33rd Annual Students' Symposium

(9th – 10th January 2020)

INDIAN INSTITUTE OF SCIENCE
भारतीय विज्ञान संस्थान

Materials Engineering

Book of Abstracts

Hierarchical Arrangement in PVDF/PMMA blends with an Active Polyamide-Graphene Oxide Quantum Dot Surface towards Forward Osmosis Desalination

*Subhasish Maiti [a#], Paresh Kumar Samantaray [b#], and Suryasarathi Bose[*a]*
[a] Department of Materials Engineering, Indian Institute of Science, Bangalore, Karnataka, India-560012
[b]Centre for BioSystems Science and Engineering, Indian Institute of Science, Bangalore, Karnataka, India-560012
Email id: subhasishappchem@gmail.com

In this work, to enhance the desalination performance, unique thin-film composite membrane was designed by insitu assembly of polyamide (PA)-graphene oxide quantum dot (GQDs) framework. This unique assembly was supported on a templated hierarchical porous membrane derived from de-mixing of a classical UCST (upper critical solution temperature) system (polyvinylidene fluoride (PVDF) and polymethyl methacrylate (PMMA)). The de-mixing was achieved by melt processing the blends above the UCST (in the miscible state) and quenching it below UCST. The pore size was controlled by varying the composition in the blends and by etching the PMMA phase. A sandwich architecture was developed by stacking different membranes using polyacrylic acid to achieve a gradient in pore size. Pure water flux, dye removal & desalination experiments were carried out to study the efficacy of this strategy. The stacked membrane showed moderate dye rejection (about 50%) and poor desalination performance. In order to improve the desalination, the membranes were suitably modified to deposit a layer of polyamide, -GQD framework obtained using interfacial polymerization. This strategy resulted in efficient salt (more than 94% and 98% for monovalent salt and divalent salt respectively) and dye rejection (more than 90% and 85% for methylene blue and congo red respectively). Moreover, the antifouling properties of the PA-GQD modified membranes were superior (80%) as compared to the stacked membrane.

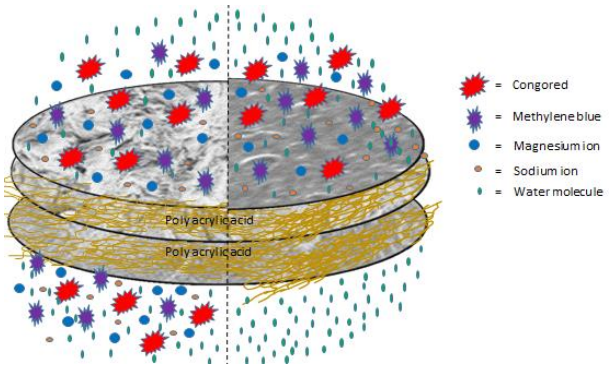


Figure 1: Hierarchical membrane for desalination

Gas powder flow in packed bed with cohesive zone

S Lakshminarasimha, G S Gupta

Experiments are carried out to study the gas-powder flow in cohesive zone of blast furnace using a 2D cold model. The combustion zone and cohesive zone in the lower part of the blast furnace are mainly responsible for productivity of it. The changes in the porosity in both the zones play a significant part in the flow of fluid. The unburnt pulverized coal accumulates in the different regions of blast furnace. Many co-relations are developed in literature to evaluate the powder holdup in packed bed with bottom inlet, lacks the raceway and its effects and also doesn't capture the maldistribution of powder occurring in packed bed with lateral inlet which is the case in blast furnace. This necessitated the study of gas powder in packed bed with the cohesive zone as the studies would more closely resemble the lower region of blast furnace. Thus, in the current study, experiments are carried out to study qualitatively and quantitatively the holdup of powder in packed bed (having cohesive zone) with changes in gas flow rate, powder flux, powder particle size and packing particle size. It was found that the power would accumulate dominantly in lower region of packed bed opposite to inlet and above some of the cohesive layers at the upper region of packed bed.

Mechanical behavior of tetra-functional epoxy composites in the presence of graphene-based core-shell nanoparticles

Radhika Wazalwar, Ashok M. Raichur*

Department of Materials Engineering, Indian Institute of Science, Bangalore 560012

* Corresponding author: Email: amr@iisc.ac.in : P: +91-80-22933238

Aircraft-grade tetra-functional epoxy was used in this work. As a consequence of its highly cross-linked network, thermosetting epoxy resin is inherently strong but highly brittle. Epoxy resin was reinforced with 0.1, 0.5 and 1.0 wt.% polystyrene-graphene oxide (PS-GO) core-shell nanoparticles in order to improve its mechanical properties with a focus on fracture toughness. 100-500 nm sized PS-GO core-shell nanoparticles were synthesized by in situ emulsion polymerization of styrene in the presence of an aqueous dispersion of GO. The core-shell nanoparticles appeared as spheres with a wrinkled surface in the scanning electron microscope (SEM) and transmission electron microscope (TEM) images, establishing that the PS spheres have been coated by the GO sheets. The fracture tests of the cured composites revealed 25% and 41% improvements in the K_{IC} and G_{IC} values respectively for the 0.5 wt.% PS-GO epoxy composite. Whereas, the compressive strength enhanced by 25% for the 0.1 wt.% PS-GO epoxy composite. At 1.0 wt.% loading, the mechanical properties were on the decline due to agglomeration leading to non-uniform dispersion of the nano-filler in the epoxy matrix. As was evident from the SEM images of the fractured surfaces, toughening in the composites occurred due to filler matrix debonding, accompanied by void formation. The glass transition (T_g) of the modified epoxy was 2.4% less than the unmodified epoxy and the thermogravimetric analysis (TGA) curves of unmodified and modified epoxy overlapped, ascertaining that the thermal stability of the epoxy resin was unharmed post PS-GO nanoparticle addition. Hence, the desired improvements in the fracture toughness and compressive strength were achieved without compromising the thermal properties.

Keywords: Polymer-matrix composite, thermosetting resin, fracture toughness, compressive strength, core-shell nanoparticle

Enhancement of piezoelectric response by tuning structural heterogeneity in $Na_{0.5}Bi_{0.5}TiO_3$ based ceramics by varying A-site stoichiometry

Anupam Mishra* and Rajeev Ranjan

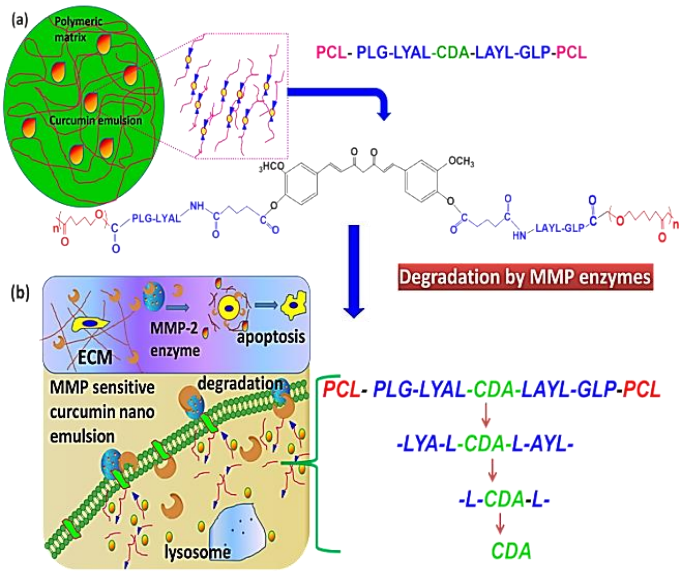
Department of Materials Engineering, Indian Institute of Science, Bangalore

Past studies have shown that certain kinds of off-stoichiometry enhance piezoelectric response in the lead-free piezoceramic $Na_{0.5}Bi_{0.5}TiO_3$ (NBT), however there is lack of clarity regarding the mechanism associated with this phenomenon from the fundamental structural viewpoint. In this abstract, we focus our energies on establishing a detailed correlation between off-stoichiometry, piezoelectricity and structure in $Na_{0.5}Bi_{0.5}TiO_3$ (NBT). Experiments were performed on two different types of off-stoichiometric samples synthesized as per the nominal formula $Na_{0.5\pm x}Bi_{0.5}TiO_3$ (Na series) and $Na_{0.5}Bi_{0.5\pm x}TiO_3$ (Bi series). A systematic increase in the piezoelectric coefficient (d_{33}), reaching a maximum ($d_{33} \sim 98$ *pC/N*) for an optimum Na-deficient composition (x=0.04) in the Na series, was recorded. To establish the structural link between off-stoichiometry and piezoelectricity, we examined the extent of structural disorder the system tends to preserve (along with the long range ferroelectric phase induced by the poling field) in the poled state using x-ray diffraction and dielectric dispersion measurements. We found that the fraction of the cubic-like phase, which is a indicator of structural disorder, increases with increasing Na-deficiency. The off-stoichiometric composition showing highest piezoelectric response is the one which retains an optimal fraction of disordered cubic phase along with the long-range ferroelectric phase (R3c), after poling. Further Na-deficiency collapses the piezoelectric response since electric field is unable to overcome structural heterogeneities and rhombohedral(R3c) distortion is not stabilized.

Cell Responsive Phytochemical Based Polyactive Nanoformulation for Targeted Delivery

Padmavathy Nagarajan and Kaushik Chatterjee*
Department of Materials Engineering; Indian Institute of Science, Bangalore-560012, Karnataka, India,
*Email: pdyvit@gmail.com; *Email:kchatterjee@iisc.ac.in*

Abstract: Phytochemicals constitute a promising class of therapeutics for the treatment of various diseases but their delivery poses significant challenges. In this work, a nanoscale polyactive emulsion was designed for smart, cell-responsive delivery of a curcumin prodrug (curcumin dicarboxylate, CDC) that was chemically conjugated to enzymatically labile oligo-peptides with polycaprolactone (PCL) as the carrier. Matrix metalloproteinase (MMP) sensitive (PLGLYAL) or non-sensitive (GPYYPLG) peptides were used as spacers for conjugating CDC and PCL. This CDC nanoemulsion incorporating the MMP-sensitive sequence showed markedly higher anti-cancer activity, cell internalization and generation of reactive oxygen species in cancer cells in vitro than the control with the non-sensitive oligopeptide. Moreover, the nanopolyactive induced minimal cytotoxicity in non-cancer cells. This work presents a unique strategy to engineer smart nano-polyactives for efficient and targeted delivery of phytochemicals.



Crystallographic orientation changes resulting from large plastic strains and complex deformation paths

B. Aashranth[1,2], Dipti Samantaray[1], Utpal Borah[1],Satyam Suwas[2]

[1] Indira Gandhi Centre for Atomic Research, Kalpakkam
[2] Indian Institute of Science, Bangalore

The imposition of stress on a crystal can result in plastic deformation only if it generates shears of adequate magnitude on appropriate slip system(s). Under a suitably high load, a crystal will change its orientation so as to optimally align the slip system with the loading axis. This could involve crystal rotation, lattice spin or both. The present work describes a scheme to describe these changes as a function of plastic deformation, with emphasis on less explored areas.

Rotation of slip systems is commonly described as rotation of slip direction towards a tensile axis (the Schmid analysis), or the rotation of slip plane normal away from a compressive axis (the Taylor analysis). However, the rotation of slip system under torsional loading, or other shears is not described by either of the above analyses. The mechanics of crystal rotation during torsion have been considered mysterious historically; this ambiguity persists today. In the era of severe plastic deformation and complex deformation paths which rely heavily on shear, it is essential to develop unambiguous and robust schemes for studying the rotation of crystals and/or slip systems. It is equally important to recognise that the additivity of strains on different slip systems during multiple slip is valid only at small strains, which may not resemble actual deformation paths.

The present scheme attempts to treat these lacunae through a generalised treatment of large plastic deformation using finite strain theory. By tracking the deformation gradient of individual lines in the crystal, rotation and the changing distance between lines are determined. The reference coordinate axes for measuring these deformations are conveniently chosen in terms of the slip system. The implementation of this scheme will tackle single/multiple slip in some deformation paths which include conventional as well as advanced techniques.

Modelling of non-steady state creep behaviour using cantilevers in bending

Priya Goel, Praveen Kumar, Dipankar Banerjee, Vikram Jayaram
Department of Materials Engineering, Indian Institute of Science, Bengaluru-560012
priyagoel@iisc.ac.in

The evaluation of material creep properties in primary stage is analyzed using cantilevers under bending. The peculiarity of bending arises from linear stress distribution along beam thickness in elastic regime, which combines with non-linear dependence of creep strain rate on stress and leads to stress redistribution at any cross-section to satisfy Bernoulli's assumption of section planarity. The stress redistribution is transient in nature as it is governed by the stress exponent in the constitutive law which takes different values for primary and secondary stages. Therefore, the analysis of bending demands a numerical technique that accounts for stress evolution in addition to microstructural evolution. In the present work, a methodology is established to calculate stress variation as a function of time and space under constant load, thereby allowing us to capture the transition between different stages and obtain the uniaxial creep constitutive law from bending deflection-time data.

The creep response of ferritic steel, commonly used in boiler tubes, shows that the transition from primary to secondary can take as long as 140 hours due to large stress redistribution time at an effective stress of 150 MPa, a stress much below the yield but relevant to applications. The model holds great significance under these conditions, when it is non-trivial to estimate the time to reach steady state in order to use analytical expressions. A greater advantage accrues for materials which do not show steady state because the analytical expressions cannot be applied at all. Herein, a unified strain – stress – strain rate constitutive relation is defined, it is assumed that the dependence of strain rate on stress is independent of strain, thus allowing replacement of strain by time in the constitutive law. It is applied to model room temperature creep response of Ti-6Al alloy, relevant to dwell-fatigue in aero-engines. It is shown that transition from elastic to primary is slow due to extremely low creep rates of the order of 10^{-8} s^{-1} even at loads close to the yield strength, stress redistribution time can be as large as around 6 hours, neglecting which can lead to significant errors in creep response. Therefore, the present work holds the potential to model the bending creep response of a range of materials exhibiting short or extended primary to only the primary stage of creep.

EMI Shielding Properties in Hybrid Polycarbonate based Nanocomposites: A Mechanistic Overview

Kumari Sushmita[a], Giridhar Madras[c], Suryasarathi Bose[b]

[a] Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore- 560012, India

[b] Department of Materials Engineering, Indian Institute of Science, Bangalore- 560012, India

[c] Interdisciplinary Center for Energy Research, Indian Institute of Science, Bangalore- 560012, India

With the increasing rate in device development and the growing demand of high-speed wireless devices, it has become imperative to suppress unwanted electromagnetic (EM) radiations which can otherwise lead to malfunctioning of electronic devices. This necessitates searching for alternate lightweight materials that can offer ease of processing, design flexibility, ease of embedding and integrating with the existing systems in place as shields to protect the precise electronic circuitry. Herein, we fabricated a lightweight Polycarbonate (PC) based nanocomposites using doped graphene derivatives and multiwalled carbon nanotubes (MWCNT) for effective shielding of EM radiation in X- and Ku- band. To get a mechanistic understanding as to how the dopant in graphene derivative influence the EM shielding properties, two dopants have been chosen; ferrimagnetic (ferrite, Fe_3O_4) and the other one as paramagnetic (Gadolinium oxide, Gd_2O_3). The doped graphene derivatives when blended with PC and MWCNTs resulted in materials that can shield the incoming EM radiation through magnetic and dielectric losses. This strategy of doping not only improves the state of dispersion of these dopants in the nanocomposites but also enhances the shielding effectiveness. At 18 GHz and with a sample thickness of 5 mm, the total shielding effectiveness (SET) of PC nanocomposites with 3 wt% MWCNT/ 5 wt% rGO-Fe_3O_4 and 3 wt% MWCNT/ 5 wt% rGO-Gd_2O_3 was measured to be -28 dB and -33 dB respectively. Our analysis further reveals that irrespective of the dopant, various losses (magnetic and dielectric) decide the shielding effectiveness in polymeric nanocomposites facilitated by the multiple internal reflections.

An Explanation of Harper-Dorn Creep

Shobhit Pratap Singh, Michael E. Kassner, Praveen Kumar

Harper-Dorn (H-D) creep, a low stress ($< 10^{-5}$ G, where G is the temperature compensated shear modulus) and high temperature (> 0.9 T_m, where T_m is the homologous temperature) deformation of high purity single and large grain sized crystals, is characterized by a stress exponent (n) of 1, an activation energy equal to the self-diffusion and the dislocation density is independent of the applied stress. Long-term annealing of high purity Al and LiF single crystals up to 1 year near their melting temperature was conducted. It is observed that a minimum saturation limit of dislocation density exists in both these systems. Observations from the present study suggests that this independence of dislocation density in H-D creep is due to the fact that the dislocation density cannot be reduced below this saturation limit resulting in a stress exponent of unity. On the other hand, a stress exponent of 3 has also been observed in this low-stress and high temperature regime. In Al, studies reporting a higher stress exponent than unity suggested an increase in the dislocation density of the crept samples compared to the initial starting dislocation densities. The initial starting dislocation densities, which reports $n > 1$, of such crystals were 2 orders of magnitude lower than the saturation limit obtained in the present study. An explanation for the observed stress exponents in H-D creep is presented based upon the behavior of dislocation density.

Fabrication of Cerium Oxide Coated Nanofibers for Cardiac Tissue Engineering

Manisha Behera[1], Aditi Jain[2], Nagalingam R. Sundaresan[2, 3*] and Kaushik Chatterjee [1, 2*]

[1] *Department of Materials Engineering; Indian Institute of Science, Bengaluru, Bengaluru-560012, Karnataka, India.*
[2] *Center for BioSystems Science and Engineering, Indian Institute of Science, Bengaluru, Bengaluru-560012, Karnataka, India.*
[3]*Department of Microbiology and Cell biology, Indian Institute of Science, Bengaluru, Bengaluru-560012, Karnataka, India.*

Abstract:

Reactive oxygen species (ROS) induce oxidative stress in biological systems, which is a critical feature of cardiovascular diseases. The chronic release of ROS from mitochondria of cardiomyocytes induce cell death associated with myocardial infraction. In order to eliminate ROS, we aimed to prepare fibrous scaffolds incorporating cerium oxide nanoparticles, which is an excellent ROS scavenger to minimize cell damage. In the present study, we fabricated nanofibers of polymer blends of polycaprolactone and gelatin by electrospinning. Cerium oxide particles were decorated on the surface of the nanofibers. Uncoated fibers were used as control. Primary cardiomyocytes extracted from neonatal rats were seeded on the cerium oxide coated nanofibers. They exhibited excellent cell attachment and viability in comparison with uncoated polymer nanofibers, which was confirmed by immunostaining of cardiac troponin I, a known cardiac marker. Thus, this study demonstrates cerium oxide coated polymer nanofibers offer a promising route for engineering biodegradable functional cardiac patches.

Keywords*: Reactive oxygen species, Cerium oxide nanoparticles, electrospinning, cardiac tissue engineering.*

Mechanical behaviour of Ni-(x)Al, x = Pt and Pd

Ananya Tripathi, Essaki Raja, Praveen Kumar and Vikram Jayaram

Diffusion aluminide coatings are an integral part of thermal barrier assembly used on the turbine blades of the hotter section of gas turbine engines. They provide oxidation resistance at high operating temperatures. These coatings comprise of β-NiAl alloy, which exists over a wide composition range (45 to 60 at % Ni). Therefore, to understand the diffusion coatings behaviour in a better way it is important to understand the properties of β-NiAl alloys. There have been innumerable studies on the β-NiAl alloy system, but the overall mechanical behaviour of this alloys is still not understood clearly because of many factors like composition, anisotropy, grain size, processing techniques etc that affect its properties. Stoichiometry affects the physical and mechanical properties of NiAl profoundly, because of the formation of different kind of defects as we move away to either side of the stoichiometry. In this work, the effect of orientation and temperature over a range of composition on the hardness and modulus of NiAl is studied. Further, addition of Pt and Pd was made to NiAl in a very systematic way to understand their effect on the modulus and hardness. It was found that overall hardness of the materials increased with little or no change in the modulus. XRD measurements were performed to explain this on the basis of site occupancy of Pt/Pd. It was also observed that the effect of composition on the hardness and modulus decreased in comparison to binary NiAl.

Ripple Flow of Liquid Metals

Vijayendra Shastri, Praveen Kumar, Rudra Pratap.

Liquid metals have been used for patterning by through processes like 3d printing, electrochemical lithography. In the similar lines we report a novel case of gallium flow on thin metal films like Pt and Au deposited on silicon substrate. Periodic Patterns produced are promising being periodic with dimensions varying from 10μm to 100nm depending on the flow parameters. The patterns with minimal post processing can be used in microfluidics, diffraction gratings and many more applications. Metal flowing on metal is always interesting research problem because of the reactive nature of the flow. The category of reactive wetting which is not well understood as compared to inert wetting which has vast literature base. To address the complexity involved we have conducted in situ study of the flow is done using environmental scanning electron microscopy (ESEM) and the flow evolution is captured. Flow involves dissolution of substrate film which is proved by Transmission electron microscopy Energy dispersive spectroscopy (TEM-EDS). Further Based on the understanding through material characterization a qualitative model is presented using COMSOL which captures the dominant behavior of the flow patterns.

Key words: Liquid metal, Thin films, Reactive/Dissolutive wetting, Patterning.

Hot deformation behavior of as cast SP-700 titanium alloy in two phase condition

Vivek Chandravanshi[1], *Nitish Bibhanshu*[2], *Vajinder Singh*[1], *Amit Bhattacharjee*[1], *and Satyam Suwas*[2]

[1]: Defence Metallurgical Research Laboratory (DMRL), Kanchanbagh, Hyderabad-58
[2:] Indian Institute of Science (IISc), Bangalore

Email of corresponding author: vivekmet@dmrl.drdo.in; vivekmet@gmail.com

SP-700 (Ti-4.5Al-3V-2Mo-2Fe) is a β rich α+β titanium alloy which was developed to improve the hot workability and mechanical properties as compared to the popular Ti-6Al-4V alloy. Due to its lower β transus ($T_\beta \approx 900$℃) temperature, this alloy shows superplastic behaviour at relatively lower temperature without much increase in the flow stresses. In the present study, hot deformation behavior of (SP-700) titanium alloy was evaluated by employing isothermal compression tests as a function of temperature (650℃-890℃) and constant strain rate of 0.001, 0.01, 0.1 and $1s^{-1}$ in as cast condition. Flow curves were generated and significant flow softening was observed at lower temperatures and slower strain rates. Also, the peak flow stress was found to be decreasing with the increase in temperature as well as decrease in strain rate. Based on the flow stress values at different temperatures and strain rates, strain rate sensitivity (SRS) map was constructed to determine the optimal processing domains. Arrhenius type constitutive equations were employed to study the relationship among flow stress, strain rate and temperature. Moreover, the effect of temperature and strain rate on hot deformation behaviour has been expressed by Zener-Holloman parameter (Z). The kinetic analysis estimated stress exponent value, n as 4.04858 and deformation activation energy, Q as 375 kJ/mol. The hot deformed materials have been subjected to microstructural characterization through Scanning Electron Microscopy based Electron Back Scatter Diffraction (SEM-EBSD) to analyse the microstructural features in detail and to correlate the features of deformed specimen with the parent microstructure.

Key words: α+β-titanium alloys, hot deformation, strain rate sensitivity maps, constitutive equations, activation energy

Organic molecule based chemiresistive sensor for the detection of hexavalent chromium

Shweta Shekar, S Subramanian and Praveen C Ramamurthy

Department of Materials Engineering, Indian Institute of Science, Bangalore 560012

The mutagenic toxicity of hexavalent chromium has resulted in significant growth of Cr(VI) sensors in the recent years. While Cr(III) is biologically stable and environmentally non-toxic, hexavalent chromium is recognized as a toxic substance. EPA and WHO have set permissible limit of 1 ppm for hexavalent chromium in drinking water.

In the recent years, several electroactive materials have been employed to probe Cr(VI) ion. 4-dimethylaminoazobenzene, 1-(2-(1*H*-imidazole-1-yl)-1-(4-methoxyphenyl)ethylidene)-2-phenyl hydrazine, 2-acetylpyridine, p-(4-Acetanilidazo)calix[4]arene, glyoxal bis(2-hydroxyanil), and tributyl phosphate are some of them. Poly-L-histidine has been successfully used to detect Cr(III) and Cr(VI) by electrochemical methods. However, there still exists a need to develop a simple, portable and miniature sensing device with high selectivity.

The present work reports the synthesis of a guanidine based small organic molecule which has exhibited potential to detect hexavalent chromium from contaminated water samples. The chemiresistor fabricated herein has shown selectivity towards chromium over other interfering anions such as carbonate, sulfate, phosphate, fluoride and chloride. The biguanide molecule also reveals fluorescence quenching in the presence of hexavalent chromium.

The bio-mimicking nature of the organic molecule synthesized is manifested by the nature of complexation of hexavalent chromium to the guanidine derivative. The thermodynamically stable chromium-histidine complex in mammalian cell shows the use of hydroxyl and amine groups acting as active sites to co-ordinate to the chromium ion. The guanidine derivative being a small molecule requires the use of a conductive filler such as carbon black to be used as an electroactive sensing material in the chemiresistor fabricated in this work. The chemiresistor evaluation shows repeatability, reproducibility, sensitivity, selectivity and a lower limit of detection of 1 ppm.

2D Materials: Covalent Cross-Linking of Phosphorene with MoS2 for Hydrogen Evolution

Nidhish Sagar, K Pramoda, Pratap Vishnoi, CNR Rao

There have been extensive investigations of various 2D inorganic analogues, since the discovery of Graphene. Of the various inorganic 2D materials, MoS2 possesses desirable structural features as well as electronic, optical, and other properties. While MoS2 exists as a semiconductor in the stable 2H-form, it is metallic in the 1T-form generated by Li-intercalation and exfoliation. Nanostructures of MoS2 in the 1T-form is probably the best material for generating hydrogen from water splitting. Nanocomposites of MoS2 sheets with other 2D layer structures, such as C3N4 and BCN, exhibit extraordinary hydrogen evolution reaction (HER) activity.

Phosphorene is found to be active for photochemical and electrochemical HER, but the activity is rather low. The use of phosphorene is made difficult by its ambient instability, and this limitation is overcome by functionalization.

In this presentation, I will talk about the process of preparation of P-MoS2 composites and its improved catalytic activity. Covalent cross-linkers were added in varying amounts to check their effect on HER activity. Different amounts of P and MoS2 were also used (1:1, 1:2, 2:1) to determine the best composite for hydrogen evolution.

Keywords: 2-Dimensional (2D) Materials, Molybdenum Disulphide (MoS2) , Hydrogen Evolution Reaction (HER), Phosphorene (P)

Solving the issues of multicomponent diffusion in Ni-Co-Fe-Cr medium entropy alloy

Anuj Dash, Neelamegan Esakkiraja, and Aloke Paul*

Department of Materials Engineering, Indian Institute of Science, Bengaluru 560012, India

Abstract: The pseudo-binary and pseudo-ternary diffusion couple methods are followed to estimate the diffusion coefficients at equiatomic composition in a NiCoFeCr medium entropy alloy. This is otherwise not possible following the conventional method in a system with more than three components. Along with the interdiffusion coefficients, we have estimated the intrinsic diffusion coefficients of all the components by designing the pseudo-binary couples such that Ni and Co develop the diffusion profiles keeping Fe and Cr fixed in one couple and Fe and Cr develop the diffusion profiles keeping Ni and Co fixed in another couple. Following, we demonstrated the calculation of the tracer diffusion coefficients utilizing the thermodynamic details. This facilitates us to compare the data estimated directly following the radiotracer method at the equiatomic composition. Subsequently, we produced three ideal pseudo-ternary diffusion couples intersecting at the compositions close to the equiatomic composition. Therefore, for the first time, we have estimated the main and cross interdiffusion coefficients experimentally at the composition of interest in an important four-component NiCoFeCr medium entropy alloy highlighting the complex diffusion interactions between the components.

Keywords: Multicomponent diffusion; Interdiffusion; Tracer diffusion; High Entropy Alloys; NiCoFeCr

Large temperature tuning of emission color of a phosphor by dual use of Raman and Photoluminescence signals

Arnab De and Rajeev Ranjan

The ability to tune the emission color of materials by external stimuli like electric field, pressure, temperature, etc., offers avenues to design light-based sensors and devices. We report here a strategy which enables large temperature tuning of the emission color of a lanthanide phosphor by combining its Raman and the photoluminescence (PL) signals. This phenomenon is demonstrated on a Eu, Er doped $BaTiO_3$, the emission color to change from orange to green when cooled down to 10 K. The large color tuning is a consequence of the synergy of two independent processes/mechanisms operating together in this phosphor system: (i) significant enhancement of the Raman signal due to structural ordering in the rhombohedral ferroelectric phase of the host $BaTiO_3$ and (ii) anomalous low temperature quenching of Eu^{+3} PL emission by trap states near the emission level. We show that this contrasting effect of temperature on the PL and the Raman signals can be used as a powerful strategy to design phosphor materials for optical thermometry with large temperature sensitivity.

Establishment of Microstructure-texture-mechanical property relationship in Electron Beam Melted 316L

Deepak Kumar[1] and Satyam Suwas[2*]

[1,2]*Dept. of Materials Engineering, Indian Institute of Science, Bengaluru - 560012*
**satyamsuwas@iisc.ac.in*

Austenitic stainless steel, 316L has been successfully manufactured using Selective laser melting (SLM) but large anisotropic microstructure and residual stress generated in this process The main reason for generation of these process related issues are extremely high cooling rate (10^5 to 10^6 Ks^{-1}), large thermal gradient and inability to heat substrate for higher temperatures (not more than 200˚C). This process related issues leads to search for the alternative additive manufacturing processes. Electron beam melting (EBM) process is gaining popularity for manufacturing of metals and alloys as this process generates comparatively lower cooling rate (~10^4 Ks^{-1}) and increased substrate heating temperature (upto 800˚C). The present paper is one of the primary studies to establish a relationship between microstructure-crystallographic texture-mechanical properties in EBM manufactured 316L.

Microstructural features which are inherited in additive manufacturing of 316L such as cell and cell wall thickness, that is a consequence of Mo and Cr segregation are coarser in EBM 316L. EBSD results has confirmed that epitaxial nature of columnar grains parallel to the build direction is retained and these grains are longer compared to SLMed counterparts. Color gradient in inverse pole figure map represents increased strain. A theory for the formation of <100> texture parallel to the build direction is proposed. These all differences are ultimately reflected in the mechanical properties. Micro hardness is lower when compared to SLM manufactured samples and the main reason is the coarser microstructure and decreased initial dislocation density that contributes to Hall-Petch and Taylor strengthening respectively.

Keywords: Electron beam melting, 316L, EBSD, texture

Effect of High-Pressure Torsion and Natural Ageing on Hardness of Commercially Pure Cu

Ajay Rijal[a], Shobhit Pratap Singh[a], Jae-Kyung Han[b], Megumi Kawasaki[b], Praveen Kumar[a,*]

[a] Department of Materials Engineering, Indian Institute of Science, Bangalore 560012 (India)

[b] School of Mechanical, Industrial and Manufacturing Engineering, Oregon State University, Corvallis, OR 97331 (USA)

Abstract

Commercially pure Cu was processed through high-pressure torsion (HPT) at a pressure of 6 GPa starting from ¼ up to 50 turns. These samples were then naturally aged for 1.75 years under the laboratory condition. Subsequently, micro-hardness was evaluated and correlated with microstructure. Grain size monotonically decreased with the number of HPT turns and became saturated at ~300 nm after an equivalent strain of ~40. Low-angle grain boundaries and sub grains were formed at onset of straining, which converted into high angle grain boundaries upon further straining. Hardness of the freshly processed samples monotonically increased with the HPT strain and saturated at the value of 155 HV; however, the samples processed to a shear strain of 2 to 20 and naturally aged by 1.75 years demonstrated a remarkable drop in the hardness values. Interestingly, the natural ageing was not effective in changing the hardness of HPT processed samples strained up to very high shear strains. Micro-hardness value is enhanced by ~ 240 % compare to annealed Cu. An overview of the observed properties, based on correlation with microstructure conducted using electron back-scattered diffraction is discussed.

Keywords : Micro-hardness; Natural ageing; Grain boundaries.

Evolution of plasma electrolytic oxidation coatings formed on Mg alloy utilizing various alkaline electrolytes with and without glycerol additive and its corrosion behavior

Ashutosh Jangde, S. Kumar

PEO coatings were synthesized by using environment-friendly alkaline electrolytes, i.e., silicate-based (Si-PEO) and phosphate-based (P-PEO) electrolytes with and without glycerol as an electrolytic additive. The formed PEO coatings were then studied for their microstructural, elemental and phase composition evolution as a function of PEO processing time. Corrosion behavior of formed coatings was evaluated as a function of PEO processing time by employing electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization. It was observed that localized microdischarges occurred at Al_8Mn_5/α-Mg interface but not at $Mg_{17}Al_{12}$/α-Mg interface for both silicate-based and phosphate-based electrolytes irrespective of glycerol addition. The glycerol addition did not have any significant effect on the coating elemental compositions for both Si-PEO and P-PEO. However, the glycerol addition resulted in the reduction of maximum pore size and coating thickness and increased the pore density and MgO phase content in the resulting coatings for both Si-PEO and P-PEO. Complete suppression of amorphous Mg_2SiO_4 phase and promotion of $Mg_3(PO_4)_2$ phase amorphization was observed for Si-PEO and P-PEO respectively due to glycerol addition. In general, the corrosion behavior of glycerol added PEO coating improved corrosion behavior for both Si-PEO and P-PEO. This can be attributed to the dense inner barrier layer and higher MgO phase content in the glycerol added PEO coatings.

Keywords: Magnesium alloy; Plasma electrolytic oxidation; Coating; Corrosion; Electrochemical impedance spectroscopy; Potentiodynamic polarization

Microstructure Evaluation of TIG-welded In617-SS304 dissimilar joint

Anbukkarasi R, S Suwas, S. Karthikeyan, S. Kumar, K Chattopadhyay
Department of Materials Engineering, Indian Institute of Science, Bengaluru-560012.

Abstract

Ni based superalloys and austenitic stainless-steel welds are widely used in high temperature applications such as steam generators and power plants, due its good strength and good corrosion resistance properties. Inconel 617 is a solid solution alloy with excellent corrosion resistance and an exceptional combination of high temperatures strength and oxidation resistance. The components made of Inconel 617 are widely used in power plants, chemical industries, aircrafts and land-based gas turbines. However, the high Ni content increases the cost of the alloy. In many cases, stainless steels are welded to Ni-base alloys when a transition is required to accommodate more oxidizing environment or superior strength requirement at elevated temperature. On the other hand, the replacement of Ni-base alloys with stainless steels can decrease material costs. In this study, a weld between In617 and SS304 alloy was carried out by GTAW technique. Then the intrinsic microstructure at different welding zones were studied and discussed here.

Key words: Dissimilar weld; GTAW; Inconel 617; Stainless-steel 304.

Exploring the oxidation mechanism of γ'-strengthened Co-Ni-Al-Mo-Ta alloy system

Saurabh M. Das, Mahander P. Singh, K. Chattopadhyay

In the present work, the oxidation mechanism of γ'-strengthened Co-Ni-Al-Mo-Ta alloy system during exposure at elevated temperatures is explored. Cross-section of the oxide scales grown with time were first characterized using SEM, and EPMA-WDS. Three different types of oxide layers were observed. The outer layer comprises of cobalt rich oxides followed by mixed oxides of other elements in the middle and inner layers. Lamellae suitable for TEM observation were lifted from middle and inner oxide interfaces using dual-beam FIB and characterized using STEM-HAADF and EDS techniques. Electron diffraction patterns are acquired to identify the crystal structure of different oxide phases formed in these layers. It shows the growth of amorphous alumina oxide along the (Co, Ni) rich solid solution grain boundaries in the base alloy Co-30Ni-10Al-5Mo-2Ta (at%) oxidized at 800ºC for 50 hours. As the oxide scale is not protective, degradation of alloy continues. Small addition of Ti and increasing oxidation temperature result in the formation of κ-Al_2O_3 along the grains of solid solution phase. However, the systematic additions of Cr (5at% and 8at%) lead to the formation of protective α-Al_2O_3 oxide scales at oxide-alloy interface. TEM analysis indicates that the addition of Cr first results in the formation of spinel $CoCr_2O_4$ oxides phases. This phase decreases the oxygen potential further into the matrix as compared to Cr-free alloys. This helps in nucleation of desired α-Al_2O_3 oxide phase and with time it forms a continuous layer. Analytical TEM analysis revealed the influence of Cr on the phase transformation mechanism of alumina oxide. These observations deliver the insights on further refinement in the compositions of these alloys system.

Keywords: γ-γ' Cobalt base superalloy, Oxidation, dual-beam FIB, (S)TEM.

Evolution of recrystallization texture in face centetred cubic material

Gyan Shankar[1], S. sanandiya, and S. Suwas[1]

[1]Department of Materials Engineering, Indian Institute of Science, Bangalore 560012, India

Abstract

Despite the substantial amount of research in the field of recrystallization, there is no general theory which deals with the evolution of microstructure and texture for various kind of materials. The present work is aimed to develop a comprehensive understanding of the effect of stacking fault energy (SFE) in face centered cubic materials on the recrystallized microstructure and micro-texture evolution. SFE is the most important parameter which decides the mechanism of deformation and formation of different kinds of heterogeneities such as deformation bands, micro-bands, shear bands, deformation twins, etc. These interfaces play a vital role during the initial stage of recrystallization and texture development henceforth.

Ni-Co and Ni-Fe alloys were chosen for this study. It is well known that nickel is a high SFE material and stacking fault energy of the alloy decreases with increase in cobalt content, whereas addition of Fe does not affect the SFE of alloy system significantly. The SFE of Ni-60wt.%Co (30mJ/m^2) being close to brass and SFE of Ni-40wt.%Fe is similar to pure nickel (high SFE) [1]. Ni-Co alloys with different Co content (0,20,40,60 Wt.%) and Ni-Fe alloy with Fe content (20,40 Wt.%) were rolled to 70% reduction in thickness and subsequently annealed above recrystallization temperature for different time. Textures were measured by SEM-EBSD and X-ray diffraction. It was found that recrystallization starts at the crossing point of micro-bands and high angle grain boundaries. There was always a trace of the orientation of new strain free grain in deformed structure. It has been seen that annealing twin is also an important factor which contributes to the formation of nuclei during early stages of recrystallization and later development of texture which was not present in the initial deformed material. A detailed micro-mechanism of annealing texture formation will be presented.

Cellular automata were used to simulate the recrystallization texture based on the experimental results [2]. Simulation results have shown good prediction of recrystallization texture in case of Ni-Co alloys.

References:

[1] Madhavan R, Ray RK, Suwas S (2014) Acta Mater 74:151–164

[2] Christian Haase, Luis A. Barrales-Mora, Günter Gottstein (2015) Acta Mater 100:155–168

On the development of γ′ coarsening resistant CoNiFeCrAlNbTi fcc-based high entropy alloys with promising high temperature mechanical properties

Sarvesh Kumar

In the present work we report a series of CoNiFeCrAlNbTi fcc-based high entropy alloys that are strengthened by the presence of $L1_2$ ordered γ′ precipitates in the disordered fcc γ-matrix. The TEM studies on as-solutionized alloys confirm the presence of very fine spheroidal γ′ precipitate distributed uniformly within the γ matrix. Further aging of alloys at 900 °C leads to evolution of cuboidal morphology of precipitates (see Fig. 1a). Composition analysis using STEM-ESD reveals preferential partitioning of Ni, Ti Al and Nb to the γ′ precipitates, whereas Co, Cr and Fe locate themselves to the γ matrix. These Ni rich $(Ni,Co,Fe)_3(Al,Ti,Nb,Cr)$ precipitates shows negative mismatch of ~ -0.65 (%) with the CoNiCr high entropy γ matrix at room temperature. These alloys show mass density in the range of 7.9 - 8.0 g/cc and γ′ dissolution temperature in the range of 1030-1090 °C.

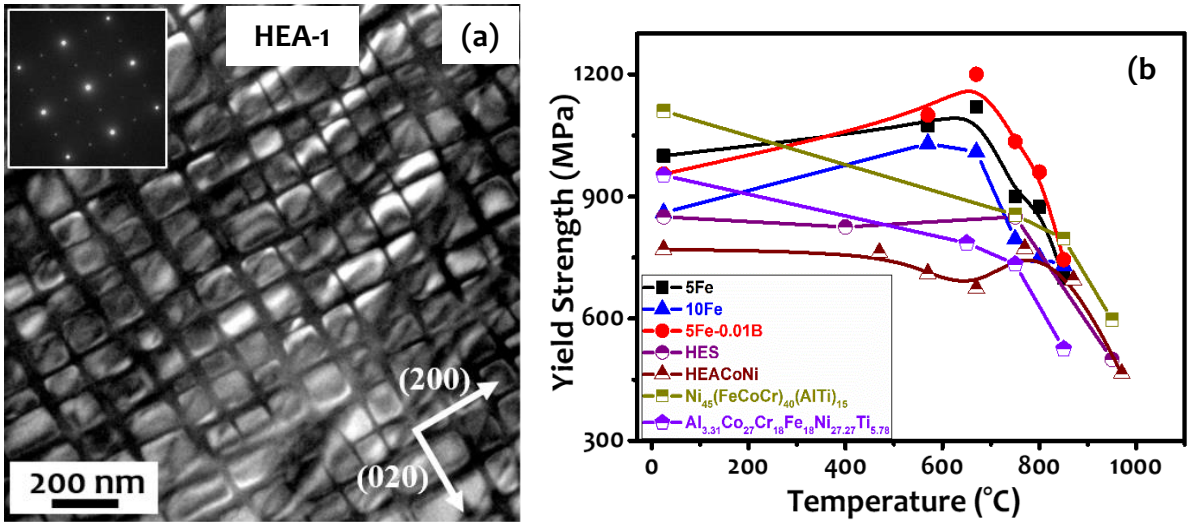


Figure 1: TEM dark-field micrograph of (a) 10Fe-0.01B alloy subjected to aging at 900 °C for 20 hours. (b) 0.2% Proof stress vs. temperature plots for 5Fe, 5Fe-0.01B, 10Fe and 10Fe-0.01B alloys and their comparison with other reported high entropy alloys.

An addition of minute amount of Boron (0.01 at. % B) to these alloys increases the high temperature strength. The presently developed HEA's show high temperature yield strength in excess of 1GPa at 750 °C, see Fig 2b. The temporal evolution of average precipitate size and number density of γ′ precipitates at 900 °C suggest classical evaporation-condensation (EC) mechanism based LSW model. The calculated γ′ precipitates coarsening rates are comparable to heavy elements (W, Re, Ta and Ru) containing Co based superalloys and other high entropy alloys.

Surface functionalization of porous poly(lactic acid) scaffolds prepared by 3D printing for bone tissue regeneration

Sagar Nilawar, Kaushik Chatterjee

Episodes of bone replacement is rising steeply all over the world owing to acute trauma and disorders associated with obesity and aging. In recent decades, scaffolds are used as an alternative for transplantation to mimic the extra cellular matrix by providing appropriate structural support and microenvironment for cells to attach, proliferate and differentiate to result in functional tissue. 3D printing is a rapid prototyping technique which generates patient specific complex scaffold with high porosity. Cerium oxide(ceria) has unique ability to switch between two oxidation states, i.e. +3 and +4 . In biomedical applications, ceria has been used mostly in the area of soft tissues and little is reported for bone tissues. Poly lactic acid(PLA) is a non-toxic degradable polymer but lacks the bioactivity for promoting osteogenesis. The objective of present study is to fabricate and characterize 3D printed PLA scaffolds decorated with nanoceria for bone tissue regeneration. In this study, we used fused filament fabrication(FFF) based printer to make 3D printed scaffolds. Circular scaffold were created in orthogonal manner to form the square pores with 500 μm diameter. After fabrication, scaffolds were hydrolyzed by sodium hydroxide (NaOH) and further conjugated with low molecular weight branched polyethyleneimine(PEI) followed by citric acid(CA) by EDC-NHS chemistry. In the final step, conjugated scaffolds were dip coated by immersing in ceria suspension prepared by oxidizing cerium chloride solution with NaOH. Scanning electron microscopy(SEM) and energy dispersive spectroscopy(EDS) confirms the intact structure of scaffold after modification also the presence of ceria particles on scaffold surface. Pore size was found to be ≈ 414 μm , mainly because of die swelling. PEI-CA conjugation facilitates the

deposition of ceria particles on the surface. Cell proliferation was studied on primary human mesenchymal stem cells (hMSCs) by using water soluble tetrazolium salt(WSTs-1) assay. WST-1 analysis shows ceria coated scaffolds supported cell proliferation. Alkaline phosphatase(ALP) and alizarin red(ARS) assay are used to analyze osteogenic differentiation. ARS and ALP result exhibits more mineralization and ALP activity on ceria coated scaffold that un-modified scaffold receptively. Further physiochemical characterizations and biological assays are currently undergoing.

Effect of scandium addition on the evolution of microstructure and texture in AA2195 aluminium alloy under high pressure torsion

Soumita Mondal[1*], Raghavendra K.G.[1], Ajit Panigrahi[2,3], Michael Zehetbauer[2] and Satyam Suwas[1]

[1]*Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
[2]*Advanced Materials Technology Department, CSIR-Institute of Minerals and Materials Technology, Bhubaneswar, India*
[3]*Physics of Nanostructured Materials, University of Vienna, Vienna, Austria*
*soumitam@iisc.ac.in

Aluminium-lithium based alloys have been under extensive research during the last few decades as they exhibit age hardenability and a high specific strength, which could enable the replacement of conventional aluminium alloys in aerospace applications. In the current investigation, the effect of Scandium (Sc) addition to AA2195 alloy on the evolution of microstructure and texture under high pressure torsion (HPT), one of the modes of severe plastic deformation (SPD), has been studied using Transmission Electron Microscope (TEM) based orientation image mapping technique called ASTAR™/ Precession Electron Diffraction (PED). The alloys studied comprised regular AA2195, AA2195-0.025wt%Sc and AA2195-0.25%Sc, and the HPT-processing was carried out at room temperature for up to 5 rotations. It was observed that the application of high strain to the Sc containing AA2195 alloys resulted in increased hardness, grain refinement and development of shear texture. Preliminary studies showed that crystallite size decreased, and dislocation density increased with increasing strain. However, with addition of Sc, the dislocation density appeared to be lowered with a slightly larger crystallite size post deformation. The reasons for these phenomena could be attributed to the precipitate morphology, shape and distribution, all of which changed with changes in Sc addition. The coherency of the precipitates was studied by High Resolution Electron Microscopy (HREM) technique. The decrease in the distribution of fine precipitates within the matrix with increase in Sc content led to easier static annealing post deformation. This led to the lower dislocation density observed in the TEM microstructures of the Sc containing alloys. The alloy containing 0.025% Sc exhibited the best microstructure and mechanical property, in terms of hardness, as compared to the alloys containing 0% Sc and 0.25% Sc.

Creep behavior of Ni-based concentrated solid solution alloys

Divya Sri. B

High Entropy Alloys (HEAs) have attracted a lot of attention recently in materials science and engineering. In these special multi-component equiatomic alloys (more than 4 elements),it is difficult to distinguish between solute and solvent atoms, which imposes challenges especially in identifying dominating deformation mechanisms at high temperatures. The current study will present a relatively simple way to evaluate deformation mechanisms, to approaching the HEAs from pure metals via concentrated solid solution (CSS) and medium entropy alloys (MEAs), which consists of 2 and 3 elements, respectively. The Ni-based CSS Ni – 33 Co and equiatomic NiCoPd are considered in the present study. There is not much change in the lattice parameter with the addition of Co to Ni, whereas the lattice parameter increased from 0.3539 nm to 0.3670 nm with Pd addition. The elastic modulus of the alloys deduced from DIC (digital image correlation), nanoindentation and immersion ultrasonic inspection techniques are in good agreement with each other. The Ni – 33 Co samples of ~ 100 μm grain size are subjected to creep deformation at 873 K and over a stress range of 30 – 90 MPa. These results suggest that high temperature climb is dominating at stresses higher than 60 MPa and there is a transition in the deformation mechanism at lower stresses. The microhardness results show an increase in hardness after creep deformation, which can be supported by an increase in dislocation density of the crept samples from EBSD – KAM maps.

Keywords: Concentrated solid solution alloys, Elastic modulus, High temperature climb, Kernel average misorientation (KAM).

Understanding the torsion behavior of cold-drawn Ni microwire

Abhinav Arya

Department of Materials Engineering, IISc, Bangalore

Starting from three different initial diameters of 1.74, 1.0 and 0.5 mm, nickel wires were drawn to a final diameter of 100 μm, corresponding to total accumulated drawing strain of 5.7, 4.6 and 3.2, respectively. Tension and torsion tests were performed on all the 100 μm drawn wires. The tensile tests showed conventional strain hardening, with the yield strength increased with an increase in drawing strain. However, the torsion tests showed an opposite trend, with the least drawn wire showing maximum yield strength. An analytical model has been developed that depends on the grain size and the texture of drawn wire to explain such torsional behavior. It is argued that the lower grain size in the more drawn wire may actually be responsible for the lower yield strength of the more drawn wires.

Keyword: wire drawing, yield strength, torsion testing, texture, grain size

Exotic structures in Sn-Te eutectic system

Aramanda Shanmukha Kiran*, Salapaka Sai Kiran, Kamanio Chattopadhyay, Abhik Choudhury

Department of Materials Engineering, Indian Institute of Science, Bangalore, India
**askiran131@gmail.com, shanmukhaa@iisc.ac.in*

Eutectics are tunable self-organizing composite materials, which can show various types of microstructural features. Microstructure evolution of eutectics is an interesting topic for physicists to study non-linear pattern formation and for materials scientists to tune the material properties. Recently, we have observed complex eutectic patterns in Sn-Te eutectic system, which consists of SnTe intermetallic compound and Te phases. In this presentation, we will explain the reasons that trigger the formation of exotic patterns in the Sn-Te eutectic system. In this work, we present morphological insights using Scanning Electron Microscope (SEM), Crystallographic relations using Electron backscatter diffraction (EBSD), compositional distribution analysis using Electron Probe Micro-Analyser (EPMA). Further we have utilized, dual beam (electron and ion beam) microscope to understand the internal structure, where ion beam has been used for milling and electron beam has been used for imaging the pattern. Using the results obtained from the characterization techniques, we elucidate the mechanisms that lead to the formation of such microstructures in eutectic systems.

Phase-field modeling of equilibrium multi-precipitate configurations

Bhalchandra Bhadak, Dr. Abhik Choudhury

Abstract:

Solid-state reactions where multiple precipitate from the matrix as here we find interesting examples of self-organized configurations. For the precipitates with coherent interfaces, there exist elastic interactions between the precipitates which influence the eventual configuration of the precipitate cluster as well as the individual shapes of the precipitates. Hence, it is important to determine these attributes of the precipitates or the cluster of the precipitates that evolve as a function of different parameters such as the anisotropy in the elastic energy and the misfit-strain, characteristic size of the precipitates, inhomogeneity in the shear moduli etc. One of such solid-state reaction is formation of core-shell microstructure from the supersaturated matrix. There is another class of solid-state reactions, where the matrix phase co-exists with clusters of different variants of the precipitates. Here, we formulate a phase-field model for the computation of equilibrium configurations of multiple phases that arise out of a solid-state precipitate reaction, in the presence of coherency stresses. Here, we utilize the phase-field framework to minimize the sum of the elastic and the interfacial energies for a given volume of the precipitates using a volume-preserved Allen-Cahn algorithm. We investigate precipitate organization for three solid-state reactions. The first is the classical two-phase precipitate reactions that lead to the formation of core-shell microstructures, where we clarify the influence of elasticity on the formation of such clusters. Following this, we investigate two symmetry breaking transitions (cubic to tetragonal) and (hexagonal to orthorhombic), that lead to the formation of multi-variant clusters where we study the organization of the precipitates as a function of the elastic properties of the phases.

Keywords: Multiphase field; coherency stresses; core-shell microstructure; multivariant precipitates.

Phase Field modelling of rapid solidification

Bikramjit Karmakar, Dr. Abhik Choudhury

Rapid solidification forms an important processing technique and modelling it bears significant technological importance in designing materials and processes. Solidification studies using phase-field modelling are generally done in the near equilibrium regime i.e. maintaining local equilibrium at the interface. This makes modifications necessary in the existing phase field models of solidification. Solute trapping is a manifestation of rapid solidification. It is used to define a process of solute redistribution at the interface, quantified by an increase in the partition coefficient k from its equilibrium value towards unity with increasing velocity v. The solute trapping effect is naturally exhibited in phase field models, however the nature of change in partition coefficient as a function of velocity [$k(v)$] is dissimilar in computational and experimental results. We make changes to a classical model to accommodate the variation. We also study the change in the nature of $k(v)$ based on the definition of partition coefficient in a diffuse interface setting. Effects of other parameters such as mobility interpolation function and interface width is also shown. A comparison with different analytical and computational models is discussed.

Atomistic Studies on Elastic and Acoustic Properties of Nanoporous Metals

Aman Gupta, Prof S. Karthikeyan

Nanoporous structure is built computationally using Exchange Monte Carlo Technique. Variation of elastic moduli and derived quantities for two different metals, Aluminum and Silver over a wide range of porosity are plotted and tested with Knudsen-Spriggs model and Phani-Niyogi model. These models are empirical/semi-empirical and are tested only for brittle solids. Results showed that, Phani-Niyogi model fits better with $\boldsymbol{R^2 > 0.98}$. Anisotropy ratio initially increases to get a maximum value and then decreases to 1 for both the metals ~80% porosity level.

Optimizing characteristics of morphology to improve the performance of polymer solar cells.

Fiyanshu Kaka, Ravi K Singh, PC Ramamurthy, Abhik Choudhury

Organic-Photovoltaics (OPVs) can potentially provide a less energy intensive means of harnessing solar energy. However, optimum OPV performance depends on understanding the Process-Structure-Property (PSP) correlation in organic semiconductors. The working of Bulk-Heterojunction (BHJ) OPVs is such that the morphology plays a key role in device performance.

It is experimentally observed that there is an optimal blend ratio of p and n-type organic semiconductor as well as annealing time with respect to device characteristics. In this work, we attempt to understand the characteristics of morphology that maximize the device performance by developing a theoretical framework. We first established process-structure correlations by generating a range of morphologies with different blend ratios of P3HT (p-type organic semiconductor) and PCBM (n-type organic semiconductor) for various annealing times. The morphologies were generated using phase-field simulations.

Secondly, we developed effective electronic properties of the morphologies which allows us to characterize the performance of each of the obtained morphologies. The structure-property correlation was derived using diffuse interface approach. This completes the theoretical PSP linkage which allows the optimization of the process parameters for device applications. We found that the necessary condition for efficient OPV device is bi-continuous network of donor and acceptor phases as that leads to percolating channels for electrons and holes to their respective electrodes. The key to an efficient solar cell is optimisation of the two important length scales involved in the working mechanism of OPV i.e., exciton dissociation and carrier conduction through the morphology to the respective electrodes. Exciton dissociation is governed by interfacial area. Efficient carrier conduction results from transportation of the electron and hole to their respective electrode via a well-connected network of phases with minimal leakage of current and recombination of charge carriers. Hence, efficient carrier conduction is governed by higher percolation fraction of the morphology.

Prediction of internal stresses in γ + γ′ phases strengthened Co-base superalloys

Shailendra K. Verma, S. Karthikeyan

The γ + γ′ phases strengthened Ni-base superalloys are used to make gas turbine blades for high temperature application due to excellent creep resistance. The remarkable property is due to two phase microstructure consisting of FCC (γ matrix) and $L1_2$ (γ′ precipitate) phases which are coherent to each other. This is due to very close lattice parameters of the two phases. This microstructure generates coherency stresses in the system. Moreover, due to cuboidal morphology of the precipitates with high volume fraction up to 50% to 70%, there is huge resistance to dislocation motion because dislocation must move through very confine γ channels.

There is combination of various strengthening mechanisms for dislocations movement in γ channels, e.g. coherency strengthening, modulus misfit strengthening, and Orowan strengthening. However, the present models available to quantify the strength are valid for low volume fraction of precipitates with spherical morphology for isotropic elasticity case. Therefore, an attempt is made to model high volume fraction of cuboidal precipitates with elastic anisotropy. In this work multiscale modelling technique is used: elastic constants were predicted using ab-initio density functional theory (DFT) and used along with lattice parameter misfit in finite element modelling (FEM). The lattice parameter misfit was obtained using XRD of three Co-Ti-V base alloys which possess γ + γ′ microstructure. The results suggest that the internal stresses increase with increase in lattice parameter misfit with less dependence on elastic modulus misfit because of almost similar elastic modulus of the two phases.

Keywords: coherency strength, $L1_2$ compound, density functional theory, finite element modeling

Role of Interfacial Energy Anisotropy in Eutectic Growth

Sumeet Khanna, A S Kiran, Abhik Choudhury

Eutectic alloys exhibit coupled growth of two or more solid phases from the parent liquid phase. Due to this concurrent growth of two phases in a binary eutectic, a diverse range of microstructures is observed. This microstructure depends upon material properties like the equilibrium composition, phase fraction, liquidus slopes, and physical properties like the interfacial energies. Here we study the influence of anisotropy in the interfacial energies on the steady state eutectic morphology. Thus, we select the Sn-Zn eutectic alloy which shows a broken lamellar microstructure contrary to the expected rod microstructure. We explain this higher stability of the lamellar morphology on the basis of the presence of anisotropy in the solid-solid interfaces. Moreover, we provide a generic discussion on the effect of strength, orientation and form of anisotropy on the microstructure evolution. We also generate a quantitative representation of the morphology using 2 point correlation statistics and principal component analysis to enable precise comparison between different microstructural patterns.

Tailoring biodegradability of nano cellulose-based materials for use in packaging applications

K N Sri Saravana, Praveen C Ramamurthy

Most of the plastics which are currently in use in many industries such as packaging are not biodegradable. Witnessing many landfills and huge garbage islands floating in Pacific, need for an alternative material had arisen. Looking for biodegradable plastics, many compounds are begin examined. Cellulose having advantages such as renewable source, and biodegradability had led to composites of cellulose, processed cellulose or its derivatives as a replacement for petroleum derived plastics. Nanocellulose is processed cellulose, with specific nano scale structure, was obtained from acid hydrolysis of cellulose, which was isolated from sugarcane bagasse. Further crosslinking of these nano cellulose enhanced its modulus and degradative properties. Polyacrylic acid was polymerized from acrylic acid, which was employed as the crosslinking agent. Various films were fabricated with different PVA, nanocellulose and crosslinking agent were characterized for chemical, mechanical, thermal, topography and degradative properties. Biodegradability of crosslinked films was studied under various conditions like in the ambient soil environment, exposure to UV and exposure to humidity with residual weight analysis and by monitoring chemical, mechanical and topographical properties over time. Results suggest that crosslinking enhanced the mechanical properties and degradation was different for different percent of crosslinking. In addition, fabricated films showed good transparency, flexibility, were compatible with printing and had surface roughness in the order of 20 nm, low density, satisfying the requirements for packaging applications. As degradation kinetics, mechanical properties can be altered by chemical modification such as crosslinking or by varying the composition, one can process to match the packaging requirement depending upon the sector.

Tailoring biodegradability of nano cellulose-based materials for use in packaging applications

K N Sri Saravana, Praveen C Ramamurthy

Most of the plastics which are currently in use in many industries such as packaging are not biodegradable. Witnessing many landfills and huge garbage islands floating in Pacific, need for an alternative material had arisen. Looking for biodegradable plastics, many compounds are begin examined. Cellulose having advantages such as renewable source, and biodegradability had led to composites of cellulose, processed cellulose or its derivatives as a replacement for petroleum derived plastics. Nanocellulose is processed cellulose, with specific nano scale structure, was obtained from acid hydrolysis of cellulose, which was isolated from sugarcane bagasse. Further crosslinking of these nano cellulose enhanced its modulus and degradative properties. Polyacrylic acid was polymerized from acrylic acid, which was employed as the crosslinking agent. Various films were fabricated with different PVA, nanocellulose and crosslinking agent were characterized for chemical, mechanical, thermal, topography and degradative properties. Biodegradability of crosslinked films was studied under various conditions like in the ambient soil environment, exposure to UV and exposure to humidity with residual weight analysis and by monitoring chemical, mechanical and topographical properties over time. Results suggest that crosslinking enhanced the mechanical properties and degradation was different for different percent of crosslinking. In addition, fabricated films showed good transparency, flexibility, were compatible with printing and had surface roughness in the order of 20 nm, low density, satisfying the requirements for packaging applications. As degradation kinetics, mechanical properties can be altered by chemical modification such as crosslinking or by varying the composition, one can process to match the packaging requirement depending upon the sector.