

## Photoluminescence of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ Quantum Well Structures

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Photoluminescence (PL) spectra of  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  multiple quantum wells (MQW) have been investigated. Strong emission bands appear for all the as-grown samples. The PL intensity is increased by a factor of 5-10 after the annealing at 600-700 °C. The annealing at 800 °C results in the low PL intensity. The dependence of the PL intensity on the excitation powers indicates that some recombination center is involved in the strong emission. This recombination center is considered to be very sensitive to the heat treatments. TEM observations show that the quality of the quantum well structures is related to the observed PL characteristics. The intense PL may be due to the two dimensional carrier confinement.

### 1. Introduction

There has been much interest recently in the optical properties of  $\text{SiGe}/\text{Si}$  heterostructures.<sup>1-5)</sup> Among them, the intense photoluminescence (PL) from  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  multiple quantum wells (MQW) reported recently by Noël et al.<sup>5)</sup> have attracted much attention because of the possibility for optoelectronic applications. They consider that the efficient PL is due to exciton accumulation in the strained  $\text{Si}_{1-x}\text{Ge}_x$  layers. However, the PL spectra of  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  MQWs have not been analyzed in detail and the origin of the intense PL is still unknown. To clear up the nature of the PL from the  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  MQWs, we have fabricated various  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  quantum well structures and investigated the dependence of the PL on the quantum well structure, the alloy composition, and the annealing condition.

### 2. Experimental

The quantum well structures were grown on  $\text{Si}(100)$  substrates by molecular beam epitaxy (MBE) at a substrate temperature of 400 °C. A typical structure of MQW consists of 30 periods of 70-Å-thick  $\text{Si}_{1-x}\text{Ge}_x$  alloy layers and 110-Å-thick Si layers. We have also fabricated single quantum well (SQW) structures each of which consists of a 70-Å-thick  $\text{Si}_{1-x}\text{Ge}_x$  alloy layer sandwiched between a Si substrate and a 2000-Å-thick Si layer. Some of the samples were annealed at 600-800 °C in  $\text{N}_2$ . The quantum well structures were examined by transmission electron microscopy (TEM).

The samples were immersed in liquid helium in a glass cryostat. They were excited by the 488 nm

line of an Ar ion laser. The emission from the sample was analyzed by a 32 cm grating monochromator with a 600 groove/mm grating blazed at 1  $\mu\text{m}$  and detected by a cooled Ge detector. The spectral response of the measurement system was calibrated using blackbody radiation.

### 3. Results and Discussion

Photoluminescence spectra of  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  MQWs are shown in Fig. 1 for the different alloy composition  $x$  of  $\text{Si}_{1-x}\text{Ge}_x$ . A small peak near 1135 nm is the band-edge emission of the Si substrate. In the first report by Noël et al.<sup>5)</sup>, strong emission was observed only for the annealed samples. However, in our work, strong emission bands has been observed for all the as-grown samples. The intensity of these emission bands is about 30 times stronger than that of the band-edge emission of the Si substrate. The peak of the emission bands shifts from 1.03 to 0.87 eV as the alloy composition is increased from 0.1 to 0.3. This corresponds to the shift of the band gap energy of  $\text{Si}_{1-x}\text{Ge}_x$ . The band gap energy of  $\text{Si}_{1-x}\text{Ge}_x$  on Si is 1.07 eV for  $x=0.1$  and 0.92 eV for  $x=0.3$  according to the theoretical calculations by People and Bean<sup>6)</sup>. The strong emission may be from the  $\text{Si}_{1-x}\text{Ge}_x$  layers.

In the case of  $x=0.1$  and 0.2, the PL spectra have a rather broad structure. The PL spectra of  $\text{Si}_{0.8}\text{Ge}_{0.2}/\text{Si}$  MQW for different excitation powers are shown in Fig. 2. For the low excitation powers, two peaks and a broad tail can be clearly observed in the spectra. The spectra are composed of at least three emission bands.

In contrast to the case of  $x=0.1$  and 0.2, only one peak can be observed in the PL spectra of  $\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Si}$

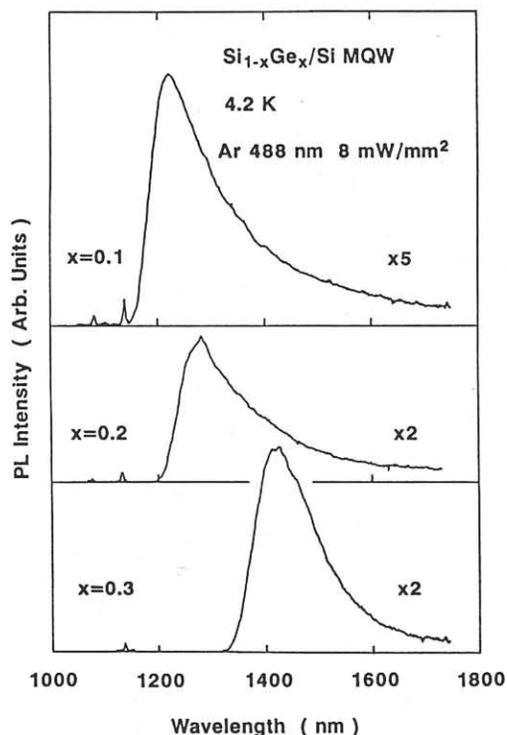


Fig. 1. Dependence of photoluminescence spectra on their composition  $x$  in  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  MQWs (as-grown). A notation "x5" indicates the original intensity is magnified by a factor of 5.

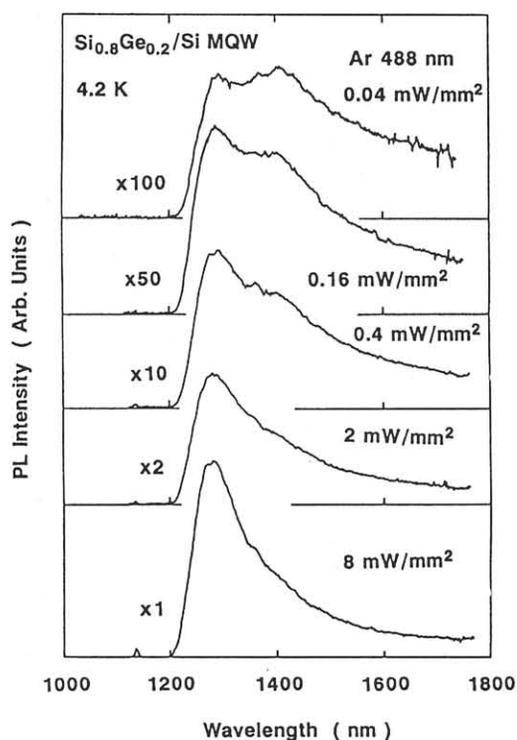


Fig. 2. Photoluminescence spectra of  $\text{Si}_{0.8}\text{Ge}_{0.2}/\text{Si}$  MQW (as-grown) for the different excitation powers.

MQW even for the low excitation powers. Moreover, the PL intensity is increased as the alloy composition  $x$  is increased. TEM observations reveal that the MQW has higher quality for  $x=0.3$  than for  $x=0.1$  and  $0.2$ . Smoother and more abrupt  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  interface can be observed for  $x=0.3$ . Anomalous contrast near the interface in the as-grown  $\text{Si}_{1-x}\text{Ge}_x$  layers was observed in the TEM image for  $x=0.1$  and  $0.2$ . This may be the fluctuation of the alloy composition in the  $\text{Si}_{1-x}\text{Ge}_x$  layers. The observed emission bands may be related to the quality of the quantum well structures.

In all cases from  $x=0.1$  to  $0.3$ , the intensity of the strong emission increases almost linear with the excitation power when the excitation power is weak. When the excitation power becomes strong, the intensity shows a sub-linear dependence, maybe due to the saturation effects. This shows that some recombination center is involved in the strong emission.

Annealing effects on the PL spectra of  $\text{Si}_{0.9}\text{Ge}_{0.1}/\text{Si}$  MQW are shown in Fig. 3. After the annealing at  $600\text{--}700\text{ }^\circ\text{C}$  in  $\text{N}_2$ , the PL intensity is increased by a factor of 5-10 and the emission band in the shorter wavelength side becomes dominant. The energy position of this dominant band is slightly lower than the band gap energy of  $\text{Si}_{1-x}\text{Ge}_x$ . The annealing at  $800\text{ }^\circ\text{C}$  results in the low PL intensity. The same effects can be observed in all cases from  $x=0.1$  to  $0.3$ .

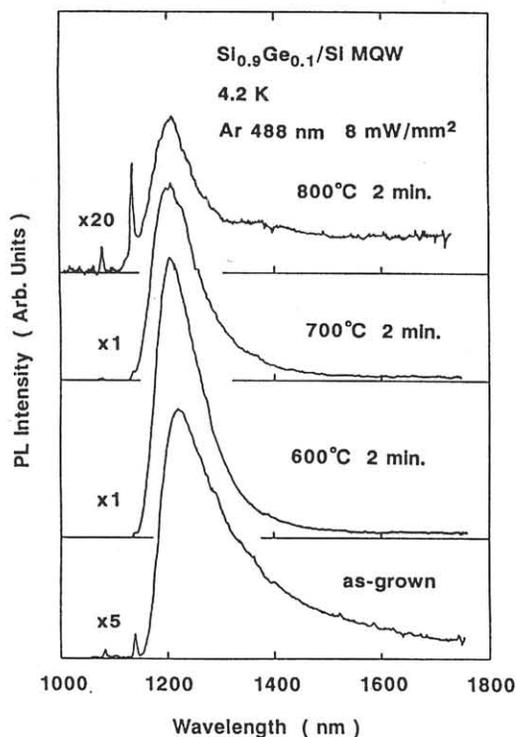


Fig. 3. Annealing effects on the photoluminescence spectra of  $\text{Si}_{0.9}\text{Ge}_{0.1}/\text{Si}$  MQW. The samples were annealed in  $\text{N}_2$ .

Noël et al.<sup>5)</sup> explained that the increased PL intensity after the annealing at 600-700 °C is due to the disappearance of the grown-in defect complexes and that the generation of misfit dislocations at 800 °C decreases the PL intensity. They consider that the efficient PL is due to exciton accumulation in the strained Si<sub>1-x</sub>Ge<sub>x</sub> layers. However, as discussed above, the strong emission is related to some recombination center. We can consider that this recombination center is very sensitive to the heat treatments. The annealing at 600-700 °C may increase the density of the recombination centers. On the other hand, the annealing at 800 °C may cause the decrease in density of recombination centers as well as the generation of the misfit dislocations.

In the TEM observations for the samples annealed at 800 °C, the degradation of the abruptness can be observed as well as the generation of misfit dislocations. The TEM observations also show the roughness of the interface and the interdiffusion of Si and Ge. The quality of the quantum well structures may also be related to the characteristics of the PL spectra.

The PL spectra of Si<sub>1-x</sub>Ge<sub>x</sub>/Si SQWs are shown in Fig. 4 for x=0.1 and 0.3. The same features as in the case of the MQWs can be observed for both the as-grown and the annealed samples. The annealing at 600-700 °C increases the PL intensity and the annealing at 800 °C results in the low PL intensity.

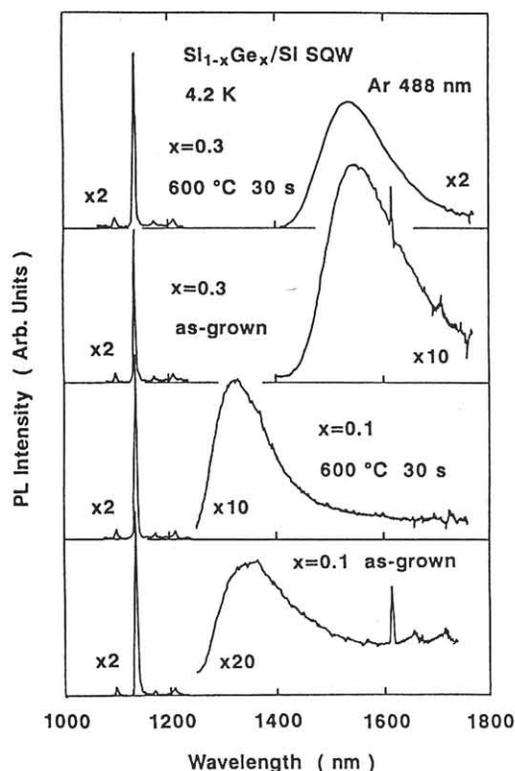


Fig. 4. Photoluminescence spectra of Si<sub>1-x</sub>Ge<sub>x</sub>/Si SQWs before and after the annealing in N<sub>2</sub>.

This indicates that the observed PL characteristics originate in the quantum well structures. In our previous work,<sup>4)</sup> thick Si<sub>1-x</sub>Ge<sub>x</sub> layers on Si substrates did not show similar emission as in the case of the MQWs. The observed PL in the MQWs and the SQWs may be related to the thickness of Si<sub>1-x</sub>Ge<sub>x</sub> layers. Strong emission is considered to be due to the two dimensional carrier confinement.

#### 4. Conclusions

Strong emission bands appear in the PL spectra of Si<sub>1-x</sub>Ge<sub>x</sub>/Si MQWs for all the as-grown samples. The PL intensity is increased by a factor of 5-10 after the annealing at 600-700 °C. The annealing at 800 °C results in the low PL intensity. For small x (about x<0.2), the PL spectra have a rather broad structure and composed of possibly three emission bands. After the annealing at 600-700 °C, the emission band in the shorter wavelength side becomes dominant. The energy position of this dominant band is slightly lower than the band gap energy of Si<sub>1-x</sub>Ge<sub>x</sub>. These features in the PL spectra of Si<sub>1-x</sub>Ge<sub>x</sub>/Si MQWs can be observed also in SQWs. The intense PL may be due to the two dimensional carrier confinement. The quality of the quantum well structures is considered to be related to the observed PL characteristics. The dependence of the PL intensity on the excitation powers indicates that some recombination center is involved in the strong emission. This recombination center is considered to be very sensitive to the heat treatments.

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