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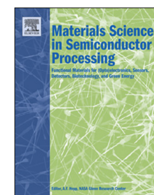

Molecular dynamics study on the thickness of damage layer in multiple grinding of monocrystalline silicon

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ABSTRACT

The molecular dynamic (MD) simulation of monocrystalline silicon under multiple grinding is carried out to study the effect of multiple grinding on the thickness of damage layer. Four grinding processes are conducted on (0 0 1) along ⟨−1 0 0⟩ direction. The depth of grinding of the first grinding is 20 Å. The subsequent grinding is machining on the machined surface with a damage layer left by the first grinding. The second grinding is a spark-out process and the depth of grinding of the third and fourth grinding increases by 5 Å compared with the previous grinding. The changes of structures and mechanical properties of the damage layer in the machined surface after the first grinding are investigated by co-ordination number (CN), the radial distribution functions (RDF) and nanoindentation. The thickness of the damage layer left by the first grinding can be reduced stably in the second and third grinding, but it will increase in the fourth grinding. Therefore, two more grinding steps between the third and fourth grinding are carried out. One is the spark-out process and the depth of grinding of the other increases by 2 Å compared with the third grinding. The results show the spark-out process can remove the springback left by the previous grinding and promote the residual compressive stress in the machined surface, which can improve the accuracy and quality of grinding. The thickness of damage layer induced by the first grinding can be reduced without new damage structures generating. However, it cannot be reduced unlimited. When the thickness of damage layer reaches half of the original thickness, a re-grinding will cause new damage structures, and the thickness of damage layer will increase. The depth of grinding is suggested to be less than half of the original damage thickness to reduce the damage layer. The research results can be applied in the ultra-precision grinding of monocrystalline silicon to control the thickness of damage layer and improve the quality of machining.

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1. Introduction

As a kind of excellent semiconductor material, monocrystalline silicon is widely used in the manufacturing of large scale integrated circuits(IC) and microelectromechanical systems (MEMS). The quality of silicon surface after processing has a great influence on the service life and performance of the devices. However, it is inevitable to cause surface and subsurface damage in the process of machining silicon [1]. In order to control the thickness of damage layer, lots of work by experiment or simulation has been done to clarify deformation mechanism and the formation mechanism of damage in processing silicon. Yan et al. [2,3] used cross-sectional transmission electron microscopy and laser micro-Raman spectroscopy to examine the subsurface structure of silicon machined by diamond tool. The results showed the machining-induced amorphous layer was related with the tool angle and depth of cut and cutting direction, and a subsurface damage model was also proposed. Zhang et al. [4,5] investigated the nanocracking in the subsurface and deformation behaviors of monocrystalline silicon after nanoscratching. Yury Gogotsi et al. [6] analyzed the pressure-induced metallization in scratching of silicon through raman microspectroscopy.

However, with the improvement of the machining accuracy, the machining process may only involve a few nanometers or even less, which makes it difficult to observe the structure change during the processing experimentally [7,8]. Therefore, some theoretical methods have been applied to study the ultra-precision machining process, in which molecular dynamics (MD) simulation has become an important and widely accepted tool. The structural phase transformations in monocrystalline silicon due to nanoindentation were studied by MD simulation commonly [9–11]. Zhang et al. [12] explores the effect of crystal plane orientation on the nanofabrication of bct-5 silicon by means of nanoscratching

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using a diamond tip with the aid of MD analysis. Li et al. [13] revealed the subsurface damage mechanism of high speed grinding process in single crystal silicon by atomistic simulations. The researches already accomplished have great significance for the study of the damage layer of monocrystalline silicon, and it is also proved that MD simulation is a reliable and effective method. However, in the real machining, the silicon wafer may go through more than once machining, such as coarse grinding, fine grinding and spark-out process. It means that the machining may be conducted on the machined surface left by the previous machining. The structure of the machined surface monocrystalline silicon has certainly changed. The change will influence its mechanical property, which will have a great impact on the subsequent machining. Moreover, with the machining proceeding, the depth of material removal in the later machining will decrease in general, so the effect of the change of machined surface will be more significant and cannot be neglected.

For the problem mentioned above, in this paper the multiple grinding MD simulation of monocrystalline silicon is established and the variation of the thickness of damage layer in the multiple grinding is investigated. First of all, the monocrystalline silicon was grinded to obtain the machined surface with a damage layer, and then the subsequent grinding processes were conducted on the damage layer. It aims to study the change regulation of the thickness of the damage layer in multiple grinding and search measures to control the damage layer to improve the process quality of monocrystalline silicon.

2. Modeling and computation

The grinding simulation model is consisted of a workpiece of monocrystalline silicon and diamond grains, as shown in Fig. 1(a). The system contains about 240,000 atoms totally, and the dimensions of the workpiece are 300 Å×150 Å ×100 Å. The detail parameters of the simulation are shown in Table 1. The workpiece is divided into three different zones which are newtonian atoms, thermostat atoms and boundary atoms. The boundary atoms are fixed and the thermostat atoms are used to ensure the outward heat conduction away from the model. The motion of the Newtonian atoms is determined by the forces produced by the

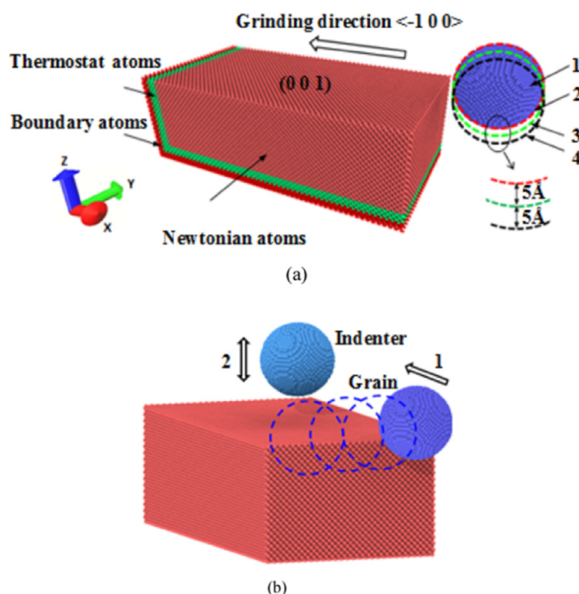

Fig. 1. The MD simulation model (a) The multiple grinding model; (b) The indentation model.

Table 1
Simulation parameters of the grinding process.

Model	Processed model
The size of model (Å)	300×150×100
Number of atoms	237,653
Grinding speed (m/s)	150
Initial temperature (K)	300
Grinding direction	⟨−1 0 0⟩
Grinding surface	(0 0 1)

Newton's equation of motion [14]. The radius of the diamond grain is 30 Å, and it is treated as rigid in the simulation. In order to study the effect of multiple grinding on the damage layer, the simulation is composed of four grinding processes. The depth of grinding of first time is 20 Å, and the damage layer will generate in the machined surface. Consequently, the next grinding processes are conducted on the damage layer. The depth of the second grinding is as same as the first time, namely a spark-out process, while that of third and fourth time increase by 5 Å compared with the previous grinding, as shown in Fig. 1(a).

In order to investigate the mechanical properties of the machined surface after grinding, the nanoindentation simulation is also carried out. The MD simulation model is shown in Fig. 1(b). Firstly, the grinding simulation is conducted on the ideal surface of monocrystalline silicon, and the depth of grinding is 20 Å. Consequently, the nanoindentation simulation is conducted on the machined surface with an indenter radius of 35 Å.

In this paper, all MD simulations are completed using large-scale atomic/molecular massively parallel simulator (LAMMPS) software. The potential functions used in the simulation are crucial to the accuracy of results. The Tersoff potential function [15] considering the effects of bond angle and covalent bonds is feasible in dealing with IV elements and those with a diamond lattice, such as Si and Ge [8], so it is used to describe the interaction between the Si atoms in this paper. On the other hand, the modified two-body Morse potential is adopted to describe the interaction between the Si and C atom, which has been applied in many simulations and shows good agreement with the experimental data [12,14,16]. The Morse potential can be expressed as

$$\phi(r_{ij}) = D\{\exp[-2\alpha(r_{ij} - r_0)] - 2\exp[-\alpha(r_{ij} - r_0)]\} \tag{1}$$

Where $\phi(r_{ij})$ is a pair-potential function, D is the cohesion energy, α is elastic modulus, and r_0 is the atomic distance at equilibrium. The value of the parameters is shown in Table 2.

3. Results and analysis

The depth of grinding of the first grinding is 20 Å, and, after the first grinding, the thickness of the damage layer generated in the machined surface is 18 Å including a springback layer size of 4 Å, as shown in Fig. 2. The thickness of the damage layer is calculated based on variations of the potential energy of atoms in the workpiece with different deformation behaviors [17]. When deformation takes place, the potential energy value of atoms will

Table 2
Parameters in Morse potential.

Parameter	C-Si
D (eV)	0.435
α (nm^{-1})	46.487
r_0	0.1947

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