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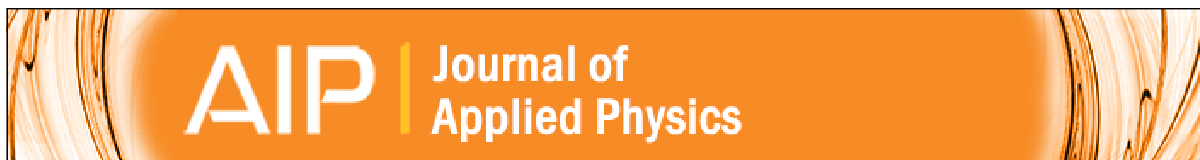

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Lin Shao, J. K. Lee, Y. Q. Wang, M. Nastasi, Phillip E. Thompson, N. David Theodore, T. L. Alford, J. W. Mayer, Peng Chen, and S. S. Lau

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Effect of substrate growth temperatures on H diffusion in hydrogenated Si/Si homoepitaxial structures grown by molecular beam epitaxy

Lin Shao,[a] J. K. Lee, Y. Q. Wang, and M. Nastasi
Los Alamos National Laboratory, Los Alamos, New Mexico 87545

Phillip E. Thompson
Code 6812, Naval Research Laboratory, Washington, DC 20375-5347

N. David Theodore
Advanced Products Research and Development Laboratory, Freescale Semiconductor Inc., Tempe, Arizona 85284

T. L. Alford and J. W. Mayer
Department of Chemical and Materials Engineering, Arizona State University, Tempe, Arizona 85287

Peng Chen and S. S. Lau
University of California at San Diego, La Jolla, California 92093

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We have investigated hydrogen diffusion in hydrogenated ⟨100⟩ Si/Si homoepitaxial structures, which were grown by molecular beam epitaxy at various temperatures. The substrate growth temperature can significantly affect the H diffusion behavior, with higher growth temperatures resulting in deeper H diffusion. For the Si/Si structure grown at the highest temperature of 800 °C, H trapping occurs at the epitaxial Si/Si substrate interface, which results in the formation of (100) oriented microcracks at the interface. The mechanism of H trapping and the potential application of these findings for the development of a method of transferring ultrathin Si layers are discussed.
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Molecular beam epitaxy (MBE) has been established as a powerful, versatile film growth technique for fabrication of nanometer scale high quality heterostructures.[1] To avoid dopant segregation and diffusion during MBE growth, low-temperature MBE (LT-MBE) has been developed to control the distribution of dopants during film growth. However, associated with the low growth temperatures employed in LT-MBE are concerns about the creation of defects in the growth layer. The dominant defects in LT-MBE-grown films are vacancy-type defects which are caused by limited adatom mobility on the epitaxial surface.[2] The presence of vacancy-type defects, including voids, in the as-grown Si films has been detected by techniques such as deep-level transient spectroscopy and positron annihilation.[2–4] Device functions can be affected by the presence of such defects, because their energy levels can provide generation-recombination centers that can quench carrier lifetime and degrade device performance.

In this study, we investigate the effects of substrate growth temperature on H diffusion and hydrogen defect formation during the hydrogenation of MBE-grown Si. Our study was motivated by the fact that hydrogen is present in virtually every step of semiconductor device processing, either as an annealing ambient, or as part of a plasma etching process, or as a chemical component for conventional wet etching or solvent cleaning.

The samples used in this work are homoepitaxial Si/Si structures. A 640 nm thick epitaxial Si layer was grown on a ⟨100⟩ 500 Ω cm *p*-type Czochralski-grown Si substrate by MBE. The substrates were given a modified Radio Corporation of America (RCA) chemical clean followed by a HF dip before being loaded rapidly into the vacuum system.[5] During growth the substrate temperature was maintained at 500, 650, or 800 °C. After MBE growth, a reactive ion etching system was used for hydrogen treatment of all samples by striking a hydrogen plasma with a bias of −500 V. For the purpose of comparison, a Czochralski-grown 15–20 Ω cm *p*-type ⟨100⟩ Si wafer was hydrogenated as a control sample. A 3 h run was performed simultaneously on all samples. The sample temperature during hydrogenation is estimated to be around 200 °C. Depth distributions of atomic H were obtained by elastic recoil detection (ERD) analysis. ERD was performed using an incident 3.0 MeV $^4He^+$ beam tilted 75° away from the sample normal. The detector was positioned 150° from the incident beam. A 15 μm thick Mylar foil was placed in front of the detector to block out elastically backscattered $^4He^+$ ions. Transmission electron microscopy (TEM) and infrared absorption (IR) measurements were used to characterize the samples before and after the hydrogenation.

Figure 1 shows ERD hydrogen depth profiles obtained from the hydrogenated Si/Si samples. The effect of surface hydrogen contamination is evident in the spectrum from the nonhydrogenated control sample. For the hydrogenated samples, the H penetrations are different for the samples grown at different temperatures. Measured at a H concentration of 1×10^{20} cm^{-3}, the H penetration depth is 360 nm for the hydrogenated control sample, 290 nm for 800 C grown

[a]Electronic mail: lshao@mailaps.org

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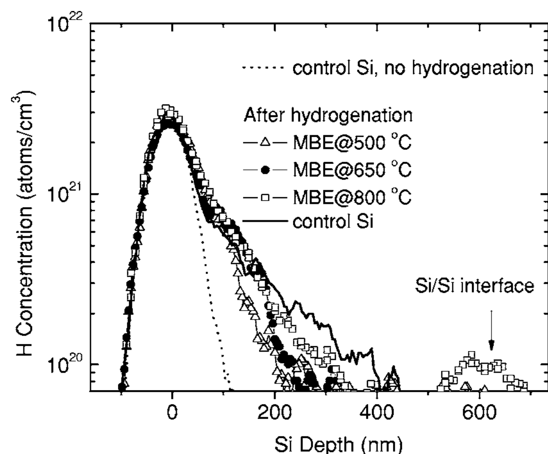

FIG. 1. ERD spectra showing H concentration vs depth for hydrogenated Si/Si samples that were grown by MBE at temperatures of 500, 650, and 800 °C, respectively.

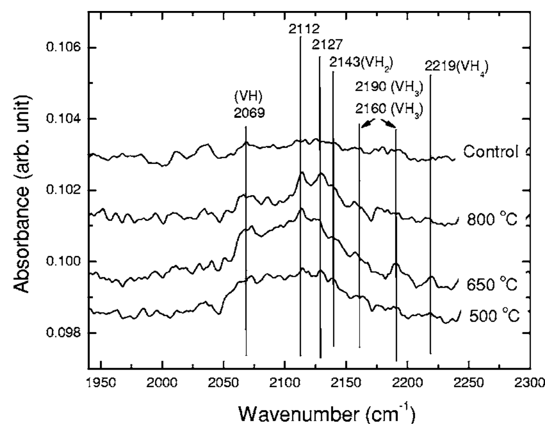

FIG. 2. Infrared absorption spectra from the hydrogenated control sample (Czochralski-grown Si) and the hydrogenated Si/Si samples which were grown by MBE at temperatures of 500, 650, and 800 °C, respectively.

Si, 220 nm for 650 °C grown Si, and 190 nm for the 500 C grown Si. H penetration is the deepest in Czochralski-grown control Si. Considering the fact that in Czochralski growth, silicon is heated to its melting point, ~1415 °C, all of the data in Fig. 1 show a systematic trend: the higher the silicon growth temperature, the deeper the H penetration.

Figure 1 further reveals that H trapping occurs in the 800 C grown Si, at a depth corresponding to the Si/Si interface. Previous study has shown the trapping of migrating Si interstitials at Si/Si interfaces during high-energy self-ion bombardment.[6] The present study shows that the Si/Si interface can be a strong trapping site for H atoms as well.

The mean penetration depth of a migrating species λ in a background field of immobile trapping centers is given by $\lambda = 1/\sqrt{4\pi a_T C_T}$,[7] where C_T is the trap density, and a_T is the effective capture radius for the trapping reaction. For a rough estimate, if we assume that a_T is a constant value for all samples and λ is the H penetration depth measured at a H concentration of 1×10^{20} cm^{-3} (from Fig. 1), the trap density, normalized to the control sample, is calculated to be around 1 for the control sample, 1.5 for 800 °C grown Si, 2.7 for 650 °C grown Si, and 3.6 for the 500 °C grown Si. For LT-MBE-grown Si, the predominant defects are believed to be vacancy-type defects.[2,3] The defect densities are expected to decrease with increasing growth temperatures. Therefore, if the extent of H penetration is trap dependent, with the predominant H trap being vacancy-type defects, we would then expect the H penetration depths to increase with increasing growth temperatures, as we observed.

Further evidence of the H interaction with vacancy-type defects is given by IR measurements. Figure 2 shows IR data from the hydrogenated MBE-grown Si samples and the control Si sample. The mode at 2069 cm^{-1} has been previously assigned to a single hydrogen atom bound to a monovacancy defect (VH).[8] The modes at 2112 and 2127 cm^{-1} are close to the assignments for symmetric and asymmetric Si–H_2 stretching modes on atomically rough (100) internal surfaces.[8] The modes at 2143 and 2219 cm^{-1} are assigned to VH_2 and VH_4, respectively.[9] The features at 2160 and 2190 cm^{-1} are attributed to VH_3 defects.[9] The MBE samples exhibit enhanced interactions of H with vacancies, as evidenced by the enhanced modes from 2050 to 2160 cm^{-1}.

It has been suggested that the microscopic structures of Si platelets are comprised of aggregated H_2^* complexes which consist of one H in a Si–Si bond center site and the other H in the antibonding interstitial site.[10] However, formation of H_2^* complexes requires the presence of both positively and negatively charged H atoms.[11] On the other hand, many experiments have provided evidence that vacancies play a central role in H-induced Si platelet formation.[9,11–14] Chemical interaction of H with dangling bonds of vacancy-type defects, and subsequent trapping of hydrogen, can lead to the formation of H-induced Si platelets. First-principles calculations have been used to examine the energetics of different hydrogen defect complexes in silicon, and it was concluded that aggregates of VH_4 (four hydrogen atoms attached to a silicon vacancy) are the precursors to Si platelet formation.[13] This picture has been supported by our recent investigation of the nucleation and growth of Si platelets in hydrogen-ion-implanted silicon.[12] Therefore, not only the H diffusion, but also the Si platelet formation will be affected by the H traps (vacancies) in the MBE grown Si. The cross-sectional TEM micrographs in Fig. 3 show the defect morphologies within the MBE samples before and after the hydrogenation. For all as-grown samples, no extended defects, or large defect clusters are observed within the Si films. In addition, it is difficult to observe the Si/Si interface in the as-grown and the hydrogenated 500 and 650 °C grown samples. For all hydrogenated samples, (111) orientated Si platelets are formed in the near surface region, consistent with the hydrogenation data of others.[13] A comparison of the data presented in Figs. 1 and 3 shows that the platelet depth distributions are correlated with the H distributions. Both the H concentration profiles and the Si platelet distributions terminate at increasing depths with increasing MBE synthesis temperatures.

One important finding revealed in Fig. 3 is that for Si/Si samples grown at 800 °C, (100) oriented microcracks are formed at the original Si/Si interface. For the samples grown at the temperature of 650 °C and below, no such interfacial cracking is observed. This is consistent with the ERD data in

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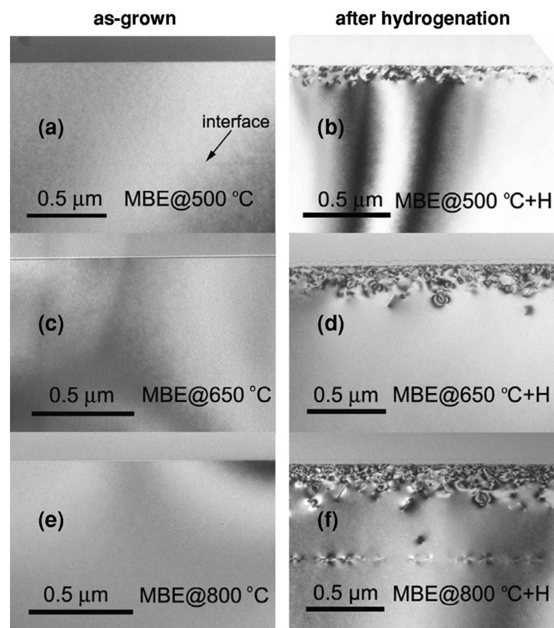

FIG. 3. Comparison of TEM micrographs of the Si/Si samples before (left column) and after the hydrogenation (right column). The Si/Si samples were grown by MBE at temperatures of [(a) and (b)] 500 °C, [(c) and (d)] 650 °C, and [(e) and (f)] 800 °C, respectively.

Fig. 1 that show trapping of H at the depth of the Si/Si interface only for the sample grown at 800 °C. These observations are also consistent with the 800 °C IR data presented in Fig. 2, which show a large enhancement in the Si–H_2 stretching modes on atomically rough (100) internal surfaces.

The formation of continuous microcracks parallel to the Si surface has potential for application in the fabrication of silicon-on-insulator wafers. In the ion-cut based technique of Si transfer, implanted hydrogen atoms (at a dose of a few 10^{16} cm^{-2}) create hydrogen-terminated cavities upon annealing that finally evolve into cracks parallel to the surface. Growth and joining of these cracks allow the surface layer to become completely separated from the substrate.[15,16] It is evident from the present study that microcracking can be controlled to arise at the interface. This controlled cracking can then be used for layer transfer. In this approach, the cleavage location is controlled by the depth of the Si/Si interface. The process has no requirement of an ion implantation step. Furthermore, using the Si/Si interface as a H trapping layer avoids contamination from implanted impurities (e.g., B and Ar) which have been used by others to create H trapping regions.[17]

We have recently reported various techniques for the lift-off of an ultrathin Si layer by growing a highly strained $Si_{1-x}Ge_x$ layer in Si as a H trapping layer.[18] We concluded that the interface, either in a homoepitaxial structure or a heteroepitaxial structure, has an appropriate microstructure to attract and retain H and thereby allow cracking to easily propagate along it. The present study shows that interfacial cracking occurs only if significant H trapping can occur at the interface. For MBE Si grown at low temperatures, the growth defects in the film limit the H penetration and the amount of interfacial H trapping. For the purpose of layer transfer, it is critical to control the growth temperature to be high enough to significantly reduce the trap density in the Si, thus making the long-range migration of H possible.

In summary, we have shown that the substrate growth temperature of MBE epitaxial Si can significantly affect the H diffusion behavior, with higher growth temperatures resulting in deeper H diffusion. We attribute this phenomenon to trap-limited diffusion of H, due to the interaction of H atoms with vacancy-type defects in the epitaxial layer. We have also shown that when the epitaxial MBE Si layer is grown on a Si substrate at 800 °C, during subsequent hydrogenation, H trapping occurs at the epitaxial Si/Si substrate interface, resulting in the formation of (100) oriented microcracks at the interface.

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