Buckled SiGe layers by the oxidation of SiGe on viscous SiO$_2$ layers

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SiGe-on-insulator structures have been fabricated by wafer bonding and layer transfer techniques. The relaxation process of the compressively strained SiGe films bonded to SiO$_2$ layers through the rapid thermal oxidation was investigated. Buckling nucleus were randomly located at the beginning of oxidation and the buckling undulation was well developed after 30 s oxidation at 960 °C. The buckling amplitude increases with the increasing thermal oxidation time. An emission peak at 1.5 μm was observed in the low temperature photoluminescence of the buckled SiGe layers. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1846937]

Strained Si on SiGe-on-insulator (SGOI) substrates is a promising technology due to the combinational advantage of mobility enhancement and device isolation.[1,2] Strain relaxation on viscous substrates can probably reduce threading dislocation density by the viscous flow of the underlying oxide layer. In recent experiments,[3] the buckling relaxation of the compressively strained SiGe films on viscous substrates has been observed by the long time furnace annealing in N$_2$ ambient with no oxidation. Note that to avoid the buckling, the strained films on reduced areas can suppress the buckling by lateral expansion.[4] Buckling is another state of semiconductor materials. The electronic and optical properties are not well known. The two-dimensional (2D) nature of buckling periodicity can be utilized as the optical grating components. In this letter, 2D buckled SiGe layers were fabricated by the oxidation of compressively strained SiGe layers on SiO$_2$ layers and the initial relaxation of the buckling process was observed. A special 1.5 μm photoluminescence (PL) emission was also observed from the buckled state, which is different from the unbuckled materials and can be potentially used as the light source.

The basic fabrication process of SGOI structures involves hydrogen ion implantation and direct wafer bonding.[5] A 100 nm defect-free pseudomorphic Si$_{0.9}$Ge$_{0.1}$ layer, capped with a 4 nm Si layer and 50 nm borophosphorosilicate glass (BPSG), was epitaxially grown on a p-type, (001) orientation Si substrate as a "host" wafer. The SiGe layer was grown by ultrahigh vacuum chemical vapor deposition (UHVCVD) at 500 °C with a Ge content of 10%, confirmed by x-ray diffraction. The hydrogen ions with a dose of 5×10^{16} cm^{-2} and the energy of 100 keV were implanted to form a deep weakened layer underneath the SiGe layers. On the other sub-strate, 700 nm BPSG was grown to form the "handle" wafer. The handle wafer and host wafer were hydrophilicly cleaned in the NH$_4$OH:H$_2$O$_2$:H$_2$O solution, and initially bonded at the room temperature.[6] The wafer pair were annealed at 800 °C for 30 min with oxygen flow to strengthen the chemical bonds and to induce layer transfer along the weakened hydrogen-implanted regions by H$_2$ blistering. The wafer was then etched by KOH solution[7] to remove the approximately 450 nm residual Si on the SiGe/BPSG stacks. Samples were then oxidized at 960 °C to induce the " Ge condensation"[8] in the remaining unoxidized SiGe layers and to enhance the buckling relaxation of SiGe on BPSG. Note that the buckling state is preferential in the thermal equilibrium for the thin SiGe film with large strain.

The lateral expansion and the counterforce by viscous BPSG produce compressive stress on SiGe layers during rapid thermal oxidation at 960 °C. One way to relieve the compressive stress in the thin strained films is to bend out of the nominal plane, since the underlying BPSG layer is soft to form a viscous state at 960 °C. The strain relaxation mechanism leads to the buckling phenomenon as shown by atomic force microscopy (AFM) in Fig. 1. This sample was oxidized at 960 °C for 300 s. Two-directional undulation on the surface is parallel to the two mutually perpendicular ⟨100⟩ directions with the period and the root-mean-square amplitude of ~6 μm and ~50 nm, respectively. The ⟨100⟩ buckling direction of the SiGe layers on viscous BPSG is due to the large shear modulus along the ⟨100⟩ direction on the (001) oriented Si substrates.[9] The initial evolution of morphology with oxidation time (1, 5, 10, and 30 s) is shown in Fig. 2. Buckling nucleus were randomly located on the strained SiGe films for 1 s oxidation. After thermal oxidation time of 30 s, the undulations were well organized.

The sinusoidal undulations are clearly observed by cross-sectional transmission electron microscopy (TEM) for

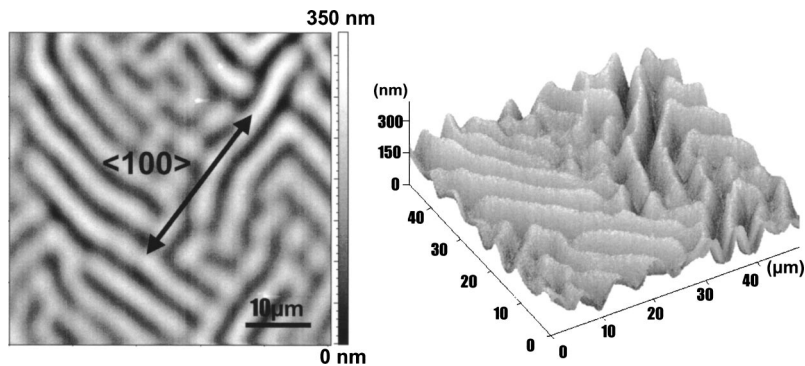[a)]Author to whom correspondence should be addressed; electronic mail: chee@cc.ee.ntu.edu.tw

FIG. 1. The AFM image of buckled SiGe layers on viscous SiO$_2$ layers. Two-directional undulating on the surface is oriented parallel to the $\langle 100 \rangle$ directions after 300 s oxidation at 960 °C with the period and the amplitude of ~6 μm and ~80 nm, respectively.

a film after 7 h oxidation shown in Fig. 3 with the peak-to-peak amplitude of ~160 nm and undulation period of ~6 μm. There is no defect or dislocation observed in the TEM pictures of buckled SiGe film in the range of 7 μm. The condensation of Ge from the oxidized SiGe layers into the underlying SiGe layer increases the Ge content and the strain, which further buckle the undulated SiGe films after continuous oxidation. The final thickness of SiGe film (T_f) is 26.5 nm after 7 h oxidation, and the final Ge fraction, x_f, is 37.7% obtained from the thickness scaling equation $x_f = x_i(T_i/T_f)$,[12] where $x_i(=10\%)$ is the initial Ge content and $T_i(=100$ nm) is the initial thickness.

Micro-Raman spectroscopy with a 514.5 nm (Ar$^+$ laser) wavelength was employed to monitor film relaxation before and after oxidation [Fig. 4(a)]. Lorentzian line shape was used to determine the peak position with respect to the bulk Si peak. The Raman shift of Si–Si phonon frequency ($\Delta\omega_{Si-Si}$) of SiGe with respect to Si substrate peak is a combinational effect of Ge content and the strain:[10]

$$\Delta\omega_{Si-Si} = -68x - 34\frac{\varepsilon}{0.0417},\qquad(1)$$

where x is the Ge fraction, and ε is the strain of the SiGe layer (negative sign for compressive strain). There was a detectable Raman peak shift (~0.5 cm^{-1}) after 30 s oxidation, indicating the Ge content and/or strain in the SiGe layers starts to change. The previous work[11] predicts that the buckled SiGe film can be even under tensile strain in some areas and the tensile strain can cause fractures. In our work, however, the fracture is not observed. Using the Ge content of 37.7% obtained from thickness scaling equation, the residual strain is almost zero in the buckled films. Therefore, the fracture is not observed.

Figure 4(a) shows surface roughness of the SGOI samples as a function of thermal oxidation time at 960 °C, measured by AFM. It shows that surface roughness increases with oxidation time due to the increase of relaxation by the increasing buckling amplitude. The amplitude reaches a stable root-mean-square amplitude of ~80 nm after 600 s oxidation. Together with Raman peak shift measured, it appears that significant buckling starts after 30 s oxidation at 960 °C.

The PL spectrum of the 2D buckled SiGe layers with 7 h oxidation time is shown in Fig. 5. At 10 K, the PL spectrum has an emission peak at 1.5 μm originated from the buckled SiGe layer, since the 1.5 μm PL peak vanishes after removal of the buckled SiGe layer on buckled BPSG. There is no PL peak of buckled SiGe layers observed at room temperature, and only a Si peak (transverse optical phonon replica) is observed at room temperature. Note that the PL of normal SiGe layers has well-known nonphonon and TO (transverse optical) phonon assistant emissions with energy around band gap.[12] The origin of the 1.5 μm PL is unknown yet. This 1.5 μm emission unlikely originates from the dislocations, since the PL of dislocations has four lines with D$_1$ line at ~1.5 μm[13] (not only one line). Since here is no Ge quantum
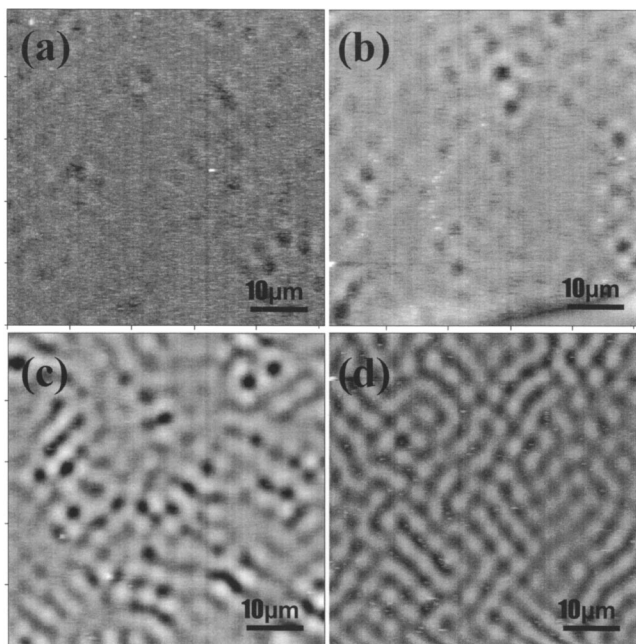

FIG. 2. Evolution of surface morphology vs oxidation time at 960 °C for (a) 1 s, (b) 5 s, (c) 10 s, and (d) 30 s. The 2D buckled SiGe layers were well organized after oxidation time of 30 s.
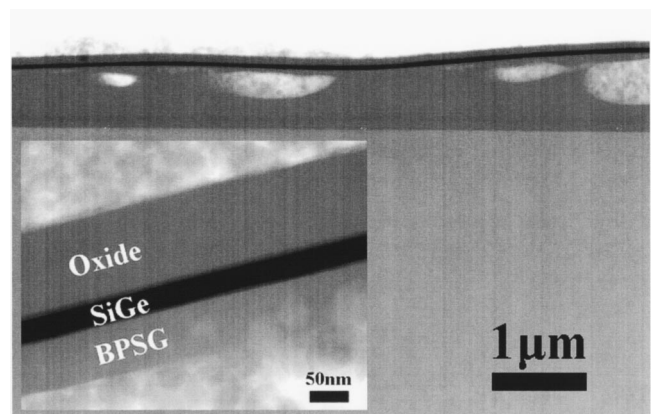

FIG. 3. Cross-sectional transmission electron microscopy of the buckled SiGe layers after 7 h oxidized at 960 °C.

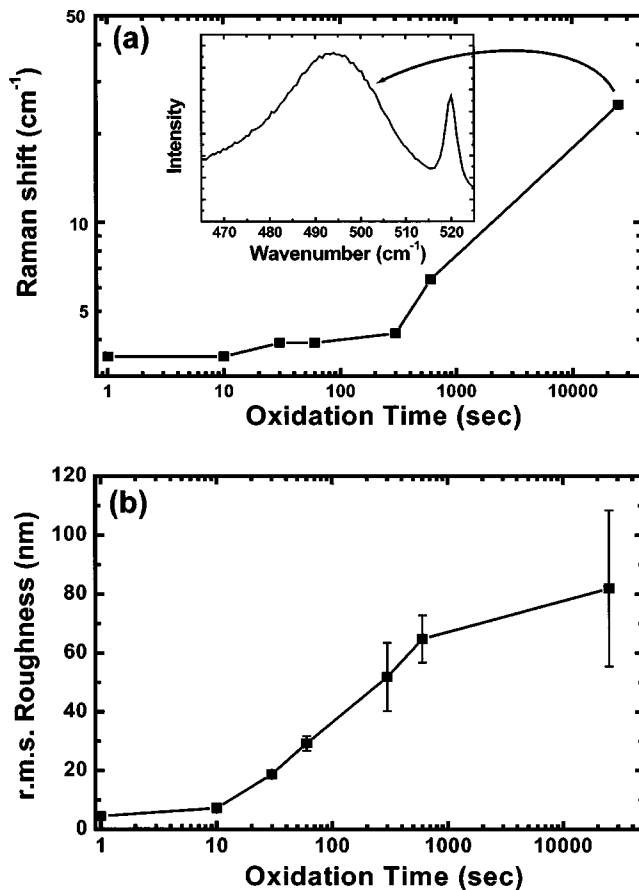FIG. 5. The photoluminescence spectra of the buckled SiGe layers.

FIG. 4. (a) Raman peak shift vs oxidation time at 960 °C. The inset is the Raman spectra of the buckled SiGe layers after oxidation, as well as original SiGe layers. (b) Surface roughness (root mean square) measured by AFM as a function of oxidation time at 960 °C.

dot observed in the TEM, the 1.5 μm PL emission is not originated from Ge dots.[14]

In summary, the relaxation of compressively elastic SiGe films on the viscous layers forms the buckled layers. Blanket films start to buckle at 960 °C after 30 s oxidation. The perturbation amplitude increases with thermal anneal time and reaches to a saturated root-mean-square amplitude of ~80 nm. There is no defect or dislocation observed in the TEM micrographs in the range of 7 μm of buckled SiGe samples. We also observed the PL spectra, indicating defect density is low enough to have sufficient radiative recombination. The PL spectrum at low temperature has an emission peak at ~1.5 μm for the buckled layers.

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