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Microstructurally based cross-slip mechanisms and their effects on dislocation microstructure evolution in fcc crystals

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Abstract—Three newly identified cross-slip mechanisms from atomistic simulations of fcc crystals, namely surface, bulk and intersection cross-slip types, were hierarchically informed into discrete dislocation dynamics simulations. The influence of each cross-slip type on the evolution of the dislocation microstructure in face-centered cubic microcrystals having different crystal sizes and initial dislocation densities was investigated. Dislocation pattern formation, surface slip localization and initial strain hardening were observed, in agreement with experimental observations, and possible explanations are given in the light of these simulations.

Keywords: Cross-slip; Dislocation dynamics; Dislocation patterning; Strain hardening

1. Introduction

Dislocations are one of the most important microstructural features governing the mechanical properties of crystalline materials. They are the main carriers of plasticity, hence most of the related phenomena (e.g. yielding, strain hardening, strain-rate dependence, temperature dependence, etc.) depend on how the dislocation microstructure evolves and how dislocations interact with other material defects [1]. The dislocation microstructure evolution is an immensely complicated phenomenon that is controlled by material properties, microstructure and boundary conditions. Several mechanisms, such as dislocation dissociation, recombination, glide, cross-slip and climb, are active during material deformation and they all contribute to the final evolved microstructure [2]. Cross-slip of screw dislocations is recognized as one of the main mechanisms controlling dislocation multiplication in crystals [3,4], strain hardening [2,5–8], stress recovery during stage-III loading [9,10] and dislocation pattern formation [11]. Cross-slip also provides an effective mechanism for dislocations to bypass obstacles [12,13].

In attempts to describe the atomic scale mechanisms associated with cross-slip in face-centered cubic (fcc) crystals, several models have been proposed (e.g. [14–17]). For a critical review of these models, the reader is referred to the article by Puschl [18]. A number of experimental [19–22] and atomistic [23–26] studies have also been conducted over the years in order to identify the atomic mechanisms and estimate the activation parameters that are involved in the process. Nevertheless, to date, there is no universal agreement on how cross-slip takes place, and direct quantitative predictions of the influence of cross-slip on the mechanical properties are still subject to intensive studies. One reason why this problem is not very well understood is that the cross-slip phenomenon spans several length scales, starting at the atomic scale and going all the way up to hundreds of nanometers. However, the majority of previous studies of this phenomenon have focused on the atomistic length scale, hence a method for bridging these findings and making connections to larger length and time scales is still necessary.

One such model that could bridge this gap is discrete dislocation dynamics (DDD) simulations, in which both the time- and length-scale limitations from atomic simulations are greatly reduced. Over the past two decades, two-dimensional (2D) and three-dimensional (3D) DDD methods have been developed to simulate plastic deformation at the mesoscale in crystalline structures by direct numerical simulations of the collective motion of dislocation ensembles according to physics-based rules [27–34]. The physics that can be incorporated in DDD simulations can range

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anywhere from the motion of simple infinite length (two-dimensional) dislocations in single crystals with periodic boundary conditions [35,36] to the complex dynamics and interactions of three-dimensional curved dislocations in single crystals or polycrystalline finite-sized materials [37]. DDD simulations were performed to study an array of material phenomena, including the response of thin films [38,39], size effects [40–43], irradiation hardening [44] and nanoindentation [45]. In addition, dislocation climb [46] and dislocation inertia effects at high strain rates [47] are among the physical behaviors that have been successfully implemented into DDD.

Cross-slip of screw-character dislocation segments in fcc crystals away from intersecting segments and forest dislocations (bulk cross-slip) was first introduced into 3D-DDD simulations by Kubin et al. [27] through a probabilistic procedure. In this approach, the cross-slip probability per time step, P_{step}, for any screw segment of length L, experiencing a local resolved shear stress on its glide plane and opposite to the applied shear stress, τ^g, is given by

$$P_{step} = \beta \frac{L}{L_o} \delta t \exp\left(\frac{(\tau^g - \tau_{III})V}{k_B T}\right) \quad (1)$$

where β is a scaling factor, L_o is a reference length of 1 μm, as defined in Ref. [27], δt is the time step, τ_{III} is the resolved shear stress at the onset of stage-III hardening for bulk crystals (i.e. parabolic hardening), V is the activation volume, k_B is the Boltzmann constant and T is the temperature. This equation was derived in accordance with the Escaig cross-slip model, which is based on a "phantom" obstacle resisting the motion of the dislocation and subsequently resulting in a constriction on the dislocation, leading to cross-slip [12]. This model has been the basis for incorporating cross-slip in most subsequent DDD simulation methods (e.g. [28,32,34,48]). It is worth noting that a similar form was used by Déprés et al. (2006); however, the resolved shear stress on the cross-slip plane was used rather than that on the glide plane [49]. A primary challenge to simulation studies using this model is that significant stresses are needed to activate the process, while generally there are no obstacles present within the idealized single crystal simulation cells to induce such stresses.

Recent molecular dynamics simulations have suggested that the activation energy of cross-slip should not be affected by the resolved shear stress on the glide plane; rather, the Escaig stress on both the glide and cross-slip planes have the dominant effect [50]. In addition, besides bulk cross-slip, a sub-group of the current authors have identified two new cross-slip mechanisms through molecular static and molecular dynamics simulations [51–55]. In the first such mechanism, intersection cross-slip, it was shown that cross-slip is preferentially observed at selected screw dislocation intersections in fcc crystals [51]. The activation energy was computed for cross-slip at attractive forest dislocation intersections and was shown to be 2–5 times lower than that for bulk cross-slip [52,53]. Furthermore, spontaneous (i.e. athermal) cross-slip was also observed to occur at mildly repulsive intersections [54]. In the second mechanism, surface cross-slip, it was reported that a negative constriction forms on screw dislocations ending at free surfaces under certain conditions and that the activation energy for cross-slip is significantly lower than that for cross-slip at attractive forest dislocation intersections [55]. These new rules promote the need to revise how cross-slip is incorporated into DDD simulations.

Accordingly, the motivation of the current work is to incorporate an atomistically informed cross-slip model into DDD simulations of fcc crystals. The details of the computational model are presented in Section 2. Simulation results of the deformation of single-crystal nickel microcrystals of various sizes and at different dislocation densities using this model are presented in Section 3. Further insights into the effect of cross-slip on dislocation evolution, microstructure patterning and slip band thickening are discussed in Section 4. Finally, a summary and conclusions are presented in Section 5.

2. Computational method

All simulations performed in this study employ the 3D-DDD open source code, ParaDiS, originally developed at Lawrence Livermore National Laboratory [33]. In ParaDis, the dislocations are discretized into short linear segments that can be arbitrarily interconnected. The open source code was modified in-house to guarantee that, for simulations of fcc crystals, dislocation collisions and glide will always remain co-planner on the correct slip systems. The code was also extended as described below to incorporate the mechanisms of bulk, surface, attractive intersection and repulsive intersection cross-slip, as identified from atomistic simulations.

In order to effectively handle the most general cases of cross-slip, a search algorithm that employs graph-theoretic approaches was used in order to detect the longest possible screw-character dislocation chains, which are sequences of dislocation segments. Here, each dislocation segment is a straight line connecting two dislocation nodes. Identifying long chains reduces the number of cross-slip events handled computationally, rather than individually computing cross-slip probabilities for several parts of the same chain. More importantly, because the probability of cross-slip increases linearly with the length of the screw dislocation chain, handling shorter chains can cause some potential cross-slip events to pass undetected. Next, the appropriate cross-slip type is identified depending on the configuration of the dislocation chain in the crystal, according to the following rules. If a screw dislocation chain intersects a free surface, it is considered a surface cross-slip type candidate. If the chain fully resides inside the crystal and it intersects with another dislocation not lying on either its glide or cross-slip plane, then it is considered to be an intersection cross-slip type candidate. Further, if the sum of the two Burgers vectors of the intersecting dislocations is $\langle 1\,1\,2\rangle$, the screw dislocation chain is determined to be a repulsive intersection cross-slip type, which is a spontaneous process that does not require any activation energy to take place [54]. On the other hand, if the sum of the Burgers vectors is $\langle 1\,0\,0\rangle$ then it is considered to be a Hirth-lock attractive cross-slip type candidate. If the Burgers vectors sum is $\langle 1\,1\,0\rangle$ and the intersecting dislocations are on $\{1\,1\,0\}$ or $\{1\,0\,0\}$ planes, then it is considered as an attractive intersection Lomer–Cottrel (LC) cross-slip type candidate. If the vectors sum is $\langle 1\,1\,0\rangle$ and the intersecting dislocations are on $\{1\,1\,1\}$ slip planes, then it is considered as an attractive intersection glide-lock cross-slip type candidate. Finally, if the screw dislocation chain does not satisfy any of the above condi-