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A dual deformation mechanism of grain boundary at different stress stages

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ABSTRACT

Molecular dynamics (MD) simulation with embedded-atom method (EAM) potential was carried out to study the structure and shear response of an asymmetric tilt grain boundary in copper bicrystal. A non-planar structure with dissociated intrinsic stacking faults was observed in the grain boundary. Simulation results show that this type of structure can significantly increase the ductility of the simulation sample under shear deformation. A dual deformation mechanism of the grain boundary was observed; the grain boundary can be a source of dislocation emission and migrate itself at different stress stages. The result of this study can provide further information to understand the grain boundary mediated plasticity in nanocrystalline materials.

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1. Introduction

Compared with conventional coarse-grained materials, nanocrystalline materials show a lot of advanced performances [1,2], which stimulated widespread interest in the mechanical properties and novel deformation mechanisms of nano-sized materials. The deformation mechanisms of metals with the average grain size in the nanometer range are studied extensively in the past two decades [3,4]. Grain boundary (GB) has been confirmed to play an important role in the mechanical behavior of nanocrystalline metals by both experimental observations and atomistic simulations. The identified deformation mechanisms in nanocrystalline metals include GB sliding [5,6], grain rotation [7–9], GB migration [10–13], dislocation sink in or nucleate from GBs [14–16].

Most of the previous work show that single deformation mechanism can be activated for a certain GB. For example, by using molecular dynamics (MD) simulation, Qi and Krajewski [6] showed that GB sliding is the primary deformation mechanism in bicrystal Al under a shear force. Cahn et al. [9] found that all of the $<0\,0\,1>$ symmetric tilt GBs in Cu can migrate coupled to a shear deformation. Zhang et al. [16] observed that dislocation nucleation dominant the mechanism of a deformed Cu with $<1\,1\,0>$ symmetric tilt GBs under tension. By using the quasi-continuum method, Sansoz and Molinari [17] correlated individual failure mechanisms to certain GBs. In tension, failure of the GBs occurred via partial dislocation nucleation and GB cleavage. In shear, they reported three different failure modes depending on the boundary structures: GB sliding by atomic shuffling, nucleation of partial dislocations from GB, and GB migration. To the best of the author's knowledge, a dual deformation mechanism of the same GB has rarely reported previously. Also, the computer modeling of GBs has been mostly focused on symmetrical GBs, which possess mirror symmetry of crystallographic planes. In contrast, very few atomistic simulations have been conducted on the asymmetric GBs. In this study, we reported a $\Sigma 11$ asymmetric GB with a non-planar structure that can play a role as dislocation source and migrate itself at different stress stages under shear deformation.

2. Methodology

Molecular dynamics simulation was carried out to study $\Sigma 11$ $(2\,2\,5)/(4\,4\,1)$ $\Phi = 54.74°$ asymmetric tilt GB in Cu bicrystal. The simulation was carried out using the parallel molecular dynamics code LAMMPS [18] with the embedded-atom method (EAM) potential for Cu developed by Mishin et al. [19]. A bicrystal model was created by constructing two separate crystal lattices with different crystallographic orientation and joining them together along the Y axis (see Fig. 1). A periodic boundary condition was applied in the *X* and *Z* directions while a non-periodic boundary condition was applied in the *Y* direction. The equilibrium structure of the GB was obtained by the energy minimization procedure and the subsequent MD relaxation in the isobaric-isothermal (NPT) ensemble at a pressure of 0 bar and a temperature of 300 K for

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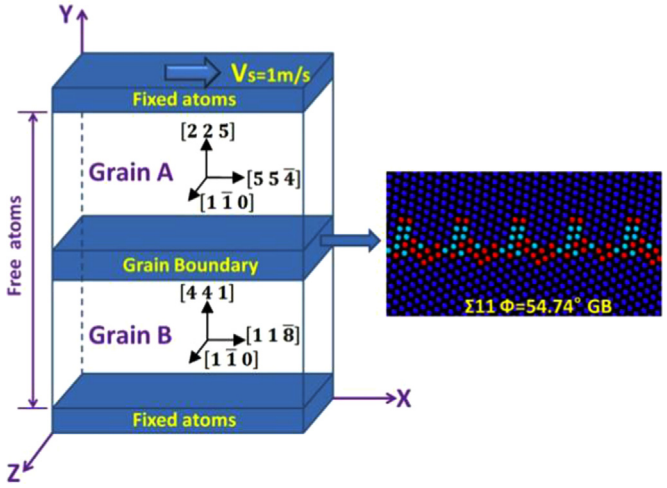

Fig. 1. Schematic of the simulation model. A constant shear velocity $V_s=1$ m/s parallel to the boundary plane was applied during the shear deformation. The atomic configuration shows the equilibrium structure of the Σ11(2 2 5)/(4 4 1) ($\Phi=54.74°$) asymmetric GB. The images are viewed along the [1 $\bar{1}$ 0] tilt axis and are colored according to the common neighbor analysis (CNA) parameter. Atoms with perfect fcc structures are colored with blue, the red atoms represent the GB plane and the dislocation core, the light blue atoms represent the stacking fault.

20 ps. As shown in the atomic configuration in Fig. 1, the equilibrium Σ11($\Phi=54.74°$) asymmetric GB shows an obvious non-planar structure with an intrinsic stacking fault that dissociated from the boundary plane.

Once the equilibrium state of GB was reached, a shear deformation was applied to bicrystal model. Atoms on the top of grain-A and atoms at the bottom of grain-B were fixed, the thickness of each fixed slab was approximate twice the cutoff radius of atomic interactions [10], while all the other atoms in the model were set free. A constant shear velocity $V_s=1$ m/s (about 4.6×10^7/s shear strain) parallel to the boundary plane was applied to the fixed area of grain-A in the $+X$ direction. Throughout the MD simulation, the NPT ensemble was adopted and the time increment of simulations was fixed at 1 fs. Stress and temperature calculations were performed on the dynamic atoms between the two fixed slabs. In atomic level, the stress is computed according to the virial theorem by the formula:

$$\sigma_{ij}=\frac{1}{V}\sum_{\alpha=1}^{N}\left(\frac{1}{2}\sum_{\beta=1}^{N}r_{\alpha\beta}^{i}F_{\alpha\beta}^{j}-m^{\alpha}v_{i}^{\alpha}v_{j}^{\alpha}\right) \quad (1)$$

Where i, j are Cartesian coordinates and α and β are atom index numbers. m and v denote to the mass and velocity of the atom. $r_{\alpha\beta}$ and $F_{\alpha\beta}$ are respectively the distance and force between two atoms with index α and β. V is the volume of the system and with number of total atoms N.

Generally, if a dislocation is subjected to stress, it tends to move through the crystal. This motion is the mechanism for plastic flow in a crystalline solid. The tendency of a dislocation to move can be described by Peach–Koehler formula [20], which states that the driving force for dislocation motion can be computed from the following equation:

$$\boldsymbol{F_L}=\left(\boldsymbol{b}\cdot\sigma_{ij}\right)\times\boldsymbol{\xi} \quad (2)$$

where $\boldsymbol{F_L}$ is the force per unit length of dislocation, this is essentially F/L for a straight dislocation where L is the length of the dislocation line; $\boldsymbol{b}$ is Burger vector of a given dislocation; σ_{ij} is the stress tensor and $\boldsymbol{\xi}$ is the line vector of the dislocation. For a mixed dislocation (with both screw and edge characteristics) of which the tangent to the dislocation line is neither parallel or perpendicular to the Burgers vector, let $\boldsymbol{b}=(b_xb_yb_z)$, $\boldsymbol{\xi}=(\xi_x\xi_y\xi_z)$ and $g=\boldsymbol{b}\cdot\sigma_{ij}$, then:

$$\begin{aligned} g_x &= b_x\sigma_{xx}+b_y\tau_{xy}+b_z\tau_{xz}\\ g_y &= b_x\tau_{yx}+b_y\sigma_{yy}+b_z\tau_{yz}\\ g_z &= b_x\tau_{zx}+b_y\tau_{zy}+b_z\sigma_{zz} \end{aligned} \quad (3)$$

and

$$\boldsymbol{F_L}=\boldsymbol{g}\times\boldsymbol{\xi}=\begin{vmatrix} i & j & k\\ g_x & g_y & g_z\\ \xi_x & \xi_y & \xi_z \end{vmatrix} \quad (4)$$

This general form of the Peach–Koehler equation is used to calculate the magnitudes of the forces on and the forces between dislocations.

3. Result and discussion

The shear stress of the bicrystal model with Σ11(2 2 5)/(4 4 1)

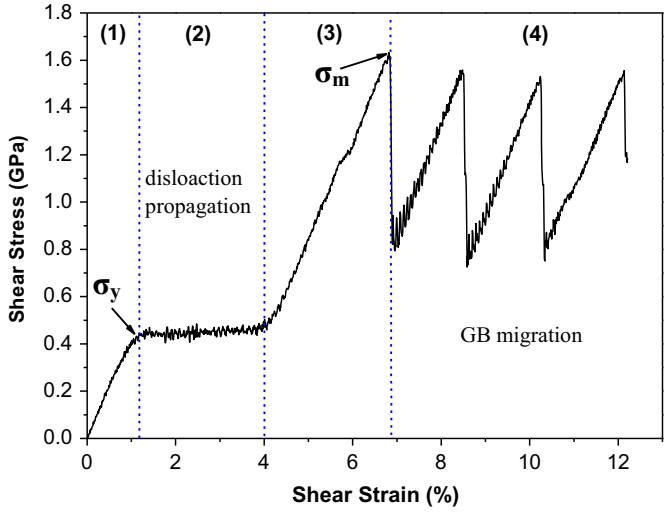

Fig. 2. The shear response of Cu bicrystal model with Σ11(2 2 5)/(4 4 1) $\Phi=54.74°$ asymmetric tilt GB at 300 K. The four deformation stages are indexed by (1) elastic (2) plastic (3) strain-hardening and (4) strain-softening.

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