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Prismatic and helical dislocation loop generation from defects

Lynn B. Munday*, Joshua C. Crone, Jaroslaw Knap

RDRL-CIH-C, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005, USA

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ABSTRACT

Plastic deformation induced by stress concentrations near crystal defects occurs through the generation of prismatic dislocation loops (PDL). The production of PDLs leads to void growth and particle decoherence. In this work we use dislocation dynamics simulations to characterize two mechanisms for PDL formation. The first mechanism corresponds to a classical model of PDL generation from dislocation nucleation. The second mechanism considers PDL generation through cross-slip of a screw dislocation intersecting the particle. We systematically study the effect of the crystal lattice and defect type on PDL generation for both mechanisms as a function of pressure. The simulations show image stresses produced by the dislocation's interaction with the free surface of a void suppresses PDL generation. The highest PDL generation rates are found for a dislocation nucleated from a void in a body-centered cubic lattice. Our simulations also show helical coiling of screw dislocations produces a continuous emission of PDLs without the need for dislocation nucleation at pressures as low as 1.0 GPa.

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1. Introduction

Plastic deformation near lattice defects is primarily dependent on locally activated modes of dislocation motion including cross-slip and nucleation [1]. These locally active dislocation mechanisms are promoted by stress concentrations arising from the lattice defects and lead to the formation of prismatic dislocation loops (PDL) around defects such as voids and misfit particles [2]. Unlike a dislocation glide loop, the Burgers vector of a PDL does not lie in the plane of the loop. This allows a PDL to displace a platelet of material relative to the defect's interface resulting in volumetric plastic deformation. In the absence of diffusion, the volumetric plastic deformation associated with the generation and emission of multiple PDL's is the primary mechanism for void growth or interface decoherence between a particle and the surrounding matrix material.

The specific mechanism for generating PDLs from a defect is dependent on a number of factors, such as, energy barriers to dislocation motion, nucleation and cross-slip as well as the initial dislocation density. Atomistic simulations tend to suggest PDL generation through the interaction of multiple dislocations nucleated on separate glide planes [3,4]. This type of PDL generation is favored under high strain rate loading where several dislocations are simultaneously nucleated on different glide planes around a defect. Still, such a mechanism may also be active at low strain rates if cross-slip of a nucleated dislocation is suppressed by energy barriers [5,6] or free surface effects [7].

In contrast, experimentally observed PDLs created at lower strain rates around submicron sized particles [8] are assumed to form through an alternative mechanism involving dislocation cross-slip. The classical model for this type of PDL generation is due to Ashby and Johnson [2]. In this model, once a single dislocation is nucleated from the surface of a lattice defect under a hydrostatic load, a PDL will always be formed through a series of cross-slip events. Thus, dislocation nucleation is considered the only barrier to PDL formation, while other barriers, such as those owing to dislocation cross-slip or free surfaces, are simply ignored. The predictions of Ashby and Johnson's model have been confirmed for PDL generation around misfit particles by means of nonlinear elastic/phase-field simulations [9] and dislocation dynamics simulations [7].

Experiments have also revealed that plastic relaxation may proceed through the formation of helical dislocations, a PDL like structure [10]. A helical dislocation appears as a long spiral of prismatic dislocation loops connected by a single screw dislocation of the same Burgers vector. Atomistic and dislocation dynamics simulations have shown the formation of helical dislocations through the interaction of a screw dislocation with prismatic dislocation loops of the same Burgers vector [11,12]. Helical dislocations have also been proposed to form in the absence of prismatic

* Corresponding author.
E-mail address: lynn.b.munday.civ@mail.mil (L.B. Munday).

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dislocation loops through vacancy assisted climb of a screw dislocation [10], a diffusion process. However, a screw dislocation under the action of the stress field produced by a misfit particle may also produce helical coils through a combination of dislocation glide and cross-slip. This alternative mechanism for PDL generation may lead to plastic relaxation near a defect without the need for dislocation nucleation.

Here, we investigate PDL generation around nanoscale defects using dislocation dynamics (DD) simulations. DD simulations are capable of accurately capturing the motion of dislocations in the vicinity of large stress gradients due to material heterogeneities [13]. Two- and three-dimensional DD simulations excluding cross-slip have been used to capture the later stages of void growth through multiplication of dislocations in the crystal [14,15]. In these simulations, the number of dislocation sources in the vicinity of a void activated by its stress concentration increases with the void size. This observation may indicate higher void growth rates for large voids. The reduction in active dislocation sources for small voids is likely to cause void growth to transition from multiplication of existing dislocations to dislocation nucleation for voids below 500 nm [15]. For voids on the order of 50 nm, three-dimensional DD simulations have shown that locally activated modes of dislocation motion, including dislocation cross-slip and nucleation, are indispensable for PDL generation [7]. These DD simulations have also drawn attention to the importance of void image stresses for cross-slip in PDL formation at low pressures. Dislocation cross-slip at free surfaces has also been shown in three-dimensional DD simulations to be an important generator of dislocation sources available for dislocation multiplication [6,16,17].

The formation of PDLs through cross-slip is largely dependent on the crystal lattice which determines both the number of secondary glide planes available for cross-slip and their orientation relative to one another. Here, we consider PDL formation in face-centered cubic (fcc), body-centered cubic (bcc), and hexagonal close-packed (hcp) lattices. In atomistic simulations of hydrostatically loaded voids, the availability of cross-slip planes leads to the formation of four-sided rhombus PDLs in fcc lattices [3] and hexagonal or triangular PDLs in bcc lattices [18,4]. The structures of PDLs in hcp lattices have not been identified through atomistic simulations and so we limit our study to dislocations with $\langle a\rangle$-type Burgers vectors in the close-packed directions. The four dominant slip planes containing the $\langle a\rangle$-type dislocation are the basal, prismatic and two different pyramidal type-I glide planes. Atomistic and DFT [19] simulations have shown cross-slip of $\langle a\rangle$-type screw dislocations between the basal, prismatic and pyramidal type-I glide planes. Based on the hcp crystallography, we would expect an eight-sided PDL to form on these glide planes.

In this article, we examine PDL generation from a spherical defect, over a range of pressures, lattice types, and initial dislocation configurations. We aim to characterize each individual factor affecting plastic deformation through PDL generation. In particular, we are interested in how these factors influence the cross-slip mechanism which we have found in our earlier work to be the dominant feature of PDL generation [7]. By considering the fcc, bcc, and hcp lattices, we determine the influence of availability of slip planes on cross-slip. Varying the type of spherical defect allows us to isolate the effects of dislocation interactions with free surfaces. The initial dislocation structure provides estimates on two sources available for PDL generation: dislocation nucleation or preexisting dislocations. Finally, pressure provides the driving force for PDL generation around the defect and our simulations will determine its dominance on cross-slip over the other factors studied.

The article is organized as follows. In section 2 we describe the DD simulation protocol. Section 2.1 addresses the finite element model and section 2.2 discusses the DD simulation. We then discuss PDL generation results in section 3. Results and discussion are given separately for PDLs generated from nucleated dislocations in section 3.1, helical coiling of the infinite screw dislocation in section 3.2, and the rate of PDL formation as a function of pressure in section 3.3. We finish with a reiteration of results in the conclusions in section 4.

2. Simulation methodology

In this work, we use dislocation dynamics (DD) simulations to capture the processes that allow PDLs to form from a dislocation interacting with a spherical defect. The material considered is aluminum with shear modulus $\mu = 27$ GPa, Poisson's ratio $\nu = 0.35$, and Burgers vector $|\mathbf{b}| = 2.86$ Å. We use these material properties for all DD simulations of PDL formation in fcc, bcc, and hcp lattices. For the hcp lattice we also define $c/a = 1.6236$, where c and a represent the vertical and lateral lattice spacing in hcp lattices, respectively. Our simulations use the DD formulation of van der Giessen and Needleman [13], where the linear elastic fields due to dislocations in an infinite bulk crystal are augmented by the linear elastic fields produced by an auxiliary boundary value problem (BVP). The boundary conditions of this BVP consist of the corrective image tractions on free surfaces and far-field loads. This simulation protocol is accomplished by coupling the DD simulator ParaDiS [20] to the corrective fields obtained from a BVP solved with a parallel finite element code [21,22].

2.1. Finite element model

The domain of our finite element model is a cube with edge length $l = 4000|\mathbf{b}|$ containing a single void at the center with radius $R_v = 100|\mathbf{b}|$. We discretize this domain with variable sized quadratic tetrahedral elements yielding a $5|\mathbf{b}|$ resolution near the void. A finely resolved mesh is needed in the vicinity of the void to resolve the image tractions and stress gradients produced by surface piercing dislocations.

Tractions are applied to the outer surface of the finite element domain commensurate with a uniform far-field hydrostatic tensile load, $\boldsymbol{\sigma}^\infty = p\mathbf{I}$, where $\mathbf{I}$ is the identity tensor and $p > 0$. In this work pressure, p, is synonymous with hydrostatic tension. No image tractions are applied to the outer surface of the cube allowing our BVP solution to produce corrective elastic fields which approximate a single void in an infinite bulk crystal. The void acts as a stress concentrator inducing shear stresses in its vicinity. Dislocation glide is driven by the resolved shear stress on its glide plane defined as $\sigma_{bn} = \widehat{\mathbf{n}}\cdot\boldsymbol{\sigma}\cdot\widehat{\mathbf{b}}$, where $\boldsymbol{\sigma}$, $\widehat{\mathbf{b}} = \mathbf{b}/\left|\mathbf{b}\right|$, $\widehat{\mathbf{n}} = \mathbf{n}/|\mathbf{n}|$ are the infinitesimal stress tensor, the unit Burgers vector and the unit normal of the glide plane, respectively. The resolved shear stress due only to the far-field loading $\boldsymbol{\sigma}^\infty$ is $\sigma_{bn}^\infty = \widehat{\mathbf{n}}\cdot\boldsymbol{\sigma}^\infty\cdot\widehat{\mathbf{b}}$ and is plotted in Fig. 1 for the (a) fcc, (b) bcc, and (c) hcp slip systems that PDLs in this work will glide on. We limit our study of hcp PDLs to those formed from an $\langle a\rangle$-type Burgers vector.

The σ_{bn}^∞ stress fields shown in Fig. 1 do not include the effect of image tractions produced by the dislocations. The image tractions change as the dislocation structure evolves. Image effects are most pronounced for dislocations intersecting the surface where image stresses are shown to strongly influence cross-slip [16,7]. The fine mesh needed to resolve these image stresses results in a finite element model with 500,000 degrees of freedom. In order to keep the corrective stress field in correspondence with the dislocation's configuration, the BVP must be solved with updated image traction boundary conditions at every dislocation dynamics time step. Owing to the fact that the finite element mesh and its stiffness matrix remain static over the course of our dislocation dynamics simulation, we efficiently solve our BVP by means of the MUMPS