Photoluminescence characterization of strained Si-SiGe-on-insulator wafers

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1. Introduction

To achieve high performance of the device fabricated on strained Si-SiGe-on-insulator (SSGOI), the high-quality wafer fabrication is desired. The SSGOI wafer can be fabricated employing the epitaxial growth of SiGe layer on Si-on-insulator (SOI) substrate, the separation by the implanted oxygen (SIMOX) technique for a thick SiGe layer grown on Si substrate, and the Ge condensation by dry oxidation of the SiGe on SOI substrate [1]. The last one is promising because the thin and high-relaxation-ratio SiGe layer on insulator (SGOI) substrate with minimum dislocation density can be achieved employing this method.

To evaluate the quality of SSGOI wafers, the application of photoluminescence (PL) is a good choice because it can provide information strongly related to electrical and optical properties. So far, some groups have performed PL characterizations for SGOI [2], SSGOI [3], and SiGe quantum wells on SOI [4]. In these studies, the SiGe layer fabrication methods are epitaxial growth [3,4] or Ge⁺ ion implantation in the over layer of SOI [2]. The PL characterization for SSGOI fabricated using the Ge condensation method has not been reported yet. In this work, we demonstrate the PL signals for SSGOI wafers with different Ge fractions (Ge%).

2. Experiment, results and discussion

The wafers were fabricated using Ge condensation by dry oxidation of intrinsic SiGe on 8-inch low-dosed SIMOX SOI substrate by chemical vapor deposition method. An intrinsic strained Si layer was epitaxially grown on SiGe for each wafer in the final step.

The as-grown wafer structure is shown in Fig. 1(a). Because the total thickness of strained Si and SiGe is only 85 nm and the diffusion length of free exciton (FE) generated by laser irradiation is at least a few μm in them,⁷ the surface recombination has a great influence on PL signals from layers above buried oxide (BOX). Thus, we performed surface passivation by SiO₂ fabricated using a thermal dry oxidation at 1000° C in O₂ ambient for 10 min, which is shown in Fig. 1(b). Approximately 20 nm SiO₂ was grown, implying approximately 9 nm of the strained Si was consumed. Since the SSGOI wafer fabrication temperature is higher than 1100°C, this passivation process would not modify the wafer crystalline quality. During the surface SiO₂ growth, the Ge atoms in SiGe layer diffused into strained Si layer simultaneously with the diffusion length of approximately 6 nm. Thus, the strained Si was completely consumed and the final wafer structure is shown in Fig. 1(c). The Ge fractions of the wafers after surface passivation are 13%, 18%, and 25%, which are referred as sample A, B, and C, respectively.

The PL measurements were carried out using a 325 nm UV line of a HeCd laser and a 514 nm green line of an Ar^+ laser. Both of the lasers are continuous waved and focused on the surface of the sample with spot areas of approximately 8×10^{-3} mm² for the 325 nm line and 3×10^{-4} mm² for the 514 nm line. The penetration depths are approximately 8 nm for 325 nm line and great than 1 µm for 514 nm line [6], which are



Fig. 1 (a) structure of the as-grown wafer; (b) surface passivation process; (c) final sample structure and penetration depths demonstration of two wavelengths from HeCd and Ar^+ lasers.

demonstrated in Fig. 1(c). PL from the samples was collected and dispersed by LabRAMHR-PL (Horiba Ltd.) system and detected by an InGaAs array sensor cooled at 180K. All of the samples were cut into small size of $4 \times 4 \text{ mm}^2$ from the position at radius of 10 cm on the wafer and set on the sample holder at the same time and cooled down to 8.5 K using cryostat to satisfy exactly the same excitation condition.

First of all, we investigated sample C by the reason of its highest defect density, consequently abundant PL signals. Figure 2 shows the PL spectrum with the excitation of the two lasers. The X-band [7] was observed under both of the excitations, and the FE transitions from Si substrate were only observed under the Ar⁺ laser excitation, which is caused by different penetration depths of the two laser beams and the isolation of the excitons by the BOX. The superscript NP indicates the no-phonon transition. TA, TO, and O^{Γ} indicate the transitions assisted by transverse acoustic, transverse optical, and zone-center optical phonon, respectively. The X-band peak is dominated by FE transition, which was verified by the detailed temperature dependence measurement. From Fig. 2, we could judge the PL signals induced by 325 nm line should only provide the information of SiGe layer. Therefore, the very broad peak (0.8-1.0 eV, so called T-band [8,9]) belongs to SiGe layer, the dislocation related peak D1 belongs to the substrate. The peak around 1.07 eV was also confirmed to be related to



Fig. 2 PL signals of sample C with (a) 325 nm and (b) 514 nm line excitations. Temperature is 8.5K and laser power is 1 mW.

defects in substrate because it survives under very low excitation power of 1 μ W, under which condition even the FE^{TO} signal can not be observed. Thus, we focused on 325 nm line excited PL signals to compare the SiGe properties in this work. In the case of defect related PL signals in the substrate, further study is needed to investigate their origins.

Figure 3 shows the 325 nm line excited PL signals from samples A, B, and C. Because the excitation conditions are exactly the same, the comparison of integrated peak intensities of the X-bands among these three samples is meaningful for wafer quality comparison. In the case of sample C, the X^{TO} peak is mixed with the T-band. Since the intensity ratio of X^{NP} to X^{TO} increases with Ge% in the Si-rich region [7], from Figs. 3(a) and 3(b) we can confirm the intensity of X^{TO} should less than that of X^{NP} for sample C. Thus, we utilized 2 times of the intensity of X^{NP} to replace the total X-band intensity for sample C. The actual total X-band intensity for sample C should be less than this value.

Fig. 4(a) shows the total X-band integrated intensities of samples A, B, and C monotonously decreased with increasing of Ge%, implying the wafer quality inversely depends on Ge%. The defect related T-band of sample C confirms its high defect density. The deep-level region PL signals from sample A and B are similar. We believe there should be more PL signals lower than 0.75 eV (which is out of detect region of InGaAs sensor) or non-irradiative centers for sample B than that for sample A.

From the X^{NP} peak energy position, we can easily obtain the X-band gap for SiGe layer [10]. The X-band gap results are shown in Fig. 4(b). The data from Ref. 7 shows the X-band gap for fully relaxed SiGe alloy at 4.2 K, which is higher than our result. Another data [11] measured by optical absorption method is in good agreement with our result. Because there is no widely accepted X-band gap data for fully relaxed SiGe alloy at 8.5 K, it is difficult to evaluate the lattice relaxation ratios of our samples. The Raman peak shift measurement shows the lattice relaxation ratios are higher than 90% for samples A and B, and the ratio is 75% for sample C.

The property of the broad peak T-band was studied by changing the laser power. Figure 5 shows the results. Under the



Fig. 3 325 nm line excited PL signals of samples A, B, and C. Temperature is 8.5K and laser power is 1 mW.



Fig. 4 (a) total integrated intensity of X^{NP} and X^{TO} peaks of samples A, B, and C; (b) X-band gaps of sample A, B, and C.



Fig. 5 Laser power dependence of T-band PLs. The laser powers are 0.01, 0.02, 0.05, 0.1, 0.2, 0.5, 1, 2, 5, and 10 mW, respectively.

minimum laser power of 10 µW, two broad sub-peaks were clearly observed. The intensities of these two peaks show sublinear dependence on laser power, implying its defect related nature. Unfortunately, the water vapor absorption [2, 12] lines just locate on the middle of T-band under the high laser power excitation, which disturb the judgment of the two sub-peaks energy positions. The blue-shift and saturation of sub-peaks energy positions with increase of laser power implies the continuous distribution of the deep levels. The two sub-peaks energy positions saturated around 0.87 eV and 0.92 eV under the maximum laser power, respectively. These two positions are close to the D2 and D3 positions of dislocation related bands. The T-bands were also observed by other groups in SGOI [2], SiGe/Si heterostructure [8], SiGe on SOI [9], and SiGe/Si/SiGe quantum well [12] structures. The origin of this band has not been clarified yet.

3. Conclusion

In summary, the X-band and deep-level PL signals was observed for three SSGOI wafers with different Ge fractions fabricated using Ge condensation by dry oxidation of the SiGe on SOI. The PL signals of wafers with 13% and 18% Ge fractions are deep-level-free, implying high wafer qualities. A defect related T-band signal could be observed for wafer with 25% Ge fraction. The saturated sub-peaks positions of the T-band are close to the dislocation related D-bands.

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