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Study of nanoindentation mechanical response of nanocrystalline structures using molecular dynamics simulations

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ABSTRACT

Molecular dynamics (MD) simulations are performed to study the nanoindentation onto three different crystal structures including the single crystalline, polycrystalline, and nanotwinned polycrystalline copper. To reveal the effects of crystal structure and twin-lamellae-thickness on the response of nanoindentation, we evaluate the evolution of crystalline structure, dislocation, strain, indentation force, temperature, hardness, and elastic recovery coefficient in the deformation zone. The results of MD simulations show that the hardness, elastic recovery ratio and temperature of those three nanocrystalline copper strongly depend on crystal structure and twin-lamellae-thickness. It is also revealed that as nanoindenter goes deeper, the extent of plastic zone becomes substantially larger. Initial dislocation always nucleates at the beneath of indenter, and the discrete drops of indentation force observed at certain indentation depths, indicates dislocation bursts during the indentation process. In particular, the twining and detwining are dominant over the dislocation nucleation in driving plasticity in nanotwinned polycrystalline during nanoindentation, which are in good agreement with the previous work. Furthermore, we find that plastic deformation has a strong dependence on crystal structure. The plastic deformation of the single crystalline copper relies on the generation, propagation and reaction of dislocations, that of the polycrystalline copper depends on the dislocation–grain boundary (GB) interactions, and that of the nanotwinned polycrystalline copper relies upon the dislocation–twin boundary (TB) interactions as well as twining/detwining. This work not only provides insights into the effects of crystal structure and two-lamellae-thickness on the mechanical properties of copper under nanoindentation, but also shed lights onto the guideline of understanding other FCC nanocrystalline materials.

1. Introduction

Nanocrystalline materials have been a topic of interest among researchers over the past decade due to their unique mechanical, physical and chemical properties [1–3]. One of the most important applications of nanocrystalline materials lies on nanoscale surface finishing and micro-nanometric geometrical configuration. In order to realize that application, it is necessary to get a fundamental understanding of the deformation processes and mechanical properties of nanocrystalline materials during machining. Nanoindentation, which uses indenter with a known geometry to drive into a specific site of the specimen by applying load with increasing magnitude, is one of the most important methods to estimate mechanical properties at nanoscale. This method is widely used to obtain the elasticity modulus, hardness, and yield stress of nanocrystalline materials [4–6]. When it comes to elemental materials like single crystals and polycrystalline materials, nanoindentation simulations were mostly performed to study those materials [7,8]. However, nanoindentation simulations of nanotwinned polycrystalline materials with high strength, intermediate ductility, and high electric conductivity [9] are reported rarely. The twin-lamellae-thickness strongly affects the competition of various plastic deformation mechanisms, which in turn changes the mechanical properties of nanotwinned materials via its interactions with the microstructures [10–13].

MD simulations have been commonly used to study the indentation process. For example, plastic deformation initiated by the indentation process was studied [14]. The dislocation nucleation

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and the pileup material are observed during nanoindentation of the single crystal iron. The plastic deformation of the nanocrystalline tantalum during nanoindentation is regulated by deformation twin in terms of surface topography and hardness measurements [15], thereby pointing out the fact that the maximum shear stress in the deformation zone is larger than the theoretical shear strength on the (010) orientation but lower than the theoretical shear strength on the (110) and (111) orientations. Using MD simulations, the size of the generated plastic zone during the nanoindentation of the FCC and BCC metals is analyzed. Also, MD simulation was used to investigate the size of plastic zone, which is generated by a spherical indenter during nanoindentation onto FCC and BCC metals. It was found that the plastic zone size does not strongly depend on crystal structure, surface orientation and indentation parameters [16]. There are also reports of machining induced defect in the nanocrystalline [17–20] which adds to more confusion. Also, a large volume data for nanocrystalline materials under various conditions is presented [21–24]. However, single crystal structure is rarely seen in real materials. Instead, polycrystalline material is widely used in industry application. Yamakov et al. [25] use large-scale MD simulations to elucidate this intricate interplay during room-temperature plastic deformation of model nanocrystalline Al microstructures, and illustrate that mechanical twinning may play an important role in the deformation behavior of nanocrystalline Al. Ma and Yang [26] study nanoindentation induces versatile deformation mechanisms in nanocrystalline Cu by means of parallel MD simulations. They find that the burst and arrest of stacking faults hold the key for the plastic deformation of nanocrystalline Cu under nanoindentation. Kim et al. [27] investigate dislocation interaction with a GB in nickel single crystal and a nickel bicrystal with a vertical GB, and show that the indentation nucleated dislocations in the shape of prismatic loops and they propagated along the slip system. Hereafter, much work was conducted on polycrystalline material [28–30]. With the improving technology and experimental method, more results from different studies can emerge and a better understanding is dispensable in the nanocrystalline materials to obtain more highly optimized materials. The above mentioned mainly focuses on the plastic deformation of the nanocrystalline materials during nanoindention, but less work systematically analyzes the difference among single crystalline, polycrystalline, and nanotwinned polycrystalline copper under nanoindention via MD simulation.

In this paper, we focus on the study of the subsurface deformation of three different crystal structures including the single crystalline, polycrystalline, and nanotwinned polycrystalline copper where both the loading and unloading processes are evaluated. To achieve that goal, the MD simulations of indentation are studied considering the importance of crystal structure and twin-lamellae-thickness in controlling mechanical response of indentation. Considering the evolution of defect structure, such as dislocation GB and TB, together with loading force, hardness and elastic recovery are shown in detail at the atomic level. We employ the results of this combined MD simulation to suggest a picture of nanoscale deformation which exhibits the dependency of mechanical properties on crystal structure and twin-lamellae-thickness.

2. MD modeling and computational details

MD simulation is employed to study the mechanical behavior of the nanocrystalline metals during nanoindentation [14–17]. The MD simulation model consists of the nanocrystalline copper workpiece and nanoindenter, as shown in Fig. 1, where the workpiece has a size of 22 nm × 22 nm × 22 nm and radius of indenter is 5 nm. The three different crystal structures are studied, which include the single crystalline, polycrystalline, and nanotwinned polycrystalline copper. In particular, the model of the polycrystalline copper substrate contains the nine randomly orientated grains with mean grain sizes of 10 nm, and is generated by using the Voronoi code. For the nanotwinned polycrystalline copper, twins in each grain are inserted by mirroring a portion of the matrix with respect to a twin plane [31–33]. In addition, three kinds of atoms are used to construct copper substrate: boundary atoms, thermostat atoms, and Newtonian atoms [18–24]. The bottom layers of atoms in the workpiece are fixed in space, and the layers adjacent to them are kept at a constant temperature of 293 K to imitate heat dissipation in a real nanoindentation condition [18–22]. The rigid

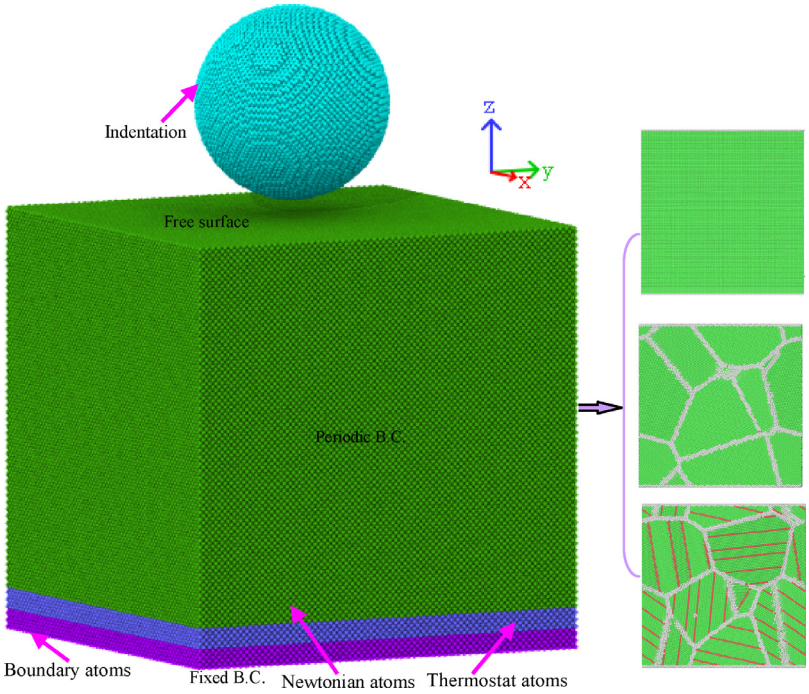

Fig. 1. Schematic of indentation using the MD simulation.