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e-Poster

## **Material Science 2018**



International Conference on

Materials Science and Engineering July 23-25, 2018 | Moscow, Russia



## Materials Science and Engineering

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### The effects of microalloying elements and temperaging treatments parameters on Nb-V containing cast microalloyed steels

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In this study. base composition without alloying elements and three microalloyed steels containing 0.06% wt V and 0.06% wt Nb-0.1% wt V in induction furnace. in controlled condition. Were casted. Temperaging were carried out on all of specimens for precipitation strengthening. For studying the influence of temperaging time and temperature. specimens with different chemical compositions were temperaged at 400,500,600 and 700 C for 1,3 and 5 h. All of specimens in as-cast condition were studied using optical microscope and hardness tester. Results showed that as-cast specimens having ferrite-pearlitic microstructures. Nb-bearing specimens shows acicular microstructures. The heat-treated samples were studied using Electron Microscope Analysis and hardness tester. Studying of mechanical properties of heat treated specimens, showed that because of precipitation strengthening, hardness of samples increased. By increasing of temperaging temperature in a constant time, hardness has an optimum value.

#### **Speaker Biography**

Farnaz Einkhah is an Iranian university teacher at Rasht, in the north of Iran. She was graduated in the Foundry field at Tehran University and earned master degree in 2005. She began to work as Research and Development Unit Manager at Gilan Steel Complex in 2006 and simultaneously Taught Corrosion in the building, Steel Project, Principles Of Building Maintenance in University of Applied Science and Technology of Rasht Academic Center for Education. In recent fourteen years she has taught many courses in Karaj House of Worker University of Applied Science and Technology, Rasht Academic Center for Education and Mouj Nonprofit University. She has codified 5 single course and one single Module In University of Applied Science and Technology that is in the stage of Approval.

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Notes:



## Accepted Abstracts

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### **Evolution of soil stabilization using Nanomaterials**

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he construction industry is increasingly turning to the use of environmentally friendly materials in order to meet the sustainable aspect required by modern infrastructures. Consequently, in the last two decades, the expansion of this concept, and the increasing global warming have raised concerns on the extensive use of Portland cement/ fly ash due to the high amount of carbon dioxide gas associated with their production. Soft clays are associated with low compressive strength and excessive settlement. This reduction in strength due to moisture leads to severe damages to buildings and foundations. The soil behavior can be a challenge to the designer build infrastructure plans to on clay deposits. The damage due to the expansive soils every year is expected to be \$1 billion in the USA, £150 million in UK and many billions of pounds worldwide. The damages associated with expansive soils are not because

of the lack of inadequate engineering solutions but to the failure to identify the existence and magnitude of expansion of these soils in the early stage of project planning. The development of nanotechnology and nanomaterials offer promising signs for a change in the way of construction and geotechnical projects. Nanotechnology, as a new industrial revolution, has brought numerous opportunities to a variety of scientific, engineering and technological sectors. The bottom-up synthetic strategy in the transitional zone between atom and molecule creates Nano-dimensional materials with novel physical and chemical properties. Hence, soil improvement with nanomaterials is a new technique to tap the significant advances made in nanotechnology which has made nanomaterials cheaper and robust material to compare with traditional methods in the future.

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### The effect of annealing temperature on structural and optical properties of ZnGa<sub>2</sub>O<sub>4</sub>: Cr<sup>3+</sup> synthesized by citrate sol-gel method

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This paper reports the material properties of  $Cr^{3+}$  (1 mol %) doped  $ZnGa_2O_4$  nano-powder prepared by citric acid assisted sol-gel method. The effect of annealing temperature on optical, structural and morphological properties of  $ZnGa_2O_4$ : $Cr^{3+}$  (1mol %) nano-sized particle were investigated. The x-ray diffraction (XRD) results showed that the synthesized nano particles are cubic structured and the annealing temperature did not affect the crystal structure. The average crystallite size of  $ZnGa_2O_4$ :  $Cr^{3+}$  was observed to increase from 11.85 nm to 30.88 nm as the annealing temperature increased from 600 to 1000 °C. The analysis of high resolution transmission electron microscope (HR-TEM) show that with increase of annealing temperature the average particle size increase and also the HR-TEM image show clear lattice fringe which is indicative of increase in crystallity with increase in annealing temperature. Ultraviolet–visible (UV-Vis) spectrophotometer measurement shown an increase in reflectance in visible region and also energy band gap found to be increase with increase of annealing temperature. The photoluminescence (PL) intensity was found to be maximum with sample annealed at high temperature (1000 °C) and least with sample annealed at low temperature (600 °C). An increase in annealing temperature leads significantly increment in PL intensity. The degree of crystallinity also increased with annealing temperature from XRD, SEM and HR-TEM analysis. The emission spectra, photoluminescence lifetimes and particle size are comparable with reports on bio imaging applications.

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### High-performance anode materials for next generation Na-ion batteries

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ecause of their high energy density, Li-ion batteries have Battracted attention as a large energy storage system over their traditional use for portable and electric vehicle applications. However, there are concerns about the scarcity, uneven global distribution and high cost of lithium resources. Compared with Li, Na has the advantages of natural abundance and low cost. Furthermore, Na and Li are in the same main group, exhibiting similar chemical properties, which translates to a resemblance between operational characteristics in Li-ion batteries and Na-ion batteries. Therefore, Na-ion batteries have been suggested for the alternatives to Li-ion batteries for largescale systems. For the practical use of Na-ion batteries, studies for finding suitable electrode materials with high energy density, good cyclability and rate performance for Na-ion batteries have been actively conducted. Although several cathode materials have been suggested, the anode choices are severely limited because of the unique characteristic of Na. Na-ions cannot be stored in the commercial layered graphite because of their large

radius. Si based materials are expected to be the most promising anode for Li-ion batteries, but it is electrochemically inactive with Na. To explore a high-performance anode materials for Na-ion batteries, we synthesized i) pure Sn electrodes with various structures such as Sn nanofibers, Sn multilayer, and Sn foam ii) MoS, MoO (2<x<3) composites using one-step electrodeposition process. The Sn electrodes exhibited a high reversible capacities and excellent cycle performances. After cycling, the Sn electrodes exhibits no loss of active materials and it was attributed to the pore volumes in the electrodes which accommodated the volume change during sodiation/ desodation, and structural stabilities of them. The MoS<sub>3</sub>/MoO<sub>2</sub> showed highly reversible capacity and superior cycling stability. After cycling, the electrode material showed almost no crack or fracture and well maintained the contact with substrate, which are attributed to the buffering action of MoO, phase during sodiation/desodiation of Na<sup>+</sup> in MoS<sub>2</sub> phase.

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### Novel conductive adhesive films materials for electronics packaging applications

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ue to the increasing demand for higher performance, greater flexibility, smaller size, and lighter weight in portable, wearable, and display electronic products, there have been growing needs of various electronic packaging products and interconnection technologies now and in near future. To realize various portable, wearable, and display electronic products, ultra-fine pitch and flexible packaging & interconnection technologies are needed. As one of the promising ultra-fine pitch and flexible interconnection technologies, electrically conductive adhesive films materials such as ACFs (Anisotropic Conductive Films) and NCFs (Non-Conductive Films) are widely used. However, ACFs have two technical limitations such as ultra-fine pitch and current handling capability. For ultra-fine pitch applications, novel Nano-fiber ACFs and APL (Anchoring Polymer Layer) ACFs have been successfully invented by KAIST for less than 20-micron pitch COG (Chip on Glass), COP (Chip on Polymer), and COF (Chip On Flex) applications. In addition, for high current handling applications, new solder ACFs have been also newly introduced by KAIST to replace the conventional metal particles based ACFs materials.

By solder ACFs, 30% lower contact resistance, 4X higher current handling capability, and excellent reliability were successfully achieved compared with conventional ACFs. Furthermore, ACF interconnection method can provide the excellent flexible interconnect solution for OLED COP and COF/CIF (Chip in Flex) packages to realize totally wearable electronic products.

Recently new interconnection materials, NCFs, are introduced for stacking semiconductor chips in 3-dimensional (3-D) way using the TSV (Through Silicon Via) technology. In the 3D-TSV vertical interconnection, Cu pillar/Sn-Ag eutectic solder bump combined with NCFs materials are the most promising bonding and interconnection method. Recent HBMs (High Bandwidth Modules) used as high-speed memory modules for AI (Artificial Intelligence) and Cloud computing have been packaged by NCFs materials. In this presentation, the novel ACFs materials for various ultra-fine pitch interconnection and the NCFs for 3D-TSV chip stacking applications will be introduced.

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### Molecular dynamics studies of temperature and grain size effects on mechanical properties of Nanocrystalline tungsten

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The elastic moduli of nancrystalline tungsten have been calculated from elastic constants by molecular dynamic simulation using embedded atom model. The Nanocrystal containing 16 grains with average diameters ranging from 4, 2 to 8, 9 is made using the Voronoi construction. We have been interested in the investigation of both temperature and

grain size effects on elastic moduli. A softening of material was observed with the temperature increase and the grain size decrease. The anisotropy calculations have shown that the material becomes more isotropic in high temperature. The found results are in good agreement with the literature.

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### Binary blended small-molecule cathode buffer layer materials for highly efficient organic photovoltaic cells

Chuanlang Zhan Chinese Academy of Sciences, China

In this topic the concept of design rational, and the photovotaic properties from a series binary blended small-molecule cathode buffer layer (CBL) maetrials for fabricating highefficiency organic photovoltaic cells has presented. As an example, I herein show that the old and famous dye, N719, can be utilized as high-efficiency, alcohol solution-processible cathode buffer layer (CBL) material. N719 and the binary N719:PrC<sub>60</sub>MAI CBL, respectively, affords 10.50% and 11.46% efficiency, single-junction ternary polymer solar cells. The work function of the Al cathode can be modulated between -3.3 eV and -3.9 eV simply by controlling the binary components weight ratios, which is due to the weight-ratio dependent rearrangment between the four kinds of cations and anions. With this binary blend as the CBL, a PCE of 11.3% was achieved from a new nonfullerene small-moelcule acceptor. The synthesis to this C<sub>60</sub> derivative is relatively complicated and this inevitably increases the cost, while the future application for commercialization requires low-cost but high performance CBL materials. We therefore turn a cheap phosphorous derivative, tetraphenylphosphonium bromide (QPhPBr), with which and its binary blend with N719 as the CBL, high-efficiency fullerene and nonfullerene polymer solar cells have been realized

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### Metal-Graphene hybrid materials as heterogeneous catalyst for carbon-carbon and carbon-heteroatom cross coupling reactions

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Graphene, one of the most promising materials in nanotechnology. Its unique physical, chemical and mechanical properties are outstanding and could allow the preparation of hybrid materials with unique characteristics. From the theoretical point of view, it provides the ultimate twodimensional model of catalytic support. This study, the thirteen nanohybrids based on graphene as support were designed and synthesized as well as heterogeneous catalysts used in the carbon-carbon and carbon-heteroatoms coupling reactions. All nanohybrids were characterized by X-ray diffraction, Raman scattering, transmission electron microscopy, scanning electron microscopy, energy-dispersive X-ray spectroscopy, X-ray photoelectron spectroscopy.

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### Two-dimensional lattice thermal transport in graphene using phonon scattering mechanism: Application as heat management material

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The extremely high electrical and thermal conductivity observed in graphene make it a suitable candidate as heat management material for various applications. Two-dimensional lattice thermal transport in bilayer graphene is investigated using phonon scattering mechanism. In the plane layer of carbon atoms the thermal conductivity ( $\kappa$ ) is demonstrated by incorporating the phonon- defect, phonon-electron, phonon-grain boundaries, phonon-phonon umklapp scatterings and out-of-plane phonon scattering process in the model Hamiltonian. A typical T<sup>1.5</sup> dependence of thermal conductivity at observed at low temperatures (lower than 150 K) is the resultant of various operating phonon scattering mechanisms. Above room

temperatures, the thermal conductivity decreases and follows almost T<sup>-2</sup> dependence which is an artifact of the dominant Umklapp phonon scattering at higher temperatures. The phonon peak appear at around 225 K is due to the competition between the increase in the phonon population and decrease in phonon mean free path due to umklapp phonon scattering with increasing temperature. The results obtained from present model are in good agreement with the available experimental data and reflect the two-dimensional nature of phonon transport in graphene which is dominated by phonon scatterings

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### The new generation of materials for off-earth mining

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he boundaries of human exploration have been expanded to the space and a Mars colonisation process is imminent in the next decades. Due to the harsh environment and the lack of biological resources, to colonise the red planet is not a trivial task, yet it shares similarities with many terrestrial colonisation processes happened during the last centuries. Initial colonisation cargo delivered to Mars should contain essential supplies to support the life of small crews but just for limited time because of the complexity of the interplanetary supply chain which is highly dependent on the launching weight. The launching of the Big Falcon Rocket inserted a new milestone on space cargo capacity; however, having a massive rocket is not enough to sustain human life on Mars because an "ideal" continuous interplanetary supply of materials is limited by physics, financial and technical constrains. Thus, in an analogous way that many colonisation processes occurred on Earth, In-Situ Resources Utilisation via off-Earth Mining (OEM) activities will be fundamental to sustain human life on Mars. OEM should not only assure a secure supply of essential elements for human survival such as water and oxygen, but also extract essential minerals to be used as a raw material for infrastructure and power generation. Design, construct and maintenance of OEM equipment is a challenging task due to the elevated level of uncertainties regarding the Martian environment and its geology; therefore, they need to be lights, efficient, versatile, enduring and cheap. To fulfil these requirement, there is no other better source than the development of new materials. This presentation explores the evolution of space exploration, reveals the main challenges and risks associated to the Martian colonisation process and the technical requirements for the new generation of materials that OEM needs to expand human presence in the solar system

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### From porous to dense nanostructured β-Ti alloys through high-pressure torsion

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**β**-Ti alloys have low elastic modulus, good specific strength and high corrosion resistance for biomaterial applications. Noble elements, such as Nb, Ta and Mo, are used to obtain β-Ti due to their chemical biocompatibility. However, due to their refractory nature, β-Ti requires specific processing routes. Powder metallurgy (P/M) allows for the development of new β-Ti alloys with decreasing costs but dealing with highelemental-content alloys can lead to a lack of diffusion and grain growth. One method to refine the structure and improve mechanical properties is a severe plastic deformation technique through high-pressure torsion (HPT). The aim of this work was to evaluate the conversion of P/M porous β-Ti-35Nb-10Ta-xFe

alloys to dense nanostructures through high-pressure torsion in one deformation step and the influence of the structure variation on the properties and microstructure. TEM analysis and ASTAR crystallographic mapping was utilized to characterize the nanostructures, and the properties of P/M  $\beta$ -Ti-35Nb-10Ta-xFe alloys processed by HPT were compared. The initial microstructure consisted mainly by the  $\beta$ -Ti phase with some  $\alpha$ -Ti phase at the grain boundaries. The HPT process refined the microstructure from 50  $\mu$ m (P/M) down to nanostructured grains of approximately 50 nm.

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### Microstructure and mechanical behavior of Zr–Mo Biomedical alloys

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**Z**r-Mo alloys show low elastic modulus and low magnetic susceptibilities which are ideal for biomedical applications. In this work Zr-xMo (x = 0, 1, 3, 7.5, 10, and 15 wt.%) alloys were investigated. Ingots were arc melted and subjected to homogenization heat treatment, hot rolling process, solution heat treatment followed water quenching. Water quenched samples were characterization by XDR, visible light microscopy, and Vickers hardness. Microstructural results (i.e. XRD and visible light microscopy) showed that the martensite  $\alpha'$  phase was the dominant form for pure Zr and Zr-1Mo content in the water quenched alloys. The  $\beta$  and  $\omega$  phases were formed in Zr–3Mo alloys while only  $\beta$  phase was observed in Zr-7.5Mo and Zr-10Mo. The Mo2Zr compound was observed in Zr-15Mo alloy. Vickers hardness results showed the lowest value for pure Zr samples (174 HV) whereas Zr-3Mo ( $\beta$  +  $\omega$  phases) presents the higher hardness (440 HV) due the brittle  $\omega$  phase. High  $\beta$ -stabilizer samples Zr-7.5 to Zr-15Mo showed values around 300 HV.

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### Multifunctional Micro and Nanoencapsulation approaches with remote controlled delivery and release properties

**Gleb B Sukhorukov** Queen Mary University of London, UK

ne of the challenges in the (bio)-nanotechnology field is development of micro or nano-sized delivery systems comprising different functionalities. These systems should be able to ship and to carry bioactive substances to pre-defined site and unload it in designed time and place predominantly with remote physical signalling. Layer-by-layer assembled capsules have been intensively studied in recent years owing to their ability to encapsulate a wide range of chemicals from complex biomacromolecules to small water-soluble compounds, for their permeability to be modified and their responsiveness to different factors and functionalities to be tailored in one capsule entity. Current research leads to the fabrication of carriers with remote guiding and activation by optical, magnetic and ultrasound addressing, what envisages unique applications as multifunctional biomaterials, including intracellular entering and in-vivo delivery with remote controlled release of micro packaged (bio)-chemicals. Release and encapsulation of materials by light and/or ultrasound and their navigation with magnetic field is a particularly interesting topic for chemical and biomedical applications. Microcapsules display a broad spectrum of qualities over other existing micro delivery systems such as high stability, longevity, versatile construction and geometry of micropackeging and a variety of methods to retain

and release the substances. The talk highlights recent advances in polyelectrolyte multilayers relevant to in vivo delivery of capsule to side of interest by magnetic field as well as make the cells magnetic upon their uptake by various cells lines. Another particular attention in areas of polyelectrolyte multilayers is given on formation of defined microstructures on patterned surfaces. Polyelectrolyte multilayers can be deposition onto widely used PDMS stamps forming, so called, microchamber arrays enabled to accommodate various biologically active molecules. These chambers can be sealed over with another thin made of polymeric layers and resulted structure is pulled off to form free standing microchambers. Entrapment of water soluble molecules into sealed chambers is performed by depositing hydrophobic layer polylactic acid on the top of multilayers and water-soluble molecule make precipitate inside wells upon drying. Sealing results on formation of microsized air-bubble what can keep water soluble molecules inside the chamber until it released upon remote signalling via ultrasound or light. The perspectives of biomedical application of remote activation and microchambers and capsule delivery and microchamber activation are discussed.

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### NOx reduction via selective catalytic reduction with NH3 over Cu-ZnO loaded onto core-shell Al-MCM-41: The effect of metal loading

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Aseries of Cu-ZnO/core-shell Al-MCM-41 catalysts having different metal loadings of 3, 5, and 7 wt% (with Cu:ZnO ratio of 1:1) was studied for NOx reduction via selective catalytic reduction (SCR) with NH3 at 300 °C. Copper was loaded onto core-shell Al-MCM-41 by a combination of three methods like substitution, ion-exchange, and impregnation to obtain various forms of copper species, while zinc was loaded by impregnation method to obtain ZnO form only. The physicochemical properties of the prepared catalysts were investigated by N<sub>2</sub> physisorption, transmission electron microscopy (TEM), X-ray diffraction (XRD), temperature programmed desorption of NH<sub>3</sub> (NH<sub>3</sub>-TPD), H<sub>2</sub> temperature programmed reduction (H<sub>2</sub>-TPR), X-ray adsorption spectroscopy (XAS), and X-ray photoelectron spectroscopy (XPS). TEM images reveal that the core-shell structure of the catalysts was remain intact after metal loading. H2-TPR profiles indicated that the Cu reducibility decreased with increasing metal content, which agreed with XPS results, as the peak shifting to higher binding energy. The catalytic performance test demonstrated that Cu-ZnO/core-shell Al-MCM-41 with total metal content of 5 wt% exhibited the best catalytic activity, as it possessed a proper amount of Cu<sup>+</sup> ion, which is the active species for this reaction. The average NO conversions based on the reaction time of 3 h of 1.5Cu-1.5ZnO/Al-MCM-41, 2.5Cu-2.5ZnO/Al-MCM-41, and 3.5Cu-3.5ZnO/Al-MCM-41 were 80, 87, and 73 %, respectively. The effects of Cu:ZnO ratio was also studied based on Cu content of 2.5 wt%. However, it was found that the optimum ratio of Cu:ZnO ratio was 1:1.

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### Designing polymeric membranes for biomedical applications

Laís Pellizzer Gabriel, André Luiz Jardini and Rubens Maciel Filho State University of Campinas, Brazil

One of the current challenge of Tissue Engineering is to produce a new generation of polymeric membranes to mimic the extracellular matrix, generating an extensive network of cells. In this field, electrospinning and rotary jet spinning techniques are highlighted due to the possibility of control the membrane pore size, surface area, and fiber alignment. This research explores both processing techniques in order to obtain polyurethane membranes with different fiber morphologies to explore the mechanical properties and in vitro cells studies. The implants characterization showed that the morphology and aligned of attachment cells influenced the cells viability, and also showed an appropriate mechanical strain capable to support cells attachment and proliferation. It was observed that adequate polymer microsurfaces structures with aligned architectures can promote cell proliferation and tissue repair mimicking the extracellular matrix

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### Perovskites photophysics: Half-organic, half-inorganic and a quarter of magic

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ybrid organic-inorganic metal halide perovskites represent a remarkable success story in recent materials science applied to optoelectronic devices, thanks to the demonstrations of solution- process solar cells with conversion efficiencies in excess of 20% and very promising LEDs. The peculiarities of perovskites are thought to stem from a blend of organic materials features, like easy fabrication and bandgap tuneability, with inorganic semiconductor properties, particularly large carrier mobilities. We will show however that concerning excited state photophysics, hybrid perovskites are a unique class of materials. Ultrafast spectroscopy demonstrates that, unlike organics, perovskites are free carrier seminconductors: the prevalent excited state species are free electrons and holes in all conditions relevant for device operation, without noticeable presence of bound excitons. As a consequence. radiative efficiency increases with the excited-state density, approaching unity at high excitation when optical gain and lasing are observed. The exciton binding energy is however an important parameter, as it turns out to be larger than in most III-V inorganic semiconductors, generating an excitonic correlation strong enough to boost optical absorption and

emission close to the bandgap; furthermore excitons become favoured over free carriers at low temperatures and high excitation levels. In spite of the large trap concentrations in solution-process perovskite films, optical excitations can be long-lived and radiative recombination efficient. we explore the recombination processes and demonstrate an optical technique to measure the ideality factor without any current flowing through the film, identifying and distinguishing recombination in the bulk and at each of the interfaces selectively. A picture emerges of selective traps creating unbalanced free electron and hole populations, a feature that appears to be universally shared by perovskite materials with various compositions and fabrication routes. Prospects of widespread perovskite optoelectronics are contingent on the ability to exploit their unique photophysics. As it turns out, perovskite materials may be not only a cheaper or better performing alternative to established materials, but able to perform qualitative different functions, such as vectorial charge trasnsport or density-dependent charge separation and recombination.

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### Thermomechanical surface treatment of metallic materials

#### Patiphan Juijerm Kasetsart University, Thailand

t is established that the fatigue lifetimes of metallic materials can be enhanced using mechanical surface treatments, such as shot peening or deep rolling processes. A crack initiation, as well as propagation, can be retarded by generated compressive residual stresses at the surface and in near-surface regions. However, compressive residual stresses can be relaxed as well as deceased during cyclic loading. Dislocation movements, rearrangements or annihilation are the cause of residual stress relaxation. Thus, a stability of compressive residual stresses is crucial for superior fatigue lifetimes as well as performances of mechanically surface treated components. Thermomechanical surface treatments (warm shot peening or high temperature deep rolling) was developed from conventional mechanical surface treatments to stabilize the compressive residual stresses using the dynamic strain ageing concept. Accordingly, dislocations are pinned by solute atoms as well as very fine carbides during the thermomechanical surface treatments. In this presentation, concept, processing and effects of the mechanical and thermomechanical surface treatments will

be addressed. The method to optimize the temperature of the thermomechanical surface treatments will be introduced. Afterwards, some examples of the fatigue performances of various metallic materials, e.g., austenitic stainless steel AISI 304, plain carbon steel AISI 1045, non-precipitationhardenable aluminium alloy AA5083 and precipitationhardenable aluminium alloy AA6110 after high-temperature deep-rolling at elevated temperatures will be presented and compared with the conventional deep rolled condition (deep rolling at room temperature). It can be concluded that the thermomechanical surface treatment effectively enhances the fatigue performance of metallic materials having interstitial solute atoms, such as steels. However, for aluminium alloys, the beneficial effects of high-temperature deep rolling are not pronounced due to the different strengthening mechanisms in aluminium alloys having major substitutional solute atoms or precipitates, which need more time to develop.