

High-germanium-content SiGe islands formed on compliant oxide by SiGe oxidation

Haizhou Yin^{a)}

Center for Photonics & Optoelectronic Materials and Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544

K. D. Hobart and F. J. Kub

Naval Research Laboratory, Washington, DC 20375

S. R. Shieh and T. S. Duffy

Department of Geosciences, Princeton University, Princeton, New Jersey 08544

J. C. Sturm

Center for Photonics & Optoelectronic Materials and Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544

(Received 18 November 2003; accepted 19 March 2004; published online 20 April 2004)

The oxidation of $\text{Si}_{1-x}\text{Ge}_x$ islands on a compliant viscous borophosphosilicate glass (BPSG) was utilized to achieve nearly fully relaxed $\text{Si}_{1-x}\text{Ge}_x$ with germanium content up to 57%. After $\text{Si}_{1-x}\text{Ge}_x$ islands were formed on BPSG by layer transfer, dry oxidation was carried out to form pure silicon dioxide on the top and to increase germanium content in the $\text{Si}_{1-x}\text{Ge}_x$ layer. Surface roughening and the nonuniformity of the enhanced germanium content during the SiGe oxidation were improved by depositing a silicon dioxide capping layer before oxidation. The strain arising from the increase of germanium content was relaxed by lateral expansion of the SiGe islands, showing that dislocations were not required in the process. © 2004 American Institute of Physics. [DOI: 10.1063/1.1738514]

Relaxed $\text{Si}_{1-x}\text{Ge}_x$ with high germanium content has drawn attention for various applications. High-quality pseudomorphic germanium can be directly deposited on relaxed $\text{Si}_{1-x}\text{Ge}_x$ with high germanium content to serve as the conduction channel for high-performance *p*-type metal-oxide-semiconductor field-effect transistors.¹ Due to its large lattice constant, which is closer to that of III-V semiconductors than that of silicon, relaxed $\text{Si}_{1-x}\text{Ge}_x$ with high germanium is often used as a buffer layer for integrating III-V semiconductors with silicon substrates.² Conventionally, relaxed $\text{Si}_{1-x}\text{Ge}_x$ with high germanium content has been obtained by growing compositionally graded $\text{Si}_{1-x}\text{Ge}_x$ much thicker than critical thickness so as to introduce dislocations to relax strain in the $\text{Si}_{1-x}\text{Ge}_x$.³ Although the density of dislocations in relaxed SiGe by this approach has been greatly reduced over time, the control of dislocations is still challenging and requires optimization for dislocation suppression. In addition, the thick $\text{Si}_{1-x}\text{Ge}_x$ films needed for strain relaxation through dislocations (on the order of a few microns, with a typical grading rate of 10% germanium increment per 1 μm) poses a serious bottleneck for throughput.^{2,3}

An approach for achieving high germanium content in relaxed $\text{Si}_{1-x}\text{Ge}_x$ has been reported that takes advantage of the selective removal of silicon atoms from a SiGe film on insulator by $\text{Si}_{1-x}\text{Ge}_x$ thermal oxidation (Fig. 1).⁴ The SiGe-on-insulator (SGOI) structure can be made by separation by implanted oxygen (SIMOX) on SiGe/Si-substrate⁵ or germanium diffusion into silicon-on-insulator.⁶ When the supply of silicon atoms by diffusion from the SiGe to the oxidation interface can meet the consumption of silicon atoms during oxidation, only the silicon atoms are oxidized because silicon

oxidation is preferred to germanium oxidation,⁷ leading to an increased germanium content in the $\text{Si}_{1-x}\text{Ge}_x$ layer as the film is thinned down. However, film quality degrades considerably as the added strain, which arises from the germanium content enhancement, is relaxed by dislocation formation during the oxidation and subsequent annealing.⁴

In this work, we obtained high-quality relaxed SiGe on oxide with high germanium content by combining SiGe oxidation and the use of SiGe layers on insulating borophosphosilicate glass (BPSG) compliant substrates. Compliant BPSG substrates have recently been utilized to relax the strain in SiGe without dislocations.^{8–11} When BPSG becomes viscous at high temperature, the SiGe layer, patterned into islands after transfer from a Si substrate, can freely expand to relax strain (Fig. 2 inset). Dislocations are not required in the relaxation process, making this approach a promising way to realize high-quality relaxed SiGe for electronic applications. The compliant BPSG, replacing the thermal silicon dioxide in SGOI, served as an excellent substrate to relax the strain introduced by germanium enhancement in the oxidation. Deposited oxide caps are shown to be critical to achieving high quality in the final layer.

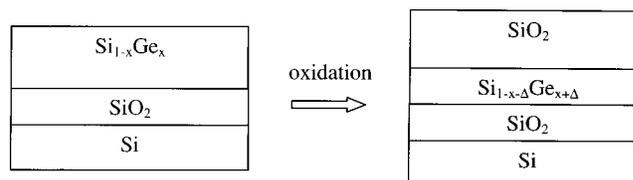


FIG. 1. Schematic for the enhancement of germanium content by SiGe oxidation. Oxidation of SiGe produces pure thermal SiO_2 and the germanium content in the remaining SiGe film increases as a result of the conservation of germanium atoms.

^{a)}Electronic mail: hyin@princeton.edu

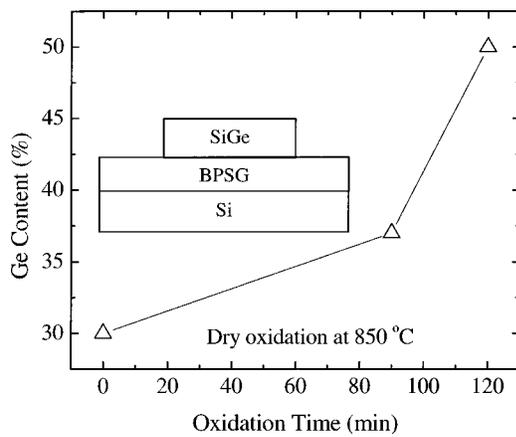


FIG. 2. Germanium content as a function of dry oxidation time at 850 °C, performed on 30 nm $\text{Si}_{0.70}\text{Ge}_{0.30}$ square islands of width 20 μm on 200-nm BPSG.

The SiGe on BPSG structure was fabricated by wafer bonding, Smart-Cut®, and patterning, as described in Ref. 9. Two samples with different germanium content and thickness were studied. One consisted of fully strained 30-nm $\text{Si}_{0.7}\text{Ge}_{0.3}$ islands on BPSG and the other of fully relaxed 55-nm $\text{Si}_{0.84}\text{Ge}_{0.16}$ islands on BPSG, formed through germanium diffusion between a bilayer of 30-nm $\text{Si}_{0.7}\text{Ge}_{0.3}$ and 25-nm Si upon annealing at 850 °C for 16 h. The square island size varied from 10 to 500 μm . The strain and germanium content in SiGe and Si films were locally measured by micro-Raman spectroscopy. The Si–Si phonon frequency $\omega_{\text{Si-Si}}$ and the Si–Ge phonon frequency $\omega_{\text{Si-Ge}}$ were employed to extract germanium content x and biaxial strain σ as follows:¹²

$$\omega_{\text{Si-Si}} \text{ (cm}^{-1}\text{)} = 520 - 68x - 815\sigma, \quad (1)$$

$$\omega_{\text{Si-Ge}} \text{ (cm}^{-1}\text{)} = 400.5 + 14.2x - 575\sigma. \quad (2)$$

The rms surface roughness of the SiGe films was measured by atomic force microscopy (AFM).

We first examined the direct oxidation of SiGe on BPSG. Square islands with 20- μm edges of 30 nm $\text{Si}_{0.7}\text{Ge}_{0.3}$ on BPSG were annealed at 800 °C in forming gas for 30 min to reach full relaxation, which was confirmed by micro-Raman measurements. Subsequently, dry oxidation was carried out at 850 °C on the relaxed islands. In this condition, we expected pure silicon dioxide to be formed.¹³ The germanium content of the sample as a function of oxidation time is shown in Fig. 2. After a 2-h dry oxidation at 850 °C, the germanium content increased to 50% from 30%. The germanium content of a 200- μm island with initial 55-nm $\text{Si}_{0.84}\text{Ge}_{0.16}$ on BPSG reached 36% after 4-h dry oxidation at 850 °C. The surface quality of the SiGe islands after this direct oxidation was poor [Fig. 3(a)]. After oxidation, the 200- μm island has a surface roughness of more than 4 nm. In addition, the variation of germanium content across the island is more than 10%. Figure 3(b) shows an 80- μm island with initially 55 nm $\text{Si}_{0.84}\text{Ge}_{0.16}$ after 3-h dry oxidation at 850 °C, oxide removal by hydrofluoric (HF) wet etch, and another 2-h dry oxidation at 850 °C. The final germanium content was $\sim 65\%$, but it varied from 50% to 80% across the island, and the surface roughness was larger than 15 nm. The rough surface and nonuniform germanium content on

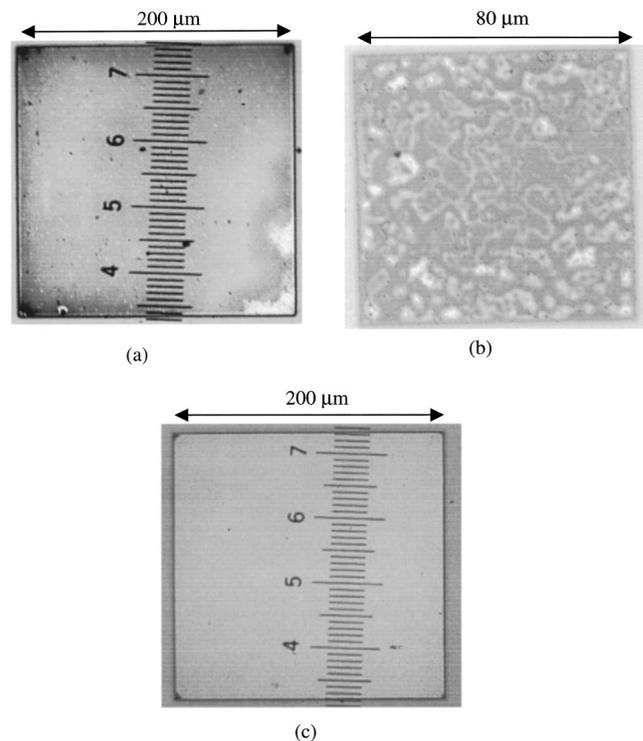


FIG. 3. Optical micrographs of 55-nm $\text{Si}_{0.84}\text{Ge}_{0.16}$ islands on BPSG after dry oxidation. (a) A 200 $\mu\text{m} \times 200 \mu\text{m}$ island after a 4-h dry oxidation at 850 °C. The germanium content reached 36% and the surface roughness was larger than 4 nm. (b) A 80 $\mu\text{m} \times 80 \mu\text{m}$ island after a 3-h dry oxidation at 850 °C, SiO_2 etch by HF, and another 2-h dry oxidation at 850 °C. The germanium content was around 65% and the surface roughness was larger than 15 nm. (c) A 200 $\mu\text{m} \times 200 \mu\text{m}$ island, capped by 70 nm PECVD SiO_2 , after dry oxidation at 850 °C for 3.5 h and at 900 °C for 2.5 h, and annealing in nitrogen at 875 °C for 5.5 h. The germanium content and strain were 57% and -0.27% , respectively. The surface roughness (rms) was less than 2 nm.

islands after oxidation probably originates from the strain-induced surface roughening on compliant BPSG (similar to buckling observed during strain relaxation of SiGe islands on BPSG⁹) and/or a nonuniformity of the oxidation rate. It has been observed that oxidation rate depends on stress,¹⁴ and surface roughening can cause variation of stress across SiGe islands on BPSG.¹⁵

To improve uniformity of the oxidation rate across islands, a 70-nm silicon dioxide capping layer was deposited on 55 nm $\text{Si}_{0.84}\text{Ge}_{0.16}$ before oxidation using plasma-enhanced chemical vapor deposition (PECVD) at 250 °C. For such a thick silicon dioxide cap, the oxidation rate is mainly controlled by the oxygen diffusion time through the silicon dioxide cap, which is determined by the thickness of the cap. Thus, the oxidation rate will have a weak dependence on the surface reaction rate, which depends on strain and surface condition of the remaining SiGe layer. In our earlier work, silicon dioxide caps have been used to suppress buckling of SiGe islands on BPSG.¹¹ The underlying mechanism is an increased film rigidity with a silicon dioxide cap, which makes strain relaxation by buckling less likely. Therefore, besides controlling oxidation rate, the silicon dioxide caps have a second benefit: a smoother SiGe surface, which in turn leads to less strain variation across islands, reducing strain-induced oxidation variation across islands.

The oxide-capped sample was oxidized in dry oxygen for 3.5 h at 850 °C and then 2.5 h at 900 °C [Fig. 3(c)]. The

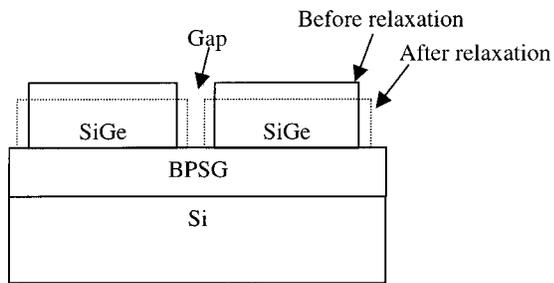


FIG. 4. Schematic illustration of lateral expansion measurement of SiGe islands after strain relaxation.

longer time and higher temperature were required because of a lower oxidation rate. The sample was then further annealed in nitrogen for 5.5 h at 875 °C to relax strain. The improvement in film quality was dramatic. The surface roughness was less than 2 nm [Fig. 3(c)]. The germanium content increased to 57% and was uniform ($\pm 3\%$) across the island. The strain in SiGe was -0.27% and, therefore, its in-plane lattice constant was the same as fully relaxed SiGe with germanium content of 52%. The layer was nearly fully relaxed despite the thick oxide cap, which should inhibit relaxation by stress balance.¹⁰ Note that the compressive strain in the thermal silicon dioxide as a result of volume expansion during oxidation is small and has a negligible effect on stress balance. The decoupling of the oxide cap from the underneath SiGe layer is fortuitous, and we think it is caused by the creation of an ultralow viscosity slippage plane during oxidation between SiO₂ and SiGe layers as a result of stress-reduced viscosity.¹⁶

The compressive strain in SiGe islands, caused by Ge enhancement during oxidation, could relax by dislocations or by the simple lateral expansion of the islands, a process that does not require dislocations. If the islands relax the compressive strain by simply expanding laterally on the BPSG, the island size would increase. If the mechanism is by dislocations, no lateral expansion would be expected. To determine the relaxation mechanism, the lateral expansion of the islands was measured by AFM. The gap between adjacent 100- μm islands was chosen to be $\sim 2 \mu\text{m}$, comparable with the magnitude of island expansion. The small amount of island expansion could be inferred from the shrinkage of the island gaps more accurately than by the direct measurement of the island size (Fig. 4). 100- μm islands with initial 55 nm Si_{0.84}Ge_{0.16} were dry oxidized at 870 °C for 80 min, followed by an anneal in nitrogen at 850 °C for 2 h to facilitate strain relaxation. The final strain and Ge content, measured by Raman spectroscopy, were 0.07% ($\pm 0.06\%$) and 27% ($\pm 0.8\%$), respectively. This is equivalent to fully relaxed SiGe with a germanium content of 25% ($\pm 1.5\%$). Lateral expansion to relax the strain would require an island expansion of 390 nm (± 60 nm). After discounting the thickness of the oxide grown on island sidewalls, the observed island expansion was 345 nm (± 50 nm) (averaged over six locations), which was near that expected for relaxation by lateral expansion. This shows dislocations do not play a dominant role in the strain relaxation process (Fig. 5).

In summary, the combination of SiGe oxidation and compliant BPSG substrates allows the enhancement of the

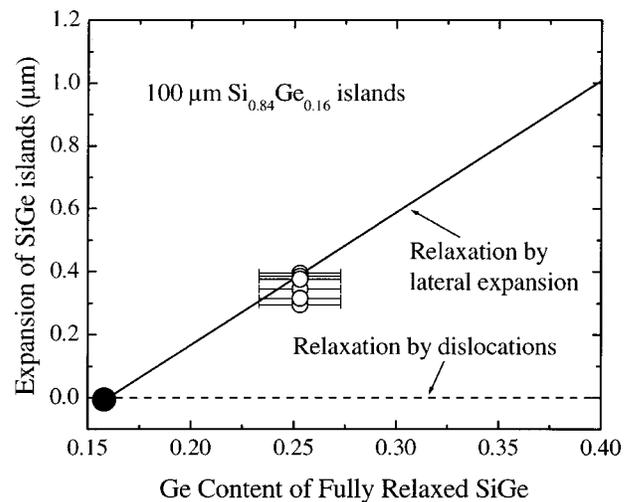


FIG. 5. Lateral expansion of SiGe islands as a function of germanium content for 100 $\mu\text{m} \times 100 \mu\text{m}$ islands with initial fully relaxed Si_{0.84}Ge_{0.16}. The solid line is a prediction assuming that all strain caused by germanium enhancement is relaxed by lateral expansion, and the horizontal dashed line assumes all strain relaxation is through misfit dislocations. The open symbols are experimental data, measured on islands after dry oxidation at 870 °C for 80 min and annealing at 850 °C for 2 h.

germanium content of SiGe on insulator, with high-quality films of germanium content as high as 57% achieved. Surface roughening and nonuniformity of germanium enhancement during SiGe oxidation on BPSG have been improved by a SiO₂ capping layer. AFM measurement confirms that lateral expansion leads to the relaxation of the strain accumulated from germanium enhancement.

This work is supported by DARPA (N66001-00-10-8957) and ARO (DAA655-98-1-0270).

- M. L. Lee, C. W. Leitz, Z. Cheng, A. J. Pitera, T. Langdo, M. T. Currie, G. Taraschi, E. A. Fitzgerald, and D. A. Antoniadis, *Appl. Phys. Lett.* **79**, 3344 (2001).
- E. A. Fitzgerald, Y.-H. Xie, D. Monroe, P. J. Silverman, J. M. Kuo, A. R. Kortan, F. A. Thiel, and B. E. Weir, *J. Vac. Sci. Technol. B* **10**, 1807 (1992).
- E. A. Fitzgerald, Y.-H. Xie, M. L. Green, D. Brasen, A. R. Kortan, and J. Michel, *Appl. Phys. Lett.* **59**, 811 (1991).
- T. Tezuka, N. Sugiyama, T. Mizuno, M. Suzuki, and S. Takagi, *Jpn. J. Appl. Phys.* **40**, 2866 (2001).
- N. Sugiyama, T. Mizuno, M. Suzuki, and S. Takagi, *Jpn. J. Appl. Phys.* **40**, 2875 (2001).
- T. Mizuno, N. Sugiyama, T. Tezuka, and S. Takagi, *Appl. Phys. Lett.* **80**, 601 (2002).
- S.-G. Park, W. S. Liu, and M.-A. Nicolet, *J. Appl. Phys.* **75**, 1764 (1994).
- K. D. Hobart, F. J. Kub, M. Fatemi, M. E. Twigg, P. E. Thompson, T. S. Kuan, and C. K. Inoki, *J. Electron. Mater.* **29**, 897 (2000).
- H. Yin, R. Huang, K. D. Hobart, Z. Suo, T. S. Kuan, C. K. Inoki, S. R. Shieh, T. S. Duffy, F. J. Kub, and J. C. Sturm, *J. Appl. Phys.* **91**, 9716 (2002).
- H. Yin, K. D. Hobart, F. J. Kub, S. R. Shieh, T. S. Duffy, and J. C. Sturm, *Appl. Phys. Lett.* **82**, 3853 (2003).
- H. Yin, R. Huang, K. D. Hobart, J. Liang, Z. Suo, S. R. Shieh, T. S. Duffy, F. J. Kub, and J. C. Sturm, *J. Appl. Phys.* **94**, 6875 (2003).
- J. C. Tsang, P. M. Mooney, F. Dacol, and J. O. Chu, *J. Appl. Phys.* **75**, 8098 (1994).
- F. K. LeGoues, R. Rosenberg, T. Nguyen, F. Himpsel, and B. S. Meyerson, *J. Appl. Phys.* **65**, 1724 (1989).
- J. Y. Yen and J. G. Hwu, *J. Appl. Phys.* **89**, 3027 (2001).
- J. Liang, R. Huang, H. Yin, J. C. Sturm, K. D. Hobart, and Z. Suo, *Acta Mater.* **50**, 2933 (2002).
- H. Yin, K. D. Hobart, S. R. Shieh, T. S. Duffy, and J. C. Sturm, *MRS Fall Meeting*, Boston, MA, 2002 (Materials Research Society, Pittsburgh, 2002).