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Kinetics of dislocation cross-slip: A molecular dynamics study

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ABSTRACT

The kinetics of cross-slip and annihilation of a screw dislocation dipole in face-centered cubic (FCC) copper crystals were studied by multiple molecular-dynamics simulations of long (200**b**) dislocations at selected stresses and temperatures with the aim to account for the thermally activated nature of the cross-slip process. A novel cross-slip mechanism was identified; this mechanism required the formation of a finite length constriction before cross-slip could be initiated. It was shown that point constrictions are not the transition state of cross-slip. A study of the kinetics confirmed that cross-slip is a first-order process. By fitting the rate constant to an Arrhenius form, the activation energy was found to be 1.05 eV ± 15%. The activation volume for the Escaig stress in the glide plane was in the range of 5–40$\mathbf{b}^3$, and the prefactor for the rate constant was evaluated to be 1 THz/**b**.

1. Introduction

The plastic deformation of crystalline materials is known to be dependent both on dislocation dynamics and on kinematics. Processes such as fatigue and dynamic recovery and all stages of the plastic deformation curve (in particular stage III) are controlled by the dynamic behavior of dislocations, including motion, multiplication, cross-slip and annihilation, with cross-slip – and to some extent annihilation – being the subject of the present study.

Both the kinematics and the kinetics of the cross-slip process are of interest to the materials science community. The kinematics of cross-slip, i.e., the mechanism or the path in configuration space along which the dislocation cross-slip, has been the subject of multiple conjectures, as reviewed thoroughly by Püschl [1]. Among the mechanisms reviewed, three are of particular relevance to the present study, namely, the Friedel-Escaig, Schoeck-Seeger-Wolf, and Fleischer mechanisms. The Friedel-Escaig mechanism regards the cross-slip process as beginning with the formation on its glide plane of a point constriction of the dissociated dislocation, which then re-dissociates on the cross-slip plane. The model of Schoeck, Seeger and Wolf proposes the formation of a line constriction, which bows out into the cross-slip plane and then dissociates, possibly with a minimal (critical) constriction length. Finally, the Fleischer mechanism postulates a continuous process without constriction. Elastic continuum studies cannot determine the validity of the proposed mechanisms, and earlier atomistic studies [2,3] have concluded that the cross-slip mechanism is the Friedel-Escaig mechanism with point constrictions.

The kinetics of the cross-slip process is typically assumed to be first-order, with the rate constant following an Arrhenius form. Most kinetic studies have thus focused on estimating the activation energy. Cross-slip is a thermally activated process that may require relatively long waiting times in the nano-second regime [3]. Most computational studies of cross-slip therefore avoid the direct calculation of the dynamics. Instead, the configuration space is sampled at 0 K, and the pathway with the lowest energy barrier is identified as the physical pathway, with the molecular-statics-based NEB (nudged elastic band) technique being a commonly used method [1,2,4–17]. The NEB technique allows easy and efficient access to molecular pathways with high activation barriers which are not easily accessible by direct simulation methods. However, the NEB technique, like other molecular-statics methods, has some inherent disadvantages: such methods must assume a final state of the cross-slip process, as well as a specific intermediate configuration to serve as the transition state. Finally, static methods are able only to infer information (e.g., the barrier height) about the cross-slip system kinetics. In contrast to molecular-statics methods, molecular dynamics (MD) is a robust approach to sample the phase space in that it requires none of the above presumptions to describe finite temperature phenomena, albeit at a much greater computational cost which may be prohibitive in some cases. Such an approach has been applied to study dislocation motion (e.g., [18–23]), and in particular cross-slip kinematics and kinetics [2,3,16].

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Due to the statistical nature of the cross-slip phenomenon, direct simulation of the process requires extensive sampling to obtain meaningful data. Previous attempts to obtain cross-slip activation parameters by MD calculations were limited by computational resources, and consequently such studies were able to address only relatively short dislocation lines, and even for those only a limited number of simulations were feasible. These limitations suggest that not all of the possible dynamical pathways in the phase space have been explored, and that fictitious correlations may possibly have been introduced due to the imposition of periodic boundary conditions (PBC). An additional problem is that the quality of the interatomic potentials in these earlier studies has left room for improvement in the quantitative modelling of physical properties. Therefore, new and more extensive calculations are required to properly model the cross-slip phenomenon.

To some extent, there is a gap between the scales accessible by experimental means and those accessible by atomistic simulations. Among the calculation approaches that are being developed to fill this gap are line dislocation dynamics (DD) and Monte-Carlo methods [24], which may be combined to form multiscale models; see for example [25]. Such approaches may use the parameters obtained from MD simulations as input data, e.g., drag coefficients are often employed for the description of dislocation kinematics. In cases where cross-slip events are expected to occur, as in face-centered cubic (FCC) metals, the activation energy and the kinetic prefactor must also be incorporated into the DD model [26–28].

In the present report, we used Cu as a case study for investigating the dynamics of dislocations in FCC crystals. We performed extensive MD simulations of dislocation cross-slip for long dislocations, repeated multiple times to obtain good statistics for the kinetic processes. We simulated the cross-slip process using a dipole structure in PBCs and studied the convergence with respect to the periodic boundary conditions The kinetics of the cross-slip process was analyzed, and both the rate constants and the activation enthalpies were calculated as a function of stress at several temperatures. These results facilitate an evaluation of the cross-slip activation energy and volumes and provide a new insight into the cross-slip kinematics.

2. Methods

MD calculations and system setup were performed with the LAMMPS package [29]. Visualization and some post processing procedures employed the OVITO package [30]. The embedded-atom method (EAM) potential of Mishin et al. [31] was chosen as the inter-atomic interaction potential. To simulate dislocations in FCC metals, it is necessary to reproduce the stacking-fault energy, which dictates the spreading of the dislocation's core through the interaction of the Shockley partials [32]. The selected potential had a value of 44.4 mJ/m^2, which agrees well with the experimental value of 45 mJ/m^2 [31]. All MD simulations were carried out in the NPT ensemble using a Nose-Hoover barostat with a time-step of 1 fs. Under applied shear, the ensemble becomes NσT by altering the relevant shearing component of the stress tensor.

To simulate a dislocation in a bulk crystal, PBCs were imposed in all three dimensions. This, in turn, required the insertion of at least two (perfect) dislocations with opposite Burgers vectors **b** so as to maintain a net Burgers vector of zero. Alternative configurations such as a quadrupole [33] do not obviously lend themselves to kinetic studies as additional interactions need to be considered. Consequently, the simulation box contained two infinite straight parallel dislocations forming a dipole. Fig. 1 illustrates the construction of a simulation box with screw dislocations. The crystallographic orientation of the simulation box was chosen to be $\hat{x}:[1\,\bar{1}\,2]$, $\hat{y}:[1\,1\,0]$, $\hat{z}:[\bar{1}\,1\,1]$ such that in our Cu FCC system the

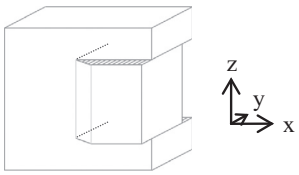

Fig. 1. Simulation box setup for a screw dipole configuration. $\hat{\boldsymbol{x}}:[\mathbf{1}\,\bar{\mathbf{1}}\,\mathbf{2}]$, $\hat{\boldsymbol{y}}:[\mathbf{1}\,\mathbf{1}\,\mathbf{0}]$, $\hat{\boldsymbol{z}}:[\bar{\mathbf{1}}\,\mathbf{1}\,\mathbf{1}]$.

axes corresponded to the glide plane and direction $\{1\,1\,1\}$ and $\langle 1\,1\,0\rangle$, respectively. Upon application of a shear stress, σ_{xz} was the activated component.

The screw dipole configuration was created by displacing a block of atoms by a unit Burgers vector as shown in Fig. 1, where the displacement was incremental across several atomic layers. This initial configuration was followed by relaxation of the atomic positions by a conjugate gradient energy minimization algorithm.

Convergence with respect to supercell parameters was ensured in the present study, by choosing the standard length dimension along the dislocation line to be 200**b** ($\sim$50 nm), facilitating the capture of the full three-dimensional behavior of the nucleation process into the cross-slip plane. In the z direction, the height of the simulation box was close to 40 nm, with a 5-nm separation between the two dislocations (dipole height) that suppressed image interactions due to the PBCs. Previous studies have considered the effect of choice of supercell configuration on the convergence of the interactions due to periodic boundary conditions [23,34–36]. Convergence with respect to dipole height is considered explicitly in the Results. Consequently, the simulation box contained 3.6 million atoms. Simulations were allowed to run for 5 ps before applying shear stress so as to enable the barostat and thermostat to stabilize the system. Following the temperature stabilization, an Escaig constriction shear stress (*xz* component) was applied to reduce the nucleation enthalpy and to allow cross-slip to occur in a reasonable time for MD calculations. The damping parameters of the barostat of the MD-code were tweaked to ensure that the stabilization times of the new stress state were much shorter than the waiting times for cross-slip; Our simulations were optimized such that the target pressure tensor was achieved in <5 ps, such that *xz* component increased from zero to 90% of the target stress within 3 ps and to 99% within 4 ps. We note that the Escaig stress only constricts the dislocation and does not induce motion.

Time to nucleation on the cross-slip plane was determined as the instant at which the first atoms to be recognized as part of the HCP stacking fault were identified outside the primary glide plane (*xy*). Simulations at different temperatures were repeated multiple times (more than 30) for each stress-temperature combination (different distributions of the initial velocities in each simulation) in order to obtain statistically significant data.

Post processing of the coordinates data to identify the initiation of cross-slip employed the Common Neighbor Analysis (CNA) [37] method, which allows for the identification of bounded stacking faults in-between the partial cores. Burgers vectors and dislocation lines were identified with the Dislocation eXtraction Algorithm (DXA) [38]. This algorithm first performs a CNA calculation, and then scans the simulation box to find and define the existing dislocation segments by systematically constructing Burgers circuits.

3. Results

3.1. Cross-slip kinematics

A typical event of cross-slip initiation and subsequent annihilation is presented in Figs. 2 and 3, respectively (10 ps record