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ARTICLE

Molecular Dynamics Simulation and Experimental Study of Single Crystalline Germanium Cutting Process

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Abstract: In order to understand the nanoscale cutting characteristics of single crystal germanium and improve the optical surface quality of the nanoscale germanium, three-dimensional molecular dynamics (MD) simulations were carried out to study the contact and sliding processes between diamond points and surfaces of single crystal germanium. The material deformation, cutting force, chips pile-up, surface morphology size, and the sliding friction process were investigated. The simulation results show that the cutting force, surface morphology size, and chips pile-up increase during the contact process with the increasing vertical force, and there is no obvious correlation with the cutting speed. The fundamental reason for the fluctuation of the cutting force in the cutting process is the generation of phase transition and the energy fluctuation caused by the destruction of the lattice of single crystal germanium. In order to verify the correctness of the simulation results, nanometer cutting experiments on single crystal germanium were carried out using nano-scratch tester. The experimental results are in agreement with the simulation results, which verify the correctness and effectiveness of the MD model.

Key words: molecular dynamics; single crystal germanium; cutting force; vertical load; cutting speed

As a typical infrared optical hard and brittle material, monocrystalline germanium has important applications in the fields of national defense, military and aerospace. Single point germanium has the characteristics of fragility, high hardness and high difficulty in processing. It is easy to destroy the surface of the single point diamond turning on the surface of the single point diamond, which makes it difficult to obtain the perfect optical quality surface. Therefore, in order to obtain high surface quality micro and nanoscale germanium devices, it is necessary to further study the micro and nano cutting mechanism of germanium.

In recent years, some scholars have begun to use atomic force microscopy (AFM) to process various kinds of nano devices, and to improve the processing efficiency[1-4]. By this way, the nanoscale groove with high surface precision can be obtained, and the cutting mechanical properties of the material can be well reacted. However, this method is serious damage to the diamond tip during the processing of hard and brittle materials, which is not suitable for mass production. Nano scratch tester is a common equipment to test the mechanical properties of materials. It can obtain the macroscopic information about the local region's hardness, modulus of elasticity, friction coefficient and so on. It also can be combined with SEM, TEM and Raman spectroscopy to determine the chip, dislocation, phase transition and so on in the nano indentation and scratch test[5-8]. Because germanium is a rare metal with high price, a lot of economic loss can be caused by the frequent use of experimental methods, and it is difficult to observe the dynamic change process in the process of micro-nano cutting. Molecular dynamics (MD) method is considered to be an effective method for exploring atomic microfabrication process because it can effectively simulate the structure of micro and nano-scale[9,10]. In recent years, because of the rapid development of computer, MD methods have been widely used in micro- nano cutting and indentation. Many scholars have applied the method of molecular dynamics simulation to simulate the process of a large number of nanoscale cutting and indentation[11-15].

In the present paper, MD method is used to process the

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nanoscale groove of single crystal germanium. The change of the cutting force, the size of the surface morphology and chip accumulation form under different vertical loads, cutting speed are analyzed. In order to verify the correctness of the simulation results, nano-scratch tester, scanning electron microscope (SEM) and atomic force microscope (AFM) were used to investigate the nanoscale cutting process of single crystal germanium. The experimental conclusion is consistent with the simulation results, which provides a theoretical and experimental basis for the production of single crystalline germanium micro-nano device.

1 Simulation Model and Experimental Equipment

As shown in Fig.1, the three-dimensional MD model consists of a single crystal germanium substrate and a rigid diamond probe. The matrix box size is $15a\times20a\times12a$, where a is the lattice constant of Ge (a=0.556 7 nm). The three orientations of the substrate are x-[100], y-[010], z-[001]. According to the boundary conditions of MD modeling presented by Belak et al[16], three kinds of zone are included in substrate. As shown in Fig.1, the three kinds of zone are:

(1) The boundary zone: the three atomic layers at the bottom of the substrate. These were kept fixed during the simulated process;

(2) The thermostat zone (heat affected zone): the five atomic layers adjacent to the boundary atoms. The temperature of the system was kept constant and initial temperature of the matrix was 293 K, the temperature of thermostat atoms was controlled at 293 K by Nose-Hoover method;

(3) The Newtonian zone: the substrate atoms above the thermostat zone. The motion of thermostat atoms and Newtonian atoms obeys classic Newton's second law. The Newton's equations of motion were integrated using the Velocity-Verlet algorithm with a time step of 1 fs. The initial velocity of thermostat atoms and Newtonian atoms was set by the Maxwell distribution. Moreover, the periodic boundary conditions were imposed on the x and y directions to reduce the effects of simulation scale.

The angle of rigid cone tip is 30° and tip radius of curvature is 1.0 nm. The initial distance from the top cone to upper plane of matrix (001) is 1.0 nm.

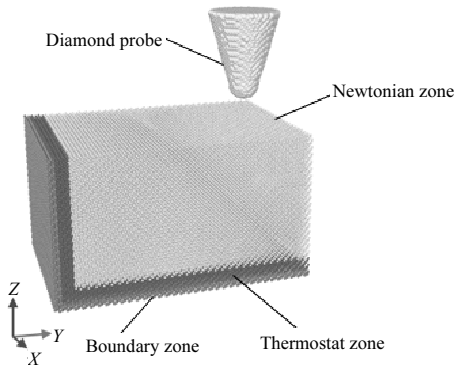

Fig.1 Model of MD simulation

There are three different atomic interactions, the Ge-Ge interactions, C-Ge interactions, and C-C interactions. As the probe is treated as a rigid body, the C-C interactions between probe atoms are ignored[17]. The 3-body Tersoff potential has been widely imposed in MD simulation of nanocutting for Ge-Ge interactions between the substrate atoms. The interaction between Ge-C atoms is calculated by Morse potential, with the corresponding parameters of D=0.125 778 eV, α=25.821 9 nm^{-1} and r_0=0.223 24 nm. The simulation parameters are listed in Table 1.

In order to verify the correctness of the simulation results, the matrix material used in the experiment is the single crystal germanium. The crystal face orientation is (100), and the sample size is 10 mm×10 mm×0.5 mm. The surface roughness of the sample is less than 0.5 nm, and the cleanliness is about 1000 (made in the super clean studio). The sample was polished on one side and the polishing surface was used as the surface of the experiment. Before the experiment, the samples were pretreated, and the samples were soaked in acetone and ethanol for 10 min for decontamination, and then the surface of the sample was preheated.

The nano-scratch tester used in the experiment has a displacement resolution of 0.01 nm and a load resolution of 0.02 μN. The radius of the diamond tip is 2 μm, and the scratching length is 200 μm. The effects of these parameters on the surface morphology of single crystalline germanium nano-scale were studied by setting different vertical loads and cutting speeds. Its specific parameters are set as shown in Table 1.

A focused ion beam scanning electron microscope (TESCANLYRA3 FEG-SEM/FIB), was used to observe the surface morphology of the samples obtained from the scratch test of single crystal germanium in a vacuum environment. The atomic force microscope (Bruker Dimension ICON) was used to observe and measure the three-dimensional shape and size of single crystal germanium nanogrooves. Five locations were randomly selected on each nano groove to measure the depth and width, and the average value was taken as the effective value.

Table 1 Parameters of MD simulation

Scratch test parameter	Value
Model size	$25a\times35a\times30a$, (a=0.565 7 nm)
Vertical load/nN	50, 100, 150
Scratch velocity/$m\cdot s^{-1}$	2, 5, 10, 20
Scratch distance/nm	0~12
Potential	Ge-Ge: Tersoff, Ge-C: Morse
Initial temperature/K	293
Sliding direction	(100)
Curvature radius/nm	1
Angle of tool, θ/(°)	30

2 Results and Discussions

2.1 Effect of cutting velocity and experiment verification

To explore the effect of cutting velocity on the cutting process, MD simulations of nanometric cutting were performed for different cutting velocities. Fig.2a~2c show the cross-sectional views of the *x*-*z* plane during the cutting process for the cutting velocities of 400, 600 and 800 m/s, respectively. The vertical load is 50 nN and the tool angle is 30°. It can be seen that the cutting velocity has a little effect on the cutting process. From Fig.3, 4, there is no change in chip volume with a higher cutting velocity. Fig.5 shows the curve of normal force and sliding distance for the different cutting speeds. It can be seen that the cutting force has little change with the increase of cutting velocity, and the average cutting is 70 nN.

For verification of the MD simulated cutting speed in this study, mechanical experiment of nanoscale cutting with single crystal germanium were conducted. Three single crystal germanium nanoscale grooves were processed with different cutting speeds. The applied vertical loads were all 30mN, and the cutting speed was 300, 400, 500 μm/min. Fig.6 shows SEM images of nanoscale grooves (20000 times magnification). It can be seen that there is no obvious change in the morphology of the groove surface as the cutting speed increases, and the evenness of each groove is very high, and there is no accumulation of chip on both sides of the groove. In order to obtain accurate size information of the width and depth of nanoscale groove, an AFM is used to measure the width and depth of the groove as show in Fig.7. The relationship between the grooves surface morphology size and the cutting speed is shown in Fig.8. It is found that the cutting speed has little effect on the width and depth of the nanoscale

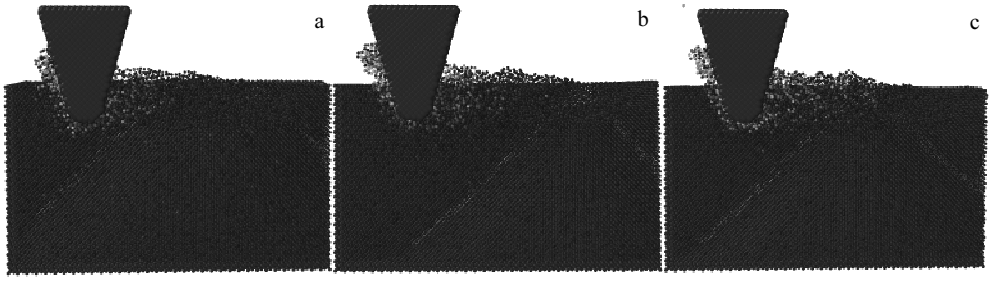

Fig.2 Cross-sectional views of *x*-*z* plane for different cutting speeds at the sliding distance of 12.0 nm: (a) 400 m/s, (b) 600 m/s, and (c) 800 m/s

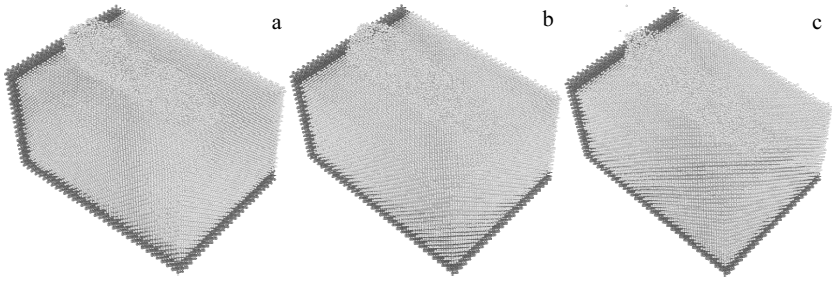

Fig.3 Images of surface wear when the sliding distance is 12.0 nm for different cutting speeds: (a) 400 m/s, (b) 600 m/s, and (c) 800 m/s

Fig.4 Images of chip when the sliding distance is 12.0 nm for different cutting speeds: (a) 400 m/s, (b) 600 m/s, and (c) 800 m/s

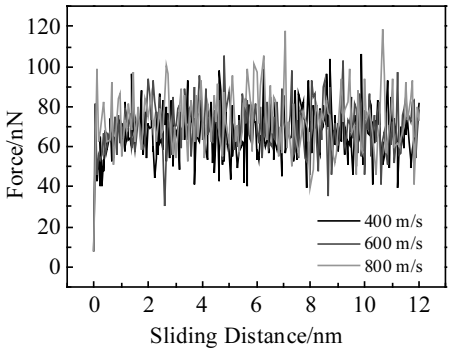

Fig.5 Relationship between normal force and sliding distance for different cutting speeds by MD simulation

groove. With the change of the cutting speed, the depth range of the nanoscale groove is 1.959~2.142 nm, and the width of the groove is 4.632~4.723 μm. Fig.9 is the experimental curves of cutting force and sliding distance for different cutting speeds, which is in good agreement between the MD simulated and experimental results.

2.2 Effect of vertical load and experimental verification

MD simulations were carried out to study the effect of cutting depth on the cutting process. Fig.10a~10c show the cross-sectional views of the *x*-*z* plane at a cutting distance of 12 nm for the cutting vertical load of 50, 100, 150 nN, respectively. The cutting velocity is 400 m/s and the tool angle is 30°. It can be seen that as the vertical load increases, more workpiece atoms deform around the tool and the chip becomes

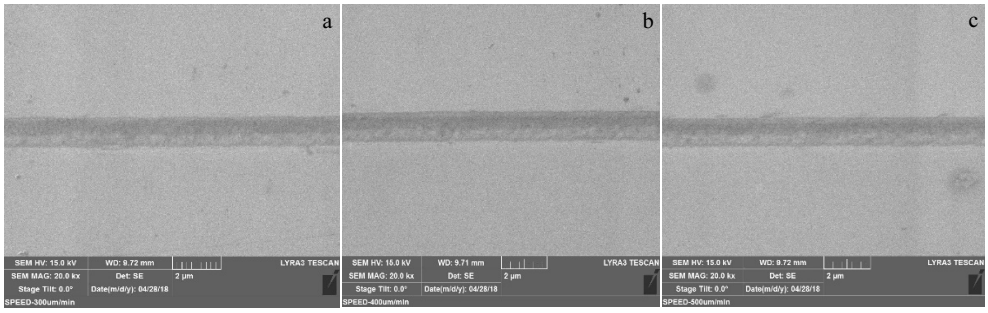

Fig.6 SEM morphologies of nanogrooves scratched with normal force of 30 mN at different cutting speeds: (a) 300 μm/min, (b) 400 μm/min, and (c) 500 μm/min

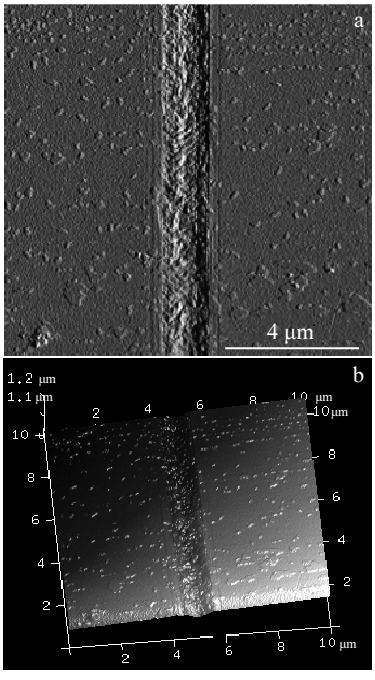

Fig.7 AFM morphologies of nanogrooves at scratching velocity of 300 μm/min with normal force of 30 mN: (a) 2D and (b) 3D

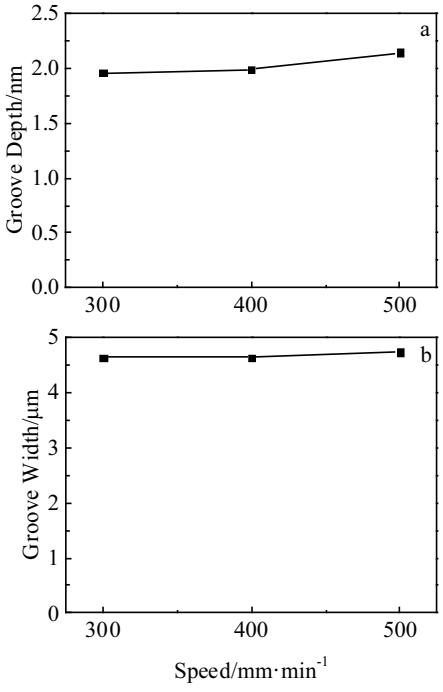

Fig.8 Relationship between depth (a), width (b) of groove and cutting speed

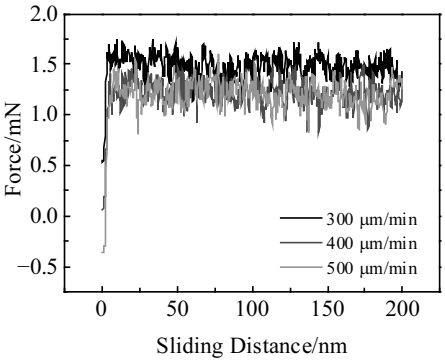

Fig.9 Relationship between normal force and sliding distance for different cutting speeds by experiment

larger. From Fig.11, 12, it can be seen that the vertical load has a significant effect on the cutting process. A higher vertical load results in a larger chip volume. The variations of cutting force during cutting process for the three vertical loads are shown in Fig.13. It can be seen that a bigger vertical load results in a bigger cutting force. And the smaller the vertical load, the earlier the cutting reaches the steady state. The bigger the vertical load is, the more workpiece atoms the tool contacts, which results in more material deformation and larger chip volume. Therefore, bigger forces are required.

The experiment applied three groups of different vertical loads to scratch three nanoscale grooves. The three groups of loads were 10, 20, 30 mN, and the calibration speed was 200 μm/min. Fig.14 is the SEM images of the nanoscale groove

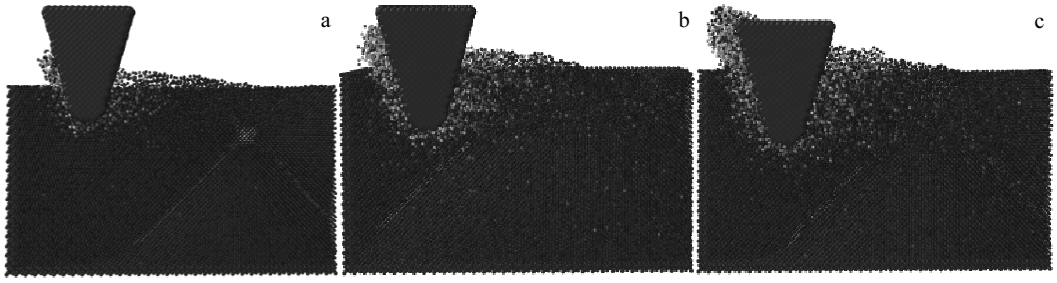

Fig.10 Cross-sectional views of *x*-*z* plane for different vertical loads at the sliding distance of 12.0 nm: (a) 50 nN, (b) 100 nN, and (c) 150 nN

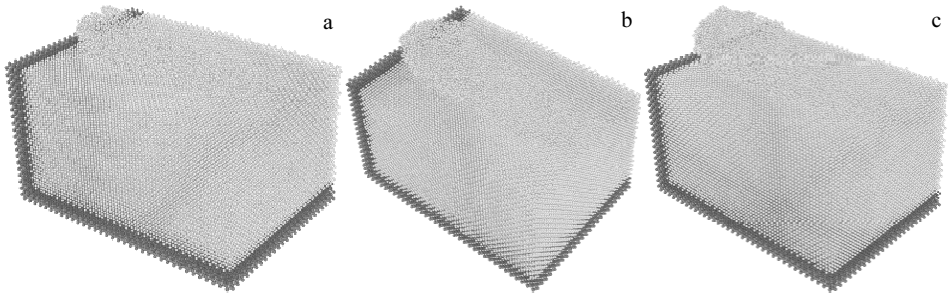

Fig.11 Images of surface wear when the sliding distance is 12.0 nm for different vertical loads: (a) 50 nN, (b) 100 nN, and (c) 150 nN

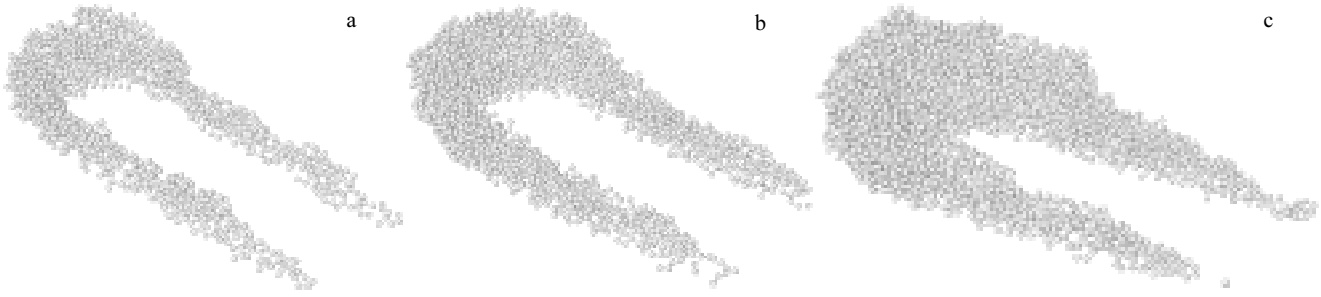

Fig.12 Images of chip when the sliding distance is 12.0 nm for different vertical loads: (a) 50 nN, (b) 100 nN, and (c) 150 nN

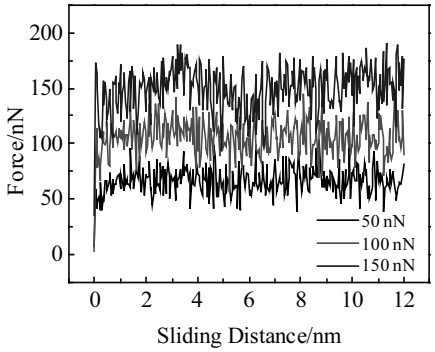

Fig.13 Relationship between normal force and sliding distance for different vertical loads by MD simulation

(amplification factor of 20 000 times). It can be clearly seen that the width of the nanoscale groove increases with the increase of the vertical load, and the chip accumulation around the groove is more and more obvious, but there is no crack, indicating that the groove is produced by the plastic deformation and does not produce brittle fracture. The relationship between the groove surface morphology size and vertical load is drawn as shown in Fig.15. It is found that when the load is changed in 10~30 mN, the depth of the groove is 3.52~4.28 nm and width is 5.7~10.4 μm. Fig.16 is the experimental curves of cutting force and sliding distance for the different vertical loads. It can be found that with the increase of vertical load, the cutting force is also increasing, which is in good agreement between the MD simulated and experimental results.

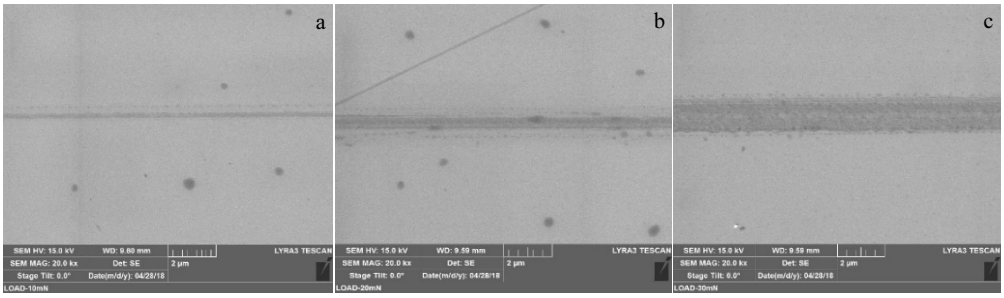

Fig.14 SEM morphologies of nanogrooves scratched with scratching velocity of 200 μm/min at different vertical loads: (a) 10 mN, (b) 20 mN, and (c) 30 mN

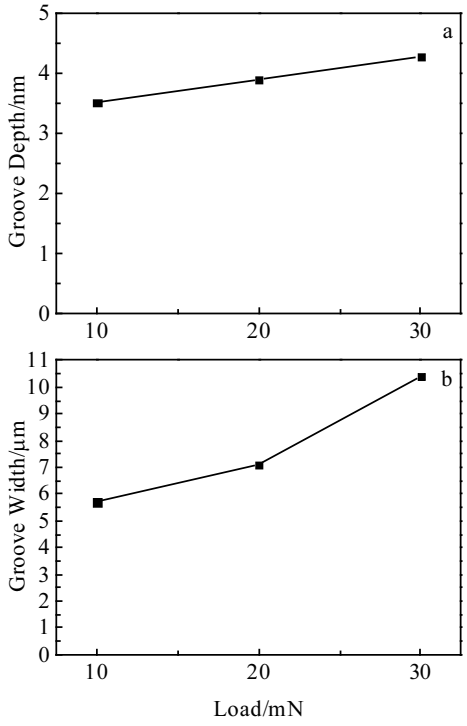

Fig.15 Relationship between depth (a), width (b) of groove and vertical load

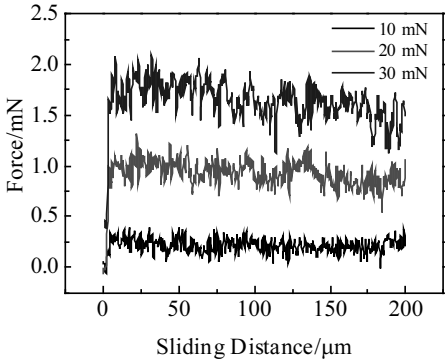

Fig.16 Relationship between normal force and sliding distance for different vertical loads by experiment

3 Conclusions

1) The simulation results show that the cutting speed has little effect on the three-dimensional size of the single crystal Ge nanoscale. With the increase of the cutting speed, the surface morphology of the nanoscale groove is almost unchanged, and the configuration of the chip accumulation is almost unchanged. The fluctuation of the cutting force is caused by the energy fluctuation due to the slip of the phase

transition in the cutting process and the destruction of the crystal lattice of single crystal germanium atoms. The width of the surface is 4.632~4.723 μm, the range of depth is 1.959~2.142 nm, and the change trend is in accordance with the simulation results.

2) The vertical load is the key factor affecting the size change of the three dimensional groove of single crystal germanium. With the increase of the vertical load and the number of characterizations, the depth and width of the nanoscale groove gradually increase. With the increase of vertical load, the cutting force is increased, only because the larger the cutting force is, the deeper the cutting depth is, and the process hardening and dislocation accumulation are caused during the cutting process. The depth range of grooves is 3.52~4.28 nm and the width range is 5.7~10.4 μm, and the experiment is in accordance with the simulation results.

3) The molecular dynamics method is an effective method to describe the microscopic phenomena. The correctness of the simulation is verified by the nanoscale scratch test experiment, which provides the theoretical basis and experimental basis for the processing of higher surface quality of the nano germanium devices.

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单晶锗纳米切削过程分子动力学仿真与实验研究

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摘　要：为深入理解单晶锗纳米切削特性，提高纳米锗器件光学表面质量，采用三维分子动力学（MD）模拟方法研究了单点金刚石压头与单晶锗表面的接触和滑动过程。研究了压头在滑动切削过程中的材料变形、切削力、切屑堆积、表面形貌尺寸。仿真结果表明，随着垂直载荷的增加，切削力、表面形貌尺寸、切屑堆积在接触过程中逐渐增加，且与切削速度无明显关联。切削过程中切削力波动的根本原因是由于单晶锗晶格破坏引起相变的产生和能量波动。为了验证仿真结果的正确性，使用纳米划痕仪对单晶锗进行了纳米切削实验。实验结果与仿真结果一致，验证了 MD 模型的正确性和有效性。

关键词：分子动力学；单晶锗；切削力；垂直载荷；切削速度

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