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Response of machining-damaged single-crystalline silicon wafers to nanosecond pulsed laser irradiation

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Abstract

Ultraprecision diamond-machined silicon wafers have been irradiated by a nanosecond pulsed Nd:YAG laser. The results indicate that at specific laser energy intensity levels, the machining-induced subsurface damage layer of silicon has been reconstructed to a perfect single-crystalline structure identical to the bulk. Laser irradiation causes two effects on silicon: one is the epitaxial regrowth of the near-surface amorphous layer, and the other is the complete removal of the dislocations from the crystalline layer. It is the dislocation-free crystalline region that serves as the seed layer to recrystallize the amorphous layer, enabling excellent crystalline perfection. These findings may offer practical alternatives to current chemo-mechanical processing methods for silicon wafers.

1. Introduction

The manufacturing of high-quality silicon wafers is indispensable for production of micro-mechanical, optical, optoelectronic and electronic parts from silicon. Usually, silicon substrates are manufactured by mechanical machining processes such as slicing, cutting, grinding and lapping followed by polishing. It has been technologically possible for these processes to produce super smooth surfaces with nanometric surface roughness. However, these material removal processes involving mechanical contacts between tools and workpieces will inevitably cause subsurface damages to the lattice structure of silicon.

Previous works have revealed that subsurface damages of silicon due to machining include microstructure changes (or alternatively termed phase transformations) and dislocations [1–6]. For precision cutting and grinding processes, a submicron-thick amorphous layer will be formed just beneath the silicon surface, below which is a crystalline region with dislocation loops. Phase transformation has also been confirmed in other silicon machining processes such as slicing and dicing [7]. While the issue of the origin of structural changes during silicon machining is a complicated one and is still under investigation, a possible reason may be the high pressures (∼10 GPa level) resulting from the tool–workpiece contact [8, 9].

Removing the subsurface damages from silicon substrates is essential for producing high-reliability silicon parts [10]. This issue has become a subject of concentrated research interests from multidisciplinary research communities and industries. Currently, after the machining processes, etching and chemo-mechanical polishing (CMP) processes are carried out to remove the subsurface damaged layers. However, due to the poor controllability of processing depth, the deterioration of substrate form accuracy becomes a big problem. Other issues, such as increase in production cost, and environmental pollution due to the chemical waste fluids, are also serious problems.

In this work, we attempted to investigate the feasibility of reconstructing the lattice structure of the damaged layer by laser irradiation. Laser irradiation, from a few decades ago, has been used as a surface processing method for silicon. One of the widespread laser processing techniques is laser annealing [11–23]. After selected dopant impurities have been implanted into silicon wafers as energetic ions, the disordered silicon surfaces can be restored to crystalline perfection by laser. It has been demonstrated that laser can crystallize sputtered, ion-implanted, vapour-deposited or hydrogenated amorphous silicon thin films on substrates of glass, sapphire and silicon

[11–23]. These crystalline silicon thin films have important applications in solar cells, transistors, flat panel display drivers, and so on. On most occasions, the laser-crystallized silicon thin films have poly-crystalline structures where the grain size depends on the irradiation conditions; whereas no literature can be found on the formation of single-crystalline structures.

The purpose of the present work is to generate perfect single-crystalline structure on a machining-damaged substrate using laser shots. Two effects are expected to occur in the laser irradiation process: one is the recrystallization of the near-surface amorphous layer, and the other is the elimination of the dislocations in the dislocated crystalline region beneath the amorphous layer. The best result is that these two aspects are accomplished simultaneously during one single pulse laser irradiation.

2. Experimental results

To make a test sample, an electric device grade n-type single-crystal silicon (1 0 0) wafer was machined by the slanted plunge-cut method on an ultraprecision lathe, Toyoda AHN-05, produced by JTEKT Corporation (Nagoya, Japan). The machine has a stepping resolution of 1 nm under four-axis numerical control. The cutting tool is a single-crystal diamond tool having a nose radius of 10 mm. To generate a thick subsurface damage layer to the silicon wafer, tool rake angle was set to -60°, higher than usually used negative rake angles. Depth of cut was changed continuously from 0 to 500 nm and cutting speed was fixed to 500 mm min^{-1}. Machining was done along the [1 1 0] direction of the wafer.

The machined sample was then irradiated by the QuikLaze-50 Nd:YAG laser machining system produced by New Wave Research, Inc. (Fremont, USA). This system employs a flash lamp-pumped Nd:YAG rod in a thermally compensated three bar invar resonator to generate radiation at 1064 nm. The 1064 nm laser pulse passes through an angle tuned KTP crystal and generates the second harmonic at 532 nm. The XY aperture shapes the beam to the rectangular size. The maximum opening of the XY aperture is 3×3 mm^2 which becomes a maximum cut size of 50×50 μm^2 with a $50\times$ objective lens on an FS60/70 microscope made by Mitutoyo Corporation (Kawasaki, Japan). In the present experiment, the XY apertures were both set to 40%, enabling a 20×20 μm^2 square irradiation area. The single pulse mode was used and the pulse width was 3–4 ns. The laser spot was pointed to the ductile-regime machined region where the depth of cut was around 100 nm and the surface roughness was 2 nmRy. The laser beam was horizontally shifted 100 μm between spots in order to obtain individual irradiations under various conditions. The incident energy level of one laser pulse was changed from 0.5 to 30 μJ, leading to a change in energy intensity from 0.125 to 7.5 J cm^{-2}.

After laser irradiation, the sample was observed with a Nomarski microscope at first to examine the surface appearance. When the energy intensity was lower than 0.2 J cm^{-2}, no change could be detected. However, when the energy intensity was higher than 0.5 J cm^{-2}, a slight change in contrast between the irradiated regions and the surrounding area could be seen. When the energy intensity was further increased to 2.5 J cm^{-2} or higher, square pits were formed on the surface; around the pits is some tiny debris.

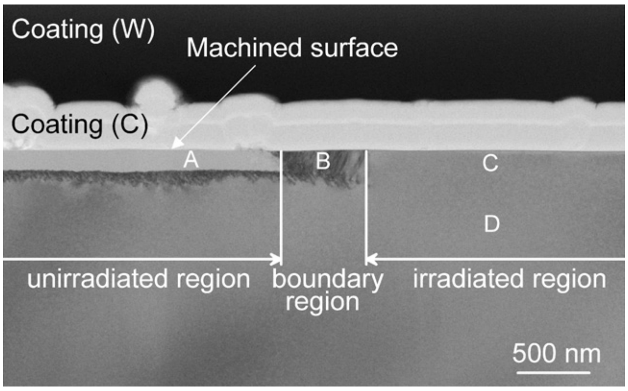

Figure 1. Bright field cross-sectional TEM micrograph of the diamond-machined silicon sample partially irradiated by nano-pulsed laser. Region A is the unirradiated region showing subsurface damage layers generated by machining. Region B is the boundary region with intensive dislocations. Region C is the laser-irradiated region, where the subsurface damages have disappeared. Region D is the original bulk single-crystalline region.

Next, a laser micro-Raman spectroscope NRS-3100, produced by JASCO Corporation (Tokyo, Japan), was used to characterize the sample. The wavelength of the laser in the micro-Raman tests was 532 nm and the focused laser spot size was 1 μm. It was found that for the unirradiated regions, broadband peaks at 470 cm^{-1} were significant in the Raman spectra, whereas no peaks could be observed at 521 cm^{-1}. This fact indicates that the near-surface layer of silicon has been completely transformed into the amorphous state during machining [5]. However, after laser irradiation at 0.5–2.5 J cm^{-2}, well-defined crystalline silicon peaks at 521 cm^{-1} were observed in the Raman spectra, whereas the response at other Raman shifts was negligibly low.

In order to confirm the changes in microstructures caused by laser irradiation, cross-sectional observations of the sample were performed with a transmission electron microscope (TEM). The sample was processed by focused ion beam (FIB) technique to prepare the TEM samples. The TEM we used was H-9000NAR, produced by Hitachi Ltd. (Tokyo, Japan). The conditions used for TEM observations were acceleration voltage 300 kV, direct magnification from 50 000 to 200 000 times. To protect from possible damages from the FIB, carbon (C) and tungsten (W) coatings were made on the samples.

Figure 1 shows a bright field cross-sectional TEM micrograph of the sample. The left side of the sample is the ductile-machined area without laser irradiation; the right side is the area irradiated at an energy intensity of 2.35 J cm^{-2}. It is clear that on the left side, beneath the machined surface, there is a 150 nm thick grey layer, below which is a dislocated layer about 50–100 nm deep. This kind of subsurface structure is very similar to those of diamond-turned silicon wafers in other previous works [2, 4, 6], and the grey layer is supposed to be the machining-induced amorphous layer. However, after laser irradiation, as shown on the right side of the figure, both the grey layer and the dislocated layer have disappeared. The machining-damaged layer has been transformed to a structure identical to the bulk material.

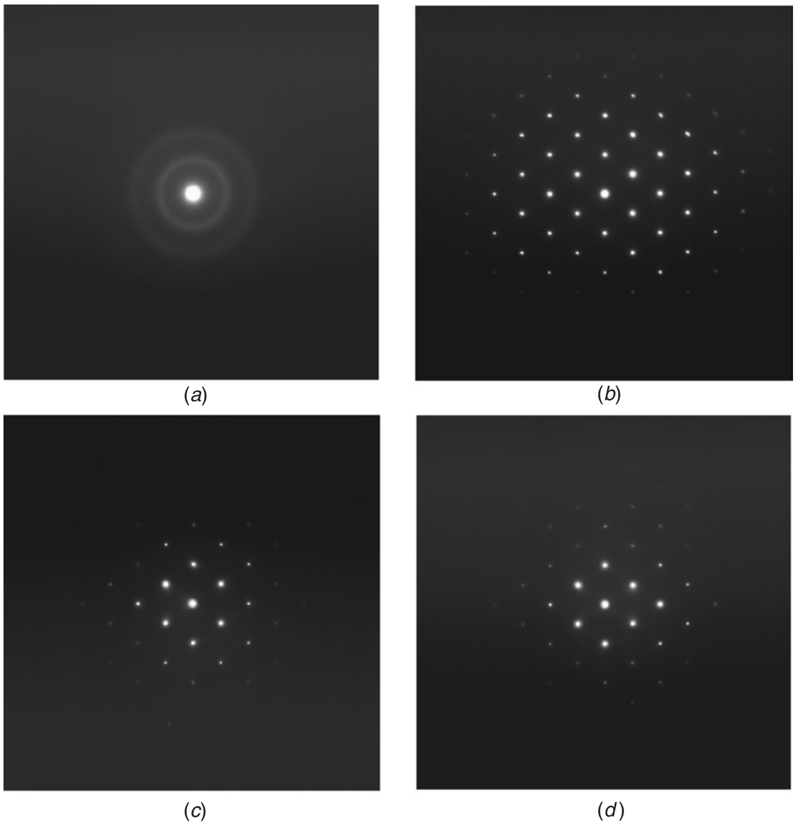

Figure 2. Selected area diffraction patterns of the individual regions marked in figure 1. In (*a*) the unirradiated region, only halo rings can be seen, indicating that the near-surface grey layer is amorphous. In (*b*) the boundary region, (*c*) the irradiated region and (*d*) the original bulk region, clear diffraction spots are shown, which demonstrates single-crystalline structures.

To further characterize the lattice structures, selected area diffraction (SAD) analysis was done with the same TEM. The diffraction area was 100 nm in diameter at a camera length of 1 m. Figures 2(*a*)–(*d*) show the SAD patterns of regions A, B, C and D, respectively, as marked in figure 1. In figure 2(*a*), only halo rings are shown, verifying that the grey layer just beneath the machined surface is amorphous. In figure 2(*b*), clear diffraction spots of [1 1 0] incidence can be seen, indicating that the boundary between the unirradiated and the irradiated region is crystalline; although dislocations can be seen in this region from figure 1. The result in figure 2(*c*) also shows clear diffraction spots of [1 1 0] incidence, which is completely the same as that of the original bulk region as shown in figure 2(*d*). Similar results were confirmed for other TEM samples under the same conditions. From these results, we can conclude that by laser irradiation the machining-damaged layer has been completely reconstructed to the original single-crystal structure.

3. Discussion and conclusions

The mechanism of the lattice structure reconstruction during laser irradiation is still unknown and under further investigation. Previous studies on laser annealing have found that the crystallization of amorphous silicon thin films results from the sudden melting of silicon due to the high energy of laser irradiation and subsequent epitaxial regrowth during cooling [11–15]. Although there are differences in wafer subsurface structures and laser irradiation conditions between laser annealing and the present work, similar mechanisms might occur in the present work. The microstructure change of the silicon wafer during laser irradiation is schematically shown in figure 3(*a*)–(*f*). Since amorphous silicon (a-Si) has a higher absorption coefficient of laser than the crystalline silicon (c-Si), there will be enough absorption of the laser light in the amorphous layer to form a thin liquid silicon film. The liquid silicon layer is metallic and has much higher absorption, thus a deeper liquid layer will be formed that extends into the dislocated crystalline region. Under high temperature conditions, the mobility of dislocations can be significantly elevated and the dislocations will be transported towards the solid–liquid interface, leaving a completely defect-free crystalline substrate. Then after the laser pulse, cooling will result in epitaxial regrowth from the defect-free crystalline layer. This layer serves as a seed layer to crystallize the liquid layer; thus can yield excellent crystalline perfection. The heating–cooling rate is extremely high and the recrystallization is an instantaneous process. In laser annealing, the duration of liquid silicon was estimated to be ranging from 10 ns to μs level, depending on the laser pulse width and other conditions [11–15].

It is thought that, provided the laser energy intensity is not too high, the lattice structure reconstruction process may be a self-stopping process. In other words, the single-crystalline region has a low-absorption coefficient thus can withstand the laser pulse without damage. If the laser energy intensity is

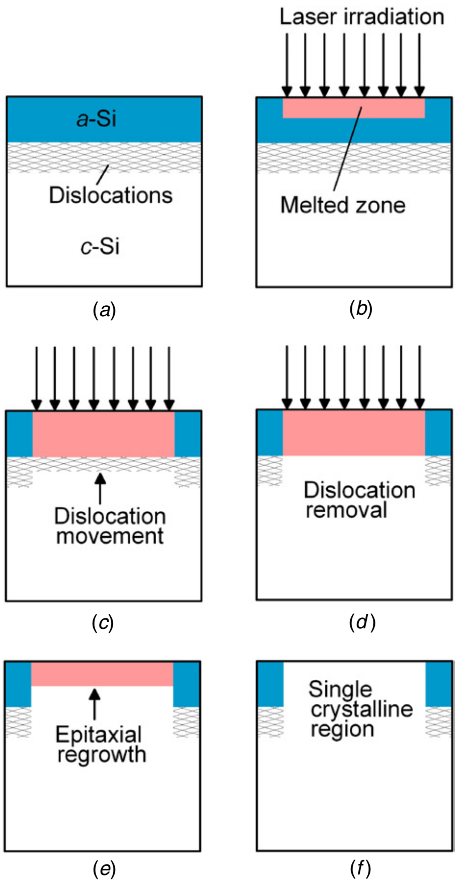

Figure 3. Schematic models of the response of a machining-damaged silicon wafer during laser irradiation. (*a*) Due to diamond machining, a subsurface amorphous layer and a dislocation layer are generated to the silicon wafer. (*b*) At the beginning of laser irradiation, a thin melted zone is formed in the amorphous layer. (*c*) The melted zone keeps growing downwards until the amorphous layer is completely melted; at the same time, the dislocations begin to move towards the liquid–solid interface. (*d*) Dislocations are completely removed before the laser pulse is over. (*e*) After the laser pulse, epitaxial regrowth begins from the liquid–solid interface. (*f*) The machining-induced damages are completely removed and the silicon wafer is reconstructed to perfect single-crystalline structure.

(This figure is in colour only in the electronic version)

excessively high, however, the molten silicon liquid might be boiled and splashed, leading to visible damages. The processing of machine-damaged layers of different depths can be realized by varying the laser energy intensity, pulse width, or the number of pulses.

In conclusion, we have demonstrated that a perfect single-crystalline structure can be obtained on a machining-damaged silicon substrate through a single nanosecond pulse laser irradiation. This finding provides the feasibility for processing silicon wafers by laser irradiation after machining processes instead of the current chemical processing. This technique offers a number of advantages. First, it does not involve material removal, thus maintains the form accuracy of the machined workpiece. Second, because the laser pulse width is extremely short, by using a high-frequency pulse laser and high speed stages for moving large-diameter workpieces, very high throughput can be realized. Third, this process is a clean process with no pollution and contamination. Another feature is that the processing area is selective, which enables fabrication of crystalline surface structures and patterns by fine spatial controls. Further investigation in this area may lead to significant technical revolutions in the semiconductor manufacturing industry.

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