Acta Materialia 101 (2015) 10–15

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Screw dislocation cross slip at cross-slip plane jogs and screw dipole annihilation in FCC Cu and Ni investigated via atomistic simulations

S.I. Rao [b,e,*], D.M. Dimiduk [c], J.A. El-Awady [d], T.A. Parthasarathy [b], M.D. Uchic [a], C. Woodward [a]

[a] Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/RXCM, Wright-Patterson AFB, OH 45433-7817, United States
[b] UES, Inc., 4401 Dayton-Xenia Rd, Dayton, OH 45432-1894, United States
[c] BlueQuartz Software, LLC, 400 S. Pioneer Blvd, Springboro, OH 45066, United States
[d] Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD, United States
[e] Institute of Mechanical Engineering, EPFL, Lausanne 1015, Switzerland

ARTICLE INFO

Article history:
Received 12 August 2015
Revised 13 August 2015
Accepted 29 August 2015

Keywords:
Cross-slip
Jogs
Screw dipole annihilation
Atomistic simulations
Nickel
Copper

ABSTRACT

Using atomistic simulations, the effect of jogs on the cross-slip of screw character dislocations and screw-dipole annihilation was examined for both FCC Cu and Ni. The stress-free activation energy for cross-slip at jogs is close to 0.4 eV in Cu, determined using a nudged elastic band method. This value is a factor of 4-to-5 lower than the activation energy for cross-slip of screw dislocations in the absence of a jog. Similar results were obtained for Ni. Molecular dynamics simulations were used to study the annihilation of a jog-containing screw dipole. The critical Escaig stress on the glide plane for dipole annihilation drops quickly from the 0 K value of ~400 MPa and, dipole annihilation is nearly athermal at room temperature. At 5 K, Escaig stresses on the cross-slip plane are a factor of 1.5 less effective than Escaig stresses on the glide plane and, glide stresses on the cross-slip plane are a factor of 3 less effective for dipole annihilation by cross-slip. The activation volume for cross-slip of screw dislocations at jogs with respect to these three stress components range from 6 to 20b^3. These results have been found to be useful in physics-based modeling of bulk cross-slip in higher length scale 3D dislocation dynamics simulations investigating dislocation pattern formation and fatigue structures in FCC crystals.

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1. Introduction

Cross-slip of screw character dislocations is an elementary thermally-activated mechanism that is all prevalent in plastic deformation. The consequences of cross slip are recognized as the most important single process underlying complex spatiotemporal development of dislocation microstructure leading to hardening, pattern formation and dynamic recovery [1,2]. The early work of Escaig remains the most widely cited and used model for cross-slip [3–7]; however, this model poses several difficulties with respect to quantitative simulations [8–12]. Previously, atomistic simulations (molecular statics) were used with embedded atom potentials to evaluate the activation barrier for a screw dislocation to transform from fully residing on the glide plane to fully residing on the cross-slip plane, where the screw dislocation was intersecting a mildly-attractive 120° forest dislocation forming Glide locks (GL), Lomer–Cottrell (LC) locks, or Hirth locks, in both Ni and Cu [8,9]. The cross-slip process was also explored at mildly-repulsive screw dislocation intersections [12]. In these simulations, the Burgers vector of the intersecting dislocation forming mildly attractive GL or LC locks was reversed. The activation energies at attractive intersections were computed using two different techniques: (a) determine the equilibrium configurations (energies) when varying pure tensile or compressive stresses that are applied along the [111] direction on the partially cross-slipped state, and (b) the classical nudged elastic band method. The cross-slip activation energies at the attractive intersections were found to be a factor of 3–20 lower than the energy for cross-slip at an isolated screw dislocation. At mildly repulsive intersections, cross-slip nucleation was found to be spontaneous and athermal, with zero cross-slip activation energy [12]. These findings provide a better physical basis to represent local cross-slip processes in larger-scale, discrete dislocation-dynamics simulations, enabling more realistic simulations of the evolution of the dislocation substructure. Such simulations should result in improved statistical representation of cross-slip effects during monotonic or cyclic deformation.

In addition, previously Vegge et al. considered cross-slip nucleation and screw dipole annihilation at two types of atomic jogs in FCC Cu [13,14]. They evaluated the activation energy for cross-slip

* Corresponding author at: Institute of Mechanical Engineering, EPFL, Lausanne 1015, Switzerland.
E-mail addresses: car894@aol.com, raosatish806@gmail.com (S.I. Rao).

http://dx.doi.org/10.1016/j.actamat.2015.08.070
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at atomic jogs using a nudged elastic band method, and found that the activation energy for cross-slip decreases by a factor of 3 as compared to cross-slip of screw dislocations in isolation. The results were identical for both types of jogs. They also evaluated the critical dipole annihilation distance of jogged-screw dislocations and found it to be 4 nm at 0 K. However, these calculations were performed using an interatomic potential that does not give the correct elastic constants and stacking fault energy of Cu (shear modulus 20% higher and stacking fault energy 30% lower than experimental values). Also, the temperature and stress dependence of cross-slip nucleation and dipole annihilation at jogged-screw dislocations was not considered.

In this study, cross-slip nucleation is examined at atomic jogs on screw dislocations using Mishin's interatomic potentials for Ni and Cu, which give elastic constants and stacking fault energies close to experimental values. The line direction of the jog resides on the cross-slip plane. It is argued that all types of atomic jogs on screw dislocation can be decomposed into a jog on a cross-slip plane plus a kink on the glide plane. Therefore, we have only considered one type of atomic jog on a cross-slip plane for calculating the cross-slip activation energy, as well as for the screw-dipole annihilation simulations. The annihilation of jogged-screw dipoles having initial separations of 14 and 44 nm were also simulated. The critical Escaig stresses for cross-slip nucleation and screw-dipole annihilation, as a function of temperature, were determined using molecular dynamics simulations. The remainder of this paper is organized as follows. Section 2 describes the simulation technique, the interatomic potentials used in the simulations, and briefly describes the method used to both analyze and visualize the core structures. Section 3 contains the results of the simulations, Section 4 presents a brief discussion of the results, and Section 5 gives a summary of the results.

2. Simulation technique

The atomistic simulations described here employed the 3-dimensional (3D) parallel molecular dynamics code, LAMMPS [15], developed at Sandia National Laboratory. The dimensions of the simulation cell were 200.0 × 20.0 × 100.0 nm along the *x*-, *y*-, and *z*-axes, respectively. The *x*-axis was aligned parallel to the [785, −783,2] crystallographic direction, which corresponded to the line direction of a screw direction [1–10] offset by a ½[0 1 1] vector resolved on the (1 1 −1) cross-slip plane. The *z*-axis was aligned parallel to the (1 1 −1) cross-slip plane normal, and the *y*-axis was aligned along the [−781, −787, −1568] direction. In total, the simulation cell had approximately 34 million atoms. Periodic boundary conditions were applied along the *x* direction.

A single screw dislocation having a Burgers vector ½[1 −1 0] was inserted into the simulation cell to examine the effect of jogs on the energetics of cross-slip. The elastic center of the initial anisotropic displacement field was selected such that the screw dislocation, upon molecular statics relaxation using fixed boundary conditions along the *y* and *z* directions, dissociates into Shockley partials on the (1 1 1) glide plane. Since the periodic direction is offset by a jog vector on the (1 1 −1) cross-slip plane, with respect to the screw direction, a jog on the cross-slip plane naturally forms upon such relaxation.

Selected loading configurations were used to calculate the energetics associated with cross-slip at the atomic jog. Uniaxial stress along the cross-slip plane normal, [1 1 −1] direction, was applied to generate Escaig stress on the (1 1 1) glide plane. The Escaig stresses act to expand or constrict the Shockley partials, depending on the sense of the stress, independent of the glide or cross-slip plane stresses. Note that uniaxial stress along this particular crystallographic direction results in no Escaig stress component on the (1 1 −1) cross-slip plane as well as no glide stresses on both the glide and cross-slip planes. Similarly, uniaxial stress along the glide plane normal, [1 1 1] was applied to generate Escaig stress on the (1 1 −1) cross-slip plane without any Escaig stress on the (1 1 1) glide plane, as well as no glide stress on both the glide and cross-slip planes. Equal uniaxial stresses along the [1 0 −1] and [0 −1 1] directions were used to generate pure glide stresses on the (1 1 −1) cross-slip plane without any glide stresses on the (1 1 1) glide plane, as well as no Escaig stress on either glide or cross-slip planes. Such uniaxial stresses were applied using appropriate uniform straining of the dislocated lattice, and using fixed boundary conditions along the *y* and *z* directions.

To examine the effect of atomic jogs on the energetics of cross-slip annihilation of screw dipoles, a pair of oppositely-signed screw dislocations was inserted into the simulation cell separated along the *y* direction by 14 or 44 nm. In some simulations, the screw dislocations were also offset along the [1 1 −2] direction on the (1 1 1) glide plane, such that they tended to move toward each other on their respective glide planes under the action of both interaction and applied forces. For these simulations, the dimension of the simulation cell along the *z* direction was increased to ∼100.0 nm, corresponding to a total of ∼170 million atoms in the simulation cell. In addition, a different simulation cell was used to examine screw dipoles where a jog was present on only one of the dislocations. In this case, the *x*-axis was aligned along the [1 −1 0] direction and the *y*-axis along [−1 −1 −2]. On one half of the simulation cell, as described previously, a pair of oppositely-signed screw dislocations was inserted separated along the *z* direction by 14 or 44 nm. On the other half of the simulation cell, one of the screw dislocations was displaced with respect to the other half by a jog vector on the cross-slip plane while the other screw dislocation was continuous with the other half. Each half-cell was relaxed separately using periodic boundary conditions along the *x* direction. Finally, the two halves were brought together and relaxed using fixed boundary conditions along the *x* direction. This procedure generated a jog vector on only one of the screw dislocations.

In the molecular dynamics (MD) simulations, free-surface boundary conditions were applied along the *y* and *z* directions. Additional forces were applied on atoms in a thin layer (twice the range of the interatomic interactions in the EAM potential) at both boundaries along the *y* and *z* directions. The sum of the individual atom forces at each boundary along the *y* and *z* directions was equal and opposite and, corresponded to the applied stress state in the initial molecular statics simulation cell. The initial conditions for the MD simulations were a molecular statics relaxed cell under stress.

2.1. Interatomic potentials

The embedded atom interatomic potentials used for the simulations are those developed for FCC Ni and Cu by Mishin et al. [16,17]. Table 1 shows the lattice parameter, cohesive energy, elastic constants and stacking fault energy produced by the Ni and Cu potentials. The Shockley partial spacing width, *d*, for the screw dislocation is $d/b = 4$–5 for the Ni potential and $d/b = 6$ for the Cu potential, where *b* is the magnitude of the Burgers vector, **b**, of the screw dislocation. The lattice parameter, cohesive energy, elastic constants and stacking-fault-energy values are very near experimental values, and therefore the results from using these potentials should be representative for these metals.

2.2. Depiction of core structures

For depiction and visualization of the dislocation core structures, we used the method developed by Stukowski and Albe [18] to analyze the atomistic simulations. The method extracts dis-

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