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Atomistic simulations of surface cross-slip nucleation in face-centered cubic nickel and copper

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Abstract

In this manuscript, embedded atom potentials are used to determine the various core structures of glide screw-character dislocations intersecting free surfaces at right and inclined angles in face-centered cubic Ni and Cu. It is shown that the negative constriction forms at free surfaces under certain conditions. The role of various factors affecting the formation of negative constriction at the free surface, negative constriction energy, ledge annihilation and screw dislocation rotation due to Lothe's forces are discussed. The activation energy for surface cross-slip nucleation when the screw dislocation intersects the free surfaces at right angles, in the absence of ledge annihilation forces, is shown to be 0.05 eV in Ni and 0.09 eV in Cu. The activation-energy values obtained via the nudged elastic band method are significantly lower than the activation energy for cross-slip at attractive forest dislocation intersections in these materials. The present results are expected to be useful in understanding the mechanical behavior of micron-sized pillars under pure tension and compression.

Keywords: Surface cross-slip; Atomistic simulations; Embedded atom potentials; Nickel; Copper

1. Introduction

There is increasing recognition of the need to incorporate physics-based models of deformation in the design of structural components. While models for predicting yield strength and creep behavior are beginning to incorporate significant physics, models for fatigue, ultimate strength and ductility remain mostly empirical. This is because strain-hardening and fatigue resistance are strongly influenced by dislocation micromechanisms, especially cross-slip, and including physics-based cross-slip processes in mesoscale simulations has been difficult. The early work of Escaig remains the most widely cited and used model for cross-slip wherein the screw dislocation locally constricts and immediately redissociates on the cross-slip plane [1]; however, this model poses several difficulties with respect to quantitative simulations. The model is highly sensitive to choice of parameters that have thus far been difficult to quantify. For example, the constriction width required for cross-slip is unknown but significantly influences the energetics of the cross-slip process [2]. This difficulty has led to an ad hoc postulate that obstacles always exist in materials and that they enable sufficient dislocation core constriction under normal stresses, thereby ensuring cross-slip [3]. Aside from being unsatisfactory, this forces cross-slip models (particularly for single crystals) to make arbitrary assumptions about dislocation obstacle spacings. Advances in atomistic simulations offer the possibility of gaining insights into the cross-slip process that may serve to enable mesoscale simulations to accurately capture the atomic-level physics of a dislocation process.

Atomistic simulation studies from the late 1990s were limited to calculating constriction energies and energetics of cross-slip using a single dislocation in a periodic unit cell [2,4]. These simulations helped to unravel some interesting and useful aspects of cross-slip which were unanticipated.

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The most important finding was that configurations exist for which one of the pair of constrictions has a negative energy [2,4]. Thus spontaneous nucleation of cross-slip is possible so long as only one constriction is needed, as is the case for surface nucleation. However, previous atomistic simulations [4] of a screw-character dislocation intersecting free surfaces at right angles in face-centered cubic (fcc) Cu have shown that the screw dislocation prefers to reside on a {1 1 1}-type plane parallel to the surface ledge on which it was created, without easy cross-slip nucleation. This is in contrast to recent atomistic simulation results of screw-character dislocations intersecting mildly attractive and repulsive forest dislocations in the bulk in fcc Ni, where cross-slip has been shown to occur easily [5–8]. In this work, the possibility of cross-slip at dislocation–surface intersections in fcc Ni and Cu was examined using large-scale atomistic simulations. A glide screw dislocation that intersects two free surfaces perpendicularly as well as in an inclined fashion is modeled and it is shown that several conditions exist where surface cross-slip can nucleate easily. This, we believe, has the potential to explain dislocation multiplication in low-density micron-sized fcc pillars subjected to a uniform tensile or compressive loading.

We have performed molecular statics simulations of screw dislocation intersections with free surfaces for the [1 1 1] and [1 0 0] orientations, with the screw dislocation having a Burgers vector of 1/2 [1 $\bar{1}$ 0]. Section 2 describes the simulation technique and the interatomic potentials used for the simulations, Section 3 presents the core structures obtained from atomistic simulations. Section 4 describes activation energy calculations for surface cross-slip when the screw dislocation intersects the free surfaces at right angles, in the absence of ledge annihilation forces. Finally, Sections 5 and 6 give a discussion and summary of the results, respectively.

2. Simulation technique

The atomistic simulations described here employed the three-dimensional (3-D) parallel molecular dynamics code, LAMMPS [9], developed at Sandia National Laboratory. The simulation cell is a rectangular parallelepiped, with the z-axis oriented along the [1 1 1] or [1 0 0] directions. For the z-axis oriented along [1 1 1], the dimensions of the simulation cell along the z-axis was ~15 nm, the dimension along the x-axis was ~30.0 nm and along the y-axis ~15 nm. For the z-axis oriented along [1 0 0], the dimensions of the simulation cell along the z-axis was ~40 nm, the dimension along the x-axis was ~14 nm and along the y axis ~14 nm. This corresponds to approximately 1 million atoms in the simulation cell. A 1/2 [1 $\bar{1}$ 0] screw dislocation is inserted in the middle of the simulation cell using its anisotropic elastic displacement field [10]. Unless otherwise specified, the plane of the cut performed to generate the screw dislocation was the (1 1 1) glide plane. In the activation energy calculations, the cube plane cut was used. The origin for the initial anisotropic displacement field of the screw dislocation was varied to obtain several different core structures for the screw dislocation interaction with the free surfaces. Fixed boundary conditions were applied along the z and y directions and energy minimization was performed using the conjugate gradient technique. Free surface boundary conditions were applied along the x direction.

2.1. Interatomic potential

The embedded atom potential used in the simulations is the potential developed for fcc Ni by Angelo, Moody and Baskes [11] (hereafter termed the Moody potential) based on the Voter and Chen format as well as the embedded atom potential developed for fcc Ni by Mishin [12]. For fcc Cu, an embedded atom potential developed by Mishin et al. is used [13]. Table 1 gives the lattice parameter, cohesive energy, elastic constants and stacking fault energy given by the Mishin and Moody potentials for fcc Ni as well as the Mishin potential for fcc Cu.

2.2. Depiction of core structures

In some figures, to depict core structures we use the method developed by Stukowski and Albe [14] which extracts dislocation lines and their associated Burgers vectors from 3-D atomistic simulations. It is based on a fully automated Burgers circuit analysis, which locates dislocation cores and determines their Burgers vector. The transition from the atomistic system to a discrete dislocation representation is achieved through a subsequent vectorization step.

In order to illustrate the relaxed screw dislocation geometries, in some figures, we take advantage of the increase in atomic energy produced by the strain field of the partial dislocations. By plotting the atoms with assigned energies within LAMMPs of greater than −4.42 eV (Ni) or 3.52 eV (Cu) (the energy of atoms in the stacking fault region), the partial dislocations can be imaged easily even in these large simulation cells [5–7]. In order to illustrate the cross-slipped-segment products of the screw dislocation, the positions are shown in a [1 1 $\bar{2}$] projection as well as the [1 1 1] projection. In the [1 1 $\bar{2}$] projection segments spread on the initial (1 1 1) plane appear as a single line and cross-slipped segments (i.e. on a (1 1 $\bar{1}$) plane) appear

Table 1
Lattice parameter, a_0, cohesive energy, E_c, elastic constants, C_{11}, C_{12} and C_{44}, and stacking fault energy, γ, given by the Moody embedded atom potential for Ni, and the Mishin embedded atom potentials for Ni and Cu.

Property	Ni (Mishin)	Ni (Moody)	Cu (Mishin)
a_0 (A)	3.52	3.52	3.615
E_c (eV)	−4.45	−4.45	−3.54
C_{11} ($\times 10^{11}$ N m^{-2})	2.41	2.46	1.70
C_{12} ($\times 10^{11}$ N m^{-2})	1.51	1.47	1.23
C_{44} ($\times 10^{11}$ N m^{-2})	1.27	1.25	0.76
γ (mJ m^{-2})	134	89	44