Simulation Analysis of Nanocutting on The Surface of Sapphire

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Abstract - The three-dimensional quasi-steady molecular statics nanocutting model developed by this paper carries out simulation analysis of nanocutting of sapphire substrate in order to explore the effects of tools with the same tip radii of probe and straight-line cutting at different cutting depths, on cutting force. The three-dimensional quasi-steady molecular statics nanocutting sapphire workpiece model first assumes the trajectory of each atom of the sapphire workpiecs being cut whenever the diamond cutter goes forward one step. It then uses the optimization search method to solve the force equilibrium equation of the Morse force in the X, Y and Z directions when each atom moves a small distance, so as to find the new movement position of each atom, and step by step calculates the behavior during cutting. And from the simulation results of cutting force, down force and side force, it is found that under the actions of cutting tools with the same tip radius of probe, cutting force enlarges with the increase of cutting depth. This result is identical to the actual experimental phenomena of nanocutting. From this, it is known that the simulation model developed in this study is reasonable.

Keywords *- quasi-steady molecular statics, sapphire substrate, nanocutting.*

I. INTRODUCTION

The theory of molecular mechanics was first proposed by Irving and Kirkwood [1]. It is mainly the use of a potential energy function model that dominates the action force between molecules, and the calculation of movement equation to acquire the corresponding physical properties and dynamic characteristics. The theory of molecular mechanics is mainly composed of three parts: (1) potential energy selection model; (2) Newton movement equation, and (3) energy minimization method. Of them, the method used by scholars applying Newton movement equation is called molecular dynamics (MD), whereas the method used by scholars applying energy minimization for calculation is called molecular statics (MS). The purpose of both of them is to find the displacement of each molecule in the system according to the action force on the molecules in the system and the initial position status.

Shimada [2] used 2D models and molecular dynamics to perform dynamic simulation of orthogonal cutting and explore its relationship with formation of chips. Childs and Maekawa [3], and Stower et al. [4] employed MD theory for numerical simulation of cutting, but their model lacked complete quantitative calculation. Fang et al. [5] indicated that the nanoscale cutting action was mainly produced by extrusion, unlike the traditional cutting behavior that shear force made workpiece become deformed. Inamura et al. [6,7] considered atoms as nodes, and used the Morse potential between atoms to deduce the finite element formulation of an atomic model. They took the Morse potential between two different atoms as examples for simulation, and acquired the formation process of chips, as well as the changing process of shear force and potential energy with the movement of cutting tool. Lin and Huang [8] improved the finite element model of Inamura et al. [9], and used the Morse potential between cutting tool and workpiece atoms to govern atomic movement by MD so as to describe the entire cutting process. With atoms regarded as nodes and lattices as elements, they developed a nanoscale orthogonal cutting model equation, and calculated the displacement of each molecule on the middle cross-section of the cut workpiece. Using the calculated molecular displacement and the concept of shape function in FEM, they calculated the strain of material. Furthermore, they used the flow stress-strain relational equation obtained after regression of the stress-strain curve of numerical stretching experiment of nanoscale thin film, to calculate equivalent stress. M. Rahman [10] used the radius of the same cutting tool to explore different cutting depths of silicon workpiece, and made simulation comparison among different cutting depths and tip radii of cutting tool. As a result, two important conclusions were drawn. When cutting of Si material was performed in ductility model, the cutting depth had to be smaller than the radius of cutting tool. When the cutting tool was greater than a certain limit, ductility cutting could not be produced. Therefore, the radius of cutting tool had to be appropriately small for smooth cutting.

Nevertheless, since the time step of MD was too small, a great deal of time had to be spent on calculation in simulation process, thus creating a problem of difficult calculation. Therefore, there were scholars who gradually took molecular statics method to simulate nanoscale studies, with the expectation to improve the problems encountered in MD. Kwon and Jung [11] explored the material nature of atomic scale balance in static load, and proposed a model combining atoms and FEM. This model

was used to simulate the stretching problem of nanoscale on materials with defects. Using molecular statics (MS) method, Jeng and Tan [12] took the smallest energy principle in finite element as the structure in order to simulate the displacement and deformation process of nanoscale impress. The smallest potential energy method was mainly used. After that, displacement control iterative method in non-linear FEM was used to solve the relationship between different forces and positions of atoms. Lin and Ye [13] investigated the simulation of 2D nanocutting of different shape of diamond cutters cut the copper material, analysis the cutting action and cutting force et al. But this paper didn't consider the conditions of three dimension nanoscale cutting. Lin and Wang [14] used 3D quasi-steady molecular statics to simulate and investigate the abrasive cutting behavior on silicon wafer, and compared the simulation results with the related literature of using molecular dynamics method to prove the 3D quasi-steady molecular statics nanoscale abrasive cutting model is reasonable.

Sapphire (Al_2O_3) belongs to a rhombohedral structure. Since its optical penetration band is very wide, it has very good transmittance. Therefore, sapphire has been extensively applied to optical elements. Besides, also because of its thermostability and high degree of hardness, it is also a material being difficult for machining. Currently, there is still no related literature studying the use of sapphire to be a material for nanocutting. For general related academic references about three-dimensional nanocutting, their simulation analyses mostly used MD model. However, this method needs analysis and simulation for a long time. Therefore, this study establishes a simulation model of three-dimensional quasi-steady molecular statics nanocutting of sapphire. Focusing on the same tip radii of probe of AFM as tool and different cutting depths, this paper conducts simulation and analysis of different axial cutting forces

II. NANOCUTTING SAPPHIRE SUBSTRATE SIMULATION MODEL

This study uses three-dimensional quasi-steady molecular statics nanocutting model to simulate the cutting of a sapphire (α-Al_2O_3) workpiece using AFM diamond probe. The physical model of nanocutting is composed of 56,079 sapphire atoms arrayed in a hexagonal close-packed structure, and belongs to a rhombohedral structure, as shown in Fig. 1. The cutting tool is composed of 2,623 carbon atoms and arrayed in a diamond formation. Thus, this study carries out simulation use of the probe tool of AFM, which there is a hemisphere at the end of the tip with the radius of 2nm to establish a three-dimensional quasi-steady nanocutting model of molecular statics and perform cutting of sapphire substrate. The calculation parameters of cutting are shown in Table 1. The model of three-dimensional nanocutting of sapphire crystal structure is shown in Fig. 1. It is found that building the model of three dimensional sapphire crystal structure as Fig. 1 is more difficult than building the model of three dimensional monocrystalline silicon structure. The nanoscale cutting was simulated by displacing the diamond tool a small distance towards the negative direction of the X-axis, as shown in Fig. 2.

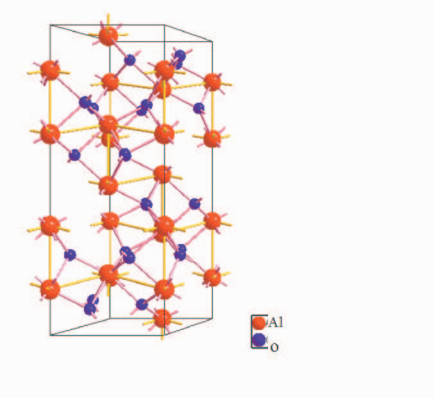

Fig. 1 Crystal structure of α-Al_2O_3

Table 1: Calculation parameters for simulation nanocutting of sapphire substrate by molecular statics

Configuration	Nanocutting
Sapphire (workpiece material) (a= 4.759Å ,c= 12.991Å) a and c are the lattice constant of sapphire	15a×8a×15c
Number of atoms in Sapphire	56,079
Number of atoms of tool (rigid-body diamond)	2,623
Tip radius of tool (nm)	2
Depth of cut (nm)	0.4, 0.5, 0.6

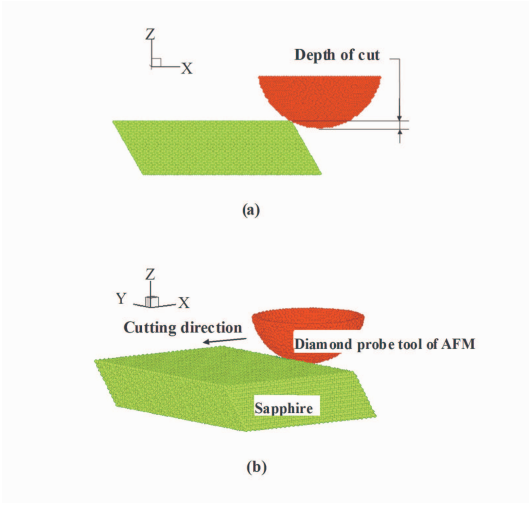

Fig. 2 Simulation model for nanocutting of sapphire substrate: (a) side view, (b) 3D image.

A. Three-dimensional quasi-steady molecular statics nanocutting simulation model

The three-dimensional quasi-steady molecular statics nanocutting model of this paper uses the adopts Morse potential energy of two-body potential energy as the basis

for calculation of the action force between molecules. The equation of Morse potential energy [15] is expressed as follows:

$$\Phi(r_{ij}) = D\left\{e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(ri_j-r_0)}\right\} \quad (1)$$

where $\Phi(r_{ij})$ is a pair potential energy function, D is the cohesion energy, α is the elastic modulus, r_{ij} is the distance between two atoms and r_0 is the particle distance at equilibrium.

For the general potential energy function, when the distance between two atoms is greater than a certain distance, the action force between these atoms will decrease rapidly. Therefore, we define such distance cut-off radius r_c, and when the distance exceeds r_c, the action force is very small so it does not need to be calculated. In this way, the calculation can be tremendously simplified. Therefore, when the distance between two atoms is within r_c and beyond r_c, Morse potentials can be furthered expressed as (2):

$$\begin{cases} \Phi(r_{ij}) = D\left\{e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}\right\} & r \le r_c \\ \Phi(r_{ij}) \cong 0 & r > r_c \end{cases} \quad (2)$$

This paper adopts Morse's two-body potential energy function to describe the interaction force between the molecules when the diamond cutter is cutting the sapphire workpiece. Since the atomic lattice structure of sapphire is more complicated than the single crystal structure of single atom, and this paper takes AFM diamond probe as a cutting tool to cut sapphire (α-Al_2O_3), the relationship between C atoms of diamond probe and the atoms of sapphire (α-Al_2O_3) workpiece has to be considered. From Table 2, the potential energy parameters, including Al-Al [15], O-O [16] and C-C [17], are all known. As to the Morse potential parameters among different atoms, such as Al-C, Al-O and O-C, the study uses Lorentz-Berthelot mixing rule [18] to calculate Al-C, Al-O and O-C Morse potential parameters, which are taken as the parameters of the nanocutting model simulated by this paper. The calculated numerical results of the Morse potential energy parameters among different atoms are shown in Table 2.

Table 2: Morse potential parameters for cutting of sapphire workpiece by AFM diamond probe tool

	Al-Al	O-O	C-C	Al-O	Al-C	O-C
D: (eV)	0.27	5.12	2.423	0.912	0.28	3.522
α: ($Å^{-1}$)	1.165	2.68	2.555	0.717	2.78	2.617
r_0: (Å)	3.253	1.208	2.522	2.231	2.20	1.865

According to the Morse potential used by this paper, the negative value of Morse potential gradient is taken to find the action force of molecules, which is expressed as (3):

$$F(r_{ij}) = -\frac{\partial\Phi(r_{ij})}{\partial(r_{ij})} = 2D\alpha\left\{e^{-2\alpha(r_{ij}-r_0)} - e^{-\alpha(r_{ij}-r_0)}\right\} \quad (3)$$

As inferred from (3), the expression of action force between atoms is shown in (4):

$$\vec{F}_i = \sum_{i=1}^{n} \vec{F}_{ij}(r_{ij}) \quad (4)$$

where i is the code number of diamond probe's atom; j is the code number of oxygen atom and aluminum atom in workpiece; n is the number of workpiece atoms; and r_{ij} is the distance between two atoms.

After action force is obtained, cut-off radius method is used to additionally judge whether the distance of r_{ij} is greater than the parameter δ of r_c. Equation (4) is rewritten as (5) in order to judge whether it is greater than r_c. When the distance of r_{ij} is greater than r_c, there is almost no potential energy action, so that let δ be zero. Contrarily, when the distance of r_{ij} is smaller than r_c, action force will be produced. By then, let δ be 1, and then calculate the action force between atoms.

$$\vec{F}_i = \sum_{i=1}^{n} \vec{F}_{ij}\,\delta(r_{ij}) \quad (5)$$

$$if \quad r_{ij_c} \ge r_c \Rightarrow \delta = 0$$

$$else \quad r_{ij} \le r_c \Rightarrow \delta = 1$$

The numerical value of the action force produced is divided into three axial component forces, F_x, F_y and F_z, with their relationship expressed in (6).

$$\vec{F}_i = \vec{F}_{x_i} + \vec{F}_{y_i} + \vec{F}_{z_i} \quad (6)$$

where F_{x_i} is the component force of action force in X direction; F_{y_i} is the component force of action force in Y direction; and F_{z_i} is the component force of action force in Z direction.

When the action forces in three axial directions produced from n grains of atoms in material being applied on m grains of probe atoms on cutting tool are added up, the total component forces in three axial directions can be obtained. F_x is the cutting force produced by diamond probe during cutting; F_z is the down force of diamond probe during cutting; and F_y is the side force of diamond probe and workpiece.

Of course, after cutting has proceeded for a certain period, the number of workpiece atoms affected by Morse force of diamond cutting tool is not only one atom. Therefore, the Morse force vector, being affected by the Morse force of diamond cutting tool, at the newly moved position of each atom in workpiece is one by one added to the Morse force of other workpiece atoms being inside cut-off radius borne by the newly moved position of each atom, so as to find the sum of Morse force vector of each workpiece atom, which is further decomposed to be Morse force component F_x in the X direction, Morse force

component F_y in the Y direction, and Morse force component F_z in the Z direction. Let each of the Morse force components be zero, and then the force equilibrium equation of quasi-steady molecular statics nanocutting model can be acquired, as shown in (7).

$$F_X = \sum_{i=1}^{m} \bar{F}_{ix}(r_{ij}) = \sum_{i=1}^{m}\sum_{j=1}^{n} \delta F_x(r_{ij}) = 0 \quad (7)$$

$$F_Y = \sum_{i=1}^{m} \bar{F}_{iy}(r_{ij}) = \sum_{i=1}^{m}\sum_{j=1}^{n} \delta F_y(r_{ij}) = 0$$

$$F_Z = \sum_{i=1}^{m} \bar{F}_{iz}(r_{ij}) = \sum_{i=1}^{m}\sum_{j=1}^{n} \delta F_z(r_{ij}) = 0$$

where

i : number assigned to all the atoms of diamond probe tool atoms that affect the Morse force of a certain workpiece atom

j : number assigned to other workpiece atoms inside the cut-off radius after removal of a certain workpiece atom affected by Morse force of probe tool.

m : quantity of all the atoms of diamond probe tool being corresponding to a certain workpiece atom affected by Morse force of probe tool.

n : quantity of other workpiece atoms inside the cut-off radius after removal of a certain workpiece atom being influenced by Morse force of probe tool.

r_{ij} : distance from the j^{th} workpiece atom in material and its corresponding i^{th} atom of diamond probe tool, and distance from the j^{th} workpiece atom and the i^{th} workpiece atom.

This paper uses Hooke-Jeeves pattern search method [19] to look for the most suitable newly displaced position of each moved atom in workpiece of each step. Since the feeding of each step in the paper does not exceed 0.002Å, and the displacement of atom cannot be too far, the paper supposes that the feeding of each search should not exceed the distance range of 1/2 lattice constant when searching the most suitable force balance transformation displacement position of each step. And Hook-Jeeves pattern search method is used to do the search. First of all, the starting point of search has to be defined. Let the workpiece atom affected by Morse force of diamond probe in each cutting step is taken as the starting point of the search. The increment of search is 0.001Å, and the convergence value of force equilibrium $\varepsilon = 10^{-6}$. By following the above logic, the point of optimal displaced position for each step can be found. It is just the point of new force balance displaced position acceptable to us. During this time, the paper calculates the total Morse force borne by the interface between the workpiece and the cutting tool in the feeding step of this time. Furthermore, the total Morse force is decomposed to be component forces in X-, Y- and Z-directions, thus achieving the cutting force (component force in X-direction), cutting side force (component force in Y-direction) and cutting down force (component force in Z-direction).

III. RESULTS AND DISCUSSIONS

Below is an analysis of this paper made on the cutting of different cutting depths on sapphire substrate workpiece by the probe tool of AFM according to the results of cutting force (F_x), down force (F_y) and side force (F_y) acquired from simulation of three-dimensional quasi-steady molecular statics nanocutting model.

A. Simulation results of 3D quasi-steady molecular statics nanocutting simulation model

This paper establishes a three-dimensional quasi-steady molecular statics nanocutting simulation model for cutting of nano groove on the surface of sapphire by a probe tool. With tip radius of probe 2nm and cutting depths 0.4nm, 0.5nm and 0.6nm, the paper conducts simulation analysis. Using the simulation results, the paper calculates the cutting force in X direction (F_x), down force in Z direction (F_z) and side force in Y direction (F_Y) under steady cutting condition. As to tip radii of probe 2nm, as well as cutting depth 0.5nm, the simulation results of different steps are shown in Fig. 3.

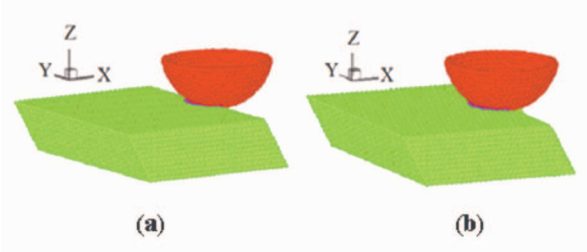

Fig. 3 Simulated results at (a) the 5000th step and (b) the 9500th step of the tip radius is 2nm and cut o.5nm.

According to the three-dimensional quasi-steady molecular statics nanocutting simulation model of sapphire developed by this paper, this paper simulates a tip radius of probe 2 nm to carry out sapphire cutting process at cutting depth 0.4 nm. The acquired results of cutting force (F_x), down force (F_y) and side force (F_y) of each step in three axial directions are respectively obtained, as shown in Fig. 4. From the simulation result, it is found that under the conditions that the same tip radii of probe and the cutting depths are different, despite the constant change of force in the Y-direction, the average value is close to zero. This is because the tool used in the simulation of cutting performed has a rounded tip, and the cutting path is a straight line. Therefore, the contact areas at its two sides during cutting are the same, and the resultant action force at each of the ends is zero.

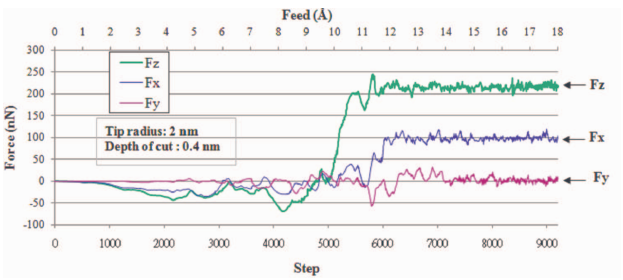

Fig. 4 Three axial action forces when the tip radius of probe is 2 nm and cutting depth is 0.4nm.

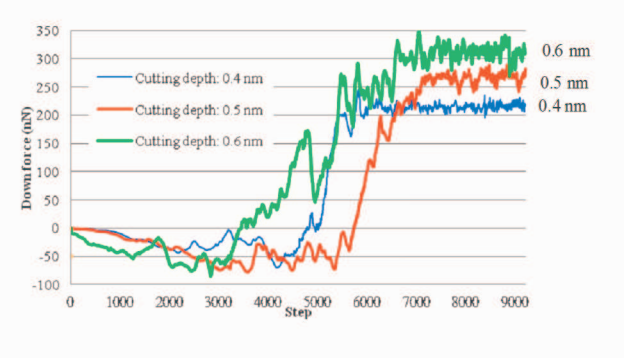

Fig. 5 Variations of down force during cutting process for the cutting depths of o.4nm,0.5nm and o.6nm, respectively.

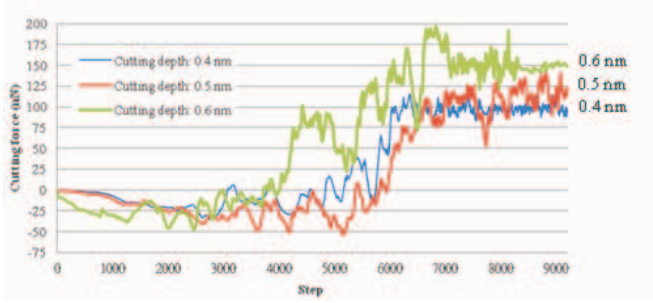

Fig. 6 Variations of cutting force during cutting process for the cutting depths of o.4nm,0.5nm and o.6nm, respectively.

From Fig. 4, it is also found that the absolute values of down forces of different cutting depths in the Z-direction are greater than the absolute values of cutting forces in the X-direction, because, when the probe tool begins cutting the workpiece, the projected contact area in the Z-direction is greater than the projected contact area in the X-direction. Therefore, in the initial cutting stage, the attraction force (negative value) in Z-direction is greater than the attraction force (negative value) in X-direction. As the probe tool gradually cuts the workpiece, a repulsive force is produced between the cutting tool and the workpiece. At the same time, From Fig. 4 to Fig.6, it can be found that the action forces in X-and Z-directions are negative values at the beginning stage of nanoscale cutting. This is because in the initial stage of cutting, the probe tool is maintained at a small distance from the workpiece, so a mutual attraction is produced between the cutting tool and the workpiece, generating negative values. However, after the tool cuts the workpiece, such that the values of force are positive. Since the projected contact area in the Z-direction is greater than the projected contact area in the X-direction, the repulsive force is also greater. Therefore, it is found that the increase rate of the down force in the Z-direction is greater than that of the cuttinf force in the X-direction.

From Fig. 5 to Fig. 6, the simulation conditions of different cutting depths are shown. The contacted crown radii of cutting tool during simulation of cutting sapphire workpiece by the tip of probe are 1.2nm, 1.32nm and 1.43nm respectively. When simulation at the 6200th, 6800th and 7300th step, the length on workpiece cut by probe tool exceeds the crown radii respectively. During this time, the force also starts to be in steady condition. The average action force of down force F_z and the average action force of cutting force F_x, obtained under the cutting condition that different cutting depths appear to be steady, are further rearranged and shown in Table 3.

Table 3: Average down force and average cutting force under different cutting depths as simulated by this paper.

Computational parameters		Down force : Fz (nN)	Cut force : Fx (nN)
Tip radius (nm)	Depth of cut (nm)		
2	0.4	215.43	97.72
2	0.5	261.18	109.06
2	0.6	312.11	148.76

IV. CONCLUSION

This study proposes using the three-dimensional quasi-steady molecular statics nanocutting model to simulate application of probe tool to conduct straight-line nanocutting of sapphire substrate, and investigates the cutting force produced at different cutting depths. From the simulation results of cutting force, down force and side force, it is found that under the actions of cutting tools with the same tip radius of probe, cutting force enlarges with the increase of cutting depth. This result is identical to the actual experimental phenomena of nanocutting. From this, it is known that the simulation model developed in this study is reasonable. After calculation of the action forces in the three axial directions produced during the nanoscale cutting of sapphire substrate by the three-dimensional quasi-steady molecular statics nanocutting model, this study finds that during the nanoscale straight-line cutting by the probe tool of AFM, the average action forces in the different axial directions after cutting is steady, the average side force in the Y-direction is around zero, and the down force in the Z-direction is greater than the cutting force in the X-direction. This study finds that the reason is because in the cutting process of the probe tool, the projected contact area between cutting tool in the Z-direction and the workpiece is greater than the projected contact area between cutting tool in the X-direction and the workpiece.

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