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Mechanical Behavior of Nanometer Ni by Simulating Nanoindentation *

TANG Qi-Heng(汤奇恒)[1,2], YANG Tian-Yong(杨天勇)[1], DING Lan(丁斓)[3]

[1]*State Key Laboratory of Nonliear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190*
[2]*State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100080*
[3]*The School of Civil and Environmental Engineering, University of Science and Technology Beijing, Beijing 100083*

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An indentation simulation of the crystal Ni is carried out by a molecular dynamics technique (MD) to study the mechanical behavior at nanometer scales. Indenter tips with both sphere shape and conical shape with 60° cone angle are used, and simulation samples with different crystal orientations are adopted. Some defects such as dislocations and point defects are observed. It is found that nucleated defects (dislocations, amorphous atoms) are from the local region near the pin tip or the sample surface. The temperature distribution of the local region is analyzed and it can explain our MD simulation results.

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Investigation of the deformation mechanism of nanometer materials is a hot topic. Some experimental methods have been developed to measure their mechanical properties by means of atomic force microscopy (AFM).[1,2] Li *et al.* performed nanoindentation tests on silver nanowires[1] and ZnS nanobelts.[2]

The merit of atomic force microscopy (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 on deformation can be obtained. Unfortunately, the deformation mechanism by nanoindentation at the atomic scale is not well understood, and the experimental protocols are unable to display the atomic processes involved in dislocation nucleation and micro defect evolution.

The molecular dynamics technique(MD) approach has been applied to study various dynamic deformation processes on the atomic scale. da Silva *et al.*[3] investigated the structural evolution and the formation of necks induced by defects. The dependence of deformation mechanism on strain rates,[4] size and time-scale effects,[5] temperature effects,[6] and geometric shape effects[7] have been investigated in detail. Kim *et al.*[8] studied the influence of crystal orientation on the plough force of a pin tool, and revealed a relation between an extensive dislocation and the plough direction of the pin tool.

In this Letter, MD simulations of the canonical ensemble (NVT) are applied to study the nucleation and evolution of dislocations and other defects in monocrystal Ni during the indentation process. Special attention is paid to the effect of temperature distribution on dislocation nucleation.

Two simulation cases are considered. In one case, the simulation system consists of both a workpiece of crystal Ni along $x[100]$, $y[010]$, $z[001]$ and an indenter tip of rigid diamond, the tip is a sphere shape with a diameter 7 nm, as shown in Fig. 1. In the other case, a workpiece of crystal Ni is along $x[111]$, $y[1\bar{1}0]$, $z[11\bar{2}]$, and the indenter tip has a conical shape.

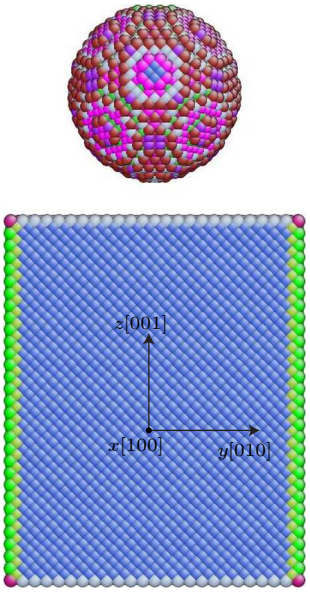

Fig. 1. Schematic of nanometer Ni indentation model for case 1.

The dimension of the Ni workpiece is constructed sufficiently large to eliminate boundary effects. According to the previous simulations,[9] the size of a workpiece of $26a_0 \times 26a_0 \times 36a_0$ along the x, y and z directions is enough, where a_0 (3.52 Å) is the crystal constant. The workpiece is made up of about 98000 Ni atoms and the tip is made of about 16000 car-

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**Email: qhtang@lnm.imech.ac.cn

bon atoms. The periodic boundary condition and free boundary condition are performed along the x and y directions, respectively. On the top surface of the workpiece the diamond tool is applied along the negative z direction, and three layers of atoms at the bottom side are fixed.

The simulation was carried out at 300 K using an embedded atom potential for Ni,[10] and the interaction between Ni atoms and the diamond atoms of the pin tool is modeled by the repulsive potential $V_p(r)$,[11] with $V_p(r) = Ar^{-n}$, where A and n are material parameters. In this work, A is chosen to be 10 nN Å^4 and n to be 3, respectively.

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.[12,13] The time integration of motion is performed by the fifth Gear's predictor-corrector method,[14] time step $dt = 1.0$ fs. The experiment shows that the Ni hardness is about 3.4 GPa and the hardness of diamond is 78.96 GPa;[15] one can assume that the diamond tip does not deform during the process of indentation.

For the first case, after 1000 MD steps of relaxation with the environment temperature 300 K, a stable structure of the workpiece is obtained. The pin tool begins to plough into the workpiece along the direction $[00\bar{1}]$ with velocity 0.176 Å/ps. Figure 2 presents the curves of stresses versus indentation depth. As the tip reaches at 1.0 nm in depth, a rapid rise in the stress σ_{zz} is observed, the stress is about 2.6 GPa. With indentation depth increasing, the compressive stresses increase slowly with fluctuations. The fluctuations may be caused by the thermal vibration of atoms surrounding the tool due to temperature, or caused by some defect evolution. During the loading process, the variation of stress of width direction is small, and it is not significant in the active research of AFM indentation.

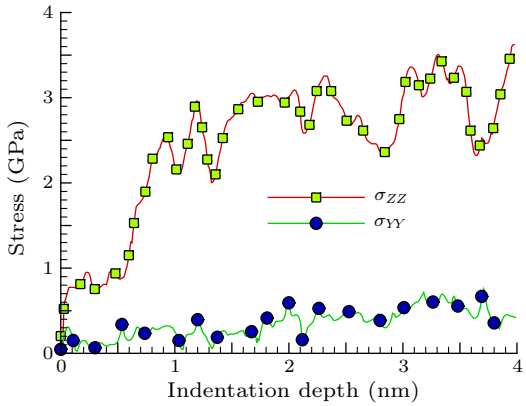

Fig. 2. Compressive stress versus depth of indentation.

Figure 3 shows four atomic configurations, the defect firstly is observed in the region near the pin tip, see Fig. 3(a), where both the pressure and temperature are higher than that of the other region. As the pin tool reaches a depth of 1.0 nm, some defects are observed. A common neighbor technology[16] is adopted to analyze the simulation results, the atoms at some perfect lattice sites are moved from Figs. 3(a), 3(b), 3(c) and 3(d), the atoms with non-perfect lattice are plotted. Some defects are generated from the surface, see Fig. 3(b), the slip planes are observed clearly from Figs. 3(c) and 3(d), and the defect evolution shows a circle structure over the substrate. Many experiments have verified that dislocations or other defects are often formed from the surface.[17,18] By comparing the ideal crystal structure, the surface atoms lose some of their neighboring atoms, therefore there are sites for defects to nucleate. Koh and Lee[19] proposed that the presence of high stresses in the surface of nanometer materials is attributed to the availability of open bonds, surface atoms are at a higher electronic state as compared to atoms situated inside the bulk and possess a higher electronic cohesive energy; this may result in surface defects being nucleated because of the formation of asymmetric bounding of surface atoms with neighboring atoms.

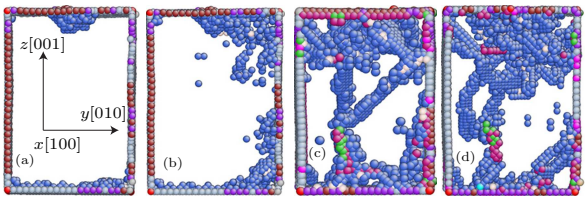

Fig. 3. Defect evolution at different depths of indentation for case 1: (a) 1.0 nm, (b) 2.0 nm, (c) 3.0 nm, (d) 4.0 nm.

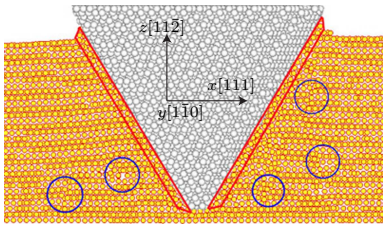

Fig. 4. Dislocations and amorphous atoms observed for case 2.

For the second case, a simulation with different crystal orientations $x[111]$, $y[1\bar{1}0]$, and $z[11\bar{2}]$ is carried out, and the conical indenter is used. From Fig. 4, several partial dislocations $\frac{1}{6}[11\bar{2}]/(111)$ are observed. For FCC crystal Ni, the partial dislocation moves on slip plane (111) are frequently observed in the experiment.[17] Carrasco *et al.*[20] made a nanoindentation experiment on Au, dislocations near the indentation site were observed. Morris and coworkers[21] developed a hybrid technique incorporating a nanoindenter into a transmission election microscope (TEM), providing in situ images of structural evolution be-

neath an indentation on Al, the initiation of dislocation activity was studied. In our study, some amorphous atoms around the indenter marked within the square lines are observed due to higher temperature, which may be caused by friction between the indenter and substrate Ni.

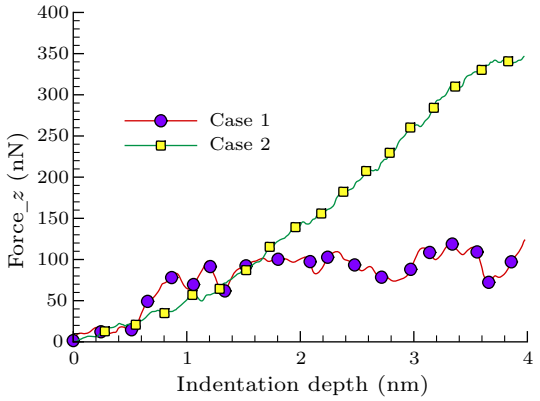

Fig. 5. Comparison of thrust force between cases 1 and 2.

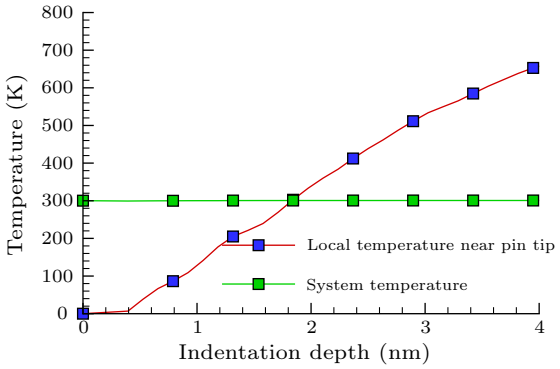

Fig. 6. Temperature versus depth of indentation.

Figure 5 shows a comparison between curves of thrust forces versus indentation depth. For the first case, when the indenter reaches the depth of 1 nm, the thrust force is about 100 nN, and it does not increase with increasing depth. For the second case, the vertical force increases with depth. When depth reaches about 4 nm, force is at 350 nN. It is deduced that the geometric shape of the indenter has an important effect on the simulation results.[7] Figure 6 displays the curve of temperature versus indentation depth, near the tool tip the local temperature reaches over 650 K after the depth of indentation reaches about 4 nm. Combining Figs. 3 and 5 with Fig. 6, it may be understood that temperature may be vital for defects (such as amorphous atoms and dislocations) to be nucleated in the relatively higher temperature region. Similar results by MD simulation are obtained by Tang[22] and Chen *et al.*[23] Rice and Beltz,[24] Meyers and Chawla[25] 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 the Arrhenius equation.[25] Recently, Zhu *et al.*[26] developed an atomistic modeling framework to address the probabilistic nature of surface dislocation nucleation. Their results show that the nucleation of surface dislocation is sensitive to temperature, and the applied load for nucleation of dislocations is reduced with increasing temperature.

In summary, MD simulations are carried out to understand the atomic scale mechanism of pin tool indentation on a nanometer Ni. The simulation shows that defects, such as dislocations and amorphous atoms, are nucleated near the tip. The local temperature near the tip is higher than that of the system, and it makes an important contribution to defect nucleation and evolution.

References

[1] Li X D, Gao H S, Murphy C J and Caswell K 2003 *Nano Lett.* **3** 1495
[2] Li X D, Wang N and Xiong Q H 2005 *Nano Lett.* **5** 1982
[3] da Silva E Z, da Silva A J R and Fazzio A 2001 *Phys. Rev. Lett.* **87** 256102
[4] Mehrez H, Ciraci S, Fong C Y and Erkoc S 1997 *J. Phys.* D **9** 10843
[5] Wang D, Zhao J, Hu S, Yin X, Liu Y H and Deng S Y 2007 *Nano Lett.* **7** 1208
[6] Mehrez H and Ciraci S 1997 *Phys. Rev.* B **56** 12632
[7] Horstemeyer M F and Baskes M I 1999 *J. Eng. Mater. Technol.* **121** 114
[8] Kim Y S, Yang S H, Kim C I and Lee S S 2003 *Mater. Sci. Forum* **426–432** 2243
[9] Fang T H, Weng C T and Chang J G 2002 *Surf. Sci.* **501** 138
[10] Voter A F, Chen S P 1987 *Mat. Res. Symp.* **82** 175
[11] Jang H Y, Seong J K, Kim J and Jang H 2004 *Mater. Sci. Forum* **449-452** 89
[12] Tang Q H 2004 *Mol. Phys.* **102** 1959
[13] Tang Q H 2008 *Chin. Phys. Lett.* **25** 2946
[14] Allen M P and Tildesley D J 2000 *Computer Simulation of Liquid* (New York: Oxford University) p 340
[15] Kim Y S, Choi S O, Lee S R and Kim J 2003 *IUTAM Sym. Mesoscopic Dynamics of Fracture Process and Materials Strength* (Osaka, Japan 6–11 July 2003)
[16] Honeycutt J D and Anderson H C 1987 *J. Phys. Chem.* **91** 4950
[17] Greer J R and Nix W D 2005 *Appl. Phys.* A **80** 1625
[18] Kiener D, Grosinger W, Dehm G and Pippan R 2008 *Acta Mater.* **56** 580
[19] Koh S J A and Lee H P 2006 *Nanotechnology* **17** 3451
[20] Carrasco E, Fuente O R, Gonzalez M A and Rojo J M 2003 *Phys. Rev.* B **68** 180102
[21] Minor A M and Morris J W 2001 *Appl. Phys. Lett.* **79** 1625
[22] Tang Q H and Chen F H 2006 *J. Phys D. Appl. Phys.* **39** 3674
[23] Chen R L, Luo J B, Guo D and Lu X 2008 *J. Appl. Phys.* **104** 104907
[24] Rice J R and Beltz G E 1994 *J. Mech. Phys. Solids* **42** 333
[25] Merers M A and Chawla K K 1983 *Mech. Metall.* (Prentice: Prentice Hall Inc.)
[26] Zhu T, Li J, Samanta A, Leach A and Gall K 2008 *Phys. Rev. Lett.* **100** 025502