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Nanometric cutting of copper: A molecular dynamics study

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Abstract

Molecular dynamics (MD) simulations were carried out to study the nanometric cutting of copper. In our approach, the many-body EAM potential was used for the atoms interaction in the copper workpiece. The effect of the tool geometry on the cutting process was investigated. It is observed that with negative rake angle, the chip becomes smaller due to the larger plastic deformation generated in the workpiece. It is shown that as the rake angle changes from −45° to 45°, the machined surface becomes smoother. Besides, both the cutting forces and the ratio of normal force to tangential force decrease considerably with the rake angle changing from negative to positive. In addition, MD simulations with the two-body Morse potential instead of the EAM potential were also carried out to study the effect of different potentials on the simulation results. It is found that there is no big difference in the simulated chip formation and the machined surface under the two different potentials. However, the Morse potential results in about 5–70% higher cutting forces than the EAM potential. It is recommended that the EAM potential should be used for the MD simulations of nanometric machining processes.

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1. Introduction

In recent years, there is an increasing demand for the manufacture of miniaturized components in the field of aviation, aerospace, medical instruments, communication systems, MEMS, etc. Tool-based micro and nanomachining are the most basic technologies to produce such miniaturized components. The ultra-precision machining with diamond tools can remove materials at nanometer scale, which has been used to produce nanometric surface finish and sub-micron level form accuracy of components. In order to fabricate well-made components, it is necessary to study the nanometric cutting mechanism and mechanics, such as the chip formation, plastic deformation, cutting forces, friction and heat dissipation.

However, as nanometric cutting involves changes in only a few atomic layers at the surface region, it is extremely difficult to observe the machining process and to measure the process parameters through experiments. Besides, the conventional theory based on "continuum mechanics", such as FEM, could not be used to analyze the nanometric cutting process due to the size limitation. Therefore, molecular dynamics (MD) simulation has become an important tool to study the nanometric cutting process.

Some typical works in the MD simulations of nanometric machining of metals include: Maekawa and Itoh [1] studied the role of friction between a single-crystal copper and a diamond-like tool in nanoscale orthogonal machining. The Morse type potentials were used for the interactions between Cu–Cu, Cu–C, and C–C atoms. Zhang and Tanaka [2] studied the wear and friction on the atomic scale and identified four distinct regimes of deformation consisting of no-wear, adherence, ploughing and cutting

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regimes. Komanduri et al. [3] have carried out MD simulations of nanometric cutting of single-crystal aluminum. They investigated the effects of crystal orientation, cutting direction and tool geometry on the nature of deformation and machining anisotropy of the material. Ye et al. [4] reported MD simulations of single-crystal copper machining with a large negative rake angle tool. In their models, the embedded atom method (EAM) potential was used to model interatomic forces. The effect of different cutting speed on the chip formation and machined surface was investigated. More recently, Kim et al. [9] used MD simulations to study the nanometric cutting in the atomic force microscopy (AFM)-based nanolithography process; and Hsu et al. [10] studied the nanoimprint process of copper with MD simulations.

From the papers published on MD simulations of nanometric machining of metals [1–10], we found that the Morse potentials were used in almost all those papers to model the interatomic force between metal atoms. Morse potential is a pair potential which considers only two-body interactions, thus it provides a rather poor description of the metallic bonding. The strength of the individual bond in metals has a strong dependence on the local environment. It decreases as the local environment becomes too crowded due to the Pauli's "exclusion principle" and increases near surfaces and in small clusters due to the localization of the electron density. Pair potentials do not depend on the environment and, as a result, cannot reproduce some of the characteristic properties of metals, such as the much stronger bonding of atoms near surfaces or in small clusters. Another shortcoming of a pair potential is that it predicts the ratio between the two elastic constants of C_{12} and C_{44} being 1 for a cubic crystal, which is a so-called *Cauthy relation*. However, experiments show that the ratio of C_{12}/C_{44} for fcc metals is generally well above 1 due to many-atoms effect. For example, the ratio of C_{12}/C_{44} for copper is about 1.5. Therefore, many-body potentials have been developed by some researchers [11,12] to solve those discrepancies.

The EAM potential, which was specially developed for metals [12,13], can better describe the metallic bonding. Therefore, it can give a more realistic description of the behavior and properties of metals. The EAM potential has been widely used in various MD simulations of metals, such as the deformation and dislocation movement [14,15], the rapid solidification and crystallization [16].

However, among all the available papers on MD simulations of metal machining, only the paper by Ye et al. [4] was found to employ the EAM potential. In their paper, the EAM potential was used to model the interatomic force between the copper atoms in the workpiece. However, they also used copper as the tool material, which is not realistic, as diamond tools are used in the real ultra-precision machining processes.

In this paper, we present the MD simulations of the nanometric cutting process of copper with a diamond cutting tool. In our simulations, the EAM potential was employed for the interaction between Cu atoms in the workpiece. As there is no available EAM potential between C and Cu atoms, we still use Morse potential for the interaction between the diamond tool and the copper workpiece. In order to employ the two different types of potentials at the same time in a simulation, our MD code had been modified to meet this requirement. We studied the effect of the tool rake angle on the cutting process. In addition, we also studied the effect of interatomic potentials on the simulation results.

2. Methodology

The simulations are based on the "orthogonal cutting", where the edge of the tool is straight and perpendicular to the direction of motion. The simulation model consists of a copper workpiece and a diamond tool as shown in Fig. 1. The workpiece consists of 10,500 atoms with the dimensions of $35a \times 15a \times 5a$, where a is the lattice constant of copper (3.62 Å). Three different tool geometries with the rake angle α being 45°, 0°, and −45° respectively, are used in the study. The tool clearance angle β is kept at 10°. The cutting speed is 100.0 m/s with the depth of cut being 1.08 nm. The cutting is in the (100) surface and along the ⟨100⟩ direction of the workpiece.

The boundary conditions of the cutting simulations include: (1) the two layers of atoms in the left side of the workpiece (lower x plane) and the bottom of the work material (lower y plane) are kept fixed; (2) periodic boundary conditions are maintained along the z direction. Similar to previous studies [3,4], we also apply a thermostat zone in the models, in order for the generated heat to be conducted away from the high temperature cutting region. The initial temperature of the workpiece is 300 K. The temperatures of the thermostat atoms are maintained at 300 K by scaling the velocities of the atoms. The simulation time step is 1 fs ($= 10^{-15}$ s).

The force acting on an individual atom is obtained by summing the forces contributed by the surrounding atoms. The forces are calculated from the interatomic potentials. The Morse potential is relatively simple and computationally inexpensive compared to the EAM potential. The Morse potential is written as

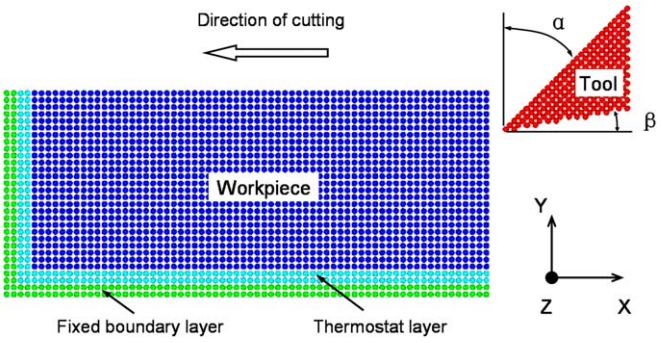

Fig. 1. Schematic MD simulation model.

$$\phi(r_{ij}) = D\{\exp[-2\alpha(r_{ij} - r_0)] - 2\exp[-\alpha(r_{ij} - r_0)]\} \quad (1)$$

where $\phi(r_{ij})$ is a pair potential energy function; D is the cohesion energy; α is the elastic modulus; r_{ij} and r_0 are the instantaneous and equilibrium distance between atoms i and j, respectively.

The EAM method, which evolved from the density-function theory, is based upon the recognition that the cohesive energy of a metal is governed not only by the pair-wise potential of the nearest neighbor atoms, but also by embedding energy related to the "electron sea" in which the atoms are embedded. For EAM potential, the total atomic potential energy of a system is expressed as

$$E_{\text{tot}} = \frac{1}{2}\sum_{i,j} \Phi_{ij}(r_{ij}) + \sum_i F_i(\bar{\rho}_i) \quad (2)$$

where Φ_{ij} is the pair-interaction energy between atoms i and j, and F_i is the embedding energy of atom i. $\bar{\rho}_i$ is the host electron density at site i induced by all other atoms in the system, which is given by

$$\bar{\rho}_i = \sum_{j \neq i} \rho_j(r_{ij}) \quad (3)$$

There are three different atomic interactions in the MD simulations of nanometric cutting processes: (1) the interaction in the workpiece; (2) the interaction between the workpiece and tool; and (3) the interaction in the tool.

For the interaction between the copper atoms in the workpiece, we used the EAM potential for copper constructed by Johnson [17]. In addition to the EAM potential, we also carried out MD simulations with the Morse potential for the copper workpiece to study the effect of the two different potentials on the simulation results. The parameters in the Morse potential for the copper were derived by Girifalco and Weizer [18] as listed in Table 1. Those parameters were later used by Inamura and Takezawa [6], Maekawa and Itoh [1] in their MD simulations, but with different r_0 values of 2.7202 [6] and 2.626 Å [1], respectively. In our MD simulations, it is found that the value of r_0 has to be modified from 2.866 to 2.78 Å in order to make the equilibrium lattice constant equal to 3.62 Å. Therefore, $r_0 = 2.78$ Å is used in our simulations.

For the interaction between the copper workpiece and the diamond tool, as there is no available EAM potential between Cu and C atoms, we still use Morse potential for the workpiece–tool interaction. The parameters used for the workpiece–tool interaction are those proposed by Zhang and Tanaka [2] and are also listed in Table 1.

Table 1
Parameters used in the Morse potential for Cu–Cu and Cu–C interactions

Parameter	Cu–Cu [18]	Cu–C [2]
D (eV)	0.3429	0.087
α (Å^{-1})	1.3588	5.140
r_0 (Å)	2.8660[a]	2.050

[a] Modified to 2.78 in our simulations.

The Morse potential is also used for the interaction between the tool atoms. As the copper workpiece is much softer than the diamond tool, it is a good approximation to take the tool as a rigid body, and so the atoms in the tools are positionally fixed relatively to each other. In this situation, the interaction force between the tool atoms will have no effect on the tool atoms in the simulations.

3. Simulation results and discussion

3.1. The simulated nanometric cutting process

The nanometric cutting processes were investigated with the MD simulations using the EAM potential for the copper workpiece. The simulated cutting processes for the different tools rake angles of 0°, 45°, and −45° are shown in Figs. 2–4, respectively. There are very obvious differences among these results with the different tool geometries. It will be shown that the tool rake angle has big effect on the chip formation, subsurface deformation, and the smoothness of the machined surface.

From the simulation results with tool rake angle 0° (Fig. 2), it can be seen that during cutting the material is deformed ahead of and in the vicinity of the cutting tool, which is similar to the conventional cutting process at larger depth of cut. It can also be seen that the uncut material in the workpiece away from the tool is almost not affected by the motion of the tool. The chip formation appears to be predominantly due to the compression and shear ahead of the tool. As the cutting proceeds, the chip moves upward along the tool surface of the 0° rake angle, and then the machined surface is formed. Besides, the material at the machined surface region below the tool undergoes plastic deformation and elastic recovery.

From the simulation results with the rake angle 45° (Fig. 3), it can be seen that although the basic cutting process is similar to that with 0° rake angle analyzed above, there are also some obvious differences resulting from the different rake angle. As the tool of 45° rake angle is very sharp, the chip mainly undergoes shear deformation and moves along the tool surface in the 45° direction. The machined surface is smoother than that with 0° rake angle.

For the rake angle −45°, the simulation results (Fig. 4) show that the chip mainly undergoes compression with the deformed chip moving along the tool surface in the −45° direction. As the material below the tool undergoes higher pressure, there is also a bigger elastic recovery. The machined surface is rougher than the cases with the tool angles of 0° and 45°. Besides, there are much more dislocations generated in the cutting region.

The cutting forces during the cutting processes were monitored in the MD simulations. Prediction of cutting forces is important as the cutting force is closely related to the cutting power and the tool life. In the MD simulation, the cutting force is the interatomic force between the workpiece and the tool, which is calculated as the summary of all the interaction forces that the workpiece atoms

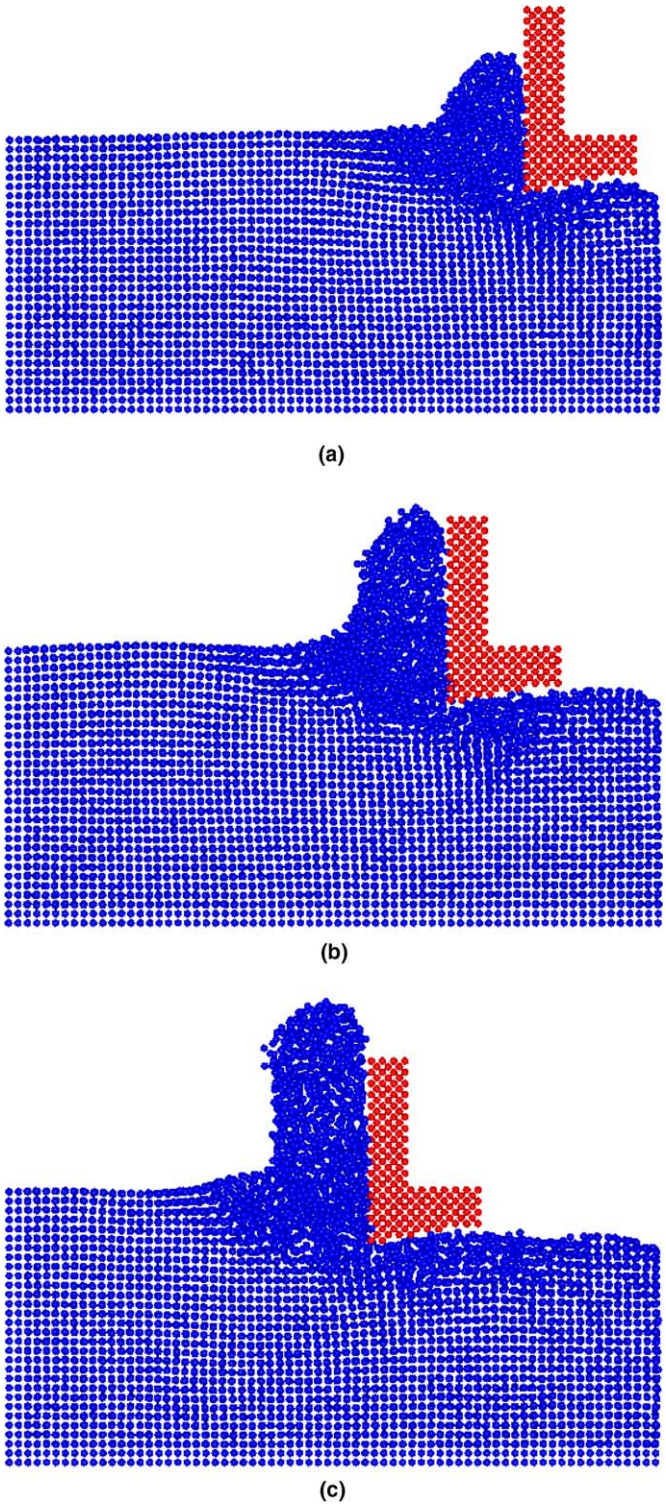

Fig. 2. Snapshots of the nanometric cutting process with the tool rake angle 0°: (a) time = 35.0 ps; (b) time = 50.0 ps; (c) time = 65.0 ps.

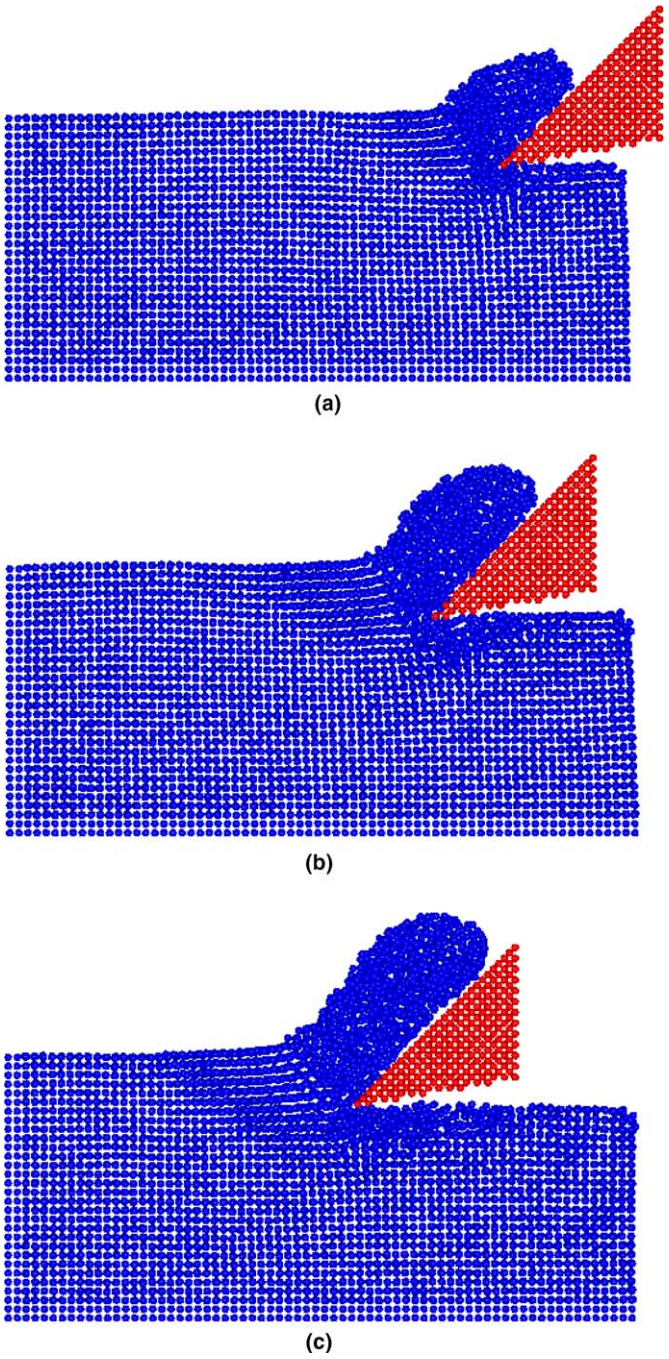

Fig. 3. Snapshots of the nanometric cutting process with the tool rake angle 45°: (a) time = 35.0 ps; (b) time = 50.0 ps; (c) time = 65.0 ps.

acting on the tool atoms. The most interested cutting forces are the tangential force F_x and the normal force F_y. Fig. 5(a)–(c) shows the variation of both the tangential and the normal cutting forces with the cutting distance for the tool rake angles of 45°, 0° and −45°, respectively.

The simulated cutting force curves shown in Fig. 5 are similar to the MD simulation results obtained by Komanduri et al. [3]. The cutting forces, though exhibit fluctuations, show a very obvious difference for the different tool rake angles of 45°, 0° and −45°. To make a comparison of the cutting forces, the mean cutting forces for the different rake angles are shown in Fig. 6. It can be seen that the rake angle has strong influence on the cutting force. As the rake angle changes from −45° to 45°, both the tangential and normal cutting forces decrease considerably. Besides, the ratio of the normal force to tangential force also decreases

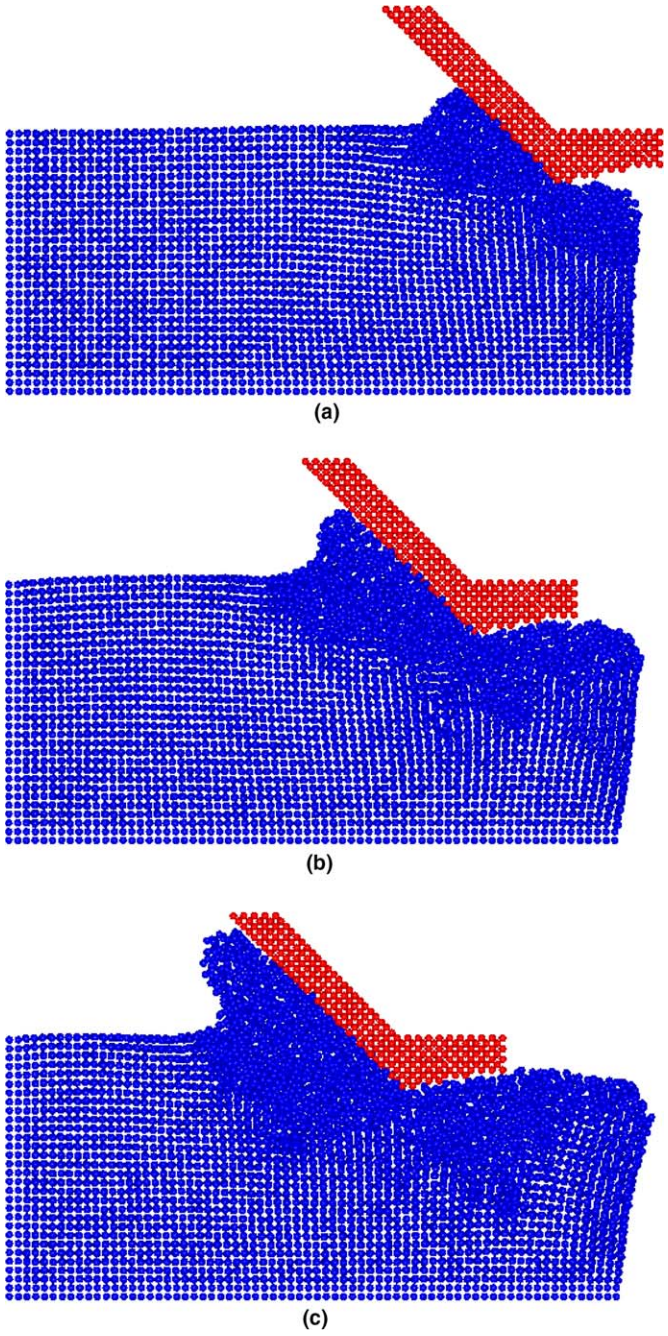

Fig. 4. Snapshots of the nanometric cutting process with the tool rake angle −45°: (a) time = 35.0 ps; (b) time = 50.0 ps; (c) time = 65.0 ps.

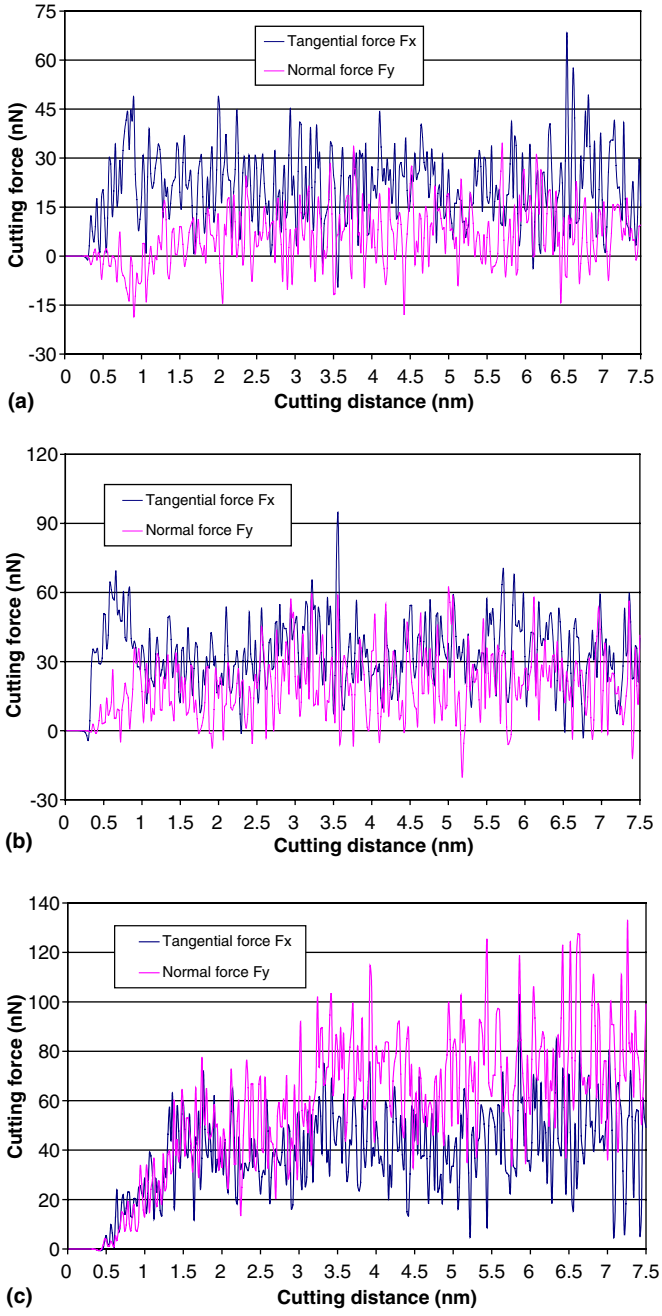

Fig. 5. Variation of the cutting forces with cutting distance for three different rake angles: (a) α = 45°; (b) α = 0°; (c) α = −45°.

as the rake angle changes from −45° to 45°, which is shown in Fig. 7. These simulation results are consistent with our knowledge and experimental results [19,20] in micro cutting.

3.2. Effect of potentials on the simulation results

In our simulations, the EAM potential was used for the copper workpiece, while in previous studies the Morse potential was used. Therefore, it is important to know whether the two different potentials will result in big difference in the simulation results of nanometric cutting process. For this purpose, we also made MD simulations with the Morse potential instead of the EAM potential for the copper workpiece. Some snapshots of the simulated cutting processes with the EAM potential and the Morse potential are shown in Figs. 8 and 9, respectively.

By comparing the pictures in Fig. 8 with the corresponding pictures in Fig. 9, it can be seen that there are no big differences between the two results in terms of the chip shape and the smoothness of machined surface, though small differences can be found. One small difference is that under the Morse potential the atoms at the chip surface are

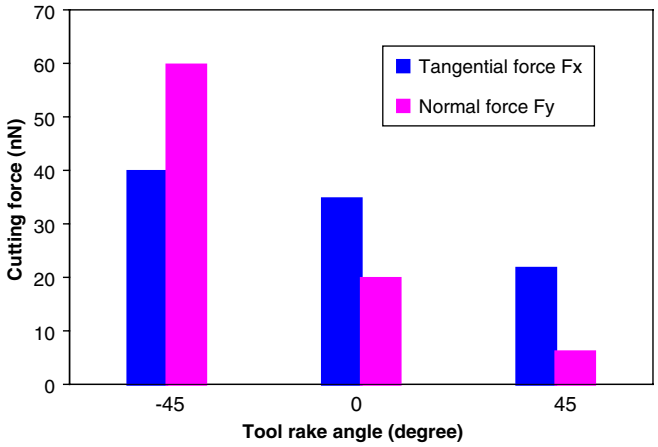

Fig. 6. The mean cutting forces for the different tool rake angles.

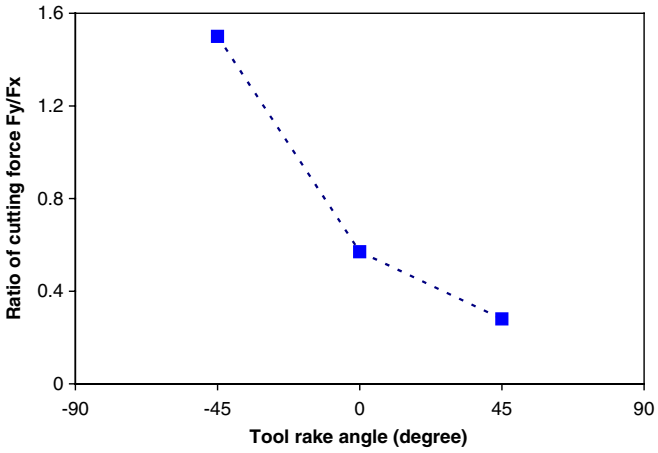

Fig. 7. Variation in the ratio of the normal cutting force to the tangential cutting force.

loosely connected to each other, while under the EAM potential the atoms at the chip surface are more closely adhesive to the surface. However, as a whole, the difference between the two simulation results is not very obvious. Therefore, it can be concluded that the two different potentials for the copper workpiece do not produce big difference in the simulated chip formation and machined surface.

The small difference in the chip surface can be explained by the metallic bonding. The special feature of metallic bonding is that the strength of the individual bond has a strong dependence on the local environment. The bonding becomes stronger at the surface due to the localization of the electron density. As the EAM potential describes the metallic bonding much better than the two-body Morse potential, the EAM potential results in stronger bonds at surface, and thus a more compact surface than the Morse potential.

The simulated tangential and normal cutting forces are shown in Figs. 10 and 11, respectively for the two different potentials in the workpiece. It can be seen that under the Morse potential both tangential and normal cutting forces are higher than that under the EAM potential. More quantitatively, the Morse potential results in about 5–70% bigger cutting force than the EAM potential.

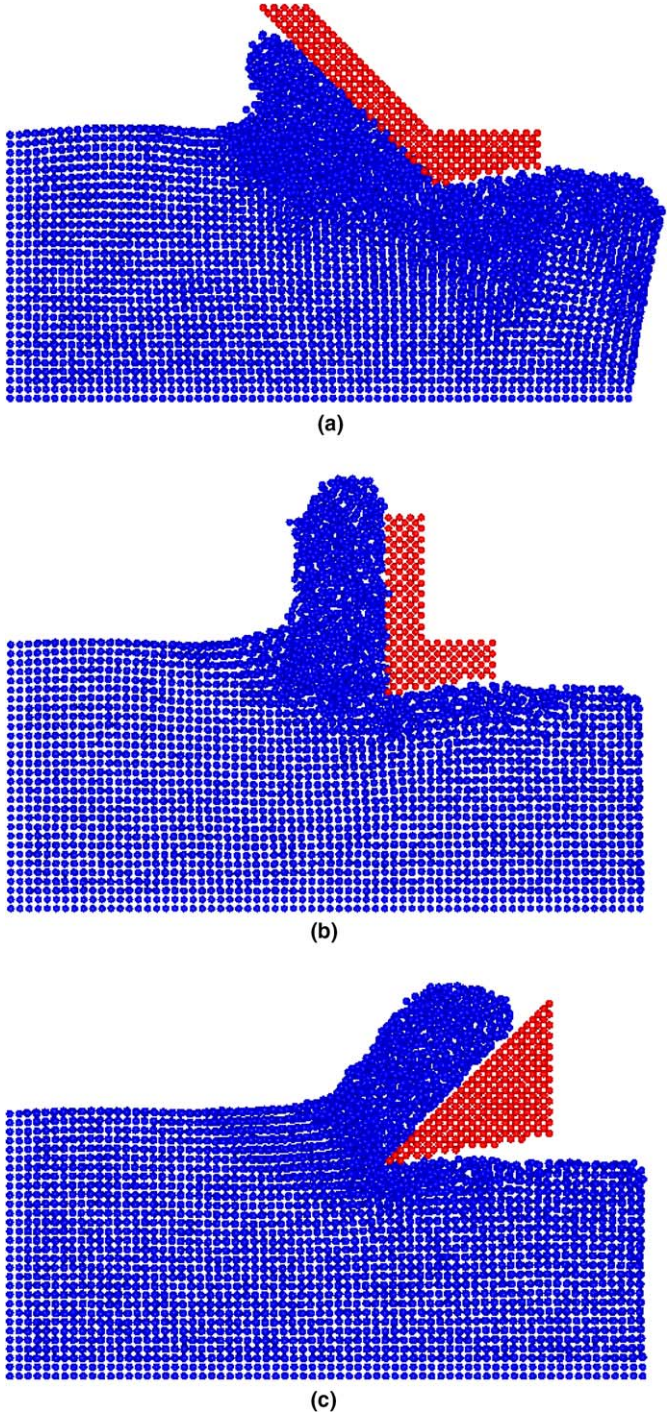

Fig. 8. Snapshots at time = 65.0 ps during the cutting processes with the EAM potential for the copper workpiece: (a) rake angle = −45°; (b) rake angle = 0°; (c) rake angle = 45°.

The bigger cutting forces with the Morse potential can also be explained by the metallic bonding. The bond strength in metallic bonding strongly depends on the local environment and becomes weaker when the local environment is more crowded. During the cutting process, the atoms at the cutting regions are very crowded, and so the

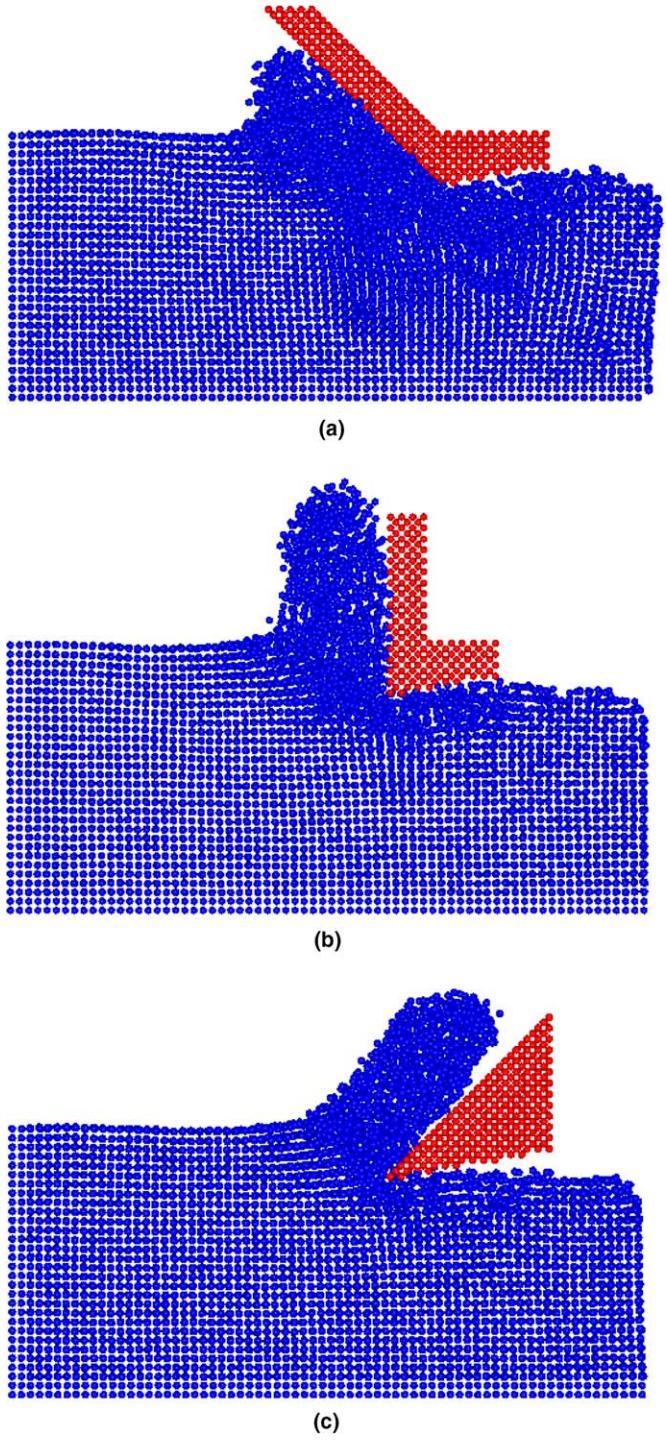

Fig. 9. Snapshots at time = 65.0 ps during the cutting processes with the Morse potential for the copper workpiece: (a) rake angle = −45°; (b) rake angle = 0°; (c) rake angle = 45°.

bonds there become weaker and easier to break than the other part of the workpiece. As the Morse potential considers only the two-body interaction and the bond strength does not depend on the local environment, the Morse potential will not result in weaker bond in more crowded region. Therefore, the simulated cutting forces under the Morse potential are higher than that under the EAM potential. This finding is very important and must be kept in mind when using MD simulation to study the nanometric machining processes. As the EAM potential describes the metallic bonding much better than the Morse potential, the EAM potential should be used for the MD simulations of nanometric machining processes.

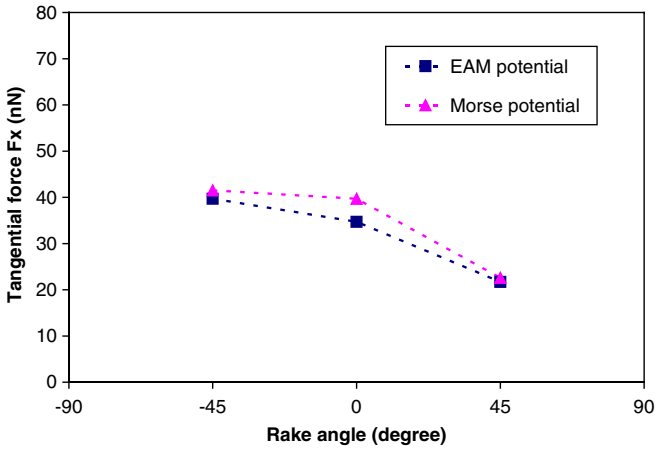

Fig. 10. Comparison of the tangential cutting forces under the EAM and Morse potential.

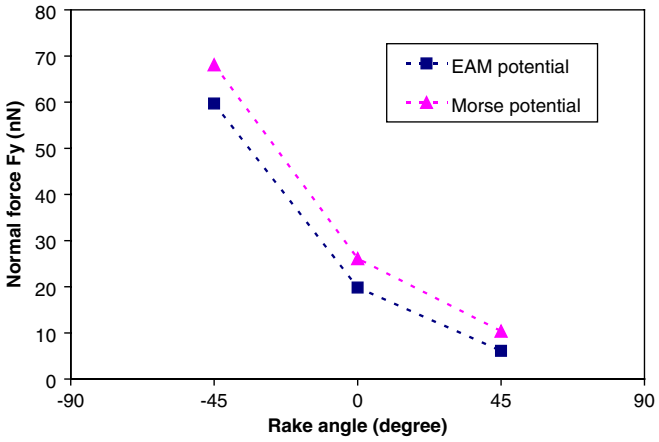

Fig. 11. Comparison of the normal cutting forces under the EAM and Morse potential.

4. Conclusions

MD simulations were carried out to study the nanometric cutting of copper. From the simulation results, the following conclusions can be drawn:

- The tool rake angle has big effect on the chip formation, subsurface deformation, and the smoothness of the machined surface. Smoother machined surface was obtained with the rake angle 45° than that with the rake angles of 0° and −45°. For the rake angle −45°, the chip is smaller due to the large plastic deformation generated in the workpiece. Besides, bigger elastic recovery was observed at the machined surface for the −45° rake angle.

- The cutting forces are strongly influenced by the rake angle. As the rake angle changes from −45° to 45°, both the cutting forces and the ratio of normal cutting force to tangential cutting force (F_y/F_x) decrease considerably.
- There is no big difference in the simulated chip formation and the machined surface between the EAM and the Morse potential. However, the cutting forces show considerable difference under the two different potentials. The Morse potential results in much higher (about 5–70% bigger) cutting forces than the EAM potential. As the EAM potential describes the metallic bonding much better than the Morse potential, the EAM potential is recommended to be used for the MD simulations of nanometric machining processes.

Acknowledgement

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