4:30 PM
High Strain-Rate Modeling of Titanium-Aluminum Laminates: *Charles Randow*[1]; George Gazonas[2]; [1]Bucknell University; [2]U.S. Army Research Laboratory

Laminate composites created by alternating layers of titanium and aluminum have shown an improved resistance to fracture with a reduction in density. In these studies, hot pressing has been used to bond the layers together, resulting in the creation of the intermetallic $TiAl_3$. In the present work, commercially pure titanium (CP-Ti) and 1100-Al are bonded using an ultrasonic consolidation process before hot pressing to form a CP-Ti/$TiAl_3$/Al laminate, with the goal of developing a system capable of withstanding the high strain-rate loads encountered in ballistic impact and blast applications. One of the difficulties in modeling such systems is the lack of information available on the high strain-rate properties of $TiAl_3$. Through the use of dynamic finite element modeling and plate impact experiments, the effect of $TiAl_3$ on the laminate strength is investigated. These results are used in predictive models of the laminate subjected to impact loading.

4:50 PM
Modeling High Temperature Strength and Flow Stress Curves of Titanium Alloys: Zhanli Guo[1]; Nigel Saunders[1]; Peter Miodownik[1]; *Jean-Philippe Schille*[1]; [1]Sente Software, Ltd.

Process design and simulation for any metals requires an understanding of their high temperature mechanical behavior, particularly with respect to flow stress as a function of temperature and strain rate. This paper describes the recent developments of JMatPro, a computer software for material property simulation, on calculating the high temperature mechanical properties of titanium alloys. Extensive validation has been carried out and shown in the present work. Good agreement between calculated and experimental results has been achieved for a variety of titanium alloys, including alpha, near-alpha, alpha+beta, and beta types, over a wide range of temperature and strain rates. The material properties calculated from JMatPro can now be passed directly into computer-aided engineering packages for process simulation.

Neutron and X-Ray Studies for Probing Materials Behavior: Scattering and Understanding of Materials Properties

Sponsored by: National Science Foundation, The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee
Program Organizers: Rozaliya Barabash, Oak Ridge National Laboratory; Yandong Wang, Northeastern University; Peter K. Liaw, University of Tennessee

Wednesday PM Room: 391
March 12, 2008 Location: Ernest Morial Convention Center

Session Chairs: Emil Zolotoyabko, Technion-Israel Institute of Technology; Gene Ice, Oak Ridge National Laboratory

2:00 PM Invited
Small-Angle Scattering of Neutrons and X-Rays in Materials Science - A Comparison: *Gernot Kostorz*[1]; [1]ETH Zurich

After a short comparison of the basic features of small-angle scattering of X-rays and neutrons, examples of recent applications will be given. Experimental rsults will be discussed, in particular those concerning phase separation of alloys, emphasizing the possibilities of spatial and temporal resolution of the decomposition process, high temperature-in-situ studies, and combinations with diffuse scattering and transmission electron microscopy. In some Al-, Cu- and Ni-base alloys, shape, volume fraction, spatial arrangement and other details of precipitates can be analyzed with great precision.

2:25 PM
Understanding Particle Morphology during High Energy Milling of Complex Metal Hydrides: *Tabbetha Dobbins*[1]; Ejiroghene Oteri[1]; Jan Ilavsky[2]; [1]Louisiana Tech University; [2]Advanced Photon Source, Argonne National Laboratory

A program comprised of ultrasmall-angle x-ray scattering (USAXS) experiments was performed at sector 33-ID at the UNI-CAT for the study of particle morphology changes in the alanates (e.g. $NaAlH_4$—both before and after transition metal salt catalytic dopant additions by high energy ball milling). The variation in surface fractal dimension and particle size with milling time and dopant content was tracked. These studies have shown that dopant content level (e.g. 2 mol % and 4 mol %) and dopant type (i.e. $TiCl_2$, $TiCl_3$, VCl_3, and $ZrCl_4$) markedly affects $NaAlH_4$ powder particle surface area (determined using surface fractal dimension). This study was able to link powder particle surface area to catalytic doping. We will report links among codopants (i.e. two dopants) and powder particle surface area studied using USAXS.

2:45 PM Invited
Diffuse Scattering and Monte Carlo Studies of Relaxor Ferroelectrics: *Thomas Welberry*[1]; [1]Australian National University

A renewed interest in the field of ferroelectricity has taken place in recent years since the finding of exceptional piezoelectric properties in the lead-oxide class of relaxor ferroelectric (RF) materials typified by the disordered perovskite $PbZn_{1/3}Nb_{2/3}O_3$ (PZN).Although PZN and numerous related materials have been extensively studied over a long period a detailed understanding of the exact nature of their polar nanostructure has still not emerged. In this paper we describe experiments in which full three-dimensional diffuse neutron scattering data have been recorded from a single crystal of PZN using the time-of-flight (tof) Laue technique. Monte Carlo simulation has been used to demonstrate that the observed diffuse patterns are due to planar nano-domains oriented normal to the six <110> directions. A simple model has been developed which explains the observed scattering.

3:10 PM Invited
Concomitant Determination of Planar Faults, Dislocations and Subgrain Size by X-Ray Line Profile Analysis: *Tamas Ungar*[1]; Levente Balogh[1]; [1]Eotvos University

X-ray line profile analysis is based on (i) the different profile shapes and (ii) the different hkl dependence of line broadening or shifts corresponding to the different types of lattice defects: (a) grain or subgrain boundaries, (b) dislocations and (c) planar defects, i.e. stacking faults and twin boundaries. It is shown that physically well established, theoretically calculated profile functions can be attributed to the three fundamental defect types, (a) to (c). These *defect-related profile-functions* have the same mathematical form for each Bragg reflection throughout the entire diffraction pattern. However, their breadths and positions are scaled by defect specific, hkl dependent scaling rules. Since the scaling rules are only weakly correlated the diffraction effects of the three different defect types can be separated and the defect properties well characterized.

3:35 PM Break

3:45 PM Invited
Probing Phonons and Phase Transitions in Solids with X-Ray Thermal Diffuse Scattering: *Tai Chiang*[1]; [1]University of Illinois

X-ray scattering by thermally populated phonons in crystals give rise to diffuse scattering. Measurements of such thermal diffuse scattering (TDS) intensities as functions of momentum transfer and sample temperature yield information about the lattice dynamics including the phonon dispersion relations. This method has a long history, and after being largely ignored for decades, it has revived and become a powerful tool with the advent of intense synchrotron x-ray sources. In this talk, we review the basics of TDS together with recent experiments of phonon studies in various systems. Issues of high order scattering and background contributions will be discussed in connection with details of data analysis. Examples will be presented to illustrate the power of TDS as a probe of phase transitions that involve phonons. The method is well suited for detailed studies of soft mode behavior and critical exponents.

4:10 PM Invited
Local Structure of Decagonal Quasicrystals by DAFS: *Hiroshi Abe*[1]; Hiroyuki Saitoh[2]; Hironori Nakao[3]; [1]National Defense Academy; [2]Japan Atomic Energy Research Institute; [3]Tohoku University

Al-Ni-Co (ANC) and Al-Ni-Fe (ANF) system is well known to be decagonal quasicrystals, which have two-dimensional quasiperiodic planes. The structures depend both on concentrations and on temperature extensively. Recently, short-range order (SRO) in quasicrystals was detected on a quasiperiodic plane by anomalous-X-ray scattering method.[1] In this study, local structure of quasicrystals was examined along the periodic direction compared with a quasiperiodic plane by X-ray diffraction anomalous fine structure (DAFS) technique. In principle, DAFS possesses site and spatial selectivity. DAFS experiment was performed on the beamline BL-4C of the Photon Factory at the High Energy Accelerator Research Organization in Japan. Apparent differences of DAFS between periodic and quasiperiodic directions were shown in ANC and ANF. [1]H. Abe, H. Saitoh, T. Ueno, H. Nakao, Y. Matsuo, K. Ohshima and H. Matsumoto, J. Phys.: Condens. Matter 15 (2003) 1665.

4:35 PM Invited
Diffuse Scattering in Quasicrystals of Icosahedral Symmetry: *Sonia Francoual*[1]; Marc de Boissieu[2]; Roland Currat[3]; Shiro Kashimoto[4]; Tsutomu Ishimasa[4]; [1]National High Magnetic Field Laboratory; [2]Sciences et Ingenierie des Materiaux et Procedes; [3]Institut Laue-Langevin; [4]Hokkaido University

According to the hydrodynamic theory of quasicrystalline materials, the long-range quasiperiodic order yields in quasicrystals new long-wavelength modes, the phason modes, in addition to the acoustic phonons. Phason excitations are diffusive and associated with internal atomic rearrangements the dynamics of which is expected to lead to a distinctive diffuse scattering signal around Bragg peaks in reciprocal space. Up to now, experimental demonstration for the existence of phason diffuse scattering was given in the enlightening single case of the Al-Pd-Mn Mackay-type icosahedral (i-) phase from which the phason elastic constants were extracted and the thermal activation revealed. In the present communication, we report on X-ray Synchrotron investigations of the diffuse scattering in the i-Zn-X-Sc (X = Mg, Ag, Co) phases and the Zn-Sc 1/1 periodic approximant bringing evidence for the presence of long-wavelength phasons also in this new class of icosahedral quasicrystals and ruling it out in the 1/1 approximant structure.

5:00 PM Invited
Towards Systematic Procedures for Interpreting Diffuse Scattering from Disordered Molecular Materials: *Hans-Beat Buergi*[1]; Christina Hoffmann[2]; [1]University of Zuerich; [2]Oak Ridge National Laboratory

Real crystals show many kinds of disorder giving rise to diffuse scattering which may cover the whole reciprocal space and is generally much weaker than Bragg scattering. However, with the advent of new, more intense radiation sources like synchrotrons and neutron Spallation sources it has become possible to measure diffuse features accurately. New X-ray and neutron single crystal diffractometers have been designed for fast data collection and repeatability of experiments at controlled conditions. X-ray and neutron experiments will be measured on the same sample by both methods, allowing to analyze the collected data simultaneously. Although state of the art computing resources allow to process the large amounts of data produced in such experiments, the methods to produce reliable models of disorder are less developed in comparison to single crystal structure analysis. Here we will sketch steps towards systematic procedures for interpreting diffuse scattering from molecular materials.

5:25 PM Invited
X-Ray Imaging for Materials and Biomedical Sciences: *Jung Ho Je*[1]; Y. Hwu[2]; G. Margaritondo[3]; [1]Pohang University of Science and Technology; [2]Academia Sinica, Institute of Physics; [3]Ecole Polytechnique Fédérale de Lausanne

Radiology is the oldest and by far the largest field of application of x-rays. In recent years, this domain has been literally revolutionized by the exploitation of the unique characteristics of synchrotron sources. The results are particularly spectacular when the high spatial coherence of the radiation is used for novel and powerful approaches to radiology. The results are very high quality microradiology and microtomograhy images and movies - taken with a limited x-ray dose – that find a variety of applications in materials science, biology and medical research. In this talk we review basic theory and selected applications of phase contrast x-ray microscopy to materials and biomedical sciences. Furthermore we introduce a new strategy of combining phase contrast radiology and diffraction x-ray microscopy to visualize atomic level defects such as misfit dislocations and micropipes in semiconductor single crystals. Finally phase contrast x-ray imaging in nanometer-resolution (<30 nm) will be demonstrated.

5:50 PM Panel Discussion:

Donald Nicholson, Oak Ridge National Laboratory

Wolfgang Pantleon, Risø National Laboratory

Gernot Kostorz, ETH Zurich

Emil Zolotoyabko, Technion-Israel Institute of Technology

Vaclav Holy, Charles University

Thomas Welberry, Australian National University

Henning Poulsen, Risø National Laboratory

Philip Withers, Manchester University

Donald Brown, Los Alamos National Laboratory

Sunil Sinha, University of California, San Diego

Ulrich Lienert, Argonne National Laboratory

Hiroshi Abe, National Defense Academy

Branton Campbell, Brigham Young University

6:20 PM Concluding Comments

Particle Beam-Induced Radiation Effects in Materials: Nanostructures

Sponsored by: The Minerals, Metals and Materials Society, American Nuclear Society, TMS Structural Materials Division, TMS/ASM: Nuclear Materials Committee
Program Organizers: Gary Was, University of Michigan; Stuart Maloy, Los Alamos National Laboratory; Christina Trautmann, Gesellschaft fur Schwerionenforschung; Maximo Victoria, Lawrence Livermore National Laboratory

Wednesday PM Room: 389
March 12, 2008 Location: Ernest Morial Convention Center

Session Chairs: Daryush Ila, Alabama A&M University; Tongde Shen, Los Alamos National Laboratory

2:00 PM
Studies of the Ion Irradiation Effects in Bulk Nanocrystalline TiNi: *Askar Kilmametov*[1]; Adam Balogh[2]; Horst Hahn[3]; Ruslan Valiev[1]; [1]Ufa State Aviation Technological University; [2]Darmstadt University of Technology; [3]Forschungszentrum Karlsruhe GmbH

Nanocrystalline intermetallic alloys, which possess a long-range chemical ordering, considered being a good object to examine irradiation effects on the stability or degradation of crystal superlattice in the ordered state. TiNi alloy as one of the most important engineering materials due to its superior shape memory and mechanical properties was studied at present work. Bulk ordered nanocrystalline samples of altered grain size values (25 and 40 nm) were processed using the method of severe plastic deformation, namely high pressure torsion technique. Ordered nanocrystalline and coarse-grained samples were subjected to 1.5 MeV Ar ion irradiation at room temperature with damage doze up to 5.6 displacements per atom. Comparative analysis of long-range disordering and amorphisation kinetics revealed the enhanced irradiation resistance of nanocrystalline TiNi alloy. It was shown that at the equal damage doze nanostructured state is able to retain a long-range ordering meanwhile the coarse-grained counterpart was just essentially amorphised.