경사진 <100> 결정립계의 계면분리 거동에 관한 분자동역학 전산모사

Decohesion of <100> Symmetric Tilt Copper Grain Boundary by Tensile Load Using Molecular Dynamics Simulation

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요 약

Debonding behavior of symmetric tilt bicrystal interfaces with <100> misorientation axis is investigated through molecular dynamics simulations. FCC single crystal copper is considered in each grain and the model is idealized as a grain boundary under mechanical loading. Embedded-Atom Method potential is chosen to calculate the interatomic forces between atoms. Constrained tensile deformations are applied to a variety of misorientation angles in order to estimate the effect of grain boundary angle on local peak stress. A new parameter of symmetric grain-boundary structure is introduced and refines the correlation between grain boundary angle and local peak stress.

Keywords: *Interface model, Copper, FCC, Cohesive zone*

1. Introduction

At nanoscale, debonding of grain boundary is one of the dominant failure mechanisms when structures are deformed. It is the high energy concentration that makes boundary surface easier to be debonded. In the present work, computational approach is used to study decohesion behavior in the copper grain boundary under tensile load.

The focus of present study is on the mechanism of interface failure behavior in <100>symmetric tilt bicrystal grain boundaries. Molecular statics and molecular dynamics simulations under tensile deforming have been performed to capture the mechanism of interface failure. The peak local stress calculated from simulation is then correlated with grain boundary angle and a new parameter of <100> symmetric tilt bicrystal structures.

2. Interface model

The present work has been performed using LAMMPS ("Large-scale Atomic/Molecular Massively

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Parallel Simulator") package for MS and MD simulation. Mishin's Embedded-Atom Method potential and virial stress were chosen to be interatomic potential and atomic stress, respectively.

2.1. Computational cell and boundary condition

The coincidence site lattice is used to generate the atomic position of grain boundary structure. At first, two identical grains are created. They are single crystals in rectangular parallelepiped shape, which has bottom face in {mn0} plane and two side faces in {001} plane. Then one grain is rotated 180° and translated to the bottom of the other so that they have identical atom arrangement in the interface. The obtained bicrystal is then called {mn0} grain boundary. All possible grain boundaries with the index $m^2+n^2 \leq 400$ is investigated in this study. At this stage, some atoms near the boundary are overlapped, i.e. too close from each other. Because overlapped atoms are physically unrealistic, some atoms near the boundary are removed in some overlap distances. For the purpose of increasing probability to access global minimum energy structure, a number of initial configurations should be considered (Wolf, 1989). In this study, 401 even overlap distances with the range from 1.2 Å to 5.2 Å are considered as initial configurations for each boundary. Removing atoms methodology to reach global minimum energy structures was introduced by Spearot. Varying the rigid-body translation of each grain was proposed as another method (Wolf, 1990).

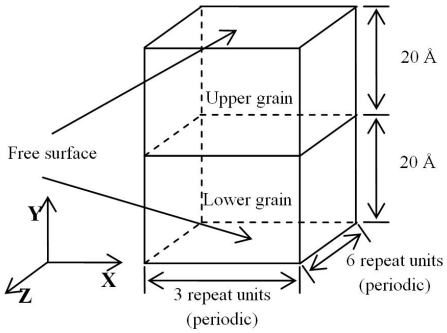

Fig. 1. Computational cell model

The geometry and dimensions of computational cell are shown in Fig. 1. Boundary condition is set to be periodic in X and Z direction. Free surface boundary condition is used in Y direction. Periodic dimensions are identified large enough to eliminate the effect of image cell on primary cell, i.e. L_x and L_z are larger than two times of cut off distance). Also L_x and L_z are taken to be multiples of periodic units because of periodic boundary condition.

2.2. Energy minimization and grain boundary energy

Energy minimization is implemented at 0 K for every overlap distances of each grain boundary seeking the lowest interface energy structure. The free surfaces are permitted to move parallel to boundary plane during energy minimization to allow volume expansion. Energy profiles of grain boundaries after minimizing energy have similar shapes. Energy at top and bottom boundary is higher due to the free surface. Near the boundary plane, energy has higher value than energy in the inner part

of each grain. In this study, interface region is defined as the region covering boundary plane and having top and bottom at 10 Å far from boundary plane. Average stress is calculated in interface region.

3. Deform interface at absolute zero

3.1 Tensile deformation installation

After minimizing energy at absolute zero, the structures are deformed but still keeping absolute zero. By fixing a group of atoms in the bottom and constantly moving a group of atoms in the top, the grain boundaries are stretched with constant strain rate $2.94 \times 10^{5} s^{-1}$ in Y-direction. The time step is 1 fs and simulation time is 1000 ps. Virial stress in Y direction is averaged in interface region and called local stress. The focus of this study is how peak value of local stress varies in the variation of symmetric tilt grain boundary.

3.1 Results and discussion

With misorientation angle smaller than 16° or larger than 83°, peak local stress shows large scatter in the variation of grain boundary angle (Fig. 2). This result could be understood as misfit angle approaches 0° or 90°, the structure approaches single crystal structure, and therefore tends to be harder to deform. This study concentrates on misfit angle from 16° to 83°, when the peak local stress mostly appears to have some correlation with the grain boundary angle. However, few grain boundaries have peak local stress fluctuate much from average tendency. The result raises a question of criterion to filter out those grain boundaries and how to calculate their peak local stress from their structure's index.

In this study, a new parameter is proposed to filter scattered peak local stress, which is named α defined as α =1/(m2+n2). With misfit angle from 16° to 83°, if angle with small α value (α <0.005) is considered only, the correlation between peak local stress and grain boundary angle is refined, expressing clearer relationship. Fitting peak local stress of small α angle by least square method, a function of peak local stress is obtained as,

$$\sigma_{\max} = a_1 + a_2\theta + a_3\theta^2 \tag{1}$$

(a_1=9.1701; a_2=0.2148; a_3=-0.0021)

To deal with scattered value of peak local stress, α is used to calculate the amount of fluctuation from the general tendency. From the graph of amount of fluctuation vs. α, linear least square method is chosen again to fit the amount of fluctuation and α.

$$Amount\ of\ fluctuation = b_1 + b_2\alpha \tag{2}$$

(b_1=0.0284; b_2=14.9533)

Combining (1) and (2), the peak local stress is then parameterized as

$$\sigma_{\max} = \left(a_1 + a_2\theta + a_3\theta^2\right) + \left(b_1 + b_2\alpha\right) \tag{3}$$

From error analysis, only two grain boundary {310} and {920} have percent of errors exceed 4%. For most of grain boundary structures, percent of errors are lower than 2%.

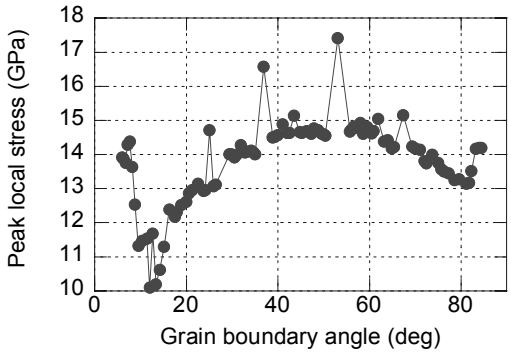

Fig. 2 Peak local stress vs. grain boundary angle on tensile loading

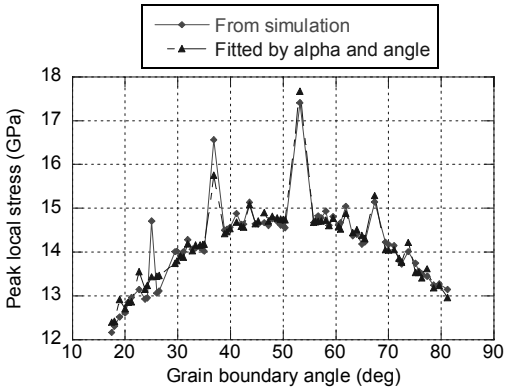

Fig. 3 Peak local stress and approximation value (4) vs. grain boundary angle on tensile loading

4. Conclusion

The methodology outlined in this paper is an initial step toward correlating the peak local stress and grain boundary structure in tensile loading. Using this methodology, the peak local stress was formulated in terms of grain boundary angle and a structure parameter, α. For the future work, local displacement and grain boundary energy evolution during deformation of grain boundary structures will be investigated. In addition, to capture the thermomechanical properties, molecular dynamics simulation will be performed at various finite temperatures.

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