

Increased critical thickness for high Ge-content strained SiGe-on-Si using selective epitaxial growth

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The onset of misfit dislocation formation, i.e., the critical thickness for heteroepitaxy, is studied for selective epitaxial growth of high Ge-content, strained SiGe on oxide-patterned Si wafers. Misfit dislocation spacing was analyzed as a function of film thickness using plan-view transmission-electron microscopy. For selective epitaxial growth at 450 °C, the critical thickness for Si_{0.33}Ge_{0.67} is found to be 8.5 nm. This is a twofold increase compared to the 4.0 nm theoretical equilibrium critical thickness and the 4.5 nm critical thickness measured for growth on bare Si wafers. The misfit dislocation density for selective epitaxial growth is strongly influenced by the shape and orientation of the growth area. © 2010 American Institute of Physics.

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High Ge-content strained SiGe-on-Si is of interest for several applications, especially as a potential channel material in high mobility SiGe-channel p-type metal oxide semiconductor field-effect transistors (p-MOSFETs).^{1,2} Strained SiGe and Ge channel p-MOSFETs have high hole mobility with an enhancement of up to ten times relative to unstrained Si.^{3,4} Hole mobility in strained SiGe-channel p-MOSFETs increases with increasing Ge composition. However, due to the 4% lattice mismatch between Si and Ge, growing SiGe on bulk Si is challenging due to the onset of misfit dislocation formation above the critical thickness T_{crit} . For SiGe-on-Si heteroepitaxy, the equilibrium T_{crit} is calculated to be 5 nm for Si_{0.5}Ge_{0.5}, 3.3 nm for Si_{0.2}Ge_{0.8}, and slightly above 2 nm for pure Ge.⁵ Because of this, for SiGe-channel p-MOSFET applications where the channel material is grown pseudomorphic to Si, it is necessary to keep the films thin to maintain the strain in the channel, and increasing the Ge composition above 70% does not yield enhanced mobility because the channel thickness is limited by critical thickness constraints.^{6,7}

Increasing the critical thickness for strained SiGe heteroepitaxy will enable thicker SiGe channels and provide a pathway to avoid the mobility degradation associated with ultrathin (<5-nm-thick) films. In addition, understanding critical thickness in selective epitaxy is of interest for epitaxial growth in small-area SiGe source/drains as means of increasing compressive strain in Si p-MOSFETs. One approach to increase T_{crit} is to grow SiGe in small areas using selective epitaxial growth (SEG). Because misfit dislocation nucleation is dominated by sources or microdefects with a fixed areal density, for small areas, it is reported that the misfit dislocation density is lower than for large areas due to the decreased number of dislocation nucleation sources and propagation length.^{8–10} Past reports showed that growing low-Ge-content (<20%) SiGe in limited areas (<50 × 50 μm²) increases the critical thickness.^{11–13} It is difficult to extrapolate those results to the high mismatch regime where different dislocation nucleation and propagation

mechanisms are expected. In this study, we have studied the critical thickness for SiGe with high Ge-content (Si_{0.33}Ge_{0.67}) on exposed Si regions on oxide-patterned Si wafers with pattern size spanning submicron to a few tens of microns.

In order to systematically study the changes in critical thickness of SiGe in small areas a mask was designed to grow epitaxial SiGe in selective areas on oxide-patterned Si wafers. Starting with a p⁻ doped 6 in. (100) Si wafer, a 40-nm-thick SiO₂ film was grown using thermal oxidation, followed by patterning using standard lithography and wet etching. The size of oxide openings ranged from 0.8 to 50 μm, and this study focused on feature sizes from 1 to 10 μm. The density of oxide openings to the field mask was kept roughly the same for all shapes and sizes to minimize loading effects during epitaxial growth. After pre-epitaxial Si surface preparation and a prebake step at a temperature of 900 °C for 5 min, SiGe is epitaxially grown to varying thicknesses up to 20 nm in a low-pressure chemical vapor deposition growth system (Applied Materials Epi Centura™). Using SiH₄ and GeH₄ as precursors, the wafer temperature was kept at 450 °C and chamber pressure at 100 Torr during growth. Blanket SiGe films of comparable thicknesses were grown under the same conditions for comparison.

After the growth, the Ge concentration in the SiGe films was first measured by spectroscopic ellipsometry and then verified to be 67% by secondary ion mass spectrometry. In order to determine whether Ge composition in the SiGe film depends on the size of the SiGe growth area, Auger electron spectroscopy was used to compare Ge composition in SiGe features of different sizes. 11-nm-thick SiGe films that were grown in 1, 3, and 10 μm square-shaped oxide openings were analyzed and compared to the data for blanket films. The Ge concentration in all samples fell within a few at. % of that measured for blanket SiGe growth. As the accuracy of the Auger technique is also a few at. %, it can be concluded that the Ge concentration for the SEG SiGe films in this study does not vary with the size of the features.

The thickness and dislocation spacing of Si_{0.33}Ge_{0.67} films were measured by transmission-electron-microscopy (TEM) techniques, using both plan-view and cross-sectional

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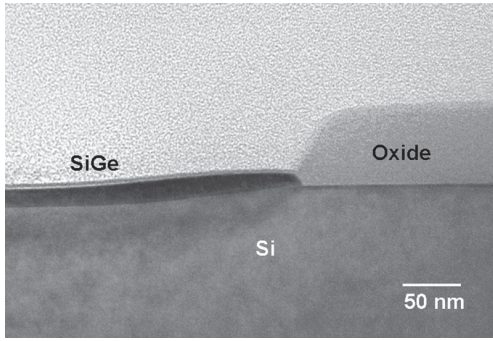


FIG. 1. A typical cross-sectional TEM image of $\text{Si}_{0.33}\text{Ge}_{0.67}$ -on-Si SEG samples. Oxide thickness is 40 nm, and $\text{Si}_{0.33}\text{Ge}_{0.67}$ film is around 10 nm. Prebake step used temperature of 900 °C for 5 min.

analyses. A standard sample preparation method by grinding and ion milling was used. Figure 1 shows a typical cross-sectional TEM image for the SEG wafers. It is observed that the SiGe film is slightly thicker within 200 nm of the oxide boundary compared to the thickness in the rest of the open area. SiGe film thickness quoted in this paper refers to that in the bulk of the film. For wafers with blanket SiGe growth, no misfit dislocations were detected when the film thickness was 4 nm, but misfits are found for SiGe films with thickness greater than 5 nm. This indicates that the critical thickness of $\text{Si}_{0.33}\text{Ge}_{0.67}$ in large areas is around 4.5 nm and is very close to the calculated equilibrium thickness of 4.0 nm.⁵ For SEG SiGe grown in 2 μm square openings, misfit dislocations were not found for 8 nm films but were detected for films thicker than 9 nm, indicating that the critical thickness is around 8.5 nm and is increased by roughly two times compared to that for large area growth. Figure 2 compares TEM images for the SEG and blanket films. Figure 2(a) shows plan-view TEM images of 10.5-nm-thick SiGe films grown in 1 and 2 μm square openings. Few dislocations are observed in such areas for this thickness, and when an area of $\sim 126 \mu\text{m}^2$ was observed, the dislocation spacing was measured to be 8.6 μm . Figure 2(b) shows plan-view TEM images of a blanket SiGe film of comparable thickness (11 nm). Misfit dislocations are easily seen, and dislocation spacing was found to be 0.25 μm for an area of observation of $\sim 144 \mu\text{m}^2$.

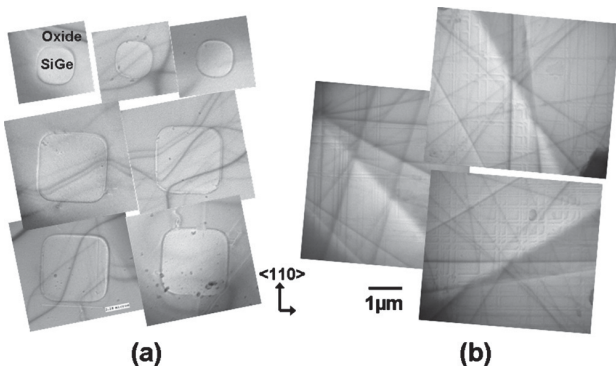


FIG. 2. Plan-view TEM images of $\text{Si}_{0.33}\text{Ge}_{0.67}$ -on-Si films illustrating the increase in critical thickness in small areas. In (a) few misfit dislocations are detected for a 10.5-nm-thick SEG film (dislocation spacing is 8.6 μm), while in (b) an 11-nm-thick blanket $\text{Si}_{0.33}\text{Ge}_{0.67}$ film shows increased misfit dislocation density (dislocation spacing is 0.25 μm). The same scale and crystallographic directions apply for both (a) and (b).

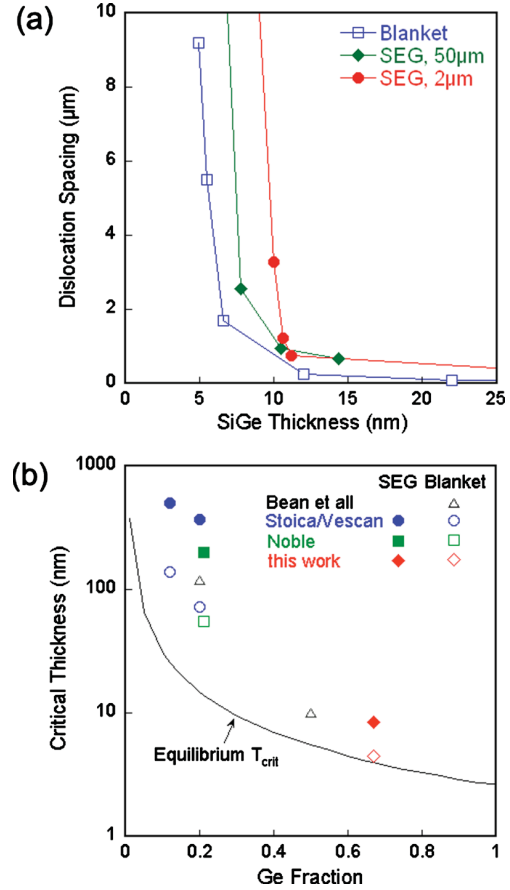


FIG. 3. (Color online) (a) Dislocation spacing vs film thickness for SEG and blanket growth for $\text{Si}_{0.33}\text{Ge}_{0.67}$ -on-Si. For SEG growth, square openings of sizes 2 and 50 μm were analyzed. T_{crit} is 8.5, 6.5, and 4.5 nm for SEG 2 μm square, SEG 50 μm square, and blanket growth, respectively. (b) Critical thickness of $\text{Si}_{1-x}\text{Ge}_x$ on Si as a function of Ge fraction, x . Calculated equilibrium critical thickness is shown by a solid line, and experimental data from previous publications are also plotted (Refs. 5 and 10–14).

Misfit dislocation spacing was measured for SiGe films of different thicknesses, and the results are summarized in Fig. 3(a). While the blanket film shows a critical thickness (asymptote where dislocation spacing increases to infinity) similar to the calculated equilibrium thickness, SEG SiGe shows a larger dislocation spacing for a given thickness, which translates into fewer misfit dislocations per unit area. The critical thickness is increased by 1.5 $\times$ for 50 μm openings and 2 $\times$ for 2 μm openings from the calculated equilibrium thickness for $\text{Si}_{0.33}\text{Ge}_{0.67}$. Figure 3(b) shows the critical thickness for SEG and blanket growth from this work, and compares the data to previously reported experimental data and to the calculated equilibrium limit.^{11–14} It is noted that for all Ge ranges, T_{crit} for SEG is larger than the equilibrium critical thickness. However, while a factor of 3 to fivefold increase in T_{crit} is found for SEG of SiGe with low-Ge composition, for high Ge-content, the increase in T_{crit} in small areas is a factor of 2. This may be related to the higher mismatch and driving force for dislocation formation. It is observed that as Ge concentration is increased, the experimental T_{crit} approaches the equilibrium critical thickness, and for $\text{Si}_{0.33}\text{Ge}_{0.67}$, T_{crit} for blanket growth is only 4.5 nm, close to the equilibrium critical thickness of 4.0 nm.

The SEG mask also includes various shapes such as squares, circles, diamonds, and long rectangular openings to

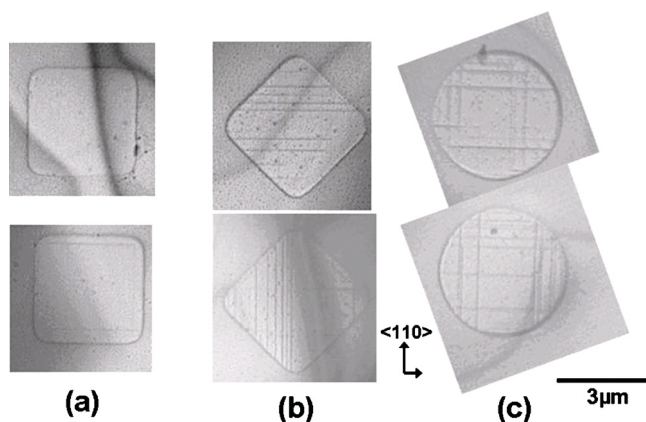


FIG. 4. (Color online) Plan-view TEM of $\text{Si}_{0.33}\text{Ge}_{0.67}$ that was grown in (a) $\langle 110 \rangle$ square oxide opening, (b) 45° rotated feature (sidewalls along $\langle 100 \rangle$), and (c) circular feature. (b) and (c) show higher misfit dislocation density. All SiGe films are ~ 10 nm thick. Scale bar and crystallographic directions apply to all figures.

study the influence of feature orientation on the critical thickness. It is observed that the misfit dislocation density for SEG growth is strongly influenced by the shape and orientation of the growth area. Figure 4 shows 10-nm-thick $\text{Si}_{0.33}\text{Ge}_{0.67}$ films, where the sample in Fig. 4(a) was grown in square oxide openings with edges parallel to the $\langle 110 \rangle$ direction, Fig. 4(b) in squares with edges parallel to $\langle 100 \rangle$, and Fig. 4(c) in circular openings. The misfit dislocation density is much higher in Figs. 4(b) and 4(c), compared to Fig. 4(a). This dependence on feature orientation/shape could be due to microsteps at the pattern edges or faceting of the SiGe, which may influence the nucleation of dislocations at the pattern edges. This could also be affected by a slightly thicker SiGe film near the pattern edges, as observed in Fig. 1. Recent work by Menéndez¹⁵ points out that the heterogeneous density of dislocation sources n_0 depends on the growth conditions, and a study is in progress to analyze the

source dislocation density for selective growth and SEG window orientation.

In summary, the selective epitaxial growth of thin, high Ge-content strained SiGe-on-Si has been studied. Germanium percentage is found to be independent of the SEG feature size, and for $\text{Si}_{0.33}\text{Ge}_{0.67}$, the critical thickness was increased by a factor of 2 (from 4 to 8 nm) using limited area growth, for features in the size range 1–10 μm . SEG feature orientation has a strong influence on the critical thickness of SiGe films, and features with edges along $\langle 110 \rangle$ yield the lowest misfit dislocation density.

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