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**Effect of the Matrix Viscosity on the Morphology and Mechanical Properties of Polypropylene /Brazilian Organoclay Nanocomposites:** *André Rodrigues*<sup>1</sup>; Tomás Melo<sup>1</sup>; Edcleide Araujo<sup>1</sup>; Pankaj Agrawal<sup>1</sup>; <sup>1</sup>Universidade Federal de Campina Grande

In this work, the effect of Polypropylene (PP) viscosity and the Brazilian organically modified clay (organoclay) on the morphology and the mechanical properties of PP/Organoclay Nanocomposites was investigated. The nanocomposites were prepared using a co-rotating twin screw extruder. Two grades of PP with different viscosities were used as a matrix and PP-g-MA was used as a compatibilizer. The nanocomposites were characterized by X-Ray Diffraction (XRD), Transmission Electron Microscopy (TEM) and Mechanical Properties. XRD results showed that a predominantly intercalated nanocomposites were formed. The nanocomposites formation was not affected by the PP viscosity. These results were confirmed by TEM. Mechanical properties results showed that the elastic modulus and the tensile strength were improved.

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**Influence of Processing Conditions on Development of PE/PE-g-MA/Organoclay Nanocomposites:** Luana Kojuch<sup>1</sup>; Renata Barbosa<sup>1</sup>; Edcleide Araújo<sup>1</sup>; Tomas Melo<sup>1</sup>; <sup>1</sup>Universidade Federal de Campina Grande

Nanocomposites developed with silicates in layers represent an alternative to the composites developed with conventional filler, because they use minimum levels of nanofiller. In this work, polyethylene/PE-g-MA/organoclay nanocomposites were produced in a Torque Rheometer Haake in these conditions: 190°C, 60 and 120rpm, for 7 and 14 minutes. The systems were characterized by X-ray diffraction (XRD). The obtained results indicated that the PE/PE-g-MA/organoclay nanocomposites presented intercalated and/or partially exfoliated structures for the 120 rpm and 7 minutes, probably due to bigger number of intercalation of polyethylene molecules between the layers of the organoclay. For the time of 14 minutes, the material showed a little degradation probably due to excessive time in the mixer.

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**Preparation and Characterization of Assymmetric Membranes Obtained of Nylon6/Brazilian Clay Nanocomposites:** *Amanda Melissa Leite*<sup>1</sup>; Larissa Maia<sup>1</sup>; Edcleide Araújo<sup>1</sup>; Hélio Lira<sup>1</sup>; <sup>1</sup>Universidade Federal de Campina Grande

A membrane is an interphase between two adjacent phases acting as a selective barrier, regulating the transport of substances between the two compartments. The main advantages of membranes technology as compared with other unit operations in chemical engineering are related to this unique separation principle, i.e. the transport selectivity of the membrane. Separations with membranes do not require additives, and they can be performed isothermally at low temperatures and compared to other thermal separation processes-at low energy consumption. In this work, asymmetric membrane of Nylon6/Brazilian clay nanocomposites using quaternary ammonium salts were obtained by phase inversion method. The membranes were characterized by SEM. The results showed that there is a significant difference in size and distribution of pores between pure nylon 6 membranes and membranes obtained from nanocomposites.

## Neutron and X-Ray Studies of Advanced Materials: Diffuse Scattering

*Sponsored by:* The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Titanium Committee  
*Program Organizers:* Rozaliya Barabash, Oak Ridge National Laboratory; Yandong Wang, Northeastern University; Peter Liaw, The University of Tennessee; Jaimie Tiley, US Air Force

Monday PM

Room: 3016

February 16, 2009

Location: Moscone West Convention Center

*Session Chairs:* Rozaliya Barabash, Oak Ridge National Laboratory; Patrice Turchi, Lawrence Livermore National Laboratory

2:00 PM Invited

**X-Ray Diffuse Scattering for The Study of the Size Distributions of Clustered Defects in Crystalline Materials:** *Bennett Larson*<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

The diffuse scattering near Bragg reflections arising from defect clusters in crystalline materials contains detailed signatures of the size, type, size-distribution, and the internal structure of clusters. In this presentation, the fundamental aspects of diffuse scattering from lattice defects will be considered within the coherent wave theory and the local-Bragg scattering interpretation in the so-called "asymptotic" diffuse scattering regime will be discussed. Detailed measurements of separate size distributions for vacancy and interstitial loops in neutron irradiated Cu and for coherent Co precipitates as a function of thermal aging in Cu(1%)Co single crystals will be presented. In addition, the use of submicron diameter x-ray microbeams to perform depth-resolved diffuse scattering measurements of vacancy and interstitial loop distributions in 10 MeV self-ion implanted silicon single crystals will be discussed. \*Research at ORNL supported by the DOE Office of Science, Basic Energy Sciences, Division of Materials Sciences and Engineering.

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**Huang-Scattering As A Probe Of Local Defect Structure:** *Branton Campbell*<sup>1</sup>; <sup>1</sup>Brigham Young University

Point-like crystal defects often give rise to anisotropic diffuse-scattering distributions that are centered around intense Bragg peaks in electron, x-ray and neutron diffraction data. These anisotropic Huang-scattering distributions are directly related to the long-range strain-fields extending outward from the defect core. By relating these strain fields to the atomic displacements within the defect core via the elastic dynamical matrix, Huang scattering can be used to indirectly probe local defect structure. We will present a convenient method of extracting local displacements from 3D Huang-scattering data that is sufficiently general to handle both arbitrary crystal symmetry and arbitrary defect symmetry. It involves first invoking the linear-continuum elastic approximation to characterize the strain fields, which are then used to extrapolate approximate local atomic displacements. In addition to exploring the strengths and limitations of this approach, we will demonstrate its application to the quantitative analysis of experimental diffuse scattering data.

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**Statistical Theory of Diffuse Scattering by Crystals with Nonrandom Precipitates:** *Rozaliya Barabash*<sup>1</sup>; Gene Ice<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

The statistical kinematical theory of diffuse scattering from precipitated alloys is reviewed. Nonperiodic potentials are used to model the scattering from different defect distributions. Fluctuating parts of the potential, resulting in diffuse scattering, is analyzed in the framework of the fluctuation wave method. Interaction of distortion fields from precipitates often causes their self-organization and nonrandom distribution. A comparison with the single defect approximation approach is performed for correlated/uncorrelated precipitates. Correlation and layered precipitates distribution in preferred crystallographic planes, results in specific features of the diffuse scattering intensity. The shape function of coherent precipitates is discussed. Experimental and simulated diffuse scattering intensity maps are used to perform quantitative characterization of the defects structure and distribution. Research is sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Science U.S. Department of Energy.

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**Elastic Diffuse Scattering Of Binary Alloys With A Large Atomic-Size Difference:** *Bernd Schönfeld*<sup>1</sup>; <sup>1</sup>ETH Zurich

Alloys with local order and a relatively large difference in atomic sizes have continued to attract interest of theoreticians and experimentalists. Here, two such alloys, Ni-Re and Ni-Pt, were investigated experimentally. Not much is known on the microstructure in Ni-Re though its fraction in Ni-based superalloys has been steadily increased. From diffuse x-ray scattering of Ni-9.4 at.% Re in combination with small-angle neutron scattering it was now established that local order is present, characterized by 1/2 diffuse maxima. For the system Ni-Pt the superstructures Ni<sub>3</sub>Pt and NiPt are known; on the Pt-rich side, however, ordered structures are unknown. A diffuse x-ray scattering experiment of Ni-87.8 at.% Pt was undertaken to investigate the possible presence of NiPt, suggested by electronic-structure calculations. With the interaction parameters obtained, Monte-Carlo simulations indicated that no NiPt<sub>2</sub> superstructure is to be expected. Species-dependent static atomic displacements also determined will be compared with values from the literature.

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**Atomic Displacements On A Si-Ge Si Rich Single Crystal:** *Jose Rodriguez-Rivera*<sup>1</sup>; *S. Moss*<sup>2</sup>; *J. Robertson*<sup>3</sup>; *Rozaliya Barabash*<sup>3</sup>; *J. Copley*<sup>4</sup>; *D. Neumann*<sup>4</sup>; <sup>1</sup>University of Maryland/National Institute of Standards and Technology; <sup>2</sup>University of Houston; <sup>3</sup>Oak Ridge National Laboratory; <sup>4</sup>National Institute of Standards and Technology

Si-Ge alloys have received a great deal of attention because of the possibility of faster devices that might employ them. However, the lattice mismatch between the two elements has made the growth of epitaxial homogeneous thin films quite difficult and various strategies have been employed to overcome this. Le Bolloc'h et al. [1] reported phonon measurements on a Si-Ge Si Rich single crystal. He also distinguishes in a radial scan of the elastic neutrons from the alloy the size effect displacement scattering. Using the Disk Chopper Spectrometer (DCS) at NIST we have measured the (110) and (001) planes which clearly shows the Huang Diffuse Scattering (HDS) and Size Effect scattering (SE) due to atomic displacements. The data also shows no SRO contribution. The data permits the extraction of HDS and SE displacements parameters.[1] Phys. Rev. B 63, 035204 (2001)

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**Structure and Dynamics of a Si-Rich SiGe Solid Solution:** *J. Robertson*<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

The SiGe system has been intensively studied because the carrier mobility is much higher than in pure silicon and this gives rise to considerable gains in electronic device performance. SiGe alloys have been the subject of intense investigation for several years. Several theoretical studies which are supported by a previous experiment on a polycrystalline solid solution predict a miscibility gap in the Si-Ge system. On the contrary, several long-range ordered structures have been reported in thin films although these were under either compressive or tensile strain as well as an XAFS study on SiGe thin films that indicates complete randomness. Thus, the study of the local atomic environments in this alloy is of fundamental importance. In this talk I will present the results of neutron and X-ray measurements on a homogeneous bulk crystal of Si<sub>0.2</sub>Ge<sub>0.8</sub> and discuss the nature of its structural disorder and dynamics.

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**Small-Angle Scattering Of X-Rays And Neutrons - Advances And Challenges:** *Gernot Kostorz*<sup>1</sup>; <sup>1</sup>ETH Zurich

Some applications of small-angle scattering in the field of materials science will be discussed. Emphasis will be on experiments pushing the spatial and temporal resolution limits of both types of radiation, exploiting their individual characteristics and their complementarity. Inhomogeneities on a scale from a few interatomic distances to several micrometers and their evolution can be studied in the bulk and at/near surfaces with good accuracy. These experiments serve to develop and test models of micro- and nanostructural features in materials.

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**"Small-Angle Scattering For Every Microstructure And Every Problem?" – A Critical Review Of Advanced Small-Angle Scattering Techniques:** *Jan Ilavsky*<sup>1</sup>; <sup>1</sup>Argonne National Laboratory

Number of small-angle scattering tools and techniques – for both X-ray or neutrons – is available today. Since some of these were developed in the last years, they may not be discussed in commonly available textbooks. Therefore many non-SAS expert researchers may not be aware of their advanced capabilities. Further, to learn these new tools and methods, one has to make use of original manuscripts, sometimes with sketchy techniques description and often-specific materials oriented. Therefore it may be difficult to generalize and apply these novel techniques to wider range of material science problems. This presentation will review different X-ray and neutron small-angle scattering techniques, such as anisotropic Porod scattering, anisotropic multiple scattering, and various types of ultra-small angle scattering. Examples of results, ranging from thermal barrier coatings to hierarchical polymer structures, will be given and applicability to assorted engineering material science problems will be discussed.

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**Chemical Order in Alloys: Current Status and Prospect:** *Patrice Turchi*<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory

The prediction of ordering trends in alloys provides valuable insight on phase formation, phase stability, and phase diagrams. In this context, neutron and X-ray scattering experiments can play a critical role in the verification and validation process, and also challenge theory. After a brief critical review of the quantum-mechanical-based approaches that are currently available for studying short-range order in alloys, examples of predictions will be discussed. They will include: transient ordering phenomenon, ordering in complex alloys such as A15 and sigma, pressure effect on chemical order, and ordering trends in some fcc and bcc-based alloys. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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**Phase Transitions In Ionic Liquid Based Mixtures Studied By Simultaneous X-Ray Diffraction And DSC Measurements:** *Hiroshi Abe*<sup>1</sup>; *Yusuke Imai*<sup>1</sup>; *Takefumi Goto*<sup>1</sup>; *Yukihiro Yoshimura*<sup>1</sup>; <sup>1</sup>National Defense Academy

Ionic liquids (ILs) are well known to be new solvents in "green chemistry". The curious nature of ILs is represented in almost zero vapor pressure. Recently, we found anomalous domain growth in [DEME][BF<sub>4</sub>]-H<sub>2</sub>O mixtures [1]. Here, three different types of the domain structures were formed with a small content of H<sub>2</sub>O. In spite of a variety of domain formations, crystal structures are the same as pure [DEME][BF<sub>4</sub>]. In addition, boundaries between complicated domain structures could not provide intrinsic strains. Subsequently, complicated phase diagram is obtained from 0 to 12 mol% H<sub>2</sub>O [2]. By simultaneous X-ray diffraction and DSC measurements, various kinds of phase transitions and phases are determined systematically. One of important solid phases is pure amorphous phase around 6 mol%. In Raman spectrum, there are "two dynamic components" in pure amorphous phase. Moreover, cold crystallization with some exothermal peak is observed upon heating above 4 mol%. The results are based on anomalous behaviors of water molecules. [1] Y. Imai et al., J. Phys. Chem. B (2008), in press. [2] Y. Imai et al., Chem. Phys. (2008), in press.

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**From Average to Local Structure: A Structural Study of Zeolite-NdY/Se System:** *A. M. Milinda Abeykoon*<sup>1</sup>; *W. Donner*<sup>2</sup>; *M. Brunelli*<sup>3</sup>; *A. J. Jacobson*<sup>1</sup>; *S. C. Moss*<sup>1</sup>; <sup>1</sup>University of Houston; <sup>2</sup>Darmstadt University of Technology; <sup>3</sup>European Synchrotron Radiation Facility (ESRF)

A challenging problem in crystal structure determination is the characterization of the atomic short-range order as observed in the diffuse scattering. The long-range order is characterized by a careful analysis of the sharp Bragg positions and intensities to obtain average atomic positions and equilibrium atom displacements. The short-range order appears as weak diffuse scattering widely distributed throughout the reciprocal space. Since many important crystalline materials have a significant disorder on the atomic scale, a method which is capable of modeling the structure of these materials is necessary. We emphasize the need of two techniques: the Pair Distribution Function (PDF) and the Rietveld method to model the structures of such systems. We will use our results of x-ray studies on zeolite-NdY/Se system to demonstrate this.