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Study on Influence Factors of Silicon Nitride Nano-cutting Process by Molecular Dynamics

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Abstract: Si_3N_4 ceramics becomes a new promising material due to its excellent physical and chemical properties. However, it is difficult to process and has high processing costs, which limits the further application of Si_3N_4 ceramics. In this paper, the molecular dynamics (MD) is employed to nano-cutting simulation of silicon nitride. The interaction forces between atoms are calculated by Tersoff potential function. The influences of cutting temperature, energy under different cutting rake angle, cutting speed and cutting depth on the cutting process are analyzed from the atom's point of view. The results show that shear effect of tangential force plays a main role on cutting process. Increasing the cutting rake angle appropriately can reduce the cutting temperature. The changes of cutting rake angle have a little effect on the potential function. The simulation results are helpful to improve the processing efficiency and reduce processing costs of the silicon nitride ceramics, which have certain guiding significance on the applications of Si_3N_4 ceramic materials.

Keywords: Si_3N_4 ceramics; Tersoff; molecular dynamics; nano-cutting.

1 Introduction

Si_3N_4 ceramics is a kind of important ceramic materials, it is widely used in industrial fields and has broad application prospects due to its excellent characteristics, such as high strength, high temperature resistance, corrosion resistance, and good thermal insulation, and so on. In the actual processing, the cutting rake angle, the cutting depth and cutting speed are difficult to change after setting due to the restriction of current experimental conditions, which has a high cost for our experimental studies. While molecular dynamics is a powerful computer simulation method, it can not only adjust the corresponding parameters according to need in the simulation program, but also can avoid various defects of workpiece covering real machining mechanism of the actual experiment, it is helpful to explain correctly for nano-machining mechanism. At home, molecular dynamics studied on nano-machining starts later. Lin Bin was engaged in the research of nano-grinding [1]. Liang Yingchun, Luo Xichun and Tang Yulan conducted a study on nano-cutting and cutter wear, and so on, which had achieved certain results [2-7].

At present, molecular dynamics studies on simple structure of single crystal materials had been some achievements, but had a little research on complex structure of compounds. In this paper, molecular dynamics was applied to simulate Si3N4 cutting process, it has characteristics of the simple modeling, fast operation, convenient use, and so on.

2 Experimental Details

2.1 The establishment of cutting model

Si3N4 ceramics is a covalent bond compounds, the basic building unit is silicon-nitrogen tetrahedron shown in Fig. 2.1, in which a silicon atom lies at the center, and four nitrogen atoms are located at each corner.

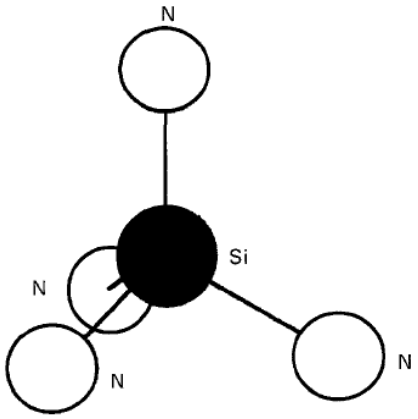

Figure 2.1: Si_3N_4 tetrahedral element

The molecular dynamics model of Si_3N_4 nano-cutting is shown in Fig. 2.2. The β-Si_3N_4 is selected as workpiece material, its crystal structure is shown in Fig. 2.3(yellow circles represent Si atoms, the blue circles represent N atoms), the diamond is used as cutter material. The workpiece is divided into three different zones, namely the Newtonian zone, the thermostat zone, and the boundary zone. The Newtonian atoms obey Newton's second law. The thermostat atoms need to be calibrated in order to maintain constant temperature in this region. The boundary atoms are fixed in their position to reduce the boundary effects and maintain proper symmetry of the lattice.

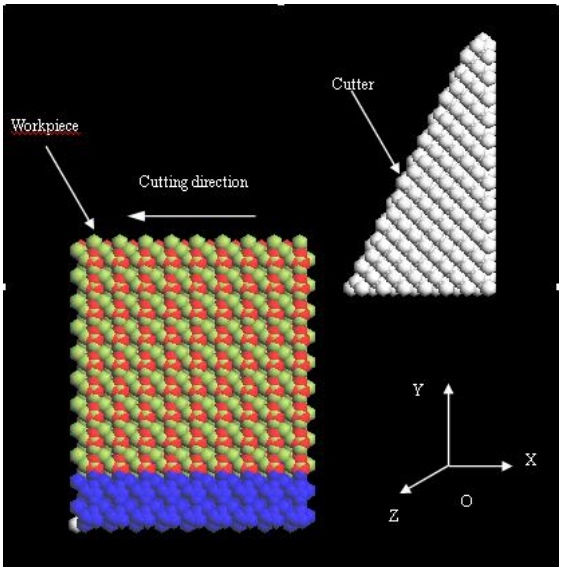

Figure 2.2: Molecular dynamics mode of Si_3N_4 nano-cutting

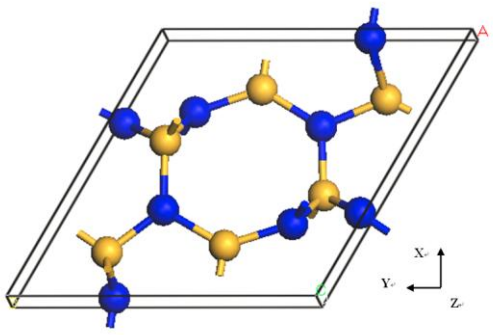

Figure 2.3: Si_3N_4 crystal structure

2.2 The choice of ensemble and potential function

The micro-canonical ensemble (NVE) [8] is employed in this simulation. When simulate the complex structure of Si_3N_4 crystal, we must consider the polyatomic interactions, so Tersoff [9, 10] potential function is used to calculate the interaction between Si atoms and N atoms and the Si-N atoms, as follows:

$$E = \frac{1}{2}\sum_{i \neq j} v_{ij} \tag{1}$$

Among,

$$v_{ij} = f_c(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right] \tag{2}$$

Where E is the total energy of system; v_{ij} is the bond energy about all the atoms; r_{ij} is the length of the ij bond, b_{ij} is the bond order term, f_R represents a repulsive pair potential, f_A represents an attractive pair potential, f_C represents a cut-off function.

2.3 The algorithm of motion equations

The Verlet algorithm is widely used due to easy use, good stability, and less storage space. In this paper, the Verlet algorithm is used to solve the equations of motion. The formula is as follows:

$$r(t+\delta t) = r(t) + v\left(t + \frac{1}{2}\delta t\right)\delta t \tag{3}$$

Among,

$$v\left(t + \frac{1}{2}\delta t\right) = v\left(t - \frac{1}{2}\delta t\right) + a(t)\delta t \tag{4}$$

2.4 The solution of processing temperature

In the microscopic simulation of cutting process, the atoms of crystal do thermal vibration in the equilibrium position. Each atom has three degrees of freedom in the thermal vibration. According to the energy equipartition theorem, the average kinetic energy of the system in each step is:

$$E_K = \frac{3}{2}NK_BT = \sum_i \frac{1}{2}mv_i^2 \tag{5}$$

Where EK is the atomic kinetic energy, N is atomic number, KB is Boltzmen constant, T is the temperature of the system. The average temperature of each time step can be calculated according to equation (5).

2.5 The simulation conditions

Table1. Conditions Simulation of Molecular Dynamics

Material	Workpiece: β-Si_3N_4	Tool: Diamond cutter
Lattice constant	a=b=7.606Å, c=2.909 Å	a=3.567 Å
Size	9a×11b×5c	
Atoms number	10511	
Potential function	Tersoff	
Time step	t=1fs	
Temperature	T_0=293K	
Cutting direction	(100) crystal face [100] anti-orientation	

3 Analysis of Simulation Results

3.1 Cutting force analysis

The cutting force is an important physical parameter for understanding the cutting process, cutting force comes from the interaction force between workpiece atoms and cutter atoms in nano-scale cutting process.

Workpiece suffers tangential force of the x-axis direction and axial force of the y-axis direction from cutter, the curves of tangential force and axial force are shown in Fig. 3.1. In the cutting process, the atomic crystal array suffer shearing action of tangential force and atomic bonds breaking, while subject to the extrusion of cutter lead to lattice deformation, lattice reconstruction and amorphous phase transition. Cutter moves forward continuously, the atoms of amorphous layer below the cutter combine to the atomic bonds of machined surface fracture by the action of axial force, forming the machined surface metamorphic layer. The atoms in ahead of the cutter are removed by the action of the tangential force. It is seen that the tangential force and axial force increase ceaselessly along with the movement of the cutter, and reciprocate fluctuations, even fluctuate severely in some places. The fluctuations have a close relationship to lattice deformation, lattice reconstruction and amorphous phase transition. And can be seen that the shearing action of the tangential force play a major role in the cutting process.

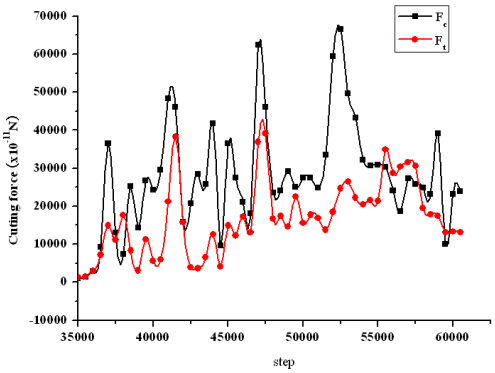

Figure 3.1: Cutting force curve

3.2 Temperature analysis

The temperature curves with different cutting conditions are shown in Fig. 3.2. It can be seen that the temperature increases rapidly when the cutter contacts with the workpiece, this is because the workpiece atoms subject to the extrusion effect of the cutter. Since the cutting force is not sufficient to destroy the atomic bonds, the temperature changes slowly. The cutting force increases gradually along with the cutting, leading to the atomic bonds break, which causes the lattice deformation, bond energy and lattice energy release, so the workpiece temperature increases gradually. When cutting into a steady state, the temperature tends to stable.

The temperature curves under the cutting speed of 109m / s, the cutting rake angle of 0°,and the cutting depth of 2.0a, 2.5a, 3.0a are shown in Fig.(a). It can be seen that the steady state cutting temperature is different under different cutting depth, and the temperature increases along with the cutting depth increases. This is because the contact area of cutter and workpiece and the pair atoms of chemical bonds increase, meanwhile the atomic lattice deformation and amorphous phase transition release more energy, thus the temperature increases.

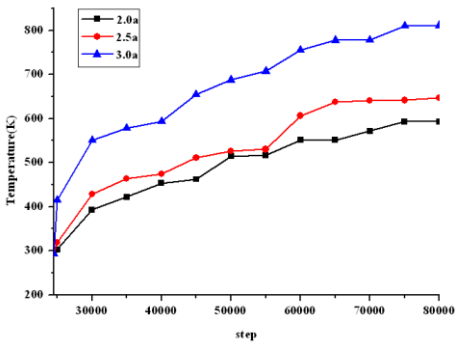

Figure (a) Temperature curves with different cutting depth

The temperature curves under the cutting thickness 2.0a, the cutting speed 109m / s, the cutting rake angle of 15°, 25°, 30° are shown in Fig.(b). It can be seen that the steady state cutting temperature is different under different cutting rake angle, and the temperature reduces with the cutting rake angle increases. This is because cutting becomes easier with the cutting rake angle increases, not only reduces the plastic deformation of the rake face extruding cutting layer, but also reduces the frictional resistance of the cutting chip flowing through the rake face. Thus the cutting heat reduces and the cutting temperature decreases.

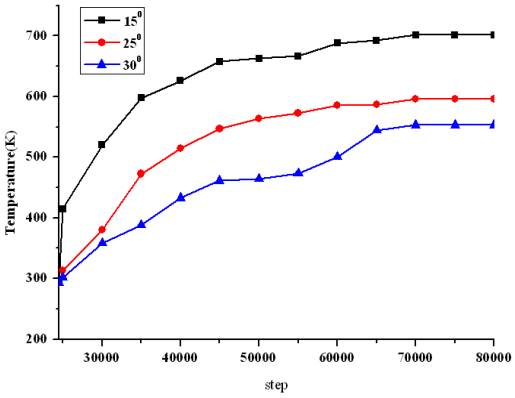

Figure (b) Temperature curves with different cutting rake angle

The temperature curves under the cutting depth of 3.0a, the cutting rake angle of 0°, and the cutting speed of 87m / s, 109m / s, 131m / s are shown in Fig.(c). It shows that the steady state cutting temperature is different under different cutting speed, and the temperature increases with the cutting speed increases. This is because the time of the cutting to reach the same molecular dynamics step reduces, and the lattice reconstruction and elastic recovery reduce, so that more energy is converted into heat and thus the temperature increases.

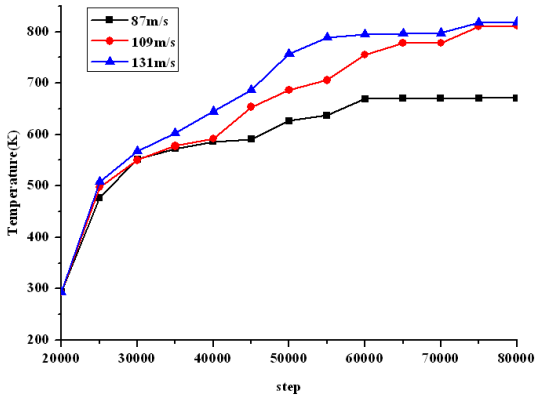

Figure (c) Temperature curves with different cutting speed

Figure 3.2: Temperature curves with different cutting conditions

3.3 Energy Analysis

The curves of kinetic and potential energy under the conditions of cutting depth 2.0a, cutting speed 109m / s, and cutting rake angle 20°,25°,45° are shown in Fig. 3.3.

The curves of the kinetic energy are shown in Fig.(a). In the relaxation phase, the kinetic energy fluctuates small and is basic to 0. When cutter contacts the workpiece, the kinetic energy increases gradually in the fluctuations. In the begining, the kinetic energy increases slowly due to the cutting force is not enough to cut off atomic bonds. The cutting force increases as the cutting progress, the atoms are subjected to the cutting action with cutter movement, so kinetic energy increases. When cutting into 60000 steps, the kinetic energy tends to maximum. Then, the kinetic energy decreases gradually in the fluctuations. When the cutting is completed, the kinetic energy is basic to 0. Comparison curves can be seen that the kinetic energy increases with the cutting rake angle increases.

The curves of the potential energy are shown in Fig.(b). In the relaxation phase, the potential energy decreases gradually due to the atoms exchange places constantly When the cutter contacts the workpiece, the potential energy increases gradually and accompanies by severe back and forth fluctuations. The potential energy increases due to the cutting action make the distance between atoms decrease, the reciprocating fluctuations have relations with lattice deformation, lattice reconstruction and amorphous phase transitions.

When cutting into 60000 steps, the potential energy tends to maximum, and then decreases gradually. When the cutting is completed, the potential energy is stabilized basically. It can be seen that the potential energy does not change significantly with the cutting rake angle increases.

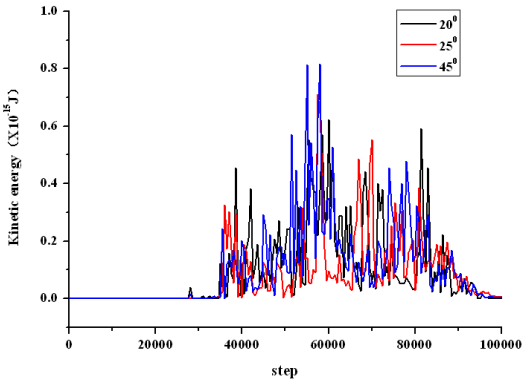

Figure (a) Kinetic energy curves

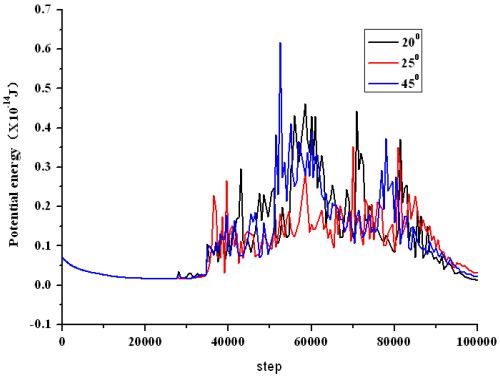

Figure (a) Potential energy curves

Figure 3.3: Energy curves with different cutting rake angle

4 Conclusion

In the simulated results, it can be seen that the shearing action of the tangential force plays a major role on the cutting due to the values of tangential force greater than the axial force. The results also indicate the temperature increases with cutting depth and cutting speed increase, the temperature reduces with the cutting rake angle increases. Therefore, appropriate to increase the cutting rake angle in nano-cutting process can reduce squeezing action of the rake face, and reduce the frictional resistance of the chip flowing through the rake face, thereby reducing the cutting temperature. Moreover, in the cutting process, the kinetic energy increases with the cutting rake angle increases, the cutting rake angle changes have little effect on the potential energy in the cutting process.

Acknowledgements

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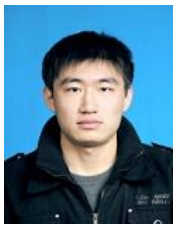

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