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Atomistic Modeling of Dislocation Slip in Alpha-Iron towards the Development of a Multi-Scale Model of Dislocation Plasticity

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Developing micro- and macro-scale models for yield in body-centered cubic (bcc) metals that capture the underlying physics is important to accurately predict performance and guide design for structural applications of these materials. This has proven challenging due to the complexity associated with the mechanisms for plastic flow in bcc metals. Among these is the observation of non-Schmid slip of dislocations, i.e. that components of the stress state other than those that contribute to the resolved shear stress affect the slip process. In addition, plasticity is known to be thermally activated, and the rate of plastic deformation can be directly connected to the activation enthalpy for dislocation motion. How this enthalpy functionally depends on both the applied stress state and the material resistance to slip is neither trivial nor obvious for materials that violate Schmid's Law.

In our efforts to develop a physically accurate yield model for bcc iron, we perform atomistic calculations to quantify the non-Schmid, stress dependent effects of slip. An atomistic potential for bcc iron is identified that captures the stable compact core dislocation core structure and single peak Peierls barrier (i.e. no metastable split core) consistent with what is predicted from *ab initio* calculations. Using this potential, we evaluate the zero temperature critical resolved shear stress (CRSS) necessary for slip to occur for a variety of different stress states. The CRSS obtained from atomistic simulations is then used to fit a generalized non-Schmid yield law that captures the dependence of the yield stress on shear stresses both parallel and perpendicular to the shear direction, as well as changes in pressure. Of particular significance, we show that atomistic results provide insight on the activation enthalpy for non-Schmid slip, and suggest a functional dependency between enthalpy, the applied stress state, and the CRSS that appears valid across a range of stress states and loading orientations.

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