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The study of void effect on the microstructure evolution process in nanoindentation

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Abstract
The void effect on the microstructure evolution and internal stress transmission of single crystal copper in nanoindentation are investigated using molecular dynamics simulation. The void is simplified to a spherical shape and is introduced beneath the free surface of the workpiece to investigate void size effect and void position effect on the plastic deformation mechanism in nanoindentation, including atomic motion process, internal stress and indentation force. The result indicates that the indentation-induced strain continuously accumulates beneath the indenter and leads to a significant plastic deformation above the void, forming a "partial-collapse", and then forming a "full-collapse". The void can block the dislocation movement and absorb the internal stress during the indentation process, which is related to the void size and void position beneath the workpiece surface. Besides that, the void in the workpiece subsurface can decrease the indentation force in the nanoindentation direction and affect the force in the orthogonal direction. The above results can be generalized to investigate the plastic deformation mechanism of the materials with irregular voids. In nanoindentation experiments, to obtain more accurate material properties, we should not only optimize the indentation parameters, but adopt the workpiece without any nanoscale irregular voids.

Nanoindentation; Void; Microstructure evolution; Internal stress; Plastic deformation; Molecular dynamics

1. Introduction

Nanoindentation which is one of the most effective methods for inducing material surface deformation by adopting concentrated local stress has been widely applied to investigate elastic/plastic deformation and mechanical properties of materials [1–3]. Generally, the indenter interacts with the workpiece surface at the micro/nano scale, which is far smaller than the average polycrystalline materials grain size. Hence the workpiece can be usually treated as the single crystal materials [4]. In this scale, the nanoindentation is easily affected by the defects in the material surface or subsurface, such as dislocation [5], impurities [6], interfaces [7, 8], alloy particle [9], or void/pore [10], hence, the internal properties of the workpiece material like subsurface damage should also be considered in nanoindentation, which would also affect the obtained material mechanical properties.

The void not only affects the plastic deformation mechanism in nanoindentation, but also the internal stress variation and indentation forces, leading to inhomogeneous distribution of the internal stress gradient in the single crystal materials. Tan et al. [11] investigated the void effect on the internal stress distribution using molecular dynamics simulation and found that the internal stress transmission was blocked and absorbed by the void which leads to a rapid increase of the compressive stress surrounding the voids. The stress concentration formed at the sharp edge of the void region, leading to a high internal stress gradient at such regions, then the "partial-collapse" happened at the high stress edge of the voids [12]. In addition, the high internal stress generally would form between the voids, leading to significant plastic deformation and a combination of the voids [13]. The void size affected the potential energy in the void region and could lead to high potential energy at the edge of the void, resulting in the dislocation would tend to nucleate in the void regions [14].

2. Method

The MD simulation is performed to study the void effect on the microstructure evolution process and internal stress transmission of single crystal copper in nanoindentation. The MD model consists of a single crystalline copper workpiece with a void beneath the workpiece surface, as shown in Fig. 1. Due to the diamond indenter is harder than the single crystal copper workpiece, the indenter is treated as a rigid body. The workpiece has a dimension of 45.0 × 45.0 × 45.0 nm^3. The workpiece is divided into three parts, namely, Newton layer, temperature layer and boundary layer, respectively. The conjugate gradient method is used to minimize the energy configuration in the workpiece system. Then, the system is relaxed using the Nose-Hoover thermostat under the isothermal-isobaric NPT ensemble for 100 picoseconds. Then, the equilibrated system is subjected to the indentation of the indenter in the NVE ensemble. The indentation direction is {100} < 100 >. The time step is 1 fs. The periodic boundary condition is set in the x-direction and z-direction. The indentation speed is 10 m/s.

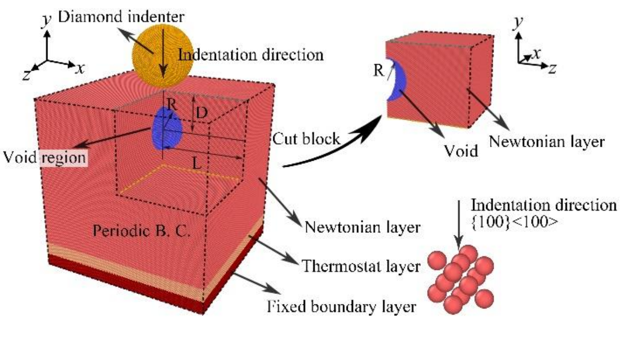

Figure 1. Nanoindentation MD simulation model

3. Results

The microstructure evolution process in the workpiece subsurface is shown in Fig. 2. It can be seen that when the indenter begins to interact with the workpiece free surface, a number of ISFs generate beneath the indenter, forming the "V-shaped" dislocation loop. When the ISFs propagate and meet the void region, the ISFs are blocked by the void, as shown in Figs. 3(a)–(b). With the increase of indentation depth, the stagnation region is pushed by the indenter and works as another indenter tip interacts with the void region, forming a "partial-collapse" at the top of the void region, as shown in Figs. 3(c)–(d). Different from the indentation process in Fig. 2, the Shockley partial dislocations induced by the indentation beneath the indenter are absorbed by the void in the subsurface of the workpiece. Stair-rod dislocations, as well as Hirth dislocation, can also be seen in the subsurface of the workpiece, which is caused by the interacted Shockley partial dislocations on different {111} crystal planes, as shown in Fig. 2(e). A number of ISFs nucleate and propagate at the other side of the void, as shown in Fig. 2(f). With the increase of the range of the collapse, the void is gradually absorbed by the subsurface of the workpiece, remaining large numbers of ISFs in the subsurface of the workpiece. Hence, the void effect could deteriorate the workpiece machined surface and affect obtained material mechanical properties by nanoindentation, especially when the void has a large range.

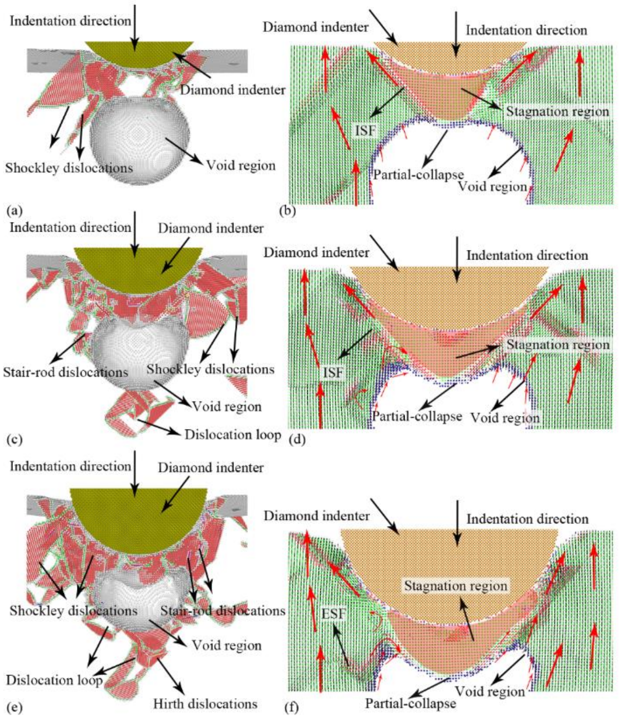

Figure 2. Microstructure evolution process and displacement vector sliced in the x-direction, at the indentation depth of 2 nm (a, b), 4 nm (c, d) and 6 nm (e, f)

To investigate the indentation-induced collapse generated at the top of the void during the indentation process, the range of the collapse region in y- and x-direction are analyzed, respectively, as shown in Fig. 3(a). The stagnation region interacts with the void region in the indentation depth of 1 nm, at which the collapse begins to generate. When the indentation depth ranges from 1 nm to 3.5 nm, the increase speed of the collapse region in x-direction keeps almost constant and then gradually decreases; however, that in y-direction gradually increases when the indentation depth increases from 1 nm to 3.5 nm and then keeps almost constant, as shown in Fig. 3(a). Hence, the indentation process can be divided into three stages: (a) no-deformation stage, (b) initial deformation stage and (c) stable deformation stage. At the no-deformation stage, the void keeps its initial shape. Then, the partial-collapse begins to form at the top of a void at the initial deformation stage and finally reaches the stable deformation stage.

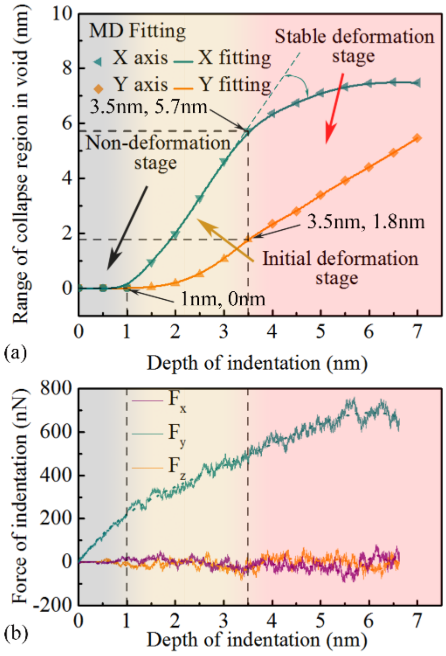

Figure 3. (a) Variation of the collapse range of the void region in x- and y-direction, and (b) variation of the indentation forces

4. Conclusions

In the nanoindentation of single-crystalline copper at {100} < 100 > crystal direction, defects nucleate and propagate beneath the indenter, forming a "V-shaped" dislocation loop. A stagnation region generates beneath the indenter and works as another indenter tip interacts with the workpiece subsurface, leading to the atoms flowing laterally to the indenter and forming the indentation surface. The position and size of the void region under the workpiece determine different plastic deformation process during the nanoindentation process. When the size of the void is larger, the void cannot be absorbed by the workpiece, and the atoms in the void region flow laterally to the partial-collapse. When the size of the void is smaller, a "full-collapse" could form in the void region, leading to the void being absorbed by the workpiece.

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