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Compliant effect of low-temperature Si buffer for SiGe growth

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Relaxed SiGe attracted much interest due to the applications for strained Si/SiGe high electron mobility transistor, metal-oxide-semiconductor field-effect transistor, heterojunction bipolar transistor, and other devices. High-quality relaxed SiGe templates, especially those with a low threading dislocation density and smooth surface, are critical for device performance. In this work, SiGe films on low-temperature Si buffer layers were grown by solid-source molecular-beam epitaxy and characterized by atomic force microscope, double-axis x-ray diffraction, and photoluminescence spectroscopy. It was demonstrated that, with the proper growth temperature and Si buffer thickness, the low-temperature Si buffer became tensily strained and reduced the lattice mismatch between the SiGe and the Si buffer layer. This performance is similar to that of the compliant substrate: a thin substrate that shares the mismatch strain in heteroepitaxy. Due to the smaller mismatch, misfit dislocation and threading dislocation densities were lower. [DOI: 10.1063/1.1337633]

High-quality relaxed SiGe layers, which are used as ‘‘virtual substrates’’ for the growth of strained Si/SiGe high electron mobility transistors (HEMT) and metal-oxide-semiconductor field-effect transistors (MOSFET)[1,2] and the integration of III–V devices on Si substrates,[3] have attracted considerable attentions. However, the large lattice mismatch (~4.17%) between Si and Ge usually results in a high density of misfit dislocations at the interface of SiGe and Si, and threading dislocations in the SiGe layers when the epilayer exceeds the critical thickness. Threading dislocations which propagate through the SiGe layer into the active region deteriorate the device performance.[4,5] Several methods have been used to grow high quality relaxed SiGe films, for example, compositionally grading,[6] compliant substrates,[7] and growth on limited areas.[8] Recent reports indicated that the use of low-temperature Si buffer (LTSi) layer could significantly reduce threading dislocation density in the SiGe layer.[9] It was speculated that the LTSi layer plays several important roles: it not only provides low energy sites for dislocation nucleation and point defects for trapping of propagating dislocations, but is also involved in strain adjustment. However, the strain adjusting mechanism of the LTSi buffer has not been shown experimentally. In this work, LTSi buffer layers were used to grow high quality relaxed SiGe films. The resulting films were studied using atomic force microscopy (AFM), photoluminescence (PL), and high-resolution double axis x-ray diffraction (DAXRD).

The samples investigated were grown by solid source molecular beam epitaxy in a Perkin-Elmer system. A 60 nm Si buffer was first grown at 600 °C, followed by a LTSi layer deposited at 400 °C, with thickness varying from 50 to 300 nm. Finally, a 200 nm $Si_{0.8}Ge_{0.2}$ layer was grown on the top of the LTSi buffer at 500 °C. The growth rate for both the Si and SiGe layers was about 1 Å/s. For convenience, in this letter, the samples with 50, 100, 150, 200, 250, and 300 nm thick LTSi buffers are referred to as samples A, B, C, D, E, and F, respectively. The surface morphology and roughness of the samples were investigated using a Park Scientific AFM in contact mode. The alloy composition and degree of strain relaxation were determined from DAXRD. Low temperature PL was measured at 4 K using an Ar^+ 488 nm laser line.

It is well known that the surface morphology of epitaxial layers is influenced by misfit and threading dislocations. Figure 1 shows the AFM images of the samples with different thicknesses of the LTSi buffer layer. The root mean squared (rms) roughness of the surface is shown in Fig. 2 as a function of LTSi buffer thickness. The roughness decreases from

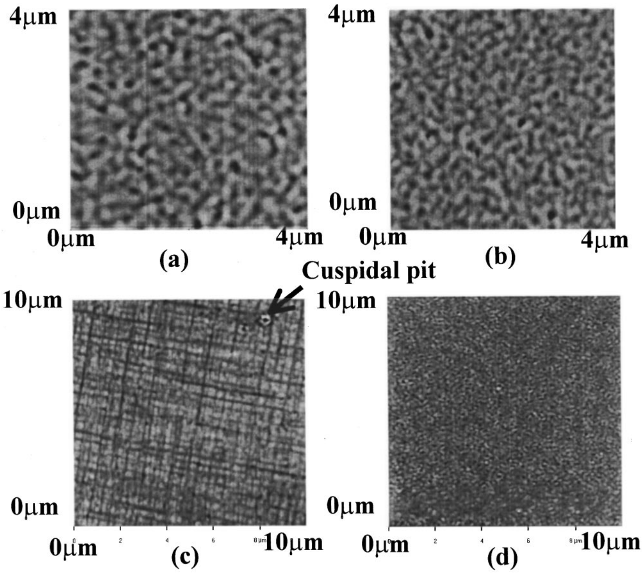

FIG. 1. AFM surface morphology of a 200 nm $Si_{0.08}Ge_{0.2}$ film grown on a 400 °C LTSi buffer with thickness (a) 50 nm, (b) 100 nm, (c) 200 nm, and (d) 250 nm.

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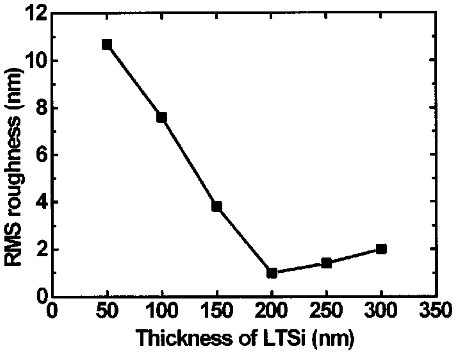

FIG. 2. rms surface roughness of the samples vs the thickness of the LTSi buffer, obtained from AFM measurement.

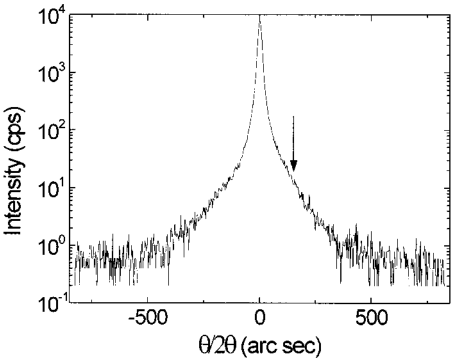

FIG. 3. $\theta/2\theta$ double-axis x-ray diffraction scan of the (004) Si peak for sample D (SiGe on 200 nm LTSi buffer). The weak shoulder to the right of the substrate peak, indicated by the arrow, is associated with a tensily strained LTSi buffer.

14 to 1 nm linearly with the LTSi thickness varying from 50 to 200 nm, then increases slightly from 1 to 2 nm when the thickness increases to 300 nm. For the 200 nm sample (D), ordered and straight crosshatch lines are observed on the surface. Though there are also some cuspidal pits on the surface, the rms roughness is only 1 nm. This roughness value is much smaller than those obtained from compositionally graded buffers and similar terminate Ge composition.[10,11] The crosshatch pattern on the surface is due to misfit dislocations traveling at the Si/SiGe interface[12] and a misfit dislocation is normally associated with two threading dislocations. As shown in Fig. 2(c), the threading dislocation density is lowest for sample D. The cuspidal pits which are observed on the surface of the samples arise from the local stress field of threading dislocations.[13] For sample D, the threading dislocation density is about the density of the cuspidal pits on surface ($\sim 10^7\ \mathrm{cm}^{-2}$). For other samples with thinner LTSi buffers, the surface is much rougher and no ordered crosshatches are observed. The huge x-ray ω-full width at half maximum (FWHM) for these samples shown later means that they have a high mosaic spread, probably due to lots of dislocations and/or 3-*d* growth (=roughness). The misfit dislocation density may be too high to observe with AFM. For samples E and F, which have buffers thicker than 200 nm, the surface is just a little rougher than for sample D, but there is no clear crosshatch observed on the surface. In this case, the point defect density in the LTSi layer may be so high that some of them annihilated and formed stacking faults before the deposition of the SiGe layer begins, then the threading density is higher and the pits on the surface distort the crosshatch lines.

The samples were measured by DAXRD to confirm the composition, relaxation, and crystal quality, and the results are given in Table I. The strain relaxation was determined by employing a high-resolution x-ray reciprocal space mapping (RSM) technique, which allows a direct elucidation of the strain status of the epilayer via a (224) reciprocal space map, independent of the composition of the SiGe layer. The composition was then determined from a scan of the (004) peak, using the measured relaxation. The SiGe peak from sample D, with a 200 nm LTSi buffer, had the smallest ω-FWHM of all the samples (ω-FWHM=1000 arcsec), indicating the lowest misfit dislocation density. The SiGe layer from sample D was determined to be 62% relaxed. It was found that too thin a LTSi buffer (50–100 nm) leads to a fully relaxed SiGe layer with very poor crystalline quality (ω-FWHM $\sim$3500 arcsec). In the (004) $\theta/2\theta$ scan of the Si peak from sample D, as shown in Fig. 3, a shoulder associated with the LTSi buffer is observed to the right of the Si substrate peak, as indicated by the arrow. The presence of the shoulder indicates that the out-of-plane lattice constant of Si buffer is smaller than that of the bulk Si, therefore the LTSi buffer layer is tensily strained. The tensile strain of the Si buffer partially compensates the compressive strain in the SiGe layer, reduces the mismatch between the SiGe layer and the Si buffer layer and substrate, and contributes to improve the quality of the SiGe layer. This mechanism is similar to that of the compliant substrate: a thin freestanding substrate that shares the mismatch strain during the heteroepitaxy.[7]

TABLE I. Ge composition, strain relaxation, and SiGe (004) peak ω-FWHM determined from DAXRD measurements for 200 nm SiGe films on different thick LTSi buffer layers.

LTSi thickness (nm)	Ge (x)	SiGe relaxation (%)	SiGe (004) peak ω-FWHM (arcsec)
50	0.16±0.01	100±20	3500±500
100	0.17±0.01	100±20	3500±500
200	0.18±0.005	62±3	1000±50
250	0.18±0.01	53±8	1100±50
300	0.19±0.005	68±8	1400±50

PL has been widely used to study dislocations and defects in SiGe alloys.[14,15] In Fig. 4(a), the high energy parts of PL spectra from the samples are shown. For samples A and B, a shoulder to the left of the strong Si TO peak from the substrate is observed (as indicated by dashed lines). For samples C, D, E, and F, the peak becomes stronger and separates from the Si TO peak. Using a Gaussian fit to these two peaks, the positions of the peaks were determined. The TO Si peak from the Si substrate remains at 1.092 eV, while the left peak changes position with the thickness of the LTSi buffer layer. The inset in Fig. 4(a) shows the shift of the left peak with respect to the Si TO peak as a function of the thickness of the LTSi buffer. At first (A–C), the redshift of the peak increases with the thickness of LTSi buffer layer, reaching a maximum value for the 200 nm LTSi buffer sample (D), then it decreases slowly (E–F). It is believed that this peak is the Si TO peak of the LTSi buffer and the tensile strain in the LTSi buffer causes the redshift. The

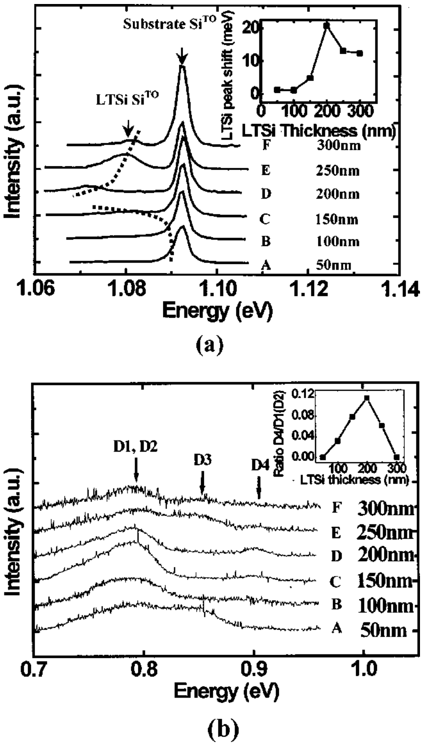

FIG. 4. (a) High energy parts of PL spectra from samples A through F in order from bottom to top. The peak to the left of the Si TO peak of the substrate may come from the LT Si buffer layer. The inset shows the shift value of the left peak (TO of LTSi) with respect to the substrate Si TO peak (b) The low energy parts of PL spectra from samples A through F in order from bottom to top. The peaks are labeled as D1/D2, D3, and D4 dislocation lines, respectively. The inset shows the integrated intensity ratio of the D4 peak to the D1/D2 peak.

maximum redshift for sample D indicates the highest tensile strain of the LTSi buffer, consistent with the DAXRD result as discussed above. The energy band gap of the strain Si on $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ is known as $E_g(\mathrm{Si})-0.4x$.[16] Thus from the redshift of the strain Si TO peak with respect to Si substrate, the strain can be estimated. For sample D, the shift of 20 meV corresponds to the strain Si on $\mathrm{Si}_{0.95}\mathrm{Ge}_{0.05}$. Since the Ge composition of the SiGe layer on LTSi layer is about 0.18, the strain of the LTSi layer is about 28% of the wholly mismatch strain between the Si and the $\mathrm{Si}_{0.82}\mathrm{Ge}_{0.18}$. Because of the smaller mismatch (28% less), the misfit dislocation density decreased.

The low energy parts of PL spectra are shown in Fig. 4(b). For clarity, the PL intensities are not to scale. For samples B, C, D, and E, a peak at about 0.9 eV is observed, which does not show up in samples A and F. This peak is attributed to the D4 dislocation line. The threading dislocations in the SiGe layers, extended straight segments of misfit dislocations, and threading dislocations in the buffer and substrate are responsible for the D4 dislocation line.[15] As the SiGe layer in our samples is only 200 nm thick, the straight segments of misfit dislocations and threading dislocations in the LTSi buffer are the dominating source of the D4 line. Additionally, the D1 and D2 line (D1, D2) is from the dislocation intersections.[15] The integrated intensity ratio of D4/D1(D2) is shown in Fig. 4(b). The highest D4/D1(D2) intensity ratio in sample D implies that the misfit dislocations are longest and/or the density of threading dislocations which are confined in LTSi buffer is highest.

LTSi buffer layer with different growth temperatures from 300 to 450 °C were studied for the growth of the SiGe films, too. It was found that the influence of the temperature on the quality of the SiGe layers is significant and 400 °C was the optimum growth temperature for LTSi buffer. Temperatures below 350 °C caused very rough surface and poor crystalline quality. Temperatures above 400 °C caused little rougher surface and more defects.

In conclusion, the use of the low temperature Si buffer layer has been shown for the growth of high quality, thin, relaxed, SiGe films, demonstrating the compliant effect. The influence of the LTSi buffer thickness on the quality of the SiGe layer was studied by AFM, PL, and DAXRD measurement. It was shown that the LTSi buffer could become tensily strained and thus reduce the lattice mismatch between the SiGe layer and the buffer layer.

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[1] K. Ismail, F. K. LeGoues, K. L. Saenger, M. Arafa, J. O. Chu, P. M. Mooney, and B. S. Meyerson, Phys. Rev. Lett. **73**, 3447 (1994).
[2] Y. H. Xie, D. Monroe, E. A. Fitzgerald, P. J. Silverman, F. A. Theil, and G. P. Watson, Appl. Phys. Lett. **63**, 2263 (1993).
[3] J. J. Welser, J. L. Hoyt, and J. F. Gibbons, IEEE Electron Device Lett. **15**, 100 (1994).
[4] R. Hull, J. C. Bean, and C. Buescher, J. Appl. Phys. **66**, 5837 (1989).
[5] L. B. Freund, J. Appl. Phys. **68**, 2073 (1990).
[6] P. Kvan and F. Namavar, Appl. Phys. Lett. **58**, 2357 (1991).
[7] Y. H. Luo, J. L. Liu, G. Jin, K. L. Wang, C. D. Moore, M. S. Goorsky, C. Chih, and K. N. Tu, J. Electron. Mater. **29**, 950 (2000).
[8] A. Nishida, K. Nakagawa, E. Murakami, and M. Miyao, J. Appl. Phys. **71**, 5913 (1992).
[9] H. Chen, L. W. Guo, Q. Cui, Q. Hu, Q. Huang, and J. M. Zhou, J. Appl. Phys. **79**, 1167 (1996).
[10] P. M. Mooney, J. L. Jordan-Sweet, K. Ismail, J. O. Chu, R. M. Feenstra, and F. K. LeGoues, Appl. Phys. Lett. **67**, 2373 (1995).
[11] J. L. Liu, C. D. Moore, G. D. U'Ren, Y. H. Luo, Y. Lu, G. Jin, S. G. Thomas, M. S. Goorsky, and K. L. Wang, Appl. Phys. Lett. **75**, 1586 (1999).
[12] E. A. Stach, K. W. Schwarz, R. Hull, F. M. Ross, and R. M. Tromp, Phys. Rev. Lett. **84**, 947 (2000).
[13] J. W. P. Hsu, E. A. Fitzgerald, Y. H. Xie, P. J. Silverman, and M. J. Cardillo, Appl. Phys. Lett. **61**, 1293 (1992).
[14] H. P. Tang, L. Vescan, C. Dieker, K. Schmidt, H. Luth, and H. D. Li, J. Cryst. Growth **125**, 301 (1992).
[15] E. A. Steinman, V. I. Vdovin, T. G. Yuhova, V. S. Avrutin, and N. F. Izyumskaya, Semicond. Sci. Technol. **14**, 582 (1999).
[16] G. Abstreiter, H. Brugger, T. Wolf, H. Jorke, and H. J. Herzog, Phys. Rev. Lett. **54**, 2441 (1985).