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Influence of the cavity on the low-temperature photoluminescence of SiGe/Si multiquantum wells grown on a silicon-on-insulator substrate

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The influences of the cavity on the low-temperature photoluminescence of $Si_{0.59}Ge_{0.41}/Si$ multiquantum wells grown on silicon-on-insulator substrates are discussed. The positions of the modulated photoluminescence (PL) peaks not only relate to the nature of SiGe/Si multiquantum wells, but also relate to the characteristic of the cavity. With increasing temperature, a redshift of the modulated PL peak originating from the thermo-optical effect of the cavity is observed. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2187433]

During the past few years, a great deal of work has been devoted to creating novel optoelectronic devices using strained SiGe/Si heterojunctions by energy-band engineering, as these devices may be monolithically integrated with mature silicon circuits.[1] To obtain good performance in such applications, a high-quality SiGe/Si heterostructure is required. Photoluminescence (PL) is widely used to evaluate the band-gap information and electronic quality of the SiGe/Si heterostructures, such as the free exciton transitions, phonon replicas, and the alignment of bound excitons.[2–7] However, due to cavity modulation to the PL spectrum, it is difficult to obtain the correct band-gap energies for SiGe/Si heterostructures grown on silicon-on-insulator (SOI) substrates. At room temperature, the effect of the cavity on the PL spectrum is easily understood and has previously been discussed in detail.[8,9] But at low temperature, this cavity effect is not so distinct and makes the determination of the band-gap energy difficult. Moreover, there are few references to discuss this cavity influence on the low temperature PL spectrum. This letter describes in detail the effect of the cavity on the low temperature PL spectrum.

All samples were grown by ultrahigh vacuum-chemical vapor deposition (UHV-CVD) on a (100) oriented SOI substrate from pure disilane and germane (Si_2H_6 and GeH_4). The SOI substrates were cleaned in an *ex situ* chemical etch process and loaded into an UHV growth chamber with a basic pressure of 8×10^{-8} Pa, and then heated up to 930 °C to deoxidize. The multilayer structures consisted of a 250 nm Si buffer layer grown at 850 °C, followed by ten bilayers consisting of 6 nm $Si_{0.59}Ge_{0.41}$ and 33 nm thick Si grown at 650 °C, and finally a 300 nm silicon capping layer to reduce nonradiative surface recombination. PL measurements were taken between 10 K and room temperature using an Ar^+ laser at $\lambda = 514.5$ nm with a power of 100 mW and a liquid-nitrogen-cooled Ge photodetector.

Figure 1 shows the PL spectrum of the $Si_{0.59}Ge_{0.41}/Si$ multiquantum wells grown on a SOI substrate at 10 K, which is similar to the typical PL spectrum of SiGe material.[10] Just according to Fig. 1, it is difficult to judge if the cavity will have an influence on the PL spectrum. So it is easily falsely believed, as we discussed in the previous works,[8] that the peaks labeled A and B should be the no-phonon transition and its TO-phonon replica of the $Si_{0.59}Ge_{0.41}/Si$ multiquantum wells respectively by the 59.2 meV separation [nearly 58 meV—the typical energy of TO-phonon replicas of Si-Si (Ref. 10)] and the peak labeled C should be the TO phonon peak of the substrate.

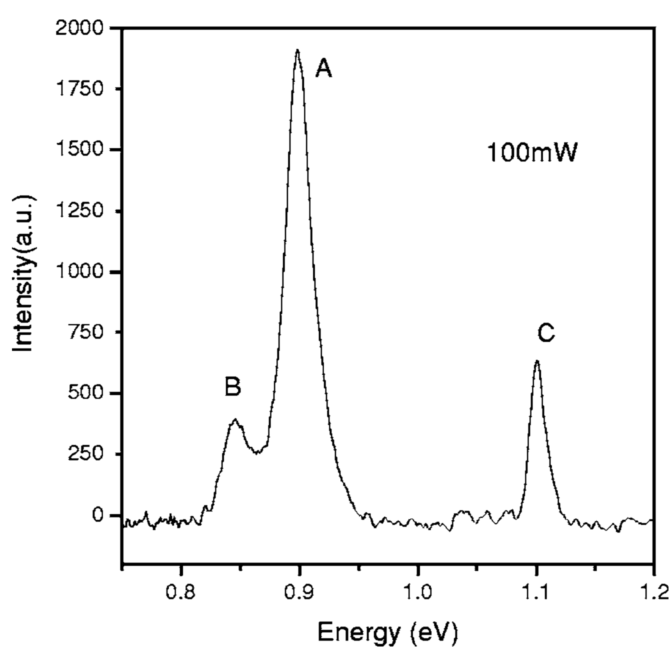

FIG. 1. PL spectrum taken at 10 K for ten $Si_{0.59}Ge_{0.41}$ (6 nm)/Si (33 nm) multiquantum wells grown on a silicon-on-insulator substrate.

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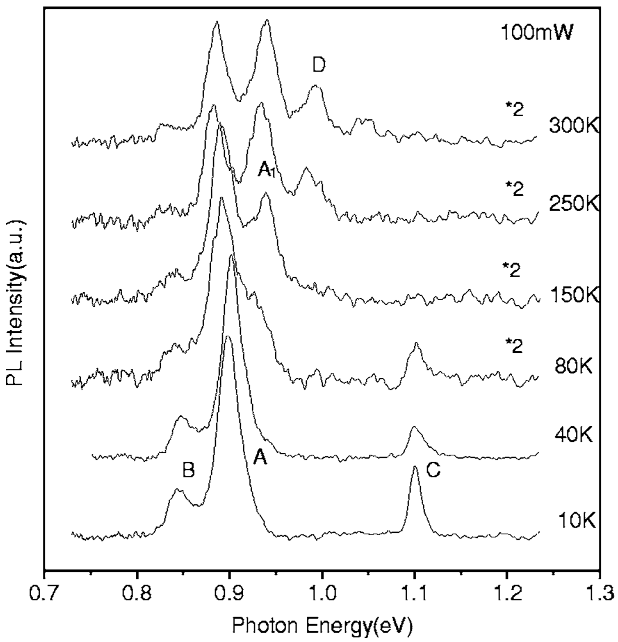

FIG. 2. PL spectrum taken at various temperatures between 10 and 300 K for ten $Si_{0.59}Ge_{0.41}$ (6 nm)/Si (33 nm) multiquantum wells grown on a silicon-on-insulator substrate.

But as the temperature is increased, there are more peaks in the PL spectrum: At 80 K, there is a shoulder on the right of the peak A and at 150 K an additional peak labeled A_1 appears, accompanied by the disappearance of peak C. When the temperature is increased to 250 K, another peak labeled D appears (as shown in Fig. 2). This is not characteristic of the PL spectrum of SiGe materials grown on Si substrates.[11,12] It is proposed that the PL spectrum at low temperature is most likely influenced by the SOI substrate.

We have previously discussed that the cavity formed by the mirrors at the surface and the buried SiO_2 interface of the SOI substrate has an influence on the room-temperature PL emission. The multipeaks in the room-temperature PL spectrum are the result of modulation by this cavity.[8,9] From this cavity effect, only when the energy of the luminescence obeys Eq. (1), can it be transmitted through the cavity and be collected:[13]

$$2\frac{2n\pi}{1.24/E}L + \Psi_1 + \Psi_2 = 2m\pi \quad (m = 1,2,3,\ldots). \tag{1}$$

Here n is the effective refractive index of the cavity, E is the energy of the PL, L is the length of cavity and Ψ_1, Ψ_2 denote phase shifts due to the penetration into the mirrors.

This equation helps explain the observed PL data shown in Fig. 2. With increasing temperature, the thermal energy of the free carriers increases and the PL peaks broaden;[11,12] the broadened PL peak is then modulated by the cavity formed by the mirrors at the surface and the buried SiO_2 interface on the SOI substrate. The higher the temperature, the more obvious the cavity modulation becomes.

The location of the PL peak of the material grown on SOI substrate not only relates to the nature of the $Si_{0.59}Ge_{0.41}$/Si multiquantum wells (the energy of no-phonon transition and its TO-phonon replica), but also relates to the properties of the cavity (such as cavity length and effective refractive index of the cavity). The former determines the general location and the latter determines the exact position of the peak. For example, no matter where the peak of no-phonon transition of SiGe material is, in peak P or peak P' (as indicated by the dotted line shown in Fig. 3), due to modulation of the cavity, the true position of this peak is located as indicated by the solid line in Fig. 3 since the true peak location is determined by the cavity characteristic according to Eq. (1). So the energy of the no-phonon in the PL spectrum of the material grown on SOI substrate is not determinable directly from the nature of the material without accounting for the effects of modulation by the optical cavity present.

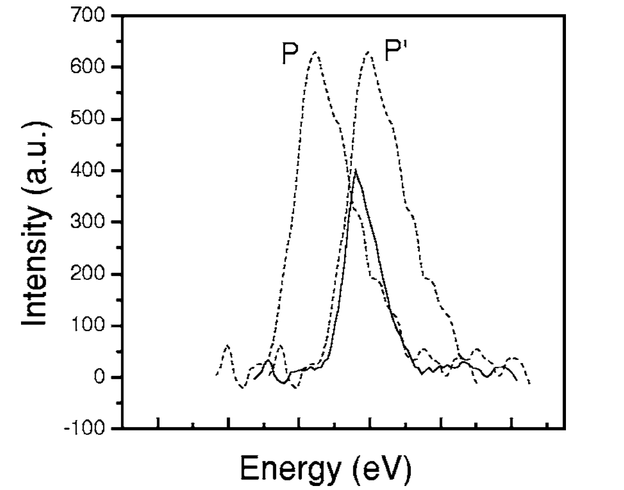

FIG. 3. A sketch to explain the modulation by the cavity to the PL spectrum. The dotted line shows the PL peak of the material as it would appear without modulation by the cavity; the solid line shows how the peak appears as a result of cavity modulation. The scales on both axes are arbitrary.

The peaks labeled A, B, and C, as shown in Fig. 1, are also the result of modulation by the cavity. The position of the PL peak is determined both by the nature of the SiGe material and the characteristics of the cavity. If this modulation by the cavity to the PL spectrum is ignored, then any interpreted optical properties of the material grown on SOI obtained from the modulated low-temperature PL spectrum would be incorrect. These facts imply that the band-gap information of the material grown on a SOI substrate cannot be singly measured using PL methods. One simple solution is to use the PL spectrum for the exact same material grown on a Si substrate.

From Fig. 2 it is apparent that with increasing temperature, there is a redshift in the peak labeled A. It is proposed here that the redshift is due to the thermo-optical effect of the cavity and not due exclusively to band-gap narrowing of the material since the PL spectrum is modulated by the cavity.

Crystalline silicon has a large thermo-optical coefficient[14,15] ($\Delta n/\Delta T$) of $1.86\times 10^{-4}\ K^{-1}$. As the temperature is increased, the refractive index of the silicon in the cavity increases correspondingly. In addition, the cavity length is also increased due to the thermal expansion of the silicon in the cavity. These combined effects contribute to the redshift of the peak labeled A in Fig. 2, since the energy of the peak position has an inverse-ratio relationship with refractive index, n, and cavity length, L, according to Eq. (1).

Between 10 and 300 K, the observed 0.012 eV redshift for peak A in Fig. 2 is consistent with calculations made using Eq. (1) taking into consideration the refractive index change of the silicon in the cavity while ignoring both the small thermal-expansion effect of the silicon in the cavity and the minor influence of the SiGe layer to the reflective index. This is additional evidence to confirm the cavity modulation to the PL spectrum.

In conclusion, the modulation of the PL spectrum by the cavity formed from $Si_{0.59}Ge_{0.41}/Si$ multiquantum wells grown on a SOI substrate at low temperature is presented. The cavity formed by the mirrors at the surface and the buried SiO_2 interface is shown to influence the PL spectrum of the SiGe material. The position of the PL peak is related to both the material and the cavity characteristics. The optical properties of the SiGe material grown on a SOI substrate can only be properly interpreted from the PL spectrum if the effects of the cavity modulation are taken into consideration. An increase in temperature from 10 to 300 K results in a 0.012 eV redshift of the modulated PL peak. This redshift is shown to originate from the increase in the refractive index of the silicon in the cavity, due to the large thermo-optical coefficient of silicon.

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