SAND2012-3643P

Atomistic motion of screw dislocations in tantalum

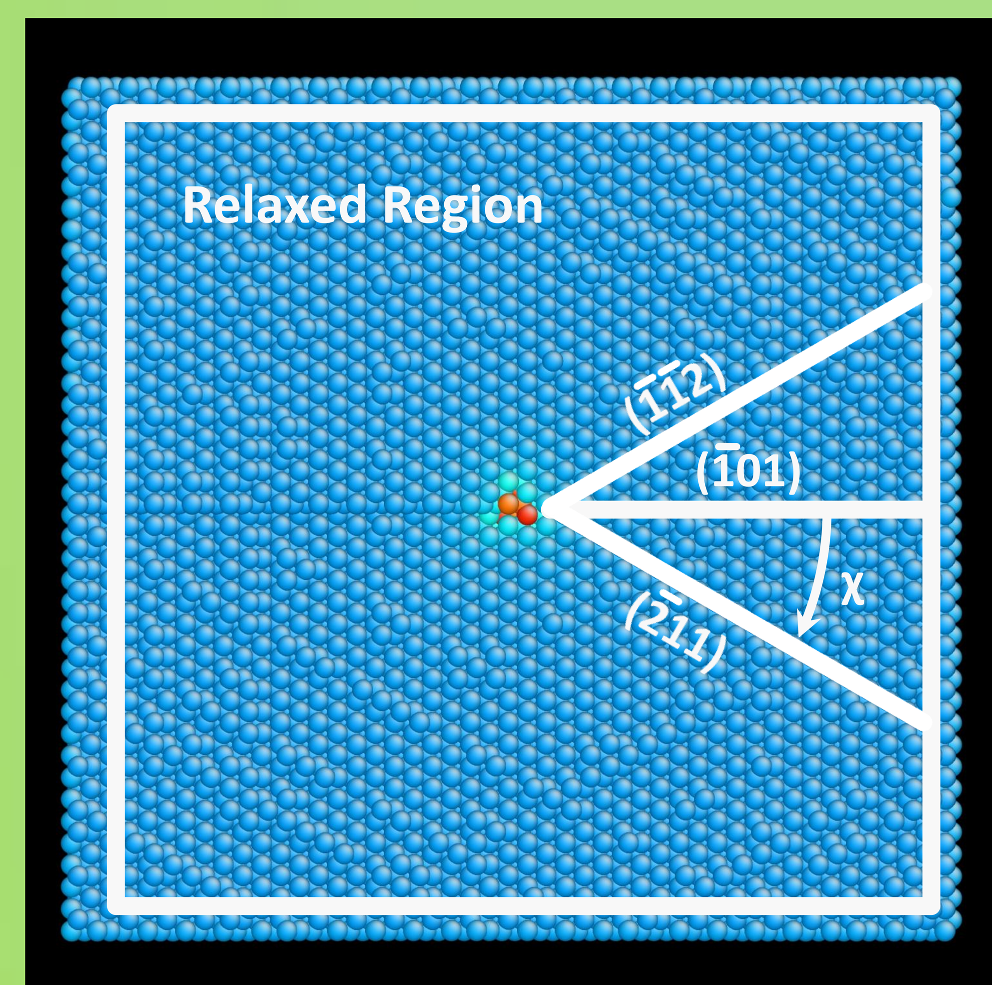
Lucas Hale, Jonathan Zimmerman, and Christopher Weinberger

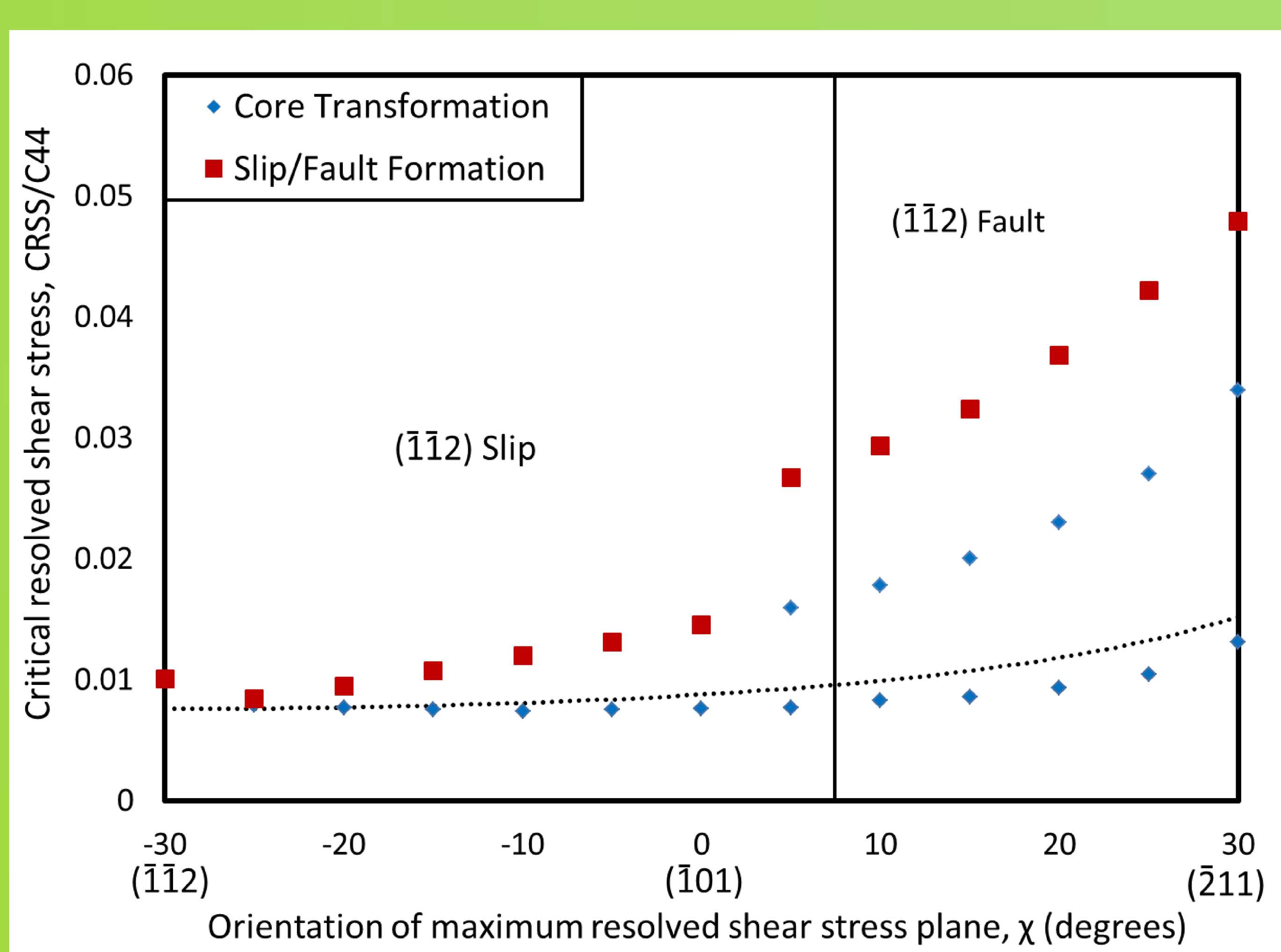
Abstract

Creating an accurate analytical model for plasticity in bcc metals has proven challenging due to the fact that dislocation slip may occur on a variety of different slip planes. Schmid's law is not adhered to as the critical shear stress for slip depends on stresses other than the resolved shear stress on the slip plane. Here, molecular dynamics simulations of dislocations in tantalum reveal that at 0 K, the dislocation core splits prior to, or in conjunction with, apparent slip on {112} planes. The relationship between the core splitting and slip is found to be highly dependent on the applied stress state resulting in discontinuities in the measured critical resolved shear stress.

Simulation Method

A single perfect <111> screw dislocation is placed in the center of a 195 Å X 185 Å X 22 Å system. The system is then incrementally deformed to obtain states of pure shear stress parallel to the dislocation line as predicted by elasticity theory. Between each increment, all but the outer 10 Å are allowed to relax. Results from multiple interatomic potentials reveal similar trends in behaviors. Only results from the ADP[1] potential are presented here.



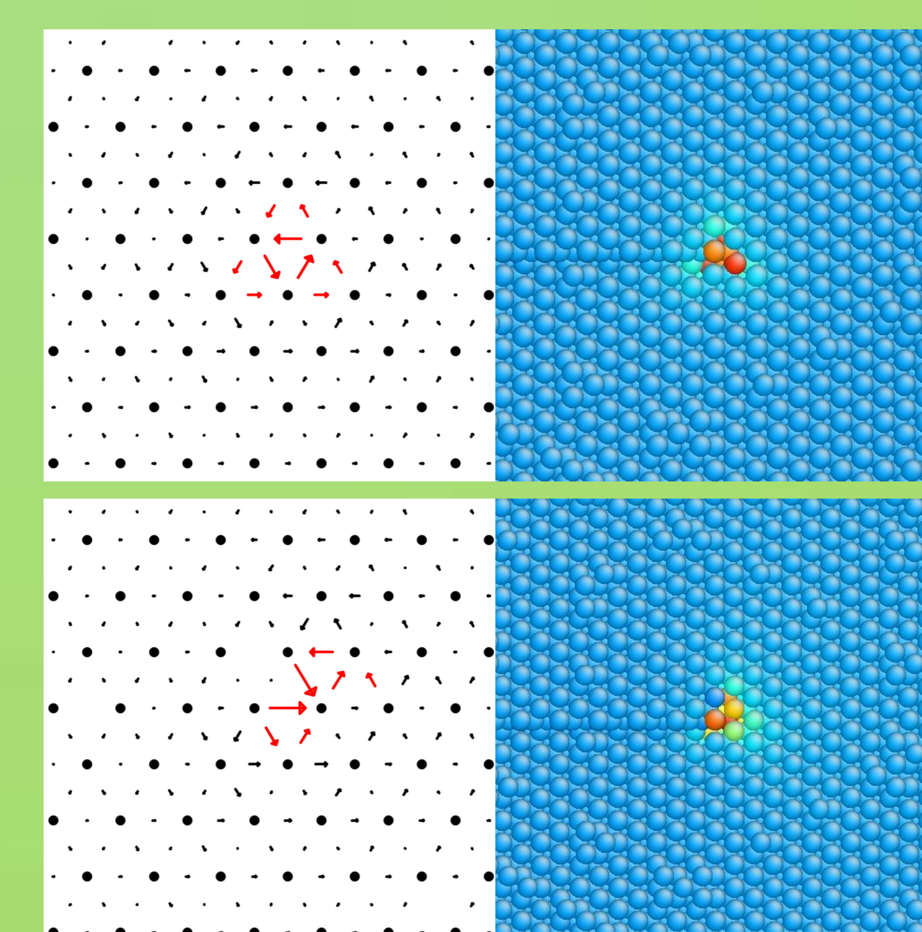


Critical Stresses

The critical stress for stress/fault formation (red squares) depends on the orientation of the plane with the most resolved shear stress. Deviation from Schmid's Law (dashed line) is observed both in trend and in the presence of discontinuities. Plotting all core transformations (blue diamonds) reveals thresholds below the critical activation.

Dislocation Morphologies

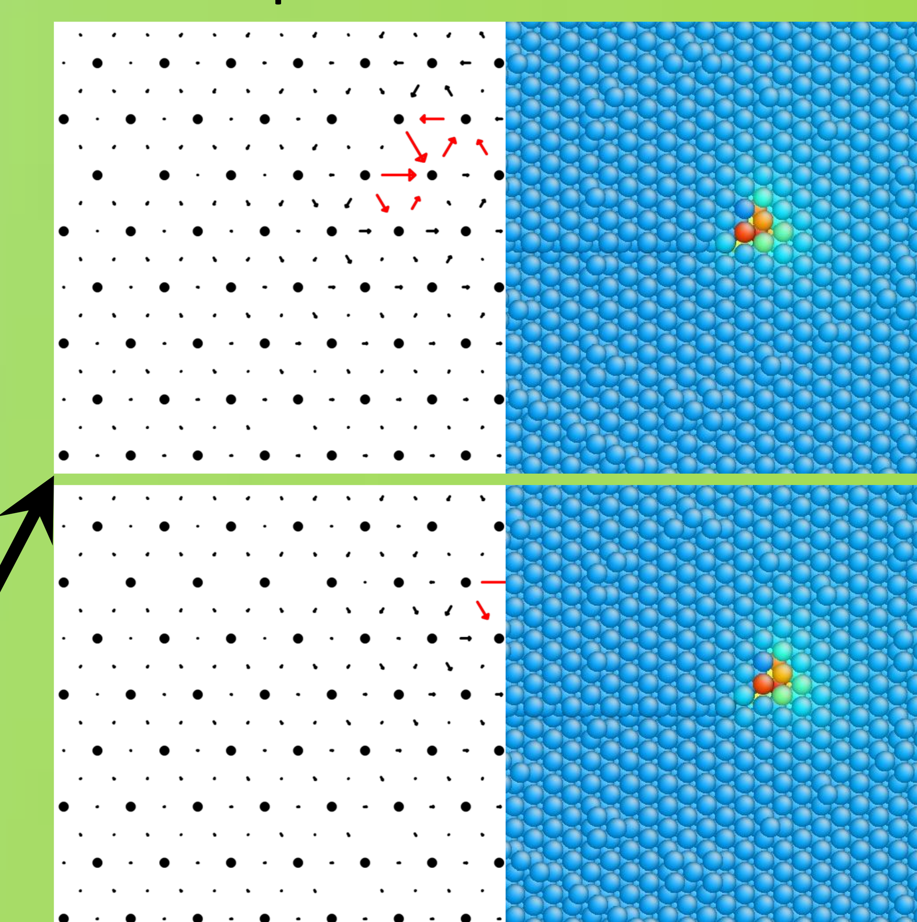
At low stresses, the dislocation core transforms from a compact (big triangle) core structure to a split core structure (two triangles). The core splitting occurs as part of the dislocation moves along a {110} plane.



A possible interpretation of the split core structure is that the dislocation has divided into two partial dislocations that remain close together. This description explains how a fault forms for the large χ angles.

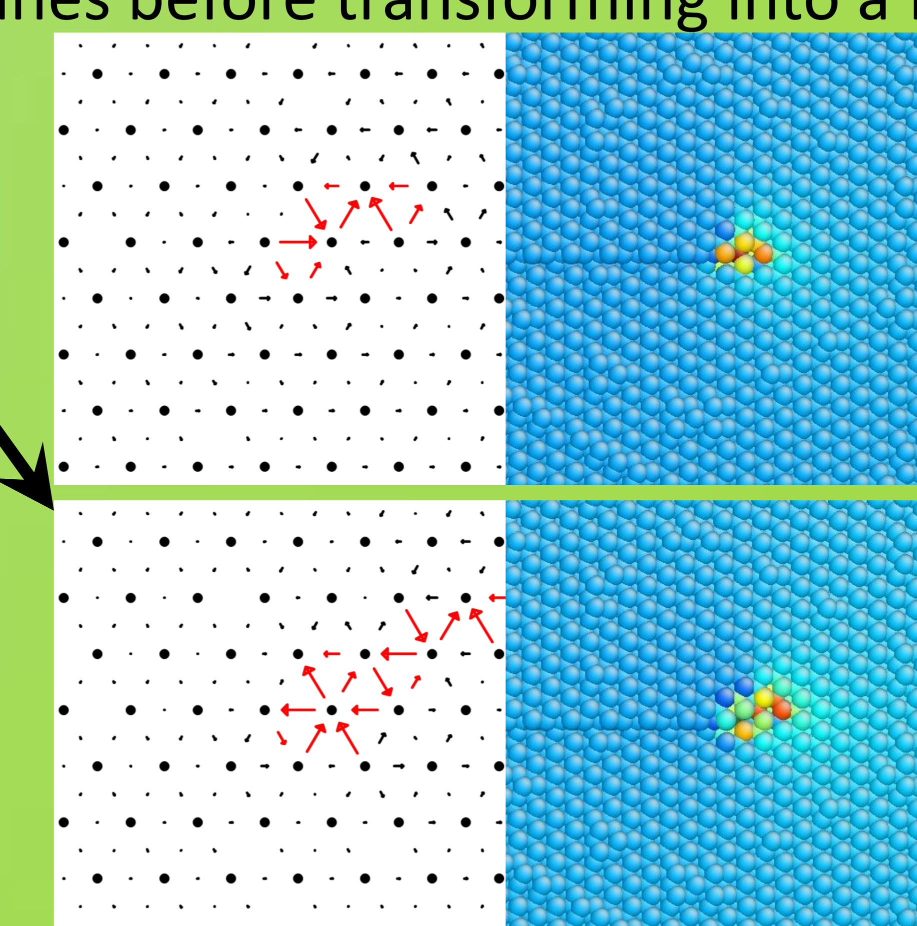
-30° ≤ χ ≤ 5°

The dislocation slips along the (1̄1̄2) plane. The split core remains after slip.



10° ≤ χ ≤ 30°

Splitting continues along alternate {110} planes before transforming into a fault.



[1] Y. Mishin and A. Y. Lozovoi, Acta Materialia **54,** 5013 (2006).

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Future Plans

1. Investigate kink formation in ambient temperature simulations.
2. Develop a yield model dependent on the total stress state acting on a dislocation.