Understanding {112} Slip in Tantalum

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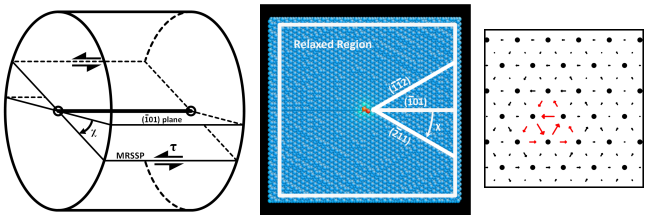
Introduction

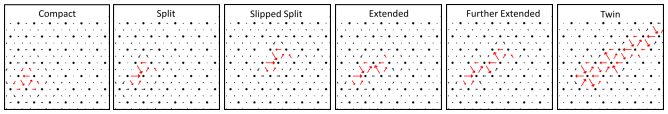
The yield behavior of body-centered cubic (bcc) metals at low temperatures is thought to be largely dependent on the motion of a/2<111> type screw dislocations. Unlike dislocations in face-centered cubic (fcc) metals, screw dislocations in bcc metals experience a large lattice resistance which results in a strong temperature and moderate strain rate dependence of plastic flow. Additionally, screw dislocations have been reported to move on multiple glide planes resulting in a complex slip behavior. Understanding yield in bcc metals is therefore dependent on characterizing the slip nature of the screw dislocations. The focus of this work is to investigate the atomic description of {112} slip in Tantalum resulting from compact core screw dislocations.

Critical Resolved Shear Stress for Ta Potentials

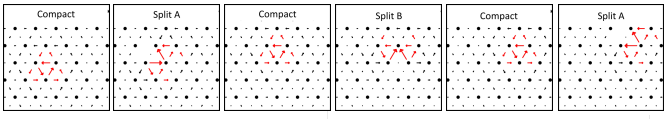
Molecular statics simulations are used to determine the critical shear stress (CRSS) required to initiate slip for an isolated screw dislocation. The CRSS is a function of χ, the angle the maximum resolved shear stress plane makes with the (-101) plane. These simulations use a thin block of atoms (24a[-12-1] x 40a[-101] x 4a[111]) containing 46,080 atoms.

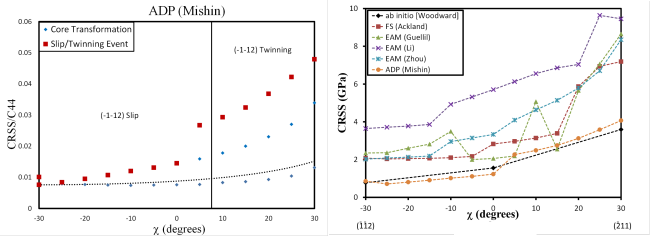


Differential displacement maps show the non-planar, compact structure of the screw dislocation in its initial state, followed by various observed structures that reflect the CRSS's dependency on χ.



Simulations reveal that the dislocation core first transforms from the compact structure to a planar, split structure. At the CRSS, the core either slips along complementary {110} planes to display an effective {112} slip (at low χ), or forms an extended core structure that later nucleates a twin (at high χ). Similar behavior was observed for three embedded atom method (EAM) potentials, the Finnis-Sinclair potential by Ackland and Thetford, and the Angular Dependent Potential (ADP) by Mishin and Lozovoi. ADP offers the best agreement with *ab inito* calculations by Woodward and Rao.





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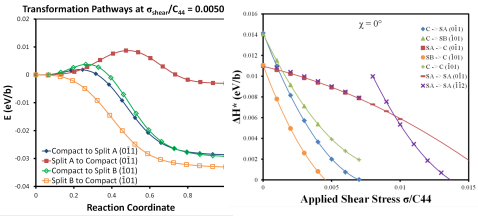
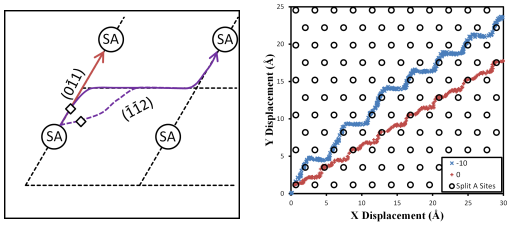
Nudged Elastic Band Estimates of Activation Enthalpy

The nudged elastic band (NEB) method is used to determine the activation enthalpy needed for dislocation core transformations and to refine the value of stress when that enthalpy is zero, i.e. the CRSS. Calculations done over a range of values of stress and χ reveal that for most orientations, the enthalpy needed for a core transformation to a split-A structure, located along a (0-11) path, is lower than that to a split-B structure, along a (-101) path. This behavior results in an effective (-1-12) slip path, even when the resolved shear is greater for slip along a pure (-101) path, such as for the case shown.

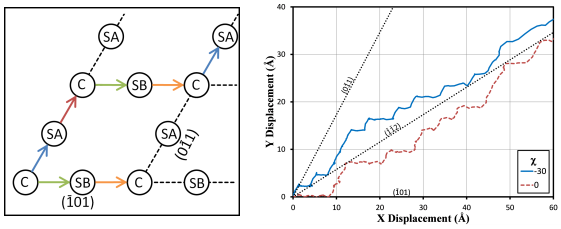


Effects of Kinking and Temperature

Molecular Dynamics simulations were done with thicker systems at both low and high temperatures to assess the role of kinks with dislocation motion. At low temperature, slip and twin transitions occur at high stress (consistent with CRSS calculations). For slip, either {112} type kinks form exclusively (for χ near 0), or in conjunction with {110} type kinks (for $\chi \leq$ -10°).



At higher temperatures, slip occurs at low stress through the thermal activation of partial kinks that form on two different {110} planes and transform the core between compact and split core structures. Cumulative {112} slip results because the compact to split transitions associated with the two {110} planes have comparable activation enthalpies.



Conclusions and Next Steps

Our simulation study of slip activation of a single screw dislocation in bcc Ta shows that both the type of critical event (core transformation, slip or twin formation) and the critical stress needed depends on orientation of the applied shear stress. All potentials studied predict that slip will occur along effective {112} planes, usually (but not exclusively) the result of composite segments of {110} planar slip. The nature of slip also depends on whether the slip is mechanically or thermally activated. Our results are consistent with previous simulations work, but some uncertainty exists with comparisons to experimental observations and *ab inito* calculations. We believe this is due to the metastable split core structure characteristic of Ta empirical potentials, and thus are conducting simulations of iron for which the split core is not metastable to verify this hypothesis.

Acknowledgements

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