Si-Ge interdiffusion and strain relaxation were studied in a metastable SiGe epitaxial structure. With Ge concentration profiling and ex-situ strain analysis, it was shown that during thermal anneals, both Si-Ge interdiffusion and strain relaxation occurred. Furthermore, the time evolutions of both strain relaxation and interdiffusion were characterized. It showed that during the ramp-up stage of thermal anneals at higher temperatures (800°C and 840°C), the degree of relaxation, \( R \), reached a “plateau”, while interdiffusion was negligible. With the approximation that the \( R \) value is constant after the ramp-up stage, a quantitative interdiffusivity model was built to account for the effect of strain relaxation and the impact of the strain relaxation induced dislocations, which gave good agreement with the experimental data.

As electronic and optoelectronic devices are continuously scaled down for better performance, novel materials and process techniques have been developed and integrated into the state-of-the-art semiconductor device manufacturing. In the last decades, SiGe alloys have been developed and integrated into the state-of-the-art semiconductor device manufacturing. In the last decades, SiGe alloys have become key materials in electronic devices. Examples are as strain relaxation is very common in semiconductor devices due to compressive stress, and also increases with ion implantation damage.10,11 Interdiffusion under partial strain relaxation was investigated. Strain relaxation was characterized using high resolution X-ray diffraction (HRXRD) and a quantitative model was built for Si-Ge interdiffusion under partial strain relaxation over a wider Ge fraction range. This model was shown to produce accurate predictions of Ge peak positions in comparison with experimental data.

**Experimental**

*Epitaxial structure growth and annealing.* — A multilayered epitaxial structure \( \text{Si}_{0.45}\text{Ge}_{0.55} / \text{Si}_{0.17}\text{Ge}_{0.83} / \text{Si}_{0.55}\text{Ge}_{0.45} \) was used for this study, as shown in Figure 1. The \( \text{Si}_{0.17}\text{Ge}_{0.83} \) layer is under the biaxial compressive strain. This structure is labeled as S4583. The epitaxial layers were grown on a 6 inch (100) Czochralski (CZ) p-type Si wafer in an Applied Materials “Epi Centura” system. In order to minimize the threading dislocation density (TDD) and its impact on Si-Ge interdiffusion in the top layers, a 5 µm graded relaxed SiGe buffer (GRB) layer was grown on the Si substrate. The Ge fraction is graded linearly from 0 to 0.45. Next a 1 µm strain-relaxed \( \text{Si}_{0.45}\text{Ge}_{0.55} \) layer was grown on the GRB layer at 900°C as the virtual substrate, to make sure the \( \text{Si}_{0.17}\text{Ge}_{0.83} \) layer of interest is far enough from the defected GRB layer. The TDD in the as-grown relaxed \( \text{Si}_{0.45}\text{Ge}_{0.55} \) layer was measured using the etch pit density (EPD) technique, and was estimated to be on the order of \( 10^4 \text{ cm}^{-2} \). Next, a thin compressively strained \( \text{Si}_{0.17}\text{Ge}_{0.83} \) layer of interest is grown at 365°C. Its thickness (9 nm) was designed to be larger than the Matthews-Blakeslee equilibrium critical thickness (5 nm), resulting in a metastable layer. It tends to relax during thermal anneals.19 On top of this compressively strained layer, another relaxed \( \text{Si}_{0.55}\text{Ge}_{0.45} \) was grown at 525°C. Finally, a thin silicon cap was grown on top at 600°C. The nominal thicknesses of the top strained Si, relaxed \( \text{Si}_{0.55}\text{Ge}_{0.45} \) and compressive \( \text{Si}_{0.17}\text{Ge}_{0.83} \) layers are 5 nm, 30 nm and 9 nm respectively. The sample structure is shown in Figure 1.

Inert anneals were performed in nitrogen ambient using an enclosed Linkam TS1200 high temperature heating stage. The annealing condition design criteria were: 1) to obtain enough diffusion for SIMS measurements and introduce sufficient strain relaxation for HRXRD to detect, and 2) diffusion should be limited such that surface transport is insignificant and can be ignored, so the mass transport is only by interdiffusion governed by Fick’s laws. A few diffusion tests were performed. The anneals at 760°C, 800°C and 840°C for 40 mins satisfied the above criteria. To investigate the time dependence of the strain relaxation and Si-Ge interdiffusion, four anneals for different times were performed at each temperature. The annealing conditions and the sample naming convention are the following: as-grown (AG), ramp up and down only (RUDO), 10-minute anneal with ramp up and down (RUD10), 20-minute anneal with ramp up and down (RUD20) and 40-minute anneal with ramp up and down (RUD40). The ramp-up and ramp down rates are 40 °C/min and 100 °C/min respectively. The temperature profiles at 800°C are shown in Figure 2.

**Depth profiling of Ge and strain analysis.** — Secondary ion mass spectrometry (SIMS) measurements were performed by Evans
Analytical Group to obtain the Ge profiles in the as-grown and annealed samples. The samples were sputtered with 1 keV Cs\(^+\) primary ion beam obliquely incident on the samples at 60° off the sample surface normal. The sputter rate was calibrated using stylus profilometer measurements of total sputtered crater depths, and corrected on a point-by-point basis for the known sputter rate variation with SiGe composition. The measurement uncertainty in Ge fraction is ±1 at.

High resolution X-ray diffraction (HRXRD) measurements were performed to characterize the biaxial compressive strain and the degree of relaxation (R) in the compressive Si\(_{1-x}\)Ge\(_{y}\) and bottom Si\(_{1-x}\)Ge\(_{y}\) layers of the as-grown and annealed samples. All the measurements were performed using a PANalytical X’Pert PRO MRD with a triple axis configuration. Symmetric (004 Bragg reflection) and asymmetric (115 Bragg reflection) scans were performed to obtain both the in-plane and out-of-plane lattice constants of the compressive Si\(_{1-x}\)Ge\(_{y}\) layer and the bottom relaxed Si\(_{1-x}\)Ge\(_{y}\) layer. This allows us to determine both the Ge fraction and strain in these layers. To eliminate the influence of the substrate wafer miscut and the tilt of the epitaxial films, XRD scans were performed with the wafer oriented at phi = 0° and 180° for both symmetric and asymmetric reflections, where “phi” denotes the angle rotation of the sample about its surface normal. The Ge fraction and strain of the Si\(_{1-x}\)Ge\(_{y}\) and bottom relaxed Si\(_{1-x}\)Ge\(_{y}\) layers were extracted by matching the average peak separation between the peaks of the layer and substrate with that simulated by the PANalytical Epitaxy software package. The thicknesses of the Si\(_{1-x}\)Ge\(_{y}\) layers used for those simulations are the full width at half maximum (FWHM) of the corresponding SIMS profiles.

Results and Discussion

Ge depth profiles measured by SIMS.— The as-grown and the annealed Ge profiles of the samples annealed at three different temperatures are shown Figure 3a. The anneal time is 40 mins for all temperatures. The Ge peak of the as-grown Si\(_{1-x}\)Ge\(_{y}\) layer has a triangle-like shape, since interdiffusion occurred during the growth of the top two layers after the Si\(_{1-x}\)Ge\(_{y}\) layer was grown. In addition, there was partial strain relaxation at the same time, as shown in Table I. The as-grown maximum Ge fraction is 0.83. This interdiffusion during the growth is hard to minimize due to the large Ge fraction and high compressive strain in the Si\(_{1-x}\)Ge\(_{y}\) layer. Simulations were conducted using two established models in Dong et al’s previous work.
work, shown in Figure 3b-3d. One model is the unified model for fully relaxed SiGe (equivalently \( R = 1 \) built over the full Ge fraction range in Ref. 15, and the other is the interdiffusivity model with full compressive strain (equivalently \( R = 0 \)) in Ref. 16. The SIMS profiles fall in between the model predictions under these two extreme strain conditions, which indicates that the strain has partially relaxed during the thermal anneals.

At each temperature, the samples were also annealed for different times: RUDO, RUD10, RUD20 and RUD40, as illustrated in Figure 2. The Ge profiles of the samples annealed with different times at 800 °C are shown in Figure 4. Comparing the SIMS profile of the RUDO sample with the as-grown one, we can see that Si-Ge interdiffusion is negligible during the ramp up and down stages, where the peak decreased by about 1 at.%, which is within the SIMS measurement uncertainty of Ge fractions. If we compare the Ge peaks after the 10, 20 and 40-minute diffusion, we see that the Ge peak drop in the first 10 minutes is much larger than that in the next 10 minutes and the next 30 minutes. As the annealing time increased, the rate of the Ge drop in the \( \text{Si}_{1-x}\text{Ge}_x \) layer became slower, which is attributed to the strong concentration and strain dependence of Si-Ge interdiffusivity. The interdiffusivity became much smaller as the Ge fraction decreased during annealing. Accordingly, the rate of the Ge peak drop was slower as the diffusion time increased.

Ge fraction and strain analysis by HRXRD.— In Figure 5, the 004 symmetric and 115 asymmetric XRD scans from samples annealed at the three different temperatures for 40 minutes are shown. The strongest peak is from the Si substrate. The second strongest peak is from the bottom \( \text{Si}_{1-x}\text{Ge}_x \) layer. The peak on the far left is from the thin \( \text{Si}_{1-x}\text{Ge}_x \) layer. The peak from the Si substrate peak is from the bottom \( \text{Si}_{1-x}\text{Ge}_x \) layer of S4583 during annealing.

![Figure 5. (a) 004 symmetric XRD and (b) 115 asymmetric scans at phi = 0° from S4583 samples. The most intense narrow peak is from the Si substrate. The second strongest peak is from the bottom \( \text{Si}_{1-x}\text{Ge}_x \) layer. The peak on the far left is from the thin \( \text{Si}_{1-x}\text{Ge}_x \) layer.](Image 63x57 to 255x201)

In addition, the time dependence of the \( R \) values for all the three annealing temperatures was characterized by the HRXRD and is shown in Figure 6. From Figure 6, we can see that the \( R \) value increased greatly at first, and went up to around 45% and gradually saturated with the annealing time, forming a plateau. The shape of the time dependence of \( R \) in S4583 is consistent with the results of the in-situ XRD measurements reported by Fischer and Zaumseil. At 760 °C, the relaxation rate was slower than the other two temperatures, and the \( R \) value reached a plateau at RUD10. In contrast, for the anneals at 800 °C and 840 °C, the \( R \) value almost reached a plateau after the ramp-up stage. Considering the slower ramp-up rate (40 °C/min) compared to the ramp-down one (100 °C/min), it is reasonable to assume that the strain relaxation happened predominantly in the ramp-up stage. After that, the \( R \) value only increased by small amounts as the anneal time increases.

Table I. Ge fraction and the degree of relaxation \( R \) in the compressive \( \text{Si}_{1-y}\text{Ge}_y \) layers and the bottom \( \text{Si}_{1-x}\text{Ge}_x \) layers from XRD measurements. The error bars of the Ge fraction and the \( R \) value are ±0.01 and ±5 respectively for \( \text{Si}_{1-x}\text{Ge}_x \) layers, and ±0.005 and ±0.5 respectively for the bottom \( \text{Si}_{1-x}\text{Ge}_x \) layers.

<table>
<thead>
<tr>
<th>Thermal condition</th>
<th>( x )</th>
<th>( y )</th>
<th>( x )</th>
<th>( y )</th>
<th>( x )</th>
<th>( y )</th>
</tr>
</thead>
<tbody>
<tr>
<td>As-grown</td>
<td>0.840</td>
<td>10</td>
<td>0.600</td>
<td>0.400</td>
<td>97.0</td>
<td>95.0</td>
</tr>
<tr>
<td>760 °C for 40 minutes</td>
<td>0.734</td>
<td>45</td>
<td>0.514</td>
<td>0.414</td>
<td>96.5</td>
<td>94.0</td>
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<tr>
<td>800 °C for 40 minutes</td>
<td>0.683</td>
<td>45</td>
<td>0.425</td>
<td>0.425</td>
<td>96.0</td>
<td>96.0</td>
</tr>
<tr>
<td>840 °C for 40 minutes</td>
<td>0.622</td>
<td>50</td>
<td>0.430</td>
<td>0.430</td>
<td>96.0</td>
<td>96.0</td>
</tr>
</tbody>
</table>

Figure 4. Ge profiles measured by SIMS for as-grown and annealed samples with different anneal times at 800 °C.

![Figure 4. Ge profiles measured by SIMS for as-grown and annealed samples with different anneal times at 800 °C.](Image 348x479 to 504x716)
interdiffusion. In other words, strain relaxation happened before Si-Ge interdiffusion in samples annealed at 800°C and 840°C.

**Interdiffusivity Modeling and Discussion**

**Modeling of lattice-mediated Si-Ge interdiffusion with partial strain relaxation.** In Dong et al’s recent work,16 we studied similar epitaxial structures with high compressive strain, which was reduced only by Si-Ge interdiffusion, with structure coherency maintained. To avoid confusion, in this work, strain relaxation only refers to plastic relaxation via dislocations, not to strain reduction by Si-Ge interdiffusion, with structure coherency maintained. To closely at high temperatures (\(T > 200 \text{ K}\)).

Thermodynamically, compressive strains play two main roles in Si-Ge interdiffusion:16

- **Driving force.** The driving force, which depends on temperature and degree of relaxation \(R\), is Young’s modulus, and \(\eta\) is Poisson ratio.

- **Impact of the biaxial strain only** on the interdiffusivity itself without the driving force impact.

Combining Equation 2 and 5, the strain energy can be ideally expressed as

\[
G_x = \frac{1}{2} V_m \sum_i \varepsilon_i \sigma_i
\]

where \(\varepsilon_i\) and \(\sigma_i\) are the biaxial strain and stress; \(V_m\) is the molar volume of the solid solution, for SiGe, \(V_m \approx 13 \text{cm}^3/\text{mol}\). Combining Equation 2 and 5, the strain energy can be ideally expressed as

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\]
The apparent interdiffusivities with different $R$ values at 800 °C and 840 °C are compared in Figure 7. The apparent interdiffusivity when $R = 0.5$ is in between those when $R = 0$ and $R = 1$. As the biaxial compressive strain reduces to $\varepsilon_0 (1 - R)$, correspondingly, the strain enhancement of interdiffusion decreases, which is consistent with the SIMS results in Figure 3. According to the model for interdiffusion with partially relaxed compressive strain in Equation 10, at 800 °C the interdiffusivity of a 10% relaxed Si$_0.17$Ge$_0.83$ (the case of the as-grown sample) is almost 100 times larger than that of a 42% relaxed Si$_0.27$Ge$_0.73$ (the case of the RUD10 sample at 800 °C). This big difference in interdiffusivity explains why the Ge peak drop is faster during the first 10 minutes in Figure 4.

Model refinement and discussion.— Based on the time dependence of strain relaxation and interdiffusion above, we see that for higher annealing temperatures (800 °C and 840 °C), the degree of relaxation $R$ reached a plateau after the ramp-up stage. Therefore, for anneals with 10 mins and longer time at the peak temperature, $R$ can reasonably be assumed to be a constant during interdiffusion as the thermal budget in the ramp-up stage is negligible for interdiffusion. Therefore, Si-Ge interdiffusion can be simulated using the model in Equation 10 with a constant $R$, and the model was implemented in TSUPREM-4, an industry mainstream two-dimension finite element simulation tool. For annealing at 800 °C with different anneal times (10 minutes, 20 minutes and 40 minutes), an average $R$ value of 42% is used; while for the anneal at 840 °C with 40 minutes, an average $R$ value of 47% is used. For the 760 °C anneals, however, the $R$ value reached a plateau at RUD10, which means that strain relaxation mostly occur in the first 10 mins anneal after the ramp-up stage, and $R$ cannot be treated as a constant after the ramp-up stage. If $R(t)$ is well characterized with much finer time steps, Equation 10 can still be applied with the measured $R(t)$. With the average $R$ values, predictions using the model in Equation 10 can be made for the anneals at 800 °C and 840 °C. The comparisons between the model predictions and the corresponding SIMS profiles are shown in Figure 8.

From Figure 8, it is demonstrated that the peak drops predicted by the model in Equation 10 match the ones from the SIMS data for all the four anneal conditions within the SIMS measurement error bar. However, in Figure 8, we can also see the peak shapes of the model predictions do not perfectly match the experimental ones, i.e., the rising and falling edges of the simulated peaks are steeper than those of the SIMS profiles. The steep edges of the model predictions are caused...
by the strong concentration and compressive stress dependence of Si-Ge interdiffusivity in the model in Equation 10. In 2002, Erdélyi et al demonstrated that if the diffusivity strongly depends on concentration, the interface can become sharper on nanoscale. Based on Fick’s first law, $J = -D \frac{∂C}{∂z}$, the diffusion flux is decided by both the diffusivity and the concentration gradient. From the as-grown SIMS profile of S4583, we can see the rising and falling edges are close to linear, so the concentration gradient doesn’t change dramatically along the rising and falling edges at time $t = 0$. Therefore, the diffusion flux is primarily determined by the interdiffusivity. At the locations with a larger Ge fraction and thus higher compressive strain and higher interdiffusivity, the diffusion flux is much larger. For S4583, the diffusion flux has a very strong Ge concentration dependence, which is illustrated in Figure 9.

According to the model in Equation 10, at higher Ge concentrations, the diffusion is much faster than at lower Ge concentrations. As time increases, the rising and falling edges should get steeper. However, this is not what we observed from the SIMS data. The edges of all the SIMS Ge peaks were flatter and went farther than the edges of the simulated Ge peaks, and the Ge peaks did not get steeper as Equation 10 predicted. This issue can be explained by the dislocation-mediated interdiffusion, which is not included in Equation 10. Equation 10 only accounts for the point-defect mediated interdiffusion (lattice diffusion), and the interdiffusivity associated with that is $D_{\text{lattice}}$. Strain relaxation in SiGe multi-layers is mainly ascribed to the formation of misfit dislocations at the interfaces and their following movements during thermal anneals. Misfit dislocations are often associated with threading dislocations, which act as fast diffusion paths. The dislocation density is expected to be higher for samples with strain relaxation, such as S4583, compared to those without strain relaxation as in Ref. 16. In order to estimate the collective impact of the relaxation induced dislocations, an additional term $\tilde{D_{\text{dislocation}}}$ is added to $D_{\text{lattice}}$ in calculating the total interdiffusivity $\tilde{D_{\text{total}}}$ as Gavelle et al did for modeling Si-Ge interdiffusion in highly defected Ge/Si heterostructures. Therefore, the total interdiffusivity can be expressed as

$$\tilde{D_{\text{total}}} = \tilde{D_{\text{lattice}}} + \tilde{D_{\text{dislocation}}}, \quad [11]$$

where $D_{\text{lattice}}$ is the diffusivity in Equation 10 for lattice mediated interdiffusion, and $\tilde{D_{\text{dislocation}}}$ is the collective diffusivity contributed from relaxation induced dislocations.

In Gavelle et al’s study, they used an Arrhenius term to describe the impact of the relaxation induced dislocations on Si-Ge interdiffusion. In this work, a similar Arrhenius expression is used to estimate the impact of dislocations analytically.

$$\tilde{D_{\text{dislocation}}} = D_{\text{dis}}^{0} (x_{\text{Ge}}) e^{\frac{-E_{\text{dis}}}{kT}} \quad [12]$$

where $D_{\text{dis}}^{0}$ and $E_{\text{dis}}$ are the prefactor and activation energy respectively. In Ref. 42, $D_{\text{dis}}^{0} = 0.01 \exp(2.5x_{\text{Ge}})$ and $E_{\text{dis}} = 3.1eV$. “dis” denotes relaxation induced dislocations.

In order to quantify the impact of the dislocations in the tail regions of S4583, the parameters in Equation 12 were extracted by fitting the SIMS profiles, as shown in Figure 10. 

![Figure 10](image1.png)

Figure 10. Best fittings to the SIMS profiles for the extraction of $D_{\text{dis}}^{0}$ and $E_{\text{dis}}$ of $\tilde{D_{\text{dislocation}}}$: (a) RUD10 at 800 °C; (b) RUD20 at 800 °C; (c) RUD40 at 800 °C and (d) RUD40 at 840 °C.
expressed as \(0.017 \exp(x_{Ge})\) and the activation \(E_{\text{dis}}\) is 3.15 eV, and this set of parameters can generate good fittings to all measured SIMS profiles as shown in Figure 10. Compare to the parameters extracted in Ref. 42, where \(D^{0}_{\text{dis}} = 0.01 \exp(2.5x_{Ge})\) and \(E_{\text{dis}} = 3.1\text{eV}\), we can see that the activation energy is very close, but \(D^{0}_{\text{dis}}\) is quite different. It should be noted that the structures in Gavelle et al’s work in Ref. 42 were highly defected relaxed Ge films on Si. The dislocation density was shown to reach 10^11 cm^-2. For these anneals, the strain relaxation happened before Si-Ge interdiffusion. With the approximation that \(R\) value is constant after the ramp-up stage of the anneals at 800°C and 840°C, the \(D_{\text{lattice}}(R)\) model gave close predictions of the Ge peak drop in the compressive Si1−yGe y Ge layer. In addition, the impact of the dislocation mediated interdiffusion \(D_{\text{dislocation}}\) was quantified, which is significant for interdiffusivity at lower Ge fractions. A two-term model that combines \(D_{\text{lattice}}\) and \(D_{\text{dislocation}}\) was shown to be very successful in explaining the data of Si-Ge interdiffusion with strain relaxation.

Conclusions

In summary, this work focused on Si-Ge interdiffusion in epitaxial SiGe heterostructures with partial strain relaxation. As SiGe with strain relaxation is common for SiGe devices such as devices with SiGe heterostructures under biaxial strain, this work is of great relevance to the semiconductor industry. Based on diffusion theories, a model for point defect mediated Si-Ge interdiffusion \(D_{\text{lattice}}(R)\) was established to include the impact from the degree of strain relaxation \(R\). Experimentally, structure S4583 with a metastable compressive Si1−yGe y Ge layer was grown and annealed. Characterized by HRXRD, the compressive layer was shown to relax during the anneals, and \(R\) value reached about 45% after the anneals. Furthermore, it was found that \(R\) values reached a “plateau” quickly during the ramp-up stage of the anneals at 800°C and 840°C. For these anneals, the strain relaxation happened before Si-Ge interdiffusion. With the approximation that \(R\) value is constant after the ramp-up stage of the anneals at 800°C and 840°C, the \(D_{\text{lattice}}(R)\) model gave close predictions of the Ge peak drop in the compressive Si1−yGe y Ge layer. In addition, the impact of the dislocation mediated interdiffusion \(D_{\text{dislocation}}\) was quantified, which is significant for interdiffusivity at lower Ge fractions. A two-term model that combines \(D_{\text{lattice}}\) and \(D_{\text{dislocation}}\) was shown to be very successful in explaining the data of Si-Ge interdiffusion with strain relaxation.

Acknowledgments

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References


Figure 11. Comparison between the total interdiffusivity \(D_{total}\) and \(D_{lattice}\) for RUD40 at 840°C.