

Chapter 1. Microscopic Mechanisms Underlying Macroscopic Response of ASCI Materials

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1.1 Project Description

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The goal of the MIT-DOE Advanced Strategic Computing Initiative (ASCI) collaboration is to understand how body-centered cubic (bcc) metals behave under extreme conditions, particularly how these materials bend and distort under extreme mechanical stress. The focus of the study is on two bcc metals with very different responses to stress: tantalum (Ta), a very ductile material which tends to "bend" (undergo plastic flow) under stress, and molybdenum (Mo), which is very brittle and tends to fracture instead.

To connect such macroscopic behavior to the quantum mechanical behavior of the trillions of atoms contained in a macroscopic sample, the MIT-ASCI project applies a mechanical analog of Fermi liquid theory. The key idea is that to understand the behavior of a complex system consisting of many particles, one needs to focus only on the behavior of the lowest energy excitations of the system, referred to as the "elementary excitations." In the context of mechanical properties, these elementary excitations are grain boundaries and dislocations. The focus of the project is to study these two classes of defect from both the atomistic and electronic structure perspectives.

1.1.1 Dislocations

The latest results of the project show that proper treatment of mechanical effects radically changes the picture previously developed of how the dislocations behave for even the most basic excitation controlling plastic flow, the (111) screw dislocation. Previous models indicated two possible structures for this defect, the so-called "hard-core" and "easy-core."

Moreover, the ground state, "easy-core" structure was thought to spontaneously break its S_3 symmetry, reducing its symmetry to C_3 . Using first principles electronic structure calculations, however, the MIT group has established that (1) the "hard-core" structure is not even mechanically meta-stable in Mo and that (2) the "easy-core" does not spontaneously break symmetry in either Mo and Ta. These results radically reduce the spectrum of possible excitations which may be involved in the motion of the dislocations; thus these results will have a profound impact on future understanding of the motion of dislocations and thereby, ultimately, the plastic deformation of the material.

The electronic structure results also give estimates for the Peierls barrier for motion of the dislocations, a key quantity for developing quantitative, predictive theories of the plasticity of the material. Intriguingly, the electronic structure results are factors of from two to three lower than previous expectations, thereby suggesting much greater mobility in the dislocations than previously thought.

1.1.2 Grain Boundaries

One goal is to better understand grain boundaries in Mo material and their relation to mechanical failure under the tensile stresses created during the propagation of shock waves (spall). Therefore, the group has also carried out an atomistic, survey study of

nearly the entire phase space of possible ground states for each boundary in the class of boundaries which make up the recrystallization texture of the material. Apart from a wealth of quantitative information on grain boundary ground state energies, these results have led to a new hypothesis for the initiation of spall via micro-void formation near grain boundaries. It appears that many grain boundaries are spontaneous emitters of large numbers of vacancies into the bulk of the material when they are exposed to tensile stresses within a factor of two of where spallation is known to occur experimentally. These results are currently under deeper investigation.

1.2 Connections

In addition to such fundamental investigations, the MIT effort is working very hard to develop connections between the resulting fundamental information and the ultimate macroscopic behavior of the material. With regard to the particularly challenging task of micro-meso connection, we report progress on two fronts:

1.2.1 Atomic Modes of Single Dislocation Mobility

Mechanisms of how dissociated dislocations glide in crystals with high-lattice resistance now can be studied in full atomistic details using appropriate inter-atomic potential models and efficient relaxation and sampling techniques. We have determined low-energy pathways for the generation, annihilation, and motion of the in-core defects in diamond-cubic silicon and characterized the various defect reactions in terms of bond breaking, bond switching, and bond exchange processes. The atomic-level analysis revealed new features pertaining to dislocation mobility, such as left-right asymmetry in the kinetics of kink propagation and a strong binding of the antiphase defect-kink complex. Combining these results with a kinetic Monte Carlo description leads to

a method for predicting dislocation velocity in the range of temperature and applied stress where measurements have been made.¹ Extension of this approach to bcc transition metals Mo and Ta is underway.

1.2.2 Dislocation Junctions and Single-Crystal Plasticity

Plastic deformation is a common phenomenon for which fundamental advances in understanding and analysis would hold great scientific and technological interests. A quantitative description on the basis of inter-atomic interactions has not been feasible for lack of atomic-level knowledge of the underlying processes, for example, how dislocations interact through the formation and destruction of junctions or nodes. In order to achieve detailed understanding of the evolution of dislocation microstructures, one must be able to study the behavior of an assembly of dislocations evolving under stress. Dislocation dynamics therefore controls such fundamental materials behavior as strain hardening and dynamic recovery. From the standpoint of a mechanism-based treatment, the essential process which must be considered is the interaction between two dislocations to form a junction which then acts as an obstacle impeding further mobility. From a large-scale molecular dynamics study of fracture in a mono-atomic FCC lattice, we have been able to observe directly the formation of a junction in the plastic zone near the crack tip and its subsequent destruction. This particular process has provided new mechanistic details to be incorporated into mesoscale simulations. This first demonstration of the micro-to-meso connection points to the feasibility of elucidating the deformation behavior of dislocation assemblies on the experimentally accessible micron scale to the atomic-level processes which can be analyzed using first principles quantum mechanical methods on the angstrom scale.²

1 W. Cai, V. Bulatov, J. Justo, S. Yip, and A. Argon, MRS Fall Meeting, *MRS Symposium Proceedings Series*, vol. 538, 1998, forthcoming.

2 V. Bulatov, F. Abraham, L. Kubin, B. Devincre, and S. Yip, *Nature* 391: 669 (1998).