Computational Materials Science 95 (2014) 484–490

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Effects of twist twin boundary and stacking fault on crack propagation of nanocrystal Al

L. Gao [a], H.Y. Song [a,b,c,*], Y. Sun [a], Y.G. Zhang [a]

[a] School of Science, Xi'an University of Posts and Telecommunications, Xi'an 710121, China
[b] College of Materials Science and Engineering, Xi'an Shiyou University, Xi'an 710065, China
[c] School of Aeronautics, Northwestern Polytechnical University, Xi'an 710072, China

ARTICLE INFO

Article history:
Received 16 May 2014
Received in revised form 6 August 2014
Accepted 10 August 2014
Available online 6 September 2014

Keywords:
Twin boundary
Stacking fault
Crack propagation
Molecular dynamic simulation

ABSTRACT

The effect of twin boundary (TB) and stacking fault (SF) with different twist angles subjected to tension loading on crack propagation of nanocrystal Al is investigated using molecular dynamics simulation. The study reveals that the twist angle of grain boundary (GB) may have particular effect on crack growth, and that the GB with an appropriate twist angle may hinder the propagation of crack effectively. The results also indicate that for the models with twist TBs, the TBs with negative twist angles are more effective on obstructing crack propagation. Meanwhile, we found that the SF with positive twist angles hinder crack propagation more effectively than that of negative twist angles. It also shows that the GB disappeared during the deformation of the samples with SF twisted at −25° and −35°. Moreover, it is investigated from the results that the crack propagation rate varies with different temperatures, while the deformation mechanism is nearly unchangeable with the influence of the temperature. The study also demonstrates that the crack growth is related to nucleation of dislocations and twinning, as well as the deformation of GB.

© 2014 Elsevier B.V. All rights reserved.

1. Introduction

Since the criterion of brittle fracture was proposed by Griffith [1], fracture mechanism has been extensively investigated because of the fundamental role in deformation behavior of material [2–5]. Moreover, as one of the most important factors in fracture behavior of material, the crack propagation has been studied by various kinds of simulations and numerical experiments [6–10]. In recent years, the molecular dynamics (MD) has been widely used to investigate crack propagation process. Many studies indicate that the crack propagation and dislocation emission strongly depend on crack orientation due to different slip plans in front of crack tip induced by different crack orientation [11–16]. Therefore, there were more works focused on the effects of crack orientation on crack propagation [17–21]. However, previous studies also indicate that, despite the orientation of crack, there are many other factors can influence the growth of crack. Rafii-Tabar et al. [22] studied crack propagation in Ag plates containing different metallic nanoscale clusters of impurities located in the vicinity of the crack tip loaded by mode I. They found that the introduction of a hard obstacle in the vicinity of the crack tip results in an increase in the required critical load. Musazadeh and Dehghani [23] investigated the crack propagation as the crack tip located different types of impurities (Ag, Au, Cu and Pd). This study shows that when the shape of impurity is short cylinder, the rate of releasing energy during the crack propagation did not depend on the type of impurity. In addition, grain boundary (GB) also plays an important role in determining the nucleation and propagation of the dislocations [24]. Therefore, the effect of GB on the cracking mechanisms was taken into consideration. By simulating the crack crossed the GB, Xie et al. [25] found that the sliding of the {001}/{110} type and {110}/{111} type GB can improve the impact toughness. Recently, two special GBs, twin boundary (TB) and stacking fault (SF) have drawn considerable interest and have been extensively studied because of their unique characteristics [26–29]. Their studies show that TB and SF can obviously improve the mechanical properties of metals and they also find that these two boundaries have other unique characteristics. However, the studies on the effect of the relationship between crack propagation and twist TB or SF are still very rare. Here, we analyze the crack growth process in nanocrystal Al with edge crack and twist TB or SF by using MD with different twist angles subjected to uniaxial loading on crack propagation. The present study aims to reveal the effect of two kinds of GB with different twist angles on crack propagation. The study results show

* Corresponding author at: School of Science, Xi'an University of Posts and Telecommunications, Xi'an 710121, China. Tel.: +86 29 88166050.
E-mail address: gsfshy@sohu.com (H.Y. Song).

http://dx.doi.org/10.1016/j.commatsci.2014.08.016
0927-0256/© 2014 Elsevier B.V. All rights reserved.

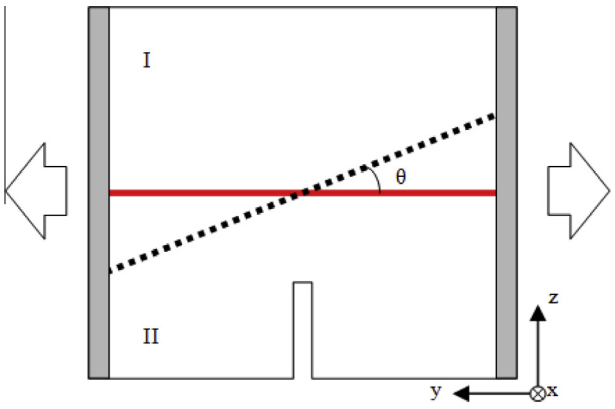

Fig. 1. Schematic of a simulated sample. The red interface represents the GB for the case of 0°, while the dashed line stands for the GB which twists of angle θ. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

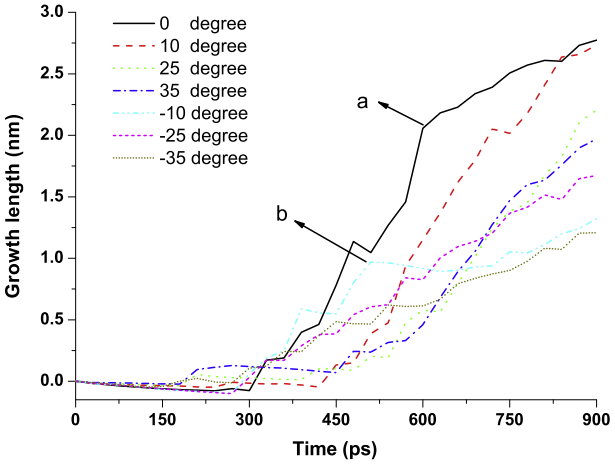

Fig. 2. The crack propagation distance as a function of loading time for the models with TBs twist different angles.

that twist GB plays an important role in hindering the propagation of crack. This work may be helpful to further understand the propagation behavior of crack in nanocrystal Al.

2. Model and method

As is indicated in Fig. 1, there are two kinds of GB: TB and SF. Both boundaries are twisted of angle θ ($\theta = 0°$, 10°, 25°, 35°, −10°, −25°, −35°). The length along X, Y and Z directions of the models are about 2.9 nm, 17.4 nm and 16.5 nm, respectively. An edge crack along Z-axis in grain II is introduced by removing the corresponding atoms. The size of the crack is about 2.9 nm(X) × 0.9 nm (Y) × 4.1 nm(Z). The number of the atoms in our models is about 49,000. Periodic boundary condition is applied in X-direction, while free boundary conditions are used in the Y- and Z-direction. Here, the embedded-atom-method (EAM) potential developed by Cleri and Rosato [30] is used to describe the interactions among Al atoms. This potential has been used to describe many fcc and hcp materials [21,26,29] and successfully reflect the mechanical properties. The potential equation is expressed by:

$$E_{tol} = \sum_i \sum_{j \neq i} A \exp\left[-p\left(\frac{r_{ij}}{r_0} - 1\right)\right] - \sum_i \left[\sum_{j \neq i} \xi^2 \exp\left[-2q\left(\frac{r_{ij}}{r_0} - 1\right)\right]\right]^{1/2} \quad (1)$$

where the former is related to the interaction between a pair of atoms and the latter stands for the interaction of each atom with the local electrons with respect to the remaining atoms in the system. The parameters for the interactions between Al atoms are given in Ref. [30]. A time step of 3 fs is used in all MD simulations. In addition, a constant force $\Delta F = 0.016$ nN per step is applied to the samples along Y directions in mode I on the two gray parts. For the purpose of visualizing defects in the nanocrystal Al, colors are assigned to the atoms according to a local crystallinity classification visualized by using common neighbor analysis (CNA) [31], which has the capability of detecting whether an atom is in a hexagonal close-packed (hcp) environment or in a face-centered cubic (fcc) environment. The Open Visualization Tool (OVITO) [32] is used to

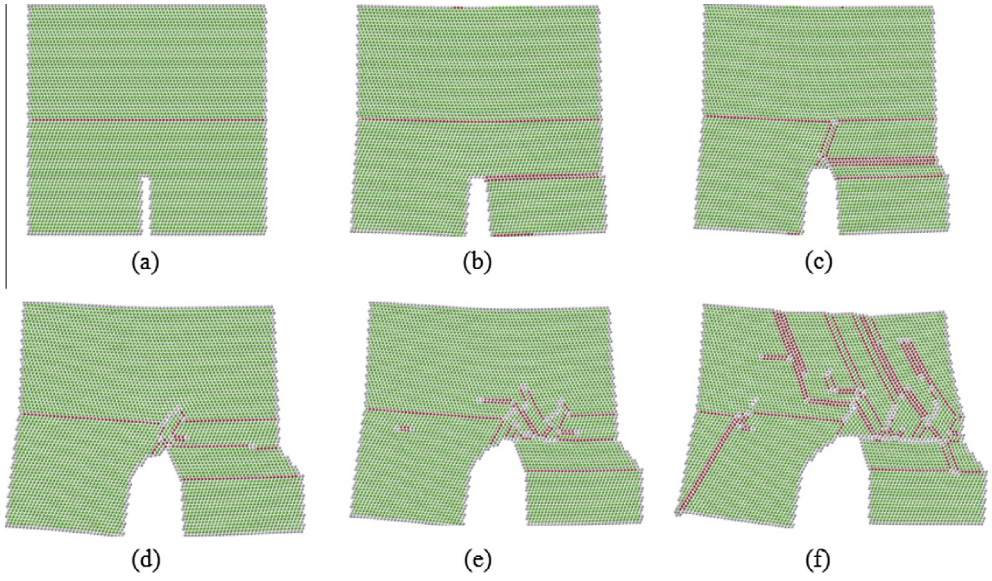

Fig. 3. Atomic structure configurations of Al with TB twists at angle 0° under tension loading: (a) 0 ps, (b) 300 ps, (c) 429 ps, (d) 600 ps, (e) 669 ps and (f) 813 ps. Atoms are colored by using common neighbor analysis method, where the hcp is red, the fcc is green and the non-structured atom is white, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Download English Version:

https://daneshyari.com/en/article/1560674

Download Persian Version:

https://daneshyari.com/article/1560674

Daneshyari.com