Atomic subsurface integrity improvement for curved and micro-structured silicon surface by laser irradiation

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Abstract

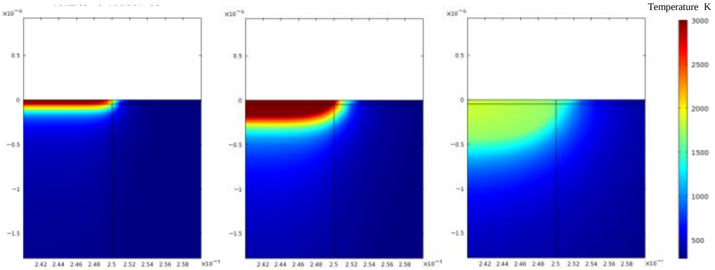
Pulsed laser irradiation was used to recover subsurface damage and to improve subsurface integrity of curved and micro-structured silicon surfaces. A multi-axis laser processing system was developed for laser irradiation tests. The subsurface microstructural changes due to laser irradiation were characterized by cross-sectional transmission electron microscope (XTEM). The damage recovery process was modelled using finite element (FE) and tight-binding quantum chemical molecular dynamics (TB-QCMD). The results demonstrated the possibility of generating atomic level single-crystalline structures on damaged silicon surfaces by a single laser pulse.

1 Introduction

The manufacturing of defect-free silicon substrate is indispensable for production of precision dark-field optics, optoelectronic elements, and micro electromechanical systems. Conventionally, silicon substrates are machined by slicing, cutting, grinding and lapping, and then the machining-induced subsurface damage is removed by chemical etching and/or chemo-mechanical polishing. The chemical processes face problems such as poor controllability in processing depth, deterioration of form accuracy, and environmental pollution due to waste fluid disposal, etc.. In this study, laser irradiation method will be used to recover, rather than remove, the subsurface damage. This technique offers a number of advantages: (i) It involves no material removal thus preserves the dimensions of the workpiece; (ii) It generates no pollutants; (iii) It enables selective processing and processing of complex shapes like aspherical and diffractive optical elements and micro-structured surfaces.

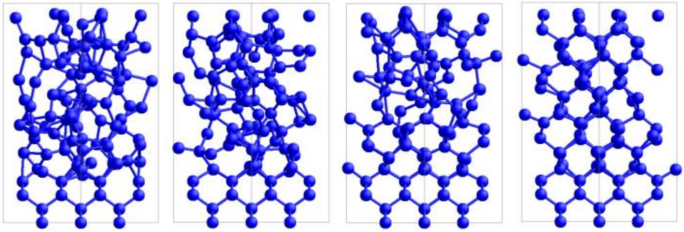
2 FE and TB-QCMD modelling of processing mechanism

Typically, subsurface damage of silicon in ultraprecision machining includes an amorphous near-surface layer and dislocations beneath the amorphous layer [1, 2]. Therefore, in this study we need to recover both the amorphous region and the dislocations. First, FE simulation was performed to illustrate the temperature change at the a-Si/c-Si interface due to laser irradiation. As shown in Fig. 1, there is sufficient absorption of laser in the near-surface layer because amorphous silicon has a remarkably higher absorption coefficient of laser light than crystalline silicon. Due to the significant temperature rise, a thin liquid silicon film will be formed which is metallic and has a much higher absorption rate. The top-down melted liquid phase finally extends below the deeper dislocated region.



1 ns 3 ns 10 ns

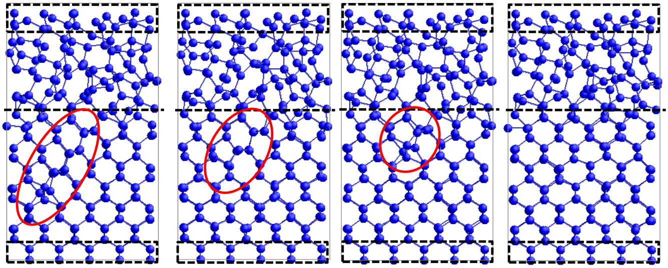
Fig.1 FE simulation of temperature change during a single laser pulse.



initial 8 ps 16 ps 24ps

Fig.2 TB-QCMD simulation of epitaxial crystal growth from undamaged bulk.

Next, TB-QCMD simulation was conducted to clarify the microstructural change of silicon caused by laser irradiation. As shown in Fig.2, after the laser pulse, environmental cooling of the melted amorphous silicon will result in a bottom-up epitaxial regrowth from the defect-free crystalline region which serves as a seed for crystal growth. Fig.3 shows the behaviour of dislocations during laser irradiation. It was found that short dislocations moves towards the liquid/solid interface and rapidly disappears by the end of the laser pulse, whereas for long dislocations there is not sufficient time to completely disappear by the end of the laser pulse. In this case, it is necessary to use a higher laser energy density to melt not only the amorphous layer but also the dislocation layer. In this way, a perfect single-crystalline structure with atomic surface integrity can be achieved.



initial 4 ps 12 ps 16 ps

Fig.3 TB-QCMD simulation of dislocation movement due to thermal effect.

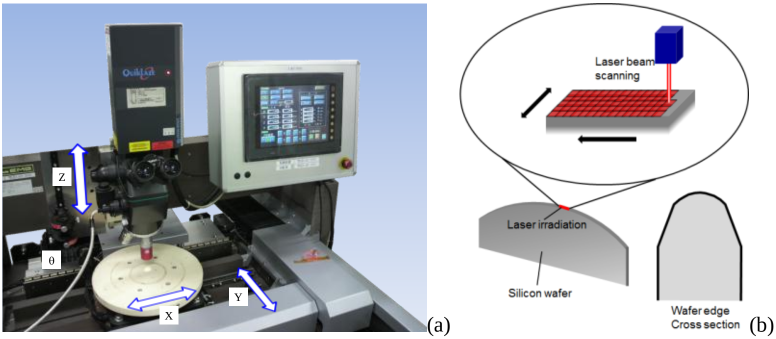
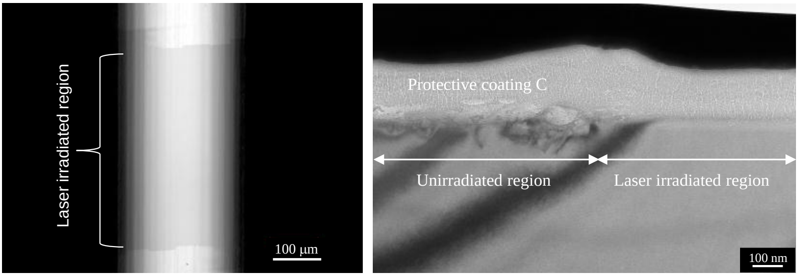


Fig.4 (a) Photograph of experimental system and (b) schematic of workpiece.

3 Experimental results and discussion

Laser irradiation experiments were carried out on silicon aspherical lenses, wafer edges, and micro grooves. In this paper, the results of silicon wafer edge, which is a complicated curved surface, are presented. The workpiece was prepared by diamond grinding. The silicon wafer was vacuum-chucked on a rotary table which can rotate along the θ axis, and irradiated by a laser-diode exited Nd:YAG laser system which has a wavelength of 532 nm and a laser pulse width of 3-4 ns. The laser oscillator was mounted onto a specially developed four-axis (XYZθ) numerical control precision stage made of ceramics (see Fig.4). The XY tables of the stage were driven by linear motors on air slides, enabling a maximum speed of 0.5 m/s. The movement of the tables was feedback-controlled by linear scales with a resolution of 0.1 μm.



(a) (b)

Fig.5 (a) Nomarski micrograph and (b) XTEM micrograph of silicon wafer edge.

Fig. 5 shows a Nomarski micrograph and an XTEM micrograph of the silicon wafer edge. In Fig. 5(a), it is seen that the laser irradiated region becomes darker than the unirradiated region, indicating that the surface roughness becomes smaller after laser irradiation. In Fig.5(b), we can see that before laser irradiation, there is an amorphous layer beneath the ground surface, and below the amorphous layer there is a layer of dislocations. After laser irradiation, however, the amorphous layer and the dislocations have completely disappeared, indicating that the recrystallization of silicon was performed successfully. A perfect single crystalline structure identical to that of the bulk material has been achieved. From the XTEM micrographs, we can also see that after laser irradiation, the surface roughness has been remarkably improved. That is, the grinding-induced tool marks on the wafer surface have been significantly flattened. The surface flattening phenomenon might be a result of surface tension effect of the melted silicon during the laser pulse. The experimental results are consistent with the simulation results and strongly demonstrate that atomic level subsurface integrity has been achieved in single-crystalline silicon after laser irradiation.

References:

[1] K. E. Puttick, L. C. Whitmore, C. L. Chao and A. E. Gee: Philos. Mag. A, 69, 1 (1994) 91-103.

[2] J. Yan, T. Asami, H. Harada, T. Kuriyagawa: Prec. Eng., 33, 4 (2009) 378-386.