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ARTICLE

A Molecular Dynamics Investigation of Stress Distribution into Nanoscale Cutting Process of Monocrystalline Germanium

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Abstract: The molecular dynamics method was used to simulate the stress field distribution of material atoms and the influence of different tool angles on stress distribution. The average stress value of hydrostatic and von Mises at various time during the cutting process was calculated by the nearest neighbor average method. The results show that during the nano-cutting process of monocrystalline germanium, the maximum average stress value is concentrated in the subsurface region of the tool tip, and the maximum stress is 8.6 GPa. There is also a high stress in the chip, which is around 4.2 GPa. In addition, the angle of the tool also has an influence on the distribution of the stress field. The cutting force curves of different tool angles were drawn. It is found that the tool rake angle has a significant influence on the cutting force. The cutting force is the largest when cutting with a negative rake angle, while the relief angle has no effect on the cutting force, which is consistent with the macro cutting theory.

Key words: monocrystalline germanium; stress distribution; molecular dynamics; tool angle

As a typical hard-brittle infrared optical material, monocrystalline germanium is widely used in chip fabrication, military, aerospace and other important scientific fields. Since monocrystalline germanium is fragile and difficult to process, it can be machined by diamond turning, but it is easy to become debris in optical processing because of its strong brittleness. Traditional cutting methods cannot produce devices that meet the requirements.

Monocrystalline crystal germanium is prone to brittle fracture during cutting, which results in poor surface quality. With the progress and development of micro-nano cutting technology and ultra-precision machining technology, the material of monocrystalline germanium cutting layer is removed plastically when milling with tens to hundreds of nano-cutting thickness, which makes the processing quality meet the requirements of infrared optical high-precision devices. However, this plastic removal process is carried out at the micro-nano scale, so the deformation law of materials is quite different from that of conventional continuum mechanics model. At the micro-nano scale, the mechanical properties of materials may change. Brittle-hard materials exhibit unique plastic deformation characteristics at the micro-nano scale for infrared optics playing a key role to the processing accuracy and surface quality of the device.

The material is regarded as the interaction between atoms or molecules in a small contact area in the micro-nano cutting process. The material of the cutting layer is removed by discrete atomic or atomic layers in the cutting process. In essence, cutting is a discrete physical phenomenon of atoms. Therefore, the finite element method and cutting theory based on the traditional continuum mechanics are not applicable to explain the nano-cutting mechanism in the nano-cutting process, so it is necessary to study the nano-cutting mechanism from the molecular and atomic point of view. Molecular dynamics is a simulation method that can describe the interaction between atoms. It has higher accuracy and effectiveness in calculating the micro-properties, especially for many micro-details related to atoms that cannot be obtained in

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experiments, but can be easily obtained in computer simulation. Therefore, molecular dynamics has become a powerful tool to study the micro-properties of materials and an indispensable means to study many physical and chemical phenomena in micro-nano cutting process[1,2].

At present, many studies focused on the plastic materials[3-6] such as Cu, Al and hard-brittle materials[7-10] such as mono-crystalline Si, SiC during studying the cutting process of materials using molecular dynamics, but relevant literature of monocrystalline germanium is very limited. Fang and others[11] have studied the cutting deformation mechanism of monocrystalline germanium nanoparticles. It is found that there is a direct amorphous transformation of single crystal germanium under stress state, and the regional distribution of phase transformation and the path of phase transformation are greatly affected by crystal planes through nano-indentation simulation of monocrystalline germanium with different crystal planes. Zhang et al[12] carried out cutting characteristics analysis of monocrystalline germanium based on molecular dynamics. Molecular dynamics method was used to simulate indentation of monocrystalline germanium by Mao et al[13], the strain changes of (111) crystal plane under different crystal planes and downward loads and modulus of elasticity were analyzed. It was found that (111) crystal plane had smaller modulus of elasticity and hardness than other crystal planes. In the actual processing, the (111) crystal surface of monocrystalline germanium can be chosen as the processing surface to obtain higher surface processing quality. Zhu et al[14] used molecular dynamics method to study plough friction coefficient and adhesion friction coefficient in cutting process of monocrystalline germanium for the first time. Stress is one of the important mechanical parameters in material cutting. At the macro scale, the finite element method is usually used to calculate the stress by plotting elements. However, the finite element method based on continuum mechanics fails at microscopic scale. It is difficult to obtain the stress distribution in the cutting process. Most of the micro-nano scale stress studies are focused on Si, SiC[15-17] and Cu[18-20], but the stress field distribution of germanium has seldom been studied.

Dai[20] established the molecular dynamics model of monocrystalline silicon, and used different structure tools to process nanotrenches of monocrystalline silicon. Von Mises stress and hydrostatic stress in the cutting process were calculated. It was found that the shape of the tool had a great influence on the stress field distribution of monocrystalline silicon. A structured nanoscale tool in machining brittle material silicon causes a smaller hydrostatic stress, a less compressive normal stress, a lower temperature and a smaller cutting force. Luo[21] studied the effect of crystal (010, 110, 111) on temperature and stress filed in nanometric cutting process of SiC by MD. It was found that the anisotropy in the cutting force, specific cutting energy, yielding stress and temperature were observed to increase with the increase of machining temperature. Wang[22] established the nano-cutting model of single crystal copper and polycrystalline copper in vacuum and water medium. By compiling calculation program, the distribution of stress field and temperature field in the nano-cutting process of single crystal copper was calculated, and the dislocation structure formed in the cutting process was analyzed in detail. The results showed that the maximum stress reached 9 GPa, and the maximum tensile stress exceeded 5 GPa.

Therefore, in order to improve the fabrication and surface precision of the nano-crystalline germanium devices, the molecular dynamics method was used to simulate the cutting process of single crystal germanium nanoparticles, and the cutting model of single crystal germanium nanoparticles was established. The temperature distribution of monocrystalline germanium and the effect of anisotropy on cutting temperature in nano-cutting process was obtained using the spatial lattice average method, which provides a reference for further understanding the nano-cutting mechanism of single crystal germanium.

1 Method

1.1 Molecular dynamics model

The molecular dynamics nanometric model of monocrystalline germanium materials is shown as Fig.1. The model consisted of a monocrystalline germanium substrate and a rigid diamond probe. The dimension of germanium substrate is 20 nm×12 nm×3 nm along the *X*, *Y*, and *Z* direction. All of the machining tools are applied along the *–X* direction on the (100) surface of workpiece. The periodic boundary (PBC) is set in *Z* direction, the F boundary (non-periodic and fixed) are set in *X* and *Y* direction. The monocrystalline germanium substrate includes three layers of atom: boundary layer, thermostat layer, Newtonian layer. The boundary layer is kept fixed to reduce the boundary effects and prevent the substrate from translating the simulated process. The thermostat layer is kept at a constant temperature of 293 K by Berendsen method. The motion of Newton layer atoms obeys the classical Newton's second law, which are mainly involved in computation. There is different rake and clearance angle in tools and the tool is treated as a rigid body in the simulations since the diamond is much harder than the germanium.

The Morse and Tersoff hybrid potential is applied in this study, and there are three different atomic interactions in the current simulation of machining process. A Tersoff-type three-body potential is employed to express the interaction between germanium atoms[23-26]. The interaction between germanium atoms and diamond atoms is modeled by a Morse type two-body potential as follows:

$$E(r) = D\mathrm{e}[\mathrm{e}^{-q\alpha(r-r_0)} - q\mathrm{e}^{-\alpha(r-r_0)}] \quad (1)$$

where, $E(r)$ is a pair potential energy function; D is the cohesion energy; q is the atomic interaction strength; α is the elastic modulus; r and r_0 are the instantaneous and equilibrium distance between two atoms, respectively. Details parameters

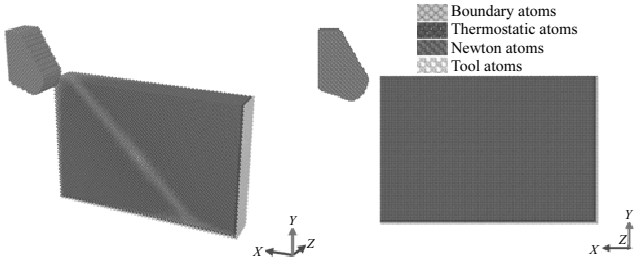

Fig.1 Three dimensional nanometric cutting model of monocrystalline germanium

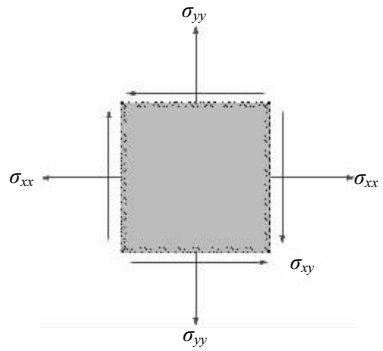

Fig.2 Stress components in the machining

are D=0.125778 eV, α= 25.8219 nm^{-1}, r_0=0.22324 nm.

The interaction between diamond atoms is ignored because the tool is treated as a rigid body[27]. The detailed parameters used in the nano cutting of single crystal germanium are shown in Table 1.

1.2 Calculation method of stress distribution

Stress is a basic parameter describing the mechanical behavior of materials in the process of material removal. Its second-order tensor reflects the interaction and deformation process between materials in the region. Stress distribution and evolution are of great significance for analyzing and predicting internal defects of workpiece. Continuous medium is generally used for Cauchy stress calculation, while virial stress is widely used in discrete atomic systems. The stress components within the workpiece in a machining operation are defined in Fig.2.

The stress tensor for atom i is given by the following formula, where a and b take on values x, y, z to generate the 6 components of the symmetric tensor:

Table 1 Details of the MD simulation model and the cutting parameters used in the study

Parameter	Value
Workpiece material	Single crystal germanium
Workpiece dimension/nm	20×12×3
Number of silicon atoms in the workpiece	65529
Tool material	Diamond
Cutting edge radius (tip radius)/nm	2
Cutting plane	(100)
Rake angle	0°, 30°, –30°
Clearance angle	10°, 20°, 30°
Temperature of thermostat layer/K	293
Cutting speed/m·s^{-1}	200
Timestep/fs	1
Potential energy function used for nanometric cutting	Tersoff and Morse

$$
\begin{aligned}
S_{ab} = -[&mv_{\mathrm{a}}v_{\mathrm{b}} + \frac{1}{2}\sum_{n=1}^{N_{\mathrm{p}}}(r_{1a}F_{1b} + r_{2a}F_{2b}) + \\
&\frac{1}{2}\sum_{n=1}^{N_{\mathrm{b}}}(r_{1a}F_{1b} + r_{2a}F_{2b}) + \\
&\frac{1}{3}\sum_{n=1}^{N_{\mathrm{a}}}(r_{1a}F_{1b} + r_{2a}F_{2b} + r_{3a}F_{3b}) + \\
&\frac{1}{4}\sum_{n=1}^{N_{\mathrm{d}}}(r_{1a}F_{1b} + r_{2a}F_{2b} + r_{3a}F_{3b} + r_{4a}F_{4b}) + \\
&\frac{1}{4}\sum_{n=1}^{N_{\mathrm{i}}}(r_{1a}F_{1b} + r_{2a}F_{2b} + r_{3a}F_{3b} + r_{4a}F_{4b}) + \\
&K_{\mathrm{space}}(r_{ia}, F_{ib}) + \sum_{n=1}^{N_{\mathrm{f}}} r_{ia}F_{ib}
\end{aligned}
\tag{2}
$$

where, m is the atomic mass; v_{a} is the velocity of a atom; v_{b} is the velocity of b atom; N_{p} is the number of pair interaction atoms; N_{b} is the number of bond interaction atoms; N_{a} is the number of angular interaction atoms; N_{d} is the number of dihedral angular interaction atoms; N_{i} is the number of improper interaction atoms; N_{f} is the number of constrained atoms; K_{space} is the long-range coulomb interaction.

The first term is a kinetic energy contribution for atom i, the second term is a pairwise energy contribution where n loops over the N_{p} neighbors of atom i, r_1 and r_2 are the positions of the 2 atoms in the pairwise interaction, and F_1 and F_2 are the forces on the 2 atoms resulting from the pairwise interaction. The latter term is the contribution of bond, angle and other factors to atom i, which are not considered in this paper. In this paper, stress analysis is based on the following formula[28,29].

$$
\sigma_{\alpha\beta} = \frac{1}{v}\left(\sum_i m_i v_{i\alpha} v_{i\beta} + \frac{1}{2}\sum_{i\neq j} v_{ij\beta} F_{ij\alpha}\right) \tag{3}
$$

where, $\sigma_{\alpha\beta}$ is the virial stress i, α, β=x, y, z is the Cartesian components. V stands for the volume of domain within the cut-off distance of atom i. m_i, $v_{i\alpha}$ and $v_{i\beta}$ are the mass, the α-component and β-component of the velocity of atom i, $r_{ij\beta}$ is the β-component of the vector r_{ij}, r_{ij} is the distance between atom i and atom j. $F_{ij\alpha}$ is the α-component of the interaction force on atom i action by atom j.

Von Mises stress and hydrostatic stress were studied during nanometric cutting of monocrystalline, in which 6 stress

components (σ_{xx}, σ_{yy}, σ_{zz}, σ_{xy}, σ_{xz}, σ_{yz}) were calculated. Von Mises stress and hydrostatic stress can be expressed as:

$$\sigma_{\text{von}} = \sqrt{\begin{matrix}3(\sigma_{xy}^2+\sigma_{yz}^2+\sigma_{xz}^2)+\\(1/2)[(\sigma_{xx}-\sigma_{yy})^2+(\sigma_{xx}-\sigma_{zz})^2+(\sigma_{zz}-\sigma_{yy})^2]\end{matrix}} \quad (4)$$

$$\sigma_{\text{hydro}} = (1/3)[(\sigma_{xx}+\sigma_{yy}+\sigma_{zz}) \quad (5)$$

In this paper, the stress distribution of each atom in volume is calculated by the nearest neighbor average method. The principle diagram is shown in Fig.3. The stress of all atoms in the nearest neighbor spherical region with the radius of atom i, r_c, in space is superimposed and then divided by the volume of the sphere. The formula is as follows:

$$S_i = \frac{\sum_i \sigma_{\alpha\beta}}{\frac{4}{3}\pi r_c^3} \quad (6)$$

where, S_i is the stress distribution of atom i in the box, $\sigma_{\alpha\beta}$ is the virial stress i, α, β=x, y, z is the Cartesian components, r_c is the search radius with a value of 5 nm in the neighbor region.

In this paper, the LAMMPS developed by Sandia National Laboratory is used to simulate the nanometric cutting process of monocrystalline germanium. The atomic trajectories x, y, z and the σ_{xx}, σ_{yy}, σ_{zz}, σ_{xy}, σ_{xz}, σ_{yz} of atoms are calculated, in which atomic information are imported into program complied by the formula to obtain von Mises and hydrostatic stress distribution, and then the atom information and stress distribution were visualized through the software OVITO.

2 Results and Discussion

2.1 Stress distribution during nano-cutting process

Fig.4a, 4b show the von Mises and hydrostatic stress distribution inside the workpiece during the nano-cutting process of monocrystalline germanium. The cutting speed is 200 m/s, the radius of the cutting edge is 1 nm, the cutting depth is 1 nm, and the time step is 25000. Hydrostatic stress is a quantity associated with volume change leading to classic thermodynamic phase transitions in continuous matter, whereas von Mises stress measures shear deformation that governs shape change usually by the activation of defect transport mechanism[30]. Von Mises equivalent stress criterion is a very commonly used yield criterion for predicting material yield.

In order to clearly display the stress distribution inside the workpiece, the atomic stress of the workpiece is calculated according to the statistical stress, and the different values of atomic stress are colored according to different colors. Fig.4 shows that the overall stress of the workpiece presents a concentric gradient distribution, centering on the knife-chip interaction zone. The high stress area is mainly located near the cutting edge and subsurface. The highest stress of the workpiece is generated at the region shear area in contact with tool and the highest stress is 2.6 GPa.

There is also a high stress region in the shear zone, the inner part of the workpiece is close to the boundary, the stress is lower, and the stress gradient is larger. The highest stress of the chip is due to the maximum deformation of the chip, the maximum lattice deformation energy of the atoms in the chip, and the stress is related to the energy released by the atoms. The frictional zone on the back face of the workpiece is also severely affected by the extrusion and friction of the cutter. The deformation of the workpiece atoms is relatively large, and the energy of the atoms in this region is larger, so the temperature in this region is also higher. The stress of the region near the boundary layer in the workpiece decreases rapidly.

Cutting force is the resistance of the workpiece to the deformation caused by cutting when cutting metal workpiece. The cutting force clearly reflects the chip removal process, which is an important physical parameter to understand cutting phenomena. Different from the macroscopic cutting force sources, the whole cutting process is carried out in the lattice due to the small cutting scale in ultra-precision cutting. The cutting force mainly comes from the interaction between the workpiece atom and the tool atom. The magnitude of cutting force can reflect the intensity of movement between atoms in the process of cutting. Fig.5 shows that the force in three directions varies with the timestep in the cutting process. The normal force (f_y) is the force perpendicular to the cutting direction. The lateral force (f_z) comes from the extrusion action of the atoms on both sides of the tool. The main cutting force (f_x) comes from the resistance of the tool along the cutting direction.

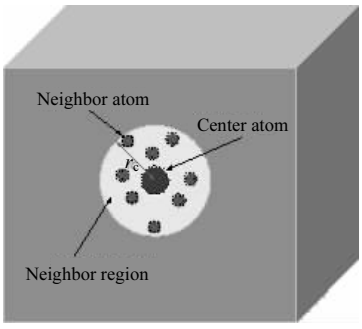

Fig.3 Calculation method of mean stress distribution: the nearest neighbor average method

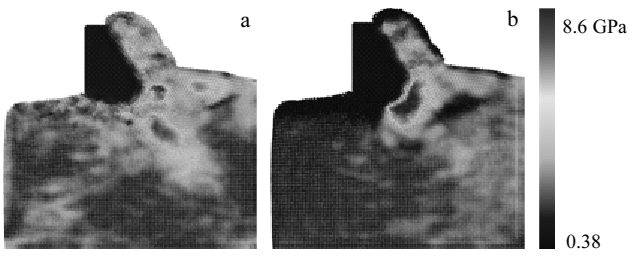

Fig.4 Stress distribution of monocrystalline germanium workpiece in nano-cutting process: (a) von Mises stress and (b) hydrostatic stress

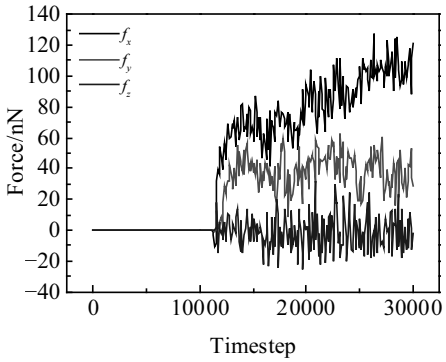

Fig.5 Cutting force-timestep curves by MD

Potential energy function reflects the change of system energy during cutting process. As shown in Fig.6, the 0~10000 step is the relaxation phase of the system, and the interatomic interaction gradually tends to be stable. The energy of the system is basically stable when it reaches the 10000 step. From 10000 to 25000 steps, the tool approaches the workpiece atom gradually, the lattice between atoms is destroyed gradually during the contact between the tool and atom, and a large amount of energy is released, which results in the potential energy of the system increasing gradually, and the degree of energy increase also reflects the severity of the cutting process. The potential energy of the system increases sharply from 25000 steps, which is due to a large number of dislocations in the system, dislocations are slipping and accumulating during the continuous cutting process as the cutting degree becomes more and more severe. As the chip atoms accumulate more and more in the cutting process, the tool movement needs to overcome greater resistance, which is also the reason for the increase of the potential energy of the system. In addition, phase transformation will occur in the single crystal germanium workpiece with diamond structure in the cutting process, which is also the reason for the fluctuation of cutting force and energy curve.

2.2 Influence of different tool angles on stress distribution

It is very difficult to change the tool angle in nano-scratch experiment. Molecular dynamics can establish various tool shapes and tool angles. The influence mechanism of tools angle on stress distribution during the cutting process of monocrystalline germanium nanoparticles is studied. In order to study the influence of different tool rake angles and clearance angles on stress distribution in nanometric process of monocrystalline germanium, six groups of cutting models with different tool angles were established. In Fig.7a~7c, the tool clearance angles are 20°, the tool front angles are 0°, 30°, −30°, respectively, and in Fig.7d~7f, the tool front angles are 20°, and the tool back angles are 10°, 20° and 30°, respectively. The cutting speed is 200 m/s, the cutting depth is 1 nm, the radius of tool tip is 1 nm, and the cutting surface is (100) crystal.

It can be seen from Fig.8 that different tool angles lead to different hydrostatic stress. The maximum hydrostatic stress value is concentrated near the front end of the tool radius. It can be seen from Fig.8a~8c that the maximum hydrostatic stress distribution occurs when the tool rake angle is 0°, and the smallest static stress distribution occurs when the tool rake angle is positive 30°. This is because the contact area between the tool and the chip increases when the tool angle is 0°, and the chip accumulation increases to make it work piece. The increase of atomic force makes the internal atom activity more intense, resulting in the increase of hydrostatic stress.

The von Mises stress distribution of six different tool angles is shown in Fig.9. It can be seen that the tool angle has a great influence on the von Mises stress distribution in the workpiece. When the rake angle of the tool is 0°, the maximum von Mises stress value is distributed in the undeformed zone along the cutting direction of the tool; when the rake angle of the tool is 30°, the maximum stress value is distributed in undeformed zone and subsurface layer of the tool; when the rake angle of the tool is −30°, the von Mises stress in the workpiece is lower, and the maximum stress is distributed in the chip and subsurface layer. From Fig.9d~9f, it can be seen that the clearance angle of the tool also affects the stress distribution of von Mises. The larger the clearance angle, the more concentrated the maximum stress value along the cutting direction of the tool and the chip area. Fig.10 shows that the

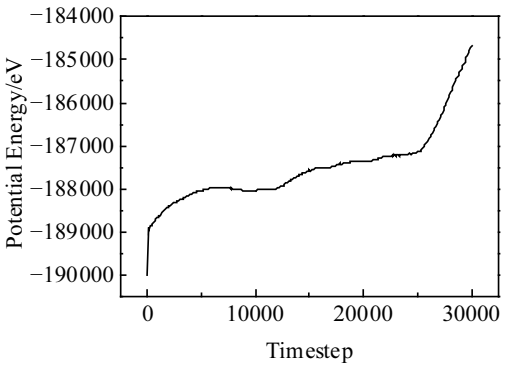

Fig.6 Cutting energy-timestep curves by MD

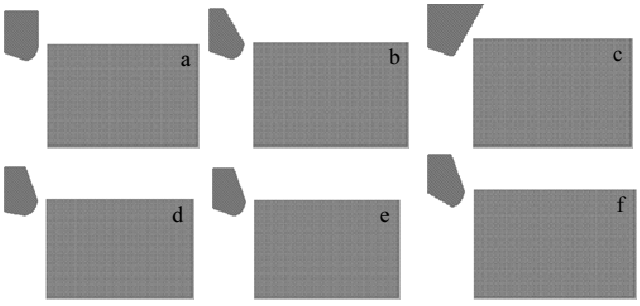

Fig.7 Cutting model of monocrystalline germanium with different tool angles: (a~c) clearance angle 20°; rake angle 0°, 30°, −30°; (d~f) rake angle 20°; clearance angle 10°, 20°, 30

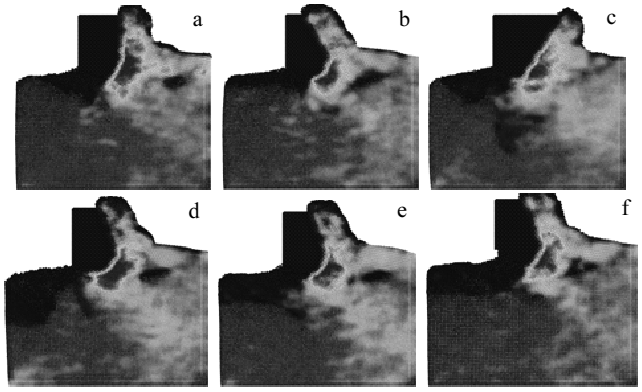

Fig.8 Hydrostatic stress distribution with different tool angles during the nanometric cutting: (a~c) clearance angle 20°; rake angle 0°, 30°, −30°; (d~f) rake angle 20°; clearance angle 10°, 20°, 30°

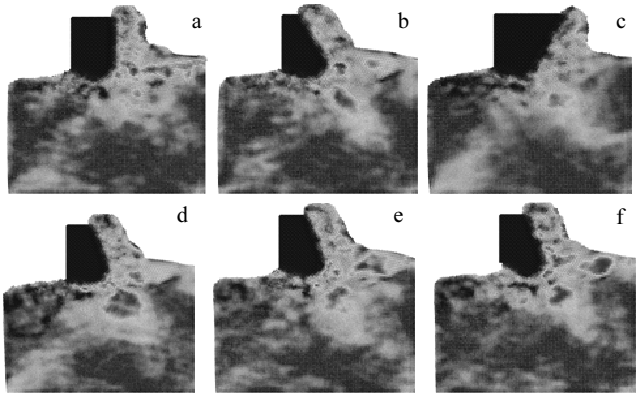

Fig.9 Von Mises stress distribution with different tool angles during the nanometric cutting: (a~c) clearance angle 20°; rake angle 0°, 30°, −30°; (d~f) rake angle 20°; clearance angle 10°, 20°, 30

rake angle of the tool has a great influence on cutting. At the same cutting speed and depth, when the rake angle of the tool is −30°, the cutting force is the largest, and the cutting force is the smallest when the rake angle of the tool is 30°. In actual machining, the purpose of taking the negative rake angle is to improve the force condition and heat dissipation condition of the edge and to improve cutting strength and impact resistance, but the contact area between tool and workpiece will increase, which will lead to the increase of cutting force and the decrease of surface quality.

The purpose of positive rake angle is to reduce the elastic deformation of the chip when it is cut off and the friction resistance between the chip and the front when it flows out, so as to reduce the cutting force and heat, make the cutting lighter and improve the quality of the machined surface, which is consistent with the macro simulation results. The clearance angle has no effect on the cutting force. The

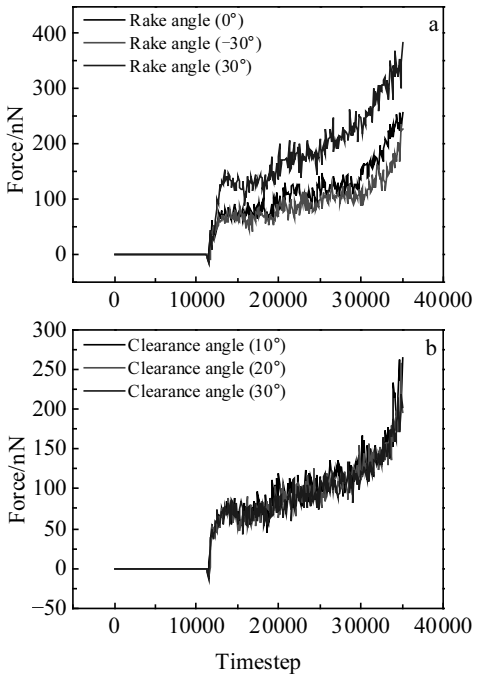

Fig.10 Cutting force-timestep curves for the different tool rake angles (a) and clearance angles (b) by MD

function of the tool's clearance angle is to prevent friction between the cutter and the machined surface, which does not affect the cutting force of the cutter in actual cutting.

3 Conclusions

1) The highest stress of the workpiece is generated at the region shear area in contact with tool and the highest stress is 8.6 GPa, and there is also a high stress in the chip, which is around 4.2 GPa. The cutting force curves in three directions and energy curves in the cutting process are obtained. The fluctuation of cutting force and energy mainly comes from the stacking of dislocations, the slip of dislocations and the phase transition of crystals in nano-cutting process.

2) Six kinds of monocrystalline germanium nanometric cutting models with different tool angles were established, and the von Mises and hydrostatic stress distribution of six models was obtained. The tool angle has a great influence on the stress distribution. The maximum stress values are mainly distributed in 3 regions: (1) inside of the chip, (2) in the unprocessed area, (3) in the subsurface area beneath tool. The clearance angle of the tool affects the stress distribution of von Mises. The larger the clearance angle, the more concentrated the maximum stress value along the cutting direction of the tool and the chip area.

(3) The cutting force is greatly influenced by the rake angle of the tool. When the rake angle of the tool is −30°, the cutting force is the largest, and the cutting force is the smallest when the rake angle of the tool is 30° and the clearance angle has no

effect on the cutting force. The cutting clearance angle affects the surface quality and residual stress of the machined plane, and has no effect on the cutting force, which is consistent with the macro cutting theory.

References

1 Xu Feifei, Fang Fengzhou, Zhang Xiaodong. *Computational Materials Science*[J], 2018, 143: 133
2 Xu Feifei, Fang Fengzhou, Zhang Xiaodong. *Applied Surface Science*[J], 2017, 425: 1020
3 Chocyk D, Zientarski T. *Vacuum*[J], 2018, 147: 24
4 Dreher M, Pauly F, Heurich J *et al. Phys Rev B*[J], 2005, 72(7): 075435
5 Mojumder S. *Physica B: Condensed Matter*[J], 2018, 530: 86
6 Dong G J, Wang X, Gao S D. *The International Journal of Advanced Manufacturing Technology*[J], 2018, 96: 1123
7 Liu Yao, Li Beizhi, Kong Lingfei. *Computational Materials Science*[J], 2018, 148: 76
8 Zhao Hongwei, Shi Chengli, Zhang Peng *et al*. *Applied Surface Science*[J], 2012, 259: 66
9 Goel S, Kovalchenko A, Stukowski A *et al*. *Acta Materialia*[J], 2016, 105: 464
10 Goel S, Luo X C, Agrawal A *et al*. *International Journal of Machine Tools & Manufacture*[J], 2015, 88: 131
11 Fang Fengzhou, Lai Min. *Scientia Sinica*[J], 2014, 44(10): 1052
12 Zhang Wentao, Mao Jiewei, Liu Wenhao. *Tool Engineering*[J], 2012, 9: 54
13 Mao Jiewei, Liu Wenhao, Wang Zengpeng. *Nanotechnology and Precision Engineering*[J], 2015, 6: 454
14 Zhu Pengzhe, Hu Yuanzhong, Ma Tianbao *et al*. *Tribology Letters*[J], 2011, 41: 41
15 Chavoshi S Z, Luo X C. *Computational Materials Science*[J], 2016, 113: 1
16 Chavoshi S Z, Luo X C. *Materials Science & Engineering A*[J], 2016, 654: 400
17 Wang Quanlong, Bai Qingshun, Chen Jiaxuan *et al*. *Nanoscale Research Letters*[J], 2015, 10(1): 1
18 Liang Yingchun, Wang Quanlong, Chen Jianxuan *et al*. *Key Engineering Materials*[J], 2013, 562: 1308
19 Wang Quanlong, Bai Qingshun, Chen Jiaxuan *et al*. *Applied Surface Science*[J], 2015, 355: 1153
20 Dai Houfu, Chen Genyu, Zhou Cong *et al*. *Applied Surface Science*[J], 2017, 393: 405
21 Chavoshi S Z, Goel S, Luo X C. *Journal of Manufacturing Processes*[J], 2016, 23: 201
22 Wang Quanlong, Bai Qingshun, Chen Jiaxuan *et al*. *Applied Surface Science*[J], 2015, 344: 38
23 Tersoff J. *Phys Rev B*[J], 1989, 39: 5566
24 Zhu P Z, Fang F Z. *Appl Phys A-Mater*[J], 2012, 108: 415
25 Lai Min, Zhang Xiaodong, Fang Fengzhou. *Nanoscale Research Letters*[J], 2013, 8: 353
26 Lai Min, Zhang Xiaodong, Fang Fengzhou. *Nanoscale Research Letters*[J], 2013, 8: 13
27 Belak J, Glosli J N, Boercker D B *et al*. *MRS Online Proceedings Library*[J], 1995, 389: 181
28 Wang Y, Shi J, Ji C. *Appl Phys A*[J], 2014, 155: 1263
29 Cheong W C D, Zhang L C. *Nanotechnology*[J], 2000, 11(3): 173
30 Cross G L W. *Nature Nanotechnology*[J], 2011, 6: 467

单晶锗纳米切削过程应力场分布的分子动力学研究

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摘　要：采用分子动力学方法研究了材料原子的应力场分布以及不同刀具角度对应力分布的影响。采用近邻平均法计算了切削过程中不同时刻的 hydrostatic 应力和 von Mises 平均应力值。结果表明，在单晶锗的纳米切削过程中，最大平均应力集中于刀具尖端的亚表面区域，最大应力值为 8.6 GPa。在切屑中也有很高的应力值，在 4.2 GPa 左右。此外，刀具的角度也对应力场的分布有很大影响，绘制了不同刀具角度的切削力曲线。发现，刀具前角对切削力有显著影响。刀具采用负前角切削时切削力最大，而刀具后角对切削力没有影响，这与宏观切削理论相一致。

关键词：单晶锗；应力分布；分子动力学；刀具角度

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