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THREE-DIMENSIONAL PHASE FIELD MODELING OF DISLOCATION DISSOCIATION, GLIDE AND TWINNING IN FCC MATERIALS

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The motion and evolution of a dislocation network is one of the main mechanisms for inelastic deformation in a variety range of metals. The energetically favored state of a dislocation line or loop in close-packed metals is its dissociated state, consisting of leading and trailing partial dislocations bounding a stacking fault. A dynamic phase-field model for {111} dislocation glide in fcc single crystals is formulated in the current work based on the Khachaturyan-Shalatov approach (e.g., [1,2]) for the elastic behavior of periodic defective systems. In this approach, (Frank) dislocations lines are represented via their (residual) strain fields which depend on corresponding scalar-valued phase fields $\boldsymbol{\phi} = (\phi_1, \ldots)$. These mediate the transition of dislocations between thermodynamic states of "unslipped" and "slipped". As usual in the phase field approach, a model $\psi = \psi_{\rm E}(\boldsymbol{E}, \boldsymbol{\phi}) + \psi_{\rm C}(\boldsymbol{\phi}) + \psi_{\rm G}(\nabla\boldsymbol{\phi})$ for the free energy density ψ of the material is central. For the current class of materials, this consists of (lattice) elastic $\psi_{\rm E}$, "crystal" $\psi_{\rm C}$ and "gradient" $\psi_{\rm G}$ parts, where $\boldsymbol{E}$ is the strain. In turn, ψ determines the stress $\boldsymbol{T} = \partial_{\boldsymbol{E}}\psi$ and so mechanical equilibrium $\operatorname{div}\boldsymbol{T} = \boldsymbol{0}$ as well as the Ginzburg-Landau relaxational dynamics $\dot{\phi}_a = m_a\,(\operatorname{div}\partial_{\nabla\phi_a}\psi - \partial_{\phi_a}\psi)$ of each phase field $\phi_a \in \boldsymbol{\phi}$ in terms of the corresponding mobility m_a. In particular, for the case of dislocation lines, $\psi_{\rm C}$ depends on the energy needed to create stacking faults or stacking fault energy (SFE) which can be calibrated or identified with the help of ab initio results from density-functional theory (DFT: e.g., [3,4]). In addition, $\psi_{\rm G}$ represents the energy of this dislocation core.

Given such a model, processes such as dislocation dissociation and stacking-fault formation, as well as dislocation-based glide or twinning deformation, can be simulated in specific materials, depending in particular on the details and "level" of the corresponding SFE. The current work focuses on a comparison of the (relatively) "low" SFE material Cu with a (relatively) "high" SFE material Al. Consider for example the case of dissociation of a single dislocation loop under no external loading and corresponding stacking-fault

formation as shown in Figure 1. Because the energy cost of forming a SF in Cu is relatively

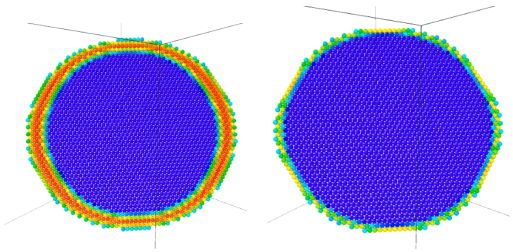

Figure 1: Dislocation loop dissociation in Cu (left) and Al (right). Points shown are those of the spatial computational grid and the colors indicate the corresponding solution field values. Blue: ideally slipped crystal. Red: partially slipped crystal (SF). Green: dislocation line.

low, an initially ideal dislocation loop in Cu dissociates (Figure 1, left) into leading (outer green ring) and trailing (inner green ring) partial dislocations bounding a relatively wide SF (red band $\approx 4a_0$ wide, a_0 equilibrium lattice spacing). On the other hand, because the energy cost of forming a SF in Al is larger, the corresponding SF is thinner ($\approx 1a_0$, not resolved on the scale of Figure 1, right). Another application of the current model is the simulation of dislocation-based glide and twinning in dislocation networks under external loading; an example of this for Cu and Al is shown in Figure 2. As shown, in case of Cu,

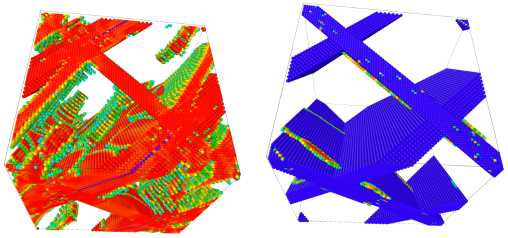

Figure 2: Loading of dislocation network in Cu (left) and Al (right). Color coding is same as Figure 1.

loading results in the formation of multiple SF layers and twinning. On the other hand, in Al, the deformation is completely governed by ideal dislocation glide.

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