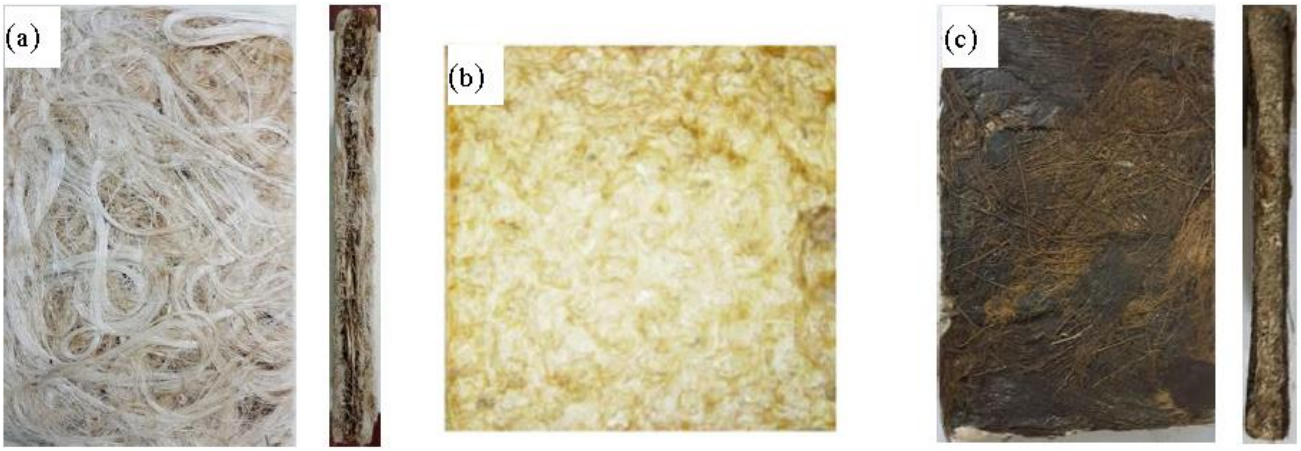

Figure 1. Different specimens of agro wasted materials (a) Hybrid agave and wheat straw, (b) Apple of Sodom fibers, and (c) Hybrid of Apple of Sodom and palm tree surface fibers.

CMSE4347

Mechanical Properties of a Wide Range of Pipe Steels under Influence of Hydrogen Pure or Blended with Natural Gas

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FM.C Silly sur Nied, France

Abstract. Hydrogen economy considers hydrogen as a substantial fraction of a nation's energy and services. This happens in future if hydrogen can be produced from domestic energy sources economically and in an environmental-friendly manner.

Hydrogen can also be used as fuel in stationary fuel cell systems for buildings, emergency power or distributed generation. Hydrogen transport is generally made by pipelines. This solution is preferable than transport on road by truck for security reasons.

The addition of hydrogen in natural gas could have an impact on the degradation over time of the materials currently used for the storage, transport, distribution and use of natural gas. The compatibility of these materials with natural gas including of hydrogen is dependent on the proportion of hydrogen added to the gas and is assessed with regard to several criteria:

-permeation of hydrogen through metallic materials;
-loss of integrity of these materials and adaptation of follow-up actions in service, surveillance and maintenance of equipment.
This paper is devoted to the effect of hydrogen embrittlement (HE) by adding hydrogen into natural gas network on design, maintenance, supervision and maximum allowable service pressure (MAOP) for smooth and damaged pipes.

Keywords: Hydrogen, Pipes, Design, Maintenance

CMSE4359
Iron and Steel in the Roman World

Janet Lang
Department of Scientific Research, British Museum, UK

Abstract. Classical writers give some useful perspectives on Roman metallurgy, but excavation provides more direct information about iron production and artifact manufacture. A wide range of Roman iron objects have been examined. This makes it possible to characterize them metallographically and attempt to evaluate their effectiveness. Iron was made by the direct (bloomery) process and is normally heterogeneous.

Wrought and phosphoric irons and low-, medium-, and some high-carbon steels were produced and utilized. Manufacturing techniques included forging, forge welding, cutting (using chisels and possibly shears), punching, filing, grinding, carburizing, quenching, and auto or slack quenching. The quality of the materials and fabrication treatments was very varied.

Ferrous materials were used extensively in the Classical world. Iron was mentioned by the Classical authors, such as Pliny. Excavations have explored Roman extraction sites and manufacturing areas. Experimental work on reconstructed furnaces has given some insight into the processes and possible outputs. Although many excavated objects, especially fine tools, are often in a poor state of preservation, sometimes metallographic examinations can be carried out. From these studies it is possible to see that different alloys were used for different applications and treatments such as carburisation and quenching were employed. Ferrous metals were widely used in buildings, agriculture, craft tools and of course, for weapons and armour.

Part V Poster Session

Poster Presentation Preparation

- There is no size constraint for the e-poster, if you have difficult to decide one, then A1 size (594mm×841mm) is recommended.
- Please send the poster at **.PDF** format. The Poster would be updated on the conference website after pre-review and confirmation.
- The Poster could design as you like with requirements as below:
  - ✧ The conference logo should be clearly shown in the header.
  - ✧ Title, presenter, and affiliation information should be well indicated.
- Signed and stamped electronic presentation certificate would be issued via e-mail after the conference.

Best Poster Presentations Selection

- One best Poster presentation will be selected based on the "**Votes**" received on the website.
- This award consists of a certificate and free attendance to CMSE2021.

Selection Criteria

- ✓ Research Quality
- ✓ Poster Design

Selection Procedure

- All poster presentations will be updated on the conference website;
- Audience could select best poster presentations by clicking "**Vote for the Best Presentation**", and votes from the same IP would be counted only one time for each presentation;
- Three poster presentations will be selected based on the number of "**Votes**" till **December 5, 2020**.
- CMSE2020 General Chair will choose the **ONE** best poster presentation among the three selected posters. Final result will be demonstrated on the website on **December 10, 2020.**

List of Posters

Time: 15:40-16:40, November 23, 2020. Eastern European Time (EET)- UTC +2

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****Should you have any questions on the posters, please feel free to write down in the notebox of each poster at CMSE2020 official website. The presenter will answer your questions as soon as possible.***

CMSE4237	Study on Effect of Rare Earth Y Refinement on Microstructure Simulation of AlSi7Cu3Mg Alloy Based on Cellular Automata *Mr. Yanzhu Jin, Jilin University, China*
CMSE4292	Use of Infrared Thermography for On-line Characterizing the Impact Damage of CFRP *Dr. Yuan-jia Song, China Aerodynamics Research and Development Center, China*
CMSE4320	Random Processes Imitation in the Problem of Fatigue under Variable Loading *Dr. Irina Gadolina, Russian Academy of Sciences, Russia*
CMSE4332	Synthesis of Hydrogrossular and Hydroxysodalite from Blast Furnace Slag using Alkali Fusion for Fixation of HCl Gas *Prof. Takaaki Wajima, Chiba University, Japan*
CMSE4333	Recycling of Waste Glass Fiber-Reinforced Plastics Using Pyrolysis with KOH *Mr. Masayuki Miyazawa, Chiba University, Japan*
CMSE4351	Accuracy Analysis of Classical Lamination Theory and Finite Element Method for Fiber-Reinforced Composites under Thermomechanical Loading *Mr. Junho Park, Portola High School, USA*
CMSE4352	Effect of Inversion Asymmetry on Quantum Confinement of Dirac Semimetal Cd_3As_2 *Mr. Christopher Chou, Washington High School, USA*
CMSE4369	A Microporous Polymer Ultrathin Membrane for the Highly Efficient Removal of Dyes from Acidic Saline Solutions *Mr. Yang Lu, University of Science and Technology of China, China*
CMSE4371	Low-cycle Fatigue Behavior and Surface Integrity Evolution of AISI 316 Steel with a Gradient Structured Surface Layer *Dr. Hsin Shen HO, Zhengzhou University, China*
CMSE4374	An Examination and Comparison the Zinc Phosphate Coatings Microstructure on the Shot Blasted, Sandblasted and Raw Steel Surfaces *Ms. Beata Herbath, BPW-Hungária Ltd. Hungary*
CMSE4375	TiO_2 Thin Films for Visible Light Photodegradation of Wastewater Pollutants *Dr. Cristina Coromelci, "Alexandru Ioan Cuza" University of Iasi, Romania*
CMSE4413	Superplastic Forming Technologies for Propulsion Components of Launcher *Prof. Ho-Sung Lee, Korea Aerospace Research Institute, South Korea*
CMSE4421	Advanced Characterizations of Sri Lankan Roof Tile Clays for more over Industrial Uses *Mr. Suresh Aluvihara, University of Peradeniya, Sri Lanka*

Abstracts of Posters

CMSE4237 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

CMSE4242

Multinary Bismuth Oxyhalides Composites: Synthesis, Characterization, and Photocatalytic Activity for Removal of Carbon Dioxide, Crystal Violet Dye, and 2-Hydroxybenzoic Acid

Yu-Chen Zhou[1], Ming-Jie Su[2], You-Siang Chen[2], Huai-Sheng Lin[2] and Chiing-Chang Chen[1,*]
[1]*Department of Science Education and Application, National Taichung University of Education*
[2]*National Chung Hsiang High School*

Abstract. Semiconductor photocatalysis driven by visible light has sparked enormous research interest because it provides a promising pathway for solving energy supply and environmental pollution problems. A novel multinary bismuth oxyhalide composite (BiOX/BiOY, X≠Y, X, Y= F, Cl, Br, I) photocatalysts were prepared using a controlled and non-template hydrothermal technique with $Bi(NO_3)_3{\cdot}5H_2O$, KF, KCl, KBr, and KI as the starting material. The pH, temperature, and KX:KY molar ratio for the reactions were adjusted to control the compositions and morphologies of multinary bismuth oxyhalide composites. The composite photocatalysts were characterized through XRD, FE-SEM-EDS, HR-TEM, XPS, DR-UV-vis, BET, PL, EPR, and UPS. Under the optimal synthesis conditions, the photocatalytic activity of BiOCl/BiOI composites was much higher than that of BiOCl and BiOI. Under 25°C, 1 atm, and 432-nm visible light irradiation at, the optimized BiOCl/BiOI increased the rate (at 161 ppm) of photocatalytic conversion from CO_2 to CH_4. Therefore, BiOCl/BiOI is superior for CH_4 production and has great potential as CO_2 photoreduction catalysts. In addition, the photodragrdation activities are evaluated against the decolorization of crystal violet (CV) and 2-Hydroxybenzoic Acid (HBA) in aqueous solution under visible light illumination. The order of rate constant is as BiOCl/BiOI > BiOF/BiOI > $Bi_4O_5Br_2$/$Bi_{24}O_{31}Br_{10}$/BiOI for CV photodegradation. The photocatalytic activity of BiOCl/BiOI reaches the maximum rate constant of 0.2625 h^{-1}, 3.3 times higher than that of BiOF/BiOI, and 3.8 times higher than that of $Bi_4O_5Br_2$/$Bi_{24}O_{31}Br_{10}$/BiOI, respectively. Our findings are useful for BiOX/BiOY synthesis and in its future green energy and environmental applications, particularly in solar fuels.

Keywords: Bismuth oxyhalide, Methane, Composite, Photocatalytic, Crystal violet, 2-hydroxybenzoic acid, CO_2

CMSE4292 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

CMSE4320 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

CMSE4332 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

CMSE4333 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

CMSE4351

Accuracy Analysis of Classical Lamination Theory and Finite Element Method for Fiber-Reinforced Composites under Thermomechanical Loading

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Abstract. The most commonly used composite structure is fiber-reinforced composite, which comprises of matrix and fiber. Due to their superior longitudinal strength but poor transverse strength, layers of composites are stacked in different angular orientations to form laminates, further enhancing the mechanical properties in multiple directions. Hence, laminated composites are being utilized for various applications such as infrastructure and automobile structure; thus, it is important to accurately assess the overall laminate performance under various loading situations. However, most common approaches for structural analysis of laminated composites such as finite element method and classical lamination theory yield approximate values. In this study, we explored the accuracy discrepancy between finite element method, classical lamination theory and experimental data. We applied thermomechanical load in different directions on fiber-reinforced single ply and laminated ply with [0, 90, 0], $[\pm 45]_4$ and $[0,90]_4$. Then, we analyzed the stress-strain, strain-strain and strain-temperature curve to highlight the discrepancy by comparing the slope values.

CMSE4352 To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

CMSE4369

A Microporous Polymer Ultrathin Membrane for The Highly Efficient Removal of Dyes from Acidic Saline Solutions

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Abstract. Thin film composite (TFC) membranes formed by interfacial polymerization on top of a porous support membrane, are commonly used for highly effective separation. To treat textile industry wastewater efficiently, TFC membranes with excellent water permeance and high dye removal efficiency are urgently desired. However, the high acidity and salinity usually exist in textile

wastewater, which will decrease dye removal efficiency for conventional polyamide-based TFC membranes. This study presents a type of acid-tolerant polyarylate (PAR) TFC membrane to tackle such a problem. The PAR active layer is produced *via* interfacial polymerization using 5,5',6,6'-tetrahydroxy-3,3,3',3'-tetramethyl-1,1'-spirobisindane (TTSBI) and isophthaloyl dichloride (IPC) as monomers, and formed on top of a single-walled carbon nanotube (SWCNT) nanofilm. The ultrathin PAR active layer was obtained, and the PAR TFC membrane exhibited the extremely high membrane permeating flux of ~210 L m^{-2} h^{-1} bar^{-1}, while the negatively charged surface of the PAR active layer made a high dye rejection of >99% at a wide range of feed solution pH and salinity possible. In addition, a high selectivity for dye and NaCl was observed with a stable NaCl rejection of ~10%, when the membrane was tested at a pH ranging from 2 to 9 and feed NaCl concentration ranging from 1000 to 5000 ppm. The PAR TFC membrane is therefore a promising tool for the highly efficient treatment of acidic and high salinity textile dye wastewaters.

Keywords: Composite membrane, Dye removal, Acid tolerance, Interfacial polymerization

CMSE4371

Low-cycle Fatigue Behavior and Surface Integrity Evolution of AISI 316 Steel with a Gradient Structured Surface Layer

Hsin Shen HO
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Abstract. Owing to the superior properties of AISI 316 austenitic stainless steel, it is one of the most widely used stainless steel in engineering applications. Inspired by earlier work, the present work thereby aims to investigate the low-cycle fatigue behavior and surface integrity evolution of such steel with a gradient structured (GSed) surface layer produced by conventional shot peening, the most commonly used surface severe plastic deformation (SPD) method in automotive industries. The main works are as follows: firstly, examine the effect of GSed surface layer on cyclic stress response; and secondly, evaluate the changes of surface integrity, described in terms of residual stress, microstructure, surface finish and hardness, at different fatigue life stages. The fatigue analyses show that all alloys possess three principal cyclic evolution stages: initial cyclic hardening (stage I), cyclic stabilization (stage II) and secondary cyclic hardening (stage III). The GSed surface layer can accelerate the transition between stage I and stage II and decelerate the transition between stage II and stage III. The surface integrity analyses show that the presence of GSed surface layer with the increase of number of cycles causes not only the occurrence of a complete compressive residual stress relaxation and austenitic to martensitic phase transformation, but also increased surface roughness and decreased surface hardness. The obtained results are useful for providing a design guideline for engineering industries. H.W. Huang et al., Acta Mater 2015;87:150-160. S. Bagherifard et al., Int J Fatigue 2014;65:64.

Keywords: Shot peening, Low-cycle fatigue, Surface integrity

CMSE4374

An Examination and Comparison the Zinc Phosphate Coatings Microstructure on the Shot Blasted, Sandblasted and Raw Steel Surfaces

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[2]*University of Pannonia, Institute of Materials and Mechanical Engineering, Veszprém, Hungary*

Abstract. In vehicle manufacturing, mechanical surface cleaning is often used as a surface preparation before painting. The blasting is used for cleaning and the blasted surface is a very clean surface and providing excellent mechanical adhesion for the paint layers. Media selection plays an important role in effective blasting. Shot or sand- blasting can be widely used to remove rust, oxides, scales. Its main scope is to provide surfaces free of adhesion preventing materials. The increased surface roughness provides good adhesion for the first layer of the coating.

However, the clean raw surface which was created by the two media (shot and sand) does not behave equally during chemical pretreatments.

In this studies were compared the difference between the surface structure of the sample plates after shot blasting and sandblasting as mechanical surface pretreatment with the structure of a raw sample plate without mechanical surface pretreatment and with a Q-Panel sample plate, witch representing the ideal surface, based on digital light microscope images. The surface roughness (R_z as maximum peak to valley height of the profile, within a single sampling length) was measured by surface profile measurement is made with a MAHR profilometer according to DIN EN ISO 4287.

The chemical composition of the surfaces was determined by energy dispersive X-ray spectroscopy (EDX) and spark excitation optical emission spectroscopy (OES) measurements.

The sample plates were treated by zinc phosphating process with a dipping and spraying system, and microstructural characterization and surface properties of zinc phosphated steel were examined by scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDX).

Keywords: Zinc phosphate conversion coating, Shot blasting, Sandblasting, Surface roughness, Steel and iron surface

CMSE4375

TiO_2 Thin Films for Visible Light Photodegradation of Wastewater Pollutants

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[2]*Department of Chemistry, "Alexandru Ioan Cuza" University, Iasi, Romania*

Abstract. Due to the industrial progress during the past decades, two of the most important issues of human life are water recycling and air cleaning. This is why applications of self-cleaning materials have become a subject of increasing interest in the last years. During this study, two different

deposition methods (dip-coating and spin-coating) of TiO_2 and various types of supports were employed for self-cleaning film preparation. Both commercially available anatase and synthesised TiO_2 using ultrasound assisted sol-gel method were used. Morphological and structural characterization of the films was performed in order to establish the effects of film deposition techniques on crystal structure, microstructure and optical properties of the films, using XRD, AFM, SEM and UV–vis spectrophotometer. The end-use properties of the obtained films were studied. After morphological and structural characterization of the films, mechanical properties, such as resistance, thickness, roughness (surface profilometry) and hydrophilicity (contact angle measurement) were determined. The photocatalytic degradation of wastewater contaminants was measured using an UV–Vis absorption spectrometer and a Total Organic Carbon (TOC) analyser, notable results being obtained for both UV and Visible light activation.

Keywords: Photocatalysis, Thin films, Self cleaning surfaces

Acknowledgements: This work was supported by a grant of Ministery of Research and Innovation, CNCS – UEFISCDI, project number PN-III-P1-1.1-PD-2016-1316, within PNCDI III

CMSE4413
Superplastic Forming Technologies for Propulsion Components of Launcher

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Launcher Structure & Materials Team, Korea Aerospace Research Institute, South Korea

Abstract. This study presents superplastic forming and diffusion bonding technology to manufacture aerospace propulsion components. The method to produce integral configuration from superalloy or titanium pressure bottles by superplastic forming shows it has been successfully demonstrated for near net shape forming of lightweight components with internal cavity. The combustion temperature in the typical combustion chamber reaches very high temperature and pressure. Diffusion welding of copper and stainless steel was necessary to manufacture a scaled combustion chamber. The outer skin of stainless steel is formed by superplastic forming and then bonded with copper inner skin with cooling channels. It is shown that solid state welding of dissimilar metals of Cu and Steel can be successfully applied to fabricate lightweight aerospace parts. Since the forming temperature is high, the forming dies are manufactured with CRES (corrosion-resistant steel). Diffusion welding of titanium is combined with superplastic forming process and produce lightweight pressure bottles.

Keywords: Aerospace, Superplastic Forming, Diffusion Bonding, Duplex Stainless Steel, Titanium, Combustion Chamber, Pressure Bottles

Part VI Call for Papers for Peer Review Journals

Part VII Acknowledgements

On behalf of the CMSE2020 Organizing Committee, we would like to take this opportunity to express our sincere gratitude to our participants. Without their support and contributions, we would not be able to hold the conference successfully in this special year. We would also like to express our acknowledgements to the Technical Program Committee members who have given their professional guidance and valuable advice as reviewers. For those who contribute to the success of the conference organization without listing the name here, we would love to say thanks as well.

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