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# Influence of the anisotropy in lattice friction on the macroscopic behavior of magnesium single crystal: A study by discrete dislocation dynamics

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ABSTRACT

It is known that the lattice friction in hexagonal close-packed (hcp) Mg crystals is anisotropic and depends on the family of slip systems. In this study, the relation between the lattice friction and the single mechanism involving the reaction between dislocations from different families of slip systems, as well as the relation between the lattice friction and the macroscopic behavior are analyzed using discrete dislocation dynamics simulations.

In this work, it is demonstrated that for small values of the friction stress, the recombination stress is controlled by the line tension of dislocations, while for large values of the friction stress, the recombination stress is controlled by the lattice friction. Further, for low values of the lattice friction, the macroscopic behavior is controlled by the well known forest mechanism, while when increasing the lattice friction (which can be viewed as a decrease in the temperature), the macroscopic behavior is controlled by the lattice friction itself.

## 1. Introduction

Metals with a hexagonal close-packed (hcp) crystal structure have a wide variety of mechanical and physical properties, and understanding the links between atomic properties, microstructure, and mechanical properties can pave the way for new applications. Opportunities for the design of new materials based on an hcp crystal structure can be escalated from the use of hierarchical scale-bridging strategies. For example, magnesium's good mechanical properties, such as low density and high specific strength, make its alloys become potential candidates for replacing steel and other heavier materials [1], particularly for structural components in the transportation industry [2,3]. Such a switch to magnesium and its alloys in the design of motor vehicle components will become progressively more important as the demand for lighter weight and more fuel efficient vehicles increases.

However, deformation mechanisms in metals crystallized with hcp lattice are complicated, and competition between dislocation plasticity and twinning plasticity occurs. For example, $\langle \mathbf{a} \rangle$ and $\langle \mathbf{c}+\mathbf{a} \rangle$ dislocations and tensile twins can be activated to accommodate the deformation of Mg single crystal [4]. Over the years, the mechanical properties of Mg and its alloys were investigated at different length scales, ranging from the electronic scale [5,6] up to the mesoscopic level [7–9]. In the work by Jain and Agnew [7] and references therein [10–12], it was indicated that, in Mg alloys, the initial critical resolved shear stress (CRSS) of the dislocation lying in the basal slip system is one order of magnitude lower than the initial CRSS of the dislocation lying in the prismatic slip system. They also reported that, when increasing the temperature from 20 °C to 200 °C, the initial CRSS in the prismatic slip system decreases from 3.2 times to 1.8 times of the initial CRSS in the basal slip systems. At a lower length scale, Capolungo et al. [13] studied the effect of elastic anisotropy on the collective behavior of dislocations using discrete dislocation dynamics (DDD) simulations in which $\langle \mathbf{c}+\mathbf{a} \rangle$ dislocations were implemented. They showed that isotropic elasticity was suitable to model the dislocation behavior in Mg as its anisotropic factor [14] is close to 1. However, for simplicity these authors did not include any effect of the anisotropy in the friction stress between slip systems. Using molecular dynamics, Groh et al. [15] and Yasi et al. [16], reported a large anisotropy in friction stress between the basal and the prismatic slip systems. These authors reported a friction stress for basal dislocations to be two orders of magnitude lower than the friction stress for prismatic dislocations. However, they did not investigate the evolution of the friction stress with respect to the temperature. Such a study was carried out by Nogaret et al. [17], who quantified that the friction stress for edge and screw $\langle \mathbf{c}+\mathbf{a} \rangle$ dislocations decreases from a few hundred MPa to a few MPa when the temperature was raised

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from 0 K to 300 K. They reported a relatively large friction stress, and a strong temperature dependence of the friction stress in the prismatic slip systems.

In this paper, DDD simulations were performed to investigate the influence of the anisotropy in lattice friction on the macroscopic behavior of Mg single crystal. Firstly, the role of the anisotropy in lattice friction was identified on the formation and destruction of dislocation junctions. To this end, a geometric model describing the annihilation distance in the presence of anisotropic friction stress was derived. This model is presented in Section 2 and then validated in Section 3. Secondly, massive calculations on the strain-path changes from the basal slip systems to the prismatic slip systems are also included in Section 3. A discussion of the findings of the present study is given in Section 4, while concluding remarks are outlined in Section 5.

## 2. Method and model

DDD simulations using the mM[1] software [18,19] are used to model the effect of the anisotropy in friction stress on (i) the single mechanism, such as the collinear interaction resulting from the reaction between dislocations on the basal and prismatic slip systems, and (ii) the macroscopic behavior of Mg single crystal submitted to the strain-path changes. In the DDD framework, the anisotropy of the lattice friction is taken into account through the mobility rule. Assuming that the resolved shear stress on the slip planes consists of various components (the Peach–Koehler force, $\tau_{\mathrm{PK}}$, the line tension, $\tau_{\mathrm{lt}}$, and the friction force, $\tau_{\mathrm{friction}}$), the effective resolved shear stress, $\tau^*$, is given by:

$$\begin{cases} \tau^{**} = \tau_{\mathrm{PK}} + \tau_{\mathrm{lt}}, \\ \tau^{*} = |\tau^{**}| - \tau_{\mathrm{friction}}. \end{cases} \tag{1}$$

Depending on the sign of the effective resolved shear stress, the velocities of the dislocations are given by:

$$\begin{cases} v_i = 0 & \text{if } \tau^* < 0, \\ v_i = \mathrm{sign}(\tau^{**})\frac{\tau^* b}{B} & \text{if } \tau^* \geqslant 0, \end{cases} \tag{2}$$

where $B$ is the drag coefficient factor. Its value was obtained at the atomistic level for both basal and prismatic slip systems [15], and an average value between the two slip systems was taken for this study. Although the velocity rule has a simple form and does not explicitly take into account the temperature effect, such a rule allows the modeling of the temperature effect in an indirect way by changing the value of the friction stress. Furthermore, the anisotropy of the velocity as a function of the dislocation character revealed by Groh et al. [15] is not taken into account in the present work. In the following, a simple model to investigate the influence of the anisotropic lattice friction on the single mechanism of the collinear interaction will be introduced in Section 2.1. Additionally, the massive model to investigate the influence of the anisotropic lattice friction on the macroscopic response will be given in Section 2.2.

### 2.1. Geometry of the collinear interaction under anisotropic lattice friction

As demonstrated by Madec et al. [18], the collinear interaction, which corresponds to the interaction between two dislocations with collinear Burgers vector gliding in intersecting slip planes, is the strongest reaction that can occur between dislocations during deformation. For this reason, to amplify the effect of the initial anisotropy of the CRSS, this work focuses on the collinear interaction between the basal and the prismatic slip systems in hcp Mg. In 2006, Monnet and Devincre [20] investigated the effect of irradiation in steel by uniformly changing the lattice friction on all slip systems. With such a strategy, these authors characterized the intrinsic annihilation reaction and the recombination stress, which is the critical shear stress required to destroy the collinear interaction, as a function of the lattice friction. However, in hcp crystals, an anisotropy of slip was demonstrated by molecular dynamics (MD) calculations, and therefore, the geometry of the junctions and their strengths must be characterized as a function of non-uniform lattice friction. In the presence of different lattice frictions on intersecting slip planes, Fig. 1 illustrates the initial configuration of the dislocation reaction and the geometry of the collinear interaction, respectively. In Fig. 1(a), $2L_1$ and $2L_2$ are the lengths of the initial dislocation lines on the prismatic and the basal slip systems, respectively. $\beta_1$ and $\beta_2$ are the angles between the dislocation lines and the intersection line of the slip planes. $b$ is the Burgers vector. In the present work, a dislocation with line direction $1/3[\bar{1}\,\bar{1}\,2\,0]$ from the basal plane making an angle $\beta_2 = 60°$ with the reaction direction, $1/3[2\,\bar{1}\,\bar{1}\,0]$, intersects a dislocation line with line direction $1/3[2\bar{1}\bar{1}\bar{3}]$, lying in the prismatic slip system and making an angle $\beta_1 = 58.5°$ with the reaction direction, $1/3[2\,\bar{1}\,\bar{1}\,0]$. The initial lengths for both dislocation lines are set to 3.9 μm. As shown in Fig. 1(b), without external loading, the dislocation tree segments (the segments from the intersected point to the endpoint of the dislocation line) bend against the friction stress into a circular arc of radius $R$, joining smoothly at the original straight position [21,22]. The annihilation distance, $X$, can be found by deriving an expression for the angle, $\varphi$, for both slip systems as a function of the initial dislocation orientations, $\beta_1$ and $\beta_2$, the length, $L_2$, and the radius of the curvature on the prismatic slip systems, $R$. The annihilation distance is then given by numerically solving the following equation:

$$\pi - \beta_1 - \arccos\left(1 - \frac{X}{2}\frac{1}{R}\sin\beta_1\right) = \arctan\frac{L_2 \sin\beta_2}{L_2\cos\beta_2 - X/2}. \tag{3}$$

Based on the work of Lavrentev et al. [21], the radius of the arc in Eq. (3) can be expressed as:

$$R = \frac{T}{\tau^{\mathrm{prismatic}}_{\mathrm{friction}} b} \approx \frac{\alpha\mu b}{\tau^{\mathrm{prismatic}}_{\mathrm{friction}}} \quad \text{with } \alpha \approx 0.5\text{—}1.0. \tag{4}$$

Although $\alpha = 1$ was considered in the work of Monnet and Devincre [20], a value of $\alpha$ between 0.5 and 1 may be considered to account for the dislocation character involved in the junction [23]. In that case, the model presented by Monnet and Devincre [20] is an upper bound for the prediction of the annihilation distance as a function of the lattice friction. The lower bound is then given when $\alpha = 0.5$. When considering the hcp crystal structure, the anisotropy in the lattice friction results in different magnitudes of the radius of the arc on the basal and the prismatic slip systems. As the lattice friction of Mg basal slip systems is small compared to the one acting on other slip systems, the radius of the arc is large on the basal slip system and therefore, the dislocation tree segments on the basal slip system can be assumed to be straight and only the radius of the arc on the prismatic slip systems is taken into account in the present study.

In finding a numerical solution for Eq. (3), one can find the annihilation distance as a function of the friction stress exerting on the prismatic slip system. Unlike the model reported for the isotropic friction stress [20], which predicts linear variations of the annihilation distance with respect to the inverse of the friction stress, the annihilation distance does not increase linearly with decreasing friction stress when anisotropic lattice friction is considered.

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[1] "mM" is an open source code for DDD simulations originally developed at the Laboratoire d'Etude des Microstructures (CNRS-ONERA) and now available under the terms of the GNU GPL.