

Temperature control of silicon-germanium alloy epitaxial growth on silicon substrates by infrared transmission

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We report the application of the technique of infrared transmission to measure the temperature of silicon wafers during the growth of silicon-germanium alloy heteroepitaxial layers in a rapid thermal processing system. The silicon-germanium alloy layers have negligible absorption at 1.3 and 1.55 μm over wide ranges of thickness, composition, and strain condition. The substantial improvement of the uniformity of layers grown using the technique to measure the temperature for feedback control of the lamp power has also been demonstrated.

The silicon-germanium alloy material system has recently received great attention for silicon-based heterojunction devices such as heterojunction bipolar transistors (HBT's).^{1,2} One promising technique for the growth of these structures involves a combination of rapid thermal processing (RTP) and chemical vapor deposition (CVD), such as limited reaction processing.³ Because of the low growth temperatures ($\sim 600^\circ\text{C}$) which make pyrometry unreliable, results to date have been obtained without any monitoring of the wafer temperature during growth cycles. In this paper, we report the use of the *in situ* measurement of infrared absorption at 1.3 and 1.55 μm to accurately monitor and control the wafer temperature during silicon-germanium growth cycles. The effect of absorption from the silicon-germanium alloy layers has been quantitatively investigated, and improved depth uniformity from feedback-controlled growth cycles has been obtained.

In a previous publication,⁴ the use of *in situ* measurement of infrared absorption was used to infer the temperature of silicon wafers inside a quartz-walled rapid thermal processing chamber in the 400–800 $^\circ\text{C}$ temperature range. In brief, photons from modulated semiconductor lasers at 1.3 and 1.55 μm were projected onto the sample wafer, and the transmitted photon signal was recovered using a lock-in amplifier to eliminate interference from the tungsten-halogen heating lamps. The signal was normalized (divided) by its room-temperature value to remove any dependence on laser power, detector efficiency, scattering from the rough wafer backside, etc. It was found that a change in the sample temperature of 1 $^\circ\text{C}$ caused a relative change in transmission of several percent, which is easily detected by simple electronics.

Assuming an $e^{-\alpha d}$ dependence of the transmitted signal on absorption coefficient α and wafer thickness d , it can easily be shown from the data of Ref. 4 that a $\pm 5 \mu\text{m}$ uncertainty in the thickness of a nominally 450- μm -thick wafer would cause an error in the temperature extracted from the normalized infrared transmission of $\sim 1^\circ\text{C}$. Based on this latitude in thickness, we have routinely applied the technique for the growth of silicon homoepitaxial layers of up to several microns in thickness. Silicon-germanium alloys have a bandgap less than that of silicon, varying from between 1.12 and 0.67 eV.^{5,6} Because of the lower band

gap, and hence increased free-carrier concentration, both the band-to-band and free-carrier absorption of infrared radiation is expected to be larger than that in silicon, which makes the applicability of this technique to the growth of $\text{Si}_{1-x}\text{Ge}_x$ alloys uncertain. As an empirical test, the transmission versus temperature characteristics of a lightly doped (*p*-type, $> 10 \Omega \text{ cm}$) 440- μm -thick wafer was measured in the experimental RTP chamber (Fig. 1). The temperature was measured directly using a tungsten-rhenium thermocouple integrally welded to the center of the wafer. 540 \AA of $\text{Si}_{0.67}\text{Ge}_{0.33}$ was then grown on each side of the same wafer at 625 $^\circ\text{C}$. After the growth of the layer, the transmission versus temperature was again measured using the thermocouple to determine the absolute temperature (Fig. 1). The two sets of data (before and after the $\text{Si}_{1-x}\text{Ge}_x$ growth) were identical to within the stability of the experimental system ($\sim 10\%$).

Although no transmission electron microscopy or x-ray diffraction experiments were performed on this sample, based on our experience with other samples we estimate that the SiGe layer was mostly strained with a relatively small number of misfit dislocations. (The strained state is expected to be a worst case for the technique because of the smaller bandgap compared to the unstrained state.) Since upper limits to the Ge fraction and the alloy thickness for HBT applications are roughly 0.2 and 1000 \AA , respectively, this experiment demonstrates that the technique is applicable to the growth of HBT structures.

After the above experiment, a further 1360- \AA of $\text{Si}_{0.67}\text{Ge}_{0.33}$ was grown on each side of the wafer, and another transmission versus temperature scan was performed. Again the results were indistinguishable from those original substrates, although in this case the layer was probably mostly relaxed. The results of this experiment and several other similar experiments are summarized in Table I. The error bars in the germanium fractions and thicknesses are ± 0.05 and $\pm 20\%$, respectively. For all $\text{Si}_{1-x}\text{Ge}_x$ samples tested (up to 1100 \AA of strained $\text{Si}_{0.55}\text{Ge}_{0.45}$ and 1.1 μm of unstrained $\text{Si}_{0.57}\text{Ge}_{0.43}$) less than a 20% effect was found on the optical transmission near 1.3 and 1.5 μm .

The upper limits of allowable thicknesses were not reached experimentally, but can be estimated by calcula-

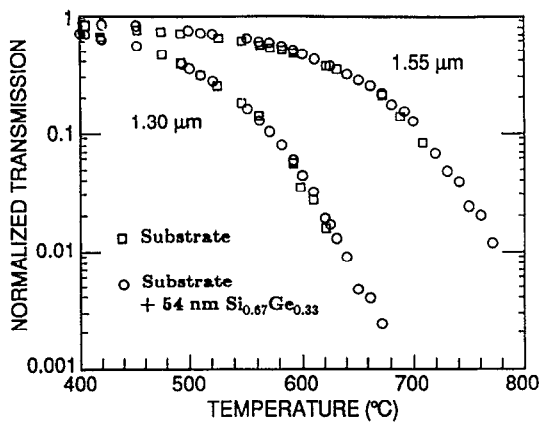


FIG. 1. Normalized transmission (at 1.3 and 1.55 μm) vs temperature for a 450 μm sample before (squares) and after (circles) the growth of 540 $^{\circ}\text{C}$ of $\text{Si}_{0.67}\text{Ge}_{0.33}$ on both sides of the wafer.

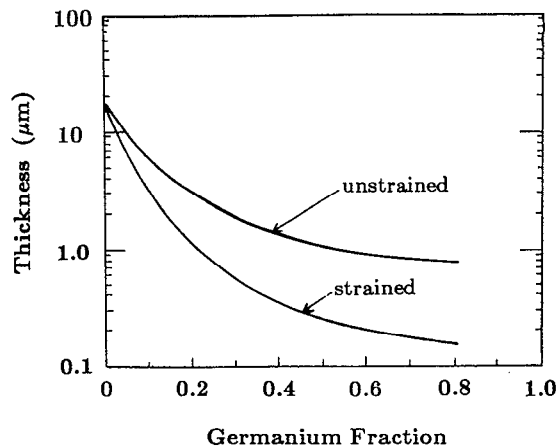


FIG. 2. Predicted thicknesses for a 10% reduction in the 1.3 μm transmission for strained and unstrained $\text{Si}_{1-x}\text{Ge}_x$ layers on silicon substrates at 625 $^{\circ}\text{C}$.

tions. Since the absorption in silicon near 600 $^{\circ}\text{C}$ at 1.3 μm is much greater than that at 1.55 μm ,⁴ absorption at 1.3 μm probably proceeds by a band-to-band process. Assuming that $\text{Si}_{1-x}\text{Ge}_x$ alloys have a band structure similar to that of silicon, one can estimate the 1.3 μm absorption coefficients in $\text{Si}_{1-x}\text{Ge}_x$ using the analytical formula for band-to-band absorption in silicon of Macfarlane *et al.*,⁷ which was simplified by Jellison and Lowndes.⁸ This formula was applied to silicon-germanium alloys by assuming a band structure identical to silicon but with bandgaps smaller than silicon by amounts which do not depend on temperature. Using the bandgap reductions of $\text{Si}_{1-x}\text{Ge}_x$ (compared to that of Si) of Braunstein⁵ and Van de Walle and Martin,⁶ one finds the absorption lengths (inverse of absorption coefficient) presented in Table I. (Since strain in $\text{Si}_{1-x}\text{Ge}_x$ splits band-edge degeneracies to lower the band-edge densities of states, we have probably overestimated the absorption in the strained layers.) A $\sim 10\%$ reduction in transmission could be expected when the total SiGe thickness reached 10% of the absorption length. If the 1.3- μm signal is used to measure temperature near 625 $^{\circ}\text{C}$ on wafers of $\sim 500 \mu\text{m}$ thickness, a 10% reduction in transmission would lead to an overestimation of temperature of $\sim 3^{\circ}\text{C}$. Note that the thicknesses of samples 1–4 in Table I are all indeed less than 10% of the calculated

absorption length. As a guide to future application of the technique, this thickness limit of 10% of the absorption length near 625 $^{\circ}\text{C}$ is plotted versus germanium fraction for both strained and unstrained layers (Fig. 2).

Pure germanium was also grown on a silicon sample with a welded thermocouple at $\sim 625^{\circ}\text{C}$ (sample 4, Table I). In this case a substantial decrease in transmission was already seen at a thickness of 240 \AA . If all of the decrease in transmission is attributed to absorption, the absorption constant of Ge at 625 $^{\circ}\text{C}$ is $\sim 10^5 \text{ cm}^{-1}$. Some of this decrease may have been due to an increase in surface scattering since this growth resulted in a “hazy” surface. (All other films were specular). However, germanium does have an optical transition from a direct bandgap with an energy of only $\sim 200 \text{ meV}$ above the indirect gap (0.9 vs 0.7 eV).⁹ This would cause the strong absorption which would reduce the transmission. Assuming that this direct band-gap scales linearly with the Ge content from its silicon value of 4.1 eV to its germanium value of 0.9 eV, and also assuming a shrinkage of this bandgap with temperature like that of the Ge indirect gap ($\Delta E_G = 340 \text{ meV}$ at 625 $^{\circ}\text{C}$),¹⁰ the direct gap would be accessible at 625 $^{\circ}\text{C}$ to the 1.3 μm photon (956 meV) at a composition of $\text{Si}_{0.12}\text{Ge}_{0.88}$. Beyond this composition one would expect excessive absorption above that predicted by the Macfarlane

TABLE I. Effects of $\text{Si}_{1-x}\text{Ge}_x$ layer growth on transmission at 1.3 and 1.55 μm near 625 $^{\circ}\text{C}$. (s) and (us) indicate layers which are probably strained and unstrained, respectively. Predicted absorption lengths are based on the band gaps in Refs. 5 and 6 and the formulae in Refs. 7 and 8. The thicknesses are the sum of growth on both sides of the wafer. Sample no. 2 consists of 18 SiGe layers in a multiple quantum well structure to preserve strain.

Sample No.	Germanium fraction	Total thickness (μm)	Effect at 1.3 μm	Effect at 1.55 μm	Calculated L_{abs} at 1.3 μm 625 $^{\circ}\text{C}$ (μm)
1	0.33 (s)	0.11	< 20%	< 20%	4.6
1	0.33 (us)	0.38	< 20%	< 20%	16
2	0.45 (s)	0.11	< 20%	< 20%	2.7
3	0.43 (us)	1.1	< 20%	< 20%	13
4	1.0 (us)	0.024	– 25%	< 20%	...
4	1.00 (us)	0.048	– 50%	– 25%	...
4	1.00 (us)	0.096	– 75%	– 45%	...

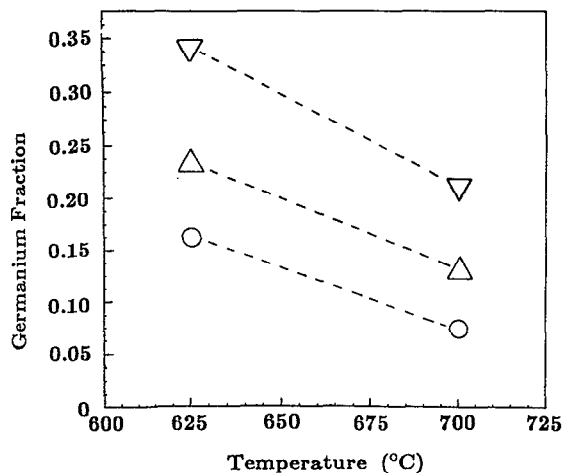


FIG. 3. The effect of growth temperature on atomic germanium fraction for three different growth conditions.

model for indirect absorption. Therefore the predictive application ranges of Fig. 2 have not been extended past a composition of 85% Ge.

The accurate control of the sample temperature during the CVD growth of silicon-germanium alloys is crucial for controlling the growth rate, which in the range of 600–700 °C is in the strongly temperature-dependent surface-reaction-limited regime. Furthermore, the temperature also has a strong effect on the germanium fraction of the grown layers.¹¹ Figure 3 presents data for the germanium fraction for three different gas flow conditions for growth at both 625 and 700 °C. The germanium fraction is substantially lower at higher growth temperatures. The advantage of active temperature control using feedback from infrared transmission during the growth of $\text{Si}_{1-x}\text{Ge}_x$ alloys is evident in Fig. 4. This figure shows secondary ion mass spectroscopy (SIMS) profiles of two samples with buried $\text{Si}_{1-x}\text{Ge}_x$ layers grown near 625 °C. During the alloy growth in each sample the gas flows were held constant. In the sample where a fixed lamp power was used without any

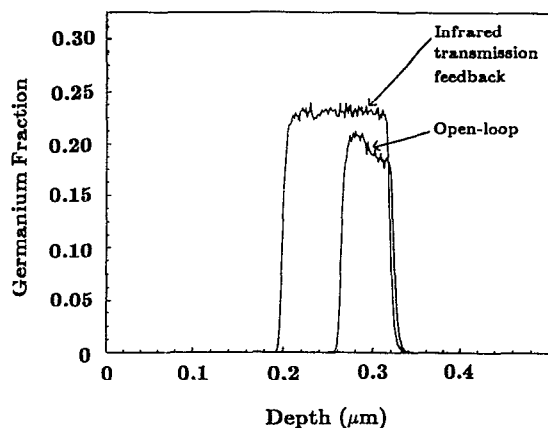


FIG. 4. SIMS profile of Ge concentration in layers grown at fixed power ("open-loop") and in layers grown with temperature control feedback.

active temperature control (open-loop), a gradual increase in the germanium content (0.18–0.21) was observed. According to the data in Fig. 3, this increase in germanium fraction can be explained by a ~ 20 °C drop in the wafer temperature over the duration of the growth (~ 5 min). This slow drop in temperature is understandable since immediately before the alloy growth a high-temperature growth cycle (~ 1000 °C) was performed, and there would be a slow cooling of the reactor background. In contrast, a second layer was grown under similar conditions except that the wafer temperature, as measured by infrared transmission technique, was held constant by using feedback to control the lamp power. The improvement in the layer uniformity is obvious. Note that if the SiGe alloy had caused excessive extra absorption of the infrared signal, the control system would have compensated by reducing the wafer temperature to increase transmission, and an increase in the germanium fraction would have been noted. That this does not occur is consistent with the data presented earlier.

In summary, the technique of temperature measurement by infrared transmission has been applied to the RTP-CVD growth of $\text{Si}_{1-x}\text{Ge}_x$ alloys on silicon substrates. The alloys have negligible effect on the transmitted photon intensity at ~ 625 °C for strained $\text{Si}_{0.55}\text{Ge}_{0.45}$ layers up to at least 0.11 μm thick and unstrained $\text{Si}_{0.57}\text{Ge}_{0.43}$ layers up to at least 1.1 μm thick. For pure Ge layers, an upper thickness limit of 0.02 μm has been established. Application of the technique to temperature feedback yields improved sample uniformity compared to samples grown at a fixed lamp power.

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