



Effects of normal stresses on the homogeneous nucleation of a basal dislocation in magnesium



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ABSTRACT

A quantitative evaluation of the deformation of metals is usually based on the critical resolved shear stress (CRSS), in which the influence of the normal stresses is not taken into account. Although it is plausible to use the CRSS for a quantitative evaluation of the deformation mode, some previous studies show that the CRSS depends on other stress components. In this work, atomistic simulations are performed to study the influence of the normal stresses on the nucleation of basal dislocations in a magnesium single crystal. We found that the activation free energy of dislocation nucleation decreases as the normal stress applied in the $[1\ 1\ 2\ 0]$ direction decreases, or that in the $[000\ 1]$ direction increases. This tendency is consistent with the dependence of CRSS on the loading direction found in a previous work done by Barrett et al. (2012) on molecular dynamics simulations of tensile deformation tests of a magnesium single crystal.

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1. Introduction

Magnesium (Mg) is strongly expected to be applied to various industrial products because of its light weight and rich remaining reserve in the Earth. However, the hexagonal close packed (HCP) structure of Mg causes a strong anisotropy of deformation in comparison with face-centered cubic metals. Hence, it is important to understand the deformation behavior of Mg in detail for further application of it. Some experimental works [1–5] are devoted to the elucidation of the deformation mode in Mg. In laboratory experiments, the critical resolved shear stress (CRSS) provides a quantitative indicator of the ease of occurrence of each deformation mode. Furthermore, the Schmid factor plays an important role in understanding the active deformation mode when a load is applied to a single crystal. However, in experiments on the biaxial loading of a zinc single crystal [6], it is observed that the normal tensile stress on the slip plane decreases the CRSS by approximately 30%. In addition, recent work on the uniaxial tensile deformation of a Mg single crystal via molecular dynamics (MD) simulation shows that the nucleation of a slip dislocation and a twin in Mg does not obey the Schmid law; that is, the resolved shear stress when the crystal begins plastic deformation depends on the loading direction, even if the same deformation mode

becomes active [7]. There are other works supporting the fact that stress components other than the resolved shear stress affect plastic deformation [8–10], but a role of these stress components during plastic deformations is still unclear.

In the present study, we focus on the nucleation of a basal dislocation loop in a Mg single crystal when a normal stress in one direction and a shear stress in the slip direction on the basal plane are applied. To this end, we performed atomistic simulations of a Mg single crystal without any defects under the applied stresses. To evaluate the activation free energy of the nucleation of a dislocation loop, the MD simulation is combined with the metadynamics method [11,12] with one collective variable, which was developed in previous works [13,14].

The rest of this paper is organized as follows. The models used in this work and some details of the simulation procedure are described in Section 2. Section 3 is devoted to an analysis of the simulation results. We discuss the dependence of the activation free energy of dislocation nucleation on the normal stress from point of view of energetics of dislocations. Moreover, we show that the results of our analysis are consistent with the non-Schmid behavior observed in an MD simulation of the tensile deformation of a Mg single crystal [7]. Section 4 is a conclusion.

2. Model and simulation procedure

Hereafter, the $[1\ 1\ 2\ 0]$, $[\bar{1}\ 1\ 0\ 0]$, and $[000\ 1]$ directions are designated as the x , y , and z directions, respectively. First, a Mg single

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crystal whose dimensions are L_x , L_y , and L_z in the x , y , and z directions, respectively, is prepared. N Mg atoms are placed at the regular positions of the HCP structure in region D_0 , which is defined by

$$D_0 = [-0.5L_x, 0.5L_x] \times [-0.5L_y, 0.5L_y] \times [-0.5L_z, 0.5L_z], \quad (1)$$

and the periodic boundary conditions are applied in all directions in order to eliminate the effects of free surfaces. In the present work, we set $(L_x, L_y, L_z) = (100a, 50\sqrt{3}a, 10\gamma a)$, where a and γ are the lattice constant and the axis ratio of Mg, respectively. Then, $N = 2 \times 10^5$ atoms are contained in D_0 . Below, $\mathbf{r}_i \in D_0$ ($i = 1, 2, \dots, N$) signifies the position of the Mg atom labeled i . The equations of motion are integrated by the scheme developed by Shinoda et al. [15], where the temperature T , which is set to 300 K in this work, is maintained via N ose–Hoover’s thermostat [16,17] and, as in the Parrinello–Rahman method [18,19], the strain energy due to the deformation of the simulation box is taken into account in order to maintain each stress component $\sigma_{\alpha\beta}$ ($\alpha, \beta = x, y, z$) at the designated value. The system is equilibrated at $T = 300$ K and zero hydrostatic pressure before the application of stresses.

The interaction potential V_{int} among Mg atoms is evaluated via the embedded atom method [20], which takes following form:

$$V_{\text{int}}(\mathbf{R}) = \sum_{i=j+1}^N \sum_{j=1}^N \phi(r_{ij}) + \sum_{i=1}^N F(\rho_i), \quad (2)$$

where $\mathbf{R} \equiv \{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N\}$, r_{ij} is the distance between the atoms labeled i and j , and ρ_i is expressed as

$$\rho_i = \sum_{j=1, j \neq i}^N \rho(r_{ij}). \quad (3)$$

Several sets of functions $\phi(r)$, $F(\rho)$, and $\rho(r)$ are proposed for Mg [21–23] according to properties that one wants to reproduce by the potential. In the present work, we use functions proposed by Sun et al. [21], which are obtained on the basis of the force matching method [24]. This potential results in many material properties that are consistent with experiments or first-principles calculations [21], e.g., $a = 0.3184$ nm and $\gamma = 1.628$ at $T = 0$ K. Moreover, this potential enables the successful reproduction of the structure of basal dislocation cores obtained from first-principles calculations [25].

In general, dislocations can be nucleated with the aid of thermal fluctuation, even if the applied stresses are insufficient to overcome the barrier for dislocation nucleation. However, the MD simulation is originally not suited for an analysis of the thermal activation observed in laboratory experiments because of the time-scale restriction. To overcome this difficulty, we adopted the metadynamics method [11,12], which is often used for the analysis of various thermal activation phenomena in the fields of chemistry and biology. In previous works [13,14], the metadynamics method was applied to dislocation nucleation, and it was confirmed that dislocations were successfully nucleated. Here, we briefly explain the method used in those works.

In the metadynamics method, to accelerate the dynamics of the collective variable \mathbf{X} , which is chosen in advance, the following history-dependent bias potential is added to the system:

$$V_{\text{bias}}(\mathbf{X}; n_{\text{MD}}) = h \sum_{j=1}^{n_{\text{meta}}} \exp \left(- \sum_{k=1}^d \frac{(\tilde{X}_k(jn_{\text{add}}) - X_k)^2}{2\delta X_k^2} \right), \quad (4)$$

where n_{MD} is the number of MD steps; n_{add} is the interval of the MD steps over which the bias potential is accumulated; n_{meta} is defined by the quotient of n_{MD} and n_{add} ; $\tilde{X}_k(jn_{\text{add}})$ is the value of the k th component of \mathbf{X} at jn_{add} MD steps; and h and δX_k are the height and width of the Gaussian function, respectively. The bias potential

accumulated until the occurrence of the activation phenomenon enables us to evaluate the activation free energy.

To realize a desirable phenomenon by the metadynamics method, it is important to select the appropriate \mathbf{X} depending on the problem. In our previous works [13,14], which treat the nucleation of a dislocation in a Mg single crystal, the following one-dimensional collective variable is adopted:

$$X(\mathbf{R}) = \sum_{i=1}^N (\mathbf{r}_i \cdot \mathbf{e}_s) \left[\frac{1_{D_u}(\mathbf{r}_i^0)}{N_u} - \frac{1_{D_l}(\mathbf{r}_i^0)}{N_l} \right], \quad (5)$$

where D_u (D_l) represents the region just above (below) the nucleation site, which is designated as the origin in this study; \mathbf{r}_i^0 is the regular lattice point of the atom labeled i ; \mathbf{e}_s is the unit vector along the slip direction; and $1_D(\mathbf{r})$ signifies the indicator function

$$1_D(\mathbf{r}) = \begin{cases} 1 & \mathbf{r} \in D \\ 0 & \mathbf{r} \notin D \end{cases}. \quad (6)$$

N_u and N_l are defined by

$$N_u = \sum_{i=1}^N 1_{D_u}(\mathbf{r}_i^0), \quad N_l = \sum_{i=1}^N 1_{D_l}(\mathbf{r}_i^0).$$

The intent behind the use of Eq. (5) is that the bias potential tries to force the atoms included in D_u to separate in the slip direction from those in D_l . According to Ref. [14], D_u and D_l are set to

$$\begin{aligned} D_u &= D(R) \times [0, 0.5\gamma a], \\ D_l &= D(R) \times [-0.5\gamma a, 0], \end{aligned} \quad (7)$$

where the two dimensional region $D(R) = \{(x, y) | x^2 + y^2 \leq R^2\}$. Previous study [14] shows that the activation free energy evaluated by the metadynamics method is not sensitively dependent on R . In this work, we choose R so that N_u and N_l are between 100 and 500. This choice of D_u and D_l leads to successful reproduction of homogeneous nucleation of dislocation as shown in Fig. 3 in Ref. [14]. In the next section, we discuss the dependence of the activation free energy of the nucleation of a basal dislocation loop on the normal stress applied to the crystal.

3. Results

In Fig. 1, we plotted the behavior of the activation free energy of the nucleation of a basal dislocation loop when the normal stress in one direction is applied in addition to the shear stress σ_{xz} . If the normal stress is fixed, the activation free energy monotonically decreases as σ_{xz} increases. When σ_{xx} is applied, the activation free energy of the nucleation of a dislocation increases with σ_{xx} . In other words, the compressive stress in the x direction decreases the activation free energy, whereas the tensile stress increases it. In contrast, when σ_{zz} is applied, the activation free energy decreases as σ_{zz} increases. However, the activation free energy is relatively insensitive to σ_{yy} in comparison with that for cases of σ_{xx} and σ_{zz} .

We discuss interpretation of the tendency observed in Fig. 1 from point of view of energetics of dislocations. The energy E_{dl} of a partial dislocation is simply divided into three contributions, that is, the elastic energy E_{el} due to the strain induced by the dislocation, the work E_{work} done by the applied stress, and stacking fault energy E_{sf} . E_{el} and E_{work} are dependent on the magnitude of the Burgers vector. When normal stresses whose magnitudes are not too large are applied to the crystal, it elastically deforms, which leads to a change in the spacing between atoms while preserving the regularity of the configuration. In Fig. 2, we plotted the dependencies of the magnitude b of the Burgers vector for basal slip, i.e., the distance between two adjacent atoms in the slip direction, and the spacing h between two adjacent basal planes on the normal

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