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Transformation of shear loop into prismatic loops during bypass of an array of impenetrable particles by edge dislocations

Sébastien Groh*

Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, Germany

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ABSTRACT

Particle strengthening resulting from the interaction between edge dislocations and impenetrable particles is investigated by molecular statics in the framework of the (modified-) embedded atoms method for magnesium. The dynamics of the bypassing mechanism have been identified as a function of the number of glide dislocations interacting with the particle. Qualitatively, it was found that the first glide dislocation bypassed the impenetrable particle by an Orowan mechanism. The net result of the first dislocation bypass was a straight dislocation line and a particle encircled by a non-planar Orowan loop. Furthermore, when a second glide dislocation interacted with the particle encircled by a non-planar Orowan loop, the molecular statics calculations revealed a bypassing mechanism occurring through a series of dislocation cross-slips. The net result obtained after the bypass of a particle with diameter between 2 nm and 8 nm by two glide dislocations is two prismatic loops on one side of the particle and a glide dislocation carrying two super jogs and a prismatic loop on the other side of the particle. Quantitatively, the stress required by a first glide dislocation to bypass an impenetrable particle was in good agreement with continuum predictions from the literature. A systematic decrease of the shear stress needed for a second glide dislocation to bypass an impenetrable particle encircled by a non-planar Orowan loop was found. Such a decrease of the bypassing stress is interpreted as the evidence that the bypass of the second dislocation by cross-slip maneuvers is a stress relief mechanism.

1. Introduction

Since the mid-1950s, the interaction between dislocations and impenetrable particles in precipitation-hardened alloys has been subject of intense investigations (i) experimentally, using transmission electron microscopy ([14,15,17,32,8,20]), (ii) theoretically, using elasticity theory ([5,6,13,21]), and (iii) numerically, using either dislocation dynamics ([27,33,34,35,25]) or molecular dynamics ([12,24]). The understanding of the dislocation–precipitate interaction and its effect on the plastic behavior of precipitation-hardened alloys might help the design of new materials as well as their manufacturing routes.

From a mechanical point of view, if one assumes an ideally plastic matrix reinforced by perfectly rigid particles, it has been demonstrated that in the absence of stress relief mechanisms (plastic relaxation), two types of stresses are present in the system: (i) large stresses in the neighborhood of the particles and (ii) long range stresses also referred as back stresses. While the large stresses are characterized by zero mean value, and contribute to the source shortening effect [4], long range stresses arise from the relaxation of external boundaries. Analyzed using dislocation physics in absence of plastic relaxation, glide dislocations can bypass perfectly rigid particles by leaving arrays of Orowan loops around the particles, and therefore, enhancing the source shortening effect. As a result, the applied stress required to move glide dislocations through an arrangement of particles increases linearly with increasing number of Orowan loops ([13,25]). As a consequence, if a mechanical model does not include plastic relaxation mechanisms, the work hardening is predicted as linear ([5,13]). On the other hand, by adding stress relief mechanisms in the neighborhood of the particles ([15,17,6]) it was shown that the large stresses in the neighborhood of the particles were lowered. In such configuration, it was shown that forest interaction was the main contributor to the hardness of the deformed material leading to a quasi-parabolic strain-hardening.

In magnesium single crystal deformed under large shear strain, Hirsch and Lally [15] observed experimentally by transmission electron microscopy (TEM) analysis the presence of a large number of prismatic loops generated in front of unidentified particles. The formation of the rows of prismatic loops was explained based on the bypassing mechanism proposed by Hirsch [14], and referred to later as the Hirsch mechanism. The Hirsch mechanism involves a series of cross-slip operations that lead to the formation of a prismatic loop on one side of the precipitate and two super-jogs carried away by the glide dislocation on the

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* Tel.: +49 37 31 39 41 38; fax: +49 3731 39 3455.
E-mail address: Sebastien.Groh@imfd.tu-freiberg.de

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other side. In Cu-based alloys, Humphreys and Hirsch [17] hypothesized a variant of the Hirsch mechanism. The variant mechanism involves a pre-existing Orowan loop encircling the particle. Under the influence of the stress field of a glide dislocation, the Orowan loop transforms into two prismatic loops located on each side of the precipitate. After recombination of the glide dislocation with the newly formed prismatic loops, the net result obtained within this mechanism is that after the passage of two dislocations, one prismatic and one Orowan loop are left behind. The formation of Orowan loops and their involvement in the bypassing mechanism is a valid hypothesis assuming that climb and pipe diffusion are two possible explanations for the disappearance of the Orowan loops between straining testing at low temperature and TEM analysis and room temperature [13]. In addition, Vivas et al [32] observed the formation of dislocation loops induced by cross-slip as well as a few Orowan loops using transmission electron microscopy in-situ straining technique in aluminum alloys. By means of full three-dimensional dislocation dynamics simulations based on the level set method, Xiang et al. [33,34,35] examined the bypassing mechanisms of particles of different natures (penetrable and impenetrable, with and without misfit). These authors reported classical and new bypassing mechanisms. However, it should be noted that none of the new mechanisms reported by Xiang et al. [33,34,35] were confirmed experimentally or by means of atomistic calculations. Although the dislocation–particle interaction has already been intensively studied at the atomistic scale (see [3] for a literature survey), very limited work was given to dislocation – impenetrable particle, and to the author's knowledge, the works of Hatano [12] and Proville and Bakó [24] are the only ones available in the literature. Hatano [12] revealed the dynamics of the Hirsch mechanism at finite temperature using molecular dynamics in fcc copper crystal modeled in the framework of the embedded atoms method. He concluded that the bypassing mechanism (either Orowan or Hirsch) depends on nature of the boundary conditions: the Orowan bypassing mechanism being recovered when the shear was applied symmetrically with respect to the middle of the specimen while Hirsch mechanism being recovered when the symmetry was broken by fixing the bottom of the specimen and applying a constant velocity on the top layers. Proville and Bakó [24] reported some calculations where a second glide dislocation interacted with a spherical precipitate encircled by an Orowan loop resulting from the bypass of the precipitate by a first glide dislocation in fcc nickel reinforced by Ni_3Al nanophases with $L1_2$ crystal structure modeled in the framework of the embedded atoms method. Although Proville and Bakó [24] observed a decrease of the bypassing stress by a few percent and two jogs were reported in the second passing dislocation, the nature of the dislocation left around the particle was not reported, and the authors did not discuss the bypassing mechanism.

The objective of this work is to numerically reveal the transformation of a shear loop into prismatic loops during the bypass of an array of impenetrable particles by edge dislocations and to quantitatively compare the Orowan and the transformation stresses against continuum predictions from the literature. To this end, a summary of the method used to set up the simulation cell is given in Section 2. The dynamics of the bypassing mechanism and the quantitative analysis are reported in Section 3 followed by a discussion in Section 4. Concluding remarks are given in Section 5.

2. Method

In this work, we simulate by means of molecular statics (MS) calculations [23] the process of a dislocation bypassing impenetrable particles in the model of hexagonal close packed crystal in the framework of the (modified-) embedded atom method ([30,19,18]). The potentials were fit to the elastic, structural, and energetic properties of Mg. Although not included in the materials database for the fitting of the potentials, the dislocation core structures for edge and screw characters from the basal and prismatic slip systems have been reported in the literature ([11] and [36]). It was shown that dislocations from the basal slip systems were dissociated into two Shockley partials bonding a stacking fault, while dislocations from the prismatic slip system were compact. In terms of energy, this finding signifies that the core energy of basal dislocations is lower than the core energy of prismatic dislocations with same Burgers vector.

Basal edge dislocations were introduced in the system using the methodology proposed by Osetsky and Bacon [22] to build a periodic array of infinite dislocations. Periodic boundary conditions were applied in directions carrying the dislocation line and the Burgers vector referenced by ***l*** and ***b*** in Fig. 1. As a consequence of the periodic boundary conditions along ***b***, the dislocation in the computational cell experiences a shear stress σ_{bn} due to its image in all periodic cells. The largest value (obtained when only one of its nearest-neighbor images was considered) is in the order $\mu b/l_b$ where μ, b, and l_b are the shear modulus, the magnitude of the Burgers vector, and the dimension of the cell along the ***b*** direction, respectively. Although the net shear stress is zero for a straight dislocation (the contributions from images on the right and on the left sides of the simulation cell are of opposite signs), the contributions from the nearest images are non-zero for curved dislocations. However, the contributions of the nearest images have not been quantified in this study, and it is assumed that these contributions remain small compared to the bypassing stresses [3]. Free surfaces were assumed at the top and bottom of the simulation cell in the direction normal to the slip plane. After relaxation of the dislocation core by means of the conjugate gradient minimization technique, an impenetrable precipitate was modeled by immobilizing a group of atoms included in a sphere of radius R_p [12]. As the atoms describing the precipitates are kept immobile during deformation, glide dislocations cannot bypass the precipitate by shear. The experimental values of the Young's modulus and yield stress of $Mg_{17}Al_{12}$ [9] validate the assumption of non-deformable precipitates modeled by freezing a group of atoms. The motion of the edge dislocation was then generated by applying rigid displacements in the direction of the Burgers vector on the top and bottom surfaces in opposite directions with respect to each other. The shear state was therefore symmetric with respect to the slip plane. The application of shear deformation induced elastic deformation of the crystal until a critical stress was reached, at which point the dislocation core started to move until it was blocked by the particle. The dislocation bypassed the particle after increasing the elastic deformation of the crystal.

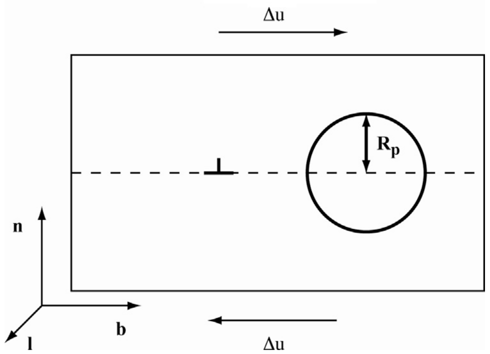

Fig. 1. 2-D projection of the simulation cell with an edge dislocation and an impenetrable particle.