SiGe relaxation on silicon-on-insulator substrates: An experimental and modeling study

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The strain relaxation behavior of $\text{Si}_{0.82}\text{Ge}_{0.18}$ films on silicon-on-insulator (SOI) substrates was investigated for films grown beyond the critical thickness and strain-relaxed during growth and metastable films, grown beyond the critical thickness, which relaxed during subsequent thermal annealing. The thickness of the top silicon layer of the SOI substrate was varied over a range from 40 nm to 10 μm . In all cases, the SiGe film relaxation occurred via the nucleation and propagation of dislocations with the same onset of film relaxation and same relaxation rate for both SOI and bulk Si substrates. The SOI substrate does not serve as a compliant substrate but does alter the dislocation structure and motion. The buried amorphous oxide layer in the SOI substrate leads to the relaxation of the dislocation strain field through the removal of the dislocation line tension. This removal of the dislocation line tension drives dislocation motion and leads to the development of strain in the thin Si layer of the SOI substrate. Models of this dislocation behavior for SiGe growth on the SOI substrate are presented and calculation of the equilibrium strain of the thin Si substrate layer closely fits the measured strain of several SOI substrates. The article addresses the implications of the modified dislocation structure and kinetics for film relaxation on SOI substrates. © 2003 American Institute of Physics. [DOI: 10.1063/1.1628406]

I. INTRODUCTION

Film strain is a critical parameter controlling the electrical and optical properties of epitaxial semiconductor thin films. A wide range of properties within the same materials system can be accessed by manipulating strain in addition to film composition. Strained-layer structures have been used in a wide variety of device structures in both elemental and compound semiconductor materials. In the case of Si β SiGe technology, the modification to the local electronic structure has been effectively used in heterojunction bipolar and heterojunction field effect transistors. Two key heterojunction device parameters are band offsets and carrier mobilities, and both parameters are controlled by the detailed strain state of the heterojunction layers.^{1,2} The choice of substrate and film composition will determine the strain in the device structure. As an alternative to a Si substrate, compositionally graded strain-relaxed layers of SiGe, grown on a Si substrate, can be used to adjust the lattice parameter of the surface layer to possess a value between that of Si and Ge. Such substrates offer opportunities in device design and materials integration. This lattice constant increase and film relaxation results from the formation and motion of dislocations. Pseudomorphic Si- and Ge-rich films can then be deposited, strained to the lattice constant of the relaxed buffer layer. A Si-rich SiGe

film grown on a relaxed SiGe film will be under a tensile strain with a band offset to the SiGe layer that allows for electron confinement in the Si layer. Conversely, holes will be confined in Ge-rich layers that are the compressively strained relative to a lower Ge composition SiGe relaxed film. This ability to control carrier placement has been exploited to form modulation-doped field effect transistors as well as electron- and hole-based resonant tunneling diodes.^{2–4} In addition, the lattice matching of relaxed Ge to GaAs has been utilized to fabricate InGaP visible light-emitting diodes on Si substrates.⁵

The increase in the lattice constant of an epitaxial SiGe film, as it develops from a pseudomorphic to a partially or fully strain-relaxed layer, is accomplished by the introduction and extension of misfit dislocations at the film/substrate interface. The total length of the misfit dislocations at this interface governs the absolute amount of film relaxation. The ends of these misfit dislocations terminate at the film surface by means of threading segments. These threading segments extend from the plane of the interface to the surface with a change in the dislocation line direction. These threading segments can penetrate active device areas in subsequently grown layers and degrade carrier mobility, increase junction leakage currents, and produce variations in the threshold voltage of field effect transistors.^{6–8} Numerous research efforts have pursued threading dislocation reduction over the past decade and have demonstrated considerable achievements. A wide variety of growth methods involving the

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growth of different buffer layer structures, altering growth temperatures, and the use of surfactants have reduced the threading dislocation density (TDD) of films containing 20%–30% Ge to 10^4 – 10^5 cm $^{-2}$.^{9–12}

In this study, we have investigated the influence of a silicon-on-insulator (SOI) substrate on the SiGe film relaxation process. Reports have indicated reductions in the TDD by a factor greater than 10^5 between identical growths on bulk Si and SOI substrates.^{13–15} Explanations for this behavior have differed. Legoues, *et al.*^{13,14} described the improvement as due to compliant substrate effects, where the buried SiO $_2$ layer allows the top Si and SiGe layers to share the misfit strain decoupled from the underlying thick substrate. The dislocation image force derived from the buried oxide layer was also suggested as playing a key role.¹⁵ Both of these sets of experiments employed SOI substrates having a top Si layer, which will be referred to as the Si–SOI layer, that was less than 60 nm thick. Both mechanisms for the defect reduction are also critically dependent on the Si–SOI being thin, either near the film critical thickness (22 nm for 18% Ge) or within the range of the image force, <40 nm. In order to determine the specific dislocation mechanisms occurring during film relaxation, we have focused on SOI substrates having a wide range of Si–SOI layer thicknesses, i.e., 40, 70, 330, or 10 000 nm and the use of ultrahigh vacuum chemical vapor deposition for SiGe growth.¹⁶

Throughout this investigation, a single composition, Si $_{0.82}$ Ge $_{0.18}$, was studied. The film composition of $\sim$ 18% Ge was chosen in order to allow control over the growth morphology for the range of growth temperatures used here. SiGe growth at high temperatures or at a high Ge film composition favors a three-dimensional (3D) island growth mode.¹⁷ An islanded surface lowers the activation barrier for dislocation nucleation and leads to the rapid formation of a high density of dislocations.¹⁸ By maintaining a smooth film, dislocation nucleation is kinetically limited and dislocation-free films can be grown well beyond the critical thickness for dislocation formation allowing for the exploration of the influence of the SOI substrate under a variety of growth and processing conditions.

Several aspects of dislocation motion and the associated strain relaxation of a SiGe film on a SOI substrate were investigated. Companion samples of identical SiGe films grown on bulk Si substrates were used throughout the study as a control and for comparison. The role of growth morphology, specifically the transition from two-dimensional (2D) to 3D growth modes, was investigated. The strain relaxation of pseudomorphic SiGe films through postgrowth *ex situ* high-temperature annealing was determined. These results are compared to the experimentally determined film relaxation processes occurring during the growth of substantially thicker films, grown above the thickness for dislocation introduction during growth. Throughout the study, x-ray diffraction was used to measure the strain state of the various SiGe and Si layers. Atomic force microscopy (AFM) quantified the surface morphology of the films at various stages of growth and annealing. The dislocation distribution throughout the samples was determined by cross-sectional transmis-

sion electron microscopy (XTEM) and plan-view transmission electron microscopy (PVTEM)

A major experimental finding in this study was that the Si–SOI layer becomes strained following relaxation of the SiGe films. This strain is a product of dislocation motion in the Si–SOI layer. The extent and details of this motion is the result of the interaction of the lattice-mismatch-derived dislocations with the amorphous oxide. This interaction results in the removal of the dislocation strain field present at the Si–SOI–oxide interface. In addition to producing strain in the Si–SOI, the reduced dislocation line tension removes the critical thickness condition and increases dislocation velocities.

II. EXPERIMENTAL PROCEDURES

A. SiGe growth and growth morphology

Film growth was carried out in a cold-wall, ultrahigh vacuum chemical vapor deposition system using 10% SiH $_4$ and 5% GeH $_4$ diluted in H $_2$ at 23 mTorr.¹⁹ Films were grown having a composition of $\sim$ 18% Ge. The composition reproducibility of this growth system for these samples is $x_{\text{Ge}} = 0.18 \pm 0.005$. This film composition allows for control of the growth morphology with temperature. SiGe films were grown to a thickness of 150 nm at 550, 630, and 670 °C, whereas the film grown at 700 °C roughened immediately and was only grown to 6 nm. The SiGe film surface was monitored during growth with differentially pumped reflection high-energy electron diffraction (RHEED).²⁰ Following growth, AFM was used to measure the surface roughness and the size and distribution of the island.

B. *Ex situ* film relaxation

Metastable and pseudomorphic Si $_{0.82}$ Ge $_{0.18}$ films were grown to 150 nm on bulk Si, 40 nm SOI, and 70 nm SOI substrates. All of the SOI substrates used in this work were bonded, not separation by implantation of oxygen- or SIMOX-based, SOI wafers. This film thickness of 150 nm is seven times greater than the critical thickness of 22 nm, yet the films remain fully strained, as verified by x-ray measurements. Following growth at 630 °C and the initial x-ray characterization, these films were annealed under N $_2$ for 1 h at temperatures as high as 1050 °C to induce relaxation and after which they were again characterized by x-ray diffraction. Reciprocal space maps (RSMs) of the (004) reflections were used to measure the film relaxation and associated lattice tilts. A slit in front of the x-ray detector limited the detector acceptance angle to 325 arc sec during the acquisition of the RSMs.

C. *In situ* film relaxation

In the another set of experiments, uniform Si $_{0.82}$ Ge $_{0.18}$ films were relaxed *in situ* by growth at 630 °C to a substantially greater thickness than used in the *ex situ* studies. Substrates for these films included bulk Si, 40 nm SOI, 70 nm SOI, 330 nm SOI, and 10 000 nm SOI. A film thickness of 150 nm, 340 nm, 765 nm, and 1200 nm was selected to span the realized levels of film relaxation from 0% to 80%. Analysis of the grown layers consisted of x-ray diffraction, AFM,

FIG. 1. AFM scans of 150 nm SiGe samples grown at 550 °C (a), 630 °C (b), 670 °C (c), and 700 °C (d). All the images are $10 \times 10 \mu\text{m}$ and plotted on a 15 nm height (grayscale) scale. The rms roughness of the samples is 0.3, 0.4, 0.7, and 3.0 nm exhibiting an increase with growth temperature. The insets to (c) and (d) are *in situ* [110] RHEED diffraction patterns.

and transmission electron microscopy (TEM). Film relaxation was calculated using the film-to-substrate peak separation from the [004] data and the composition from the 150 nm nonrelaxed samples grown under identical growth conditions. Only the thicker films from this sample set provided sufficient x-ray diffracted intensity to allow the acquisition of RSMs with the higher resolution analyzer crystal ($< 5 \text{ arc sec}$).

III. EXPERIMENTAL RESULTS

A. Control of SiGe islanding through growth temperature

The relationship between growth morphology and growth temperature observed for a series of 150 nm thick SiGe films is shown in the AFM images of Fig. 1 for films grown at different temperatures. These surfaces, as measured by AFM, have a root-mean-square (rms) roughness of 0.3, 0.4, and 0.7 nm for growth at 550, 630, and 670 °C respectively. The insets in Figs. 1(c) and 1(d) present the *in situ* RHEED diffraction patterns from the SiGe 150 nm films. The films grown at a temperature below 670 °C yielded the same RHEED diffraction pattern as shown in the inset of Fig. 1(c). The single intensity maximum on each vertical streak indicates diffraction from a flat 2D surface. The RHEED pattern from the film grown at 700 °C, [Fig. 1(d) inset] exhibits multiple maxima on each streak, indicating 3D diffraction and hence the presence of island growth. This surface roughness develops after only 6 nm of film growth in contrast to the smooth surface achieved on the 150 nm thick

FIG. 2. RSMs of the (004) reflection of 150 nm SiGe films on both bulk Si [(a), (b), and (c)] and 40 nm SOI [(d), (e), and (f)] substrates after annealing. SiGe film relaxation is observed following annealing at 950 °C and 1050 °C.

TABLE I. Summary of x-ray data from annealed films listing percent relaxation, (FWHM), and the percent strain in the Si–SOI layer for the substrates studied.

Anneal temperature (°C)	Substrate type	SiGe film thickness	SiGe film % relaxation	SiGe film FWHM	Si–SOI % in-plane strain
875	Bulk Si	150 nm	0	78.8 ± 1.3	...
875	40 nm SOI	150 nm	0	73.5 ± 0.7	0
950	Bulk Si	150 nm	15 ± 2	212 ± 11.0	...
950	40 nm SOI	150 nm	11 ± 2	185 ± 7.0	-0.037 ± 0.004
950	70 nm SOI	150 nm	14 ± 2	219 ± 12.0	-0.027 ± 0.004
1050	Bulk Si	150 nm	51 ± 2	850 ± 22.0	...
1050	40 nm SOI	150 nm	46 ± 2	822 ± 11.0	interdiffused

film grown at lower temperatures. AFM micrographs of the sample shown in Fig. 1(d) reveals a dense network of SiGe islands populating the surface with an rms roughness of 3 nm after only 6 nm of film growth. While film strain provides a driving force for roughening, the slow surface diffusion at growth temperatures below 700 °C preserves smooth film morphology. The film-islanding occurring at 700 °C leads to the rapid nucleation of dislocations. In order to reduce the dislocation nucleation, all subsequent film growths were carried out at 630 °C. This temperature represents a balance between the low temperatures needed to achieve a smooth surface, and hence control over dislocation nucleation, and the elevated growth temperatures required for a high dislocation velocity.

B. Ex situ film relaxation

Film relaxation due to postgrowth annealing was monitored through changes in the x-ray RSMs. A summary of the x-ray diffraction RSMs of the metastable films following annealing is presented in Fig. 2. A slight initial angular tilt (± 500 arc s) across the oxide of the bonded SOI substrate is apparent and allows the bulk Si substrate and the Si–SOI layer to be measured independently. This tilt is a result of the small difference in alignment between the orientation of the handle wafer and the Si–SOI layer during manufacture of the SOI substrate. At annealing temperatures of 875 °C, film relaxation was not observed on either the bulk Si or SOI substrates. Strain relaxation was observed as movement of the SiGe diffraction peak apparent in the RSMs for samples undergoing the 950 °C and 1050 °C anneals. The x-ray data are summarized in Table I. The film relaxation leads to an increase in the crystal tilts within the SiGe layer, producing a broadened peak width and crosshatch that is apparent in AFM images of the film surface in Fig. 3. The progression from a metastable to a relaxed film occurs at the same rate and temperature for the bulk Si, 70 nm SOI (not shown), and 40 nm SOI substrates. The surface morphology of these samples is unchanged between the initial growth surfaces [Figure 1(b)] and after annealing at 875 °C [Figs. 3(a) and 3(d)]. These metastable films, after annealing, exhibit the very initial stages of crosshatch associated with the strain relaxation processes, with trenches extending hundreds of micrometers in length at a spacing of tens of micrometers. Samples annealed at 950 °C possessed a densely crosshatched surface, seen in Figs. 3(b) and 3(e). The cross-

hatched film surface, when combined with the film relaxation observed in the x-ray diffraction of Figs. 2(b) and 2(e), indicates that a large misfit dislocation density is present in the SiGe films.

Additional information can be gained through monitoring the peak shift in the RSM of the Si–SOI layer. After annealing at 875 °C, the Si–SOI layer has the bulk lattice constant of Si. Following the anneal at 950 °C, the SiGe film peak broadens and surface crosshatch appears, due to the introduction and motion of dislocations. The 950 °C annealed SOI samples also exhibit a small amount of in-plane strain in the Si–SOI layer of 0.047% and 0.035% for the 40 and 70 nm SOI substrates. It is interesting to note that if this tensile strain in the Si–SOI layer were attributed to purely compliant substrate effects, associated with a “compliant” oxide layer, a much greater strain would be predicted. A model of a purely compliant substrate would predict strain partitioning between the SiGe and Si–SOI layers which would leave the Si–SOI layer with a tensile strain of 0.16% and 0.11% for the 40 and 70 nm SOI substrates, respectively. The observed strain is approximately four times less than that predicted through a purely compliant substrate model. Additionally, the strain in the Si–SOI layer only appears with the onset of dislocation-based relaxation of the SiGe film and not simply through thermal annealing alone, as would be expected when the oxide serves to form the compliant medium within the compliant substrate structure.

FIG. 3. AFM micrographs of the films after annealing. Crosshatch is observed in samples on both bulk Si and SOI substrates which received the 950 °C and 1050 °C anneals.

FIG. 4. Cross-sectional micrographs of the (a) bulk Si and (b) 40 nm SOI samples following 950 °C annealing. An arrow indicates the placement of the SiGe–Si interface. Substrate dislocations extend several microns into the bulk Si, while on the SOI substrate they cross the SOI layer and terminate at the oxide. Dislocation contrast is not observed at the buried oxide interface of the SOI substrate.

After annealing at 1050 °C, the diffraction peak from the Si–SOI layer diminished greatly in intensity and the peak shifted toward the SiGe diffraction peak. This peak shift is due to significant interdiffusion between the SiGe and Si–SOI layer that is apparent after annealing at 1050 °C. Numerical simulations of the interdiffusion process confirm that the interdiffusion would lead to a Ge compositional gradient across the Si–SOI layer from 18% Ge at the SiGe–Si–SOI interface to at least 1% Ge at the oxide interface after a 1050 °C anneal.

The X-ray diffraction and AFM measurements have confirmed the presence of dislocations that relax the SiGe film. XTEM was also carried out on samples annealed at 950 °C to determine the distribution of these dislocations within the material. Dislocations are easily observed in films on both bulk Si and SOI substrates as shown in Fig. 4. For films grown on the bulk Si substrate [shown in Fig. 4(a)] dislocations loops appear at least 2 μm into the Si substrate. Pairs of associated dislocations on parallel glide planes are observed in the substrate as previously described in Ref. 20. The substrate dislocations in the SOI substrate simply cross the 40 nm Si–SOI layer to the buried oxide. There is no dislocation-based contrast along the Si–SOI/SiO₂ interface in the TEM micrographs. This lack of contrast in the TEM micrographs has been directly observed at room temperature for dislocations at metal/amorphous material interfaces.^{21–23} In these previous studies, the dislocation core was found to dissipate by core-spreading at the interface, reducing the elastic distortion and energy of the dislocation core. This core-spreading is likely to be taking place at the Si/SiO₂ interface in this study. The amorphous layer is able to reorient, on the atomic scale, to absorb the displacement of the core leading to a final result that is very similar to the behavior of a dislocation reaching or interacting with a free surface.

While a larger density of dislocations is observed extending into the Si–SOI layer than into the companion bulk Si substrate under similar growth conditions, no film threading dislocations were observed in the small areas of the Si–SOI layer probed by the XTEM, putting an upper limit on the threading dislocation density near 10^7 per cm². An

equivalent density of threading dislocations is observed in the film grown on the bulk Si substrate.

C. *In situ* film relaxation

In the previous series of samples, the 150 nm films grown on the bulk Si or SOI substrates remain fully strained following growth and cooling to room temperature. An increase in the film thickness to 340 nm however leads to the initiation of film relaxation on all the substrates during the growth process. The Pendellosung thickness fringes present in the RSMs of Figs. 2(a) and 2(d) diminish in intensity and the SiGe peak broadens as a result of the *in situ* strain relaxation. The misfit dislocation density is still too low, however, to cause a measurable shift in the diffraction peak position. Film growth to 765 nm and 1200 nm did result in observable amounts of strain relaxation as indicated by peak shifts in the respective RSMs. The triple crystal RSMs from these films, grown on a bulk Si substrate, 330 nm and 40 nm SOI substrates, are presented in Fig. 5. The degree of film relaxation, as indicated in the peak shift and peak width, is nearly identical for the 765 nm and 1200 nm thick films grown on all the various substrates. The only variation in the RSMs with a substrate is the shift in the position of the Si–SOI diffraction peak. The peak from the bulk Si substrate is also broadened upon the growth of the SiGe film, similar to the 330 nm Si–SOI layer, whereas the 40 nm Si–SOI diffraction peak is below the detection limits of the x-ray measurement system. It is notable from these RSMs that the peak position of the 330 nm Si–SOI peak is shifted to positive Bragg angles. Analysis of the 40 nm and 70 nm SOI samples, with the lower resolution but higher signal intensity detector slit, allows the shift of the diffraction peak from the thin Si–SOI layer to positive Bragg angles to also be observed. This peak shift was not detectable in the 10 000 nm SOI sample. A larger Si–SOI peak shift is observed for the 1200 nm film over the 765 nm film as expected from the greater strain relaxation in the 1200 nm film. This positive shift of Bragg angle indicates a reduction in the Si–SOI out-of-plane lattice constant and a resultant tensile strain. Table II contains a summary of the x-ray data for the *in situ* relaxed samples. The full width at half maximum is measured in the tilt direction of Fig. 5.

TEM micrographs from the *in situ* relaxed samples confirm the presence of dislocations. Dislocations are also indicated by the crosshatch and the increased x-ray peak breadth observed for these samples. XTEM micrographs in Fig. 6 show a high density of misfit dislocations at the SiGe/Si interface. Film threading dislocations are observed in all the samples as well as a high density of dislocations that extend and terminate at the buried oxide. As with the annealed samples, the dislocations that reach the oxide do not show any contrast in the TEM micrograph indicating that the strain field associated with the core of the misfit dislocations at the Si/SiO₂ interface has been largely dissipated. Additionally, stacking faults are present in all the thick relaxed films grown on both bulk Si and SOI substrates. The presence of stacking faults has been previously reported when relaxing highly strained films, such as Ge on relaxed Si_{0.70}Ge_{0.30},²⁴

FIG. 5. Triple crystal RSMs of the (004) reflection of *in situ* relaxed films. The upper and lower rows were obtained from films grown to a thickness of 765 nm and 1200 nm, respectively. From the left- to the right-hand side, the RSMs were determined from samples are grown on a bulk Si substrate, 330 nm SOI substrate, and 40 nm SOI substrate.

and in a graded SiGe buffer layer grown with a grading rate above $>27\%$ per μm .²⁵ In the XTEM micrograph of Fig. 6(b), a stacking fault with at least six associated dislocations is observed. The density of dislocations indicates that the stacking fault strongly interacts with the threading dislocations. The PVTEM micrographs of the 1200 nm films relaxed on bulk Si, 300 nm SOI, and 40 nm SOI, are shown in Fig. 7. These specimens were prepared by thinning from the substrate side so that only the SiGe film is imaged by TEM. All three samples have stacking faults and threading dislocations present. The blocking of dislocation motion by stacking faults, prevalent on all the substrates, increases the TDD

TABLE II. SiGe and Si-SOI layer strain data.

Film thickness (nm)	Substrate	SiGe film relaxation (%)	SiGe in-plane % strain	Dislocation density (μm)	Si-SOI in-plane % strain	Dislocation density at film/substrate interface (μm)	Dislocation density at Si-SOI/SiO ₂ interface (μm)
340	330 nm SOI	0	-0.67	0	0	0.0	0.0
340	Bulk Si	0	-0.67	0	...	0.0	0.0
765	40 nm SOI	76	-0.16	27	0.196	10.0	17.0
765	70 nm SOI	67	-0.22	23	0.133	6.9	16.1
765	330 nm SOI	72	-0.20	24	0.0501	2.6	21.4
765	Bulk Si	70	-0.21	24	...	...	...
1200	40 nm SOI	75	-0.167	26	0.218	11.0	15.0
1200	70 nm SOI	84	-0.054	32	...	...	...
1200	330 nm SOI	81	-0.120	29	0.0693	3.6	25.4
1200	10 μm SOI		-0.154	27	0.0		
1200	Bulk Si		-0.074	32	...	...	...

FIG. 6. Dislocation are observed in the XTEM micrographs obtained from the 1200 nm SiGe films grown on (a) bulk Si and (b) 330 nm SOI substrates. An arrow indicates the placement of the SiGe-Si interface. The stacking fault in (b) has accumulated at least six dislocations that have glided to it from the right-hand side.

which ranges from 10^8 cm^{-2} on bulk Si, to $5 \times 10^7 \text{ cm}^{-2}$ on 330 nm SOI, and $2 \times 10^7 \text{ cm}^{-2}$ on 40 nm SOI.

Many of the dislocations in the PVTEM micrographs lie on common glide planes. This arrangement is the product of a dislocation multiplication process during film relaxation, which has been previously observed in SiGe films.^{20,26} The buried oxide of the SOI substrate does not appear to interfere with these multiplication processes.

The AFM micrographs of all the *in situ* relaxed films exhibit the dislocation-derived crosshatch, as shown in Fig. 8. These films have a similar rms roughness ranging from 4.9 to 6.4 nm. Morphological differences are observed, however, on a finer scale. All of the surface trenches run the full width of the scan range for the SiGe films grown on the bulk Si substrates. This behavior is also present on the 10 000 nm SOI, which also has a high density of surface mounds. On the 330 nm and 40 nm Si-SOI substrates, only the deepest trenches run the length of the $10 \mu\text{m}$ scans. Many shallow trenches run only a short distance. This is contrasted with the crosshatch structure of the films that relaxed during the *ex situ* annealing shown in Fig. 3. All of these *ex situ* annealed films exhibited very long uniform trenches, which were only present on the *in situ* relaxed bulk Si and 10 000 nm SOI samples. Similar *in situ* observations were made using low-energy electron microscopy, as described in Ref. 27.

IV. DISCUSSION AND MODELING

A. Film relaxation on silicon-on-insulator substrates

The dependence of the SiGe film relaxation on both the temperature and film thickness for Si and SOI substrates, whether induced by high-temperature annealing or during growth, is essentially identical. In all cases, a large density of misfit dislocations at the Si/SiGe interface are inferred from the increased x-ray diffraction peak width, the surface crosshatch, and, more directly, in the TEM micrographs. These

FIG. 7. PVTEM micrographs of the 1200 nm SiGe films grown on (a) bulk Si, (b) 330 nm SOI, (c) 40 nm SOI substrates in which the shaded rectangular regions are stacking faults present in these films.

results cannot be attributed to a compliant substrate mechanism, which would relax the film without the introduction of dislocations in the SiGe film. In addition, the amount of strain transfer to the Si-SOI layer, required by the compliant substrate mechanism, was not observed in the x-ray diffraction. Compliant substrate theory predicts a tensile strain in the Si-SOI layer. This tensile strain is only observed in this study after extensive dislocation-based film relaxation. In both the *ex situ* and *in situ* samples, an appreciable dislocation density is also apparent from the diffraction peak width.

Compliant substrate strain sharing between the SiGe film and the Si-SOI layer was not present in any of the growth or annealing experiments. Film relaxation was only observed due to dislocation nucleation and propagation. Dislocations nucleate and propagate across the sample relaxing the film, with segments extending into the substrate. The dislocations in either the bulk Si or Si-SOI layers are the product of the

FIG. 8. AFM micrographs obtained from the *in situ* relaxed SiGe layers which were 1200 nm thick and grown on substrates consisting of (a) bulk Si, (b) a 10 000 nm SOI substrate, (c) a 330 nm SOI substrate, and (d) a 40 nm SOI substrate. The long, even trenches apparent in Fig. 6(a) are contrasted with the much shorter shallower trenches in (c) and (d).

strong dislocation interactions, which push dislocations into the underlying layers. These dislocation interactions have been observed and modeled for a variety of cases including dislocation multiplication processes during perpendicular and parallel crossings of dislocations.²⁰ The strain field interaction between dislocations provides the driving force to move the dislocations into the Si–SOI layer and has a far greater influence on dislocation motion than the dislocation image force attributed to the buried oxide.¹⁵ On the SOI substrates, the dislocations penetrating into the Si–SOI layer can reach the buried amorphous Si–SOI/oxide interface. The substrate dislocations, pictured in the XTEM of the 40 nm Si–SOI layer in Fig. 4(b), all directly cross the layer and terminate at the oxide. In the 330 nm Si–SOI layer in Fig. 6(b), the majority of the dislocations continue to reach the buried oxide layer. Throughout these series of samples, no dislocation-based contrast was observed at the Si/SiO₂ interface in the TEM micrographs. Therefore, the growth temperature of 630 °C is sufficient for substantial dislocation core-spreading to occur during the film growth at this interface.

This change in the dislocation structure occurs with no observed changes in the onset of film strain relaxation or the relaxation rate. This result suggests that the rate limiting steps governing film relaxation are largely taking place in the film and not in the substrate or at the film–substrate interface.

B. Strain in the Si–Si-on-insulator layer

Dislocation core-spreading has been observed, *in situ*, at interfaces between metals and amorphous layers.^{28–31} The lack of an extended crystal structure in the amorphous layer enables atomic motion, transforming the large and very local displacement of the dislocation core into smaller displacements spread along the interface through plastic deformation of the amorphous layer.^{32,33} This accommodation of the dislocation by the oxide reduces the strain, and ultimately removes the strain associated with the dislocation core and the accompanying dislocation line tension. This reduction in the dislocation line tension drives dislocation motion through the Si–SOI layer.

The amount of misfit dislocation length transferred from the SiGe/Si interface to the Si/SiO₂ interface can be experimentally determined from the change in strain of the layers. Each dislocation changes the lattice constant by an amount equal to the pure edge component of the Burger's vector in the plane of the interface. The 60° dislocations found in the SiGe system have a Burger's vector of the type $a/2[011]$, and the relevant edge component is $a/\sqrt{2}[110] = 0.193$ nm. The average spacing of these dislocations can be determined from the change in in-plane strain of the layer.⁹

$$\text{Dislocation Density} = \frac{\Delta \epsilon}{|b_{\text{edge}}|}. \quad (1)$$

The calculated dislocation density is included in Table II. The observed 75% relaxation of the 1200 nm film on the 40 nm SOI substrate requires 26 dislocations per micron. The dislocation density can also be calculated for the dislocations that have moved across the Si–SOI layer. The production of 0.22% strain in the Si–SOI layer requires 11 dislocations per micron to have moved to the oxide interface, which leaves 15 dislocations per micron at the film/substrate interface. Similar dislocation densities exist at both interfaces, however, the dislocations at the crystalline interface are clearly visible in the XTEM micrographs, while they are not visible at the amorphous interface. The dislocation density at the amorphous interface varies between 2.6 to 11 per micron for the samples examined.

The dislocation loops extending into the bulk substrate will also cause a tensile strain to develop in the top microns of the Si substrate. In this case, there will be a broad distribution of strain states present in depth into the bulk Si substrate. Observation of this strain with an x ray is difficult due to the broad distribution of strain states over the diffraction sampling depth of tens of microns. In Fig. 5, the bulk substrate diffraction peak is clearly broader than the handle substrate of the SOI wafers. The diffracted intensity in the tail of the Si substrate peak is not symmetric with intensity broadening toward tensile-strained Si, i.e., positive Bragg angle.

C. Equilibrium strain of Si–Si-on-insulator

A schematic layout of the film and SOI substrate with respect to dislocation propagation is depicted in Fig. 9. A segment of the dislocation loop in the SiGe film has moved down to the SiO₂ interface. The threading dislocation (TD) segments are labeled TD_F and TD_S, which cross the SiGe

FIG. 9. Plot of the strain observed in the Si-SOI layers following SiGe relaxation. The critical strain of Eq. (3) closely fits the data. The strain from neglecting the presence of the oxide layer is drawn dotted as well as the compliant substrate model, both overstate the observed strain.

film and Si-SOI layer respectively. The film misfit dislocation (MD_F) is the conventional misfit dislocation lying at the SiGe/Si interface, while MD_{OX} is the misfit dislocation at the SiO₂ interface. The right-hand side of the loop shows the possibility of TD_F and TD_S merging and removing MD_F from the interface. The dislocation energetics and resulting critical or equilibrium strains in the layers are discussed below.

The line tension of MD_F must be known in order to calculate the equilibrium strain of the Si-SOI layer. The conventional dislocation line tension is defined by having the dislocation adjacent to a free surface and within an infinite substrate:

$$F_{MD_F} = \frac{\mu |\mathbf{b}|^2 [1 - \nu \cos^2(\alpha)]}{4\pi(1 - \nu)} \ln\left(\frac{h_F}{|\mathbf{b}|}\right), \quad (2)$$

where α is the angle between the Burger's vector and the dislocation line, μ is the shear modulus, $|\mathbf{b}|$ is the magnitude of the Burger's vector, ν is Poisson's ratio, and h_F is the film thickness. It is important to note that the equations for the dislocation line tension are accurate to $\sim 20\%$.

The dislocation line tension will be reduced by the local presence of the SiO₂ layer on the SOI substrate, which has a smaller shear modulus, 0.333 GPa, than Si, 0.681 GPa. Dislocation core-spreading further reduces the strain in the oxide and decreases the dislocation line tension. Three different line tensions are calculated and evaluated against the experimental data. Equation (2) represents the upper limit for the line tension and is termed model 1. The smaller shear modulus of the oxide can be accounted for in an approximate manner in model 2 by using the average shear modulus of the oxide and Si in Eq. (2). In model 3, the oxide interface is described as a free surface that is able to completely absorb the dislocation strain field while the core is tens of nanometers from the oxide interface. The line tension for this case of a dislocation in a free plate has been calculated to be:³³

$$F_{MD_F} = \frac{\mu |\mathbf{b}|^2 [1 - \nu \cos^2(\alpha)]}{4\pi(1 - \nu)} \ln\left(\frac{h_S h_F}{|\mathbf{b}|(h_S + h_F)}\right), \quad (3)$$

where h_S is the Si-SOI thickness. In the limit of a conventional substrate, $h_S \gg h_F$, Eq. (3) reduces to Eq. (2).

FIG. 10. Schematic of a misfit dislocation half-loop penetrating into the substrate. The threading and misfit dislocations are labeled, TD and MD respectively. Motion of the TDs determines the strain of the layers and the MD lengths.

The net force associated with the Si-SOI layer strain, and the line tension of both MD_{OX} and MD_F determine the motion of TD_S in the Si-SOI layer. Initially, the strain in the Si-SOI layer is zero, and the dislocation core spreading of the oxide reduces MD_{OX} to zero. Therefore TD_S will move to the left-hand side in the diagram of Fig. 9.

The SiGe film relaxation evolves by moving TD_F to the left-hand side schematically in Fig. 9, which increases the in-plane lattice constant of the film. Left-hand sideward motion of TD_S within the Si-SOI layer in Fig. 9 also increases the in-plane lattice constant of the Si-SOI layer, subsequently producing a tensile strain in the Si-SOI layer. This dislocation motion is the source of the tensile strain present in the Si-SOI layer observed in Fig. 5. Misfit dislocation length will continue to be transferred from MD_F to MD_{OX} as TD_S moves across the Si-SOI layer, until the strain in the Si-SOI is large enough to impede and stop the motion of TD_S . The force on the threading dislocation from the film strain, F_{TD_S} , is given by⁹

$$F_{TD_S} = \frac{\mu(1 + \nu)}{(1 - \nu)} \varepsilon_s |\mathbf{b}| h_S, \quad (4)$$

where ε_s is the strain in the Si-SOI layer. Equilibrium is established and TD_S stops moving when F_{TD_S} equals F_{MD_F} . For model 3, where F_{MD_F} is the line tension for a dislocation in a free plate, Eq. (3), the equilibrium strain is given by

$$\varepsilon^* = \frac{|\mathbf{b}| [1 - \nu \cos^2(\alpha)]}{4\pi h_S (1 + \nu)} \ln\left(\frac{h_S h_F}{|\mathbf{b}|(h_S + h_F)}\right). \quad (5)$$

A higher or lower strain state in the Si-SOI layer would lead to TD_S motion allowing the layer to approach this equilibrium strain state. The calculated equilibrium strain according to these three models is plotted with the measured strain from the Si-SOI layers in Fig. 10. The lower three lines correspond to the three models presented above to describe the line tension of MD_F . The solid dark line in Fig. 10 represents the results of model 3 in which the oxide behaves as a free surface represented in Eq. (5). The dotted line uti-

lizes the average shear modulus of the oxide and the Si described in model 2, and the dashed line is for the case of an infinitely thick Si substrate, model 1. The equilibrium strain of a perfectly compliant substrate, where the SiGe film and Si-SOI layers are decoupled from the substrate, is also plotted in Fig. 10. In a compliant substrate, the mismatch strain is divided between the layers such that the strain of the SiGe and Si-SOI layers is given by³⁴

$$\varepsilon_S = -\varepsilon_m \frac{h_F}{h_S + h_F}, \quad \varepsilon_F = \varepsilon_m \frac{h_S}{h_S + h_F}, \quad (6)$$

where ε_m is the mismatch strain between Si and the SiGe film. A compliant substrate model predicts a much higher strain level in the Si-SOI than was observed.

The equilibrium strain for the case of the infinite Si substrate, as well as the incorporation of the reduced shear modulus due to the softer oxide, over predict the observed strain. The best fit is obtained for model 3, which treats the oxide as a free surface. Several important conclusions can be reached from this analysis. The oxide is able to remove the line tension of MD_{OX} at the oxide interface, and the fit of model 3 to the data suggests that the oxide is able to reduce the strain field of the dislocations that remain within a distance of 40 and 70 nm from the oxide interface. In order for these effects to occur, atoms in the oxide must be able to move and remove the strain in the oxide layer attributed to the line tension and strain field of the misfit dislocation. When the dislocation reaches the oxide interface, the oxide will be locally displaced by the length of the Burger's vector, 0.38 nm. The oxide is capable of this local atomic-scale motion, evidenced by the lack of dislocation contrast at the amorphous interface in the XTEM micrographs. The atomic displacements at the oxide interface, resulting from dislocations at or near the oxide interface, need only be of the magnitude of a fraction of an Angstrom. The fit of model 3 suggests that the oxide is also able to undergo these small displacements at the growth temperature of 630 °C.

D. Critical thickness for misfit dislocation formation

A stated benefit of a compliant substrate has been the increase of the SiGe film critical thickness. Changes in the dislocation structure in the SOI substrate are not due to such compliant substrate behavior, but due to the buried oxide affecting the detailed energy and force balances governing dislocation motion. By reducing the MD_F line tension, the oxide stabilizes the formation of the misfit dislocation through the decrease in its energy, which has the effect of actually reducing the film critical thickness. Beyond a critical thickness, TD_F will glide and extend MD_F. The forces on TD_F are the line tension of the MD_F, from Eq. (3), and the film strain from Eq. (4). Equating these forces determines the critical thickness, h_F^* , to be

$$h_F^* = \frac{|\mathbf{b}|[1 - \nu \cos^2(\alpha)]}{4\pi\varepsilon_F(1 + \nu)} \ln\left(\frac{h_S h_F^*}{|\mathbf{b}|(h_S + h_F^*)}\right). \quad (7)$$

The resulting critical thickness is plotted in Fig. 11 for Si-SOI thicknesses of 5 nm, 15 nm, and a conventional substrate thickness of 500 μm . The reduction in the Si-SOI

FIG. 11. Plot of the critical thickness for a strained film on a SOI substrate. Thinner substrate layers decrease the film critical thickness. The % reduction of the critical thickness by a 5 nm is plotted in (b).

thickness decreases the film critical thickness by stabilizing the misfit dislocation formation. The percent of reduction of the critical thickness by the 5 nm Si-SOI substrate is plotted in Fig. 11(b) and ranges from 35% to over 60%.

E. Relaxation without misfit dislocation formation

The values of the critical thickness or strain of the SiGe film and Si-SOI layer are derived from a force balance between the respective threading dislocation and MD_F. These values will be altered if MD_F is not present and TD_S and TD_F merge into a single segment. In this case, there are no misfit dislocations at the Si/SiGe interface as schematically described in the right-hand side half of Fig. 2. The layers will subsequently have a common in-plane lattice constant and the strain in the two layers would sum to the original mismatch strain between the Si and SiGe

$$\varepsilon_m = \varepsilon_{\text{SiGe}} - \varepsilon_{\text{Si-SOI}}. \quad (8)$$

Strain is transferred between the layers as a single threading segment moves within the bilayer. The equilibrium strain distribution is determined from the force balance on the TD in each layer coupled through Eq. (8). This result is the same equilibrium strain as the compliant substrate case of Eq. (6). The compliant substrate strain distribution is derived by setting the sum of the compressive and tensile stresses of the two layers to zero at equilibrium³⁴

$$\frac{2\mu(1 + \nu)}{(1 - \nu)} \varepsilon_S h + \frac{2\mu(1 + \nu)}{(1 - \nu)} \varepsilon_F h = 0, \quad (9)$$

allowing the mechanical constants to be the same for the SiGe and Si.

The force on the TDs is this derived stress multiplied by the Burger's vector and the geometrical factor as expressed in Eq. (4). Since the Burger's vector and the TD orientation is the same in both layers, these terms cancel out, leading to the same strain distribution between the layers which is identical to the compliant substrate case. While the final strain

FIG. 12. Plot of strain as a function of thickness for a $\text{Si}_{0.82}\text{Ge}_{0.18}$ film on a 40 nm Si-SOI layer. The top half is the film strain, which is reduced due to dislocation motion with and without formation of a MD. The lower graph is the strain that develops in a 40 nm Si-SOI layer.

states achieved for the compliant substrate and the model presented here are the same, the pathways to energy reduction are quite different.

The buried oxide, which allows TD motion and film relaxation without the formation of a misfit dislocation at the SiGe/Si-SOI interface, removes the constraint of a critical thickness for film relaxation. At any film thickness, it is energetically favorable to move dislocations and redistribute the strain according to Eq. (6). The SiGe film will initially relax by transferring strain to the Si-SOI layer through the movement of the dislocation to the oxide interface. The SiGe is pseudomorphic to the Si-SOI during this stage of relaxation, and the in-plane lattice constant of both layers is increasing from the value for bulk silicon. Further deposition and relaxation of the strained film will exceed the critical strain of the Si-SOI layer resulting in the extension of misfit dislocations at the Si/SiGe interface instead of the oxide interface. At this point, the system is transitioning from the right- to the left-hand side half of Fig. 9.

Figure 12 is a plot of the possible strains for a $\text{Si}_{0.82}\text{Ge}_{0.18}$ film grown on a 40 nm Si-SOI layer as a function of SiGe film thickness. The solid line is the mismatch strain between Si and $\text{Si}_{0.82}\text{Ge}_{0.18}$. The dotted line of Fig. 12 traces the strain distribution according to Eq. (6), while the dashed line is the equilibrium strain of the layers due to misfit dislocation extension, Eq. (5). The system will follow the pathway of least energy or strain. At the onset of growth, the strain in the SiGe layer will relax as the Si-SOI becomes strained following the dotted lines in Fig. 12. The Si-SOI layer reaches its critical strain level at a SiGe film thickness

of 13 nm. TD_S of Fig. 9 will stop gliding, while TD_F continues to glide, which extends MD_F . The layer strains are now following the dashed lines as MD_F extends at the SiGe/Si-SOI interface.

Thinner Si-SOI layers will have the effect of shifting the crossover point to a greater film thickness. A 20 nm Si-SOI layer would shift the point to 25 nm of SiGe film thickness while an 11 nm Si-SOI layer would remove the crossover all together. At 11 nm, the strain of an infinitely thick $\text{Si}_{0.82}\text{Ge}_{0.18}$ film can be transferred to the Si-SOI without the formation of a misfit dislocation at the SiGe-to-Si-SOI interface.

The dislocation nucleation process is often a kinetically limited process, preventing film relaxation from following such equilibrium predictions. However, when threading dislocations are already present, the critical thickness is an accurate predictor of misfit dislocation formation.³⁵ SiGe-on-Insulator (SGOI) substrates have a TDD of $\sim 10^6$ per cm^2 and have been fabricated as thin as 9 nm.³⁶ A strained Si film deposited on this SGOI substrate would be expected to follow the relaxation behavior described in Fig. 12.

F. Effect on dislocation velocity

The reduction in the dislocation strain field and line tension due to the buried amorphous layer can reduce the SiGe critical thickness and film strain. This phenomenon will also affect dislocation velocities in the layers. The equilibrium or critical strain occurs when the layer stress equals the line tension of the misfit dislocation. When these values are not equal, TDs in the layer move, bringing the layer toward the equilibrium strain state. The TD velocity is proportional to the difference between the film stress and line tension of the dislocation, which is defined as the excess stress.^{37,38} By decreasing or removing the line tension of the misfit dislocation, the buried amorphous oxide increases the magnitude of the excess stress and hence the dislocation velocity.

The buried amorphous layer will also increase the dislocation mobility, in addition to increasing the driving force for threading dislocation glide. Dislocation glide occurs by the nucleation of kinks, both by pairs of kinks within the film and single kinks from the film surface. The buried oxide provides a second interface for single kink nucleation. The oxide both increases the ease of kink formation as well as the driving force for kink formation, contributing to an increased dislocation velocity. Higher dislocation velocities will allow film relaxation to occur with a lower density of dislocations, providing for a reduced final threading dislocation density in the SiGe film.

These processes may explain the dislocation motion results of Dehm and Arzt.³¹ Their *in situ* TEM experiment observed dislocation loops in Cu meeting an amorphous SiN_x interface. The Cu/ SiN_x interface was described as a dislocation sink, removing dislocations from the TEM micrographs. The dislocation velocity was estimated at 3–25 nm/s, while moving and expanding within the Cu film. The dislocation velocity accelerated to greater than 50 nm/s when the dislocation reached the SiN_x interface. The change in excess stress resulting from dislocation core spreading and addi-

tional kink formation would lead to such an increase in dislocation velocity.

V. CONCLUSIONS

We have studied the SiGe relaxation on SOI substrates utilizing high temperatures to initiate relaxation of metastable films, as well as *in situ* relaxation of films by growth of the SiGe film to a thickness well beyond any critical thickness. SOI substrates used in this study had a thickness of 40 nm, 70 nm, 330 nm, or 10 000 nm. On Si and SOI substrates, film relaxation was initiated at the same thickness or temperature, progressed at the same rate, and developed a cross-hatched surface. The film TDD had a modest reduction from 10^8 cm^{-2} on bulk Si to $5 \times 10^7 \text{ cm}^{-2}$ on 330 nm SOI, and $2 \times 10^7 \text{ cm}^{-2}$ on 40 nm SOI. No evidence of compliant substrate behavior was observed. While the crosshatch occurring for SiGe growth on a bulk Si substrate involves trenches running hundreds of microns in length, the crosshatch on SOI included some short trenches that were only a few microns in length. A primary structural difference between growths on bulk Si versus Si-SOI layers was the development of strain in the Si-SOI layer, which varied inversely with Si-SOI layer thickness from 0.17% for the 40 nm Si-SOI to 0 for both the 10 000 nm SOI and bulk Si substrates. The strain in the Si-SOI layer was modeled by describing the dislocation structure for the case where the SiO_2 layer behaves as a free surface. Atomic motion within the oxide near the Si-SOI/oxide interface would remove the dislocation strain field for dislocations at the oxide interface and within the Si-SOI layer. The reduction in the dislocation strain fields decreases the dislocation line tension stabilizing misfit dislocation formation. The removal of the line tension of the dislocation at the oxide interface results in TD motion and film relaxation occurring without encountering an initial critical thickness limitation. The dislocation motion, changes in critical thickness, and the increased dislocation velocity derived from the response of the amorphous layer to the dislocation strain field should be observable in other heteroepitaxial systems incorporating strain and a buried or surface amorphous layer.

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