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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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Motivation

Developing micro- and macro-scale models for yield in body-centered cubic (bcc) metals that capture the underlying physics is challenging due to the complexity of plastic flow mechanisms 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. To develop a physically accurate yield model for bcc iron, we perform atomistic calculations of screw dislocation glide to provide quantitative insight on how the activation enthalpy for slip depends on both the applied stress state and the critical resolved shear stress (CRSS), which itself is stress-dependent.

Theory

Thermal and stress-activated rate of slip — $\dot{\gamma} = \dot{\gamma}_0 \exp\left(\frac{-\Delta H}{k_B T}\right)$

Kocks model of activation enthalpy — $\Delta H = \Delta H_0 \left(1 - \Theta^p\right)^q$

Criterion for onset of dislocation slip — $\tau_{cr} \leq \mathbf{P}_S : \boldsymbol{\sigma} + \mathbf{P}_{nS} : \boldsymbol{\sigma}$

Schmid and non-Schmid stress projection tensors —

$$\mathbf{P}_S = \frac{1}{2}\left(\mathbf{m} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{m}\right) \qquad \mathbf{P}_{nS}^{\mathrm{uv}} = \mathbf{u} \otimes \mathbf{v}$$

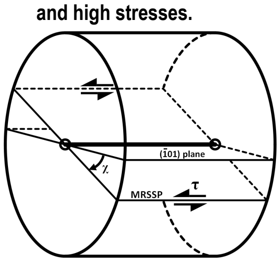
$$\mathbf{P}_{nS} = c_1 \mathbf{P}_{nS}^{\mathrm{tm}} + c_2 \mathbf{P}_{nS}^{\mathrm{tn}} + c_3 \mathbf{P}_{nS}^{\mathrm{nn}} + c_4 \mathbf{P}_{nS}^{\mathrm{tt}} + c_5 \mathbf{P}_{nS}^{\mathrm{mm}}$$

Ratio of resolved shear stress to athermal slip resistance —

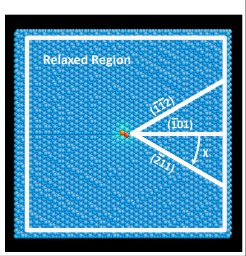
$$\Theta = \frac{\tau^{MRSSP}}{CRSS\left(\boldsymbol{\sigma}\right)} = \frac{\mathbf{P}_S : \boldsymbol{\sigma} + c_1 \mathbf{P}_{nS}^{\mathrm{tm}}}{\tau_{cr} - c_2 \mathbf{P}_{nS}^{\mathrm{tn}} - c_3 \mathbf{P}_{nS}^{\mathrm{nn}} - c_4 \mathbf{P}_{nS}^{\mathrm{tt}} - c_5 \mathbf{P}_{nS}^{\mathrm{mm}}}$$

Simulation Setup and Methodology

- Molecular statics used to estimate the critical shear stress (CRSS) required to initiate slip for an isolated a/2[111] screw dislocation.
- The CRSS is a function of χ, the angle the maximum resolved shear stress plane (MRSSP) makes with the (-101) plane.
- System dimensions 24a[-12-1] x 40a[-101] x n*a[111], where n = 4 (46,080 atoms) or n = 48 (552,960 atoms) and a = 2.865 Å.
- Fixed(periodic) BCs used for planar(out-of-plane) boundaries.
- EAM potential by Chamati *et al.* predicts correct equilibrium dislocation core structure, correct shape of Peierls potential, and {110} slip at both low and high stresses.

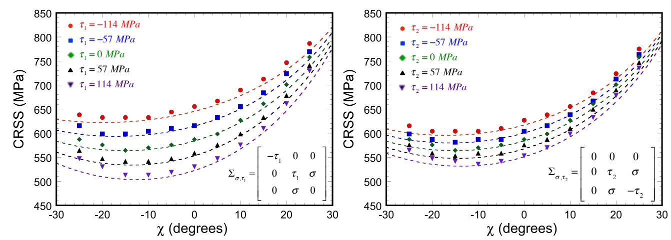


Schematics showing the orientation of the applied stress, the slip plane and the MRSSP. [adapted from Fellinger, PRB 2010].

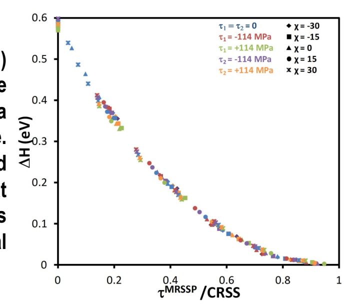


Calculation of Critical Resolved Shear Stress

- Stress is applied through displacement control: fixed boundary atoms are moved according to anisotropic elasticity for a particular stress state.
- Combinations of hydrostatic and shear stress are used to characterize the dependency of CRSS on stress.



- Calculated CRSS values are used to fit the non-Schmid constants: c_1 = 0.27, c_2 = 0.15, c_3 = 0.31, c_4 = -0.23, c_5 = 0.02 and τ_{cr} = 584 MPa.
- Nudged elastic band (NEB) calculations are used to calculate the activation enthalpy as a function of the entire stress state. These calculations consider end states with dislocation cores at neighboring stable positions subject to the same subcritical strain state.



- Examination of NEB results for several definitions of Θ shows that the ratio of τ^{MRSSP} to CRSS(σ) exhibits close to universal behavior of the Kocks model with regard to arbitrary stress state, using p = 0.9, q = 2.0 and ΔH_0 = 0.6 eV

Conclusions

- Our expression for Θ is consistent with classical theory with τ^{MRSSP} equivalent to the driving force given by the Peach-Koehler equation.
- This driving force on a screw dislocation is independent of the slip plane, and crystallographic information manifests only in the lattice resistance.
- This insight helps explain bcc slip at low temperatures having clearly defined slip systems, while at high temperatures slip closely follows the applied shear, e.g. pencil glide.

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