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Molecular Dynamics Simulations of the Nanoindentation for Aluminum and Copper

Xiaozhi Tang[1], **Yafang Guo**[1] **and Yu Gao**[1]

Abstract: Atomistic simulations were performed to study the nanoindentation for two kinds of FCC metals, aluminum and copper. Due to the higher stacking faults in aluminum than in copper, two different deformation mechanisms were observed in our simulation under exactly the same simulation condition. Aluminum and copper also showed different mechanical properties in the unloading stage. The influence of stacking sequence along the loading direction on deformation mechanism was also investigated in this paper.

Keywords: Atomistic simulation, stacking fault, dislocation, nanoindentation, FCC metal.

1 Introduction

As an effective tool to bridge the simulation and the experiment [Lilleoddena, E.T.; Zimmermanb, J.A.; Foilesc, S.M.; Nixa, W.D. (2003)], nanoindentation simulation using molecular dynamics became more and more important on many fields of research [Liu, D. S.; Tsai, C.Y. (2009)][Munteanu, L.; Chiroiu, V. (2009)]. For FCC metals, deformation mechanism in nanoindentation process will be different according to properties of material and atomistic structure in the simulation model.

In this paper, molecular dynamic simulations by using LAMMPS MD code [Steve Plimpton (2002)] were conducted with the aim of investigate different deformation mechanisms of indentation in FCC metals. Two types of metals, copper and aluminum were selected in this work.

2 MD simulation model

The orientation of whole model is included in Fig.1: the substrate was constructed with 78408 atoms in an 8α*40α*60α cell, here α means the lattice constant. For the convenience of deformation mechanisms observing, period boundary condition

[1] Institute of Engineering Mechanics, Northern Jiaotong University, Beijing 100044, China

was applied along x axis, which means the [1 0 0] direction. We had 16 layers of atoms in the period boundary condition for the substrate. The indenter was modeled by a rigid cubic with its side length of 8a. And it was initially placed above the substrate at a distance slightly larger than the cutoff distance of the potential. In all of the simulations, isothermal-isobaric (NPT) ensemble was adopted, and the pressure along the x axis we controlled was zero and the temperature was 5K.

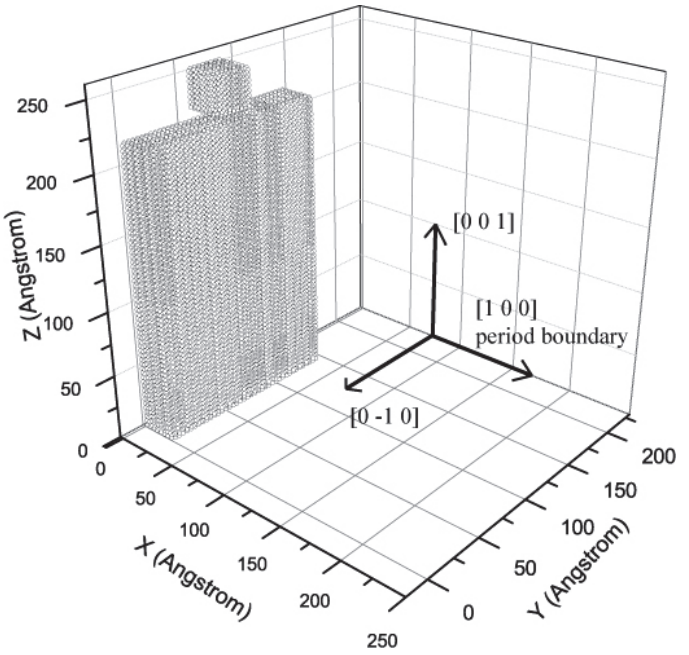

Figure 1: Simulation model

In the simulations, we have a loading stage and an unloading stage. Between the loading stage and the unloading stage, we have a relaxation stage for relaxing the system for 5,000 steps. The indenter moved into the substrate gradually along [0 0 $\bar{1}$] direction with a constant velocity of 22 m/s in the loading stage, while four bottom atomic layers in the substrate were fixed in order to avoid the displacement in loading direction.

It is known that in FCC metals the atoms align in layers along the [0 0 1] direction periodically with the sequence of ...ABAB... So in this paper two different cases with different stacking sequence among the indenter and the substrate are studied. As shown in Fig.2 for case 1, the bottom layer of indenter is A, and the top layer of substrate is B, which keeps the stacking sequence of ...ABAB... among the

indenter and the substrate. While for case 2, the bottom layer of indenter and the top layer of substrate are both A, the periodically repetitive structure does not exist between the indenter and the substrate.

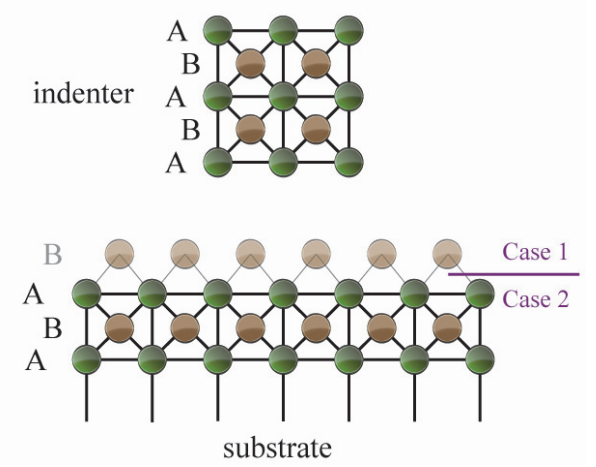

Figure 2: Stacking sequence

3 Results and discussion

3.1 Different deformation mechanisms for copper and aluminum

Fig.3 and Fig.4 present the atomistic configuration of copper and aluminum separately when loading stage ended. The pictures were illustrated by AtomEye [Ju Li (2003)]. As it is shown, the deformation mechanisms are totally different for copper and aluminum. For the case of copper, a series of highly organized stacking faults in ($\bar{1}$ 1 1) and (1 $\bar{1}$ 1) planes appeared gradually below the indenter in loading process. These stacking faults became interlaced in the central plane of substrate below the indenter. However, for the case of aluminum, only dislocations and very small short-lived stacking faults were found during the whole loading process. This phenomenon could be explained by the higher stacking fault energy in aluminum [Muzyk, M.; Pakiela, Z.; Kurzydlowski, K.J. (2011)] than in copper. After a relaxation stage of 5,000 steps, all the stacking faults disappeared completely in unloading stage for copper, and further simulation showed that, this reversibility of stacking faults will not exist when load is much larger. While for aluminum, the dislocations remained where they were and the trapezoidal deformations they coursed on the substrate surface would not disappear.

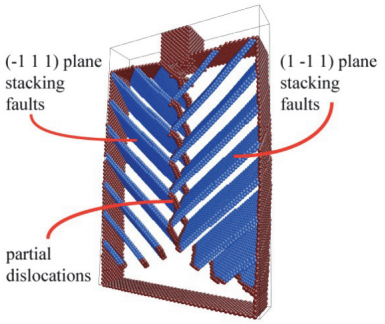

Figure 3: Deformation in copper

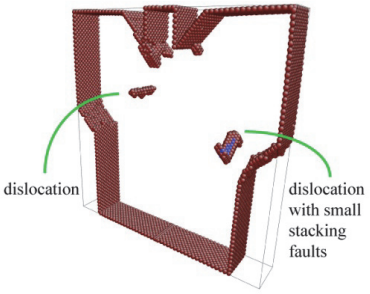

Figure 4: Deformation in aluminum

Load-displacement curves containing the unloading stage in copper and aluminum are shown in Fig. 5 and Fig. 6. In both simulations, the first maximum of the curves represent that substrate suffered an attractive force from the indenter. After the actual contact between indenter and substrate, both curves presented periodically wave-motion due to the form of stacking faults in copper and dislocations emitting in aluminum. In copper, when curve rose, stacking fault extended in the substrate with partial dislocations along their edges, which caused the pressure decreasing. Because two or more stacking faults formed nearly under the indenter at the same time, the load-displacement curve did not fluctuate so regularly that each extension of stacking faults could be marked. The curve of unloading stage was nearly the same as loading stage in copper. In aluminum, there was a downtrend about 15GPa in the curve which means compression pressure increased rapidly when the indenter moved only about 8 angstroms deeper. During this downtrend process, no deformation was observed. The first dislocation emitted when the curve suddenly decreased to about 10GPa. And then, in the rest of the loading stage, the continuous nucleation of dislocations kept the curve fluctuating around this pressure. The dislocations always appeared in pair and moved along [0 $\bar{1}$ $\bar{1}$] and [0 1 $\bar{1}$] directions to the substrate surfaces.

3.2 Influences of the stacking sequence

For copper in case 2, when both the bottom layer of indenter and the top layer of substrate are atoms A, the stacking faults only extended in ($\bar{1}$ 1 1) plane, as shown in Fig. 7. But for aluminum, there was no such difference between two cases. So, the stacking sequence among the indenter and the substrate only has an effect on stacking faults obviously. The load-displacement curves for two cases show nearly the same tendency. Due to the command of LAMMPS code, to create case 2 will

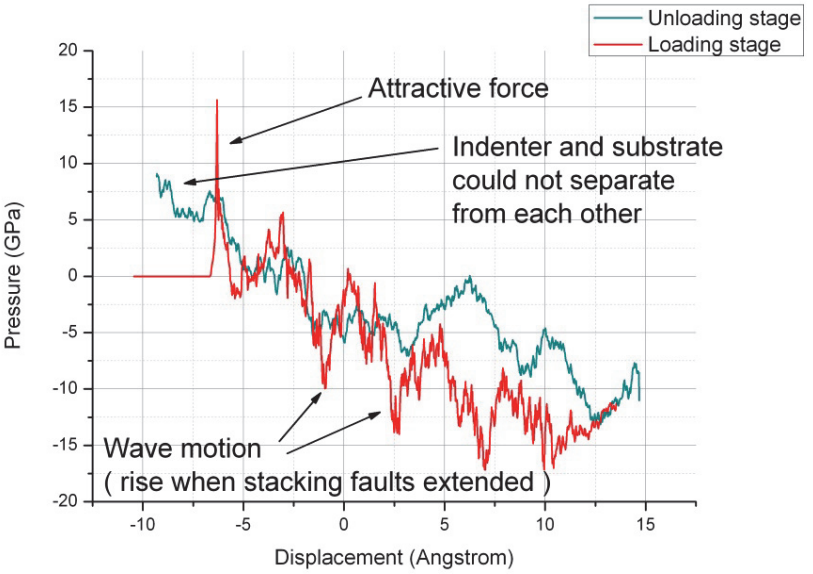

Figure 5: Load-displacement curve of copper

results in shortage of the distance between indenter and substrate, so the curve will show that they attracted each other earlier than that for case 1.

4 Conclusions

In this paper, we found that stacking fault is the main deformation mechanism for copper in indentation simulation, but only dislocations found in aluminum substrate because of the higher stacking fault energy in aluminum. This will cause a reversible loading process in copper which means stacking faults totally disappeared when completely unloaded, but dislocations in aluminum could not. It was also found that stacking sequence among the bottom layer of indenter and the top layer of substrate in loading direction will change the form of stacking faults.

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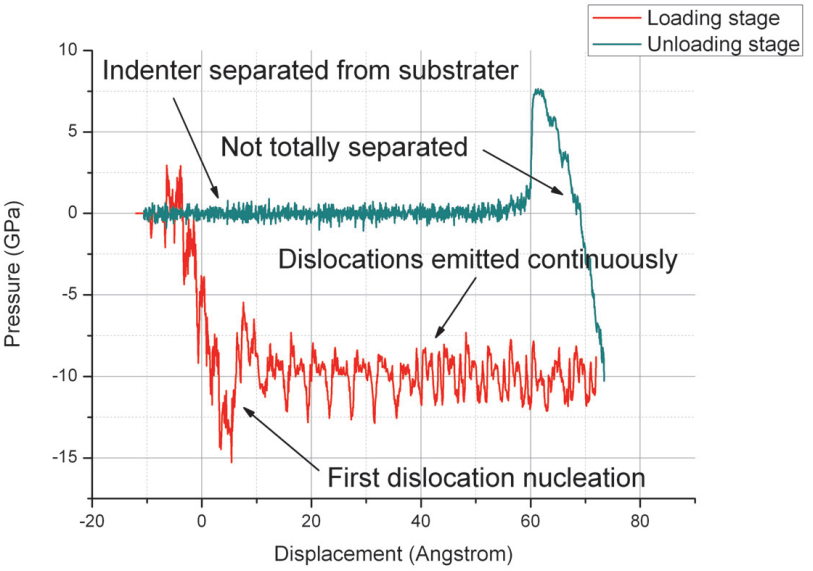

Figure 6: Load-displacement curve of aluminum

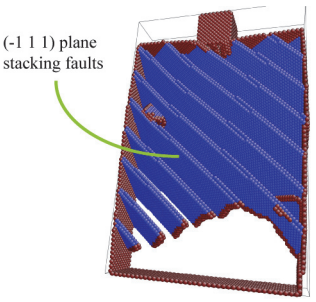

Figure 7: Deformation in copper in case 2

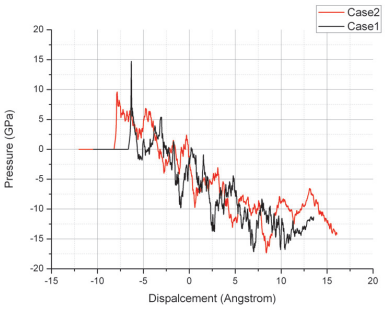

Figure 8: PH curves for two cases

References

Ju Li (2003): AtomEye: an efficient atomistic configuration viewer. *Modeling and Simulation in Materials Science and Engineering, Vol.11, pp. 173-177.*

Liu, D. S.; Tsai, C.Y. (2009): Estimation of thermo-elasto-plastic properties of thin-film mechanical properties using MD nanoindentation simulations and an in-

verse FEM/ANN computational scheme, *CMES: Computer Modeling in Engineering & Sciences, Vol.39, No.1, pp. 29-48, 2009.*

Lilleoddena, E.T.; Zimmermanb, J.A.; Foilesc, S.M.; Nixa, W.D. (2003): Atomistic simulations of elastic deformation and dislocation nucleation during nanoindentation. *Journal of the Mechanics and Physics of Solids, Vol.51, pp. 901-920.*

Munteanu, L.; Chiroiu, V. (2009): Shell Buckling of Carbon Nanotubes Using Nanoindentation, *CMES: Computer Modeling in Engineering & Sciences, Vol. 48, No. 1, pp. 27-42, 2009.*

Muzyk, M.; Pakiela, Z.; Kurzydlowski, K.J. (2011): Ab initio calculations of the generalized stacking fault energy in aluminum alloys. *Scripta Materialia, Vol.64, pp. 916-918.*

Steve Plimpton (2002): Fast parallel algorithms for short-range molecular dynamics. *Journal of Computational Physics, Vol. 117, pp. 1-19.*