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Shearing single crystal magnesium in the close-packed basal plane at different temperatures

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ABSTRACT

Shear behaviors of single crystal magnesium (Mg) in close-packed (0001) basal plane along the $[\bar{1}2\bar{1}0]$, $[1\bar{2}10]$, $[10\bar{1}0]$ and $[\bar{1}010]$ directions were studied using molecular dynamics simulations *via* EAM potential. The results show that both shear stress-strain curves along the four directions and the motion path of free atoms during shearing behave periodic characteristics. It reveals that the periodic shear displacement is inherently related to the crystallographic orientation in single crystal Mg. Moreover, different temperatures in a range from 10 to 750 K were considered, demonstrating that shear modulus decreases with increasing temperatures. The results agree well with the MTS model. It is manifested that the modulus is independent with the shear direction and the size of the atomic model. This work also demonstrates that the classical description of shear modulus is still effective at the nanoscale.

1. Introduction

Magnesium (Mg), as a common and lightweight metal, can potentially be more widely used as a structural material in applications especially when weight-saving is crucial. However, mechanical properties and applications accordingly of wrought Mg are somewhat restrict due to the lack of deformability caused by the inherent limited number of slip system in the hexagonal-close-packed (hcp) crystal structure [1–6]. On this account, it is important to study the deformation and process of such materials to explore their wider applications. It is well known that dislocations and stacking faults are crucial effects on the plastic deformation for metallic materials [7,8], where the shear modulus is a vital parameter in describing the characteristics of the two effects. Therefore, a fundamental knowledge of shear modulus is thus significant for describing plastic behaviors of such materials in their response to dislocations and/or stacking faults.

For now, several works have been carried out to study the elastic properties of Mg and Mg-alloys. Counts et al. [5] used *ab initio* simulations to calculate the elastic parameters for designing bcc Mg-Li alloys. Groh et al. [9] studied evolution of the elastic properties including elastic constants, bulk, and shear moduli, and anisotropic index of hcp Mg-Ti-B alloy by using first-principle simulations. Yamagishi et al. [10] determined the mechanical properties of extruded pure Mg during tension-tension low-cycle fatigue using ultrasonic testing. In addition, many theoretical methods have been investigated to show the temperature-dependent behavior of shear modulus. Varshni et al. [11] proposed the mechanical threshold stress (MTS) model to describe the evolution of shear modulus with respect to temperature. In our previous works, shear moduli of hcp Ti [12] and fcc Ni [13] and Cu [14] crystals have been investigated in different orientations and temperatures by using Molecular dynamics (MD) simulations. To our knowledge, little work has been done for shear behaviors of hcp Mg at different temperatures using MD simulations. Additionally, the applicability of a classical description for shear modulus of hcp crystal structure at nanoscale still needs more evidence.

In this work, the MD method was applied to investigate shear behaviors of single crystal hcp Mg along the $[\bar{1}2\bar{1}0]$, $[1\bar{2}10]$, $[10\bar{1}0]$ and $[\bar{1}010]$ directions at different temperatures. We show that shear stress-strain curves are of periodic characteristics, and that shear behaviors are anisotropic in the two orthogonal (e.g. $[\bar{1}2\bar{1}0]$ and $[10\bar{1}0]$) directions. Shear modulus obtained from the curve shows a size-independent feature and a decrease tendency with increasing temperatures. Those simulation results are in good agreement with the MTS model.

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2. Model and simulation method

A three-dimensional (3D) orthogonal simulation box for shear test was built with cross-sectional area in 3.5 nm × 3.1 nm, while the dimension in the [0001] direction varies for each simulation case, as shown in Fig. 1. Atoms in the top and bottom three layers were held fixed, named fixed layers, while the remaining part was simulated as in free motion, namely free layers, respectively. Shear experiments were carried out by displacing the top fixed layers parallel to the bottom fixed layers in the close-packed (0001) crystallographic plane along $[\bar{1}2\bar{1}0]$, $[1\bar{2}10]$, $[10\bar{1}0]$ and $[\bar{1}010]$ directions, respectively. Periodic boundary conditions were utilized to the system in directions parallel to shear plane.

MD simulations were implemented by LAMMPS code [15]. The forces between atoms in the simulation system were calculated using an EAM potential, which was specially developed for metals [16,17] and was proved to be able to well describe the metallic bonding in crystal Mg [18]. In the simulations, the equations of motion were integrated with a time step of 0.5 fs. A constant strain rate of 0.005% ps^{-1} was applied to displace the top fixed atomic layers horizontally in four shear directions. After each imposed displacement increment, the structure was relaxed for a time of 5 ps. Shear tests were carried out at 10, 150, 300, 450, 600, 750 K, respectively. In all simulations, the system temperature was controlled by rescaling the velocities of atoms. In this paper, shear modulus is calculated from classical description. The detailed method has been reported elsewhere [12–14].

3. Results and discussion

Shear behaviors of hcp single crystal Mg with various sizes at low temperature (i.e. 1.0 K) was explored firstly. Fig. 2 shows the shear stress-strain curves along the $[\bar{1}2\bar{1}0]$, $[1\bar{2}10]$, $[10\bar{1}0]$ and $[\bar{1}010]$ directions of Mg with different number of free atomic layers along the [0001] direction. It can be seen that shear stress increases with increasing strain up to a critical value, and then drops gradually with a further increase of strain, followed by oscillations around zero. It should be mentioned that the curves perform periodic behaviors along with shearing in these four directions. Here only first period is illustrated for a clear vision. Similar shear performance has also been observed in fcc and hcp Ti crystals during shearing process [12–14], which shed deep insight into the inherent relationship between periodic displacement and atomic distance in corresponding crystallographic orientation in these materials.

As seen from Fig. 2(a) that when a shear is carried out along the $[\bar{1}2\bar{1}0]$ direction the shear stress-strain curve behaves one period with the strain $\varepsilon = 0.62$ for Mg with one free atomic layer; however, the period

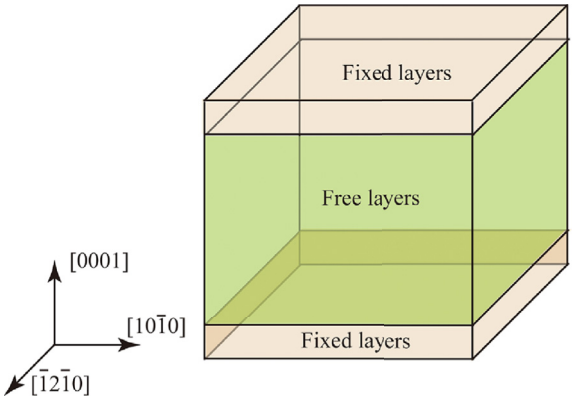

Fig. 1. Shear setups with fixed layers on top and bottom regions, and the remaining part in light green is free layers. Shear tests were carried out in the $[\bar{1}2\bar{1}0]$, $[1\bar{2}10]$, $[10\bar{1}0]$ and $[\bar{1}010]$ directions, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

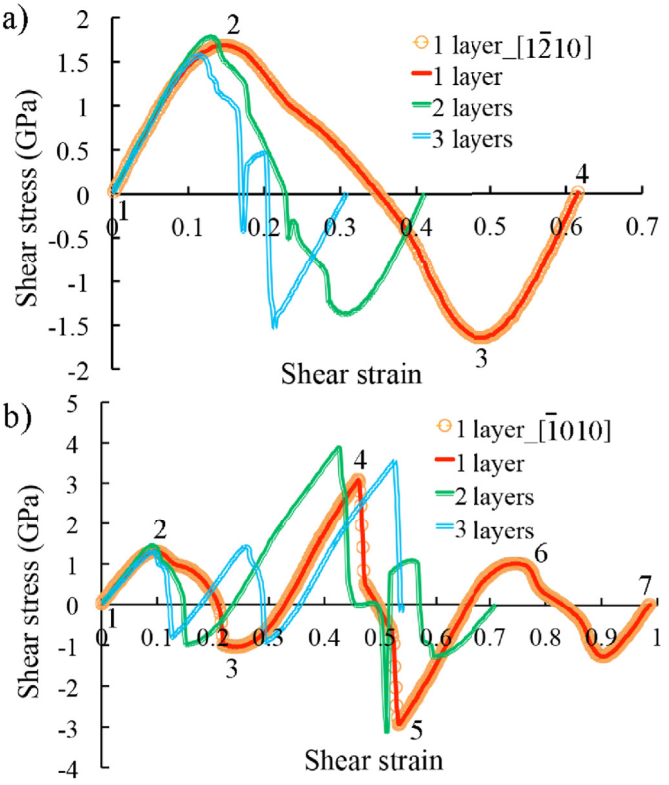

Fig. 2. Shear stress-strain curves of single crystal Mg at 10 K with different number of free atomic layers when shear is imposed along the (a) $[\bar{1}2\bar{1}0]$ and opposite, (b) $[10\bar{1}0]$ and opposite directions, respectively. The signs with numerical numbers denote the special points in the curves.

shortens to be $\varepsilon = 0.41$ and 0.31 for models with two and three free atomic layers, respectively. Interestingly, the periodic strain corresponds to the same shear displacement a, where a denotes the lattice constant. When shearing along the $[10\bar{1}0]$ direction, a similar periodic phenomenon occurs, i.e. the periodic strain of the shear stress-strain curve decrease with increasing model layers, as shown in Fig. 2(b). Here, one period of the strain corresponds to the same shear displacement $\sqrt{3}a$. It should be noted that these shear displacements (i.e. a and $\sqrt{3}a$ along $[\bar{1}2\bar{1}0]$ and $[10\bar{1}0]$ directions) are the same with distances between two neighboring atoms along corresponding directions. This can be interpreted from the perspective of the atomic configuration of hcp Mg. Fig. 3(a) illustrates a close-up 3D view of a normal hcp lattice of Mg. The *ABAB* … basal planes are marked with different colors. In Fig. 3(b), we take the projection view along the [0001] direction (perpendicular to the c axis). It can be seen that the distances between two neighboring atoms are arranged to be a and $\sqrt{3}a$ along $[\bar{1}2\bar{1}0]$ and $[10\bar{1}0]$ directions, respectively. In other words, shear displacement for one period of shear stress-strain curve is equal to the atomic arrangement period in corresponding crystallographic orientation in hcp crystals.

It also can be seen from Fig. 2 that shear stress-strain curves of $[\bar{1}2\bar{1}0]$ and $[10\bar{1}0]$ directions are totally the same with their counterparts of opposite directions, indicating that shear behaviors are the same along opposite directions in close-packed (0001) basal plane. Moreover, the curves in $[10\bar{1}0]$ and $[\bar{1}010]$ directions shown in Fig. 2(b) perform obviously more perturbations than those in $[\bar{1}2\bar{1}0]$ and $[1\bar{2}10]$ directions shown in Fig. 2(a), which relates to atomic paths during shear process.

For a better interpretation of the different shear stress-strain response, the trajectory of free atoms along the $[\bar{1}2\bar{1}0]$, $[1\bar{2}10]$, $[10\bar{1}0]$ and $[\bar{1}010]$ directions is traced during shear process, as illustrated in Fig. 4. It can be seen that the red atom initially located at site 1 where is the center of the triangle formed by three atoms underneath, corresponding to the origin