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ARTICLE

Titanium Nanometric Cutting Process Based on Molecular Dynamics

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Abstract: Based on the molecular dynamics simulation (MDS) method, this paper built up a molecular dynamics (MD) model of titanium nanometric cutting. It chose representative cutting conditions, to obtain the instantaneous image of atomic position through simulation and analyzed the material removal phenomenon, the surface formation process, the change rules of system potential energy and workpiece temperature in cutting process. It is found that the formation of the chips and the machined surface in cutting process are caused by the release of lattice energy and the lasting expansion of dislocation. The elastic recovery and the lattice reconstruction of the machined surface can slow down the increasing trend of total potential energy and temperature, accompanied by slight fluctuations.

Key words: titanium; nanometric cutting; molecular dynamics; cutting parameters

With the development of computer science and technology, analog computation can provide the information that is unavailable or difficult to obtain during the experiment. Molecular dynamics simulation (MDS) is becoming the basic method to connect microscopic information and macroscopic properties of materials[1]. In the nanometric cutting process of some metals, workpiece material is removed in the form of discrete atoms or atomic layer. As a result, the finite element method and the macroscopic solid mechanics model based on the traditional continuum mechanics are difficult to exactly explain the various phenomena and internal mechanism produced in this process. While MDS method can easily change the cutting conditions, the geometric shapes of tools and the characteristics of materials to analyze the cutting process from the microscopic perspective of molecules and atoms[2].

Currently, the researches on MDS of ultra-precision machining surface formation mechanism, indentation phase change and cutting process about single crystal silicon, single crystal aluminum, single crystal copper and some other metals have been widely studied. Scholars like Hoover, Belak, Ikawa and Shimada[3-5] as well as some domestic scholars such as Luo Xichun, Liang Yingchun, Liu Fei, Zhang Junjie and Zhang Wentao[6-9] have done some concerned researches in this aspect.

In comparison, the researches on ultra-precision machining and nanofabrication of titanium are fewer now and so are the related articles. As a new functional material and important biomaterial as well as the "third metal" after iron and aluminum, titanium is widely used in industrialized countries because of its good characteristics of low density, good corrosion resistance, high specific strength and specific stiffness and so on[10]. Production and life in modern time need a high machining precision for the components of titanium and its alloys. Because the traditional classical cutting theory built on macroscopic continuum mechanics is not suitable for the explanation of titanium nanometric cutting process, this paper researched titanium nanometric cutting process from atomic scale based on the MDS method.

1 Theoretical Basis and Model Building of MDS in Titanium Nanometric Cutting Process

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The basic principle of MDS is to describe the interaction characteristics between molecules or atoms detailedly and accurately to achieve the understanding of some material's properties. For microscopic physical system, this principle gives the interaction potential between particles in the system, creates a set of motion equations that each particle is considered to obey the classical Newtonian mechanics laws, and then gets the coordinates and momentum of each particle at different time by numerical solution. That is the motion trajectory in phase space[11]. Based on the trajectory, it can reasonably explain the removal mechanisms and machining process of material in nanometric cutting process.

As is shown in Fig.1, the cutting model consists of titanium workpiece and diamond tool. According to the conditions of the computer's hardware, the number of workpiece material atoms is set as 2035, and that of tool atoms is 258. When cutting, the tool is supposed as rigid body. Workpiece material is in turn divided into three layers which are the boundary layer, thermostatic layer and Newton layer. Atoms in the Newton layer and the thermostatic layer follow the classical Newtonian mechanics equations to participate in simulation while the boundary atoms are always stationary. In the simulation process, it is necessary to conduct a speed calibration to the atoms in thermostatic layer every 20 step.

If we use MDS method to do a computer simulation, the key of whether the result is accurate or not depends on the selection of interatomic potential function[12].

The potential function between Ti-Ti selects an embedding atom method (EAM). The expression for total energy E of atom i is as follow:

$$E=\sum_i F_i(\rho_i)+\frac{1}{2}\sum_{ij(i\neq j)}\phi_{ij}(r_{ij}) \quad (1)$$

$$\rho_i=\sum_{j(j\neq i)} f_j(r_{ij}) \quad (2)$$

where, F_i is the embedding energy of atom i whose electron density is ρ_i; ϕ_{ij} is the relative potential energy of atom i and atom j; r_{ij} is the distance between atom i and atom j; ρ_i is the sum of electron cloud density produced by all other atoms' extranuclear electron to atom i; $f_j(r_{ij})$ is the electron density produced by atom j whose distance from atom i is r_{ij}.

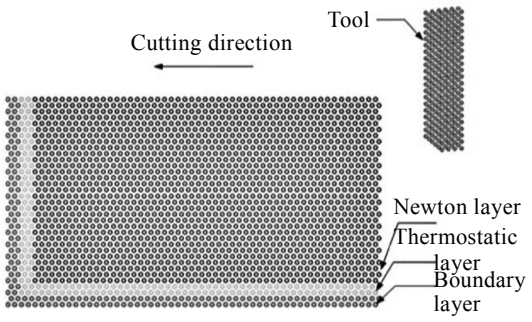

Fig.1 MDS model of titanium nanometric cutting

Because the parameters of Morse potential function between workpiece material and tool material can't be obtained directly from the literature, this paper uses the following method to calculate the parameters of Morse potential function of Ti-C.

$$\varphi_{\text{Ti-Ti}}(r_{ij})=D_{\text{Ti}}\left[\exp(-2\alpha_{\text{Ti}}(r_{ij}-r_{\text{Ti}}))-2\exp(-\alpha_{\text{Ti}}(r_{ij}-r_{\text{Ti}}))\right] \quad (3)$$

$$\varphi_{\text{C-C}}(r_{ij})=D_{\text{Ti}}\left[\exp(-2\alpha_{\text{C}}(r_{ij}-r_{\text{C}}))-2\exp(-\alpha_{\text{C}}(r_{ij}-r_{\text{C}}))\right] \quad (4)$$

We use the following similar Morse potential function to describe the interaction potential between Ti-C:

$$\varphi_{\text{Ti-C}}(r_{ij})=D_{\text{Ti-C}}\left[\exp(-2\alpha_{\text{Ti-C}}(r_{ij}-r_{\text{Ti-C}}))-2\exp(-\alpha_{\text{Ti-C}}(r_{ij}-r_{\text{Ti-C}}))\right] \quad (5)$$

In the formulas above, $\varphi_{\text{Ti-Ti}}(r_{ij})$ is Morse potential function of Ti-Ti; $\varphi_{\text{C-C}}(r_{ij})$ is Morse potential function of C-C; $\varphi_{\text{Ti-C}}(r_{ij})$ is Morse potential function of Ti-C; α is gradient coefficient of potential energy curve and D is binding energy coefficient.

Parameters of Morse potential function of Ti-C can be calculated by Eqs. (3)~(5):

$$D_{\text{Ti-C}}=\sqrt{D_{\text{Ti}}D_{\text{C}}} \quad (6)$$

$$\alpha_{\text{Ti-C}}=\sqrt{\alpha_{\text{Ti}}\alpha_{\text{C}}} \quad (7)$$

$$r_{\text{Ti-C}}=\sqrt{r_{\text{Ti}}r_{\text{C}}} \quad (8)$$

where $D_{\text{Ti-C}}$, $\alpha_{\text{Ti-C}}$, $r_{\text{Ti-C}}$ are the binding energy coefficient, gradient coefficient of potential energy curve and equilibrium distance of Ti-C, respectively. We can substitute the parameters' values into formula (6)~(8) to get:

$D_{\text{Ti-C}}$=0.982 eV, $\alpha_{\text{Ti-C}}$=22.83 nm, $r_{\text{Ti-C}}$=0.1892 nm

Specific cutting conditions are shown in Table 1.

2 Result Analysis of Titanium Nanometric Cutting Process

Table 1 Cutting conditions of titanium nanometric cutting simulation model

Material	Titanium	Diamond
Number of atoms	2035	258
Potential function	EAM (Ti-Ti)	Morse (Ti-C)
System temperature/K	300	
Time step/fs	2	
Cutting speed/m·s^{-1}	300	
Cutting depth/nm	3	
Rake angle/(°)	0	
Relief angle/(°)	5	
Cutting edge radius/nm	1.068	
Cutting plane	(0001)	