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Study on machinability of silicon irradiated by swift ions[☆]

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ABSTRACT

Diamond cutting of hard and brittle materials is difficult owing to poor surface quality and severe tool wear. It has been clear that ion implantation can be used to improve the machinability. In previous studies, surface modification is realized by the nuclear collision cascade that induces phase transition during the implantation. Except for the nuclear collision process, electronic interaction between the incident particles and the target material, such as ionization, also occurs particularly during a high-energy ion implantation. However, the influence of ionization on the machinability has not been studied. In this paper, modification on the nanocutting of silicon by MeV oxygen ions is studied. Molecular dynamics simulation is conducted to reveal the nanocutting process on silicon with irradiation damages. Experiments show an enhancement in the critical undeformed chip thickness that is crucial in machining of brittle materials.

1. Introduction

Ductile-regime machining of hard and brittle materials has been investigated at least for two decades. The most commonly used method is abrasive grinding followed by fine polishing. Besides, diamond turning technique has also been developed for ultra-precision machining, especially for the freeform optics [1]. However, high efficiency and low surface damage are still difficult to be achieved simultaneously. The main reason is that material must be removed at submicron or even nanometric scale to avoid brittle failure. In the ultra-precision machining of brittle materials, the critical undeformed chip thickness (t_c) is used to evaluate the small scale material removal, above which machining would transform from ductile to brittle mode. For example, the t_c of silicon and germanium were reported as 57 and 37 nm respectively [2]. Strictly speaking, t_c varies with process condition (e.g. tool geometry and cutting speed) and crystal orientation of the workpiece, rather than being a material constant. This is the reason for different pitting damage patterns in the crystal turning [3]. If t_c can be raised, the machinability of brittle materials will be improved significantly.

One novel approach named as “nanometric machining of ion implanted materials” (NiIM) has been proposed in improving the machinability of brittle materials [4]. In this method, ion irradiation is conducted prior to the machining process. During ion implantation, the surface layer lattice would transform from crystalline to amorphous phase (c-a transition). For the covalent solid, the amorphous structure usually has lower mechanical strength and higher fracture toughness and are isotropic in mechanical properties. Indeed, the c-a transition has already shown its validity of improving the ultra-precision machining of brittle materials. For example, the t_c of silicon was enhanced to ∼923 nm after fluorine ion irradiation [4]. Hardness, Young's modulus and tool wear were reduced obviously for the modified silicon. A decrease in the high-frequency vibration of cutting force was also reported in the micro-machining of hydrogen irradiated silicon [5]. Similarly, the t_c of germanium was enhanced to ∼730 nm by copper ion implantation [6]. Researches focusing on the effects of non-amorphizing modification and post annealing were conducted as well [7,8].

The mechanism of material modification by NiIM has been considered as the nuclear collision induced c-a transition for a long time. However, electronic interactions, such as ionization, also occur during ion implantation. After high-energy (at MeV) swift ions just enter the target, energy transfer takes place primarily through the electronic process. At this stage, few nuclear collision events occur. As ions move deeply into the solid and lose energy, they would displace the target atoms and trigger the collision cascade which induces the amorphization. In fact, the electronic interaction would also modify the lattice structure. High-energy ion implantation could induce electron excitation or ionization. The temporary positively charged lattice frame would undergo the phase transition owing to strong Coulomb repulsive force [9]. This phenomenon is also critical in the phase-change materials [10]. High-energy irradiation has been used to fabricate the optical waveguide [11]. However, it is not clear so far whether ionization could improve the machinability of brittle material.

In this paper, modification of MeV ion irradiation on the

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nanocutting of silicon is studied. After high-energy implantation, the change of material lattice is analyzed. Then, nanometric taper cutting test [12] is conducted to evaluate the t_c of modified silicon (m-Si). For a further understanding, molecular dynamics (MD) and Monte Carlo (MC) methods are also used to reveal the mechanism of nanocutting on the material with ionization induced damages.

2. Experiments and numerical simulation setup

High energy irradiation is conducted using a tandem electrostatic accelerator. Oxygen ions with 6 MeV energy and 1×10^{15} cm^{-2} dose are implanted into the (100) surface of high resistivity monocrystalline silicon (c-Si) at room temperature. There is a 7° angle between the ion beam and the sample surface to avoid the channel effect. Current of O ions is maintained at 300 nA during the implantation. To investigate the modification on the material lattice, the Raman spectrums are obtained from a Horiba iHR-550 system equipped with a 531.8 nm laser and a 1800 grooves/mm grating. The microstructure of m-Si is further observed by transmission electron microscope (TEM) and the cross-sectional sample with thickness about 70 nm is prepared using a focused ion beam and scanning electron microscope (FIB/SEM) dual beam system. As mentioned above, t_c is a critical parameter for brittle materials and is evaluated by the taper cutting test, which is realized by a commercial diamond tool and an ultra-precision lathe (Moore Nanotech-250). The tool's nose radius is 0.428 mm and the cutting velocity is 10 mm/min. All the cuttings are conducted along the same direction. Then, surface topography and t_c is measured by a white light interferometer.

MD and MC simulations are conducted to deeply study the material processes at nanoscale. MC algorithm realized by the Stopping and Range of Ions in Matter (SRIM) software [13] is used to calculate the ionization intensity and lattice damage distributions. MD simulations are used to reveal the material deformation mechanisms for c-Si and m-Si during nanocutting and the model is shown in Fig. 1. The workpiece model comprising distributed lattice damage pockets, which mimic the local phase transition induced by ionization during the high-energy irradiation [9], is constructed and relaxed to equilibrium at 293 K. Cutting speed and distance are 10 m/s and 60 nm respectively. The interatomic forces between Si-Si and C-Si atoms are described by the Tersoff type potential [14] and simulations are conducted under the microcanonical ensemble (NVE) ensemble with a 2 fs time step. MD computing is executed by the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package [15]. The Open Visualization Tool (OVITO) [16] software is also used for the visualization of MD data.

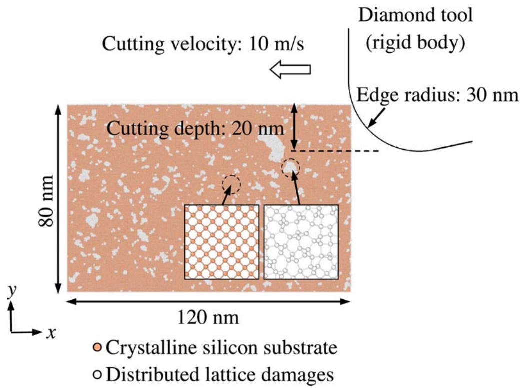

Fig. 1. Nanocutting model. The *z* dimension is orthogonal to the *x-y* plane with a scale of 0.543 nm and periodic boundary condition.

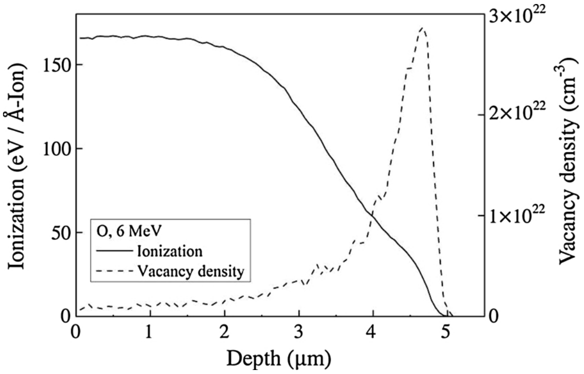

Fig. 2. Depth profiles of ionization and vacancy density calculated by MC.

3. Results and discussions

3.1. Experimental results

Fig. 2 shows the depth profiles of ionization and vacancies for the O ion implantation. It is clear that the regions with intensive electronic process (ionization) and nuclear collision (vacancy density) are well separated. In the 2 μm range, the ionization keeps at ~160 eV/Å-ion but the vacancy density is merely less than 1.3×10^{21} cm^{-3} which can be neglected. It is noted that the atom density of silicon is 5×10^{22} cm^{-3}. Therefore, electronic excitation is the dominant process which modifies the solid lattice structure of shallow surface layer.

After ion irradiation, intensity of the characteristic Raman peak of Si with diamond structure at 521 cm^{-1} decreases, which indicates the reduction in the lattice order (Fig. 3). However, the amorphous peak at 470 cm^{-1} [17] does not occur. It means the lattice has not been disordered completely. TEM image (Fig. 4(a)) indicates the occurrence of numerous nano-amorphous pockets (white dots) induced by high-energy ionization. There are also some recrystallization regions, which are formed by the dynamic self-annealing process [18] owing to the local high temperature. The bright spots and misty rings in the electron diffraction pattern (Fig. 4(b)) also imply the mixture of crystalline and amorphous structures. Fig. 5 shows the 3-D measurement of the taper cutting groove. As the cutting depth increasing, surface fracture would take place and the t_c could be evaluated. Under the cutting conditions in this work, the average value of t_c is enhanced from 52.9 nm to 87.8 nm. Consequently, the ionization induced lattice damage during high-energy irradiation can improve the machinability of brittle materials.

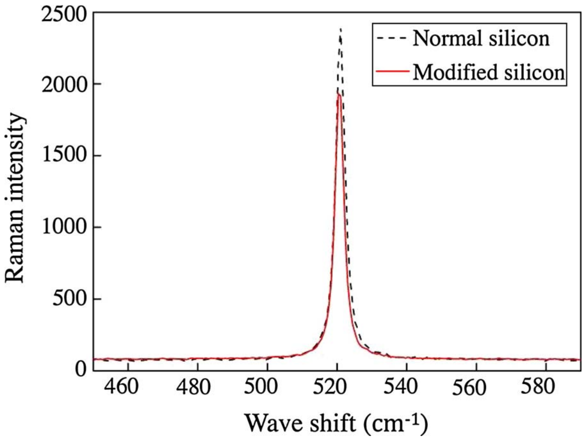

Fig. 3. Raman spectrums of c-Si and m-Si. Five points are measured on each sample and the results are averaged. The exposure time is 10 s.