

Mechanical Behavior of Nanometer Ni by MD Simulation

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Abstract. The indentation simulation of the crystal Ni is carried out by molecular dynamics technique (MD) to study the mechanical behavior at nanometer scales, the indenter tips with sphere shape is used. Some defects such as dislocations, point defects are observed. It is found that defects (dislocations, amorphous) nucleated from local region near the pin tip or the sample surface. The temperature distribution of local region is analyzed and it can explain our MD simulation result.

Keywords: Nanocrystal, molecular dynamics simulation, indentation, dislocation, surface temperature .

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1. INTRODUCTION

Investigation of deformation mechanism on nanometer materials is a hot topic. Some experimental methods have been developed to measure their mechanical properties by means of an atomic force microscope AFM-based nanoindentation technique [1-3]. Li et al. performed nanoindentation tests on silver nanowires [1], Cu₂O nanocubes [2] and ZnS nanobelts [3].

The merit of AFM-based lithography techniques is that AFM can exert a very small vertical force on the workpiece surface, which leads to a depth of cut of several nanometers, and a wealth of information of deformation is obtained. Unfortunately, the cutting mechanism at the atomic scale is not well understood, and the experimental picture cannot display the atomic process involved in dislocation nucleation and micro defects evolution.

The MD approach has been applied to study various dynamic deformation processes on the atomic scale, e.g. indentation, adhesion, friction, surface defect and cutting [4-5]. Kim et al. [6] studied the influence of crystal orientation on the ploughing force of pin tool, and revealed relation between an extensive dislocation and ploughing direction of pin tool. Yan et al. [4] simulated the effect of tool geometry on the deformation process of the workpiece. The potential energy variation of atoms in different deformed regions of workpiece such as plastically deformed region, elastically deformed region and the mixed deformation region is different.

In this paper, a MD simulation under the canonical ensemble (NVT) is applied to study the defects nucleation and evolution of monocrystal Ni during the indentation process. Special attention is paid to the effect of temperature distribution on dislocation nucleation. The plan of the paper is as follows: in the next section the details of the simulation method will be described; in section 3 the simulation results and discussion are presented and finally the conclusion will be drawn in section 4.

2. COMPUTATION AND MODELLING

2.1 Initial Model

In the current simulation, a workpiece and a pin tool are assumed to consist of a monocrystalline Ni and a rigid diamond indenter, respectively, as shown in figure 1. The dimensions of the Ni workpiece are constructed sufficiently large to eliminate boundary effects. According to the simulation of Fang et al. [7], the size of a workpiece which is $26 a_0 \times 26 a_0 \times 36 a_0$ along x, y and z directions is enough, a_0 is the crystal constant. The diamond tool is a sphere shape with $20 a_0$ in diameter. The workpiece is made up of about 98000 Ni atoms and the tool is made of about 16000 carbon atoms. The periodic boundary condition and free boundary condition are performed along the x and y directions, respectively. On the top surface of workpiece the diamond tool is applied along the negative z direction, and three layers of atoms at the bottom side are fixed.

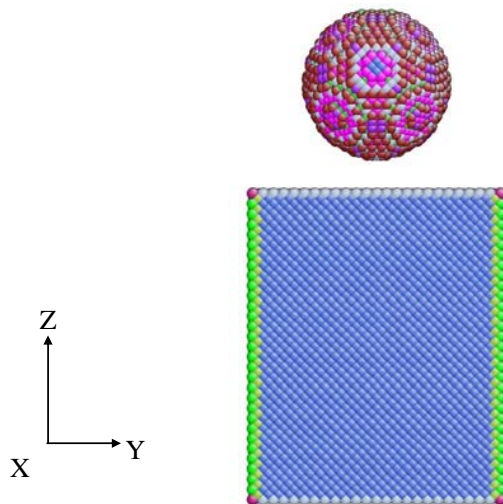


FIGURE 1. Schematic of nanometer Ni indentation model

2.2. Interatomic Potentials and Simulation Method

The simulation was carried out at 300 K using an embedded atom potential for Ni[8], and the interaction between Ni atoms and the diamond pin tool atoms is modelled by the repulsive potential $V(r)$ [9] given by , $E_p(r) = Ar^{-n}$, where A and n are material parameters. In this work, A was chosen as $10nN(\text{Angstrom})^4$ and n as 3.

Initial velocities of atoms are specified based on the Maxwellian distribution corresponding to a given temperature, $T_0 = 300$ K, and the magnitudes may be adjusted so as to keep constant temperature in the system [10]. The time integration of motion is performed by the fifth Gear's predictor–corrector method [11], time step $dt = 1.0$ fs.,

3. RESULTS AND DISCUSSION

The simulation system consists of a Ni workpiece and a diamond tool. The experiment shows that the Ni hardness is about 3~4 GPa and of diamond is 78.96 GPa [6]; one can assume that the diamond tip does not deform in the process of indentation. After 4000 MD steps relaxation with the environment temperature 300 K, a stable structure of workpiece is obtained. And the pin tool begins to plough into workpiece along the negative Z direction [00-1] with velocity 0.176 Angstrom/ps. Fig.2 presents the curves of stresses versus indentation depth. After a rapid rise in the stress σ_{zz} until tip reaches at 0.704 nm in depth, workpiece is in the stage of elastic deformation, stress is

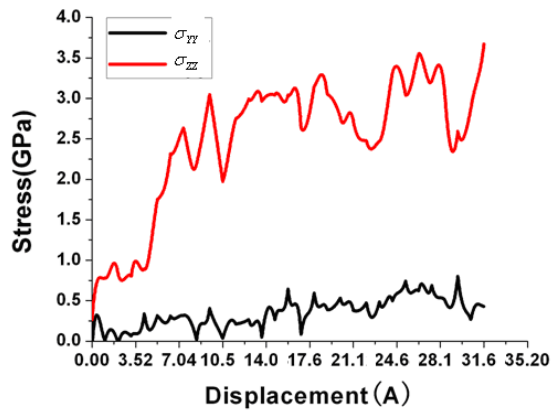


FIGURE 2. Compressive stress versus depth of indentation

about 2.6 GPa. With indentation depth increasing, the plastic deformation is observed, the compressive stresses increase slowly with fluctuations. It may be caused by the thermal vibration of atoms surrounding the tool due to temperature, or caused by some defects nucleated and evolution. During the loading process, the variation of stress of width direction is small, and it is not significant in the research active of AFM indentation.

Fig.3a-e show the atomic configurations, the defects firstly is observed in the region near the tool, see Fig.3a, where both the pressure and temperature are higher than that of other region. As the pin tool reaches at 0.704 nm, some defects are observed on the boundary, see Fig.3b and c. A common neighbor technology is adopted [12] to analyze, the atoms with perfect lattice structure are moved from Fig.3a, b, d and e, left atoms in these figures are the defects atoms, or surface atoms. Fig.3c is an atomic configuration of yz cross section, some point defects are observed, and small steps occurs in the surface, and some dislocation nucleated from surface, see sites with circle lines. Many experiments verified that dislocations and steps are often formed from surface [13-14]. By comparing the ideal crystal structure, the surface atoms lose some of their neighboring atoms, therefore it is site for defects to nucleated. Koh and Lee[15] proposed that the presence of the high stresses in the surface of nanometer materials are attributed to the availability of open bonds, surface atoms is at higher electronic state as compared to atoms situated within the interior bulk and possess a higher electronic cohesive energy, this may result in surface defects nucleated because of formation of asymmetric bounding of surface atoms with neighboring atoms.

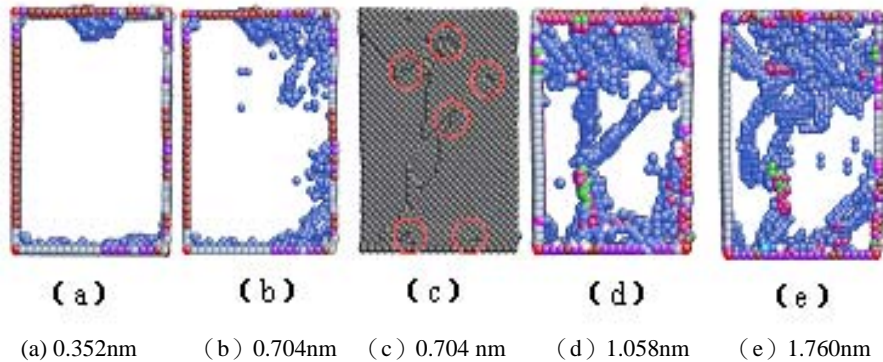


FIGURE 3. Defect evolution at different depths of indentation

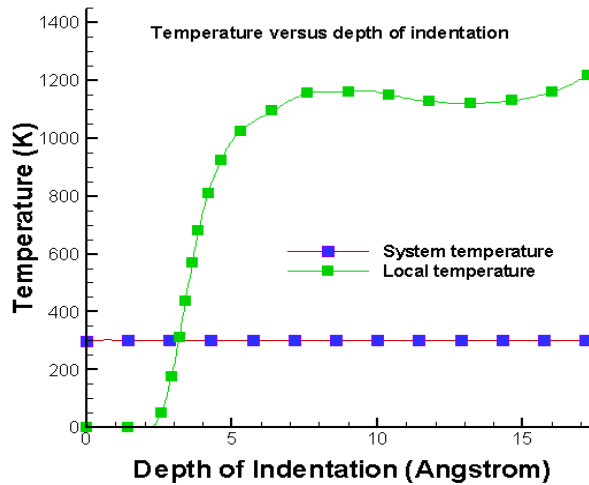


FIGURE 4. Temperature versus depth of indentation

From the atomic configuration Fig.3d and 3e, some defects are identified as point defects, amorphous and partial dislocations, and several slip planes are observed clearly. Fig.3a-3e display that defects multiply and connect from the local region to over all the region of workpiece finally leading to materials destroyed. Fig.4 displays the curve of temperature versus md steps, near the tool tip the local temperature reaches over 1000 K after the depth of indentation reaching 0.6 nm. Combining Fig.3 with 4, it may be understood that temperature may be a vital factor for defects nucleated, such as amorphous and dislocations, to be nucleated in relatively higher temperature region. Rice and Beltz [16], Meyers and Chawla [17] pointed out that the effects of thermal activation are very significant in lowering the load for dislocation nucleation, the tendency of the process of dislocation nucleation can be described by Arrhenius' equation [17]. Recently, Zhu et al. [18] develop an atomistic modelling framework to address the probabilistic nature of surface dislocation nucleation. Their results show that the nucleation of surface dislocation is sensitive to temperature, the applied load of dislocation nucleated is reduced with temperature increment.

4. CONCLUSIONS

MD simulations are carried out in order to understand the atomic scale mechanism of pin tool indentation on a nanometer Ni. Some interesting conclusions are drawn as follows.

- (1) By applying both EAM and repulsive pair potentials, the MD simulation of AFM indentation is carried out. The defects nucleated is observed near the tip firstly.
- (2) The temperature of the local region near the tip is higher than that of system, and it has an important contribution on defects nucleation and evolution.

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