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Atomic simulations of the effect of twist grain boundaries on deformation behavior of nanocrystalline copper

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ABSTRACT

The effects of twist grain boundary (GB) on the mechanical properties of two types of nanocrystalline copper (Cu) under tensile loading are investigated by molecular dynamics simulation. The results indicate that the plasticity of bicrystalline Cu with a high twist angle is much better than that of structure with low twist angle, due to the blockage of dislocations' motion by twist GBs. However, the plasticity of trifurcate crystal Cu is better in low twist angle structure. The studies demonstrate that these different deformation behaviors are associated with the nucleation and propagation of dislocations. The results also show that regardless of crystalline types, the Young's modulus of nanocrystalline Cu slightly increases with increasing twist angle. The general conclusions derived from this work may be of importance in devising high-performance face-center cubic metal with different GBs.

1. Introduction

The structure of grain boundary (GB) is generally considered to be an important factor in determining the nucleation and propagation of the dislocations. In recent years, the deformation behavior of grain boundaries (GBs) in nanocrystalline metals has drawn considerable interest, and has been extensively studied by experiments and molecular dynamics (MD) simulations [1–15]. One of the main motivations for the research comes from the expectation of unprecedented mechanical properties. Sansoz et al. [15] studied the mechanical behaviors of tilt GBs in nanoscale copper (Cu) and aluminum (Al) using molecular simulations and shown that the deformation of the boundaries is found to operate by three modes depending on the GB equilibrium configuration: GB sliding by uncorrelated atomic shuffling, nucleation of partial dislocations from the interface to the grains, and GB migration. Li et al. [16] investigated the dislocation nucleation governed softening and maximum strength in nanocrystalline Cu with a kind of special GB: nanotwins. The results indicated that dislocation nucleation governs the strength of such materials, resulting in their softening below a critical twin thickness. An and Song [17] investigated the influence of twin boundary on the crack propagation in nanocrystalline Al with different initial crack orientations, and presented that the mechanical properties are extremely different for various initial crack orientations in nanotwinned Al. Chen et al. [18] investigated the strength of a nickel bicrystal under compression. They found that the misorientation angle for the bicrystal have significant effect on the dislocations nucleation and the strength of nickel bicrystal. Wang et al. [19] simulated the mechanical deformation of bicrystalline Cu nanowires with three different boundaries. Liu et al. [20] studied the tension response of bicrystal Cu with twist GB by using MD simulation. Very recently, Trautt et al. [21] applied a combination of MD and phase field crystal simulations to investigate stress-driven motion of asymmetrical GBs between Cu bicrystals over the entire range of inclination angles. As mentioned above, the studies on the deformation mechanisms of twist GB so far are mostly focused on examining the deformation behaviors of twist GB in bicrystalline metals, where the tensile-loading direction perpendicular to GB [22–26]. However, the studies on the effect of twist GB on the mechanical behavior of bicrystalline metals, where the twist boundary does not perpendicular to the direction of tensile loading, are still very rare [21]. The deformation mechanism of bicrystalline metals under various loading conditions is different [27]. The clarification of the mechanical behavior of the bicrystalline metals under these loading conditions is crucial. Here, we investigate the effect of twist grain boundary on the tensile deformation behavior of two types of crystalline Cu (see Fig. 1 for illustration) using our MD simulation codes. The study results show that twist angle plays an important role in determining the mechanical properties of Cu.

The rest of the paper is organized in the following way. In Section 2 we describe the simulation model and method for MD simulation. Section 3 provides results and discussion. Finally, some concluding remarks are given in Section 4.

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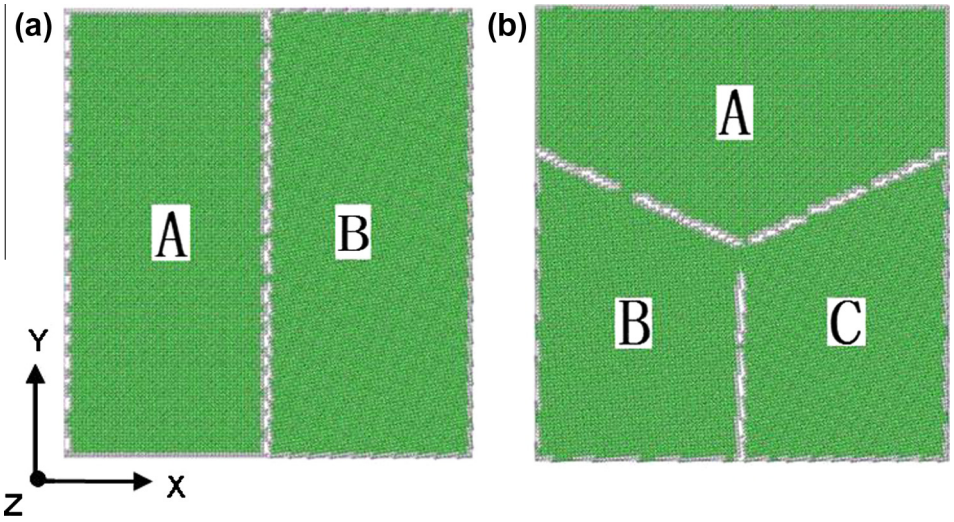

Fig. 1. The atomic structures of two types of crystalline Cu with twist grain boundary: (a) the bicrystalline Cu; (b) the trifurcate crystal Cu.

2. Simulation model and method

Here, MD simulations are performed to study the mechanical properties of two types of crystalline Cu with twist boundaries under tension loading. The initial configurations used in the present study are shown in Fig. 1. In the first structure, the bicrystal model consists of two grains labeled as Cu A and Cu B for the case of a twist [1 0 0] GB, as shown in Fig. 1. The GB plane is parallel to the direction of tension (i.e. *Y* axes). The initial orientation of the Cu B region is the same as that of the Cu A region, which is then anticlockwise rotated about the *Z* axes by an angle θ. In the second structure, trifurcate crystal Cu is labeled as Cu A, Cu B and Cu C. The misorientation angle (or twist angle) for the trifurcate crystal is obtained by fixing the Cu A, and anticlockwise rotating the Cu B and Cu C around the *Z* axes by an angle θ and 2θ, respectively. The dimensions of the simulation system in the *x*-, *y*- and *z*-directions are about 20.0, 22.0 and 3.6 nm, respectively. Periodic boundary condition is applied in *z*-direction, while free surface is used for the *x*-direction. The number of atoms in both the samples approximately is 133,500. A constant strain of 0.001 is applied to the sample in *y*-direction. Here, strain is introduced by adjusting the *y*-coordinate of five layer atoms both at the top and at the bottom during the simulation. The simulation process includes the following steps: relaxing the initial configurations to reach the equilibrium states, applying a constant strain 0.001 to the models in *y*-direction and keeping 0 bar pressure in the *x*-directions, then the *y*-direction boundary is fixed and the system is relaxed 1500 time steps to reach a new equilibrium state and a new configuration.

The tight-binding potential [28] is used for modeling the interactions between Cu atoms. The Verlet algorithm is used to integrate the equations of motion. A time step of 3 fs is used in all MD simulations. The Nose–Hoover thermostats [29] are applied so as to keep the system temperature constantly of 300 K. For the purpose of visualizing defects in the nanocrystalline Cu, colors are assigned to atoms according to the local crystal structure of atoms by common neighbor analysis [30]. This is implemented by using the Open Visualization Tool [31]. The analysis and classification of each atom according to its environment help us to identify the various deformation mechanisms during tension loading. Here, the hexagonal close-packed (hcp), face-centered cubic (fcc) and non-structured atoms (often existing on the grain boundary or at the dislocation core) are colored red, green and gray, respectively.

The average stress in current study is calculated by using the Virial theorem [32,33], which is expressed by:

$$\sigma^{\alpha\beta} = \frac{1}{\Omega}\left[-\sum_i m_i v_i^{\alpha} v_i^{\beta} + \frac{1}{2}\sum_i \sum_{j\neq i} F_{ij}^{\alpha} r_{ij}^{\beta}\right] \quad (1)$$

where the $\sigma^{\alpha\beta}$ stands for the average stress, and Ω is the total volume of all the atoms. The first part of in the right side of Eq. (1) is a kinetic energy component for atom *i*, while the second part is produced due to the inner-atom force. m_i and v_i^{α} (or v_i^{β}) are the mass and velocity of atom *i*, and F_{ij}^{α} is the force between atom *i* and atom *j*, where the indice α, β denote the Cartesian components. r_{ij}^{β} is the distance vector between atom *i* and atom *j* along coordinate β.

3. Results and discussion

The tension behaviors of two types of crystalline Cu with different twist angles are investigated using the MD simulation method for the comparison purpose. The typical stress–strain curves for the first structure and the second structure are shown in Fig. 2a and b, respectively. It can be observed from Fig. 2 that both curves show a rather abrupt drop after reaching the peak stress, regardless of twist angle and structure. For the first structure, the stress rapidly reduce to zero in the cases with twist angle 6° and 8° after the yield stress, as shown in Fig 2a. However, in the cases of the twist angle 10°, 12°, and 26°, the stress is observed to decrease gradually to an approximately steady value, after linearly increasing with strain up to peak stress, meaning an approximate stable flow stress. In another word, the flow stress for the first structure with relative high twist angle is much higher than that with low twist angle, where the flow stress is nearly zero, implying the ductility of the former is better than the latter. The results also show that the effect of twist angle on the peak stress of the first structure is not obvious when the twist angle is larger than 6°. For the second structure, the results in Fig. 2b show that the peak stress increases as the twist angle between Cu A and Cu B is increased from 5° to 6°, while there is a dramatic reduction for the peak stress as the twist angle increases to 7°. The stress transiently reduces to zero after the stress increases up to a peak when the twist angle is larger than 6°. As is shown from Fig. 2b, the plastic response of the second structure with relative low twist angle (for example 5° and 6°) is much better than high twist angle (for example 12° and 16°), where the flow stresses is nearly zero. The following illustrations