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Molecular dynamics simulations of thermal effects in nanometric cutting process

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Understanding the basic action of how material removing in nanoscale is a critical issue of producing well-formed components. In order to clarify thermal effects on material removal at atomic level, molecular dynamics (MD) simulations of nanometric cutting of mono-crystalline copper are performed with Morse, EAM and Tersoff potential. The effects of cutting speed on temperature distribution are investigated. The simulation results demonstrate that the temperature distribution shows a roughly concentric shape around shear zone and a steep temperature gradient lies in diamond tool, a relative high temperature is located in shear zone and machined surface, but the highest temperature is found in chip. At a high cutting speed mode, the atoms in shear zone with high temperature implies a large stress is built up in a local region.

molecular dynamics, nanometric cutting, temperature distribution

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1 Introduction

In recent years, nanomachining has attracted an increasing attention due to the remarkable advancement in science and technology. Therefore, it is instructive to get a better understanding of material removal mechanism in nanoscale. In nanometric cutting process, surface and subsurface atomic interactions play an important role. At such a small governing length scale, the traditional continuum representation of the problem becomes questionable. Furthermore, it is extremely difficult to observe machining phenomena and measure cutting parameters by experiment. To study such a process, molecular dynamics (MD) simulation method is more appropriate. Since the 1990s, MD has been used to study cutting mechanism in atomic scale. Much work has been preformed to study the chip formation, surface generation, tool wear, plastic and elastic deformation etc [1–7].

Some typical work has been done by many researchers. Blake et al. [8] and Ikawa et al. [9] investigated the effect of cutting edge radius and minimum cut thickness in nanometric cutting process. Komanduri et al. [10] simulated nanometric cutting under different cutting conditions to investigate the burr formation and exit failure in copper. They reported that the positive burr with no crack propagation into workpiece material was observed in more ductile material, in contrast, negative burr with crack propagation into workpiece material was observed in the not-so-ductile or somewhat brittle material. Cutting speed, crystal orientation and cutting direction have a strong effect on material deformation. Pei et al. [11] studied nanometric machining of copper with the model size of more than four million atoms, they found that as cutting depth decreases, the specific cutting force increases rapidly and a higher cutting speed results in more lattice defects at the cutting region and higher cutting forces. Lin et al. [12] investigated the effect of atmosphere in ultra-micro cutting by modifying the potential of surface

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atoms of diamond tool and silicon workpiece. The simulation results showed that principal cutting force decrease if the rake face of tool and the rear face of chips are exposed to atmosphere. Zhang et al. [13] used MD to study atomic scale deformation in silicon induced by two-body and three-body contact sliding and found that amorphous phase transformation is the main deformation mechanism.

However, the previous work mainly focused on clarifying the material removing mechanisms in nanoscale, examples can be found in discussion of tool wear, energy consumption, dislocation nucleation and emission etc, little work has been down on investigation of temperature distribution and corresponding thermal effects. In this work, the temperature distribution during nanometric cutting of mono-crystalline copper is investigated based on Morse, EAM and Tersoff potential. The simulation results are shown in 3D images and analyzed in detail.

2 MD simulation method

The simulation model for nanometric cutting includes a mono-crystalline copper workpiece and a diamond tool, as shown in Figure 1. The copper workpiece has the size of 90 a×45 a×11 a, where "a" (3.62 Å) represents the lattice constant of copper. The employed process model consists of 195309 fully dynamic workpiece and tool atoms. The workpiece is divided into three different kinds, namely, boundary atoms, thermostat atoms and Newton atoms, respectively. The initial temperature of the system is 300 K. The boundary atoms are fixed in positions to reduce the edge effects and maintain the proper symmetry of lattice. The motions of Newton and thermostat atoms obey Newton's second law, and are determined by direct integration of classical Hamiltonian equations of motion using the Velocity-Verlet algorithm. Periodic boundary condition is imposed in *Z* direction to reduce the effect of simulation scale. The top surface of workpiece is (1 0 0) plane and *X* direction is in the ⟨1 0 0⟩ orientation. The tool is divided into fix atoms and Newton atoms, respectively. The initial velocity of copper atoms is assigned based on Maxwell distribution, and the time step is set as 1 fs. Details of the simulation parameters are summarized in Table 1.

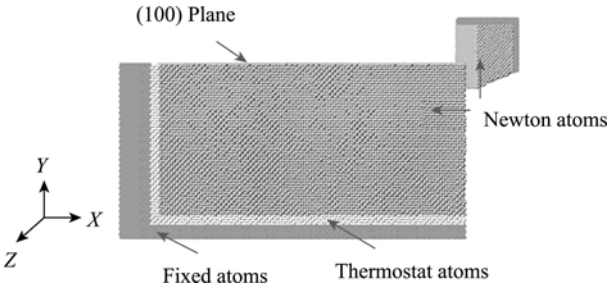

Figure 1 The MD simulation model of nanometric cutting.

Table 1 Workspace and simulation parameters

Potential for simulations	Tersoff, Morse, EAM
Workpiece material	Copper
Workpiece crystal structure	fcc
Workpiece dimensions	90 a × 45 a × 11 a
Clearance angle	15°
Rake angle	0°
Cutting directions	$[\bar{1}00]$ on (100) surface
Cutting depth	1.81 nm
Cutting speed	150–400 m/s
Initial temperature	300 K
MD time step	1 fs

There are three different atomic interactions in the current MD simulation: 1) the interactions between copper atoms (Cu-Cu); 2) the interactions between copper atoms and diamond atoms (Cu-C); 3) the interactions between diamond atoms (C-C). The interactions of diamond atoms (C-C) are depicted by Tersoff potential, which has been used successfully in nanometric cutting process [14–17]. For Tersoff potential, the total atomic potential energy of atoms in system is computed as follows

$$E = \sum_i E_i = \frac{1}{2}\sum_{i\neq j} V_{ij},$$

$$V_{ij} = f_C(r_{ij})[f_R(r_{ij}) + b_{ij} f_A(r_{ij})], \tag{1}$$

$$f_R(r_{ij}) = A\exp(-\lambda r_{ij}),$$

$$f_A(r_{ij}) = -B\exp(-\mu r_{ij}), \tag{2}$$

$$f_C(r_{ij}) = \begin{cases} 1, & r_{ij} < R, \\ \frac{1}{2} + \frac{1}{2}\cos\left[\pi\frac{r_{ij}-R}{S-R}\right], & R < r_{ij} < S, \\ 0, & r_{ij} > S, \end{cases} \tag{3}$$

$$b_{ij} = \left(1 + \beta_i^n \xi_{ij}^n\right)^{-1/2n},\ \xi_{ij} = \sum_{k\neq i,j} f_C(r_{ik})\omega_{ikg}(\theta_{ijk})$$

$$g(\theta_{ijk}) = 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h - \cos\theta_{ijk})^2}, \tag{4}$$

where E_i is the site energy, V_{ij} is the bond energy about all the atomic bonds, *i, j, k* label the atoms of the system, r_{ij} is the length of the *ij* bond, b_{ij} is the bond order term, θ_{ij} is the bond angle between the bonds *ij* and *ik*, f_R represents a repulsive pair potential, f_A represents attractive pair potential, f_C merely represents a smooth cutoff function to limit the range of the potential, and ξ_{ij} counts the number of other bonds to atom *i* besides the *ij* bond.

The Cu–Cu interactions between copper atoms are described by the EAM potential [18]. The total atomic potential energy of a system is expressed as

$$E_{\text{tot}} = \frac{1}{2}\sum_{ij}\varphi_{ij}(r_{ij}) + \sum_{i}F_i(\rho_i), \tag{5}$$

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

$$\rho_i = \sum_{j\neq i}\rho_j(r_{ij}). \tag{6}$$

For the Cu–C interactions between tool and workpiece atoms, Morse type pair potential is derived [19], the Morse potential is written as

$$\phi(r_{ij}) = D[\exp(-2a(r-r_0)) - 2\exp(-a(r-r_0))], \tag{7}$$

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

The conversion between kinetic energy and temperature of each atom can be computed at each time step, as the follows equation

$$\frac{1}{2}\sum_{i}m_i v_i^2 = \frac{3}{2}nk_B T_i, \tag{8}$$

where N is the number of atoms, v_i represents the instantaneous velocity. k_B is the Boltzmann constant and T represents the temperature of atoms. However, the kinetic energy of per atom could not be transformed into temperature immediately, the velocity of atoms should be averaged and reassigned to each atom every N steps, namely, for the sake of comparing the simulation results with macroscopic thermo-mechanism properties, and suitable data average algorithm should be taken. Furthermore, the contribution of tool movement in the cutting direction should not be included in computing the kinetic energy. The simulation results show that an average over about 2000 time steps led to significantly stable mean properties, but still provide a certain time resolution to study some dynamics of the cutting phenomena. The velocities of thermostat atoms are rescaled when the temperature departs more than 10 K of the specified temperature. This algorithm allows the transfer of heat from the machined region on the surface to the bulk of the workpiece material, similar to experiment [20]. The various temperature zones are coded by different colors to distinguish the system temperature distribution during nanometric cutting process.

3 Results and discussion

The defect-free specimen is relaxed for 20 ps to minimize energy. The variations of the average temperature of workpiece and tool with relaxation time are shown in Figure 2. The periodicity intermittence of surface atoms and the coordination number of overlapped atoms in workpiece are changed during relaxation process, and those atoms would be departed and vibrated around their lattice position to achieve a new equilibrium. From Figure 2, it can be seen that the average temperature fluctuations in both of workplace and tool becomes descending and keeps constant at about 300 K after 20 ps, which predicates the thermal equilibrium has achieved.

To study the effect of cutting speed on nanometric cutting process, simulations with cutting speeds of 150, 300 and 400 m/s have been conducted. The average temperature curves of workpiece and tool under different cutting speeds are shown in Figures 3 and 4, respectively. The corresponding cutting depth is 1.81 nm. It can be seen that the temperature in both of tool and workpiece are raised with cutting distance, the high cutting speed results in a relative high temperature in workpiece material, but the temperature in tool changes slightly. At a high cutting speed mode,

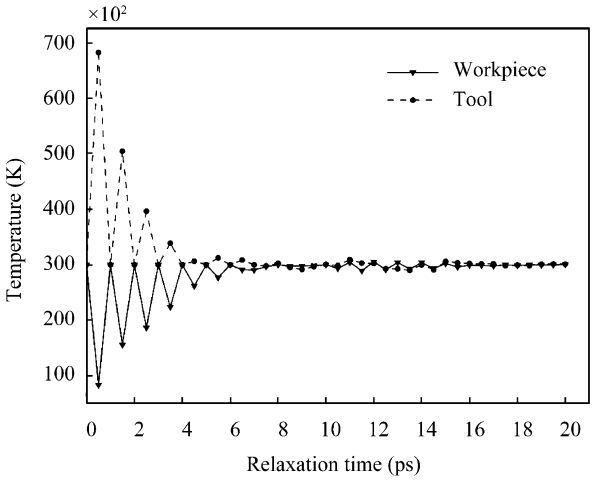

Figure 2 The average temperature-time curves during relaxation.

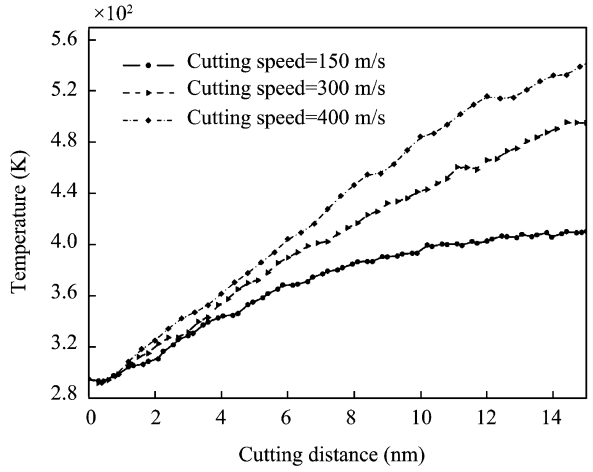

Figure 3 The average temperature curves of workpiece under different cutting speeds.

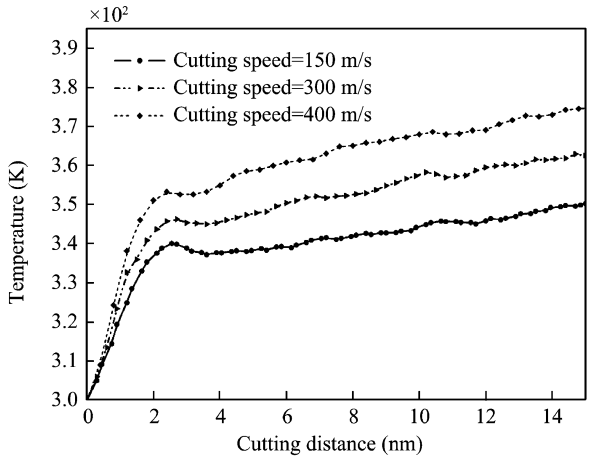

Figure 4 The average temperature curves of tool under different cutting speeds.

dislocations and the atoms in shear zone have a shorter time to rearrange, thus the dislocations pile up in the cutting region and strengthen the workpiece material, in which the extrusion and friction between atoms become more intensively. The friction and strain energy released from the deformed crystal lattice will be transformed into cutting heat, and results in a higher deformation force and generates more thermal energy. Besides, little chip is formed in the initial cutting stage, and almost all the thermal energy is concentrated in the tool-workpiece contact area, which leads to the rapid rise of the average temperature in tool as shown in Figure 4. Furthermore, it is clearly demonstrated that the fluctuation and increasing of the average temperature becomes smoothly with the increase of cutting distance, since most of heat is taken away by chips during stable cutting process. In addition, compared with copper, diamond has a much higher thermal conductivity which could transform heat faster and maintain a relative low average temperature in tool as discussed in the next part.

Figure 5 shows the side cross-sectional view of temperature distribution at cutting speed of 400 m/s, the cutting depth is 1.81 nm and the cutting distance is 15 nm. It can be seen that the temperature distribution shows a roughly concentric shape around shear zone, and a steep temperature gradient is observed in diamond tool. The temperature is about 700 K in shear zone and a relative high temperature (about 500–600 K) is remained in the machined surface, but the highest temperature lies in chip (about 1000–1100 K). In addition, from the topology of temperature distribution, it can be inferred that the temperature of some chip atoms is more than 1200 K, which is very close to the melting point of copper (1357 K), and the temperature level at the bottom of workpiece preserves about 300 K. The number of atoms in different temperature ranges is shown in Figure 6, It can be seen that when the cutting speed is 150 m/s, the atoms with temperature less than 400 K accounts for 73% and the atoms with temperature more than 700 K only holds about

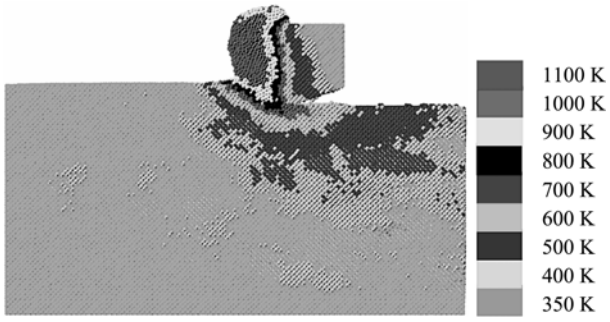

Figure 5 Side cross-sectional view of temperature distribution at cutting speed of 400 m/s.

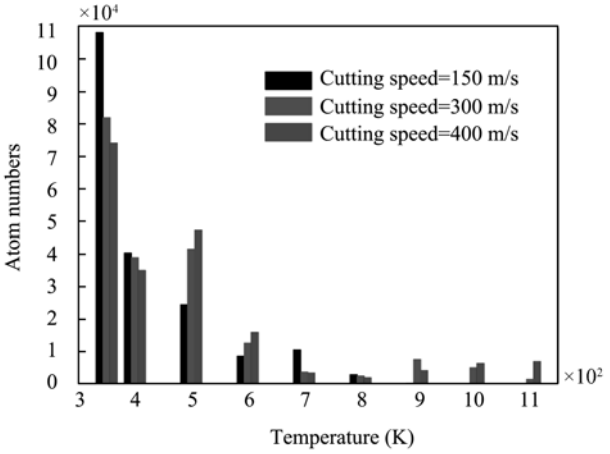

Figure 6 The number of atoms in different temperature ranges.

8%, and the highest temperature in chips is about 800 K. One can found that the number of atoms with high temperature is increased as the cutting speed increases. A significative phenomenon is that there are about two layers atoms in the surface of tool rake face, which has a considerable lower temperature than chips. Furthermore, the temperature of some tool atoms even lower than 350 K, and an obvious temperature gradient in tool can be observed. The temperature increment is a function of the relative atomic velocity and could be less in the case of smaller velocities. Additionally, diamond has a relative high thermal conductivity and could transfer heat faster. However, Newton atoms are so close to the thermostat atoms that the temperature drops obviously and results in a steep temperature gradient in tool. This similar phenomenon also is virtually all in good agree with the fact, compared with tool shank, that the volume ratio of diamond is very small.

The high temperature region in shear zone means a build up of large stress in a local region. Most of heat is generated by the friction and excursion between tool edge and workpiece atoms, and the atoms in shear zone with high temperature move along the rake face of tool forward, bonds are broken and bonds energy are released due to plastic deformation in workpiece material, and almost all the chemis-

try and kinetic energy are transformed into cutting heat. Most of heat is taken away by chips, but the relative small chip size and lack of energy conversion raised the system temperature ultimately. Furthermore, the thermostat atoms are so far away that they can not affect the temperature of Newton atoms significantly in workpiece. Although many dislocations and deformations are distributed around diamond tool, most of shear stress is concentrated in shear zone, which implies the formation of new shear plane with small effective shear angle and raises the chip cross-section [21]. Besides, the atoms vibrate more frequently and the distance between neighbor atoms increased with the raise of system temperature, which inevitably results in weakening the bonding force between atoms. Surface and subsurface atoms with high temperature in workpiece could be removed easily when external force are imposed on the tool, that is why workpiece could be deformed under a relative low cutting force as the temperature increases.

4 Conclusion

In the present work, MD simulations using Tersoff, EAM and Morse potential are conducted to study the thermal effects in nanometric cutting process. MD simulations provide a foundation insight into atomic process of cutting monocrystalline copper on (100) surface. The temperature distribution is roughly presents a concentric shape around shear zone. During cutting process there is a narrow region with the highest temperature in chip, which is nearly reaches the melting point of copper and implies that a relative high stress is generated and concentrated. Diamond has a good thermal conductivity and results in a steep temperature gradient in tool. High machining speed leads to a relative high deformation in workpiece, more chips are generated, and more kinetic energy and stress are transformed into cutting heat. At a lower cutting speed, dislocations and the atoms in shear zone have a longer time to rearrange, thus the highest temperature in shear zone is much lower and a smaller chip formation can be achieved.

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