Computational Materials Science 118 (2016) 66–76

Contents lists available at ScienceDirect

Computational Materials Science

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

A molecular dynamics investigation into plastic deformation mechanism of nanocrystalline copper for different nanoscratching rates

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ARTICLE INFO

Article history:
Received 23 December 2015
Received in revised form 27 February 2016
Accepted 4 March 2016
Available online 14 March 2016

Keywords:
Plastic deformation
Nanoscratching
Scratching rate
Polycrystalline
Twin

ABSTRACT

The plastic deformation mechanisms of nanoscratching process are investigated through the study of a rigid diamond tip sliding against nanocrystalline Cu using molecular dynamics (MD) simulation. Special attentions are paid to the scratching rate effects, as well as the crystal structural effects from single crystalline, polycrystalline and nanotwinned (NT) polycrystalline. With the increase of scratching rate, scratching force and workpiece temperature increase continuously due to severe plastic deformation and large chip volume, resulting in dislocation slip, GB slip, and twinning/detwinning. Scratching rate also governs the distributions of potential energy and kinetic energy of all the atoms, revealing the rate-dependent plastic deformation. Specifically, the plastic deformation for different scratching rates depends on the competition of scratching force, workpiece temperature and tool–workpiece contacting time that affect dislocation evolution. In addition, the results show that the plastic deformation due to scratching of single crystalline Cu is dominated by the dislocation–dislocation interactions. And the scratching induced plastic deformation of polycrystalline Cu is determined by the dislocation-grain boundary (GB) interactions. As for NT polycrystalline Cu under scratching, it is the dislocation–GB–twin boundary (TB) interactions accompanied with the twinning/detwinning process. While the presented MD simulations and the associated conclusions are based on nanocrystalline Cu, it is believed that the current deformation mechanism could also be applied to other face-centered-cubic nanocrystalline metals.

1. Introduction

Manufactured products at nanoscale are expected to demonstrate superior quality and enhanced functional performance, which can be widely used demand in micro–electro-mechanical systems (MEMS) and nano–electro-mechanical systems (NEMS) [1,2]. The functional performance of nanometer products suffered from material removal process is seriously limited by the reduced integrity and reliability of surface and subsurface layer [3–5]. Here material removal behaviors usually result from severe plastic deformation involving large strain and high strain rate in the chip [6–9]. In the past few years, much work has focused on the nature of the surface and subsurface alterations to correlate them for the better functional performance [10–16]. However, due to limited scratching depth of only a few nanometers, observation of microstructure evolution becomes extremely difficult during scratching process.

To solve this problem encountered in experiments, computational simulation can be utilized to analyze directly the nanoscratching process. Through first-principle simulation, the active role of bonds is revealed based on the implementation of free electronic degree, but this kind of simulation is time consuming [17]. In addition, finite element method (FEM) is employed to simulate nanoscale scratching process. However, its inaccuracy due to the sample phenomenological constitutive model limits its application [18]. The quasicontinuum (QC) method is also used to analyze nanoscratching process, but it fails to capture scratching-induced microstructure evolution, such as dislocation motion and phase transformation [19]. In contrast, MD simulations have been proved a reliable approach to reveal nanoscratching process, which plays a critical role in producing nanoscale components [20–22].

The constant demand for minimized subsurface damage and enhanced surface integrity of manufactured components has long acted as driving force for the continuous study of scratching-induced plastic deformation, which strongly affects the physical and mechanical properties of manufactured products [23,24].

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http://dx.doi.org/10.1016/j.commatsci.2016.03.008
0927-0256/

Significant progress has revealed a number of plastic deformation behaviors, which can be induced by dislocation [25,26], grain formation [27], grain sliding [28], twinning [29,30], asymmetrical deformation [31] and amorphous [32]. Using MD simulations and experimental techniques, Zhang and his co-workers [33–36] pioneer in the study of plastic deformation characteristics of the subsurface layer of the monocrystalline silicon by analyzing phase transformation and dislocation during scratching process. With experimental methods, Zhu et al. [37] found superior properties of nanocrystalline materials induced by severe plastic deformation, which is obtained through equal-channel angular pressing, high-pressure torsion, repetitive corrugation and straightening, friction stir processing and high speed machining. Fang et al. [38], Pei et al. [39] and Cai et al. [40] used MD simulations to study atomic scale deformation during the machining process of both brittle and ductile materials, and provided guidelines for future work [41–44]. An interesting work related to machining-induced plastic deformation has been reported by Li and his co-workers [15,16,45,46], where machining rate effects on grinding process is considered. Subsequently, characterization methods related to nanomachining have been extensively studied and reported, including X-rays, scanning electron microscope (SEM), Raman spectroscopy and photo thermal microscopy, which are used to investigate the subsurface deformation [47,48]. The above mentioned work mainly focuses on the machining-induced plastic deformation of single crystal materials, but few work study that of polycrystalline materials via MD simulation.

In this study, based on our previous work [12,15,16,45,46] we perform MD simulations to investigate scratching rate effects on plastic deformation of three different crystal structures, including single crystalline, polycrystalline and NT polycrystalline. Cu is selected as the study object, because it has not only much higher fracture toughness but also great potential for applications in microelectronics due to its high-conductivity [47,48]. Recently, NT metals are becoming more and more important research objects due to their outstanding mechanical properties, such as ultra-high strength, good ductility and high fracture toughness [49–52]. For examples, NT polycrystalline Cu has high fatigue crack growth resistance [50], and NT polycrystalline Ni nanowire subjected to tension exhibits an inverse Hall–Petch relation [51]. This is attributed to the fact that high-density nanoscale twin is introduced into grain, which confines the dislocation segment length and stores the mobile dislocations during deformation [48,52]. To obtain a fundamental understanding of scratching-induced deformation mechanism in NT metals, here scratching process of NT polycrystalline Cu is investigated in details. The deformation mechanisms of three different crystal structures at different scratching speeds are elucidated in terms of scratching force, workpiece temperature, atomic displacement, and microstructure evolution. MD simulations show that scratching speed has a strong influence on plastic deformation mechanism of nanocrystalline Cu subjected to nanoscratching.

2. Simulation methods

The MD simulation model of nanoscratching consists of a nanocrystalline workpiece and a rigid diamond tip/tool, as shown in Fig. 1. The three different crystal structures include single crystalline Cu, polycrystalline Cu, and NT polycrystalline Cu. The NT polycrystalline Cu can be constructed via this way as followed [52]: firstly, a multilayer that consists of multiple single crystal Cu layers of equal thickness is built and TB forms between adjacent layer; secondly, the angle of each grain is calculated; finally, NT polycrystalline with periodic boundary conditions is generated using Voronoi construction, which accommodates the multilayer and the obtained grain angle. The polycrystalline Cu workpiece has average grain size of 8 nm, and the NT polycrystalline Cu has average grain size of 8 nm with 2 nm twin spacing. The workpiece has a dimension of $44 \times 22 \times 22\ \text{nm}^3$, consisting of 2.8 million atoms. There are three kinds of atoms in the workpiece: boundary atoms, thermostat atoms and Newtonian atoms. Here the bottom boundary atoms are kept fixed in space to support the whole system. Initial temperature of workpiece is chosen as 293 K. The heat dissipation is achieved by keeping thermostat atoms at constant temperature of 293 K using the velocity rescaling method during MD simulation process. A periodic boundary condition is prescribed in the x-direction of workpiece to reduce the simulation scale effect. The diamond tip/tool of a spherical shape has a radius of 5 nm. The tool is treated as a rigid body since diamond is much harder than Cu [10,11,15,45]. Finally, the depth of scratching is 1 nm.

Before nanoscratching, workpiece is first relaxed to equilibrium configurations by following procedures. Firstly, the atoms in the workpiece are first relaxed to their minimum energy configurations using the fast inertia relaxation engine algorithm [53]. Secondly, workpiece is heated up to 293 K by dynamic MD simulation using the Nose–Hoover thermostat for 100 ps in the isothermal–isobaric NPT ensemble. The equilibrated Cu workpiece is then subjected to the nanoscratching of the spherical diamond tool in microcanonical NVE ensemble. During nanoscratching, the tool moves with a constant velocity along the positive y-direction.

The atomic interactions between face-centered-cubic (FCC) Cu atoms are described by the embedded atom method (EAM) potential [10–15], which is expressed as a multi-body potential energy function in the following form

$$E = F_\alpha \sum_{j \neq i} \rho_i(R_{ij}) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha,\beta}(R_{ij}) \tag{1}$$

where the total energy $E(U)$ on atom i is the sum of the embedding energy F and the short-range pair potential energy ϕ, ρ is the electron density, and α and β are the element types of atoms i and j. The embedding energy is the energy to put atom i in a host electron density at the site of that atom. The pair potential term (ϕ) describes the electrostatic contributions.

The interaction between the Cu atoms in the nanocrystalline workpiece and the carbon atoms in the diamond tool can be modeled using the pairwise Morse potential [10,11,45,46]

$$U = D\{\exp[-2\alpha(r_{ij} - r_0)] - 2\exp[-\alpha(r_{ij} - r_0)]\} \tag{2}$$

where D is the cohesion energy, α is a constant parameter, r_{ij} is the distance between the two atoms, and r_0 is the distance at equilibrium.

The stress in MD systems can be derived from viral route stress. The average viral stress in the domain can be defined as the sum of the contribution from all the atoms in the domain divided by the domain volume [10,11,15–19]

$$S = \frac{1}{\Omega} \sum_{i}^{N} \left(m_i v_i \otimes v_i + \frac{1}{2} \sum_{i \neq j} r_{ij} \otimes \frac{\partial U(r_{ij})}{\partial r_{ij}} \right) \tag{3}$$

where S is the average viral stress with six components, Ω is the volume of cutoff domain, m_i is the mass, v_i is the velocity of the atom i, $\otimes$ denotes the tensor product of two vectors, and N is the total number atoms in the domain.

To calculate scratching force, the individual interaction force on atom i due to atom j should be computed first by differentiating the potential energy over corresponding distance. The reaction force on each tool atom is computed by summing over the individual interaction force of its neighbor atoms. Finally, the scratching force in vector form can be obtained as followed [10,11,15–19]