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Contact: Email: aswath@uta.edu/Phone: 817 - 272 - 7108

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Author	Title	Time
R. Bob & P. Aswath	Introductory Speech	6:00 - 6: 15 PM
Y. Yang	Dehydration assisted nanoimprint of PEDOT:PSS nanogratings to improve organic photovoltaics	6:15 - 6:30 PM
H. Xu	Influence of dynamic recovery and recrystallization on the fatigue fracture mechanics of lead-free solder joint	6:30 - 6:45 PM
S. Vidhate	Time Depended Piezoresponse of PVDF-MWCNT Composite	6:45 - 7:00 PM
H. Yao	A New Compression Testing Technique for Anistropic Porous Materials	7:00 - 7:15 PM
J. He	Growth Mechanism of Multi-oriented Twin Domain Structure in Epitaxial $Ba(Zr,Ti)O_3$ Thin Films	7:15 - 7:30 PM
E. Erkan	Kelvin Probe Force Microscopy Study of Grain Boundaries in Chalcopyrite Thin Film Solar Cells	7:30 - 7:45 PM
Y. Xuan	Material Anisotropy Characterized by Transparent Indenter	7:45 - 8:00 PM
	Dinner	8:00 - 8:30 PM
M. Patel	Compositional and structural characterization of diesel soot and its correlation with wear of diesel engine components	8:30 - 8:45 PM
N. Gupta	Spallation of a Near Theoretical Strength Cu-Nb Multilayer Nanocomposite	8:45 - 9:00 PM
S. Katakam	Laser cladding of Fe based amorphous powder on AISI 4310 steel: A microstructural and thermal modeling study	9:00 - 9:15 PM
A. Devraj	Phase separation and second phase precipitation in beta Titanium alloys	9:15 - 9:30 PM
Y. Xiang	Computational Study on the Effect of SrO/CaO Substitution on the Structural and Diffusion Properties of Bioactive Glasses	9:30 - 9:45 PM
	Award Ceremony and Concluding Remarks	9:45 - 10:00 PM

Dehydration Assisted Nanoimprint of PEDOT:PSS Nanogratings to Improve Organic Photovoltaics

Yi Yang,[1]* Koyau Lee,[2] Kamil Mielczarek,[2] Anvar Zakhidov[1,2] and Walter Hu,[1,3]

[1]*Department of Materials Science and Engineering,* [2]*Department of Physics,*
[3]*Department of Electrical Engineering,*
The University of Texas at Dallas, Richardson, TX 75080
* *yxy081020@utdallas.edu*

In recent years, nanoimprint lithography (NIL) has emerged as an effective method to improve power conversion efficiency (PCE) for organic photovoltaics (OPV) devices by providing an ordered and continuously interdigitized morphology in active layers for both efficient charge separation and collection.[1] NIL can also be used to pattern the hole transport/electron blocking layers (HTL/EBL) in bulk heterojunction OPV and a more efficient charge carrier collection has been observed using imprinted poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS).[2] However, due to the low cohesion in PEDOT:PSS molecules, the nanostructures formed by NIL are easy to destroy during demolding.[2] Because of this limitation, the application of imprinting PEDOT:PSS for organic electronic devices is limited up to now.

In this work, we demonstrate the fabrication of PEDOT:PSS nanogratings by a dehydration assisted nanoimprint lithographic technique. Dehydration of PEDOT:PSS increases its cohesion for nanoimprint, resulting in formation of high quality fine nanogratings of 60 nm in height, 70 nm in width, and 70 nm in spacing. PEDOT:PSS nanogratings are used as HTL/EBL in blend poly(3-hexylthiophene-2,5-diyl)(P3HT): [6,6]-penyl-C61-butyric-acid-methyl-ester (PCBM) organic solar cells, showing enhancement of photocurrent and PCE in comparison to devices with non-patterned PEDOT:PSS films. Moreover, the effects of imprint temperature and pressure on PEDOT:PSS conductivity and solar cell performance are studied as well.

[1]Y. Yang, M. Aryal, K. Mielczarek, W. Hu, and A. Zakhidov, J. Vac. Sci. Technol. B **28** (6), C6M104-C6M107 (2010)
[2]J. B. Emah, R. J. Curry, and S. R.P. Silva, Appl. Phys. Lett. **93**, 103301 (2008).

Influence of Dynamic Recovery and Recrystallization on the Fatigue Fracture Mechanics of Lead-Free Solder Joint

Huili Xu, Woong Ho Bang, Choong-Un Kim, Tae-Kyu Lee, Hongtao Ma, Kuo-Chuan Liu

Materials Science and Engineering Department, University of Texas at Arlington, Arlington, TX 76019

*huili.xu@mavs.uta.edu

The mechanism of solder joint failure under various mechanical loading conditions have emerged as one of the critical research subjects in the field of microelectronic packaging as its control has been proven to be key to the success of future packaging technology and also successful migration to lead-free technology. While recent studies address a few key failure mechanisms and their relation to loading conditions, it is not yet clear how fatigue failure interacts with dynamic change in solder microstructure. With low homologous temperature, solder is expected to undergo a dynamic reconfiguration of its microstructure even at room temperature and thus has an ability of releasing the stored energy by cumulative plastic deformation. This, damage relaxation, can greatly influence the failure kinetics of solder joint, but its exact influence and its interplay with loading conditions is not well understood. Utilizing high cycle bending and shear fatigue tester, we have been conducting series of investigations to understand the prevailing damage relaxation mechanism in lead-free solder and its impacts on the fatigue failure. Our study reveals that 1) dynamic recovery is the most active form of damage relaxation at room temperature while recrystallization is more prevailing mechanism at higher temperature; 2) the damage relaxation by such mechanisms (and thus retardation of failure) is effective only when the kinetics of such processes can keep up with the damage accumulation rate. This paper presents supporting evidence of our findings along with mechanistic analysis of fatigue fracture process.

Time Depended Piezoresponse of PVDF-MWCNT Composite

Shailesh Vidhate,[1] Jaycee Chung,[2] Vijay Vaidyanathan,[1] Nandika D'Souza[1]

[1]Department of Materials Science and Engineering, University of North Texas, Denton, TX 76201, USA [2]Global Contour Ltd., Rockwall, TX 75087, USA

Multiwall carbon nanotubes filled polyvinylidene fluoride (PVDF) nanocomposites were prepared by melt blending. Time dependent piezoresistance was investigated as a function of concentration. In the quasi-static case, a transition from negative pressure coefficient (NPC) to positive pressure coefficient (PPC) behavior was observed with the PPC effect being negligible at high concentrations. Initial resistive response decreased and the magnitude of the decrease scaled with concentration. However, long term creep response was resistive for low concentrations while conductive at high concentrations. A model based on a Maxwell and Kelvin elements was utilized to describe the strain dependence and an equivalent model using resistances and capacitances were examined for fractional resistivity-time dependence. Correlating the results with Raman mapping based analysis of dispersion, the results indicated increased dispersion and MWCNT-MWCNT contact area result in a transition from matrix based resistive response to filler based conductive response.

A New Compression Testing Technique for Anistropic Porous Materials

Hang Yao and Wei Tong

Bobby B Lyle School of Engineering,
Southern Methodist Univeristy, Dallas, TX

A new compression testing technique has been developed for anisotropic porous materials with 3D full-field surface strain measurement using "two-camera two-mirror" setup. Two cameras took images of four surfaces using two 45-degree inclined mirrors. The whole-specimen apparent strain was measured using video extensometer, and the full-field local strain was measured using digital image correlation technique. Not only the apparent stress-strain curve, but also the Poisson's ratios and the volumetric strain can be measured through data post-processing. Moreover, the local strain mapping of each surface can be obtained to observe local strain distribution and concentration. Sawbones solid rigid polyurethane foams were tested to verify this compression testing technique. This new technique provides a prompt and accurate approach to calibrate and validate micro-finite element models of biological materials such as trabecular bone.

Growth Mechanism of Multi-oriented Twin Domain Structure in Epitaxial $Ba(Zr,Ti)O_3$ Thin Films

Jie He and Efstathios Meletis

Materials Science and Engineering Department, University of Texas at Arlington, Arlington, TX 76019

The research is focused on understanding the growth mechanism of epitaxial perovskite-type oxide thin films via microstructure analysis at the atomic/nano scale. Perovskite epitaxial oxide thin films, especially formed in 1-D nanocolumns, possess novel properties and are considered as one of the most important material families to meet advanced nanotechnology material challenges. Epitaxial $Ba(Zr,Ti)O_3$ (BZT) and 2%Mn-doped $Ba(Zr,Ti)O_3$ (Mn:BZT) thin films grown by pulsed laser deposition (PLD) on (001) MgO substrate were selected as a model system. The microstructures of the films were studied using conventional transmission electron microscope (TEM) and high-resolution (HR) TEM. It was observed that initially both films grow by forming a continuous epitaxial layer from the substrate followed by the formation of twin-coupled nano-pillars. The electron diffraction patterns (EDP) of such a complex structure composed of an epilayer and twin domains with specific crystallographic orientation relationship to the substrate show characteristics/features similar to those of single crystal EDPs. The microstructure evolution from the epilayer to nanopillar is accomplished by alternatively introducing {111} and {110} plane twin boundaries, resulting in gradual shrinking/enlarging of the lateral size of the epitaxial grains/twin-coupled nanopillars.

Preliminary results show that the BZT20 ($Ba(Zr_{0.2}Ti_{0.8})O_3$) thin films possessing such complex structure exhibit a nonuniform polarization switching behavior. Since the properties of thin films strongly depend on the domains, twinning, grain boundaries and defects at the nanoscale level, the present effort can provide the framework to produce new materials with greatly improved properties via fundamental understanding of their growth mechanism.

Kelvin Probe Force Microscopy Study of Grain Boundaries in Chalcopyrite Thin Film Solar Cells

Eray Erkan and Michael Jin

Materials Science and Engineering Department, University of Texas at Arlington, Arlington, TX 76019

Thin film solar cells have been attracting attention since they can be produced by low-cost and high-rate processes over large areas, and due to their light weight. Particularly, effort has been put on polycrystalline chalcopyrite Cu(In, Ga)Se2 (CIGS)-based thin film solar cells which are the most promising group among other thin film solar cells. Despite the extensive research being done to increase the efficiencies of CIGS solar cells, fundamental properties of CIGS is not yet well understood. For instance, one of the biggest question marks is on the role of grain boundaries in CIGS solar cells. It is not clear to us yet that how the polycrystalline CIGS solar cells have reached power conversion efficiencies of 20.3% despite the GBs they have, whereas their single crystalline counterparts have shown only around 13% power conversion efficiency [1, 2]. This is not intuitive since it is well known that the GBs in semiconductor materials, such as Si and GaAs, are defect sites and act as recombination centers for photogenerated carriers.

Kelvin probe force microscopy (KPFM) is an atomic force microscopy (AFM) based technique which is used to extract the contact potential difference between the sample and the conductive AFM tip with nanoscale resolution. Therefore, it is possible to obtain a work function map of a material by using KPFM which makes it very suitable to study the electrical properties of GBs in CIGS solar cells.

In this study, we used KPFM to study the electrical properties of GBs in CIGS thin films. KPFM results show that there is a reduction in work function over GBs relative to the grain interiors, which is interpreted as band bending at the GBs. The band bending at the GBs can help photogenerated charge carrier separation instead of causing their recombination, and might be one of the possible reasons for high performance of polycrystalline CIGS-based solar cells.

References

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Material Anisotropy Characterized by Transparent Indenter

Yue Xuan and Wei Tong

Bobby B. Lyle School of Engineering, Southern Methodist University, Dallas, TX

Anisotropy is a common property for soft materials including biomaterials and biological materials according to their complex microstructures. Indentation testing has been used to characterize the multiple mechanical properties of soft materials. However, there are still some issues hindering the application of indentation testing on soft materials. A simply transparent indenter measurement system has been designed and built to test mechanical property of soft polymers and tissues. It enabled the direct view and accurate measurement of the contact area. With the transparent indenter feature, the mapping of local surface deformation profile was also achieved. Since soft tissues and biomaterials are characterized by nonlinear and anisotropic properties, the shape and area of the contact reflect the corresponding anisotropy. The elliptical contact areas were measured. The direction of the axes of the ellipse was correlated to the surface geometry profile as well as the anisotropic structure.

Compositional and Structural Characterization of Diesel Soot and its Correlation with Wear of Diesel Engine Components

Mihir Patel, Pranesh Aswath

Tribology Lubrication and Coating Laboratory, Materials Science and Engineering Department,, University of Texas at Arlington, Arlington TX 76019

An important theme of the twenty first century is to achieve a clean environment. One of the prime concerns to achieve a clean environment is to reduce emission of NOx from diesel engines. Worldwide, governments have implemented various mandates with allowable limit of emission of NOx, which is significantly less than previous centuries. As a result, diesel engine manufacturers experience greater stress to develop new protocols to comply with stringent mandates. Various protocols have been designed such as optimized combustion timings using retarded injection timings and exhaust gas recirculation (EGR). These techniques have proved as effective strategies to curb the emission of NOx but have plagued engine with enormous amount of soot in the crankcase of diesel engine and increase wear of engines and hence significant reduction on drain interval. Reduction in drain interval increases wear of engine components and the cost of operation of diesel engine. Hence, the need has been felt to understand the wear mechanism of diesel soot fundamentally to help lubricant additive and engine manufacturers to optimize their products and to provide sufficient anti wear properties to protect the diesel engine as well as to comply with emission standards to protect the environment. Researchers have attempted to understand the diesel soot wear mechanism and have proposed various phenomenological models, but fundamental wear mechanism has not been comprehended thoroughly in order to improve the engine performance along with reduced emission of pollutants.

The study had been conducted to comprehend the fundamental wear mechanism of the diesel engine in presence of diesel soot. This study was approached to investigate changes in soot structures and chemistry to correlate with wear results using third generation synchrotron facility using synchrotron radiation. X-ray Absorption Near Edge Spectroscopy (XANES) using synchrotron radiation was employed as a high resolution surface analysis technique to understand the chemical modification in the soot. Furthermore, Raman Spectroscopy and Transmission Electron Microscopy were employed to understand structural changes in the soot. Synchrotron X-ray diffraction was employed to characterize the crystalline phase change in the soot.

Keywords: Diesel Engine, Lubrication, Diesel Soot, XANES, and Exhaust Gas Recirculation

Acknowledgements: XANES experiments were conducted at SRC in Wisconsin, Madison and CLS at Saskatoon, Saskatchewan, Canada.

Spallation of a Near Theoretical Strength Cu-Nb Multilayer Nanocomposite

Niraj Gupta, Srinivasan G. Srivilliputhur

Department of Materials Science and Engineering, University of North Texas

Spallation is an important mode of failure in high strain rate deformation. We study this phenomena in Copper-Niobium nanoscale layered composites conforming to a Kurdjimov-Sach's orientation using multi million atom molecular dynamics simulations. The copper and niobium atoms are immiscible and the orientational relation of their lattices creates an interface that act as an effective sink for dislocations and vacancies. In this talk we will focus on understanding the role played by Cu-Nb interfaces and layer morphology on the void nucleation, growth, and their ultimate effect on spall strength of the multilayered composites. The target structures consisted of varying numbers of alternating copper and niobium layers with thicknesses varying from 1 nm to 22 nm. Flyer velocities ranged from 3.5 to 11.5 Å/ps, corresponding to an approximate strain rate of 10^9 /s. Spallation occurs in the vicinity of the Cu-Nb interface, and always in the copper layer. We compare these results with spallation processes in single crystal Cu.

Laser cladding of Fe based amorphous powder on AISI 4310 steel: A microstructural and thermal modeling study

Shravan Katakam, Sameer R. Paital, Junyeon Hwang, Rajarshi Banerjee, Narendra B. Dahotre

Department of Materials Science and Engineering, University of North Texas

Iron based amorphous materials owing to its very high hardness, elastic modulus, wear and corrosion resistance can be a potential material for surface modification and engineering of many structural alloys. To achieve such a functional surface, in the current work an iron based ($Fe_{48}Cr_{15}Mo_{14}Y_2C_{15}B$) amorphous precursor powder was cladded on AISI 4310 steel using a continuous wave diode-pumped ytterbium laser. The coatings were characterized by different techniques like XRD, SEM and TEM. SEM and TEM studies indicated the presence of Fe based nanocrystalline dendrites intermixed within an amorphous matrix. A three dimensional thermal modeling approach based on COMSOL Multiphysics was used to approximately predict the temperature evolution and cooling rates achieved during laser processing. The effect of temperature evolution and cooling rates on the microstructural and phase evolution within the coatings is studied.

Phase Separation and Second Phase Precipitation in beta Titanium Alloys

Devaraj Arun, N. Gupta, S. Nag, H. L. Fraser*, R. Banerjee and S. G. Srinivasan

Department of Materials Science and Engineering, University of North Texas
** Ohio State University*

The early stages of phase transformation in materials systems ultimately dictate their final microstructure and the attendant properties. This talk focuses on omega precipitation within the beta matrix of simple model binary titanium-molybdenum (Ti-Mo) alloys. Direct atomic scale observation of pre-transition omega-like embryos in quenched alloys, using aberration-corrected HRSTEM coupled with 3DAP tomography will be presented. First-principles computations using the Vienna *ab initio* simulation package (VASP) is used to determine the minimum energy path for the beta to omega transformation in Ti-Mo alloys with up to 16.66at%Mo. The results of these computations are compared and contrasted with the experimental results to elucidate a novel mechanism for the beta to omega transformation in Ti-Mo alloys. The overall goal of these investigations was to obtain fundamental insights into the mechanisms of solid-state transformations in metallic systems by capturing the earliest stages of nucleation at atomic to near atomic spatial and compositional resolution.

Computational Study on the Effect of SrO/CaO Substitution on the Structural and Diffusion Properties of Bioactive Glasses

Ye Xiang and Jincheng Du

Department of Materials Science and Engineering, University of North Texas

Bioactive glasses have been applied in a variety of biomedical applications. Strontium-containing bioactive glasses have attracted considerable recent interests due to the additional beneficial effect of enhanced bone growth introduced by strontium ions. However, rational design of strontium containing glass compositions requires detailed understanding of the atomic structure and especially the strontium environment in these glasses. In this talk, I will present the effect of strontium substitution for calcium on structure and properties in the 45S5 glasses obtained using molecular dynamics (MD) computer simulations. The series of $46.1SiO_2 \cdot 24.4Na_2O \cdot$ (26.9-x) $CaO \cdot 2.6P_2O_5 \cdot xSrO$ (x=0, 1, 5, 10, 15) compositions have been simulated with effective partial charge potentials and a combination of constant temperature and pressure (NPT) and microcanomical (NVE) ensembles. The substitution effects on the local environment around strontium and other cations were analyzed by studying the partial pair distribution functions, bond angle distributions, coordination number and its distribution. Change of the medium range structures were characterized by Q_n distributions and network connectivity, cation-cation distribution, modifier ion preference distributions and aggregation. Ionic diffusion behaviors of strontium doped glasses have also been studied using MD simulations. The diffusion coefficients and energy barriers have been obtained for these series of glasses. The results show that strontium ions have an average coordination number of 7 and an average Sr-O bond length of 2.59 Å. Increase of strontium concentration leads to an increased level of clustering of calcium ions. Diffusion coefficients of ions at different temperature have been obtained and energy barrier of each ionic species calculated as a function of composition.