Analysis of the influence of tool radius on single crystal silicon cutting process based on Molecular dynamics

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Abstract. In this paper, a molecular dynamics method is used to construct a simulation model for cutting single crystal silicon with a tool. Through the analysis of phase transition, instantaneous atomic position, temperature, Wigner-Seitz defect and other variables, the influence of tool radius on material deformation is studied. The results show that in the process of cutting single crystal silicon, the contact area between the cutting edge and the single crystal silicon workpiece is the main area of cutting heat generation, and the phase change process from the atomic crystalline state to the amorphous state is reflected in the cutting process of different tool radii. The difference is that the amorphous atoms are removed in the form of chips during the cutting process of the sharp-angle tool, while the amorphous atoms are further compressed directly under the tool in the round-angle tool, causing subsurface damage. The chip removal mechanism of sharp tools is shear, and the chip removal mechanism of round tools is shear and extrusion. As the radius of the tool increases, the more atoms are compressed directly below the tool, the worse the surface quality of the machined surface.

1. Introduction
In recent years, the manufacturing process has higher requirements for surface quality and machining accuracy, and micro-manufacturing will also become one of the future manufacturing trends [1-3]. In nano-cutting, the cutting measure and the tool radius are usually between several nanometers [4], and a series of special physical phenomena will appear, for instance: size effect [5,6], micro-wear [7,8] etc., correspondingly, the influence of the tool radius on the quality of the machined surface cannot be ignored [6].

As the most important semiconductor material in modern industry, single crystal silicon is a typical representative of brittle materials [9-11]. According to the principles of fracture mechanics, process-singe brittle materials will be accompanied by brittle-plastic transformation [12], and it will exist in the crystal as crack extension. CAI et al. [13] used the residual stress in the local deformation zone to explain the plastic-brittle conversion problem during the cutting of single crystal silicon. F. Z. Fang et al. [14] believe that the difference between the shearing mechanism of single crystal silicon under nano-scale and traditional cutting conditions is that it is removed by extrusion. Tang Yulan et al. [15] found that there is no obvious dislocation and elastic recovery in the amorphous phase transformation of single
crystal silicon. Tangential force promotes the formation of amorphous phase transformation, and normal force makes the amorphous state expand. Ji Chunhui et al. [16] studied the stress distribution in the chip contact area and found that the shear stress in the chip area gradually decreases with a regular waveform. Shi Liqiu et al. [17] established cutting tools of different shapes to cut single crystal silicon, and found that tools with negative rake angles will help improve the quality of the processed display.

The above studies [12~17] mostly used two-dimensional or quasi-three-dimensional tool models when molecular dynamics methods were used to study the mechanism of nano-cutting, but none of them considered more realistic three-dimensional tool models. Previous research helps to understand the nano-cutting process. However, they mainly study the effect of tool cutting edge radius and rake angle on the material removal mechanism. There is no systematic research on the influence of nano-cutting tool radius and other tool geometric parameters on the material surface integrity and the deformation of the workpiece material. In this work, we will consider the influence of the tool radius and conduct a series of large-scale molecular dynamics (MD) simulations on the nano-scale cutting of single crystal silicon with diamond tools. In addition, this chapter establishes a single-crystal silicon nano-cutting model with tool fillet, and investigates the single-crystal silicon nano-cutting process from the perspectives of workpiece morphology change, cutting force and energy evolution, so as to study the mechanism of tool fillet nano-cutting of single-crystal silicon Impact.

2. Single crystal silicon nano-cutting simulation model

Single crystal silicon is composed of a face-centered cubic lattice. The four silicon atoms in the lattice are located at 1/4 of the different diagonals of the cube, and form a diamond structure in the form of covalent bonds with the adjacent four atoms. After the simulation model is established, the system needs to reach a steady state and make it go through a relaxation process. In order to reduce the influence of the size effect, free boundary conditions are applied in the x and y directions, and periodic boundary conditions are applied in the z direction. The simulation conditions of the cutting model are shown in Table 1.

| Processing parameters | Single crystal silicon nano-cutting |
|-----------------------|-----------------------------------|
| Workpiece material    | Monocrystalline silicon           |
| Tool material         | Diamond                           |
| Workpiece size        | 22.263 nm × 19.548 nm × 9.774 nm  |
| Tool rake-angle       | 20°                               |
| Tool relief-angle     | 20°                               |
| Tool cutting edge radius | 0、2nm                         |
| Cutting speed         | 200m/s                            |
| Depth of cut          | 18nm                              |
| Time Step             | 1fs                               |

In this paper, MD simulations are performed by using large atom/molecule massively parallel simulators (LAMMPs) (USA) [18]. The Stillinger-Weber potential is used to describe the interaction between single crystal silicon atoms, which has been used to predict the mechanical properties of silicon atoms in previous studies [19]. The Lennard-Jones potential and the modified Terrsoff multibody empirical potential are used to describe the atomic interaction between single crystal silicon and diamond, which has been verified in our previous work [20, 21]. Before cutting, the conjugate gradient method is used to minimize the system energy, and the time step has set to 1 fs. The molecular model of single crystal
silicon nano-cutting is shown in Figure 1 (a), (b). The single crystal silicon model is divided into three zones, namely the boundary zone, the constant temperature zone, and the Newton zone. The outermost atoms in Figure 1 are boundary zone atoms, the atoms next to the boundary zone are constant temperature zone atoms, and the innermost atoms are Newton zone atoms. The movement of atoms in the Newton zone and the constant temperature zone conforms to the classic Newton's law of motion. In order to ensure a constant temperature during the cutting process, each atom in the constant temperature zone undergoes a speed calibration for every step of calculation. The ratio \( r = \frac{R}{h} \) is a key parameter in the process of controlling material removal. Among them, \( R \) tool radius, \( R \) tool radius, \( h \) cutting thickness, as shown in Figure 1(c), the tool radius discussed later is characterized by the tool radius \( R \).

3. Analysis of MD simulation results

3.1. Instantaneous atomic position analysis

The migration of a large number of microscopic single crystal silicon atoms constitutes the macroscopic plastic removal process in nano-cutting. For the convenience of display, the mid-plane view in the Z-axis direction in the three-dimensional model is intercepted.
In order to have an intuitive understanding of the nano-cutting process, the central symmetry parameter (CSP) of each silicon atom is calculated according to the description formula of the central symmetry parameter, and it is colored according to the numerical value, as shown in Fig.2, the different cutting in the simulation process Instantaneous atomic image at distance.

It can be seen from the figure that as the tool moves, when the tool starts to cut the single crystal silicon substrate, the matrix atoms in front of the tool push away. The main reason is that the tool gradually moves forward, and the force between the single crystal silicon atoms near the outermost layer of the tool and the diamond tool atoms is transformed from attractive force to repulsive force between the two. At the same time, the internal atoms of the single crystal silicon also have a certain force on the outermost atoms. On the one hand, because the bonding energy between the diamond tool atoms is relatively large, the energy required to break the bond energy between them is relatively large. And in the simulation, the diamond tool atoms are set as rigid bodies, and no wear occurs during the cutting process. Because the repulsive force acting on the outermost single crystal silicon atoms plays a major role, on the other hand, due to the binding energy ratio between the single crystal silicon atoms. The bonding energy between the diamond cutter atoms is much smaller. Therefore, the single crystal silicon atoms move forward, and shear extrusion occurs under the action of the cutter.

![Fig 3. The state diagram of each area when the rounded tool cuts chips](image-url)

One of the characteristics of extrusion is the appearance of stagnation points [22]. According to the definition, it is a spatial position, only the material above the spatial position can be moved into the chip, and the material below is pressed down to form a machined surface. As shown in Figure 3, the instantaneous position of the atoms in the region I did not change during the cutting process, the original crystal lattice was retained and some of the atoms moved along the rake face into the chip with the movement of the tool. We call the region I the stagnation zone. There is a region II near the contact edge of the tool and the workpiece in a highly compressed and sheared state. The material lattice in this region is deformed, and for hard and brittle materials such as silicon, since the strain energy is released through phase change rather than fracture, ductile processing is guaranteed. These amorphous structures are only distributed in the area close to the contour of the tool, where the stress is high enough, and the crystal lattice is quickly destroyed. Therefore, the work done by the diamond tool on the workpiece will be dissipated due to high plastic deformation, which is also the reason for the low stress state in the amorphous phase near the edge. Due to direct contact, these highly localized amorphous structures evolve into chips, stagnant zones and machined surfaces through complex plastic deformation according to their positions. We call area II a contact-type amorphous area. Area III is the atomic movement zone, which indicates the direction of the atom movement in the next stage. We call region IV the strained amorphization region. From Fig. 3, it can be seen that the atoms in region IV are mainly distributed below the processed surface. Due to the large elastic modulus and bulk modulus of silicon, the stress is concentrated and the deformed lattice is stored a large amount of strain energy, and then the phase change releases high strain energy, causing damage to the workpiece under the machined surface.
3.2. Workpiece temperature analysis

It can be seen from Fig. 4 that the contact area between the cutting edge and the single crystal silicon workpiece is the main area of cutting heat. This is because the single crystal silicon atoms undergo amorphous phase transition and a small amount of dislocation under the action of the cutting edge. The potential energy is converted into kinetic energy and released in the form of heat, which in turn affects the lattice deformation and lattice reorganization of single crystal silicon atoms. As a result, the amorphous atoms under the front of the cutting edge continue to extend and expand, and combine with the broken atomic bonds of the processed surface layer, forming a processed surface metamorphic layer that is not in front of the tool but in front of the cutting edge. Pressing and shearing action, accumulation and formation of chips. At the same time, some dislocations inevitably form atomic "saw teeth" on the machined surface. The height of these "saw teeth" remaining on the workpiece surface can be considered as the surface roughness that can be achieved by nano-cutting.

3.3. Wigner-Seitz defect analysis

Take simulation models of different tool radii and cutting thicknesses to analyze the Wigner-Seitz defect. In order to ensure the principle of unique variables, the cutting thickness is 12nm when cutting with different tool radii, and the sharp corner tool is selected for different cutting thickness. As shown in Figure 5(a). Taking 100ps as the end point of the simulation, the number of defects caused by the deviation of atoms from the original lattice in the workpiece is 55256 when the tool simulation process with R=35nm produces the most; the tool simulation process with R=15nm produces the least one, 47331 One. high2, high3, high4, and high6 represent different cutting thicknesses respectively, which are 16nm, 14nm, 12nm and 8nm in sequence. The number of defect atoms generated during the simulation process is 52178, 52146, 49119, 47894 in sequence. As the cutting thickness decreases, the generation of defective atoms also decreases, and the energy stored in the damaged lattice decreases, which helps to improve the quality of the machined surface.
Take the defect analysis simulation diagram at the time when the defect atom number generation rate is faster, Fig. 9(b)~(m), corresponding to 6, 8, 10, 14, 32ps, and 94ps as the stable time point of the defect atom number, respectively. Corresponding to cutting distance 1.2nm, 1.6nm, 2.0nm, 2.8nm, 6.4nm, 18.8nm. The larger the initial R of the cutting tool, the less defective atoms will be produced. This is because the larger the R corresponds to the larger the radius of the tool, the more atoms are squeezed by the tool, and the material removal process has not yet been carried out. As the cutting prog-

Fig 5. Wigner-Saitz defect analysis simulation diagram (a) The number of defective atoms generated under different cutting conditions; (b)~(g) and (h)~(m) are the analysis under the conditions of R15 and R35, respectively. Simulation diagram

resses, the squeezed atoms increase, and the energy stored in the lattice increases until the lattice is destroyed and the energy is released. At this time, the atoms undergo a phase change and gradually diffuse into the depth of the workpiece in a shape similar to a tool arc. Atoms leave the original crystal
lattice, creating atomic vacancies in their original positions, severely destroying the quality of the sub-surface underground. Compared with the tool with small R, the number and extent of atoms leaving the original lattice are larger. When R is small, shearing is used to participate in the material removal process at the beginning of cutting, the number of extruded atoms is small, and the vacancies mostly exist in the contact area between the tool and the workpiece, the diffusion of phase change is shallow, and the surface quality is better.

4. Conclusion
In this study, the influence of the tool radius at the nanometer scale on the deformation of the workpiece was studied. The cutting process has two new features: analysis of amorphous regions and analysis of stress changes. They provide more details for revealing the mechanism of nano-cutting, and it is convenient to study the influence of tool radius on workpiece deformation. Clarified the cutting process of sharp corners and fillets from a basic perspective. The main results are summarized as follows:

a. There is a phase change in the cutting process of sharp and rounded tools. The contact-type amorphized atoms and strain-type amorphized atoms generated during the cutting of the sharp-angle tool are moved to the chip to be removed, and the strain-type amorphized atoms form a shear band; above the stagnant zone during the cutting process of the round corner tool. The amorphized atoms are continuously removed, and the underground subsurface damage is caused by the strain-type amorphized atoms.

b. The contact area between the cutting edge and the single crystal silicon workpiece is the main area of cutting heat. The single crystal silicon atom undergoes an amorphous phase transition and a small amount of dislocation under the action of the cutting edge, and a large amount of potential energy is converted into kinetic energy. The form is released.

c. The cutting mechanism of sharp-corner tools is shear, and the cutting mechanism of round-corner tools is extrusion and shear. As the cutting thickness decreases, the generation of defective atoms also decreases, and the energy stored in the damaged lattice decreases. Helps improve the quality of the processed surface. The larger the tool radius R, the more uncut thickness, which means that more material will be squeezed to form strain-type amorphous atoms, resulting in serious underground subsurface damage.

Acknowledgments
This work was financially supported by National Natural Science Foundation of China (51505241), Fujian Natural Science Foundation (2018J01509) fund, Ningde Normal University New Energy Vehicle Motor drive system design and intelligent manufacturing collaborative innovation center(2017Z01), Ningde Normal University Mechanical Engineering Intelligent Design and manufacturing innovation team(2019T04).

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