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ARTICLE

Nano-cutting Temperature Field Distribution and the Influence of Anisotropy on Cutting Temperature of Single Crystal Germanium

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Abstract: In order to understand the nano-cutting properties of single crystal germanium and improve the optical surface quality of nano-germanium devices, the three-dimensional molecular dynamics (MD) method was firstly applied to investigate the temperature distribution of the material atoms during the nano-cutting process of single crystal germanium. The anisotropy effect of Ge (100), (110) and (111) on the cutting temperature and the influence of cutting temperature on cutting force were investigated. The results show that the highest cutting temperature during the cutting process is distributed among the chips, reaching 460 K. There is also a high temperature region in the friction zone of the tool back face, and the highest temperature is above 400 K. Among the three different crystal planes, the highest cutting temperature exists on the surface of Ge (111) crystal. Atomic arrangement is the most intensive in Ge (111), namely, Ge (111) is the densely packed surface of the single crystal germanium, which releases the most energy. What's more, cutting temperature has also made an impact on the cutting force. As the cutting temperature increases, the cutting force of the material atoms is reduced.

Key words: single crystal germanium; anisotropy; molecular dynamics; cutting temperature; cutting force

Single crystal germanium is a typical representative of infrared optical hard and brittle materials. It can be used in both long-wave infrared band and medium-wave infrared band. The refractive index of single crystal germanium is large, which is good for reducing aberration. It is quite beneficial for designing optical devices. It has important applications in aerospace, military equipment and other high-tech fields, for example, infrared detectors installed on space stations and space shuttles. Single crystal germanium devices are used in individual night market systems on military infrared equipment, tank infrared night vision systems, warship infrared thermal imaging weapon defense systems, infrared guided missiles, infrared tracking systems and infrared surveillance systems. In addition, single crystal germanium is also used in civil infrared optical equipment. Civil infrared optical lens is mainly used in fire, power, manufacturing and medical industries. In recent years, single crystal germanium is also used in solar cells. Compared with the traditional monocrystalline silicon cell, the photoelectric conversion efficiency of germanium substrate cell is excellent, and its life is also better than that of silicon cell.

In the metal cutting process, the work done by the shearing deformation of the chip and the friction between the front and the rear of the tool are all transformed into heat. The heat carried by the chip is the largest, and the heat transmitted to the tool is small, but the temperature at the front and the rear affects the cutting process and the wear of the tool. Therefore, it is very necessary to understand the change law of the cutting temperature. However, as the nanoscale cutting involves only a few nanometers or less on the material surface, it is very difficult to observe the temperature field distribution by experiments. MD simulation as a theoretical investigation method is a very useful tool in studying the nanometric cutting process[1-3]. Many scholars have applied the method of

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molecular dynamics simulation to simulate the process of a large number of nanoscale cutting and indentation[4-8]. Wu[4] studied the effects of individual layer thickness, indentation velocity, and temperature on the mechanical properties under indentation by MD simulations based on many-body embedded-atom potential, and the results show the average required indentation force increases with increasing the indentation velocity or decreasing the temperature. Chavoshi[9-11] employed MD simulation to explore elevated temperature cutting anisotropy of single crystal silicon, and made a series of achievements. Wang[12-15] studied the nano-cutting process of single crystal copper by the molecular dynamics method and the temperature distribution, stress distribution, phase structure change and dislocation defect of single crystal copper were studied.

According to the published literatures, we found that few studies focus on the effect of cutting temperature distribution on the nanometric cutting process. The distribution of cutting temperature in monocrystalline germanium nanometric cutting process has seldom been reported before. Therefore, in order to improve the fabrication and surface precision of the nano-crystalline germanium devices, the three-dimensional molecular dynamics (MD) method was firstly applied to investigate the temperature distribution of the material atoms during the nano-cutting process of single crystal germanium, and the cutting model of single crystal germanium was established. For the first time, 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 Simulation Methodology

Fig.1 shows the MD simulation model of nanometric cutting of single crystal germanium. The model consists of a single crystal germanium workpiece of diamond structure and a diamond tool. Table 1 summarizes the computational parameters used in the MD simulations. The size of the workpiece is 20 nm×12 nm×3 nm. The cutting is conducted along the -X direction on the surface of the workpiece in Fig.1. The workpiece includes three kinds of atoms: boundary atoms, thermostat atoms and Newtonian atoms. The motions of thermostat atoms and Newtonian atoms obey classical Newton's second law. The Newton's equations of motion are integrated with a velocity-Verlet algorithm with a time step of 1 fs. The three layers of boundary atoms at the left and the bottom of the workpiece are kept fixed in space to reduce edge effect. The next layers of atoms adjacent to the boundary atoms at the left and the bottom of the workpiece are thermostat atoms. The bulk (initial) temperature of the workpiece is 293 K. During MD simulations, constant temperature is obtained by keeping the thermostat atoms at a

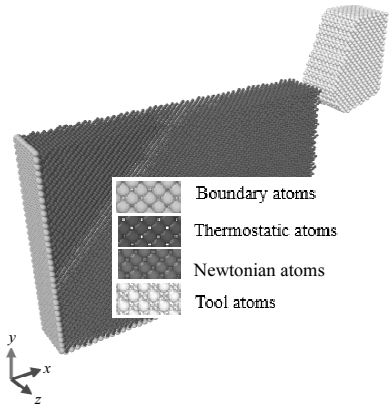

Fig.1 Schematic of the MD simulation model

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

Workpiece material	Single crystal germanium
Workpiece dimension/nm	20×12×3
Tool material	Diamond
Cutting edge radius (tip radius)/nm	2
Cutting plane	(100), (110), (111)
Rake angle of the cutting tool/(°)	30
Clearance angle of the cutting tool/(°)	20
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

constant temperature of 293 K by a velocity scaling method. Periodic boundary conditions are imposed in the *z* direction.

The diamond tool created from perfect diamond atomic lattices has a configuration with a rake 30° and clearance angle 20°. The apex of the cone is truncated by one atom. The tool is treated as a rigid body in the simulations since the diamond is much harder than the germanium.

There are three different atomic interactions in the MD simulation: (1) the interaction between germanium atoms (Ge-Ge) in the workpiece; (2) the interaction between diamond atoms (C-C) in the tool; (3) the interaction between workpiece and tool (Ge-C).

For the Ge-Ge interaction between workpiece atoms, the Tersoff potential[16-19] was used to depict the interaction among the germanium atoms of the substrate.

As the tool is treated as a rigid body, the C-C interactions between tool atoms are ignored. For the Ge-C interaction we adopt Morse 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; α is the elastic modulus; r and r_0 are the

instantaneous and equilibrium distance between two atoms, respectively. Detailed parameters are D=0.125 778 eV, α= 25.8219 nm^{-1}, r_0=0.223 24 nm.

The calculation method of temperature is to divide the bulk into small boxes of 0.4 nm×0.4 nm×0.4 nm (Space partitioning method) and to count the number of atoms in the small boxes, thus getting temperature distribution based on the relationship between temperature T and kinetic energy:

$$T = \frac{\sum_{i=1}^{N} m_i v_i^2}{3Nk_B} \quad (2)$$

where, $m_i v_i^2$ is the kinetic energy of the i atom, 3 is the Spatial freedom of atoms, N is the number of atoms in small boxes, The kinetic energy coefficient of k_B is constant.

2 Results and Discussion

2.1 Temperature field distribution of monocrystalline germanium in nano-cutting process

Fig.2 shows the temperature distribution inside the workpiece during the nano-cutting process of single crystal germanium. The cutting speed is 200 m/s, the radius of the cutting edge is 2 nm, the cutting depth is 2 nm, and the time step is 20 000. In order to clearly display the temperature distribution inside the workpiece, the atomic temperature of the workpiece was calculated according to the statistical temperature, and the different values of atomic temperature were colored according to different colors. Fig.2 shows that the overall temperature of the workpiece presents a concentric gradient distribution, centering on the knife-chip interaction zone. The highest temperature of the workpiece is generated at the chip and the highest temperature is above 460 K. There is also a high temperature region in the friction zone of the tool back face, and the highest temperature is above 400 K. The temperature of the sub-surface and the machined surface of the workpiece is about 400 K. The temperature of the subsurface and the machined surface of the workpiece is between 340~350 K. The inner part of the workpiece is close to the boundary, the temperature is lower, and the temperature gradient is larger. The highest temperature 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 temperature 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 temperature of the region near the boundary layer in the workpiece decreases rapidly, the temperature gradient is large and the temperature value is low due to the temperature regulation of the constant temperature layer.

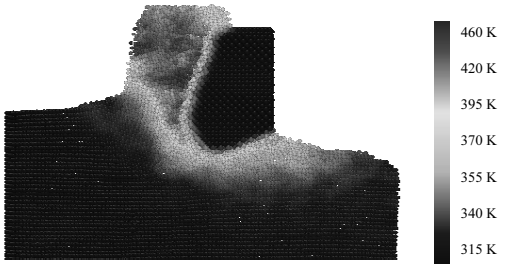

Fig.2 Temperature distribution of workpiece in nano cutting process

2.2 Influence of anisotropy on cutting temperature

A series of MD simulations with different crystal planes (100), (110), (111) are conducted to evaluate the effect of crystal direction. The cutting velocity is 200 s^{-1} and the cutting depth is 2 nm.

As a typical hard and brittle infrared optical material, single crystal germanium has anisotropic characteristics, i.e. its physical, chemical and optical properties reflected from different crystal directions are different, and the fundamental reason is that the periodicity and density of atoms arranged in different directions along the lattice are different. For a given crystal, the number of atoms per unit volume is certain as same as the volume of nodes. The minimum repetition unit volume is also certain. Therefore, the thinner the crystal plane, the more atoms on each crystal plane must be. In addition, considering that the equilibrium position of the particles in the crystal corresponds to the position where the binding energy is minimum, the arrangement of the particles should be as close as possible. It is because of the different arrangement of atoms in different crystal planes and crystal directions that the crystals are anisotropic. The larger the distance between atoms is, the larger the binding force is, and the easier it is to split. Fig.3 shows the arrangement of atoms in single crystal germanium crystals[20].

Fig.4 is the temperature-timestep curves of workpiece with different crystal directions (100), (110), (111) during the nano-cutting process of single crystal germanium. The first 10 000 steps of the system are the relaxation process of the system, so as to achieve balance and stability. As can be seen from Fig.4, when the number of cutting steps is 12 000, the tool begins to contact the workpiece, and the temperature of the workpiece increases with the distance of the tool sliding. With the increase of cutting distance, the movement of atoms in the workpiece becomes more and more intense. Dislocation

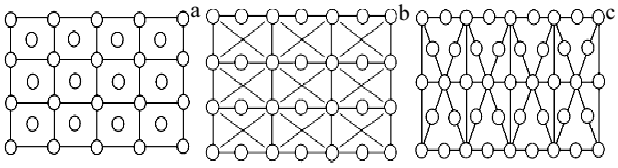

Fig.3 Atomic arrangement position of each crystal orientation of the single crystal germanium[20]: (a) (100), (b) (110), and (c) (111)

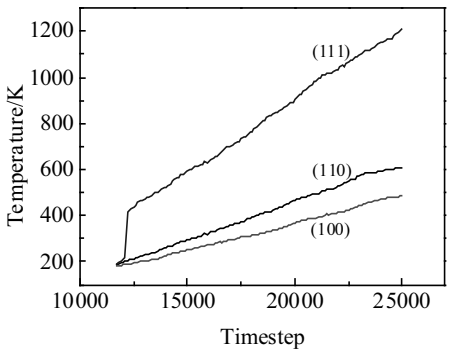

Fig.4 Curves of temperature-timestep for the different crystal planes by MD

slip, dislocation accumulation and work hardening begin to occur in the workpiece. This makes the atoms in the workpiece release a lot of lattice energy, and the temperature of the atoms in the workpiece increases gradually. It can also be seen that the temperature distributions of the three orientations are the lowest (100) and the highest (111). This can be well illustrated by Fig.3. It can be clearly seen that the atoms in the (100) lattice are the least, the atom spacing is large, and the atoms in the (111) lattice are the dense planes of atoms within the same volume. Atoms release the most energy, so the temperature of the crystal toward the workpiece is the highest.

2.3 Influence of temperature on cutting force

MD simulations were carried out to study the effect of cutting temperature on the cutting process. Fig.5a~5c show cross-sectional view of *x-y* plane for the cutting temperature of

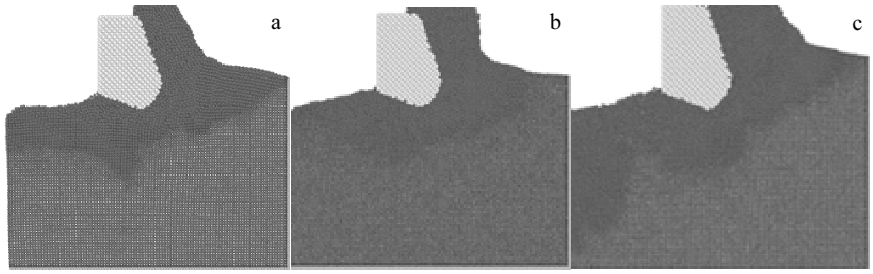

Fig.5 Cross-sectional view of *x-y* plane for the different cutting temperatures at a cutting timestep of 25 000: (a) 300 K, (b) 500 K, and (c) 800 K

300, 500 and 800 K at a cutting timestep of 25 000, respectively. The cutting velocity is 200 m/s. It can be seen that as the cutting temperature increases, more workpiece atoms deform around the tool and the chip becomes larger, chip accumulation is becoming more and more obvious. The variations of cutting force during cutting process for the three cutting temperature are shown in Fig.6. It can be seen that a higher cutting temperature results in a smaller cutting force, because as the temperature increases, the dislocation atoms inside the workpiece begin to move more and more intensely,

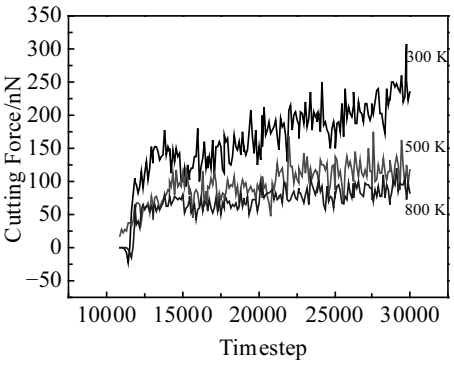

Fig.6 Curves of cutting force-timestep for the different cutting temperatures by MD

the plastic deformation of the workpiece material is easier and easier, so the cutting force will continue to decrease.

3 Conclusions

1) The temperature distribution of single crystal germanium nano-cutting process was studied. The highest temperature in the workpiece is in the chip and the highest temperature is above 460 K. There is also a high temperature region in the friction zone of the tool back face, and the highest temperature is above 400 K. The temperature of the sub-surface and the machined surface of the workpiece is about 400 K. It is also relatively high, between 340~350 K.

2) The effect of anisotropy on cutting temperature is very obvious. The temperature distributions of the three orientations are the lowest (100) and the highest (111), and the fundamental reason is the degree of intensity between the atoms in different crystal orientation. The atoms in (111) crystal plane is most closely aligned, and the energy released by the change of atomic structure during cutting is the highest, so the temperature is the highest.

3) MD simulations were carried out to study the effect of cutting temperature on the cutting forces in the nano-cutting process of monocrystalline germanium. The cutting force decreases with increasing cutting temperature, because as the temperature increases, the dislocation atoms inside the

workpiece begin to move more and more intensely, the plastic deformation of the workpiece material is easier and easier, resulting in the cutting force continuing to decrease.

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单晶锗纳米切削温度场分布及各向异性对切削温度的影响研究

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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，首次采用三维分子动力学（MD）的方法研究了单晶锗纳米切削过程中工件原子的温度分布情况，研究了晶体的各向异性(100), (110), (111)晶面对切削温度的影响及切削温度对切削力的影响。结果表明，在切削过程中最高切削温度分布在切屑当中，达到了 460 K。刀具的后刀面与已加工表面之间的区域也有较高的温度，在 400 K 以上。在 3 个不同的晶面中，(111)晶面的切削温度最高，(111)晶面的原子密度最大，即为单晶锗的密排面，释放出的能量最多。切削温度对切削力也有影响，切削温度越高，工件中原子受到的切削力越小。

关键词：单晶锗；各向异性；分子动力学；切削温度；切削力

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