The role of strain in hydrogenation induced cracking in Si/Si$_{1-x}$Ge$_{x}$/Si structures


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Hydrogenation induced cracking in molecular beam epitaxy grown Si/Si$_{1-x}$Ge$_{x}$/Si heterostructures is studied. The Si$_{1-x}$Ge$_x$ layer buried between an ~200 nm thick Si capping layer and the Si substrate is ~5 nm thick. After plasma hydrogenation, long range H migration and H trapping at the Si$_{1-x}$Ge$_x$ layer are observed. With increasing Ge concentrations, the amount of H trapping increases, cracking along the Si$_{1-x}$Ge$_x$ layer is smoother, and fewer defects are formed in the Si capping layer. The study suggests maximizing the interfacial strain to achieve the smoothest cracking with minimized radiation damage for ultrathin silicon-on-insulator technology. © 2008 American Institute of Physics. [DOI: 10.1063/1.2963489]

Silicon-on-insulator (SOI) technology is one of the manufacturing strategies employed to further minimize microelectronic device dimensions and enhance device performance. The current mainstream technique to fabricate SOI wafers is the Smart Cut™ method based on a combination of H ion implantation and wafer bonding. However, this method is limited in its ability to directly transfer a layer of sub-20 nm thickness. The primary barrier to Smart Cut™ implementation in ultrathin layer transfer is the drastic increase in both radiation damage and surface roughness of a transferred layer when ultralow energy H ion implantation is used.

Our previous studies have shown that a thin strained layer epitaxially grown inside monocrystalline Si can trap H atoms during plasma hydrogenation. Subsequent H-induced cracking can be guided along the strained layer. To utilize this technique to overcome the technology barrier for transferring an ultrathin Si layer, systematic studies are necessary to explore the fundamental mechanisms of strain effects in both H trapping and the cracking processes.

The samples used in this study were grown on Si(100) substrates using molecular beam epitaxy (MBE). A 5-nm-thick Si$_{1-x}$Ge$_x$ layer followed by a Si capping layer of ~200 nm was grown at 650 °C. Ge concentration, x, was varied from 0.05 to 0.2. The as-grown samples were then exposed to a hydrogen plasma at 250–300 °C for 1 h and then at 300–350 °C for two more hours. The applied bias during hydrogenation was ~500 V. Transmission electron microscopy (TEM) was used to characterize the sample microstructure. Depth profiles of Ge and H atoms were measured by using secondary ion mass spectrometry (SIMS) with a 1 keV Cs+ beam. The strain in the as-grown samples was measured using high resolution x-ray diffraction (XRD) analysis. A Bede D1 x-ray diffractometer was used to collect an omega scan around Si(004). High resolution strain-depth profiles were obtained by Bede RADS autofit to XRD data. The autofitting program is commercial software developed by Bede Scientific Instruments Ltd. (Durham, UK). Rutherford backscattering spectrometry (RBS) analysis was used to characterize sample structures by using a 2.0 MeV 4He+ analyzing beam.

Figures 1(a)–1(c) show SIMS hydrogen and germanium profiles obtained from the hydrogenated Si/Si$_{1-x}$Ge$_x$/Si samples. Long range H migration and H trapping by the interface are observed. A comparison among Si/Si$_{0.95}$Ge$_{0.05}$/Si [shown in Fig. 1(a)], Si/Si$_{0.90}$Ge$_{0.10}$/Si [shown in Fig. 1(b)], and Si/Si$_{0.80}$Ge$_{0.20}$/Si [shown in Fig. 1(c)] shows that (1) the H concentration peaks at the depth of the Si$_{1-x}$Ge$_x$ layer and (2) the H peak density increases with increasing Ge concentration.

![FIG. 1. SIMS H profiles from hydrogenated samples with a buried thin strained layer of (a) Si$_{0.95}$Ge$_{0.05}$, (b) Si$_{0.90}$Ge$_{0.10}$, and (c) Si$_{0.80}$Ge$_{0.20}$ respectively. Note that H trapping increases with the increase in Ge concentration.](image-url)
Both sides of the Si$_{1-x}$Ge$_x$ layer correspond in-plane tensile stress from the as-grown Si$_{1-x}$Ge$_x$. In the hydrogenated Si$_{1-x}$Ge$_x$ layer, the presence of opposing stress on either side of the interface between the Si and the Si$_{1-x}$Ge$_x$ layer results in a state of shear. As shown in Figs. 3(a)–3(c), the intensity of the interfacial shear strain increases with increasing Ge concentrations.

The above observations suggest that the buried Si$_{1-x}$Ge$_x$ layer can facilitate (100)-oriented cracking through at least three successive steps. First, the layer traps H atoms. Second, the trapped H atoms induce Si platelet formation. Third, platelets in combination with interfacial shear stress induce continuous cracking. Si platelets typically have a thickness of 1–2 nm. However, they distribute over a wide depth range in traditional H implantation. In our approach, platelets are controlled to form primarily at the Si$_{1-x}$Ge$_x$ layer; thus they greatly facilitate crack connection with reduced roughness.

Figure 2(a) shows platelet and microcrack formation in both the Si capping layer and the Si$_{0.95}$Ge$_{0.05}$ layer. As shown in Figs. 2(b) and 2(c), however, there is no direct observation of platelet formation in the Si$_{0.80}$Ge$_{0.20}$ layer or the Si$_{0.90}$Ge$_{0.10}$ layer, since these two samples have developed continuous cracking. Based on a general consensus that platelet formation is a crucial step for cracking formation, it may be concluded that platelet formation and its subsequent growth and evolution into cracking are greatly accelerated in Si$_{1-x}$Ge$_x$ layers with higher Ge concentrations.

Recently, we observed H trapping at the interface of MBE deposited Si layer and Si substrate, even without the presence of Ge atoms or a SiGe strain layer. In this situation, the trapped H peak concentration at the Si/Si interface was $1 \times 10^{20}$ cm$^{-3}$, an order of magnitude less than that shown in Fig. 1. For the Si/Si interface, H trapping is likely due to the interaction of H atoms with impurities or impurity induced defects. Here, the term “impurities” refer to contaminants such as C, O, and F. These contaminants are introduced during the surface cleaning process and have been detected by SIMS analysis (to be published elsewhere).

While our previous results showed that interfaces are effective at trapping H, the present work shows that a strain layer produces much more trapping. The most likely explanation is that the in-plane stress present in the SiGe strain layer facilitates the nucleation and growth of platelets.
which are even stronger H trapping centers than are interfaces alone. Previous studies by Grisolia et al. have shown that the growth of the platelets follows a conservative ripening,\textsuperscript{5} which suggests that the binding energy of H atoms is bigger in larger platelets. In the present study, it is hypothesized that an increase in the amount of Ge in the strain layer results in an increase in in-plane compressive stress, which facilitates the growth of platelets, resulting in more H trapping.

In Si/Si$_{1-x}$Ge$_x$/Si samples, the presence of strain at the interface contributes an additional component to fracture through the following equation:\textsuperscript{10}

\[
J = \frac{(1 - v^2)}{E} \frac{4}{\pi} P^2 a + \sigma^2 h,
\]

where $J$ is the amount of energy released, $E$ is Young's modulus, $v$ is Poisson’s ratio, $P$ is the pressure inside the platelet, $\sigma$ is the in-plane compressive stress in the strain layer, $a$ is the radius of the platelet, and $h$ is the thickness of the strained layer. Once the energy $J$ exceeds the energy required to form a new surface, the platelets will crack. Therefore, with the highest strain in the Si/Si$_{0.80}$Ge$_{0.20}$/Si sample, cracking starts early and propagates easily along the interface.

Figure 4 shows channeling RBS spectra obtained from Si/Si$_{0.80}$Ge$_{0.20}$/Si samples before and after hydrogenation. The sample before hydrogenation shows a typical surface peak. There is no detectable damage at the interface of Si/Si$_{1-x}$Ge$_x$ layers. For the hydrogenated sample, the shadowed region corresponds to backscattered yields from dislocations at the Si/Si$_{1-x}$Ge$_x$ interface. Continuous cracking is equivalent to creating two new surfaces Si$_{1-x}$Ge$_x$ faces on either side of the crack. It is expected that for atoms on the two internal surfaces, both surface atomic relaxation and cracking-induced atomic position shifts will displace and expose surface atoms to the channeled beam. These displaced atoms will serve as direct scattering centers for incident beams and contribute to an interface peak. If the cracking is zigzaglike and has large roughness, the interface peak will be very wide. If significant damage is created at the interface, the interface peak yields will be very high. As shown in Fig. 4, the interface peak (after subtracting the background) in the hydrogenated sample is comparable to the surface peak in the as-grown sample, in both peak yields and width. Consider that the surface peak of a virgin as-grown sample represents an atomic scale smooth surface with a few monolayers of displaced atoms, Fig. 4 suggests that, in addition to forming new surfaces, there is no significant damage at the cracking interface, and cracking roughness is small.

Because of interface cracking, the hydrogenated sample develops a convexly curved surface, thus resulting in high RBS yields in the top Si layer. In the present study, the beam is aligned to obtain minimum yield from a given wafer orientation. Over a curved surface (over a region of $\sim 4$ mm$^2$), the incident beam experiences angular deviation from perfect alignment. Therefore, dechanneling becomes significant. The top 200 nm thick Si capping layer is granular and similar to, for example, a silicide layer, which consists of domains with well defined but slightly different orientations with respect to the sample normal direction.\textsuperscript{11} For this reason, it is difficult to extract damage information in the top Si layer by using channeling RBS analysis. Rather, we conclude that the highest strained sample has the least damage, based mainly on the TEM studies.

In summary, we have systematically studied the role of strain intensity in the phenomenon of strain-facilitated cracking. For the MBE grown Si/Si$_{1-x}$Ge$_x$/Si sample containing a 5 nm thick Si$_{1-x}$Ge$_x$ layer, when Ge concentration increases from 0.05 to 0.20, it was found that (1) interfacial shear stress increases, (2) the amount of trapped hydrogen decreases, (3) defects in the top Si layer decrease, and (4) cracking is smoother. The results of this study could have a beneficial impact on development of the strain-facilitated layer transfer technique.

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