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Atomistic simulation of nanoindentation on incipient plasticity and dislocation evolution in γ/γ′ phase with interface and void

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ABSTRACT

Nanoindentation of γ/γ′ phase in Ni-based single crystal alloy is simulated by the molecular dynamics method. The perfect γ/γ′ phase model and the defective model with a void in the γ phase are researched respectively. Center-symmetry parameter is used to analyze the incipient plasticity and the dislocation evolution during the nanoindentation process. The results show that the incipient plasticity begins with the nucleation of dislocations in both two models. However, there are some different phenomena between the two models. Firstly, the elasticity stage of the defective model is much shorter than the perfect model since the presence of a void and the decrease of indentation load in the defective model is much more conspicuous. Secondly, the nucleation of new dislocations in the defective model is later than in the perfect model as the collapse of the void consumes the accumulated strain energy. Moreover, the stacking faults form at the indentation depth 1.32 nm in the perfect model while no stacking faults are found at the same indentation depth in the defective model. At last, none of dislocations moves into the γ′ phase because of the existence of the misfit dislocations in the γ/γ′ phase interface in both models. The dislocations tangle around the void in the defective model when the indentation depth arrives 1.6891 nm, which causes a lower indentation load contrasting to the load of the perfect model at the same depth.

1. Introduction

Study on the elastic limit and incipient plasticity of materials in nanoscale is beneficial for the optimization of material properties. Since 1968, researchers have focused on the detection and understanding of plastic yield of fundamental material using nanoindentation [1]. Nowadays, with the rapid development in nanotechnology and computer technology, experiments and simulations of nanoindentation-induced defect mechanism have become more and more popular, which facilitate better understanding of atomic-level mechanism of plastic deformation. Compared with experiments, atomistic simulation provides invaluable physical insight to nanoindentation for scientists to probe the nanodeformation mechanism. Van Vliet and Li et al. [2,3] proposed a position-sensitive criterion based on elastic stability to predict the initiation location of plasticity. Lilleodden et al. [4] presented a simulation study of the initial stages of indentation. Lee et al. [5] investigated the defect nucleation and evolution in Al single crystal under nanoindentation. Saraev et al. [6] used molecular dynamics simulations to elucidate details of plastic deformation and the underlying deformation mechanisms during nanoindentation of thin copper films with epitaxial nickel coatings.

Up to now, most materials simulated in nanoindentation are mainly single phase without considering the phase interface [2,4,7–11]. For two phase mosaic structures like γ/γ′ phase of Ni based single crystal alloy, which has been widely used in producing aero-engine turbine blades because of good mechanical properties, are rarely considered in nanoindentation, especially for incipient plasticity analysis. The microstructure of Ni based single crystal alloy consists of a high volume fraction (70% or even higher) of fine and ordered γ′ precipitates embedded in γ matrix. The mosaic structure has great impacts on the mechanical properties of the single crystal alloy. So atomistic simulation ought to be implemented to figure out the influence of γ/γ′ phase interface on the nanoindentation-induced plasticity for Ni based single crystal alloy.

Moreover, most atomistic simulation just focused on the mechanical properties of perfect material models while neglecting defects in materials such as grain boundary, surface steps and voids. Therefore, it's necessary to perform nanoindentation simulation to investigate the effects of defects on materials' properties.

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Shan et al. [12] researched the effect of spherical voids on the first dislocation emission of single crystal Cu in nanoindentation by atomistic simulation. Yu and Shen [13] used multiscale simulations to study the effects of a nanocavity on nanoindentation of copper film, focusing on the shape of the cavity and its geometrical parameters and location. Tan and Jeng [14] observed a stress concentration at the internal surface of the void in all simulations cases. Njeim and Bahr [15] discussed the effect of vacancies on dislocation nucleation in iron by means of molecular dynamics atomistic simulations at low temperatures.

In this paper, molecular dynamics simulation is employed to investigate the nanoindentation-induced plasticity of γ/γ' phase in Ni based single crystal alloy. Furthermore, a void is taken into consideration to see the difference between perfect materials and defective materials under nanoindentation. Emphasis is paid on the initial dislocation nucleation and the development of defect structures, aiming to better understand the atomic-level mechanism of plastic deformation of Ni-based single crystal alloy. The nucleation of dislocations and the motion of dislocations are investigated, and the comparison between perfect materials and defective materials is presented.

2. Modeling and simulation

In this work, the MD model consists of γ/γ' phase of Ni-base single crystal and a diamond indenter (R = 2.5 nm). Fig. 1 shows the sketch of nanoindentation model, while Table 1 gives the detail information of the computational model. The axis X, Y, Z represent for crystal orientation [100], [010], [001] respectively. The size of the γ (Ni) phase is $67a_1 \times 67a_1 \times 8a_1$, where a_1 is the lattice constant of γ (a_1 = 0.352 nm). Besides, the size of the γ' (Ni_3Al) phase is $66a_2 \times 66a_2 \times 8a_2$, where a_2 is the lattice constant of γ' (a_2 = 0.3573 nm). There are 157 thousands atoms and 153 thousands atoms in γ phase and γ' phase respectively. For the detective material, a spherical void is embedded in the atoms just underneath the indenter with a certain radius r = 0.8 nm. The distance between the up surface of γ phase and the top point of the void is H. Since our attention is on the difference between perfect materials and defective materials about the onset of plastic deformation and dislocation motions, here H is just taken as 1.5 nm. These two simulation models are presented in Fig. 2. The bottom surface of the γ' phase is fixed along [001] orientation to avoid rigid displacements. To eliminate the effect of boundary conditions on the side faces, periodic boundary condition is added along [010] and [100] orientation [16]. The model is divided into three layers as Newtonian, thermostat and rigid atoms along [00$\bar{1}$] orientation. Since the influence of temperature on dislocations is not considered in this work, microcanonical ensemble is taken during the simulation process. And the temperature of thermostat atoms is controlled by rescaling the atoms velocities [17]. The initial temperature of the matrix is 1 K. The speed of indenter belongs to 1–100 m/s normally [5] and in this paper is defined as 30 m/s with the maximum indentation depth 1.75 nm. The step time used was 2×10^{-15} s.

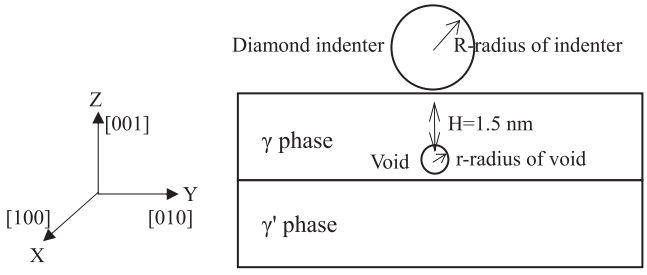

Fig. 1. Sketch of model.

According to the study of Geng et al. [18], there are three different atomic configurations at γ/γ' (001) interphase in Ni based single crystal alloy and the configuration II has the maximum probability to appear, as shown in Fig. 3. Therefore, the configuration II was employed in this work.

Interatomic interactions in classical molecular dynamics simulations are usually represented by empirical potentials. It's confirmed that the embedded-atom method (EAM) potential proposed by Mishin et al. [19] is appropriated for Ni–Ni and Ni–Al. The Morse potential [20] was chosen for C–C, C–Ni and C–Al.

Technique to selectively visualize interior defects is very important in the atomistic simulation of defect nucleation and evolution. Center symmetry parameter (CSP) was chosen in this paper which had been proven effective for the visualization of dislocation nucleation and evolution [4,21]. For fcc crystals, the CSP value of each atom, which is represented by P in this paper, could be defined by formula (1):

$$P = \sum_{i=1,6} |R_i + R_{i+6}|^2, \tag{1}$$

where R_i stands for the nearest-neighboring atoms and R_{i+6} stands for the opposite ones. If there exists a defect in a material, the CSP value P of the atoms in the vicinity of the defects will be greater than the perfect ones. When P is less than a cutoff value, which is equal to 0.5, the corresponding atom will be eliminated from visualizing the simulation results.

3. Analysis of incipient plasticity and dislocations evolution

In this section, incipient plasticity caused by indenting γ/γ' phase along [001] orientation is discussed with the analysis of dislocations evolution. After the relaxation, γ/γ' phase is in an equilibrium state with the potential energy vibrates in a small scale below 3 eV. Misfit dislocations are found at the γ/γ' phase interface, as shown in Fig. 4. The misfit dislocations are the main difference contrasting with single phase materials like Ni, Al and Cu, which will inevitably influence the mechanical properties of materials [22,23]. The movement of dislocations will be affected strongly by the misfit dislocations. Detailed discussion will be presented later.

The interaction force among atoms can be obtained by derivation of the potential equation. Here we considered the summation of the vertical components of the interaction force among atoms underneath the indenter as the indentation load. Fig. 5 gives the relationship between indentation load and depth before plastic deformation, while the whole indentation load–depth curve is shown in Fig. 6. The instants marked by A–I represent the significant changes in deformation or defect structure respectively. Besides, Fig. 7 gives the snapshots of dislocation structures at these marked instants separately. Note that perfect atoms are eliminated by controlling the CSP value.

As illustrated in Fig. 5, the indentation load grows smoothly and quickly before it reaches point A, where the first "pop-in" event [24] has been found at the indentation load–depth curve. And it does mean the initiation of plastic deformation which has been confirmed by a lot of literature [25]. The indentation load suddenly decreases by 4% from 69.63 nN to 66.853 nN. As shown in Fig. 7(a), dislocation embryos nucleate beneath the intenter at the instant of A in Fig. 5. These embryonic dislocations keep their shapes until the indentation depth reaches 0.3196 nm at the instant of B, where they transform into the tetrahedral sessile lock of Fig. 7(b).

After the tetrahedral sessile lock is formed, the indentation load goes on a glacial stage until the partial dislocation loops emanate