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CMSN Newsletter

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Department of Physics
University of Washington, Seattle

CMSN News

On June 16-18, 2005, a workshop on “X-rays and neutrons: essential tools for nanoscience research” will be held in Washington, D.C. The workshop is sponsored by the Science and Engineering and Technology Committee's Subcommittee on Nanoscale Science, Engineering and Technology (NSET) and the National Nanotechnology Initiative (NNI). This workshop is expected to play a role in setting national nanoscience technology policy for the future. A summary report will be issued after the workshop’s completion.

The following is copied from the workshop’s website, at http://www.sns.gov/workshops/nni_05/index.html

Summary

Virtually all of the grand challenges in nanotechnology have as overriding themes the need to determine the structure over a wide range of length scales and to understand how the combination of the structure and dynamics leads to their unique properties. Both x-rays and neutrons cover all the length scales of interest in nanoscience, from the atomic structure of individual building blocks to the configuration of assembled, functional structures, making them essential tools for the elucidation of these challenges.

The workshop is one of a series of workshops in support of the National Nanotechnology Initiative (NNI) Strategic Plan prepared by the Nanoscale Science and Engineering and Technology Subcommittee (NSTC), recently updated in December 2004 as part of the 21st Century Nanotechnology Research and Development Act (Public Law 108-153).

As called for in the Strategic Plan, the workshop will provide a guiding strategy to policy makers for the development of essential scattering tools for R&D in nanotechnology. The workshop report will be developed by internationally renowned participants who will identify frontier problems in their fields from experimental and theoretical perspectives by addressing the essential questions:

- Which of the outstanding problems in nanoscale synthesis, structure, dynamics and properties can be addressed using X-ray and neutron techniques such as scattering, imaging and spectroscopy, and how can these techniques help illuminate the important and urgent issues at the nanoscale?
- How might the current resource base in X-ray and neutron scattering techniques be augmented and used in solving outstanding problems in nanoscale science?

A scholarship program will also provide the opportunity for selected early career researchers to participate fully in the workshop and the development of the ensuing report.

Projected Outcomes

The workshop will bring together established experts and young scientists from the x-ray, neutron, and nanoscience/nanotechnology communities to discuss future research directions and opportunities. The goal of the workshop is to identify and promote the innovations in scattering techniques and related instrumentation required to tackle the exciting challenges of nanotechnology research now and for the future. The focus of this workshop will be to identify frontier problems in nanoscience such as understanding interfacial structures, nano-systems, confinement, and self-assembly of hard materials, soft materials, and biomaterials which can be elucidated through the use of x-ray and neutron scattering techniques.

After these research opportunities are identified, the workshop report will outline a roadmap for the prioritized development of these critical resources. Specifically, the workshop report will address the following goals:

- Identify the challenges in characterization at the nanoscale for the next 5-10 years that may be addressed using x-ray or neutron scattering techniques.
- Identify the instrumentation and techniques that must be developed to meet these challenges and allow research in nanoscience to advance.
- Identify both short and long term R&D in areas such as beam optics, detectors and in-situ characterization that will be required to support this vision.

The workshop report will be an effective tool for funding agencies, principal investigators, academia and industry to coordinate their long term investment strategies.

Supported by

- U.S. Department of Energy, Office of Basic Energy Sciences
- National Institute of Standards and Technology, NIST Center for Neutron Research
- National Science Foundation, Division of Materials Sciences

Workshop Chairs

- Ian Anderson (Oak Ridge National Laboratory, Spallation Neutron Source)
- Linda Horton (Oak Ridge National Laboratory, Center for Nanophase Materials Sciences)
- Eric Isaacs (Argonne National Laboratory, Center for Nanoscale Materials, and University of Chicago)
- Mark Ratner (Northwestern University)

Workshop Organizers

- Ian Anderson (Oak Ridge National Laboratory, Spallation Neutron Source)
- Kristin Bennett (U.S. Department of Energy, Office of Basic Energy Sciences)
- Al Ekkebus (Oak Ridge National Laboratory, Spallation Neutron Source)
- Pat Gallagher (National Institute of Standards and Technology)

- Phillip Lippel (National Nanotechnology Coordination Office)
- Linda Horton (Oak Ridge National Laboratory, Center for Nanophase Materials Sciences)
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Research Highlights

In this issue of the *CMSN Newsletter*, we feature a research highlight from our Fundamentals of Dirty Interfaces team. titled "Calculation of grain boundary stiffness from boundary fluctuations," by Stephen M. Foiles (Sandia).

Calculation of Grain Boundary Stiffness from Boundary Fluctuations

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Summary: *Cross-fertilization between work on solid-liquid and solid-solid interfaces during CMSN meetings has resulted in the successful calculation of mobility and interfacial stiffness based on fluctuations of the position of grain boundaries during MD simulations.*

The understanding and mesoscale simulation of polycrystalline microstructures depends on a fundamental understanding of the mechanisms and driving forces of grain boundary motion. Boundary motion is driven by a combination of local curvature of a boundary and by thermodynamic driving forces resulting from spatial variation of the local free energy in the bulk material due, for example, to inhomogeneous strain. In the case of purely curvature driven motion, the boundary velocity is given by $v = M\Gamma k$ where M is the boundary mobility, $\Gamma = (g + g'')$ is the boundary stiffness and κ is the local curvature [Herring, 1951]. Due to a lack of knowledge of the stiffness, it has often been assumed that the stiffness can be approximated by the boundary free energy, γ, and that the contribution of the second derivative of the boundary free energy with respect to orientation, g'', can be ignored. However, recent collaborative work of CMSN team members in this project has shown that it is essential to include the full stiffness in order to understand both experimental results and simulations based on a two-dimensional Ising model [Lobkovsky, *et al.*, 2004; see also previous highlight at http://www.phys.washington.edu/users/cmsn/FDI_highlight.html]. Here we present the first calculation of the boundary stiffness for a realistic grain boundary model.

The calculation of both interfacial mobility and interfacial stiffness from atomistic simulations has been considered recently for the case of solid-liquid interfaces where this information is crucial for the simulation of solidification [Hoyt, *et al.* 2001; Hoyt, *et al.* 2003]. One of the methodologies developed is based on the analysis of the equilibrium fluctuations of the solid-liquid interface. Here we show that the same strategy is applicable to the calculation of the mobility and stiffness of a grain boundary. The same approach has recently been applied to boundaries in a 2-D Ising model [Traut and Upmanyu, 2005]. The boundary considered here is an asymmetric $\Sigma7$ <111>-tilt boundary in Ni modeled with an embedded atom method potential. The atomic-level motion of the boundary is simulated using standard isothermal molecular dynamics. A snapshot of such a simulation is shown in figure 1. The color of the atoms corresponds to the crystal orientation its local geometry is closer to. From these simulations the coarse-grained interfacial position can be determined as a function of time and of position within the boundary. The stiffness can be obtained from the resulting fluctuation spectrum through the equation

$\left\langle \left| A(\vec{k}) \right|^2 \right\rangle = \dfrac{k_B T}{L_x L_y \Gamma(\hat{k}) k^2}$ where $A(\vec{k})$ is the Fourier transform of the interface height and L_x and L_y are the lengths of the cell in the boundary. The mobility can be determined from an analysis of the time correlation function of the fluctuations, $\left\langle A(\vec{k},0) A^*(\vec{k},t) \right\rangle = \left\langle \left| A(\vec{k}) \right|^2 \right\rangle e^{-t/t}$. The mobilities deduced are comparable to mobilities deduced in other atomistic simulations of mobility [Schönfelder, *et al.*, 1997; Zhang, *et al.*, 2004].

Figure 2 shows values of the stiffness for various values of k as a function of the direction within the boundary computed for both 1250 K and 1400 K. For this potential these temperature are 0.80 and 0.89 T_M, respectively. Also included in the figures are fits to the data of the form $\Gamma(q) = A + B\cos(2q + d)$, which is the simplest form consistent with the fact that opposite directions must have the same stiffness. Note that as the temperature increases the average stiffness decreases. This is consistent with the temperature dependence of grain boundary free energy. The important observation is that the stiffness varies substantially with direction in the boundary. This was not expected *a priori*. This fact indicates that the contribution of g'', the second derivative of the boundary free energy with respect to orientation, is substantial since the grain boundary free energy contribution, γ, to the stiffness is independent of direction within the plane. This observation is consistent with the conclusion of Lobkovsky and coworkers [2004] based on the 2-D Ising model of using the full expression for the stiffness. The implications of this strong orientation dependence of the boundary stiffness on mesoscale dynamics of boundary growth are currently unknown. Future work will examine the behavior of the stiffness for other grain misorientations and boundary orientations. These results demonstrate that computational methods developed to gain fundamental insights into solid-liquid interfacial properties also have direct applications to grain boundaries. Hence they highlight the importance of studying both types of interfaces within a broad collaboration, which is made uniquely possible in this CMSN project.

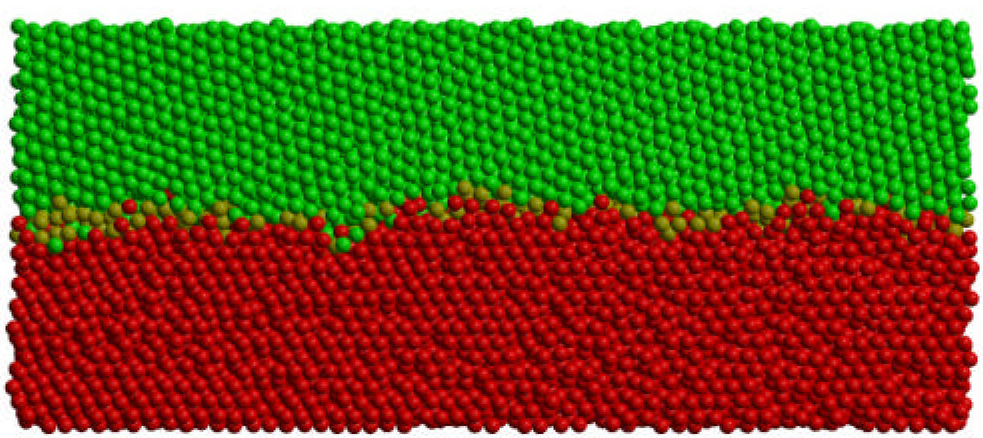

Figure 1. Snapshot of molecular dynamics simulation of an asymmetric S7 <111>-tilt boundary in Ni at 1400 K. The color indicates the crystal orientation assign to each atom with red and green being the two crystals and the orange atoms having an indeterminate assignment.

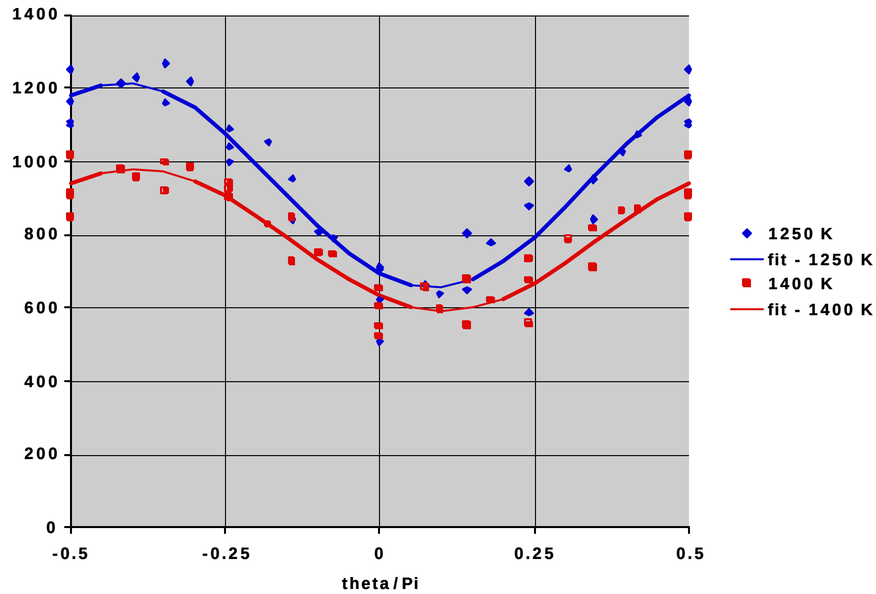

Figure 2. Computed grain boundary stiffness, G, as a function of the direction within the boundary plane at 1250 K (blue) and 1400 K (red). The points represent computed values for individual wave vectors and the solid curves are fits to the data (see text).

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Meetings

Fall Coordination Meetings are presently in the planning stages for all CRTs.

1. The Fundamentals of Dirty Interfaces CRT held its most recent Coordination Meeting at Northeastern University on May 12-13, 2005.
2. The Excited States CRT will likely hold its Fall Coordination Meeting at Vanderbilt University in mid-October 2005, although plans have not yet been confirmed.
3. Workshop on "X-rays and Neutrons: Essential Tools for Nanoscience Research," to be held June 16-18, 2005 in Washington, D.C. See above for more details.

The Summer and Fall/Winter editions of the *CMSN Newsletter* will contain more information on the meetings. In the meantime, please consult the CMSN website for updated information on meetings, job postings, and other information, at http://www.phys.washington.edu/~cmsn/.

CMSN Information

CMSN's teams, oversight, and administration are listed below.

Cooperative Research Teams	Leaders
Magnetic Materials Bridging Basic and Applied Science	Bruce Harmon (Ames) and Malcolm Stocks (ORNL)
Excited State Electronic Structure and Response Functions	John Rehr (Washington) and Steven Louie (UC-Berkeley)
Fundamentals of Dirty Interfaces: From Atoms to Alloy Microstructures	Alain Karma (Northeastern) and Anthony Rollett (Carnegie-Mellon)
Microstructural Effects on the Mechanics of Materials	Dieter Wolf (ANL) and Richard Lesar (Sandia)
Predictive Capability for Strongly Correlated Systems	Richard Scalettar and Warren Pickett (UC-Davis)

CMSN Oversight

CMSN Scientific Advisory Committee	Ellen Stechel (chair) (Ford) Samuel Trickey (Florida) Juan Sanchez (Texas) James Davenport (Brookhaven) George Samara (Sandia) Hamish Fraser (Ohio State) Roberto Car (Princeton)
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