Materials Science & Engineering A 606 (2014) 334–345

Contents lists available at ScienceDirect

Materials Science & Engineering A

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

Deformation and failure mechanisms of nanotwinned copper films with a pre-existing crack

L.G. Sun [a], X.Q. He [a], J.B. Wang [b], J. Lu [c,d,*]

[a] Department of Civil and Architectural Engineering, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong
[b] School of Naval Architecture & Civil Engineering, Zhejiang Ocean University, Zhoushan 316000, China
[c] Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong
[d] Centre for Advanced Structural Materials, City University of Hong Kong, Shenzhen Research Institute, 8 Yuexing 1st Road, Shenzhen Hi-Tech Industrial Park, Nanshan District, Shenzhen, China

ARTICLE INFO

Article history:
Received 3 December 2013
Received in revised form
24 March 2014
Accepted 25 March 2014
Available online 2 April 2014

Keywords:
Nanotwinned copper film
Molecular dynamics simulations
Thickness
Crack location
Crack tip microstructure

ABSTRACT

Molecular dynamics simulations are adopted to analyze the deformation and failure mechanisms of nanotwinned copper films with a pre-existing crack and a twin plane. Evolution of the microstructure is examined with consideration of the effects of certain factors such as thickness of nanotwinned copper films, the location of pre-existing crack and the microstructure of the crack tip. The simulation results demonstrate that twin boundaries decohesion near the crack tip becomes harder with the increase of thickness and is replaced by crack tip decohesion. The crack propagation along the twin plane is very special. On the other hand, the easier formation of dislocations, single vacancies and stacking faults with the increase of thickness causes a transition from brittle to ductile. In addition, location of the pre-existing crack and microstructure of the crack tip also contribute to the transition from brittle to ductile, which is closely related to easy stacking faults formation and crack tip decohesion blockage. Furthermore, the scaling-up models are studied and the results show the transition from brittle to ductile is only related to the absolute thickness.

1. Introduction

Traditionally, properties of nanocrystalline materials are related to their microstructures such as precipitates, dislocation forests and grain boundaries (GBs). However, when the size of materials studied is below submicroscale or nanoscale, it is essential to take size effect into consideration because physical mechanisms at nanoscale [1–3] are different from the traditional mechanisms. Therefore, it is critical to develop a fundamental understanding of the mechanisms for deriving mechanical properties and deformation behaviors. More recently, engineering coherent internal boundaries at the nanoscale has been regarded as an efficient way to achieve high strength while maintaining substantial ductility [4–6]. Nanotwinned metals demonstrate the highly desirable combination of superior strength and high ductility [7–9]. Further studies in recent years have revealed that properties of nanotwinned metals are closely related to grain size, twin spacing, twin distribution and dislocation density, etc. Tensile tests of nanotwinned copper [7] reveal the maximum yield strength at a critical twin spacing around 15 nm which is closely related to grain size. With decrease in grain size, this critical twin spacing is also reduced. Metal nanopillars, metallic bulk materials and nanowires with nanosized twin structure have ultrahigh strength and acceptable or increased plasticity [6,10–13].

Recently, dislocation nucleation from crack tips in metallic materials has been studied widely. Fracture failures in ductile materials have been studied extensively by modeling, simulations and experiments at various length scales [14–19]. Since dislocations nucleation and propagation determine the transition from brittle to ductile in crystalline materials, a variety of continuum models have been proposed to describe the dislocation nucleation from a crack tip [20–22]. Meanwhile experimental investigations of dislocation generation and propagation along slip systems leading to material fracture have also been carried out [23,24]. However, the studies mentioned above did not account for twin structures which should have great effect on properties of nanocrystalline materials. Further studies indicate that twin boundaries (TBs) have the function of blocking dislocation activities initiated from crack tip [25]. The high dislocation density near TBs can harden the material, which can enhance strength of metals.

On the other hand, nanometer-scale thick metallic films are widely used in modern technologies, such as microelectronics and nanofabrication [26]. From the perspective of safety and reliability, design of such materials is important since it affects mechanical behavior of the

* Corresponding author at: Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong.
E-mail address: jianlu@cityu.edu.hk (J. Lu).

http://dx.doi.org/10.1016/j.msea.2014.03.113
0921-5093/

films. In recent years, the plasticity of thin films has been an issue for researchers to study since plastic properties of thin films are significantly different from those of the corresponding bulk materials [27,28]. On the basis of the pioneering work of Nix [29] on single crystalline films, a large number of efforts have been made [30–32] to identify distinctive properties of films and the orientation and rate dependence of partial dislocation nucleation in Cu has been investigated [30]. In addition, Guo et al. [31] studied the tensile behavior of Cu film at various temperatures under uniaxial tensile loading, and Xu et al. [33] studied plastic characteristics of single crystalline nano-Cu films under uniaxial tension. The slip mechanism and void formation are carefully explored by describing atoms movements.

With the continued development of science and technology, it has become possible to produce nanoscale devices and models. Based on experiments, a lot of models have been formulated and tested and favorable results have been obtained. However, understanding the mechanism of deformation and failure is still lacking. Molecular dynamics (MD) simulation is a very popular method for research work related to this kind of problems involving a variety of nanocrystalline materials such as copper [10,19], nickel [34,35], gold [36,37], aluminum [38,39] and steel [40]. It is suitable for learning the mechanism because the whole process of simulation can be observed and, thus, when, where and how the nanostructures of metals adjust themselves can be known.

However, a quantitative comparison of results obtained by MD simulations [12,41,42] indicates that the strength of nanotwinned materials depends on various internal parameters, including TB spacing, the size and shape of the cross-section and twin-boundary orientation. It is noted that the peak stresses in the nanopillars obtained from MD simulations and experiments show substantial discrepancies, which might be attributable to several orders of magnitude higher strain rate used in MD simulations as compared with the experiments [10]. In spite of the demerits mentioned above, MD simulation is still viewed as a powerful tool to qualitatively expose the deformation and fracture failure mechanisms of nanocrystalline materials.

Since dislocation nucleation from crack tips in nanotwinned materials with nanotwinned structure in thin films has not been studied, this paper attempts to identify the special properties under this specific circumstance. Based on MD simulation, nanotwinned thin films of copper with pre-existing cracks are examined. The deformation and fracture mechanisms under biaxial tension are discussed in the present work. With consideration of the shape of the crack tip, thickness of the film and location of the pre-existing crack, totally different deformations and fracture mechanisms are revealed in this work.

2. MD simulation techniques

The material studied in this paper is nanotwinned copper, which has face-centered-cubic (fcc) structure, as shown in Fig. 1a. To create the twin plane in MD simulation model, *X*, *Y* and *Z* axes are oriented along $[1\bar{1}1]$, $[\bar{1}12]$ and [110] directions, respectively. The 3 outer-most layers of atoms in *X* direction are identified as the boundary, and the fixed-displacement boundary condition is applied in the simulation. The simulated model is a film with dimensions of $16a_0 \times 26b_0 \times Nc_0$ (where $a_0 = 6.26084$ Å, $b_0 = 5.90278$ Å and $c_0 = 5.11196$ Å are the lattice spacing in *X*, *Y* and *Z* directions, respectively; '*N*' represents the thickness of the models). The simulation system contains 6688*N* atoms ($N = 1, 2, 3, \ldots$). The predominant twinning system in thin copper film is $(1\bar{1}1)[\bar{1}12]$ (the light blue atoms in Fig. 1a). Several MD simulation samples are built as below:

1. Based on the model shown in Fig. 1a, there is a pre-existing crack on the twin plane (Fig. 1b) of the magnitude 6 Å $\times 3b_0$. From ultrathin to relatively thick films are studied with the thickness being equal to Nc_0 ($N = 1, 2, \ldots, 6$).
2. With the change of location of the crack, two cases are constructed: upper or lower crack (Fig. 1b and c). Different deformation and fracture mechanisms are investigated with the effect of the thickness variation being taken into account.
3. Considering the local microstructure of the crack tip, two different shapes are studied here: inverted U-type and M-type (Fig. 1d and e).
4. By proportionally scaling-up the size of ultrathin films in *X* and *Y* directions and keeping the thickness fixed, the so-called absolute thickness and model size are especially examined.

Throughout the simulations, the temperature was kept constant at 300 K by using the Nosé–Hoover thermostat [43]. The embedded atom method (EAM) potential [44] was used to calculate interatomic force. At the beginning of the simulations, the samples were relaxed and equilibrated at 300 K for 200 ps. Then a crack on the twin plane was created with another round of relaxation for 200 ps. The simulated samples were then applied biaxial tensile loading in the *X* direction under constant temperature at 300 K with the constant engineering strain rate of $4 \times 10^7\ s^{-1}$. To identify the defects in the samples, colors are characterized according to the local crystalline classification visualized by common neighbor analysis (CNA) [45]. Based on this coloring method, different atomic structures can be distinguished, for example, dark blue stands for fcc atoms, light blue stands for hexagonal close packed (hcp) atoms and red stands for disordered atoms that do not satisfy any kind of fundamental atomic structures, as shown in Fig. 1. A single layer of hcp atoms represents a TB which is the pre-existing twin plane in our samples. Note that two adjacent hcp layers stand for an intrinsic stacking fault (ISF) and the two hcp layers with a fcc layer stand for an extrinsic stacking fault (ESF) between them.

3. Results and discussions

3.1. Thickness variation with unchanged length and width

To investigate the relationship between thickness variation and the deformation and failure mechanisms, six MD simulated samples are built with different thicknesses of $16a_0 \times 26b_0 \times Nc_0$ ($N = 1, 2, \ldots, 6$). Among these samples, it is observed that two samples ($N = 2$ and 3) have special brittle failure mechanism, which is totally different from other samples. The failure initiates from the crack tip and progressively extends fast along the twin plane to the end of the sample, but this kind of straight-line failure only appears in $N = 2$ and 3 samples. Because the straight-line failure mechanisms of samples with $N = 2$ and 3 are exactly the same, sample $N = 2$ is chosen for the simulation analysis (Fig. 2). With the increase of *N*, the plastic deformation plays a dominant role during the tensile simulation. As a representative example, the simulation result is shown in Fig. 3 for the sample of $N = 4$. It can be seen from Fig. 3b that intrinsic stacking faults occur first, instead of failure at the crack tip., then the large propagation of dislocations enhances the plasticity of the sample, and defects on the twin plane finally form nano-voids on the twin plane near the crack tip with propagation of dislocations, and coalescence of voids on the twin plane dominates the deformation and failure mode (Fig. 3d, in addition, Fig. 16c presents a clearer example). In addition, the burgers vector for Shockley partial dislocation is $b_1 = 1/6[1\bar{1}2]$ in the direction in which SFs are more likely to occur. Owing to the special location of the crack and the symmetrical structure depending on the twin plane, the nucleation of partial dislocation from crack tip is blocked in this direction (Fig. 3e). It should be emphasized that only in this kind of twin structure with the specific location of the pre-existing crack can the slip from the crack tip be hindered. So the process of formation of