

First Principles-based atomistic modeling of plasticity in Ta

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Despite decades of experimental and theoretical research on the mechanical properties of materials, many questions remain open, particularly in the relation between atomistic processes and macroscopic behavior. Atomic interactions are described from first principles by Quantum Mechanics (QM). Unfortunately, despite the enormous progress in ab-initio QM methods, such calculations are computationally too demanding to study directly most processes relevant to plasticity and failure. On the other hand, macroscopic plasticity is described by a variety of meso and macroscopic models with parameters usually obtained empirically. These models and their parameters should ultimately be derivable in terms of the fundamental physics of atomic interactions. In order to bridge the gap between atomic interactions and macroscopic behavior we developed first principles-based force fields that allow large-scale atomistic simulations necessary to characterize the fundamental unit mechanisms that govern mechanical properties of materials.

Using an ab initio-based many-body potential for Ta (denoted qEAM) we characterized static and dynamical properties of dislocations ($b=1/2\langle 111 \rangle$ screw, and the $b=1/2\langle 111 \rangle$ edge on (110) planes). Using molecular dynamics we calculate core energies and their pressure dependence, Peierls stress and its orientation, temperature and strain rate dependence as well as kink properties. We propose a novel definition of Peierls stress based on the variation of the local energy of the atoms forming the dislocation core during dislocation migration that allows detailed characterization of the dislocations dynamics.

We also use atomistic modeling to study the relation between Peierls stress and core properties of the $1/2\langle 111 \rangle$ screw dislocation in bcc metals. We find that polarization in the $1/2\langle 111 \rangle$ screw dislocation (the collective translation of the central three atoms in the dislocation core) necessarily changes during migration of the dislocation and that the Peierls stress is a direct function of the core stiffness (the curvature of the core energy-polarization curve).

The materials properties obtained using the First Principles-based qEAM potential have been used with micromechanical modeling [Stainier, Cuitino and Ortiz, *J. Mech. Phys. Solids*, 50, 1511 (2002)] to predict strain-stress curves of single-crystal Ta under uniaxial tension in a wide range of temperatures and strain rates; our first principles results are in good quantitative and qualitative agreement with experiments, capturing: i) the dependence of the yield point on temperature and strain rate, ii) the presence of a marked stage I of easy glide at low temperatures and high strain rates; and iii) the sharp onset of stage II hardening.

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