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Influence of twist angle on crack propagation of nanoscale bicrystal nickel film based on molecular dynamics simulation

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ABSTRACT

Tensile deformation of nanoscale bicrystal nickel film with twist grain boundary, which includes various twist angles, is investigated via molecular dynamics simulation to obtain the influence of twist angle on crack propagation. The twist angle has a significant influence on crack propagation. At the tensile strain of 0.667, as for the twist angles of 0°, 3.54° and 7.05°, the bicrystal nickel films are subjected to complete fracture, while as for the twist angles of 16.1° and 33.96°, no complete fracture occurs in the bicrystal nickel films. When the twist angles are 16.1° and 33.96°, the dislocations emitted from the crack tip are almost unable to go across the grain boundary and enter into the other grain along the slip planes {111}. There should appear a critical twist angle above which the crack propagation is suppressed at the grain boundary. The higher energy in the grain boundary with larger twist angle contributes to facilitating the movement of the glissile dislocation along the grain boundary rather than across the grain boundary, which leads to the propagation of the crack along the grain boundary.

1. Introduction

In recent years, the development of molecular dynamics (MD) provides a more effective method for investigating the crack propagation in nanoscale. Many researchers have devoted themselves to investigating crack propagation in various materials [1–5] and at different interface [6–9] by means of MD simulation. Plenty of studies have shown that the direction of crack propagation and dislocation transmission is related closely to the orientation of preset crack. Therefore, most of the studies, which are associated with crack propagation, focus on the influence of the crack orientation on crack propagation. Sun et al. [10] investigated fracture behavior in ceria and gadolinia-doped ceria by means of MD method, where the results indicate that when no dopant is introduced, the crack propagates with the progression of local plastic deformation and no obvious dislocation emissions are observed for the cracks on the (001) and $(0\bar{1}1)$ plane, but the dislocation slip can be found during the process for crack propagation on the (111) plane. Xie et al. [11] investigated the effect of crack orientation on the twin formation from the crack tip in γ'-Ni_3Al by fabricating three types of crack and their simulation results show that (001)⟨110⟩ type crack produces two slip bands at the crack tip, while $(\bar{1}10)\langle 110\rangle$ and $(1\bar{1}\bar{1})\langle 110\rangle$ type cracks produce twins rather than slip bands at the crack tip, where the formation mechanism of the twin is based on the slipping of 1/6[112] type Shockley partial dislocations on consecutive {111} planes. Ma et al. [12] chose three typical models, in which they preset a center crack of [001](010), $[00\bar{1}](110)$ and $[11\bar{2}](111)$, respectively, in order to study the effect of orientation on fatigue crack propagation in iron single crystal, where as for the model of [001](010) crack, slip bands and cross slip are observed in front of crack tip and the corresponding slip system is ⟨111⟩{110}, while in the case of $[00\bar{1}](110)$ crack, the different slip system ⟨110⟩{110} is observed and the crack growth exhibits brittle cleavage, and for the $[11\bar{2}](111)$ crack, twins are dominant mechanism around crack tip and crack propagation rate is larger than that in the other directions. Liu et al. [13] investigated the influence of Re on the lattice trapping and fracture stress of the five orientation cracks in Ni by means of MD method and they found that Re–Ni interatomic interactions can prevent the breaking of atomic bonds and thus can heal cracks. Sung and Chen [14] investigated the crack propagation of pre-cracked single crystal nickel by virtue of MD simulation, and they found that partial dislocations begin to slip at the crack tip and propagate along the close-packed (111) plane until fracture. Wu et al. [15] investigated the growth of nanoscale fatigue crack in a single crystal nickel by introducing a cohesive zone model based on MD simulations, where the results show that under increasing strain amplitude cyclic loading, dislocations emit and persistent slip bands form around the fatigue crack tip, which plays an important role in retarding crack propagation and changing the stress distributions.

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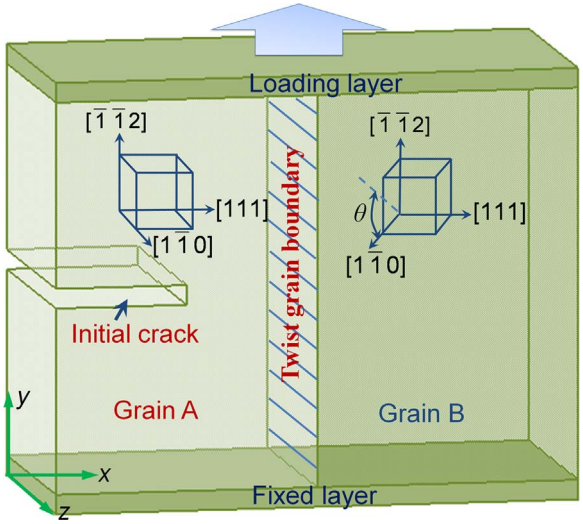

Fig. 1. Schematic diagram of nanoscale bicrystal nickel film with twist boundary used for MD simulation.

Besides the orientation of preset crack, grain boundary has a significant influence on the crack propagation as well. Zhao et al. [16] investigated the fracture behavior of several symmetric tilt grain boundaries in γ-TiAl bicrystals, where the tensile direction is perpendicular to the grain boundary, and their results show that tensile fracture mechanism of the bicrystals is that micro-cracks nucleate at the grain boundary and propagate along the interface. Adlakha et al. [17] explored the influence of grain boundary structure and the adjacent crystallographic orientation on the directional asymmetry of an intergranular crack for aluminum grain boundaries by means of MD simulation, and the corresponding simulation results from seven ⟨110⟩ symmetric tilt grain boundaries show that the grain boundary structure and the associated free volume directly influence the stress–strain response, crack growth rate and crack tip plasticity mechanisms for middle-tension crack propagation specimens. Zhou et al. [18] studied the propagation behavior of central cracks at different symmetrical tilt grain boundaries in bicrystalline copper by using atomistic simulations, and their results show that there are three different propagation modes for the interfacial crack, where the first mode is that the crack propagates in a brittle manner along grain boundary, and the second mode is that the crack propagates along with voids and coalescences ahead of the crack tip and blunts in the opposite direction, whereas the third mode is that the crack blunts at both two tips of the crack. Gao et al. [19] investigated the effect of twin boundary and stacking fault with different twist angles on crack propagation of nanocrystal Al by using MD simulation and they revealed that the twist angle of grain boundary may have a particular effect on crack growth and the grain boundary with an appropriate twist angle may hinder the propagation of crack effectively.

In the present study, influence of twist angle on crack propagation of nanoscale bicrystal nickel film with twist grain boundary is investigated based on MD simulation, which has never been reported in the literatures.

2. Simulation model and method

2.1. Simulation model

Fig. 1 indicates a three-dimensional MD model which is used for simulating influence of twist angle on crack propagation of nanoscale bicrystal nickel film with twist grain boundary. In the simulation, [111], [$\bar{1}\bar{1}$2] and [1$\bar{1}$0] directions were defined as the x-axis, the y-axis and the z-axis of the Cartesian reference frame, respectively. It is well known that nickel belongs to a face-centered cubic (FCC) structure. The size of the model is 30×35×5 unit cells, where the crystal lattice constant a is 0.352 nm for nickel. The bicrystal model is composed of grain A and grain B. An initial crack is preset in the grain A, where the length of the initial crack is 8 unit cells. A Cartesian coordinate is used in the model of interest, where the non-periodic boundary conditions are adopted. All the simulations are conducted at the temperature of 0.01 K so that thermal effects could be eliminated. The simulation process includes two steps as follows. Firstly, the initial configurations are relaxed at 0.01 K so that the energy is minimized. Secondly, a tensile loading is imparted to the system at a constant strain rate of $2.67\times10^{10}s^{-1}$. The various twist angles, which include $\theta = 0°$, $\theta = 3.54°$, $\theta = 7.05°$, $\theta = 16.1°$and $\theta = 33.96°$, respectively, are chosen in order to investigate the influence of twist angle on crack propagation of nanoscale bicrystal nickel film. In addition, bicrystal nickel film with twist angle of 0° is equivalent to a single crystal nickel film, where grain A and grain B are described by part A and part B in the following text, respectively.

2.2. Potential function

In the present study, the embedded-atom-method (EAM) potential developed by Foiles et al. [20] was used to describe the interactions among Nickel atoms. The EAM potential is expressed as

$$E_{\text{total}} = \sum F_i(\rho_{h,i}) + \frac{1}{2}\sum_i \sum_{j(\neq i)} \varphi_{ij}(R_{ij}) \quad (1)$$

where E_{total} is the total energy of the system, $(\rho_{h,i})$ is the host electron density at atom i due to the remaining atoms of the system, $F_i(\rho)$ is the energy for embedding atom i into the background electron density ρ, and $\varphi_{ij}(R_{ij})$ is the core-core pair repulsion between atoms i and j separated by the distance R_{ij}. It can be noted that F_i only depends on the element of atom i and φ_{ij} only depends on the elements of atoms i and j. The electron density is, as stated above, approximated by the superposition of atomic densities, namely

$$\rho_{h,i} = \sum_{j(\neq i)} \rho_j(R_{ij}) \quad (2)$$

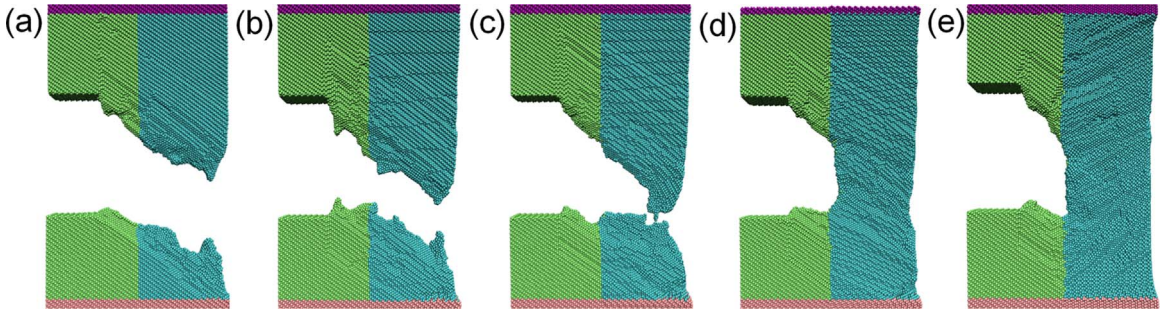

Fig. 2. Final deformation results of nanoscale bicrystal nickel films with various twist angles based on MD simulation: (a) $\theta = 0°$; (b) $\theta = 3.54°$; (c) $\theta = 7.05°$; (d) $\theta = 16.1°$; (e) $\theta = 33.96°$.