 CMES, vol.50, no.3, pp.227-252, 2009

Quasi-steady Molecular Statics Model for Simulation of Nanoscale Cutting with Different Diamond Cutters

Zone-Ching Lin[1] **and Jia-Rong Ye**[2]

Abstract: The paper develops a quasi-steady molecular statics model to analyze nanoscale cutting of copper materials by diamond cutters with different shapes. Cutting action, cutting force, equivalent strain and equivalent stress are discussed and compared. The quasi-steady molecular statics nanocutting model first assumes the trajectory of each atom of the copper workpiece 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 and Y directions when each atom moves a small distance, so as to find the new movement position of each atom. Since the force equilibrium equation of the model has two unknowns to be solved, i.e. the x and y coordinates for each position, a method in engineering optimization can be used to find the new movement position of each atom when the force equilibrium equation is satisfied. After that, the displacement of the acquired new position of each atom combined with the concept of shape function of finite element method are employed to calculate the equivalent strain of the copper workpiece during nano-cutting. By using the relationship equation of the flow stress-strain curve, the equivalent stress of the copper workpiece during nano-cutting can be obtained. The cutting forces of nanoscale cutting for a copper workpiece acquired in this paper are compared with previous results to verify that the model developed by this paper is reasonable.

Keywords: Quasi-steady molecular statics, Nano-cutting, Copper.

1 Introduction

"Nanotechnology" refers to the study of the properties and interaction of substances at nanoscale (1nm∼100nm), including properties such as action force, quantum confinement effect, size effect and surface effect. Since nanoscale interactions can produce there effects, the physical and chemical properties in the atomic grade are

[1] NTUST, Taipei, Taiwan.
[2] NTUST, Taipei, Taiwan.

different from those of substances at macroscopic scale, thus producing materials with special properties.

To understand nanotechnology properties and forming, analysis can be made through experiments and theoretical simulation. However, experiments usually need expensive equipment, and the subsequent analysis is more difficult, making theoretical analysis more attractive. Molecular dynamics is employed for nanoscale analysis, and molecular dynamics simulation is extensively applied to the studies of nanocutting, nanoindentation, nano tension, etc. With the rapid development of computer technologies, computation speed is being greatly accelerated, further enhancing the development and significance of molecular dynamics simulation in nanoscale studies.

Shimada (1990) used 2D models and molecular dynamics for the dynamic simulation of orthogonal cutting, and investigated its relation to chip formation. Childs and Maekawa (1990), and Stower et al. (1990) employed molecular dynamics theory for numerical simulation of cutting, though their model lacked complete quantitative calculation. Kim(1995) used molecular dynamics to construct a 2D cutting model of a single-crystal diamond cutter for cutting (111) copper material with the highest density plane with[110] cutting direction. That study found that an arc-shaped cutter could produce thinner chip than a sharp cutter. Fang et al.(2007) indicated that the nanaoscale cutting action was mainly produced by extrusion, in contrast to the traditional cutting action, where the workpiece is deformed by shearing. Pei et al.(2006) pointed out that the rake angle of cutter has significant influence to chip formation and the surface of workpiece. Inamura et al. (1991)(1992) 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 potentials of two different atoms as examples for simulation, and achieved the chip formation process, and the changing process of cutting force and potential energy along with movement of the cutting tool. Lin and Huang (2004) used the Morse potential between the cutter and the atoms of workpiece and used molecular dynamics to simulatet the the overall cutting process. Shen and Atluri (2004) proposed the analysis of atomic-level stress calculation and continuum-molecular system equivalence. Their paper mainly studied that "an equivalent continuum is defined for molecular dynamics (MD) particle systems, based on the definition of atomistic stress and in conjunction with the SPH technique." Besides, the case analyzed in their paper only considered the elastic fields in the discussion of uniform applied deformation. Their paper did not consider the nanocutting process.

With molecular dynamics (MD), its basic principle is the establishment of a particle system to simulate the microscopic phenomenon to be studied. The particle movement follows Newton's law of motion and when quantum effect and multi-body in-

teraction are neglected, the interaction between particles satisfies the superposition principles. Using the dynamics equations of particles, the trajectory of different particles in phase space can be determined by molecular dynamics. Furthermore, the relative properties of the system can be acquired.

Nevertheless, the time step for molecular dynamics is too small, thus creating the problems that the simulation process has to spend much time for the calculations, which are difficult.

Therefore, some researchers have used molecular statics to simulate nanoscale studies in order to rectify the problems encountered with molecular dynamics. Kwon et al.(2004) investigated material properties by using atomic model to simulate the equilibrium of static load. They proposed a model that combines the atoms with finite element formulation to simulate the nanoscale tensile problem for the defective material. Telitche and Vinogradov(2006) used quasi-static analysis to investigate the tensile problem of non-perfect lattice structure. Their paper mentioned that two different methods for solving the static equilibrium position, both used the minimum energy method and allowed the force to reach a relatively small value when atoms were moved. Each equilibrium state of the crystal was described by a linear algebraic equation. This equation had displacement interdependence, so the Inverse Broyden's Algorithm (IBA) was used to solve the atomic trajectory displacement of the system. Jeng (2004) adopted the combination of molecular statics method with the least energy principle in the finite element as the structure to simulate the displacement and deformation process of nanoindentation. The least potential energy method was primarily used, followed by the displacement control superposition method in the non-linear finite element formulation to solve the relationship between each atomic force and position. Theodosiou and Saravanos (2007), they focused on carbon nanotube to propose an analysis model of the bending deformation and stress of the nanotube of molecular mechanics based finite element after external force is borne. Their paper only considered the elastic moduli of the nanotube.

Therefore, using the molecular statics of the papers mentioned above can not to apply the step-by-step quasi-steady nanocutting by diamond cutting tool as simulated in this paper, and they also cannot analyze the chip separation and formation and the equivalent stress and equivalent strain of flow curve of the cutting workpiece and chip under the already existed similar plastic situation for nanoscale cutting.

This paper adopts the idea of molecular statics to simulate the nanocutting action. The simulation of nanocutting action uses the Morse force component of each atom in X and Y directions during cutting to establish a force equilibrium equation. By using the engineering optimization method, the most suitable displacement position of force equilibrium can be calculated. It is also confirmed that the new position

has reached a position of less energy in the entire system, so that the new position after force equilibrium is just the position of less energy, where the number of times of calculation can be decreased. In addition, the action force produced by a diamond cutter on the workpiece material can be acquired. In order to verify the rationality of the horizontal cutting force and normal cutting force acquired by the developed quasi-steady molecular statics, nano cutting model in this paper the numerical value of cutting force acquired from the simulation by a 5Å round-edge diamond cutter is compared with the results of Ikawa (1991). This demonstrates that the numerical value of cutting force acquired by the paper is reasonable. It also implies that the quasi-steady molecular statics nanocutting model developed by this paper is reasonable. In addition, this paper applies the developed nanocutting model, to obtain the displacement of the atom, and then the displacement of atoms during nanocutting is used to obtain the strain of the element which each atom is considered to be a node of element. Finally it analyzes the equivalent stress and equivalent strain, so as to observe the distribution trend of equivalent strain and equivalent stress of the cutting material in nanocutting, and complate the overall investigation of nanocutting simulation.

2 Quasi-steady molecular statics nanocutting model

The 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 [Girifalco and Weizer (1959)] is expressed as follows:

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

D: binding energy
α: material parameter
r_{ij}: distance between two atoms
r_0: equilibrium distance

For the general potential energy function, when the distance between two atoms is greater than a certain distance, the action force between atoms will decrease rapidly. Therefore, we define the 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, the Morse potential energy of the distance between two atoms inside r_c and outside r_c can be further expressed as equation (2):

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

The paper adopts Morse's two-body potential energy function to describe the interaction force between molecules when the diamond cutter is cutting a copper workpiece. The Morse potential energy function parameters used between the carbon atoms of diamond cutter and the copper (Cu) atoms of the workpiece is shown in Table 1 [Kim and Moon (1995)].

Table 1: Morse potential energy function parameters between diamond cutter and atoms of copper workpiece material.

	cu-cu	cu-c
D: binding energy (ev)	0.3429	0.087
α: material parameter ($Å^{-1}$)	1.3588	1.7
r0: equilibrium distance between atoms (Å)	2.87	2.05

According to the Morse potential used by this paper, the action force between two atoms can be expressed as equation (3):

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

The action force between two atoms acquired from equation (3) can be further divided into the components of force in two axes, $\vec{F}x$ and $\vec{F}y$, as shown in equation (4):

$$\vec{F}_i = \vec{F}x_i + \vec{F}y_i \tag{4}$$

$\vec{F}x_i$: component of force of the action force in X direction
$\vec{F}y_i$: component of force of the action force in Y direction

As shown in Figure 1, it is assumed that there is only one copper workpiece atom Cu_1 located in the cut-off radius area of the diamond cutter. The Morse force of the diamond cutter would cause a slight displacement and deformation to the copper workpiece atom Cu_1. The new displacement position of the copper workpiece atom Cu_1 is assumed to be an unknown P_0(x, y). Then, this unknown displacement position P_0(x, y) is used to calculate the r_{ij}between copper atom, Cu_1 and diamond cutter and the r_{ij} between copper atom Cu_1 and other copper atoms located inside the cut-off radius of copper atom Cu_1. The r_{ij} is then substituted in the Morse force equation of equation (3) to acquire the Morse force of the copper atom Cu_1 at the new position P_0 (x, y). This is done for each atom of the diamond cutter, and the Morse force of other copper atoms located inside the cut-off radius of the copper atom Cu_1 on this copper atom Cu_1. Then, the new Morse force components in X

direction and Y direction, $\vec{F}x_i$, $\vec{F}y_i$ can also be solved. We find the summation of the new Morse force of the abovementioned copper atom, when it is at the new position P(x, y) for each atom of the diamond cutter, and the new Morse force of each of the other copper atoms located inside the cut-off radius of the atom Cu_1 on this copper atom Cu_1 in X direction, as well as the summation of the new Morse forces in Y direction. The paper assumes that when this copper atom Cu_1 is moved to the new position P_i (x, y), the equilibrium equation of Morse force must be satisfied. The acquired new P_i (x, y) should satisfy the force equilibrium equation of Morse force. Therefore, this paper adopts a Hooke-Jeeves pattern search method to acquire the coordinates P_i (x, y) of the new position of this copper atom Cu_1, in the X and Y directions. This search method is applied to acquire the coordinates of the new position P_i (x, y), which are then substituted in the calculation of r_{ij} value. The various r_{ij} values are substituted in the calculation of Morse force, to check whether the force equilibrium equation meets force equilibrium. If the convergence value among force equilibrium is met, it indicator that the coordinates P(x, y) of the new position of the copper atom Cu_1 are where the new displacement position is. At this time, these new coordinates, P_i (x, y), of the copper atom Cu_1 satisfy the force equilibrium equation of the developed quasi-steady molecular static nanocutting model.

Of course, after cutting has proceeded for a certain period, there is not just one cop-

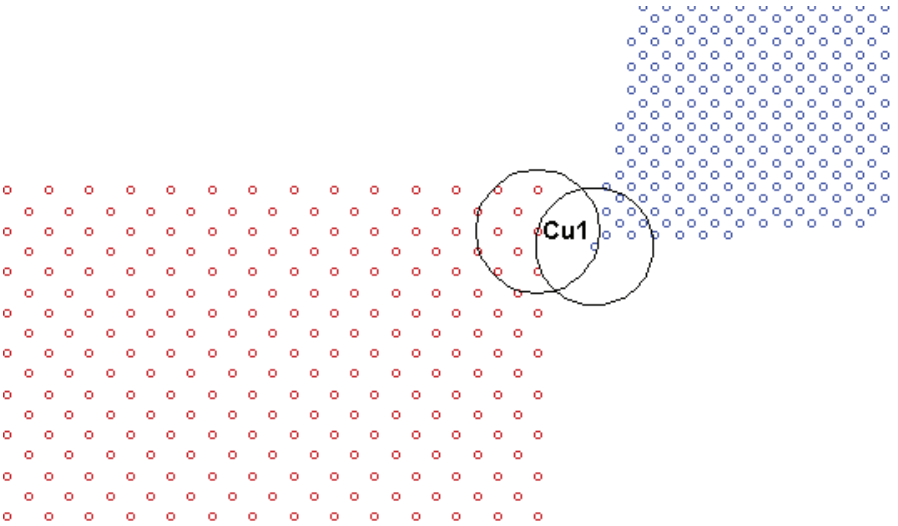


Figure 1: The area with cut-off radius of 5Å, referring to the area with copper atoms being affected.

per workpiece atom influenced by the Morse force of the diamond cutter. Hence, the Morse force vector of each copper atom of the copper workpiece being affected by the Morse force of diamond cutter after having moved to the new position, as well as the Morse force of other copper atoms inside the cut-off radius acted on by each atom after moving to the new position are used in sequential order to find the sum of Morse force vector of each copper atom. The sum of Morse force vector are further resolved as the Morse force component F_X in the X direction as well as the Morse force component F_Y in Y direction. As mentioned above, let the sum of the Morse force components in the X and the Y directions be zero respectively. Then the force equilibrium equation of the quasi-steady molecular statics nanocutting model is formed, as shown in equation (5).

$$\begin{cases} F_X = \sum_{i=1}^{m} (F_x)_i + \sum_{j=1}^{n} (F_x)_j = 0 \\ F_Y = \sum_{i=1}^{m} (F_y)_i + \sum_{j=1}^{n} (F_y)_j = 0 \end{cases} \tag{5}$$

i**:** numbers assigned to all the atoms of diamond cutters that affect the Morse force of a certain copper atom.

j**:** numbers assigned to other copper atoms inside the cut-off radius other than a certain copper atom affected by the Morse force of cutter.

m**:** quantity of all the diamond cutter atoms when corresponding to a certain copper atom affected by the Morse force of cutter.

n**:** quantity of other copper atoms inside the cut-off radius other than a certain copper atom affected by the Morse force of cutter.

r_{ij}**:** distance between the jth copper atom in the copper material and the corresponding ith atom of diamond cutter, and the distance between the jth copper atom and the corresponding ith copper atom.

To find the most suitable displacement position by optimization search method, a search area has to be defined first. Since the feed of the diamond cutter of this paper does not exceed 0.002Å at each step, and not the displacement of each atom is small, thus this paper supposes a distance area with each feed of diamond cutter not exceeding 1/2 of the lattice constant, to search the most suitable and displacement positions of force equilibrium of the atoms for the feed at each step.

The Hooke-Jeeves pattern search method in direct search method is used to search the most suitable new displacement position of each atom during the feed of diamond cutter at each step when the abovementioned Morse force equilibrium equation is satisfied.

As mentioned above, the simulation procedures of the quasi-steady molecular statics nanocutting model can be descripted as follows:

1. Define the simulated physical model.

2. Set the feed value of cutter at each step and the total feed distance.

3. For each feed of cutter at one step, find out the cutted copper atoms which are affected by Morse pforce within the distance 5Å of cutter, and induce the quasi-steady Morse force equilibrium equation of each copper atom being affected by the Morse force of cutter.

4. Use Hooke-Jeeves direct search method together with the Morse force equation and Morse force equilibrium equation to find the coordinates (x, y) of the new position of the first copper atom of cutting workpiece that satisfies the quasi-steady Morse force equilibrium equation.

5. The coordinates of the new position of the first copper atom that satisfies the Morse force equilibrium equation and the coordinates of all other copper atoms within 5Å are taken as the coordinates of the new initial copper atom. Furthermore, the coordinates (x, y) of the new position of the second copper atom that satisfies the Morse force equilibrium equation of quasi-steady cutting are calculated. Then the coordinates of the new positions of all the copper atoms within 5Å for the feed of diamond cutter at one step are sequentially calculated.

6. Furthermore, during the feed of diamond cutter at the next step according to the above steps 3$\sim$5, the new coordinates of each of all the copper atoms that satisfy the Morse force equilibrium equation of quasi-steady molecular statics nanocutting can be calculated.

7. If the diamond cutter has reached the preset feed distance, the calculations are terminated. If the preset feed distance has not been achieved, the above-mentioned calculation is continued for the next step feed.

Next, it is necessary to verify whether the new displacement position of each copper atom, which is acquired by using the Morse force equilibrium equation being satisfied, can meet the less-energy condition of the system. This paper further uses the concept of the least-energy to confirm whether the system has reached the equilibrium and steady state. The original position of a certain copper atom affected by the diamond cutter feed at each step and the 5Å area of its cut-off radius are employed to calculate the total energy of the system. After that, we use the Hooke-Jeeves

direct search method and the Morse force equilibrium equation being satisfied to acquire the position of a certain copper atom. This new position of the copper atom and the 5Å area of its cut-off radius are employed to calculate the total energy of the system. Comparing the two calculated total energy values, we can judge whether the energy of the copper atom at new position is lower than at the former position. Then, we can confirm that the condition of less energy can be met when the entire system satisfies the Morse force equilibrium equation. Furthermore, in the step of the abovementioned quasi-steady molecular statics nanocutting model, it is feasible to omit the calculation procedure that meets the condition of less energy.

Based on the above reasons, this paper takes the two cutting steps of perfect copper crystal cutting, the 99^{th} cutting step and the 500^{th} cutting step, to calculate the total energy of the system inside the cut-off radius of this copper workpiece atom, both before and when the Morse force equilibrium equation is satisfied. At the 99^{th} cutting step, the calculated total energy values of the system before and when the Morse force equilibrium equation is satisfied are -1.08614 (ev) and -1.08757(ev) respectively; and at the 500^{th} cutting step, the calculated total energy values before and during equilibrium are -1.08772(ev) and -1.08927(ev) respectively. As observed from these two cutting steps, at each step before and after the Morse force equilibrium equation is satisfied, the total energy during equilibrium is lower than that before equilibrium. Therefore, it is proved that the new position of copper atom acquired by the model of this paper by using the optimization Hooke-Jeeves search method and the Morse force equilibrium equation being satisfied, is just the position of less energy after the equilibrium of system at this step.

3 Calculation of equivalent stress and equivalent strain of the quasi-steady molecular statics nanocutting model

After the new position of each copper atom for the diamond cutter feed at each step is calculated, this paper compares the new position of each copper atom with its original position in order to acquire the copper atom displacement. Then, the relationship between the displacement and node of finite element method is applied. At this time, each copper atom regarded as the node, and the equivalent strain of copper element is calculated. After that, the relationship curve equation between the equivalent stress and equivalent strain simulated by Rau's (1999) numerical tensile value of nanoscale copper film is used to further calculate the numerical value of the equivalent stress of copper element of this time.

The above-mentioned quasi-steady molecular statics nanocutting model is used to find out the new displacement position of each copper atom of the copper workpiece being cut after the diamond cutter is advanced at each step. Then, before the analysis of equivalent stress and equivalent strain, there must be a fracture criterion

of element for making an evaluation. When the diamond cutter enters the workpiece, the cooper atom is displaced due to the cutting force. Therefore, the copper lattice element that is made up of copper atoms of workpiece is deformed. When the deformation of copper lattice element is greater than a certain extent, lift-off is caused between one element and another element, and a chip from the cooper workpiece is thus formed. Hence, there must be a fracture criterion of copper element, and then reasonable numerical values of the calculated equivalent strain and equivalent stress of copper workpiece being cut can be achieved.

According to the chip lift-off criterion of Lin and Huang (2004) that combines Morse potential with the space limitation rule of a rigid cutter, there are two conditions mentioned. When one of the two conditions is met during cutting, the element can be regarded as being fractured. The conditions of these two lift-off criteria are described as follows:

1. When any two nodes of a certain triangular element are located at the rake face and clearance face of a diamond rigid cutter respectively, it implies that the elements of these two nodes are fractured for being cut by the diamond cutter. Thus, this triangular element should be removed.

2. When the distance between any two nodes of a triangular element is greater than the distance that both can attract each other, it implies there is no interrelation between these two nodes. The distance available for mutual attraction is defined as the distance that is greater the length of 2.5 times the equilibrium distance (r_0) of copper atoms plus 1 Å. Therefore, if the distance between any two nodes of a certain triangular element is greater than the defined distance available for mutual attraction, it indicates that this element is fractured. Thus, this element will be removed.

This paper adopts the calculation model of Lin and Huang (2004) to calculate the equivalent stress-equivalent stress solution. Since the strain-displacement relationship is purely a conversion of a geometric relationship, and not a mechanics relationship, no doubt should be caused. Therefore, after quasi-steady molecular statics nano-cutting model is used to calculate the new displacement position of copper atom at each cutting step, the strain-displacement relationship equation can be used to acquire the atomic-grade equivalent strain.

This paper employs the mesh segmentation of the constant strain triangle (CST) developed by Lin and Huang (2004). Thus, the strain-displacement relationship

equation is deduced as follows:

$$\{\varepsilon\} = \begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_{xy} \end{Bmatrix} = \frac{1}{2A} \begin{Bmatrix} \beta_i & 0 & \beta_j & 0 & \beta_m & 0 \\ 0 & \gamma_i & 0 & \gamma_j & 0 & \gamma_m \\ \gamma_i & \beta_i & \gamma_j & \beta_j & \gamma_m & \beta_m \end{Bmatrix} \begin{Bmatrix} u_i \\ v_i \\ u_j \\ v_j \\ u_m \\ v_m \end{Bmatrix} = \{B\}\{\delta\} \tag{6}$$

where $\{\varepsilon\}$: strain matrix of element, $\{B\}$: displacement-strain relationship matrix, $\{\delta\}$: node displacement matrix.

It can be seen that that after the displacement component of cooper atoms has been acquired from the quasi-steady nano-cutting model, the strain of the triangular element can be obtained from equation (6). Then, from the acquired strain of element made up of copper atoms in the equation, the equivalent strain can be further calculated. Regarding the equation for the relationship curve between equivalent strain and equivalent stress, this paper uses equation (7) of the equivalent stress-equivalent strain curve acquired from Rau's(1999) simulation experiment of the numerical tensile value of nanoscale copper film, as the basis. Then, the relationship curve between equivalent stress and equivalent strain required by the paper can be acquired. According to equation (7) and the equivalent strain calculated above, the equivalent stress produced under the equivalent strain of each element can be calculated.

$$\begin{cases} \overline{\sigma} = 1.9621 + 3.2966\overline{\varepsilon}, & 0 \le \varepsilon \le 0.3 \\ \overline{\sigma} = 3.69293\overline{\varepsilon}^{0.1817}, & \varepsilon > 0.3 \end{cases} \tag{7}$$

4 Results and discussion

The quasi-steady molecular statics nanocutting model constructed by this paper simulates the cutting of copper material by a diamond cutter. The diamond cutters currently considered by this paper are the cutter being sharp and the round-edge cutters with nose radius. For sharp cutter, its rake angle is 10° and its clearance angle is 5°. The construction of sharp cutter and the copper workpiece material are shown in Figure 2. Furthermore, since the round-edge cutters with the nose radii of 10Å and 5Å are considered, their rake angle is 10° and their clearance angle is 5°, being the same as those of sharp cutter. The construction of the round-edge cutters with nose radii of 10Å and the copper workpiece material being cut are shown in Figure 3.

During nano-cutting, since the copper material being cut is much softer than the diamond cutter, this paper considers the diamond cutter as a rigid body. When

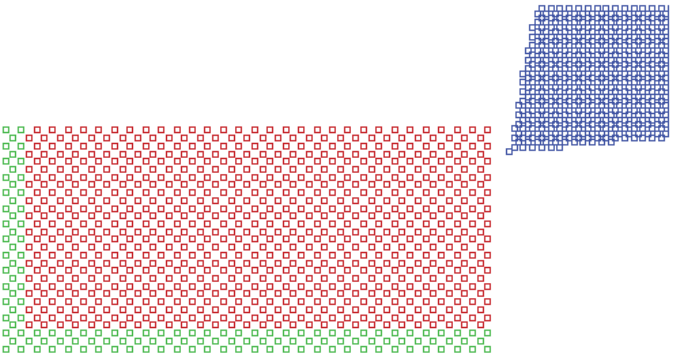


Figure 2: Sharp diamond cutter with rake angle of 10° and perfect lattice copper workpiece material.

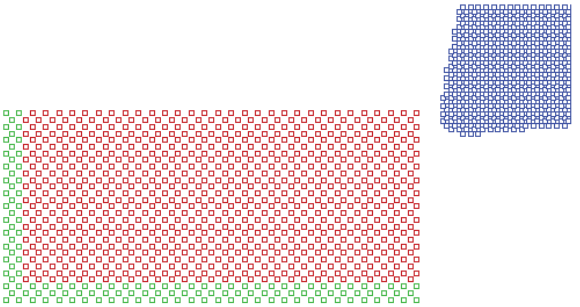


Figure 3: Round-edge diamond cutter with nose radius of 10Å and perfect lattice copper workpiece material.

the distance between two atoms reaches 5Å, the Morse potential energy function is almost equal to zero. Therefore, we take 5Å as the cut-off radius. The cutting conditions of the simulated copper workpiece are divided into a free movement zone and a fixed boundary zone. The two layers of copper atoms close to the left hand side of the cut copper workpiece material in the Y direction and the two layers of copper atoms close to the bottom of the cut copper workpiece material in the X direction are fixed, but all other copper atoms of the cut copper workpiece can move freely.

4.1 Investigation of cutting action

During the initial simulation of this paper, the cutting conditions for the coordinates of diamond cutter in X direction were preset at the distance of 5Å from the perfect lattice copper workpiece, the cutting depth was 5Å, and the feed of each step was 0.002Å. There were used to simulate the nanocutting action of perfect lattice copper material. Figure 4 (a) and (b) respectively show the cutting conditions of the sharp diamond cutter and the round-edge diamond cutter with nose radius of 10Å at the feed of 5.0Å, which was also during the time the diamond cutter exactly cut in the copper material when the feed steps of diamond cutter was 2,500 steps. Figure 5 shows the cutting conditions of these two kinds of diamond cutters at the feed of 20.0Å, which was also during the time the feed steps was 10,000 steps.

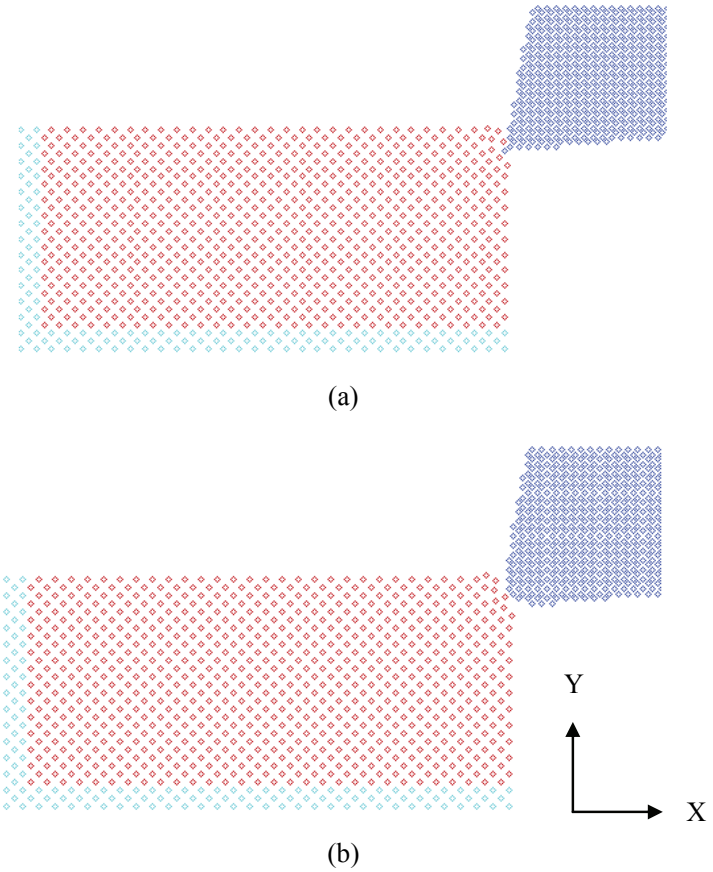


Figure 4: Cutting conditions of two cutters when feed distance is 5.0 Å: (a) sharp diamond cutter; (b) round-edge diamond cutter with nose radius of 10Å.

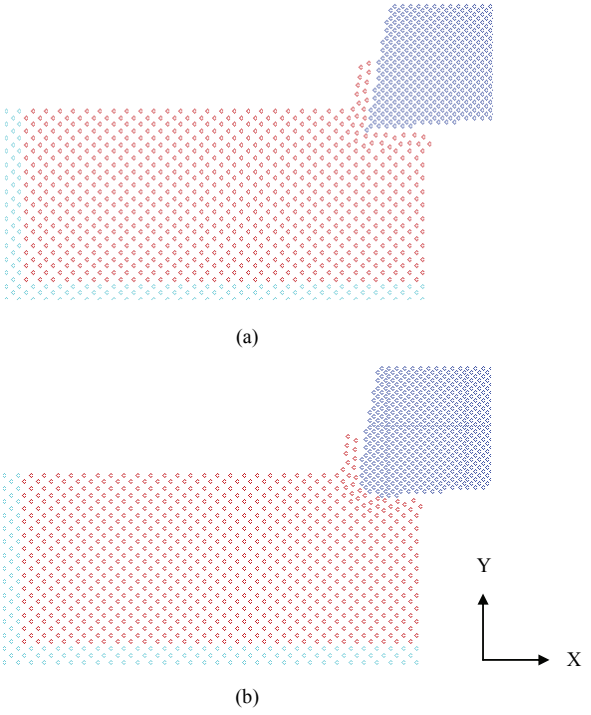


Figure 5: Cutting conditions of two cutters when feed distance is 20.0Å: (a) sharp diamond cutter; (b) round-edge diamond cutter with nose radius of 10Å.

Although the cutting depth and the cutting feed could not clearly reflect the difference in the deformation of copper workpiece when these two cutters were cutting copper material, it can be observed from Figure 5 that the chip length of copper workpiece material cut by the round-edge diamond cutter was smaller than the chip length cut by the sharp diamond cutter.

4.2 Investigation of cutting force

Figure 6 and Figure 7 respectively show the cutting force curves of sharp diamond cutter and the round-edge diamond cutter with nose radius of 10Å while nanocutting copper material. The mutually attractive force between diamond cutter and copper workpiece material is defined as a negative value, and the repulsive force between diamond cutter and copper workpiece material is defined as a positive value. The cutting force in the X direction is a horizontal cutting force, and the cutting force in the Y direction is a normal cutting force. Figures 6 and 7 show the

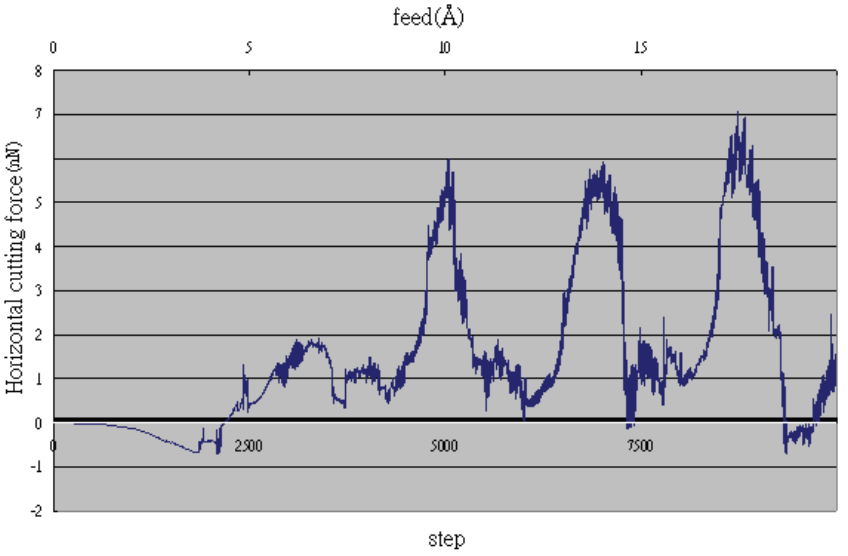
changes in cutting force of the diamond cutter caused to the copper material within the total cutting feed of 20Å. Every 2,500 cutting steps is taken as a designated point, indicating that every cutting feed of 5Å is taken as a designated point for us to observe the change of cutting force loaded by the copper material. From the figures, it can be found that when the cutter goes forward, the peak value of cutting force becomes greater. Only when until the cutting of diamond cutter enters the workpiece a certain distance does a more stable peak value appear.

It can be observed from Figure 7 that while cutting of the workpiece, there is less numerical difference between the horizontal cutting force and the normal cutting force cutting by round-edge cutter. Figure 6 reveals that the numerical difference between the horizontal cutting force and the normal cutting force from a sharp cutter is greater. From Figure 6 and Figure 7, it can be seen that the maximum values of the horizontal cutting force and the normal cutting force by round-edge cutter are both greater than those values for cutting by sharp diamond cutter

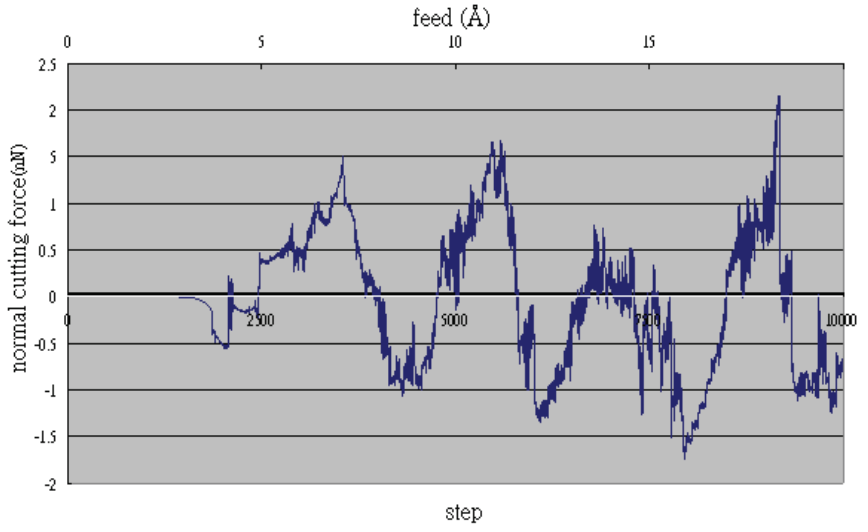
Nevertheless, to prove that the nanocutting model constructed by this paper is reasonable, this paper compares the simulation results by using the developed quasi-steady molecular statics nanocutting model with the cutting force found in Ikawa (1991) of a 5Å round-edge diamond cutter cutting the copper material at the cutting depth of 5Å. Figure 8 shows the cutting situation of diamond cutter when the feed distance is 5Å and 20.0Å, and the cutting condition when the feed steps are 2,500 and 10,000 steps. The numerical value of cutting force in Figure 9 is compared with the numerical value of cutting force in Ikawa (1991). A point around the $8{,}000^{th}$ step in Figure 9 is taken as the cutting step during the steadier situation, and the numerical values of its horizontal cutting force and normal cutting force are around 6.3nN and 4.2nN around 8000^{th} step respectively. The acquired horizontal cutting force and normal cutting force are respectively divided by the length of the lattice constant of copper material at the opted chip length. After conversion of units, the horizontal cutting force (F_t) of unit length is 0.015 (N/mm), and the normal cutting force (F_n) of unit length is 0.01 (N/mm).

The above data are then compared with the cutting force in Ikawa et al. (1991) to determine whether or not the numerical value of the cutting force of this paper is reasonable. When Ikawa et al. (1991) used the 5Å round-edge diamond cutter to cut the copper material at the cutting depth of 2.4∼5.3Å, the simulated horizontal cutting force of unit length was 0.015∼0.023 (N/mm), and the normal cutting force of unit length was 0.007∼0.013 (N/mm).

Therefore, as seen from the above mentioned simulation results using the developed quasi-steady molecular statics nanocutting model with the round-edge diamond cutter of nose radius 5Å and cutting depth of 5Å, the acquired cutting force (F_t) of unit length and the normal cutting force (F_n) of unit length do not differ

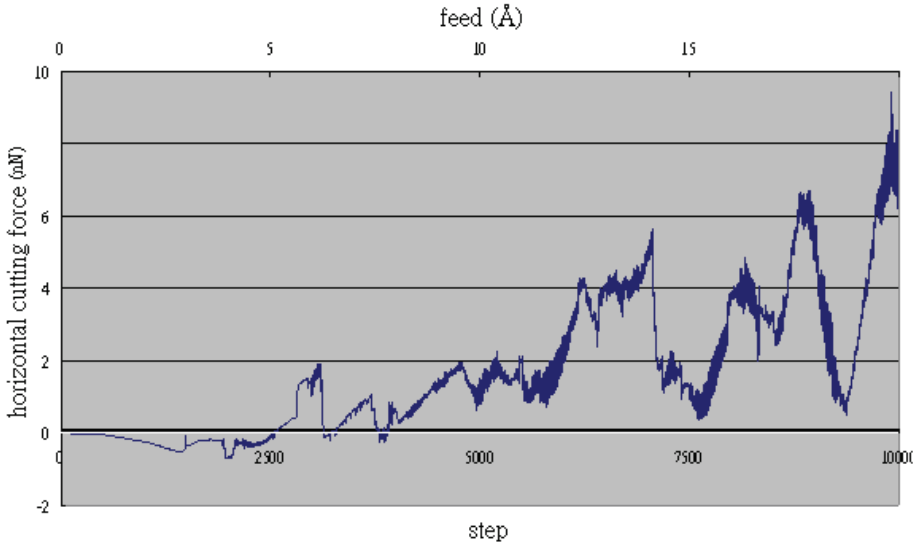


(a) Horizontal cutting force

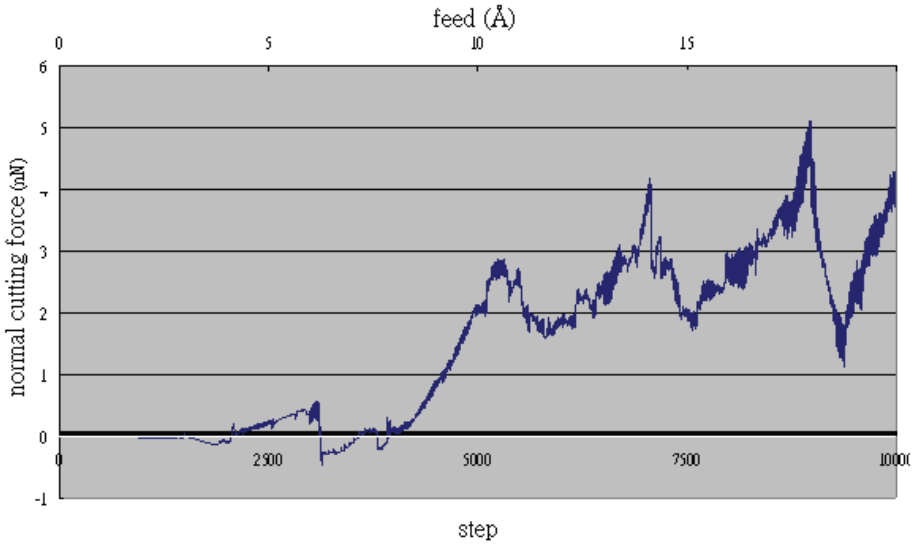


(b) Normal cutting force

Figure 6: (a) Horizontal cutting force, and (b) normal cutting force for sharp diamond cutter with a rake angle of 10°.

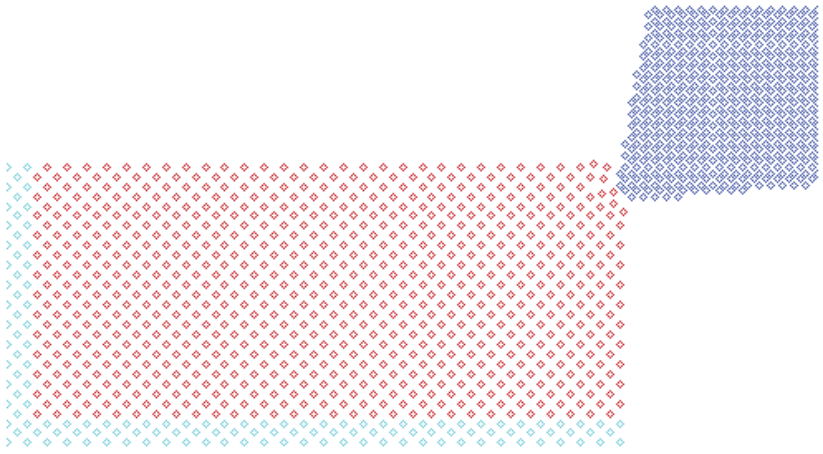


(a) Horizontal cutting force

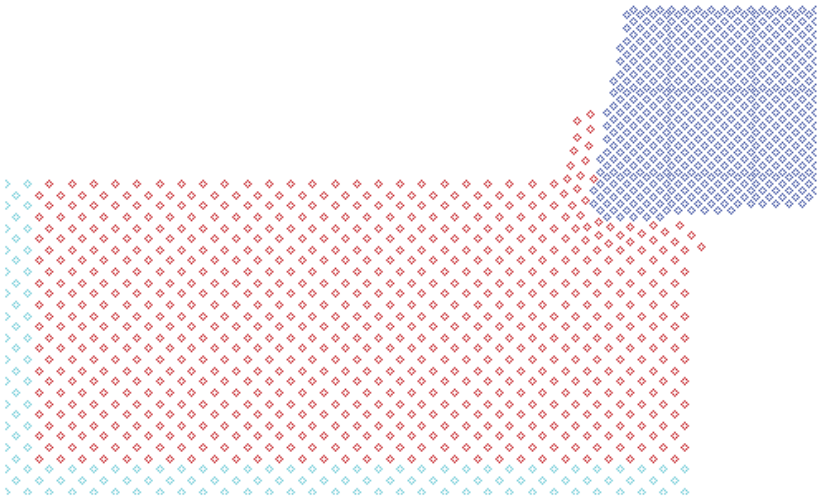


(b) Normal cutting force

Figure 7: (a) Horizontal cutting force, and (b) normal cutting force for 10Å round-edge diamond cutter.

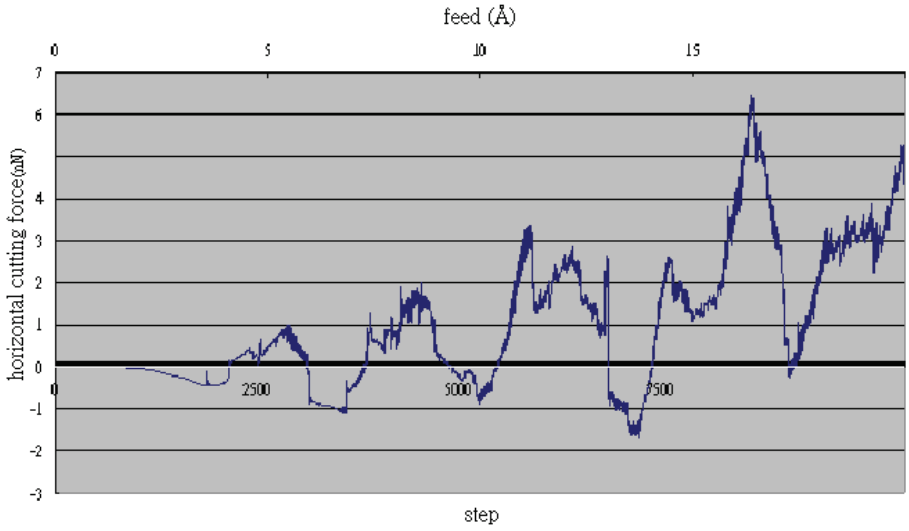


(a)

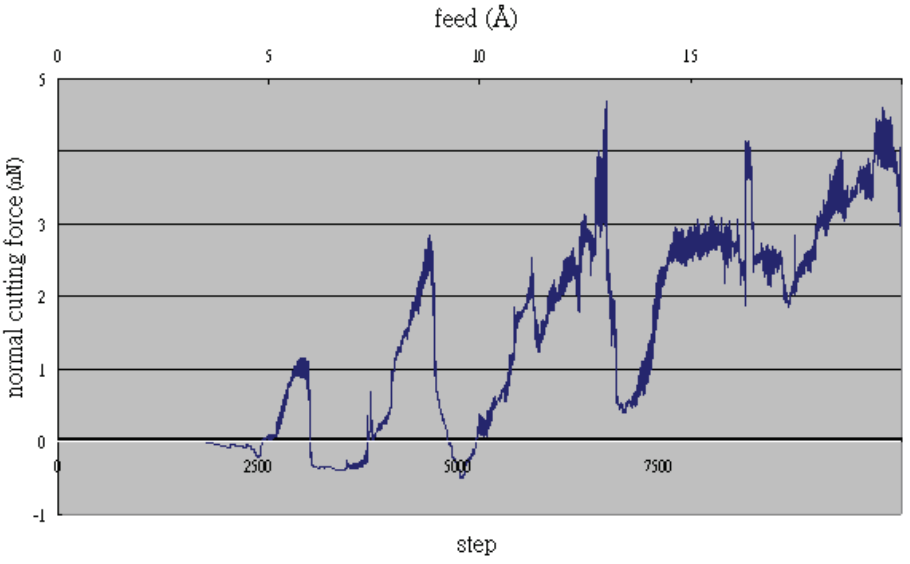


(b)

Figure 8: Cutting conditions of perfect crystal material by 5Å round-edge diamond cutter at the feed distance of (a) 5.0Å; and (b) 20.0 Å.



(a) Horizontal cutting forces



(b) Normal cutting forces

Figure 9: (a) Horizontal cutting forces, and (b) normal cutting forces of the 5Å round-edge diamond cutter at different cutting steps

significantly from the numerical values of Ikawa et al. (1991). This verifies that the quasi-steady molecular statics nanocutting model proposed have is acceptable. In addition, this paper uses a sharp diamond cutter to cut the copper material. The numerical values of the horizontal cutting force and the normal cutting force of around the $9{,}000^{th}$ step during the steadier situation in Figure 6 are around 7nN and 2.1nN respectively. The acquired horizontal cutting force and normal cutting force are divided by the length of the lattice constant of copper material. Then, the horizontal cutting force (F_t) of unit length is 0.014 (N/mm), and the normal cutting force (F_n) of unit length is 0.005 (N/mm). As shown in Figure 7, the 10Å round-edge diamond cutter is used to cut the copper material. The numerical values of the horizontal cutting force and the normal cutting force of the cutting step during the steadier situation the in Figure 7 are around 8.1nN and 4nN respectively. When the acquired horizontal cutting force and normal cutting force are divided by the length of the lattice constant of copper material, the horizontal cutting force (F_t) of unit length is 0.0146 (N/mm), and the normal cutting force (F_n) of unit length is 0.0072 (N/mm).

The cutting forces of all the above cutting conditions are presented in Table 2. It can be seen that the numerical values of the horizontal cutting force and the normal cutting force of the round-edge diamond cutter with nose radius of 10Å are also close to the numerical range of Ikawa et al. (1991). Although the horizontal cutting force and the normal cutting force of sharp cutter are smaller, they are close to the numerical range of Ikawa, and the difference is not significant.

Table 2: Comparison between cutting forces.

	Horizontal cutting force of unit length F_t (N/mm)	Normal cutting force of unit length F_n (N/mm)
Sharp diamond cutter	0.014	0.005
Round-edge cutter with nose radius 5 Å.	0.015	0.01
Round-edge cutter with nose radius 10 Å.	0.0146	0.0072
Ikawa's numerical value	0.015∼0.023	0.007∼0.013

Furthermore, this paper uses a sharp diamond cutter to cut the copper material. The numerical values of the horizontal cutting force and the normal cutting force of around the $9{,}000^{th}$ step during the steadier situation in Figure 6 are around 7nN and 2.1nN respectively. The acquired horizontal cutting force and normal cutting

force are divided by the length of the lattice constant of copper material. Then, the horizontal cutting force (F_t) of unit length is 0.014 (N/mm), and the normal cutting force (F_n) of unit length is 0.005 (N/mm). As shown in Figure 7, a 10Å round-edge diamond cutter is used to cut the copper material. The numerical values of the horizontal cutting force and the normal cutting force of the cutting step during the steadier situation in figure 7 are around 8.1nN and 4nN respectively. When the acquired horizontal cutting force and normal cutting force are divided by the length of the lattice constant of copper material, the horizontal cutting force (F_t) of unit length is 0.0146 (N/mm), and the normal cutting force (F_n) of unit length is 0.0072 (N/mm).

4.3 Analysis of the numerical values of equivalent strain and equivalent stress in a nanocutting state

Concerning on the cutting by the sharp diamond cutter with a rake angle of 10° and the diamond cutter with nose radius of 10Å up to the 5,000th step, the distribution trend of equivalent strain and equivalent stress are shown in Figure 10 and Figure 11.

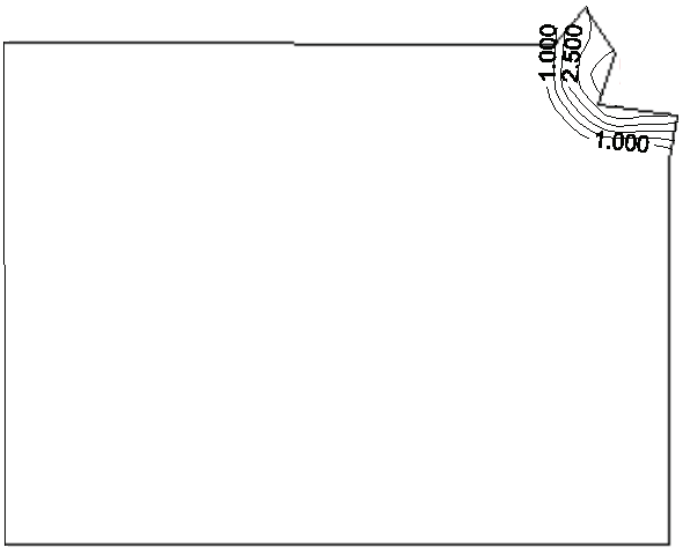
The maximum simulated numerical value of equivalent strain produced when using the sharp diamond cutter with a rake angle of 10° for cutting is around 1.2, and the maximum simulated numerical value of equivalent stress is around 3.8 GPa. The maximum simulated numerical value of equivalent strain produced when using the round-edge diamond cutter with nose radius of 10Å for cutting is around 1.1, and the maximum simulated numerical value of equivalent stress is around 3.7 GPa.

It can also be observed from Figure 10 that the equivalent strain and the equivalent stress acquired by using the diamond cutter with a rake angle of 10° for cutting have an island-shaped distribution trend on the rake face of diamond cutter. In contrast, it can be observed from Figure 11 that the equivalent strain and the equivalent stress acquired by using the round-edge diamond cutter with nose radius of 10Å for cutting have an island-shaped distribution trend at the round edge of the nose radius of the diamond cutter.

5 Conclusion

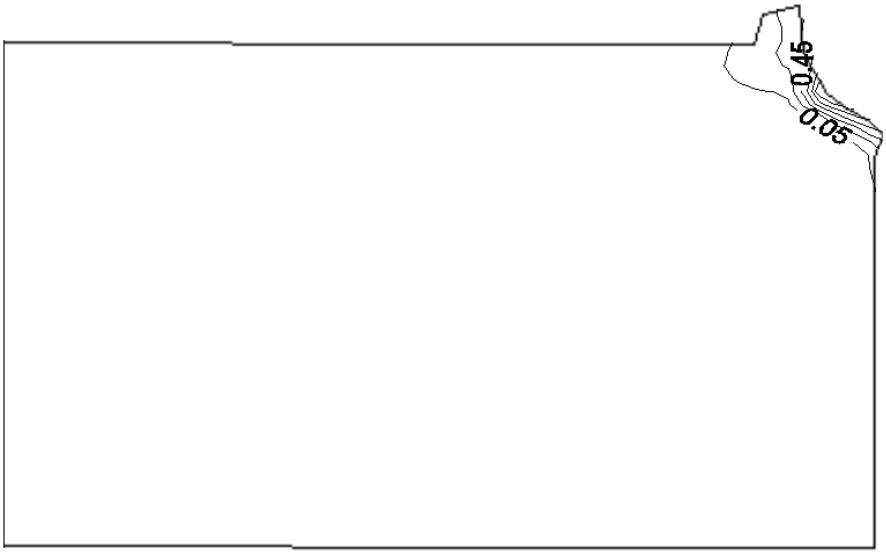
This paper presents a quasi-steady molecular statics nanocutting model to simulate the nanocutting of a perfect crystal copper material with a diamond cutter. The quasi-steady molecular statics used by this paper is the calculation of the trajectory of each atom to directly solve the equilibrium equation of the Morse force in the X and Y directions. In addition, the Mooke-Jeeves searching method in engineering optimization is used to find the displacement position of copper atoms.

(a) Equivalent strain

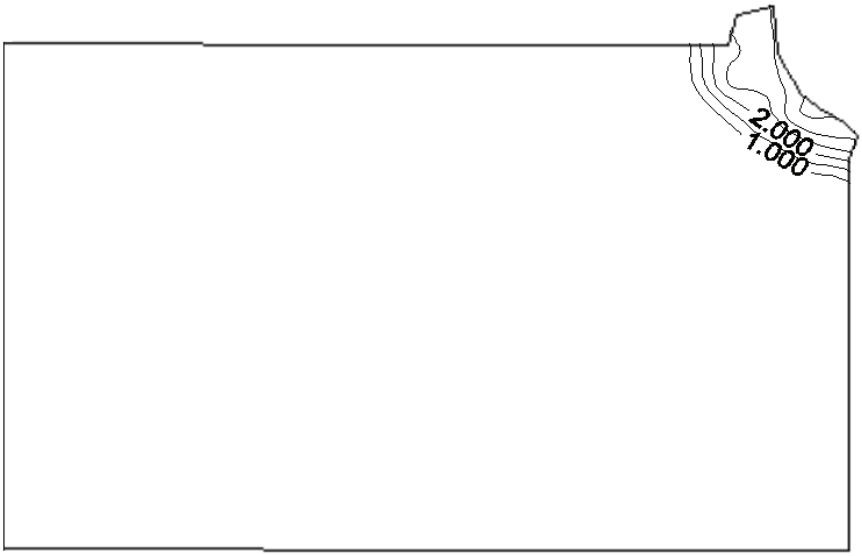


(b) Equivalent stress

Figure 10: Distribution trends of (a) equivalent strain, and (b) equivalent stress of the copper workpiece being cut when the sharp diamond cutter with a rake angle of 10° is at the $5{,}000^{th}$ cutting step



(a) Equivalent strain



(b) Equivalent stress

Figure 11: Distribution trends of (a) equivalent strain, and (b) equivalent stress of the copper workpiece being cut when the round-edge diamond cutter with nose radius of 10Å is at the 5,000th cutting step

Then, according to the displacement of copper atoms, nanoscale equivalent strain and equivalent stress are employed to analyze the distribution trend of equivalent strain and equivalent stress. According to these nanocutting simulation results, the following phenomena are drawn:

1. When a sharp diamond cutter is used for cutting copper material, its chip length will be more obvious than that when cutting by a round-edge diamond cutter.

2. The horizontal cutting force and the normal cutting force induced by using a round-edge cutter are both greater than those values induced by using a sharp diamond cutter.

3. It is also observed that the equivalent strain and the equivalent stress acquired by using the diamond cutter with a rake angle of 10° for cutting have an island-shaped distribution trend on the rake face of diamond cutter. In contrast the equivalent strain and the equivalent stress acquired by using the round-edge diamond cutter with nose radius of 10Å for cutting have an island-shaped distribution trend at the round edge of the nose radius of diamond cutter.

The quasi-steady molecular statics nanocutting model established by this study not only can be applied to simulate nanocutting of copper material by diamond cutting tool as used in this study, but also can be potential used to the cutting of single-crystal silicon material, and even extensively applied to the nanoscale abrasive cutting process of single abrasive particle for abrasive cutting copper and silicon materials in future. And the use the simulation result, it can also analyze the deformation of the abrasive cutting workpiece and the equivalent stress with the production of nanoscale flow stress. The equilibrium equation and solution of the force equilibrium equation of molecular statics used in the paper is simpler and clearer than those appeared in other references.

References

Shimada, S. (1990): Molecular Dynamics Analysis as Compared with Experimental Results of Micromachining. *Ann. CIRP* 117 - 120.

Childs, T. H. C.; Maewaka, K. (1990): Computer-aided Simulation and Experimental Studies of Chip Flow and Tool Wear in the Turning of Flow Alloy Steels by Cemented Carbide Tools. *Wear* 235-250 .

Belak, J.; Stowers, I. F. (1990): A Molecular Dynamics Model of the Orthogonal Cutting Process. *Proc. Am. Soc.*, Prec. Eng. 76-79 .

Kim, J. D.; Moon, C. H. (1995): A study on microcutting for the configuration of tools using molecular dynamics. *Journal of Materials Processing Technology*: 309-314.

Fang, F.Z.;, Wu, H.; Zhou, W.; Hu, X. T. (2007): A study on mechanism of nano-cutting single crystal silicon. *Journal of Materials Processing Technology*: 407-410.

Pei, Q..X.; Lu, C.; Fang, F.Z.; Wu, H. (2006): Nanometric cutting of copper: A molecular dynamics study. *Computational Materials Science*: 434- 441.

Inamura, T.; Takezawa, N. (1991): Cutting Experiments in a Computer Using Atomic Models of a Copper Crystal and a Diamond Tool. *Int. J. Japan Soc. Prec. Eng.*: 259-266 .

Inamura, T.; Takezawa, N. (1992): Atomic-Scale Cutting in a Computer Using Crystal Models of Copper and Diamond. *Annals of the CIRP*: 121-124 .

Inamura, T.; Takezawa, N.; Kumaki, Y. (1993): Mechanics and energy dissipation in nanoscale cutting. *Annals. CIRP*: 79-82.

Lin, Z. C.; Huang, J. C. (2004): A nano-orthogonal Cutting Model Based on a Modified Molecular Dynamics Technique. *Nanotechnology*: 510-519 .

Kwon, Y. W.; Jung, S. H. (2004): Atomic model and coupling with continuum model for static equilibrium problems. *Computational Structures Technology*: 1993-2000.

IGOR, Ye.; Telitchev; OLEG Vinogradov (2006): A method for quasi-static analysis of topologically variable lattice structures. *International Journal of Computational Methods*: 71-81.

Jeng, Y. R.; Tan, C. M. (2004): Study of Nanoindentation Using FEM Atomic Model. *Journal of Tribology*: 767-774.

Ikawa, N.; Shimada, S.; Tanaka, H.; Ohmori, G. (1991): An Atomistic Analysis of Nanometric Chip Removal as Affected by Tool-Work Interaction in Diamond Turning. *Annals of the CIRP*: 551-554.

Girifalco, L. A .; Weizer, V. G. (1959): Application of the Morse Potential Function to Cubic Metals. *Phys. Rev.*: 687-690.

Rau, J. S. (1999): A Study on Mechanical Problems of Nanoscopic Micro-structures by Molecular Dynamics Theory. Master Thesis, Department of Mechanical Engineering, National Cheng Kung University, Taiwan.

Shen, S.; Atluri, S. N. (2004): Atomic-level Stress Calculation and Continuum-Molecular System Equivalence. *CMES: Computer Modeling in Engineering and Sciences*. 6: 91-104.

Theodosiou, T.C.; Saravanos, D.A. (2007): Molecular mechanics based finite element for carbon nanotube modeling. *CMES: Computer Modeling in Engineering and Sciences*. 19(2): 121-134.