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# Photoluminescence and Raman study of a tensilely strained Si type-II quantum well on a relaxed SiGe graded buffer

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**Abstract.** We have investigated the photoluminescence and Raman scattering of tensilely strained Si quantum wells embedded in $Si_{1-x}Ge_x$ relaxed layers. The radiative recombination of excitons in the $Si_{1-x}Ge_x$ ($x \lesssim 0.3$) alloy layers and the type II transitions involving the recombination of an electron localized in the $\Delta_2$ minimum of the conduction band of the strained Si quantum well and a hole localized in the valence band maximum of the $Si_{1-x}Ge_x$ layer were observed. The influence of a graded buffer on the density of defects/dislocations and, consequently, on the optical properties was clearly observed.

## 1. Introduction

Strain has been explored as an important parameter in the band structure engineering that allows increasing carrier mobility in silicon based heterostructures [1]. In particular, silicon channels deposited on strain-relaxed $Si_{1-x}Ge_x$ layers on Si substrates showed enhanced carrier mobilities which is very important for microelectronic device applications, especially in metal-oxide-semiconductor field-effect transistors [2]. In order to tensilely strain the silicon channel, the $Si_{1-x}Ge_x$ layers must have a high Ge content, particularly with $x$ in the range $0.2 < x < 0.5$ [3]. The ideal $Si_{1-x}Ge_x$ layers should have low densities of dislocations and other extended defects, a smooth surface with low roughness and a uniform and high degree of strain relaxation. The occurrence of dislocations and defects in the layers around the buried channel create a high density of pathways for the recombination of carriers which will deteriorate the optical and electrical parameters. In this work, we study the radiative recombination of excitons in a structure containing a Si quantum well (QW) embedded in $Si_{1-x}Ge_x$ layers, as well as the influence of defects and dislocations on the optical properties of the structure.

## 2. Experimental details

Three samples with a Si quantum well (QW) embedded in a nominal $Si_{0.7}Ge_{0.3}$ layers were grown by molecular beam epitaxy on a Si (001) substrate, according to the structures shown in figure 1. Two different thicknesses of the Si QW were considered and the growth of the above structure

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was done on a compositionally-graded $Si_{1-x}Ge_x$ buffer or directly on the Si substrate. After the growth, some pieces of the samples were passivated with atomic hydrogen in a chemical vapour deposition reactor at $T \sim 100^0$ C for 30 min, in order to decrease the density of defects causing strong nonradiative recombination.

**Figure 1.** Nominal schematic drawing of the three structures studied. The difference between samples A and B is in the thickness of the Si QW, 10 and 20 nm, respectively. Sample C has a similar structure to sample A except in the absence of the graded buffer.

Photoluminescence (PL) was performed in the range from $5-300$ K, using a Fourier transform infrared Bruker IFS 66v spectrometer equipped with a Ge detector cooled to liquid nitrogen temperature. The 514.5 nm line of an $Ar^+$ laser was used as excitation source. Raman spectroscopy was performed in the visible region using a Jobin Yvon T64000 spectrometer, equipped with a 100× microscope objective and a liquid nitrogen cooled charge-coupled device. The excitation source was the 514.5 nm line of an $Ar^+$ laser. The measurements were done at room temperature in the backscattering geometry $z(x, y)\overline{z}$, where $x||[100]$, $y||[010]$, $z||[001]$.

## 3. Results and discussion

The PL spectrum observed for the as-grown sample A is dominated by two bands centred at $\sim 0.79$ and $\sim 0.85$ eV (see figure 2 a)). After hydrogen passivation, a change in the relative intensity of the bands occurs, as a result of a reduction in the number of recombination active defects. Additionally to a band at $\sim 0.796$ eV, two pairs of bands are clearly observed, one at ($\sim 1.010$ and $\sim 0.952$ eV) and another one at ($\sim 0.902$ and $\sim 0.856$ eV), denoted by pairs P1 and P2, respectively. The temperature dependence of the luminescence of the passivated sample is shown in figure 2 a). The pair P1 persists for $T \lesssim 10$ K whereas the pair P2 is observed for $T \lesssim 60$ K. With increasing temperature, the emission becomes dominated by two main transitions at $\sim 0.871$ and $\sim 0.796$ eV which are attributed to the dislocation related D2 and D1 bands, respectively [5].

A behaviour similar to the one peculiar to sample A was obtained after the passivation treatment of samples B and C as shown in figure 2 b). For sample B, just the pair P2 is observed at $\sim 0.92$ and $\sim 0.86$ eV and for sample C the emission is dominated by dislocations and a broad band suggesting a high density of defects. At higher energies, the pair P1 is observed at $\sim 1.013$ and $\sim 0.957$ eV. For this sample, the increase of the density of defects/dislocations can be attributed to the absence of the graded buffer.

The dislocation related emission depends on the sample and on the measurement temperature. In order to clearly show for sample A the superposition of the pair of bands P2 with the dislocations related emission, we tentatively took the spectrum of the sample at $T = 70$ K in the range $0.75 < h\nu < 0.95$ eV as representative of the dislocations emission and performed a simulation of the spectrum at 5 K (see figure 2 b)). The observed two pairs of bands were represented by gaussian curves. The above model can describe fairly well the total emission for the studied temperatures, showing a clear influence of defects/dislocations on the optical properties of the samples under study.

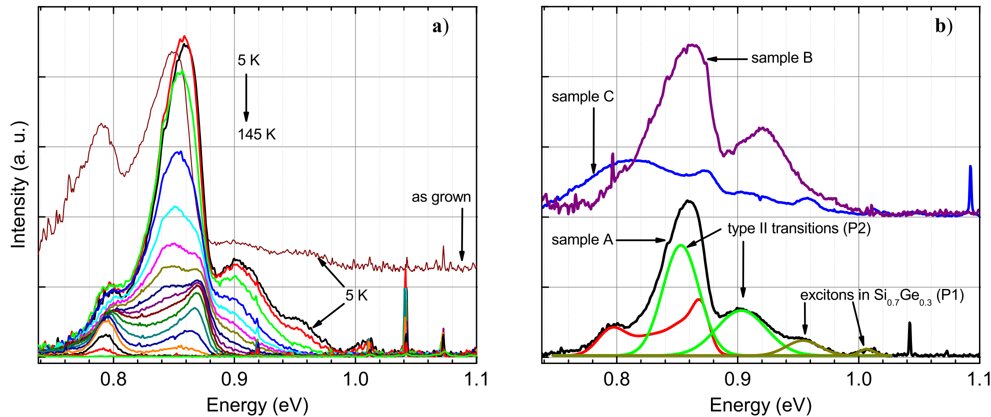


**Figure 2.** a) PL spectrum for the as grown sample A at 5 K and temperature dependence of the PL from the passivated sample A; b) comparison of the PL spectra for the passivated samples A, B and C at 5 K; a simulation of the emission of the passivated sample A at $T = 5$ K is shown.

To interpret the pairs of bands P1 and P2, we must point out that the energy separation in each pair of transitions is very close to the value of the TO phonon in Si (0.0585 eV [4]). The temperature dependence for sample A showed that the pair P1 was observed for $T \lesssim 10$ K. On the other hand, the calculation of the free exciton energy gap at low temperatures for unstrained $Si_{0.7}Ge_{0.3}$ alloy gives $E_g^{\Delta} = 1.028$ eV [6]. In this way, the pair P1 is attributed to a no-phonon (NP) and a TO-phonon assisted transitions due to the recombination of excitons in the $Si_{1-x}Ge_x$ layers. Finally, the conduction band offset between $Si_{0.7}Ge_{0.3}$ and Si is $\Delta E = 0.180$ eV [1]. So, the energy separation between an electron in the conduction band minimum of the strained Si layer and a hole localized in the valence maximum band of the $Si_{0.7}Ge_{0.3}$ layer is 0.848 eV. In view of the energy band alignment at the interface, the pair P2 is consistent with the NP and TO phonon transitions involving the type-II recombination of an electron localized in the $\Delta_2$ minimum of the conduction band of the strained Si layer and a hole localized in the valence band maximum of the $Si_{0.7}Ge_{0.3}$ layer. This type of transition was clearly established [1]. The temperature stability for the pair P2 observed for sample A is in accordance with this interpretation. The above attributions of both pairs of bands are also supported by other PL measurements in tensilely strained Si QW grown on buffers with different Ge contents [7, 8, 9].

The Raman spectra of samples A, B and C, for the $z(x, y)\overline{z}$ geometry, are shown in figure 3 and support the interpretation of the pair of bands P2 as follows. For the three samples as observed the stretching vibrations of the Ge-Ge, Si-Ge and Si-Si bonds in the $Si_{0.7}Ge_{0.3}$ alloy layer, as well as the Si-Si vibration in the strained Si QW are seen. Additionally, for sample C the Si-Si vibration in the substrate is observed. The absence of this peak in the spectra of samples A and B is due to the penetration depths of the 514.5 nm laser line in Si (3.70 $\mu$m) and $Si_{0.7}Ge_{0.3}$ (240 nm). The positions of the observed peaks are listed in table 1. The observed peaks confirm the nominal structure of the three samples. The Si-Si peaks with origins in the $Si_{0.7}Ge_{0.3}$ alloy layer and in the strained Si QW have similar frequencies in both samples A and C which are lower than those measured in sample B. Additionally, we observe a lower intensity of the Ge-Ge and Si-Ge peaks in sample B when compared to the observed in the other two samples. These results could be explained if we assume a Ge content $x < 0.3$ in the $Si_{1-x}Ge_x$ buffer of sample B. In this case, the influence of the Ge content on the Si-Si peak from the alloy layer will be lower in sample B and the relative intensity of the Ge-Ge and Si-Ge peaks will be also lower. The strain in the Si QW will be consequently smaller which results in a shift of the Si-Si peak with origin in this layer to higher frequencies (see table 1). The above evaluation of

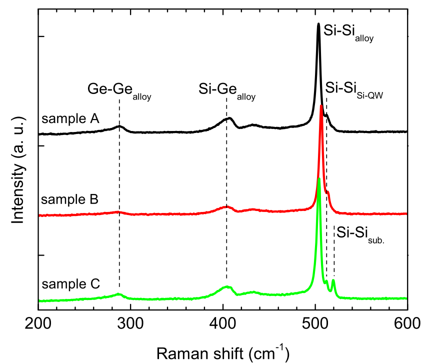


**Figure 3.** Raman spectra of samples A, B and C. The used geometry was $z(x,y)\overline{z}$. Dashed lines are used to identify the phonon vibrations with the origin in the $Si_{0.7}Ge_{0.3}$ alloy layer, Si QW and Si substrate. The peak observed in the range $432.1 - 433.5\,\mathrm{cm}^{-1}$ was related to Si vibrations in chemically different local environments within the alloy layer [10].

**Table 1.** Peaks positions for the observed phonons. The experimental error is $0.5\,\mathrm{cm}^{-1}$.

| Sample | $Ge\text{-}Ge_{alloy}$ | $Si\text{-}Ge_{alloy}$ | $Si\text{-}Si_{alloy}$ | $Si\text{-}Si_{Si\ QW}$ | $Si\text{-}Si_{sub}$ |
|---|---|---|---|---|---|
| A | 287.9 | 407.1 | 503.6 | 512.1 | |
| B | 286.3 | 404.8 | 506.5 | 513.5 | |
| C | 286.9 | 404.9 | 504.0 | 512.2 | 519.6 |

the Ge content in the $Si_{1-x}Ge_x$ buffer of sample B is in a qualitative accordance with the PL measurements: the NP transition observed in sample A at $\sim 0.902\,\mathrm{eV}$ is observed in sample B at $\sim 0.92\,\mathrm{eV}$, as expected for a lower Ge content in the $Si_{1-x}Ge_x$ buffer of sample B.

In this work, we observed the radiative recombination of excitons in the $Si_{1-x}Ge_x$ ($x \lesssim 0.3$) alloy layers and the type II transitions involving the recombination of an electron localized in the $\Delta_2$ minimum of the conduction band of the strained Si layer and a hole localized in the valence band maximum of the $Si_{1-x}Ge_x$ layer. The Raman spectroscopy delivered complementary information that allowed an evaluation of the Ge content and strain in the structures. The absence of the graded buffer results in a high dislocations density. The influence of defects/dislocations on the optical properties was shown. Finally, this work shows the importance of the optical techniques for the monitorization of the growth of structures involving strain between the different grown layers.

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