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Grain size effects on indentation-induced defect evolution and plastic deformation mechanism of ploycrystalline materials

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ABSTRACT

Using molecular dynamics (MD) simulations, the defect evolution and plastic deformation mechanism of single-crystalline and polycrystalline copper under spherical nanoindentation are investigated and compared with previous nanoindentation simulations and experiments. To reveal the grain size effects on the indentation-induced internal stress and deformation behavior, the polycrystalline copper with different grain size are adopted in nanoindentation simulations, whose grain size are follow the inverse Hall-Petch relation. To study the grain boundary network effect, the grain boundary interface is further divided into three microstructural components with different dimensions. The results show that the indentation force of single-crystalline copper is larger than that of polycrystalline copper, and that of polycrystalline copper continuously decreases with the decrease of grain size due to softening phenomenon. The defect nucleation and propagation region in both single-crystalline and polycrystalline copper appear below the tool tip, due to the high internal stress and atomic potential energy induced by nanoindentation. The horizontal propagation of defects is faster and larger than the vertical propagation of that, and such defects are limited in the grains around the tool tip due to grain boundary network. An obvious stresses and potential energy gradient exist under tool tip in single-crystalline copper, and such gradients are possibly distributed along multiply direction in the polycrystalline copper. The internal stresses and atomic potential energy in the region of VP are highest, followed by that in TJ, GB and VP, resulting in the defect nucleation and propagation are more possible occur in VP than other microstructural components.

1. Introduction

Nanomaterials range in size from 1 to 100 nm [1], which can be widely adopted demand in micro-electro-mechanical systems (MEMS) and nano-electro-mechanical systems (NEMS) [2,3]. The manufacturing of nanomaterials products are suffered from material removal process, due to the limit of understanding of the nanomechanical response of nanomaterials, especially in microstructure evolution and internal stress transmission during nano-machining process. Hence, the study on the deformation mechanical of polycrystalline materials like polycrystalline copper is necessary to improve the technology of nanomaterials manufacturing [4–10].

To solve this problem, the deformation mechanical in copper can be investigated by various experimental methods, such as nanoindentation [11], atomic force microscopy (AFM) [12], scanning electron microscope (SEM) [13], transmission electron microscopy (TEM) [14], focused ion beam (FIB) [15], X-ray diffraction [16]. However, the computational simulation methods are more suitable, due to it can directly analyze the deformation and internal stress during nano-machining process, including first-principle simulation [17] which is limited by time consuming, finite element method [18] which is limited by nanoscale model, quasi-continuum (QC) method [19] which is limited by microstructural analyze, and molecular simulation (MD) method [20,21] which have been widely used to perform an in-depth analysis of the nanoindentation process. Although many scholars have conducted studies in term of normal force [22], strain rate sensitivity [23], flow stress [24], equivalent stress [25], elastic recovery coefficient [26], elastic modulus [27] and friction behaviors [28], the effect of grain size on the defect evolution and plastic deformation of polycrystalline copper during nanoindentation is still is necessary to improve related theoretical research.

In addition, as we all know, the grain boundary network has great effect on the nano-matching behavior of polycrystalline copper [29–33]. To further study the grain boundary network, on the nanometer scale, the polycrystalline materials can be classified into various microstructural entities with different dimensionalities that contain grain cell (GC) (three dimensions) and grain boundary interface (interfaces), and the interfaces can be further divided into grain boundary

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(GB) (two dimensions, neighboring grains sharing the same area), triple junction (TJ) (one dimensions, adjacent grains sharing the same junction line) and vertex points (VP) (no dimensions, adjacent grains sharing the same point) [34,35]. In traditional approaches [36], no distinction is made between these entities and the GB, TJ, VP are usually lumped together and treated as interface. In our work, we could distinguish all the microstructural components and mark them individually.

In this study, we perform MD simulations to investigate the grain size effect on the defect evolution and plastic deformation mechanism of four different crystal structures, including a single-crystalline copper, and three polycrystalline copper with different grain size. The deformation mechanisms of the four different crystal structures are elucidated in terms of nanoindentation force, defect nucleation and propagation process, internal stress, atomic potential energy, and microstructural component effects. MD simulation clarify that grain size and grain boundary network play an important role in defect evolution and plastic deformation mechanism of polycrystalline copper subjected to nanoindentation.

2. Model and methods

The MD simulation model that contains a single-crystalline/polycrystalline copper and a rigid diamond tool/indenter, as shown in Fig. 1. The workpiece consisting of approximately 6,163,200 atoms has a dimension of $41.5 \times 41.5 \times 41.5\,nm^3$. Although various indenters that contain spherical, conical, Vickers and Berkovich can be used in nanoindentation experiment [37–39], for simulation convenience, a spherical shape diamond indenter containing 253,135 atoms with the diameter R of 14.0 nm is adopted in the MD simulation. Due to the fact that diamond is harder than copper [40,41], the tool is treated as a rigid body. The polycrystalline structures that contain grain cell (GC) and grain boundary interface (interfaces) are constructed by the Poisson-Voronoi tessellation and Inverse Monte Carlo method, then, the grain boundary interface is further divided into grain boundary (GB), triple junction (TJ) and vertex points (VP), respectively. For details, refer to our previous work in Refs. [42,43]. The main procedures are as follows. (1) We build a Voronoi cell topology model to ensure that the Voronoi cells have a grain size as close as possible to that of the real GC, and then, we fix the Voronoi cell sizes and satisfy the Monte Carlo distribution; (2) we build grains based on the atomic crystal structure of copper and fill copper atoms into the empty Voronoi cells that are built in (1). The copper atoms can also be replaced by other types of atoms to build the desired polycrystalline model; (3) we identify the microstructural components in the polycrystalline model from (2). Based on the information of the topology model in (1), the interfaces are divided into GB, TJ and VP [44]. The polycrystalline structures have 20, 50, 500 grains, and the corresponding average grain size are 19 nm, 14 nm and 6.5 nm, respectively. Here are four MD samples cases are investigated: (1) Case 1, single-crystalline copper; (2) Case 2, polycrystalline copper with average grain size of 19 nm; (3) Case 2, polycrystalline copper with average grain size of 14 nm; (4) Case 2, polycrystalline copper with average grain size of 6.5 nm. Periodic boundary condition (PBC) are prescribed in the x-direction and z-direction to reduce the simulation scale effect [45]. The workpiece is categorized into three parts, namely, Newton layer, temperature layer and boundary layer [46].

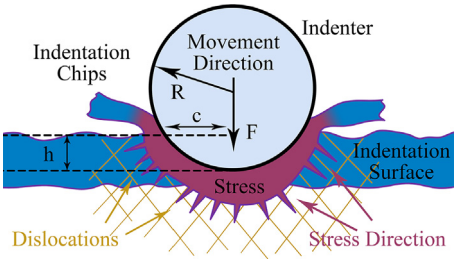

Fig. 2. Illustration of indentation-induced deformation and internal stress.

Before nanoindentation, the atoms in the workpiece are subjected to minimum energy configuration using the conjugate gradient method. Then, the isothermal-isobaric NPT ensemble is adopted to heated the workpiece up to 293 K using Nose-Hoover thermostat for 100 picoseconds. The equilibrated workpiece is then subjected to the nanoindentation of diamond tool in NVE ensemble. A time step is 1 fs. The diamond tool moves with a constant velocity of 10 m/s along the y-direction. The nanoindentation parameters used in this work are shown in Fig. 2.

The atomic interactions between face-centered-face (FCC) copper atoms are described by the EAM potential, which was developed by Daw and Baskes [47,48]. The EAM potential is shown in Eq. (1).

$$E_i = F_\alpha\left(\sum_{j\neq i}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}(r_{ij}) \tag{1}$$

where E is the total energy; i, the atom number; F, the embedding energy; ρ, the atomic electron density; ϕ, a pair potential interaction; α, β, the element types of atoms i and j, respectively.

The interaction between the copper atoms in the workpiece and the carbon atoms of the diamond tool are described by the Morse potential [49]. The Morse potential is shown in Eq. (2).

$$E(r) = D_0[\exp(-2\alpha(r-r_0)) - 2\exp(-\alpha(r-r_0))] \quad r < r_c \tag{2}$$

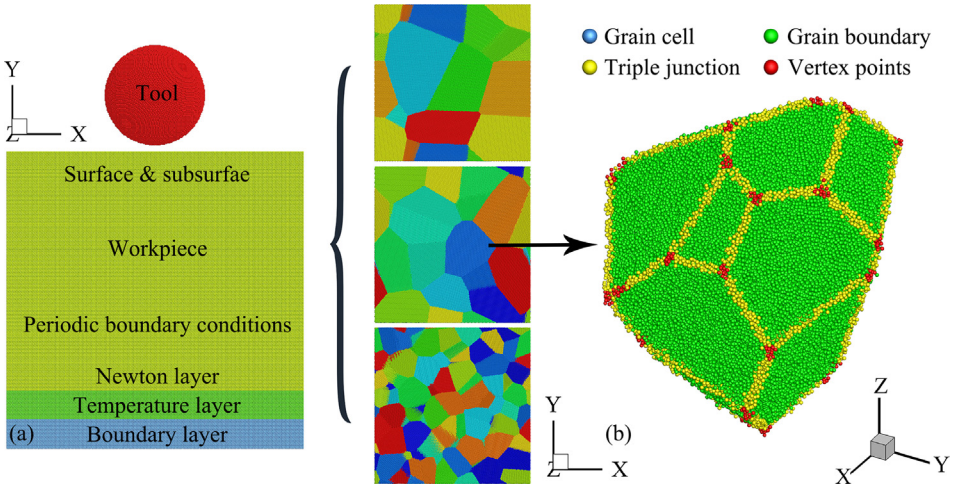

Fig. 1. Nanoindentation MD simulation model. (a) Single-crystalline and polycrystalline copper. (b) Microstructural components within polycrystalline copper.