Wear 332-333 (2015) 941–948

Contents lists available at ScienceDirect

Wear

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

Atomistic investigation of wear mechanisms of a copper bi-crystal

Junjie Zhang [a,b,*], Christoph Begau [c], Lin Geng [a], Alexander Hartmaier [c]

[a] School of Materials Science and Engineering, Harbin Institute of Technology, Harbin 15001, China
[b] Center for Precision Engineering, Harbin Institute of Technology, Harbin 15001, China
[c] Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-University Bochum, 44780 Bochum, Germany

ARTICLE INFO

Article history:
Received 22 January 2015
Received in revised form
6 February 2015
Accepted 9 February 2015

Keywords:
Copper
Grain boundary
Wear
Molecular dynamics.

ABSTRACT

In the present work, we investigate the wear mechanisms of a Cu bi-crystal containing a random high angle grain boundary by means of molecular dynamics simulations. The underlying deformation behavior of the material is analyzed and further related to the observed characteristics of mechanical response and resulting morphology of the worn surface. In particular, the grain boundary-associated mechanisms are characterized by advanced analysis techniques for lattice defects. Our simulation results indicate that in addition to dislocation slip and dislocation-grain boundary interactions, grain boundary migration plays an important role in the plastic deformation of Cu bi-crystal. It is found that the wear behavior of Cu depends on the crystallographic orientation of the worn surface and can be altered quite significantly by the presence of a grain boundary.

1. Introduction

Nanocrystalline (nc) materials possess unique mechanical, electrical and optical properties, and thus are promising candidates for the fabrication of advanced functional nanostructures [1,2]. With the demand for system-level miniaturization and increased performance of optical and electrical components/devices, the wear resistance is one important parameter that determines the performance and life cycle of nanostructures [3,4]. Therefore, a fundamental understanding of the wear mechanisms of nc materials at the nanoscale is crucial not only for the rational design of nc materials-based nanostructures, but also the optimization of their synthesis.

Nc materials have an average grain size of less than 100 nm and hence an increased volume fraction of grain boundaries (GBs) compared to their coarse-grained counterparts. Consequently, dislocation–GB interactions and GB-associated mechanisms play an increasing or even dominant role in the mechanical response of nc materials under external loads. Previous experimental, theoretical and computational studies have widely investigated the deformation behavior of nc metals under tension [5,6], torsion [7] and nanoindentation [8] tests. It is found that GBs can act as both source and sink for dislocations. Furthermore, the interactions of GBs with dislocations also result in pronounced GB-associated activities in nc metals. However, much less attention has been paid to the mechanisms occurring in nc materials during wear processes with localized multiaxial stress states. Although molecular dynamics (MD) simulation has been proven to be a powerful tool for exploring the wear process at the nanoscale, most of previous MD simulations focused on wear of single crystals [9–11]. In addition to dislocation mechanisms that exclusively govern the plastic deformation of single crystalline metals, dislocation-GB interactions, GB-associated mechanisms and deformation twinning also act as non-trivial plastic deformation modes for nc materials. Sun et al. [12] recently performed MD simulations to investigate the influence of dislocation–GB interactions on the tribological behavior of nano-grained copper. However, in their work the GB-associated mechanisms are not addressed fully. There are still some key issues remaining unknown, particularly for the wear of nc materials: what are the underlying deformation mechanisms of the materials? Particularly, what kind of role do GBs play in the wear resistance and resulting damage of the materials?

In the present work, we perform MD simulations to elucidate the wear mechanisms of a Cu bi-crystal containing a random GB. The bi-crystal model is employed not only to emphasize dislocation–GB interactions and GB-associated mechanisms, but also exclude uncertainty in analysis caused by other deformation modes, i.e., deformation twinning [13]. An advanced analysis technique for lattice defects is developed to characterize the grain boundary-associated mechanisms, such as GB migration. The microscopic deformation behavior of the material under wear conditions is examined and further related to the mechanical response and wear morphology of the material.

* Corresponding author at: Center for Precision Engineering, Harbin Institute of Technology, Harbin 15001, China.
E-mail address: zhjj505@gmail.com (J. Zhang).

http://dx.doi.org/10.1016/j.wear.2015.02.023
0043-1648/

2. Simulation method

2.1. Bi-crystal model

Fig. 1(a) shows the atomic configuration of a Cu bi-crystal substrate, which is composed of two single crystalline regions (grains) of different crystallographic orientations attached to each other. Each grain has the same dimensions of 14 nm, 10 nm and 21 nm in *X*, *Y* and *Z* directions, respectively. For comparison, two single-crystalline substrates with different orientations, i.e. Cu (010) and Cu(111), and the same dimensions as the bi-crystal are also considered. Periodic boundary conditions are applied in the lateral *X* and *Z* directions of each model. At the bottom, several atomic layers are fixed to avoid any rigid motion. The atomic interactions between face-centered cubic (FCC) Cu atoms are described by an embedded atom method (EAM) potential [14].

As depicted in Fig. 1(a), the crystallographic orientations for the Cu bi-crystal substrate are: Grain I: *X*[−1−12], *Y*[111] and *Z* [−110]; Grain II: *X*[100], *Y*[010] and *Z*[001]. The two grains are attached to each other, which results in the formation of a high angle GB located in the center of the substrate. To obtain an equilibrium configuration of the atoms, the model is first relaxed to its global minimum energy configuration using the FIRE (Fast Inertia Relaxation Engine) algorithm [15], and then subjected to isothermal–isobaric NPT relaxation under 0 bar pressure at 273 K for 50 ps. Fig. 1(a) presents the defect structures in the bi-crystal Cu after the relaxation, demonstrating that a stable structure of the planar GB is obtained. The dimensions of the single-crystalline parts joined together are chosen such that no net strain results in the simulation box, but only the typical very short-ranged strain field close to the random high-angle GB.

2.2. Wear procedure

After completion of the relaxation, the equilibrated Cu substrates are subjected to a wear process using a spherical probe in microcanonical NVE ensemble at 273 K. The utilized probe with a radius of 8 nm is represented by a purely repulsive potential in the form of $V(r) = A\theta(R-r)(R-r)^3$, where r is the distance between the atom and the center of the probe, R is the radius of the probe, θ is the Heaviside function and A is a constant with the value $A = 10$ nN/Å^2 [16]. The wear process is mimicked by penetration and following scratching stages, as depicted in Fig. 1(a). The labels shown in Fig. 1(a) schematically illustrate the positions of the probe prior to the wear (A), after penetration (B) and after scratching (C). In the penetration stage, the probe moves downwards with a constant velocity of 20 m/s to penetrate into the surface until a pre-determined penetration depth of 0.75 nm is reached. In the following scratching stage, the probe scratches a distance of 16.288 nm along horizontal direction with a constant velocity of 20 m/s. For the Cu bi-crystal, two different directional scratching routes are adopted: one is first penetrating into Grain I, and then scratching along positive *X* direction to reach Grain II (referred as to L2R); the other first penetrates into Grain II and scratches along negative *X* direction to reach Grain I (referred as to R2L). For each scratching route, the penetration position has the distance of 8 nm to the center GB. Accordingly, the scratching routes for the single crystal Cu substrates are consistent with R2L and L2R for the (010) and (111) free surfaces, respectively. All MD simulations are performed using the open source MD code IMD with a time step of 1 fs [17].

2.3. Defect analysis

Nucleation and motion of defects play a critical role in the deformation behavior of materials at the nanoscale. In the present work a modified version of the bond angle distribution (BAD) method [18,19], originally introduced by Ackland and Jones [20], is utilized to identify the location and type of defects. In contrast to the original method only the number of almost straight bonds ($\alpha > 167^\circ$) between nearest neighbor pairs are considered to distinguish FCC (six straight bonds), HCP (three bonds) and defects of which atoms with less than 10 neighbors are considered as part of the surface. For a clearer visualization of crystal defects, atoms sitting on perfect FCC lattice sites are omitted in the figures showing atomic configurations. The coloring scheme for these figures is as follows: atoms at the surface are colored in red, atoms in hexagonal close-packed (HCP) configuration in blue, and the remaining atoms are categorized as defects which include dislocation cores and vacancies.

Monitoring the change of the GB is crucial to reveal GB-associated mechanisms occurring in the Cu bi-crystal. In the present work, the atoms are labeled according to the grain in which they are originally situated. In such a way the initial grain structure can be distinguished clearly, and the migration of atoms into different grains during the wear process can be tracked

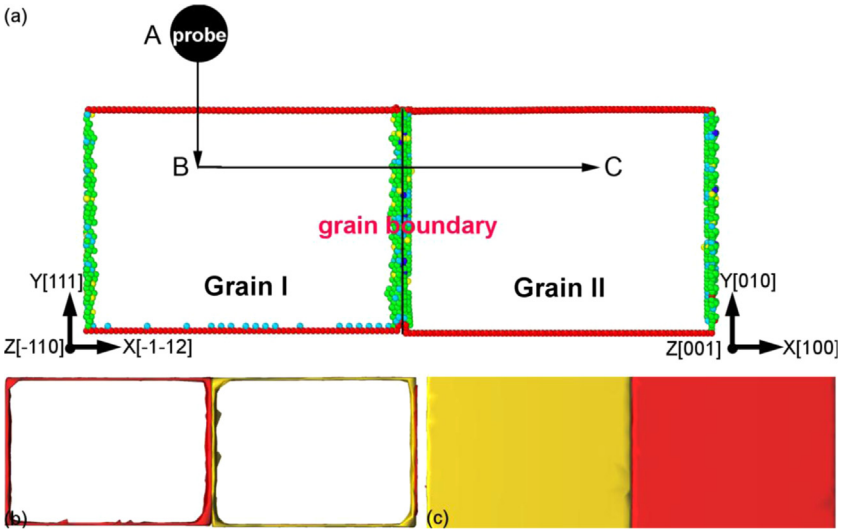

Fig. 1. (a) MD model of wear of copper bi-crystal. Atoms are color coded according to their bond angle distribution (BAD) (red, blue and other colors stand for surface, HCP and defect atoms, respectively), atoms on perfect FCC sites are not shown; (b) and (c) show side and top views of the GB representation. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).