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An effective compliant substrate for low-dislocation relaxed $Si_{1-x}Ge_x$ growth

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Abstract. An effective compliant substrate for $Si_{1-x}Ge_x$ growth is presented. A silicon-on-insulator substrate was implanted with B and O forming 20 wt % borosilicate glass within the SiO_2. The addition of the borosilicate glass to the buried oxide acted to reduce the viscosity at the growth temperature of $Si_{1-x}Ge_x$, promoting the in situ elastic deformation of the thin Si (~ 20 nm) layer on the insulator. The sharing of the misfit between the Si and the $Si_{1-x}Ge_x$ layers was observed and quantified by double-axis X-ray diffraction. In addition, the material quality was assessed using cross-sectional transmission electron microscopy, photoluminescence and etch pit density measurements. No misfit dislocations were observed in the partially relaxed 150-nm $Si_{0.75}Ge_{0.25}$ sample as-grown on a 20% borosilicate glass substrate. The threading dislocation density was estimated at $2\times10^4\,cm^{-2}$ for 500-nm $Si_{0.75}Ge_{0.25}$ grown on the 20% borosilicate glass substrate. This method may be used to prepare compliant substrates for the growth of low-dislocation relaxed SiGe layers.

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High-mobility strained Si, $Si_{1-x}Ge_x$, and Ge have attracted considerable attention for their potential applications in high-frequency devices [1, 2]. This has stimulated considerable interest in the study of relaxed $Si_{1-x}Ge_x$ buffer layers, which can be used as "virtual substrates" for the growth of high-mobility structures and the integration of III–V devices on Si [3, 4]. However, the large lattice mismatch ($\sim 4.17\%$) between Si and Ge usually results in a high density of dislocations in the SiGe buffer layer at high Ge content. Moreover, threading dislocations can propagate through the SiGe buffer layer into the active layers on top, degrading the electrical and optical performance of the devices [5, 6]. To date, several techniques have been used to grow relaxed SiGe layers having a low threading dislocation density, including graded composition growth [7], low-temperature buffer layers [8]. However, the buffer layers have to be relatively thick in order to achieve low dislocation densities for device applications. In some cases, these schemes offer inadequate improvement in the material quality required to realize significant dividends in device performance.

Recently, it was found that compliant substrates could be used for lattice-mismatched epitaxy by accommodating part of the strain in the thin substrate and absorbing the threading dislocations. The idea was proposed by Lo [9] and was attempted experimentally by Powell et al. using silicon-on-insulator (SOI) substrates at relatively high annealing temperatures [10]. Thin Si-on-SiO_2 has also been shown, at high temperature, to be a compliant substrate for SiGe and GaN growth by several groups [11–13]. In the case of SiGe, the SiO_2 is expected to be rigid in the growth temperature range necessary for SiGe epitaxy (typically between 450 °C and 700 °C). The inability of the Si layer to deform at these substrate temperatures limits the use of the Si layer for sharing the misfit strain during epitaxy. As a result, the relaxed SiGe layers grown on these types of substrates exhibited a large number of dislocations [11]. Therefore, to achieve a better compliant substrate, it is necessary to promote the in situ accommodation of the misfit. This could be realized provided that, at growth temperatures, the SiO_2 layer becomes soft and the Si layer deforms. Borosilicate glass (BSG) has been known to have a lower softening temperature than SiO_2 [14]. In this work, we used borosilicate glass to decrease the softening temperature of SiO_2 and anticipated that the Si layer on the glass could become strained during the growth to accommodate the misfit strain. For further epitaxy, the underlying thin Si layer may eventually be dislocated to accommodate the whole misfit. Substrates having different concentrations of BSG in the SiO_2 layer of SOI wafers were fabricated. These substrates are called BSG substrates in this paper.

1 Experimental procedure

The fabrication process for the BSG substrates was as follows: SOI wafers with a 60-nm Si layer and a 400-nm buried layer of SiO_2 were implanted with boron and oxygen with an implant dosage and energy selected according to the stoi-

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chiometric ratio of B_2O_3 and the target concentration by weight [15]. After implantation, a two-step annealing process was performed to form the single crystal Si layer and the BSG layer. Solid phase epitaxy was performed at 500 °C for 2 h in nitrogen ambient. The wafers were subsequently annealed at 900 °C for 5 h in nitrogen ambient to form the borosilicate glass, as well as to minimize implantation damage. The top Si layer was thinned down to about 20 nm by thermal oxidation and then dipped in 2% HF. The surface morphology was analyzed by atomic force microscopy and found to be suitable for molecular beam epitaxy, with a root mean squared roughness measured at 0.3 nm. The substrates were cleaned and immediately loaded into a Perkin-Elmer MBE system for SiGe epitaxy.

BSG substrates with three weight ratios, 5%, 10% and 20% B_2O_3, were used for SiGe epitaxy. The epitaxy sequence consisted of a 10-nm Si buffer layer and a 150-nm $Si_{0.75}Ge_{0.25}$ layer. The growth temperature for both layers was 500 °C. The nominal deposition rates of Si and Ge were 1.2 Å/s and 0.4 Å/s, respectively. The sample grown on the 5% BSG substrate is named the 5% BSG sample in this paper, and likewise for the other samples. In order to study the relaxation behavior of the SiGe layer and the formation of misfit dislocation for the samples grown on the compliant and non-compliant substrates, the annealed samples were measured.

Symmetric and asymmetric double-axis X-ray diffraction (DAXRD) measurements were used to determine the composition and relaxation of the SiGe layers. Cross-sectional transmission electron microscopy (XTEM) was used to observe the dislocation distribution and estimate the dislocation density.

2 Results and discussion

DAXRD symmetric (004) and asymmetric (113) measurement results for the as-grown 5% and 20% BSG samples are shown in Fig. 1. From the peak separation between the SiGe and Si substrate, the Ge composition and the relaxation of the SiGe layer were calculated. The scans were repeated after rotation by 180° and no tilting between the epilayer and substrate was observed. The technique of X-ray diffraction allowed measurement of the relaxation independent of the dislocation density, which could be estimated by XTEM.

The DAXRD results for as-grown and annealed samples are summarized in Table 1. For the 5% BSG sample, due to the presence of misfit dislocations at the SiGe/Si interface, as seen in Fig. 2a, the SiGe peaks were broadened as a result of the mosaic structure. After annealing, the SiGe layer became fully relaxed, just as SiGe on a planar Si substrate. For the 20% BSG sample, the much smaller full width at half maximum (FWHM) of the SiGe peaks indicates a much lower density of misfit dislocation, which was subsequently confirmed by the XTEM results. As the 20% BSG softened

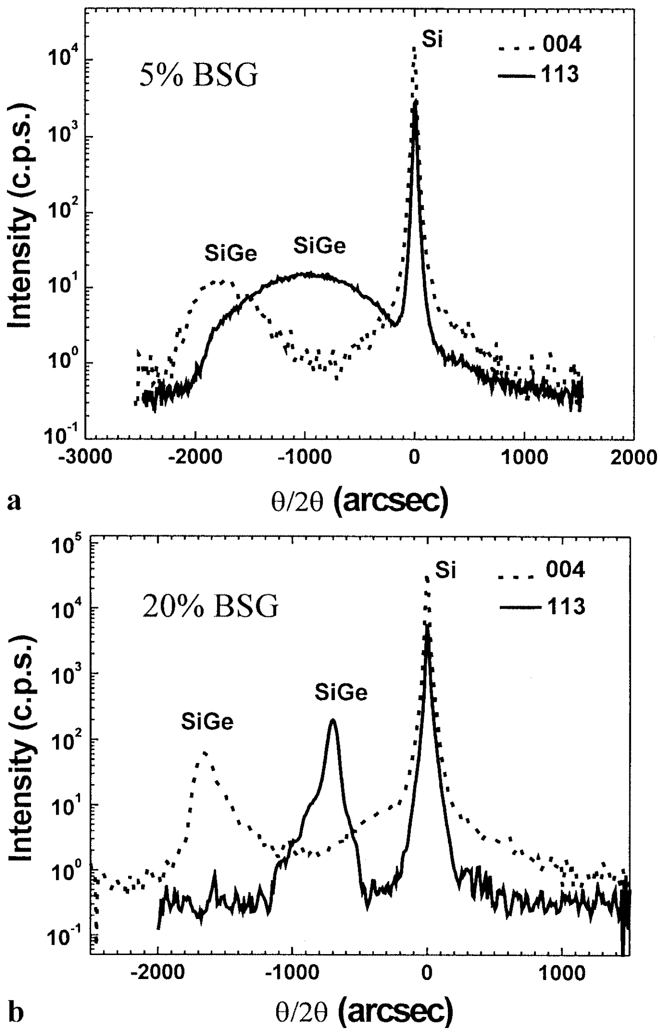

Fig. 1a,b. Symmetric (004) and asymmetric (113) DAXRD measurements for: **a** the as-grown 5% BSG sample; **b** the as-grown 20% BSG sample. The structure of the sample is 150-nm $Si_{0.75}Ge_{0.25}$/10-nm Si/20-nm Si/BSG

at the growth temperature, the thin Si layer became strained during growth and there was much less misfit between the Si layer and the SiGe layer. The relaxation of the SiGe layer after the strain equalization in the bilayer was later calculated to confirm the strain sharing between the SiGe layer and the Si layer. After annealing, the SiGe layer relaxed further, but was not fully relaxed as in the case of the SiGe layer on planar Si substrate.

The quality of the SiGe layer was further assessed using XTEM. The density of misfit dislocations was estimated from several XTEM images taken at different magnifications. The maximum range of observation was about 5 μm. For the as-grown 5% BSG sample, the density of misfit dislocation was estimated to be $8 \times 10^4\ cm^{-1}$. After having been annealed

Table 1. Ge composition, relaxation of SiGe, and FWHM of the (004) scan SiGe peak from DAXRD for 5% BSG and 20% BSG samples, before and after annealing at 850 °C

Sample	Ge composition (x)	Relaxation (%)	FWHM of SiGe Peak for (004) (arcsec)
As-grown 5% BSG	0.28 ± 0.02	79 ± 10	590
Annealed 5% BSG	0.28 ± 0.02	99 ± 3	610
As-grown 20% BSG	0.23 ± 0.01	64 ± 3	140
Annealed 20% BSG	0.23 ± 0.01	85 ± 2	233

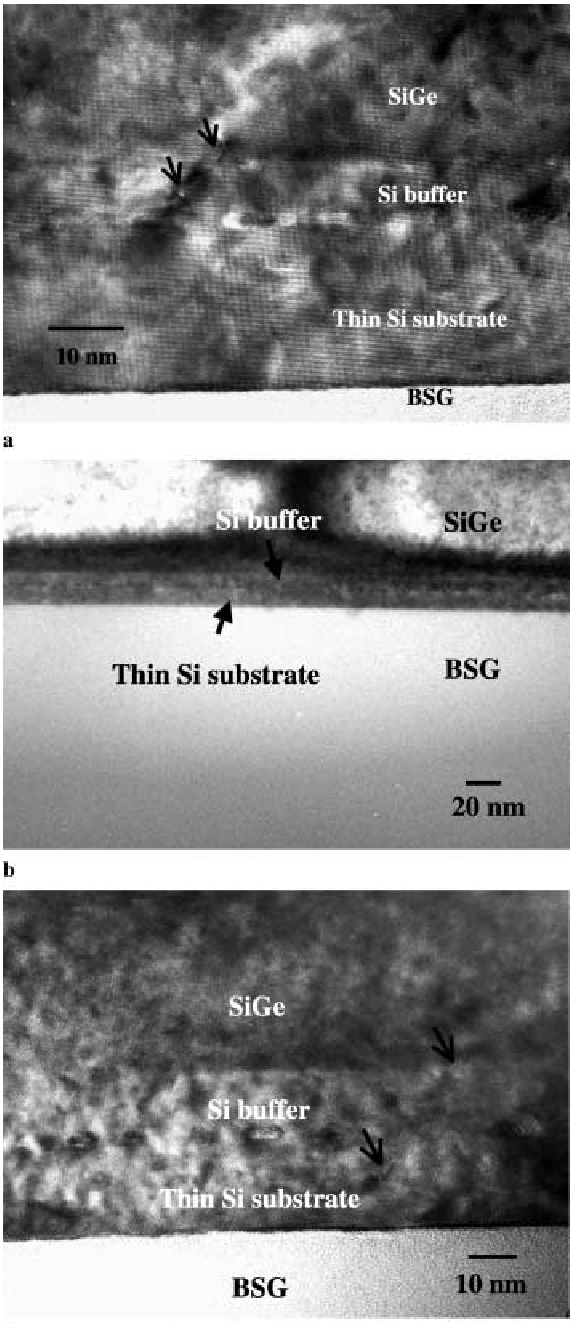

Fig. 2. XTEM image of: **a** the as-grown 5% BSG sample; **b** the as-grown 20% BSG sample; **c** the 20% BSG sample annealed at 850 °C for 30 min in ambient nitrogen. The *arrow* (→) indicates the dislocation

at 850 °C for 30 min, the density of misfit dislocation at the SiGe/Si interface increased to $1.6\times10^5\,\mathrm{cm}^{-1}$. From high-resolution XTEM images, no dislocation was observed to nucleate in the Si substrate, suggesting that the Si substrate was not strained. As the softening temperature of 5% borosilicate glass was estimated to be about 850 °C [14], which is much higher than the growth temperature of 500 °C, the Si layer was not strained in order to accommodate the misfit strain associated with the SiGe layer during growth.

For 20% BSG sample (shown in Fig. 2b), no misfit dislocation was observed at the interface between the SiGe and Si layers in any of the images, suggesting that the density was below $2\times10^3\,\mathrm{cm}^{-1}$. Compared with the as-grown and annealed 5% sample, this density is more than one order of magnitude lower. After having been annealed at 850 °C for 30 min, as shown in Fig. 2c, the density of misfit dislocation at the SiGe/Si interface increased to about $1\times10^4\,\mathrm{cm}^{-1}$ and threading dislocations propagated downwards into the Si buffer layer. No threading dislocation was observed in the SiGe layer. Combined with the DAXRD results, it may be concluded that the 20% BSG layer was softened at the growth temperature of 500 °C and the thin Si layer became strained accommodating the the misfit strain during growth. During the 850 °C annealing, the Si substrate relaxed and threading dislocations formed within it.

From the strain sharing model [16], the strain for the Si (ε_1) and SiGe (ε_2) films is given by:

$$\varepsilon_1=\frac{B_2h_2(1/a_1-1/a_2)}{a_2(B_1h_1/a_1^2+B_2h_2/a_2^2)}$$

and

$$\varepsilon_2=\frac{B_1h_1(1/a_2-1/a_1)}{a_1(B_1h_1/a_1^2+B_2h_2/a_2^2)}\,,$$

where a_1 and a_2 are the relaxed (cubic) lattice constants of Si and SiGe, respectively; and h_1 and h_2 are the thickness of the Si and the SiGe; B_1 andB_2 are material constants, given by $(2G_i(1+\nu_i)/(1-\nu_i)(i=1\sim2))$, where G_i and ν_i are the shear modulus and the Poisson's ratio of the Si and the SiGe, respectively. To minimize the total energy, $(E=B_1\varepsilon_1^2h_1+B_2\varepsilon_2^2h_2)$, the two films will reach a common lattice constant a_0. The lattice constants and elastic constants of Si and Ge from published data [17] were used and the corresponding constants for SiGe were interpolated. The equilibrium strain part of the mismatch strain in the $Si_{0.25}Ge_{0.75}$ layer was then calculated to be 32.6%. This value implied that the relaxation of the SiGe layer was about 100%–32.6% = 67.4%, which was remarkably close to the 64% relaxation in SiGe layer obtained from the DAXRD results for the 20% BSG sample. Thus, for the 20% BSG sample, the misfit strain was allowed to equalize between the SiGe layer and the Si layer during growth.

Many photoluminescence (PL) studies have been devoted to bulk SiGe alloys and thick MBE SiGe layers [18, 19]. It has been proved that PL emission is very sensitive to the relaxation of SiGe and dislocations. Chu et al. showed that a broad peak close to 0.8 eV in MBE-grown SiGe showed a different behavior to that of the compliant substrate. The peak would disappear if the thin Si layer was behaving as a compliant substrate. As a result, PL was proven to be a sensitive method to confirm the compliant effect [11]. In this work, SiGe samples grown on different substrates (SOI, BSG) were measured using PL to check their compliant effect. All measurements were performed at 4.5 K using the 488-nm line from an Ar^+ laser.

The PL results for the 150 nm $Si_{0.75}Ge_{0.25}$ samples grown on SOI and BSG substrates are shown in Fig. 3. The integrated intensity ratio of the broad peak at ~0.8 eV to the Si-Si TO peak of the substrate is shown in the inset. It was found that the ratio decreased uniformly from the SOI to the 20% BSG sample. This was because the mismatch strain between the SiGe and the Si layer was transferred to the Si layer

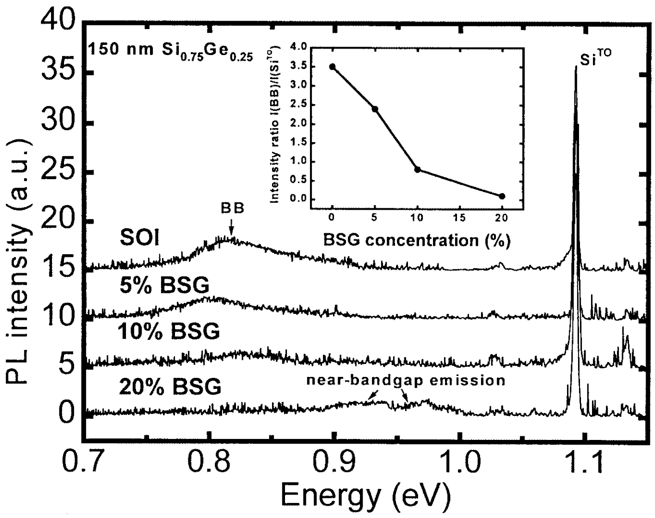

Fig. 3. 4.2 K photoluminescence spectra of the 150-nm $Si_{0.75}Ge_{0.25}$ on SOI, 5%, 10%, and 20% BSG substrates

either fully or partially, depending on the viscosity of the BSG layer. For the 20% BSG substrate, the BSG layer was so soft during growth that there was almost no mismatch strain at the SiGe/Si interface. The peaks of the near-band-gap emission of SiGe (~ 0.95 eV) were observed in the 20% BSG sample, which indicated the relatively high quality of the SiGe layer in this sample.

The final purpose of our compliant substrates was to grow high-quality relaxed SiGe films, especially those having low threading dislocation density. Thus, thicker SiGe samples were grown on different substrates to check the performance of the compliant substrate. The samples were grown on SOI, 5%, 10% and 20% BSG substrates at the same time. The epitaxy sequence consisted of a 10-nm Si buffer layer and a 500-nm $Si_{0.75}Ge_{0.25}$ layer. The growth temperature for both layers was 500 °C. Material quality was evaluated using a modified Schimmel etch [20] to reveal crystalline defects, which were observed using Nomarski interference microscopy. The micrographs are shown in Fig. 4. From the etch pits on the surface, the density of threading dislocations were estimated to be about 2×10^6 cm^{-2}, 4×10^5 cm^{-2}, 1.5×10^5 cm^{-2}, and 2×10^4 cm^{-2} for SiGe grown on SOI, 5%, 10% and 20% BSG substrates, respectively. The much lower threading dislocation density on the surface of the SiGe layer grown on the 20% BSG substrate was due to the in situ strain sharing effect of the substrate. According to Fitzgerald et al. [21], a 2.5-μm SiGe layer with compositions graded up to $Si_{0.75}Ge_{0.25}$, grown with 10% Ge μm^{-1} had a threading dislocation density of about 10^5 cm^{-2}. According to Li et al. [8], a 500-nm $Si_{0.7}Ge_{0.3}$ layer grown on a low-temperature Si buffer layer had a threading dislocation density of about 10^5 cm^{-2}. The threading dislocation density of the 500-nm $Si_{0.75}Ge_{0.25}$ on the 20% BSG substrate in this work was similar to or better than the above results.

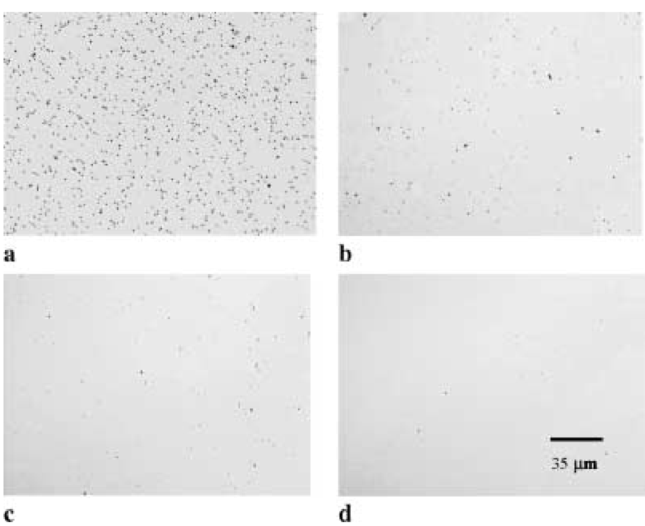

Fig. 4a–d. Nomarski micrograph showing etch pits for the 500-nm $Si_{0.75}Ge_{0.25}$ grown on: **a** SOI substrate; **b** 5% BSG substrate; **c** 10% BSG substrate; **d** 20% BSG substrate. The etch pit density is about 2×10^6 cm^{-2}, 4×10^5 cm^{-2}, 1.5×10^5 cm^{-2} and 2×10^4 cm^{-2}, respectively

3 Summary

In summary, an effective compliant substrate was successfully fabricated by forming a 20% concentration of B_2O_3 borosilicate glass in the SiO_2 layer of a SOI wafer and thinning down the Si layer. It was observed that the compliant substrate accommodated part of the misfit strain between the SiGe layer and the Si layer during growth. This kind of substrate therefore may be used to provide low dislocation density growth of relaxed SiGe layers for device applications.

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