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MD simulation of nanometric cutting of copper with and without water lubrication

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Three-dimensional molecular dynamics (MD) simulation was carried out to understand the mechanism of water lubrication in nanometric cutting. The water-lubricated cutting was compared with the dry cutting process in terms of lattice deformation, cutting force, heat and pressure distribution, and machined surface integrity. It was found that water molecules effectively reduce the friction between the tool and workpiece, the heat in the cutting zone and the pressure being generated on the tool surface, thus leading to prolonged tool life. Water molecules also enlarged the pressure-affected area, which decreased the roughness of the machined surface.

molecular dynamics, cutting tools

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1 Introduction

Nanometric cutting that has a depth of cut of several nanometres is extensively used in the manufacture of modern optic and photonic products [1]. In such cutting processes, considerably high hydrostatic pressure is distributed on the tool tip, as the contact zone between tool and workpiece is extremely small. This results in rapid tool wear, hence increases machining cost and degrades machined surface integrity [2]. Therefore, lubrication becomes indispensable in nanometric cutting to prolong tool life and achieve the required surface integrity.

In nanometric cutting, inter-atomic actions on the surface and under subsurface could become dominant. Therefore the influence of lubricant molecules on the workpiece surface generation should be taken into account. Understanding of the effect of lubricant molecules on cutting performance is a challenging issue as direct experimental observation is difficult, or even impossible, in a nanometric cutting process. For this reason, molecular dynamics (MD) simulations should be an ideal technique because it can reveal the deformation and removal mechanics that are involved in a physical process at atomic level [3]. For example, Zarudi et al. [4] suggested that the damage and change of the subsurface structure of monocrystalline silicon was highly related to the effects of water in repeated nano-indenting processes. Tang and Zhang [5] revealed that the presence of water could significantly reduce the adhesion between indenter and silicon during nanoindentation of single crystal silicon. Chen et al. [6] studied the surface damage during the impact of a large silica cluster on a crystal silicon substrate in dry and wet conditions, respectively. Their simulation results showed that the damage of silicon substrate under the dry condition was more severe than under the wet condition

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because considerably great impact energy is absorbed by the water film, which is transformed into thermal dissipation energy between the simulation ensemble and the water film. Rentsch and Inasaki [7] explored the impact of fluids on the surface generation and the tribological contact conditions on basis of MD simulation results, but they only considered simple atomic non-reacting fluid which ignores the rotational molecular momenta of inertia and didn't include the research on surface generation. Nevertheless, the lubrication effect in nanometric cutting has not been systematically studied by use of MD simulation.

This work aimed at investigating the lubrication effect of water in the nanometric cutting of copper using three dimensional MD simulations by comparing the results in terms of lattice deformation, cutting force, heat and pressure distribution and machined surface integrity under dry and wet impact.

2 Modelling and computational details

The simulations were carried out using large-scale atomic/molecular massively parallel simulator (LAMMPS) [8] which presented three parallel algorithms for classical molecular dynamics and visualised by software VMD [9] and Atomeye [10]. Figure 1 shows the MD model of the cutting system. It consists of a diamond cutting tool, a water layer, and a copper substrate with thermostat and boundary layers. The diamond tool is a rigid shell which has a rake angle of 0°, a clearance angle of 12°, a tip radius of 2 nm and is positioned 5 Å above the water molecules layer. The water molecules have a depth of 50 Å with a density of 0.977 g/mL. The copper substrate is 140*a* (where *a* is the lattice constant of copper, and equals to 3.6147 Å) long, 42*a* wide and 150*a* thick, which has a periodic boundary imposed on the *x* and *y* directions. The orientations of the monocrystalline copper along *x*, *y* and *z* axes are [100], [010] and [001], respectively. Underneath the copper substrate are the thermal and boundary layers, which ensure adequate heat conduction in the system and prevent the substrate from unexpected movements. Both the dimensions of the model and the periodic boundaries were carefully selected to avoid the boundary effect. The initial temperature of the substrate was set to be 300 K using the Nose-Hoover method [11]. During the cutting process, only the temperature of thermostat atoms were maintained at 300 K to ensure the dissipation of heat which generated due to the friction between cutting tool and the substrate. To simulate the dry cutting process for comparison, the water layer was taken off.

A three-body Embedded-Atom Method (EAM) potential [12], which has been extensively used in the MD simulation of the interaction between copper atoms, was used in this work. The Morse potential was employed to determine the interaction between the workpiece and the tool [13]. The diamond tool was treated as a rigid body while C-C interactions were neglected. Water molecules were simulated using the rigid TIP4P2005 model [14–16] to describe the intra-molecular electrostatic and Lennard-Jones water interactions that consists of four interaction sites with two positively-charged hydrogen atoms, a non-charged oxygen atom and a negatively-charged site in a planar configuration. The reaction field method which used to model the coulomb interactions between water molecules and the long-range Lennard-Jones potential was used to govern the non-bonded Cu-H_2O and C-H_2O interactions, where hydrogen atoms (intra-molecular long-ranged electrostatics) were not considered due to the insignificant role on the properties of silicon. The potential parameters used are given in Table 1.

The MD simulation was run using a timestep of 1 femtosecond. The cutting speed was 10 m/s. Water was initially relaxed to an amorphous state with a density of 0.977 g/mL at a temperature of 300 K. The model was further relaxed for 10000 timesteps to disintegrate water molecules on copper surface. A relatively thick water layer of 5 nm in depth was chosen so that there would be sufficient water-copper contact at the interface throughout the cutting process. The diamond tool initially stayed 5 Å above the water layer, and then penetrated into the water layer along the normal direction till it reached the copper surface. The tool then started to move laterally to create a taper-cutting mark before it moved tangentially to create the machined surface. The simulation without water layer was also carried

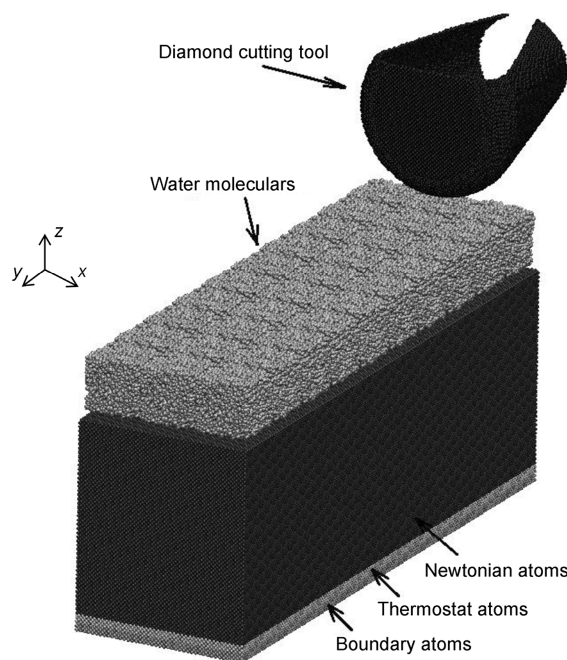

Figure 1 The MD model for water lubrication nanometric cutting.

Table 1 Parameters of the Lennard-Jones potential for interatomic pairs

Interatomic pair	ε (kJ mol^{-1})	δ (Å)
C–O	0.4785	3.275
Cu–O	0.38	2.467

out for comparison to understand the effect of water. The common neighbour analysis (CNA) [17], which is widely used to characterise the lattice deformation of perfect crystal structures, was used to measure the local crystal structure change during cutting and to visualise planar defects in copper crystals.

In MD simulation, an individual atom does not have a definite temperature, so kinetic energy of atoms is often used to determine the heat generated by friction and strain energy release involved in a cutting process. The conversion between kinetic energy and temperature can be computed using the following equation [18]:

$$\frac{1}{2}\sum_i m_i v_i^2 = \frac{3}{2} n k_B T_i, \tag{1}$$

where n is the number of atoms, v_i is the instantaneous velocity, k_B is the Boltzmann constant and T is the temperature of atoms. Based on the kinetic energy value of a similar cutting system [19], the temperature was calibrated and the temperature distribution was then generated.

To study the stress distribution in cutting area, the atomistic stress definition is used in this paper. The atomic stress i is a stress quantity at the atomic scale. It is a strength measurement of the inter-atomic interactions of the atoms with its neighbouring atoms. This atomic stress tensor is defined as [20]

$$\sigma_{\alpha\beta}(i) = -\frac{1}{2\Omega_i}\sum_{j\neq(i)}^{N} f_\alpha(i,j) r_\beta(i,j), \tag{2}$$

where N is the number of atoms in a region around atoms i within an EAM potential cut-off distance, $f_\alpha(i, j)$ is the vector component form of the interaction force exerted by atom j on atom i, $r_\beta(i, j)$ is the vector component form of the relative position form atom j to atom i, and Ω_i is the volume of atom i given by

$$\Omega_i = \frac{4}{3}\pi R_i^3, \tag{3}$$

where R_i is the radius of the atom i.

3 Experimental results

The comparison of workpiece deformation in cutting processes between dry and wet cutting condition is shown in Figure 2. In the wet cutting, when the tool penetrating into the water layer, water molecules were pushed into the copper surface and became interspersed with copper atoms, forming cavities on the copper surface around the tool-working interface. The uniformly distributed pressure introduced by the flow of water molecules did initiate stacking faults, as shown in Figure 2(b). In contrast, at the same time in dry cutting, copper surface remained intact before the tool touched the copper surface, as shown in Figure 2(a).

When the diamond tool penetrated through the water layer and into the copper, water molecules formed a thin layer which separated the tool and the workpiece, as shown in Figure 2(d). So the tool was not in direct contact with copper atoms during cutting. The dry cutting at the same time-step, as shown in Figure 2(c), started to generate stacking faults and a greater chip was formed.

During tool retrieving, as shown in Figure 2(f), because the water barrier was formed around the tool, the tool surface was clean and there was no adhesion of workpiece atoms. While in dry cutting, as shown in Figure 2(e), copper atoms attached to the tool surface.

Figure 3 shows the enlarged images of the retrieved tools after dry and wet cutting. It is clearly seen in Figure 3(a) that after dry cutting, there were a few copper atoms (red particles) resided on the tool surface, indicating the adhesion of workpiece material. In contrast, no copper atom was found on the tool surface after wet cutting in Figure 3(b), however, plenty of water molecules (pink and blue particles) left on the tool surface.

Figure 4 shows the normal and tangential forces obtained from both dry and wet cutting processes when the tool penetrated into the work surface and began to cut tangentially.

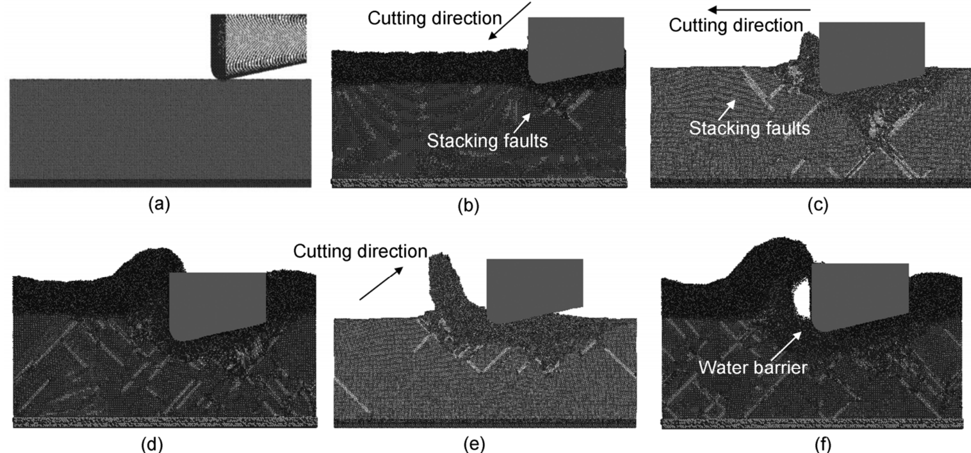

Figure 2 Comparison of cutting processes without and with water lubrication. (a) Dry cutting: prior to contact; (b) wet cutting: prior to contact; (c) dry cutting: in the cutting process; (d) wet cutting: in the cutting process; (e) dry cutting: tool retrieving; (f) wet cutting: tool retrieving.

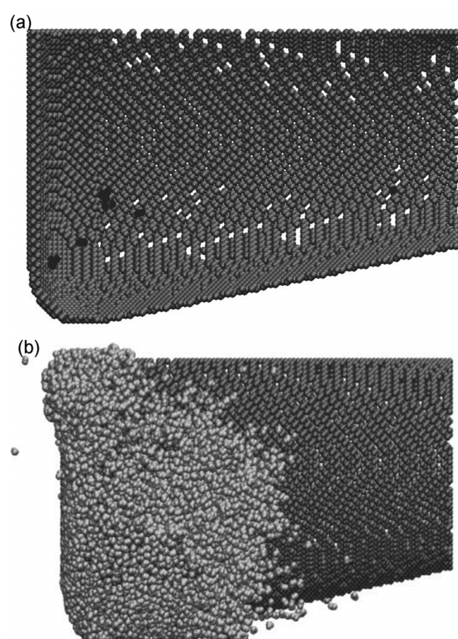

Figure 3 Comparison of tool surfaces after. (a) Dry cutting; (b) wet cutting.

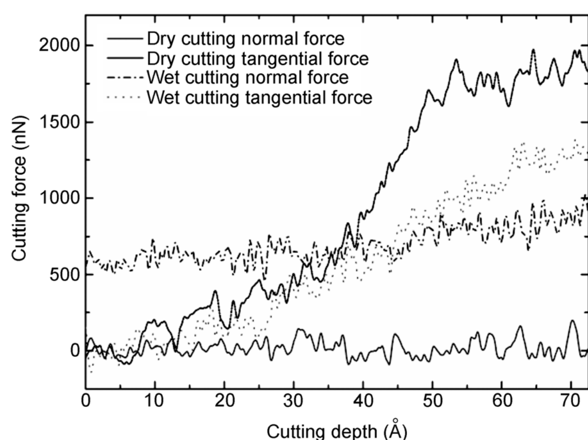

Figure 4 Comparison of forces between dry and wet cutting processes.

The normal forces involved in the wet and dry cutting processes remained almost unchanged with the progress of cutting. The normal forces were extremely small as the depth of cut was only several nanometres and the tool had already penetrated into the workpiece. The normal force in wet cutting had an offset value of about 500 nN as water molecules generated an extra force. The tangential forces in both dry and wet cutting processes gradually increased with the increased depth of cut due to the chip pile-up ahead of the rake face. The effect of water lubrication in wet cutting is obvious as the tangential force in wet cutting was 2/3 of that in dry cutting.

Figure 5 shows the temperature distribution of the workpiece during the dry and wet cutting processes. Since the water molecular can only reach 373 K which is relatively low compared to the temperature of the cutting area, the temperature distribution on water layer was not shown in Figure 5. As can be seen from Figure 5(a), in dry cutting the temperature of copper atoms near the rake face (shear zone) was 1000 to 1200 K and the temperature underneath the clearance face was 800–1000 K. The temperatures in the same areas were apparently lower for wet cutting, with only a small region of the shear zone reaching 1000–1200 K and most of the region underneath the clearance face reaching only 600–800 K, as shown in Figure 5(b).

Figure 6 shows the comparison of the stress distributions between the two processes. The hydrostatic pressure introduced by tool extrusion was concentrated on the tool tip area in dry cutting, reaching the maximum pressure of more than 10 MPa at the tip, as shown in Figure 6(a). In wet cutting, as shown in Figure 6(b), the pressure around the tool tip was effectively reduced to 8–9 MPa, although the pressure in some regions underneath the clearance face was slightly increased. Apparently, the inclusion of water molecules distributed the stress wider.

Figure 7 shows the cross-sectional views of uncut, cutting and cut surfaces in the two processes. The uncut surface without water effect was smooth, with a perfect crystalline structure, as shown in Figure 7(a), while the subsurface shown in Figure 7(b) had atomic cavities formed. During wet cutting there was a layer of water atoms surrounding the tool, forming a water barrier or lubrication film that separated the tool and the workpiece, as shown in Figure 7(d). After dry cutting, the cut depth left on the work surface was about 30 layers of copper atoms, as shown in Figure 7(e). In contrast, the cut depth after wet cutting was approximately half of what was generated by dry cutting.

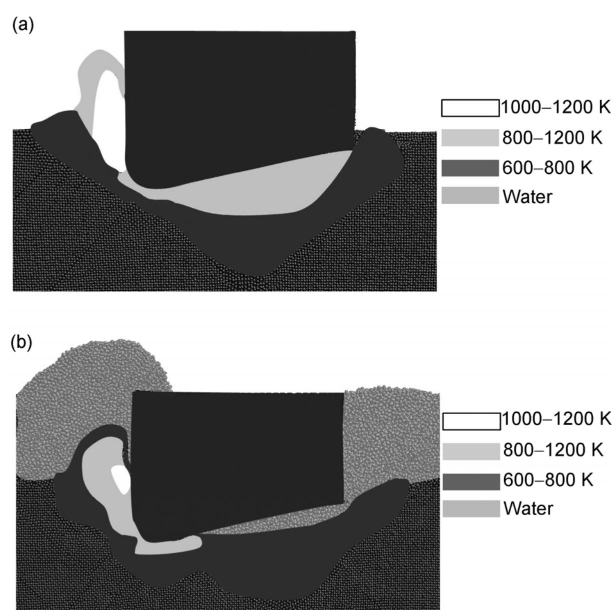

Figure 5 Temperature comparison. (a) Dry cutting; (b) wet cutting.

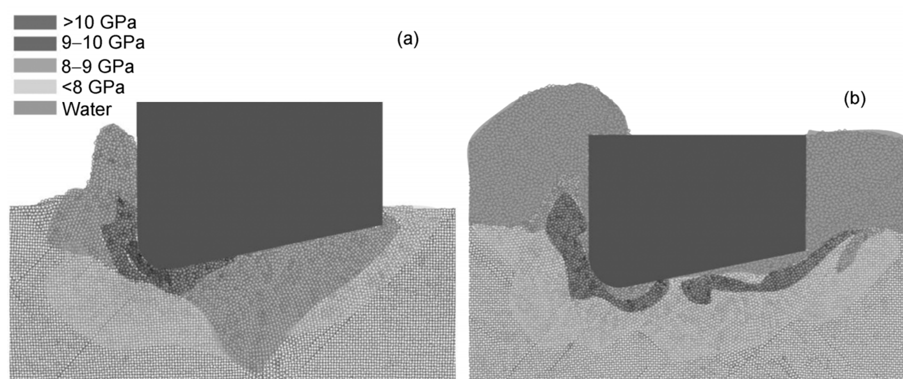

Figure 6 Stress comparison. (a) Dry cutting; (b) wet cutting.

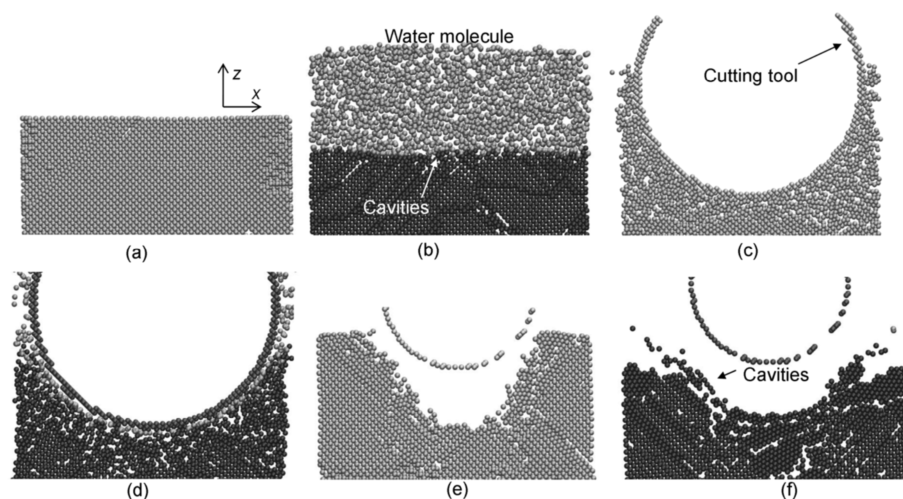

Figure 7 Comparison of work surfaces at different stage. (a) Dry cutting: uncut surface; (b) wet cutting: uncut surface; (c) dry cutting: cutting process; (d) dry cutting: cutting process; (e) dry cutting: after cutting; (f) wet cutting: after cutting.

4 Discussion

The comparison of results between the wet and dry cutting processes demonstrated that the effects of water molecules on the cutting performance were mainly through lubrication (i.e. reduction of friction), cooling (i.e. dissipation of heat), and surface pressure redistribution. When water was applied into nanometric cutting, water molecules quickly distributed at the contact area between the tool and the workpiece. As the consequence, an atomically thin layer of water film was formed around the tool, which separated the tool and the work material, as shown in Figure 7(d). Apparently, the formation of such a film reduces the friction between the tool and the workpiece during cutting as the tangential force of the water-lubricated cutting was reduced to 2/3 of the value for dry cutting, as shown in Figure 4. The formation of atomic water film around the tool also worked as a physical barrier, which prevented from the direct contact of copper atoms with the tool and reduced the heat generation by reducing the friction between them. In contrast, without the protection of water film, copper atoms would stick to the tool surface, which should increase the friction. The reduction in friction and the build-up of physical barrier due to the water addition into cutting process would certainly prolong the tool life.

The coolant effect of water on the cutting heat dissipation was obvious and expected. As shown in Figure 5, the temperatures around the cutting tool in wet cutting were apparently decreased. Water molecules flew away from the cutting zone, part of the kinetic energy of cutting was dissipated into water and taken away from the contact zone by the flow. Therefore, temperature was lowered. This also helped to reduce tool wear and improve the quality of machined surface.

Due to the interaction between water and copper molecules or the formation of water film, the pressure on the copper surface generated by the tool was spread wider, comparing to dry cutting, as shown in Figure 6. It was also found that the concentrated stress at tool tip in dry cutting was relieved in wet cutting. The reduction of stress concentrated at tool tip would significantly reduce the wear. This is

especially important as maintaining tool sharpness is critical to achieve the required surface finish, which is the top priority in nanometric cutting. As the stress was more evenly distributed around the tool in wet cutting, it is not surprising to see that the scratches left on the cut surface were shallower in this process (Figure 7(d)) than in the dry cutting (Figure 7(c)). Therefore, the use of water in nanometric cutting would definitely reduce the roughness of the machined surface, although more atomic cavities or defects were formed in the subsurface layer of several nanometres thick. As the stress distribution was altered by the inclusion of water molecules in wet cutting, the microstructure of the machined subsurface was slightly varied, in comparison to dry cutting. As shown in Figure 2(d), the area of copper amorphization [21,22] in the cutting zone was reduced in wet cutting, but the stacking faults initiated was increased, in comparison to the dry cutting in Figures 2(c) (note that the cutting conditions were the same). Since the dry cutting generated higher stress and high temperature around the tool, the stability of stacking-fault defects was lower than lubricated cutting, thus resulted in larger area of amorphization and smaller area of residual stacking faults [23]. It may be reasonable to derive that the amorphization of single crystal copper requires higher energy than the initiation of stacking faults in copper. Future studies should be carried out to verify this hypothesis.

5 Concluding remarks

The introduction of water into nanometric cutting resulted in the formation of water film at atomic scale around the cutting tool. This significantly reduced the tangential force and the heat generated during cutting. The water film also helped relieve the stress concentrated at the tool tip and prevented the chips from adhesion to the tool surface. All these effects reduced the friction between the tool and the workpiece and thus prolonged the tool life, leading to an improved surface finish. The only drawback was that more stacking faults and atomic cavities were generated in the subsurface layer of several nanometres deep.

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