Molecular Dynamics Simulation of Diamond Cutting Iron with Water Lubrication

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Abstract: The water-based cutting fluid plays an important role in cooling and lubricating during cutting process. In order to analyze the role of water in the cutting process from the microscopic view, this paper used molecular dynamics simulation to establish the cutting model with water lubrication by covering a water layer on the surface of iron workpiece. By comparing the cutting heat and friction coefficient under dry cutting and wet cutting, it is found that: water molecules will enter the gap between the tool and the workpiece, preventing the direct contact between the carbon atoms and the iron atoms, thereby reducing the friction coefficient. At the same time, wet cutting can reduce the surface temperature of the workpiece and play a role in cooling and lubricating.

1. Introduction

Diamond material is widely applied in ultra-precision machining due to the high hardness, high thermal conductivity, and low friction coefficient[1]. In ultra-precision machining, diamond tools have fast cutting speed, rapid temperature rise, and severe wear, which will shorten the service life of diamond tools and affect the accuracy of the machined surface[2]. Due to the limitation of the test conditions, the cutting test will consume a lot of resources. As a supplementary method of experimental research, molecular dynamics is widely used in the cutting simulation[3]. In recent years, there is a few papers that have done research on wet cutting in MD simulation. Therefore, this paper studies the influence of wet cutting on temperature and friction coefficient by simulating the cutting process with water lubrication. MD simulation is conducted by LAMMPS software. The visualization and analysis of simulation results are carried out by VMD software[4] and OVITO software[5].

2. Establishment of MD Model

The three-dimensional MD model of wet cutting is shown in Figure 1. The model consists of three parts: the single-crystal iron workpiece, the water layer and the diamond tool. The size of the iron workpiece is $8\text{nm} \times 12\text{nm} \times 5\text{nm}$; the size of the water layer is $8\text{nm} \times 12\text{nm} \times 1\text{nm}$; the size of the diamond tool is $3\text{nm} \times 3\text{nm} \times 3\text{nm}$. The number of water molecules in the system is 2874, and the number of Fe atoms and C atoms is 47860. The diamond tool and the iron workpiece were respectively divided into three different parts, namely the boundary layer, the thermostat layer and the Newton layer. The atoms in the boundary layer remain fixed in their equilibrium positions to simulate the boundary. The thermostat layer adopt Nose–Hoover thermal baths[6] to keep the temperature constant. The movement of atoms in the Newton layer is in accordance with Newton’s second law and is used to establish and solve
differential equations[7]. This paper used a four-point rigid water molecule model——TIP4P model, which adds an extra site compared to the traditional three-point TIP3P model. The four sites contained in the TIP4P model are two positively charged hydrogen atoms, one uncharged oxygen atom, and a massless negatively charged point. The distance between the massless negatively charged point and the oxygen atom is defined as OM distance. According to the LAMMPS manual, in the TIP4P water molecule model, the OM distance is 0.125Å. During the cutting process, the C-C interaction was described by the Tersoff potential function[8], the Fe-Fe interaction was described by the EAM potential function[9], and the C-Fe interaction was described by the LJ potential function[10]. The specific parameters are shown in Table 1.

Table 1 Lennard-Jones energies ($\varepsilon$) and distances ($\sigma$) for Fe, C and O

| Species | $\varepsilon$ (eV) | $\sigma$ (Å) |
|---------|-------------------|--------------|
| O-O     | 0.16275           | 3.16435      |
| O-Fe    | 0.06237           | 2.6405       |
| O-C     | 0.4785            | 3.275        |
| Fe-C    | 0.02495           | 3.7          |

In the simulation, the timestep was selected to be 1fs, the cutting speed was 2nm/ps, and the cutting thickness was 1nm. The initial temperature was set at 300k to simulate the actual environmental temperature. The water layer was first relaxed by Langevin thermostat to make its density 0.922g/ml, and then the water layer was relaxed under NVT ensemble to keep its temperature at 300k while fully contacting the surface of the iron workpiece. In this paper, PPF boundary conditions were selected and the periodic boundaries were used in the X and Y directions to reduce the boundary effects.

3. Simulation Results

Figure 2 shows the cutting process with water lubrication. Figure a is the state before relaxation, water molecules regularly cover the surface of the iron workpiece, and the water layer still maintains an ordered shape. Figure b shows the relaxation process. Since the size of the simulation box is slightly larger than that of the iron workpiece, water molecules can move to the side of the workpiece. When the relaxation begins, the water molecules begin to move under the constraints of the ensemble and the potential function, gradually wrapping the sides and the flank surface of the tool. As the tool feeds into the workpiece, more and more water molecules gather on the surface of the tool, wrapping the tool completely. As the cutting progresses, the diamond tool begins to squeeze and shear the Newton-layer atoms of the workpiece. Under the extrusion of the tool, shear slip and plastic deformation occur, and chips are formed in the Z direction gradually. During the cutting process, water molecules enter the gap between the tool rake face and the workpiece, and there are also water molecules gathering in the gap between the tool flank face and the workpiece, which prevents the direct contact between the carbon atoms and the iron atoms[11].
4. Analysis of Results

4.1. Influence of Wet Cutting on Temperature

Temperature is an important factor affecting graphitization of diamond tools. Therefore, it is necessary to clarify the effect of water layer on the temperature in wet cutting. Output the comparison diagram of the temperature under dry cutting and wet cutting, as shown in Figure 3. The workpiece temperature under wet cutting (blue line) is significantly lower than that under dry cutting (purple line), which is in line with forecast. The tool temperature under wet cutting (black line) is slightly higher than that under dry cutting (red line) in the early cutting stage. In the stable cutting stage, the tool temperature under wet cutting increases slowly, while the tool temperature under dry cutting maintains the previous growth rate. The reason is that in the early cutting stage, the number of water molecules in contact with the tool is small, and the water layer does not have a significant endothermic effect on the tool atoms. At the same time, since the water molecules are set as rigid water molecules, the interaction between the carbon atoms and the water molecules increases the heat released during the simulation process. Due to the large size of the workpiece, most of the water molecules are adsorbed on the workpiece surface, which can play a better role in endothermic effect.

Figure 2 Cutting process with water lubrication
4.2. Influence of Wet Cutting on Friction Coefficient
In MD simulation, the friction coefficient is defined as the ratio of tangential cutting stress to normal cutting stress[12]. The change of friction coefficient with timestep under wet cutting and dry cutting is shown in Figure 4. The friction coefficient under wet cutting is smaller than that under dry cutting in the stable cutting stage, which shows that the existence of water layer will play a role in lubricating. In wet cutting simulation, water molecules act like “rollers” in rolling bearings, which can convert sliding friction into rolling friction and reduce the friction coefficient.

5. Conclusions
In this paper, a MD simulation model of diamond cutting iron with water lubrication was established, and the cooling and lubricating effect of water molecules was studied from a microscopic point of view. The main conclusions are as follows:

(1) In the wet cutting process, the water layer will absorb the heat generated during cutting, resulting in the decrease of workpiece temperature and tool temperature.
(2) By comparing the dry and wet cutting process, it is found that water molecules will prevent the direct contact between the carbon atoms and the iron atoms, and reduce the friction coefficient.

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