Computational Materials Science 138 (2017) 236–245

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Modeling the mechanical response and microstructure evolution of magnesium single crystals under c-axis compression

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ARTICLE INFO

Article history:
Received 13 February 2017
Received in revised form 14 June 2017
Accepted 19 June 2017

Keywords:
Dislocation dynamics
Plasticity
Magnesium
Pyramidal slip
C-axis

ABSTRACT

Atomistically informed multiscale dislocation dynamics plasticity (MDDP) framework is used to investigate the mechanical response and microstructure evolution in bulk magnesium single crystals subjected to c-axis compression. The MDDP framework was modified to account for the ⟨c + a⟩ dislocation slip on the pyramidal I and pyramidal II planes. Several aspects of the ⟨c + a⟩ dislocation reactions such as the transition of pyramidal I near edge and pyramidal II pure edge segments to basal plane, and the thermally activated cross slip are considered. Additionally, a generalized mobility law and anisotropic frictional stress models are implemented based on the findings of several molecular dynamics studies. MDDP predictions of the yielding and strain hardening behaviors, as well as the maximum stress prior to failure are in good agreement with the reported experimental values. Moreover, detailed study of the dislocation microstructure evolution and the dislocation density dependence on the applied stress are presented and compared with available experimental results.

1. Introduction

In recent years, Hexagonal Close-Packed (HCP) materials such as magnesium (Mg), titanium and their alloys have attracted the attention of many research groups. Due to the ever increasing need for energy efficiency, the search for lightweight material is an active area of research. Magnesium, the lightest of all metals, provides great promise, and induce automotive and aircraft industries to replace denser materials with Mg-based alloys. Despite having many attractive properties, plastic anisotropy and the relatively low ductility influence the use of magnesium as a structural material. Therefore, detailed understanding of the relationship between the microstructure of Mg and its mechanical properties such as yielding, toughness, and strain hardening is very crucial in the design of Mg based components.

Plastic deformation in HCP metals takes place primarily by dislocation slip and twinning. Dislocation slip may occur on basal, prismatic, pyramidal I, and pyramidal II planes. Twinning on the other hand can be either compressive or tensile and forms on planes different from the dislocation slip planes. Due to the high anisotropy exhibited by HCP metals, the stress required to activate their deformation modes is very dependent on the orientation. In Mg, for example, basal slip of Burgers vector ⟨a⟩ is known to be the easiest at all temperatures [1–5]. This is also true for metals with c/a ratio less than the ideal one (1.63); such as cadmium and zinc. As the c/a ratio increase, as in titanium, prismatic planes become more closely packed than basal plane and thus prismatic slip becomes more dominant. While the ⟨a⟩ slip on the basal and the prismatic planes is fairly understood, the nature of deformation via ⟨c + a⟩ slip that may occur on the pyramidal I and pyramidal II planes is under debate. Specifically, it is of paramount interest to aluminate on slip activation and interaction under c-axis compression which is necessary to fulfill von-Mises criterion for homogeneous deformation of polycrystalline deformation [6].

Under c-axis compression, plastic deformation in Mg can be accommodated by ⟨c + a⟩ slip on pyramidal I and pyramidal II planes. Since the dislocation core structures on these two families of pyramidal planes are different, it is expected that the activation energy, Peirels barrier, and dislocation mobility will also be different. While in theory the ⟨c + a⟩ slip can be activated on both pyramidal I and II planes, most of the early experimental investigations [7–11] and some of the recent experimental [12] and molecular dynamics studies [13–17] reported that c-axis deformation in Mg single crystals can be accommodated by ⟨c + a⟩ slip on pyramidal II planes. However, recent reexaminations of slip traces pointed out on the activation of pyramidal I rather than pyramidal II slip [18]. This is also supported by recent slip trace analyses of Mg

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http://dx.doi.org/10.1016/j.commatsci.2017.06.022
0927-0256/

single crystals subjected to room temperature c-axis compression showing the activation of pyramidal I rather than Pyramidal II planes [19].

In addition to the c-axis macro-compression experiments [7,20–22] Mg single crystals have been investigated at small scale using micro-compression experiments [23–26]. In all these compression experiments, Mg exhibits unusually strong strain hardening and low ductility. This behavior is primarily attributed to the formation of sessile dislocation junction from the activated ⟨c + a⟩ dislocations [7,8,20,21]. Additionally, while strong size effect was reported in microcrystals [24,25], Byer and Ramesh [26] demonstrated that size effect may disappear in samples with high initial dislocation density.

Along with these experimental investigations, first principle [27,28] and atomistic [13–18,29–31] computations have been utilized in the hope to provide better understanding of the nature of the ⟨c + a⟩ slip on pyramidal planes. Density Functional Theory (DFT) studies of the core structures of ⟨c + a⟩ dislocations on the pyramidal II planes revealed that the critical resolved shear stress required for gliding a screw dislocation is higher than that of an edge one [27]. Itakura et al. [28] carried out large scale ab initio calculations in Mg and reported that screw dislocation is more stable on pyramidal II planes than on pyramidal I. However, they also showed that dislocation core transition to pyramidal I plane occurs during glide. Moreover, El-Awady and coworkers [18,29–31] conducted MD computations on the critical resolved shear stress (CRSS) and mobility of ⟨c + a⟩ dislocations of different characters placed on pyramidal I and pyramidal II Planes. The main findings of these investigations are; 1 – The CRSS is very sensitive to temperature, 2 – At low temperatures (below 360 K), pyramidal I near screw dislocation exhibits the lowest CRSS 3-The near edge dislocation on pyramidal I and the pure edge dislocation on pyramidal II planes always decompose. It is therefore plausible based on the slip trace analyses [18,19] and MD evidences that ⟨c + a⟩ glide is predominant of pyramidal I planes.

While atomistic simulations are crucial for understanding the underlying physics of ⟨c + a⟩ slip, they are limited in size, and thus may not be suitable to complete the picture of the observed mechanical response of HCP metals. Dislocation dynamics on the other hand, can utilize the necessary parameters obtained from atomistic simulations to accurately capture the main features of the mechanical response. Discrete dislocation dynamics (DDD) simulations have been extensively used to unravel several aspects of plasticity in both FCC and BCC metals. However, limited DDD investigations of the deformation in HCP metals have been reported. Monnet et al. [32] performed DDD simulations of single crystals zirconium for prismatic glide in which mobility law for screw and non-screw dislocations was implemented. Capolungo [33] developed an anisotropic DDD elasticity framework applicable to HCP metals and found that the difference between the anisotropic and isotropic computations is negligible. Additionally, Bertin et al. [34] carried out DDD simulations to obtain the hardening parameters of the slip systems in Mg single crystals. Recently, HCP slips have been incorporated in ParaDiS simulator in which dislocation segments are allowed to dissociate into partials coupled with a mobility law that depends on the dislocation segment orientation [35]. Aitken et al. [36] implemented HCP slip in DDD and employed it to simulate the mechanical response of Mg microcrystals. Under the assumption that pyramidal II slip is activated, they showed strong hardening and significant size effects under c-axis compression.

From the above discussion, it is obvious that the deformation mechanisms under c-axis compression in Mg single crystals are subject to discussion, as prior works have often been controversial or inconclusive. This motivates us to study the deformation and slip in Mg single crystal oriented for c-axis compression using multiscale dislocation dynamics plasticity (MDDP) analyses. MDDP was originally developed for FCC and BCC metals. In this work, the modifications incorporated in MDDP to account for slip in HCP structure are described. This include MD informed generalized mobility law and a lattice friction model [18,29–31] applicable to Mg single crystals. We then illustrate the capabilities of the developed model to predict the mechanical response of Mg undergoing c-axis compression.

2. Methodology

2.1. Multiscale dislocation dynamic plasticity (MDDP)

MDDP [37–43] is hybrid elasto-viscoplastic simulation model coupling DDD with finite element (FE) analysis. DDD is used to determine plastic deformation in single crystals by the evaluation of the dislocation evolution history. Dislocation lines and curves are represented by discrete straight segments. At each time step, the Peach-Koehler (PK) force is computed by accounting for all force components arising from: Peierls barrier ($F_{Peierls}$), dislocation-dislocation interaction (F_D), self-force (F_{self}), interaction with obstacles ($F_{obstacle}$), image forces (F_{image}), and externally applied loads ($F_{External}$). Thus the total glide force on each dislocation segment i can be expressed as:

$$F_i = F_{Peierls} + F_D + F_{self} + F_{External} + F_{obstacle} + F_{image} \tag{1}$$

The dynamics of dislocations is governed by a "Newtonian" equation of motion, consisting of an inertia term, viscous damping term, and driving force term such that;

$$m_i \dot{v}_{gi} + \frac{1}{M_i} v_{gi} = F_i \tag{2}$$

In the above equations, m_i is the effective dislocation segment mass, M_i is the dislocation mobility which depends on the dislocation segment orientation, v_{gi} is the segment glide velocity. The equation of motion is then solved to find the velocities and thus the plastic strain rate $\dot{\varepsilon}^p$ and the plastic spin W_p are evaluated respectively:

$$\dot{\varepsilon}^p = \sum_{i=1}^{N} \frac{l_i v_{gi}}{2V} (n_i \otimes b_i + b_i \otimes n_i) \tag{3}$$

$$W^p = \sum_{i=1}^{N} \frac{l_i v_{gi}}{2V} (n_i \otimes b_i - b_i \otimes n_i) \tag{4}$$

where l_i is the dislocation segment length, n_i is a unit normal to the slip plane, and V is the volume of the representative element. The above relations provide the most rigorous connection between the dislocation motion (the fundamental mechanism of plastic deformation in crystalline materials) and the macroscopic plastic strain, with its dependence on strength and applied stress being explicitly embedded in the calculation of the velocity of each dislocation.

In the macro level, it is assumed that the material obeys the basic laws of continuum mechanics, *i.e.* linear momentum balance and energy balance:

$$div\ \mathrm{S} = \rho \dot{\mathrm{v}} \tag{5}$$

$$\rho C_v \dot{T} = \eta S . \dot{\varepsilon}^p \tag{6}$$

In the above equations, S is the Cauchy stress tensor, T is the temperature, v_p is the particle velocity, ρ, C_v and K are mass density, specific heat and thermal conductivity respectively. For elasto-viscoplastic behavior, the strain rate tensor $\dot{\varepsilon}$ is decomposed into an elastic part $\dot{\varepsilon}^e$ and plastic part $\dot{\varepsilon}^p$ such that: