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Subsurface Damage in the Monocrystal Silicon Grinding on Atomic Scale*

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Abstract: A molecular dynamics (MD) simulation is carried out to analyze the effect of cutting edge radius, cut-depth, and grinding speed on the depth of subsurface damage layers in monocrystal silicon grinding processes on an atomic scale. The results show that when the cutting edge radius decreases in the nanometric grinding process with the same cut-depth and grinding speed, the depth of the damage layers and the potential energy between the silicon atoms decrease too. Also, when the cut depth increases, both the depth of the damage layers and the potential energy between silicon atoms increase. When the grinding speed is between 20 and 200m/s, the depth of the damage layers does not change much with the increase of the grinding speed under the same cutting edge radius and cut depth conditions. This means that the MD simulation is not sensitive to changes in the grinding speed, and thus increasing the grinding speed properly can shorten the simulation time and enlarge the simulation scale. In conclusion, the subsurface damage of monocrystal silicon is mainly based on the change of the potential energy between silicon atoms, which is verified by the ultra-precision grinding and CMP experiments.

Key words: molecular dynamics; grinding; subsurface damage; monocrystal silicon
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1 Introduction

Monocrystal silicon is an important material for semiconductor devices, high-density information storage devices, and micro-electric-mechanical systems. The fabrication and application of these delicate devices demand that a high surface integrity be achieved by ultra-precision or nanometric machining. Although the machining accuracy of silicon wafer has reached the nanometric level, microscopic physical phenomena that occur in nanometric machining can hardly be explained by the conventional theory based on “continuum mechanics”. Thus, further investigation and understanding of the mechanism of nanometric machining are restricted to a certain extent. Nowadays, a molecular dynamics (MD) simulation method is usually used to study the mechanism of nanometric machining, and it has proven to be a very effective tool for the prediction and analysis of nanometric machining processes on an atomic scale[1,2].

This paper aims at gaining deep insight into subsurface damage in a diamond-silicon grinding system. Emphasis will be placed on the depth of the damage layers in monocrystal silicon material. As the research interest is on the atomic and nanometric scales, the MD method will be used as a theoretical tool to simulate the grinding process of a single grain with different cutting edge radii, cut depths, and grinding speeds. Grinding and CMP experiments are carried out to examine the subsurface damage of monocrystal silicon wafer and verify the MD simulation results.

2 Method

2.1 Modeling

Models of a silicon monocrystal and diamond grain are shown in Fig. 1. Here it is assumed that the initial temperature in the grinding process is 293K and the diamond grain is absolutely rigid. As

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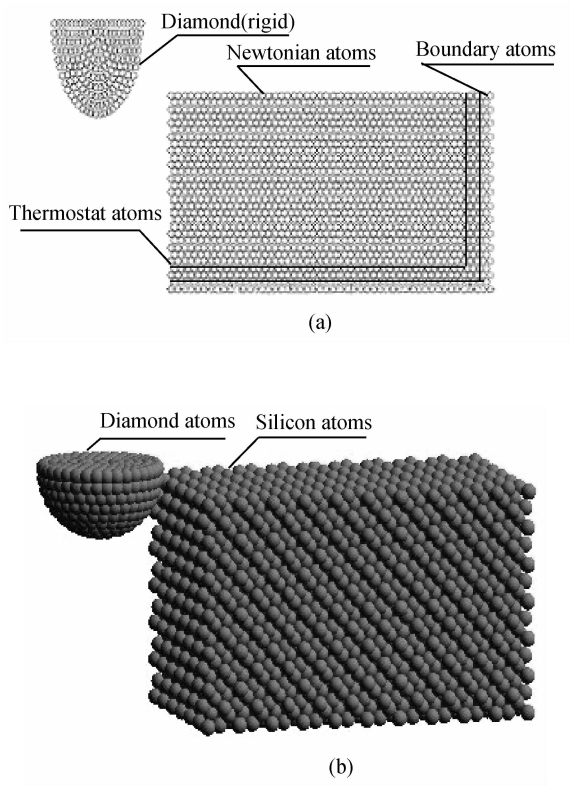

(a)

(b)

Fig.1 Schematic models of the atoms of diamond and silicon in a single grain grinding system (a) Two-dimensional model;(b) Three-dimensional model

shown in the figure, the silicon monocrystal atoms are divided into boundary atoms, Newtonian atoms, and thermostat atoms. The static boundary atoms are fixed to the rigid bases of the specimen, and the atoms in the two layers adjacent to the boundary atoms act as the thermostat atoms. The Newtonian atoms follow Newton's equation of motion, as expressed in Eq. (1). The silicon atoms are covalently bonded, so the Tersoff potential is used to describe the interactions between Si—Si, C—C and Si—C atoms[3].

$$\frac{dv_i(t)}{dt} = \frac{1}{m_i}\sum_{i<j} F_i(r_{ij}), \quad i = 1,2,\cdots,N \quad (1)$$

with

$$\frac{dr_{ij}(t)}{dt} = v_i(t) \quad (2)$$

The force function in Eq. (1), $F_i(r_{ij})$, can be derived from the partial derivative of the potential function, with respect to the atomic distance r_{ij}. As expressed by the sum of forces in Eq. (1), the resulting force on each atom is calculated as a sum of contributions from all neighboring atoms j, based on the distance r_{ij}.

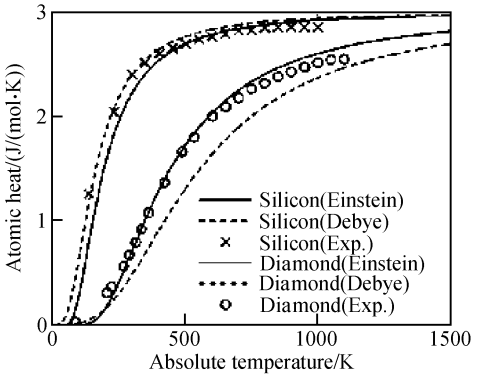

Fig. 2 A comparison of theoretical calculation of atomic heat with experimental measurement

2.2 Temperature conversion[4]

The conversion between the kinetic energy and temperature of the silicon atoms is an important factor in a successful MD simulation. At present, there are three models available for the conversion. They are the Dulong-Petit model, which takes into account the independent lattice vibration, the Einstein model, which is based on the consideration of the single characteristic frequency, and the Debye model, which involves a range of frequencies. A comparison of the theoretical calculation results with the experimental measurement is given by Sinnott as shown in Fig. 2. It is indicated that the Debye model is the best for silicon and the Einstein model is the most suitable for diamond in the temperature area encountered in the present. Thus the Debye model is used in the MD simulation.

2.3 Experiment

Experiments are carried out in two ways, i.e., ultra-precision grinding and CMP, to examine the variations of surface and subsurface microstructures of monocrystal silicon and to understand and verify the theoretical predictions of molecular dynamics analysis. The grinding experiment is performed on an ultra-precision grinding machine, VG401MK Ⅱ. The CMP experiment is conducted on a precision polishing machine. The subsurface structure is investigated by a transmission electron microscope, Tecnai 20 G2 S-Twin.

3 Simulation results and discussion

Some two-dimensional and three-dimensional

MD simulations of the grinding process of a single grain with different cutting edge radii, cut depths, and grinding speeds are carried out to gain insight into the depth of damage the layers in the diamond-silicon grinding system. All these simulation results have good agreement on the instantaneous distribution of atoms, the variance of the grinding force, and the potential energy between the atoms. This means the mechanism of chip removal and the formation and propagation of damage layers are all the same in nanometric grinding processes no matter how different the cutting edge radius, the cut depth, and the grinding speed are. Further details about the mechanism of monocrystal silicon nanometric grinding can be found in Ref.[5].

To explore surface and subsurface damage exactly, the depth of the damage layers on the atomic scale is defined as the maximum thickness of the atomic layers with atomic random arrangement in the direction of the grinding depth. Here the depth of the damage layers is calculated by means of the instantaneous distribution of atoms.

3.1 Effect of cutting edge radius on the depth of damage layers

Figure 3 shows that the depth of the damage layers gets thicker with the increase of the cutting edge radius. This means the smaller the grain size, the better the quality of surface and subsurface in monocrystalline silicon.

From the viewpoint of atomic potential, the potential energy between silicon atoms increases with the increase of the cutting edge radius. With the enhancement of the abrasive grain, the potential energy between silicon atoms increases owing to the actions of the abrasive grain, leading to deformations and phase transformations of the silicon crystal. Thus the value of the potential energy has a decisive effect on the surface and subsurface damage of the silicon crystal.

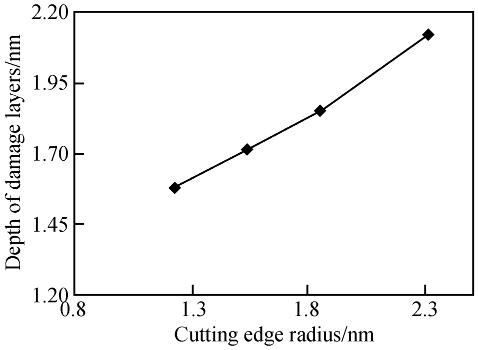

Fig. 3 Relationship between the cutting edge radius and the depth of damage layers

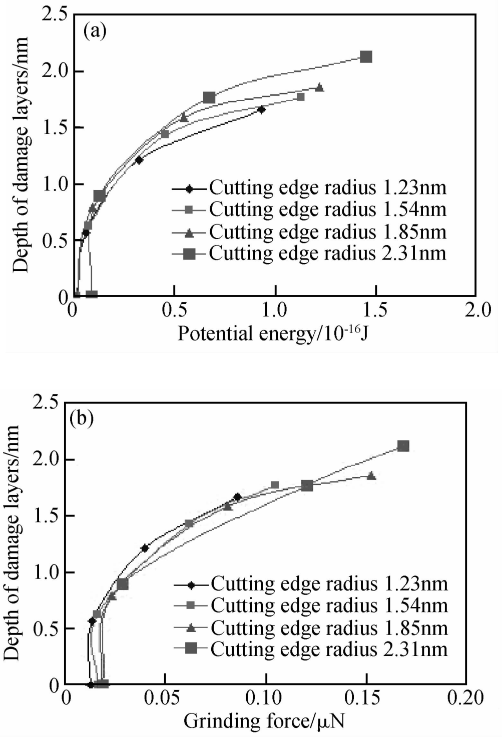

Fig. 4 Effect of the potential energy and the grinding force on the depth of damage layers (a) Potential energy; (b) Grinding force

As shown in Fig. 4, with the increase of the potential energy and the grinding force, the damage layers become thicker.

3.2 Effect of cut-depth on the depth of damage layers

As shown in Fig. 5 and Fig. 6, with the increase of the cut-depth, the depth of the damage

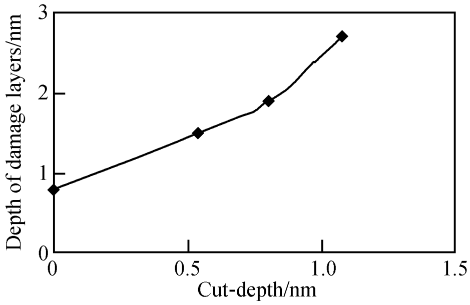

Fig. 5 Relationship between the cut-depth and the depth of damage layers

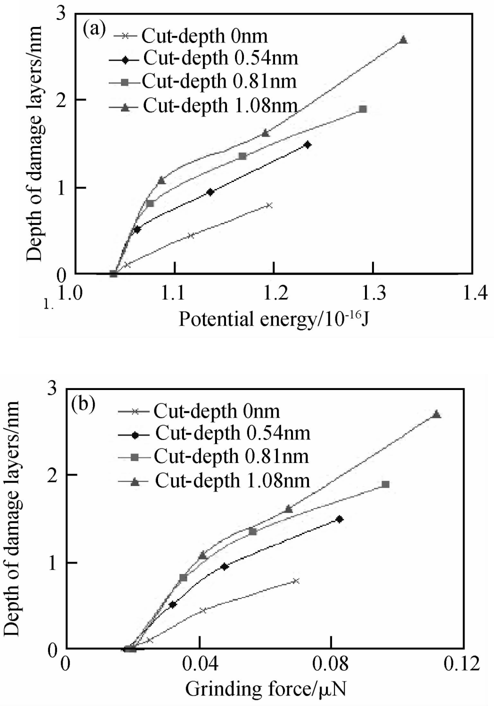

Fig. 6 Effect of the potential energy and the grinding force on the depth of damage layers (a) Potential energy; (b) Grinding force

layers, the potential energy between the atoms, and the grinding force increase. As a result, more severe surface and subsurface damages take place. The reason is that the silicon must release more potential energy by reconstruction and dislocations because of the increase of the potential energy.

3.3 Effect of grinding speed on the depth of damage layers

As shown in Fig. 7 and Fig. 8, with the increase of the grinding speed, there is almost no change in the depth of the damage layers, the potential energy between silicon atoms, and the grinding force. This means that the surface and subsurface damage is slightly affected and MD simulation is insensitive to changes in grinding speed. Thus, increasing the speed properly will save simulation time without reducing the accuracy of the simulation.

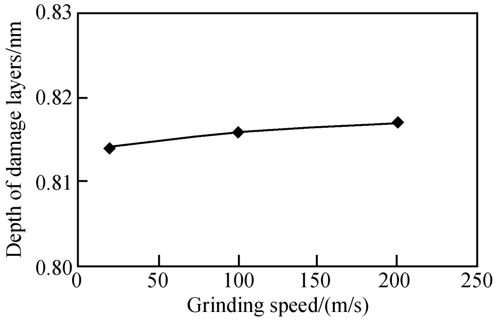

Fig. 7 Relationship between the grinding speed and the depth of damage layers

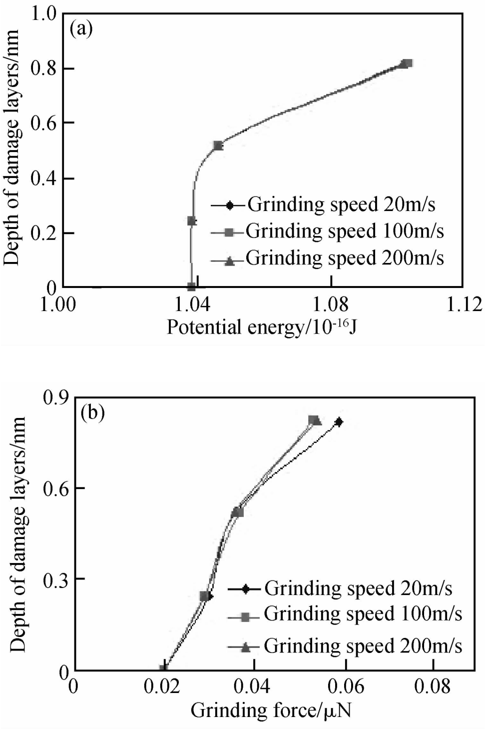

Fig. 8 Effect of the potential energy and the grinding force on the depth of damage layers (a) Potential energy; (b) Grinding force

4 Experimental results and discussion

Both the theoretical and experimental results show that there always exists a thin layer of amorphous silicon in a specimen subsurface subjected to the grinding and CMP, as shown in Fig. 9 and Fig. 10. The thickness of the layer decreases with decreasing cutting edge radius and cut-depth. Two dislocation systems can be developed in the crystal silicon below the amorphous layer with the ♯2000 grinding wheel, as shown in Fig. 9(a). When the ♯3000 grinding wheel is used, only one dislocation system appears (see in Fig. 9(b)). If the abrasive size and the cut-depth are decreased further, dislocations cannot be activated but the amorphous layer still appears, as shown in Fig. 10. This means that the MD simulation results are reliable and can be used to predict the grinding mecha-

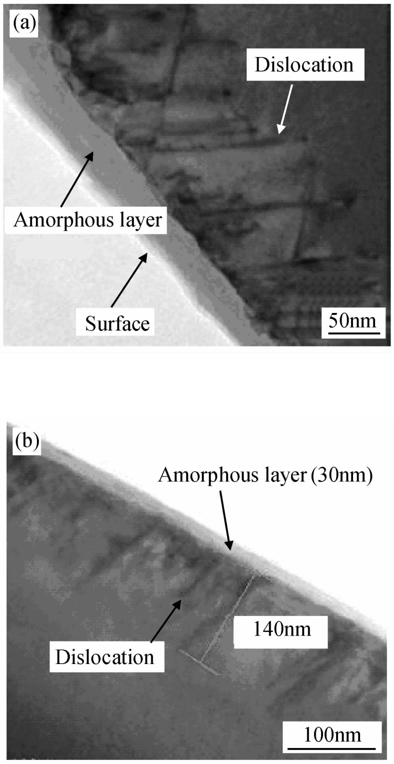

Fig. 9　TEM photo of silicon wafer specimens (grinding)　(a) ＃2000 grinding wheel; (b) ＃3000 grinding wheel

nism. It also verifies that the variance of the potential energy between silicon atoms is the most important factor leading to the subsurface damage of monocrystal silicon in grinding processes.

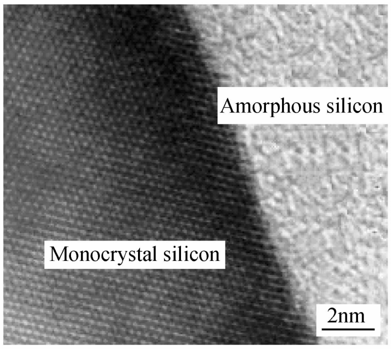

Fig. 10　TEM photo of silicon wafer specimens (CMP) with monocrystal silicon and amorphous silicon

5　Conclusions

In summary, with the aid of the MD approach and experiments, we have acquired the following understandings of the depth of damage layers:

(1) A new concept: the depth of damage layers on atomic scale is examined, which is very important to the study of surface and subsurface damage in nanometric machining.

(2) With the decrease of the cutting edge radius, the depth of the damage layers, the potential energy between silicon atoms, and the grinding force will decrease, and better surface and subsurface quality will be obtained.

(3) When the cut-depth gets deeper, the depth of the damage layers, the potential energy between silicon atoms and the grinding force increase accordingly. This means the quality of the surface and subsurface deteriorates.

(4) The depth of damage layers, the potential energy between silicon atoms, and the grinding force do not change much with increased grinding speed. That is to say, increasing the grinding speed properly does not affect the simulation accuracy. On the contrary, it reduces the simulation time.

(5) The potential energy between silicon atoms varies with grinding force and has a decisive effect on the surface and subsurface damage.

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原子量级条件下单晶硅磨削过程中的亚表面损伤*

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摘要： 应用分子动力学仿真研究了原子量级条件下磨粒钝圆半径、磨削深度和磨削速度对单晶硅磨削后亚表面损伤层深度的影响.分子动力学仿真结果表明：在磨削深度和磨削速度相同情况下，随着磨粒钝圆半径的减小，损伤层深度和硅原子间势能亦减小.随着磨削深度的增大，损伤层深度和硅原子间势能增大.在磨削深度和磨粒钝圆半径相同的情况下，在 20～200m/s 范围内，磨削速度对单晶硅亚表面损伤影响很小，说明分子动力学仿真对磨削速度的变化不敏感，因此可以适当提高仿真速度，从而缩短仿真时间和扩大仿真规模.单晶硅亚表面损伤主要是基于硅原子间势能的变化，并通过超精密磨削实验进行了实验验证.

关键词： 分子动力学仿真；磨削；亚表面损伤；单晶硅

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