Molecular-Dynamics Study of Void-Formation inside Silicon Wafers in Stealth Dicing

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Abstract. The mechanism of void formation in crystalline silicon after laser irradiation is extensively studied by molecular-dynamics simulations. When the laser-irradiated region is melted due to a rapid temperature increase, small voids are generated in that region because of large density fluctuations. Because tensile stresses are generated in the melting region, the large empty hole is formed upon cooling. When the temperature drops below the melting point, recrystallization occurs around the large void. We find that the void persists even after the recrystallization process is stopped, and that a part of the laser-irradiated region is amorphous even at room temperature. The stress distribution around the void and the amorphous region in crystalline silicon is also discussed.

1. Introduction

The process of cutting a wafer into individual IC chips, used in the semiconductor manufacturing industry, is called “dicing”. An innovative dicing method, called “Stealth Dicing (SD),” was recently developed by Hamamatsu Photonics K. K. [1-4]. In this method, a permeable nanosecond laser pulse is focused inside the wafer. The accumulation of laser energy modifies the crystalline structure in the irradiated region. By applying a tensile strain, the wafer is diced into separate chips. In this process, cracks are assumed to be initiated in the irradiated region inside the wafer and they grow toward the surface. A significant advantage of this method is that the wafer surface suffers negligible damage, while only the interior is modified.

The SD method is superior to various other dicing techniques. However, the details of the irradiation-induced microscopic processes that take place inside the wafer are still unknown. Clarifying these mechanisms is essential for establishing a more reliable dicing method. So far, the void-formation mechanism in a laser-modified region has been investigated by considering the absorption coefficient of silicon [5, 6] measured experimentally [7-12]. In addition, the crack propagation process has been analyzed in terms of fracture mechanics [13].

The purpose of our study is to clarify the mechanism of void formation. Voids appear in the laser-irradiated region, as shown in Figs. 1 and 2. The reason for the creation of a void has not been clarified since the method was invented. For this purpose, we herein present the results of computer simulations based on molecular dynamics (MD).
**Figure 1.** Cross-sectional SEM image

**Figure 2.** Magnified view of the laser-focused area in Fig. 1
2. Method of Calculation

We investigated the void-formation process by carrying out MD simulations using the micro-canonical ensemble. The Stillinger-Weber potential [14] was used to model interatomic interactions. We considered two model systems by taking into account the measured temperature dependence of the absorption coefficient of silicon [5, 6]. For the MD simulations, we set the time step $\Delta t$ to 0.4 fs and controlled the temperature by velocity scaling [15]. We used an isobaric and isothermal ensemble to obtain the volume as a function of the temperature [16-18] in Fig. 3. The following section explains the details of our model systems along with the calculated results.

![Diagram of crystalline, diamond structure, liquid, amorphous phases]

**Figure 3.** Variation of volume with temperature obtained by MD simulations using the isothermal-isobaric ensembles at ambient pressure.

3. Model systems and results

3.1. Void-formation process

To investigate the void-formation process, we were required to model the state of the material inside the wafer immediately after the laser irradiation. Our first model (‘model I’) considered the absorption coefficient, which depends on temperature. Experimental measurements showed that it increases exponentially with increasing temperature. Based on this temperature dependence, we assumed that the state of the interior of the wafer immediately after laser irradiation evolves as follows. First, the temperature rises rapidly in the laser-focused region because of the absorption coefficient and the high laser-energy density (see Fig. 4(a)). It is actually known from a thermo-elastic-plastic finite element analysis that the temperature around the laser focal point approaches 10000-40000 K due to larger absorption coefficients at higher temperatures [7]. The temperature in the surrounding region then increases as a result of thermal conduction (Fig. 4(b)). The irradiated laser energy is absorbed mainly in the region along the incident laser direction, and the temperature in this region increases rapidly (Fig. 4(c)). The region of greatest absorption shifts gradually along the incident direction because of thermal conduction and the temperature rise caused by the absorption of the laser energy (Figs. 4(d)-4(h)). It is also assumed that melting occurs in this region due to the rapid temperature increase. Based on these considerations, model I represents the shape of the melting region by a quadratic function, as shown in Fig. 5(a). The system size is $1000\times1000\times15 \, \text{Å}^3$, which included 844800 Si atoms. Starting with an initial diamond structure, the melting region was heated to...
3000 K, while the temperature of the laser-focused region was set to 10000 K. The effects of the heating details will be studied in our future work.

Large density fluctuations occur in the laser-focused region because of the rapid temperature rise at 10000 K. Figure 3 shows that the volume of liquid silicon is smaller than that of the crystalline phase, and it decreases with decreasing temperature. Therefore, small voids are generated because of volume contraction when the system cools (see Fig. 5(b)). As shown in Fig. 5(c), the void near the laser-focused region is enlarged to relax the tensile stresses, thereby forming a large empty hole, while small voids in the melting region disappear. When the temperature of the melting region drops below the melting point, recrystallization occurs instantly. Because the melting region around the large void recrystallizes quickly, the void persists even after the recrystallization is stopped as will be discussed in the subsection 3.2. When the region directly above the void becomes recrystallized, Si atoms move in the direction of the red arrow in Fig. 5(d), because recrystallization produces a lateral compression from left and right. This displacement of Si atoms results in a gradual protrusion of the melting area into the void from above, as displayed by the red circle in Fig. 5(d). The shape of this protrusion appropriately reproduces the experimental observations of Fig. 2. We conclude that this is the mechanism for the formation of the protrusions.

Figure 4. Schematic representation of the model I
Figure 5. Time progression for model I. Approximately 15 ns passed between (a) and (f).
3.2. Stress distribution around the laser-modified region inside the wafer

A few nanoseconds after the state shown in Fig. 5(d), the melting area above the void became thinner, and eventually separated from the void to give the state shown in Fig. 5(f). The atomic configuration enclosed in red box in Fig. 5(f) is magnified as shown in Fig. 6, which consists of two snapshots at 14.6 and 15.0 ns. It is clearly seen that the crystalline structure is formed below the red line, i.e. a part of the melting area was recrystallized, while the rest remained in a disordered state, namely an amorphous state, above the red line. From the time evolution of the atomic configuration from 14.6 to 15.0 ns, we see that the recrystallization was stopped because the red lines (the boundary between the crystalline and amorphous structures) are identical. For convenience, we hereafter refer to the area separated from the void, which stayed in the amorphous state when the recrystallization no longer proceeded, as the “upper melting area.” Since the density of the upper melting area increased in proportion to the volume of the void, the area had a high density and could not recrystallize completely. This is the reason why a part of the melting area remained amorphous. We conclude that the upper melting area corresponds to the laser-modified region shown in Fig. 1 and that a part of the modified region remained amorphous.

To confirm this conclusion, we compared the stress distributions of the states depicted in Figs. 5(e) and 5(f) with that of the experimentally modified region [1, 2]. Figures 7(a) and 7(b) show the $\sigma_{ss}$ stress distributions of the atomic configurations corresponding to Figs. 5(e) and 5(f), respectively. As shown in Fig. 7(a), tensile stresses formed in the upper melting area, whereas compressive stresses are formed in the upper melting area in Fig. 7(b), which is consistent with the experimental stress distribution.

To investigate the stress distribution in detail, we made a second model (‘model II’) that reproduced the behavior in the upper melting area, as shown in Fig. 8. The system size for model II was $1800\times1000\times15\text{Å}^3$, which included 1440000 Si atoms. Starting from the initial diamond structure (see Fig. 8(a)), we increased the density of an ellipsoidal region by inserting additional atoms at interstitial sites of the diamond lattice (Fig. 8(b)). The density was thus increased by approximately 8%. The ellipsoidal region was melted at 3000 K, and was recrystallized by lowering the temperature to 1200 K. The added atoms corresponded to atoms that were originally present in the void. This ellipsoidal melting area corresponded to the upper melting area (and the region modified by the laser).
Recrystallization began when the temperature decreased to 1200 K. As expected, a part of the melting region remained in an amorphous state even after recrystallization was stopped. As shown in Fig. 8(c), we created a void by extracting the same number of atoms as were inserted in the ellipsoidal region.

Figures 9(a) and 9(b) show the stress distributions for $\sigma_{xx}$ before and after recrystallization, respectively. Before recrystallization, tensile stresses formed inside and round the melting region (Fig. 9(a)). However, compressive stresses appeared after recrystallization (Fig. 9(b)), and the overall distribution was in reasonable agreement with the experiment. We believe this agreement proves that a part of the laser-modified region remains in an amorphous state, and that the void-formation process is related to the formation of the laser-modified region.

![Figure 7. Stress distributions corresponding to Figs. 4(e) and 4(f). Red and blue colors show compressive and tensile stresses, respectively.](image)

![Figure 8. Schematic representation of model II](image)
4. Summary.

We performed molecular-dynamics computer simulations for several model systems to investigate the mechanism of void formation and the stress distributions around a region modified by laser irradiation in crystalline silicon. The conclusions are summarized as follows.

(1) Melting occurs in the laser-focused region due to a rapid rise in temperature, and small voids are generated there because of large density fluctuations. The small voids are generated because of volume contraction upon cooling.

(2) These voids can lead to a relaxation of tensile stresses in the melting region, and the voids merge to form a large empty hole.

(3) When the temperature of the melting region drops below the melting point, recrystallization occurs instantly. However, the void persists even after the recrystallization process is stopped. Therefore, the density of the melting region increases in proportion to the volume of the void.

(4) The melting region near the void protrudes into the void as a result of recrystallization to form the protrusions that were observed experimentally.

(5) The melting region is not completely recrystallized because of its increasing density. We propose that a part of the region remains in an amorphous state even at room temperature and that the void-formation process is closely related to the formation of the laser-modified region.

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