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Shearing single crystal copper in molecular dynamics simulation at different temperatures

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ABSTRACT

Molecular dynamics simulations using the embedded atom method (EAM) potential were carried out to study shear behaviors of single crystal copper at different temperatures. Shear tests were set in the (1 1 1) crystallographic plane along the $[\bar{1}\,1\,0]$ and $[1\,1\,\bar{2}]$ directions, respectively. The period of shear stress–shear strain curves was observed when shear was set along the $[\bar{1}\,1\,0]$ direction. Microtwins arose during the shear process along the $[1\,1\,\bar{2}]$ direction. Shear modulus obtained from the slop of shear stress–shear strain curves is on the level of 40.0 ± 1.5 GPa at 0 K and decreases with increasing temperature, and performs insensitivity to the size of shear model and shear direction. Simulation results also indicate that the EAM potential is adequate to describe the shear behaviors of single crystal copper. In addition, this work also shows that the classical description of shear modulus is still efficient at the nanoscale, which might suggest a simple and direct way to obtain shear modulus in atomic scale.

1. Introduction

Dislocations and stacking faults are important microstructures in most metallic materials, which have well-known crucial effects on the plastic deformation of materials and the processes such as work hardening [1,2]. In the theory of deformation of crystals, both of those mechanisms intimately relate to the shear modulus. In classical theory, shear modulus is defined as the ratio of shear stress to shear strain, which measures the rigidness of materials. In materials science, shear modulus is an important parameter to describe the characters of dislocations, such as stress fields and strain energy of a dislocation, forces between dislocations, stacking fault energy. On that account, knowledge of shear modulus is fundamental for describing plastic behavior of metallic materials in their response to dislocations and stacking faults.

To date, several theoretical methods are investigated to calculate the shear modulus, such as numerical models [3,4] and molecular dynamics (MD) simulations [5,6]. Heino et al. [5] simulated shear modulus of copper at room temperature using an MD method with effective-medium theory. Luo et al. [6] applied the quantum Sutton–Chen potential *via* MD simulations to study shear modulus of nickel as a function of temperature. Varshni [3] proposed the mechanical threshold stress (MTS) model to describe the evolution of shear modulus with respect to temperature. Although some numerical modeling of shear modulus of face-centered crystals has been reported, to our knowledge little work has been done for single crystal copper at different temperatures using MD simulations with an EAM potential. Additionally, the applicability of a classical description for shear modulus at nanoscale remains unclear.

In this work, shear modulus of single crystal copper was investigated *via* MD simulations using an EAM potential at different temperatures along the $[\bar{1}\,1\,0]$ and $[1\,1\,\bar{2}]$ shear directions, respectively. We show that there is no appreciable difference of shear modulus along those two shear directions. The modulus is insensitive to the size of the shear model and decreases with increasing temperature. Those simulation results are in good agreement with the MTS model and show that the classical description of shear modulus is still efficient at the nanoscale.

2. Model and simulation method

An orthogonal simulation box for testing shear was built with cross-sectional dimension in 3.5 nm × 3.1 nm, while the dimension in the [1 1 1] direction varies for each simulation cases, as shown in Fig. 1. Atoms in the top and bottom three layers were held fixed, named rigid group and fixed group, respectively, while the remaining part was simulated as in free motion, namely free group. The rigid and fixed group in all models used in this study consist 576 atoms, respectively, while the number of atoms in free group varies around 2000 depending on the numbers of atomic

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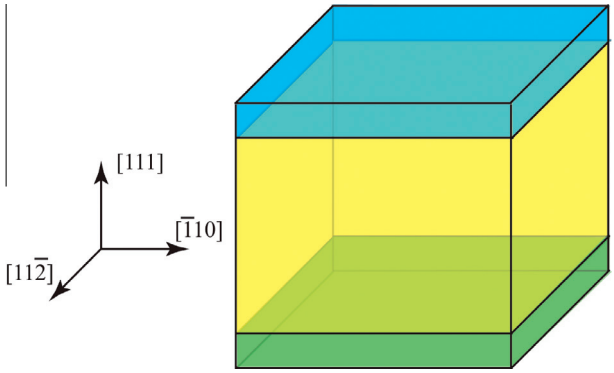

Fig. 1. Shear setups with fixed group and rigid group in green and blue, respectively. The remaining part in yellow is free group in which atoms are free to relax in time. Shear tests were carried out in the [$\bar{1}$10] and [11$\bar{2}$] directions, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

layers. Shear experiments were investigated *via* displacing the rigid group parallel to the fixed group in the (111) crystallographic plane. Periodic boundary conditions were imposed to the system in directions parallel to shear plane.

MD simulations were performed with LAMMPS, a classical MD code that models an ensemble of particles in a liquid, solid, or gaseous state. Short- or long-range forces are modeled with Newton's equations of motion for collections of atoms with a variety of initial and/or boundary condition (http://lammps.sandia.gov). A constant strain rate of 0.005% ps^{-1} was applied to displace the rigid group horizontally in the [$\bar{1}$10] and [11$\bar{2}$] directions, respectively. After each imposed displacement increment, the structure was relaxed for a time of 5 ps. The forces between atoms in the simulation system were calculated *via* an EAM potential, which was specially developed for metals [7,8] and was proved to be able to well describe the metallic bonding in single crystal copper [9]. In the simulations, the equations of motion were integrated with a time step of 0.5 fs, where the velocities of atoms were rescaled to control the temperature of the entire system.

In this paper, shear modulus is computed as following

$$G = \frac{\tau}{\varepsilon} \tag{1}$$

where τ denotes shear stress, ε is shear strain, which are defined as

$$\tau = \frac{f}{A}, \varepsilon = \frac{\Delta x}{l} \tag{2}$$

where f denotes applied shear force, A is the area that force acts on (the cross-section of model in this work), Δx is applied displacement due to applied shear force, l is the height of free group along the [111] direction in the shear model. The applied shear force in those two shear directions (fx or fy) [10] can be determined by imposing a displacement on the rigid group.

3. Results and discussion

Shear behaviors of a single crystal of copper with different heights of the free group were explored. Here the number of free atomic layers normal to the [111] direction corresponds to the height of the free group. Fig. 2 presents shear stress–shear strain curves of copper at 0 K with different specified numbers of free atomic layers when shear is set along the [$\bar{1}$10] and [11$\bar{2}$] crystallographic directions, respectively. As can be seen from Fig. 2(a), shear stress increases with increasing shear strain up to a threshold value that is defined as the shear strength, but further increase in shear strain leads to a steep drop of stress. Interestingly, the stress decreases to a negative value and oscillates around zero as shear strain increases and then presents the same tendency as initial. It can be said that the shear stress–shear strain curves behave periodically. Our calculation shows that when the shear displacement is $\frac{\sqrt{2}}{2} * a$, where a denotes the lattice constant, the shear stress–shear strain curve completes one period for a model with one free atomic layer. It should be noted from Fig. 2(a) that two and three periods occur for models with three and five free atomic layers when shear displacement is $\sqrt{2} * a$ and $\frac{3\sqrt{2}}{2} * a$, respectively, corresponding to the same shear strain ($\varepsilon = 0.62$). In other words, more periods of shear stress–shear strain curve occur, with the same shear strain, for models with more atomic layers. Note that shear distance with $\frac{\sqrt{2}}{2} * a$ results in one period of shear stress–shear strain curve, independent with the number of free atomic layers in shear model. For the cases with shearing in the [11$\bar{2}$] direction, as shown in Fig. 2(b), a different phenomenon of the shear stress–shear strain appeared. A series of vibrational perturbations emerge at the beginning of the shear stress–shear strain curve, followed by periodic variations. This behavior might be related to the atomic trajectory during shearing in the [11$\bar{2}$] direction, which will be addressed later.

The trajectory of atoms was traced during the shear procedure. Fig. 3 displays the schematic of the trajectory of a specified atom colored in red in the free group moving in the (111) plane along the [$\bar{1}$10] and [11$\bar{2}$] directions, respectively. Obviously, the red atom is initially located at the center of the blue triangle formed by three blue atoms, as indicated with site ①. With increasing shear strain, blue atoms are frozen at their ideal positions, and the red atom moves from site ① to ② along the shear direction at the beginning, where translational motion varies when shear is set along different directions. When further shear is applied along the [$\bar{1}$10] direction, as shown in Fig. 3(a), the red atom cannot overcome the obstacle formed by two blue atoms and instead moves from site ② to ③, followed by a series of deviations before returning to the original site where the shear starts, performing the same configuration as initial status, as indicated with sites ① and ⑥. This period in the trajectory of atoms corresponds to the period of shear stress–shear strain curve. By contrast, when shear is set along the [11$\bar{2}$] direction, the red atom moves in the triangle I at the beginning of shear, then traverses the barrier between the two peaks comprised of two blue atoms, and arrives at triangle II, as shown in Fig. 3(b). As shear continues, the atom moves forward the peak shaped by one blue atom, leading to increasing stress until maximum value, as indicated with label ⑥ in Fig. 2. And then the atom cannot traverse the peak and moves to triangle III through the valley between two blue atoms. Finally, it locates at the center of triangle III. Considering the periodic boundary condition in the [$\bar{1}$10] and [11$\bar{2}$] directions, the final configuration presents the same with initial one, as indicated with sites ① and ⑧. The trajectory of atoms relates to the stress they are suffering. During one period motion in [11$\bar{2}$] direction, the red atom passes three triangle areas successively with more special locations than those when shearing in the [$\bar{1}$10] direction with the same numbers of free atomic layers, which can explain why vibrational perturbations appear when shear was set along the [11$\bar{2}$] direction. It should be mentioned that twinning and stacking faults easily occur when shear is along the [11$\bar{2}$] direction [11], which was also observed in this study, as shown in Fig. 4. It can be seen that many microtwins appear during shear process in the [11$\bar{2}$] direction. Particularly, the more free atomic layers, the more opportunities for the formation of twinning and stacking faults. This might also take responsibility for vibrations of shear stress–shear strain curves and more vibrations for models with more free atomic layers, as shown in Fig. 2(b). As a result, shear stress–shear strain curves have differing characteristics at the beginning stage of the shear test along the [$\bar{1}$10] and [11$\bar{2}$] shear directions, respectively.