

## Study of the interdiffusion effect on the band structures of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ quantum wells

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(Received 16 January 2006; accepted 15 February 2006; published online 10 April 2006)

We investigated the influence of thermal interdiffusion on the band structures of  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  single quantum wells (SQWs) with a well width of 125 Å and Ge concentration  $x=0.3$ . Rapid thermal annealing with the temperatures of 750 and 800 °C leads to substantial interdiffusion indicated by a significant photoluminescence (PL) blueshift as large as 46 meV. The effect is modeled by a Si–Ge atomic interdiffusion at the heterointerface. The band structures and optical transitions of QW after interdiffusion were calculated based on an error function distribution and the 6+2-band  $k\cdot p$  method. The diffusion lengths of the intermixing process are deduced from the PL shift. The thermal dependence of the interdiffusion coefficients follows the Arrhenius law. An activation energy ( $E_a$ ) for interdiffusion of 2.75 eV is obtained. Our investigation indicates that the 6+2-band  $k\cdot p$  formalism is valid for interdiffused  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  QWs. © 2006 American Institute of Physics.  
 [DOI: 10.1063/1.2186983]

In recent years, tremendous developments have occurred in the field of SiGe heterojunctions and their applications in heterojunction bipolar transistors. Compared with higher cost III-V materials, SiGe devices are cost advantageous due to the mature and cheap silicon fabrication process. Furthermore, the indirect band gap of  $\text{Si}_{1-x}\text{Ge}_x$  spans the 1.30–1.55  $\mu\text{m}$  range, which makes Si–Ge alloys more attractive in long wavelength system-on-a-chip application.<sup>1–3</sup> Although the layers can be grown to very large thickness by symmetrically strained method,<sup>4</sup> the thermal stability through nucleation dislocation and interdiffusion of Si–Ge atoms is still a critical issue especially when the high processing temperature is unavoidable. The interdiffusion of  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  quantum wells (QWs) has been reported in several literatures. However, there exists a discrepancy in the literature on the value of  $E_a$ , which can be divided into two groups: (1) 2–3 eV, Sunamura *et al.* and Boucaud *et al.* obtained the  $E_a$  of 2.47 and 2.42 eV separately by the photoluminescence (PL) method,<sup>5,6</sup> which are fairly close to the value of Baribeau *et al.* of 2 eV.<sup>7</sup> (2) 4–5 eV, Holländer *et al.* deduced an average  $E_a$  for interdiffusion of  $\sim 4.0$  eV using the Rutherford backscattering spectrometry (RBS) method.<sup>8</sup> Prokes *et al.* and Green *et al.* reported approximate values.<sup>9,10</sup> In this work, the  $E_a$  value is reexamined by applying the PL study on interdiffusion of SiGe/Si single quantum well (SQW) undergoing a postgrowth thermal treatment and the 6+2-band  $k\cdot p$  method.

The  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  SQWs were grown by a low pressure chemical vapor deposition epitaxy system at a substrate temperature of 650 °C. The mixture of silane ( $\text{SiH}_4$ ) and germane ( $\text{GeH}_4$ ) were used as source gases for GeSi growth on (001) *n*-type Si substrate. Postgrowth annealing was carried out in a flowing  $\text{N}_2$  gas ambient of 100 s and the annealing temperatures ranged from 750 to 800 °C. The PL was mea-

sured at 4 K in standard lock-in techniques and detected with a liquid nitrogen cooled Ge detector. The PL spectra of the  $\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Si}$  SQW ( $L_z=12.5$  nm) are shown in Fig. 1. The peaks corresponding to energies higher than 1 eV are silicon related. There are two obviously observed groups of peaks from the extreme left: The first are peaks of the no-phonon (NP) transition due to alloy disorder scattering and the other from the left are transverse-optic (TO) phonon-assisted transition peaks. Both of them are associated with the SiGe layer. For the as-grown sample, the peak of the NP emission line is located at 1.329  $\mu\text{m}$  (933 meV). For the annealed samples (750 and 800 °C at 100 s), blueshifts of the NP peak energies of 8 and 46 meV, respectively, and increases of the NP peak intensity after annealing are observed. Meanwhile, decreases of the full width at half maximum (FWHM) are also found. The enhancement of the PL intensity is due to the reduction of the density of the defects in the sample by thermal annealing.

Following Ref. 6, we believe that the PL-peak shift is caused by Si–Ge atomic interdiffusion across the interface of the QW. The  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  disordered QW is modeled by set-

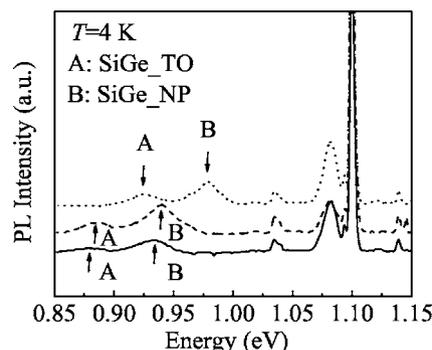


FIG. 1. Low-temperature (4 K) photoluminescence spectra of  $\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Si}$  QW as-grown sample (solid line) and the samples after RTA at 750 °C (dashed line) and 800 °C (dotted line) for 100 s.

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ting  $x'$  as the composition of Ge atom after Si-Ge interdiffusion. The interdiffusion process is normally described by diffusion length  $L_d$ , which is equal to  $(Dt)^{1/2}$ , where  $t$  is the diffusion time and  $D$  is the diffusion coefficient. The Ge composition  $x'$  after interdiffusion can be described as<sup>11,12</sup>

$$x'(z) = \frac{x}{2} \left[ \operatorname{erf}\left(\frac{L_z + 2z}{4L_d}\right) + \operatorname{erf}\left(\frac{L_z - 2z}{4L_d}\right) \right], \quad (1)$$

where  $z$  is the length along growth direction,  $x$  is the as-grown composition of Ge, and  $L_z$  is the QW width before interdiffusion. The maximum of valence bands of strained SiGe alloys occurs at  $\Gamma$  valleys ( $\Gamma_8^+$  and  $\Gamma_7^+$ ),<sup>13,14</sup> while the minimum of conduction bands occurs at  $\Delta$  valleys for alloys with Ge compositions smaller than 0.85.<sup>3</sup> We use the six-band Hamiltonian to calculate valence band energy levels and the simple-band model to calculate the conduction band energy levels at  $\Delta$  valley, which results in the 6+2-band  $k \cdot p$  method.<sup>15</sup> Since the effective mass at  $\Delta$  valley is anisotropic, we consider the matrix element  $C$  in the eight-band Hamiltonian in Ref. 15 as

$$C = E_g + \varepsilon_1(z) + \frac{\hbar^2}{2m_0} \left( \frac{k_z^2}{m_l^*} + \frac{k_x^2 + k_y^2}{m_t^*} \right), \quad (2)$$

where  $m_l^*$  and  $m_t^*$  are  $\Delta$  valley longitudinal mass and transverse mass, respectively. One should note that  $E_p$  in the expression of  $C$  equals to zero when no interaction between conduction band and valence band was taken into account. The energy gap of the unstrained  $\text{Si}_{1-x'}\text{Ge}_{x'}$  is calculated through<sup>3</sup>

$$E_g(\text{Si}_{1-x'}\text{Ge}_{x'}) = 1.155 - 0.43x' + 0.0206x'^2. \quad (3)$$

Hence the band gap energy of silicon is taken as 1.155 eV. The band alignment of SiGe/Si QW for Ge composition below 0.85 is type II, and the valence band offset considering strain is given by<sup>3</sup>

$$\Delta E_v(\text{Si}_{1-x'}\text{Ge}_{x'}) = 0.74x'. \quad (4)$$

All the other parameters for  $\text{Si}_{1-x'}\text{Ge}_{x'}$  material are obtained using a linear interpolation between the parameters of Si and Ge, respectively, as shown in Table I.<sup>3,13,16-18</sup>

Figure 2(a) shows the dependence of electron (CB), heavy hole (HH), and light hole (LH) confinement profiles of the 125 Å  $\text{Si}_{0.7}\text{Ge}_{0.3}/200$  Å Si SQW structure along the growth axis with different diffusion lengths including the strain effect. The origin is taken to be the valence band maximum after strain. The valence band edge is actually the HH band edge due to compressive strain. We derive the relationship between the HH and LH terms in the strained Hamiltonian matrix as

$$E_{\text{lh}}^s(x') = E_{\text{hh}}^s(x') + 2Q_\varepsilon(x'), \quad (5)$$

where  $Q_\varepsilon(x')$  is the shear strain energy term of  $\text{Si}_{1-x'}\text{Ge}_{x'}$ . The profile of  $2Q_\varepsilon(x')$  is shown in Fig. 2(b). Considering the interdiffusion effect, for the case of  $L_d=1.5$  nm, at the well center ( $z=0$  nm),  $E_{\text{hh}}^s$  and  $2Q_\varepsilon$  are  $-0.7$  and  $-98.5$  meV, respectively, so that  $E_{\text{lh}}^s = -99.2$  meV. As  $z$  approaches the interface in the well region ( $z=6.2$  nm),  $E_{\text{hh}}^s$  and  $2Q_\varepsilon$  are  $-111$  and  $-50.7$  meV, respectively, leading to  $E_{\text{lh}}^s = -161.7$  meV. It

TABLE I. Parameters used in the calculation.

Parameters	Si	Ge
Lattice constant $a_0$ (Å)	3.57 Å <sup>a</sup>	3.57 Å <sup>a</sup>
Spin-orbit splitting energy $\Delta_0$ (eV)	0.044 <sup>b</sup>	0.296 <sup>b</sup>
Optical matrix parameter $E_p$ (eV)	21.6 <sup>a</sup>	26.3 <sup>a</sup>
Deformation potential constant $a_c^A$ (eV)	4.88 <sup>c</sup>	2.55 <sup>c</sup>
Deformation potential constant $a_v$ (eV)	2.46 <sup>c</sup>	2.55 <sup>c</sup>
Shear deformation potential $b$ (eV)	-2.33 <sup>c</sup>	-2.08 <sup>c</sup>
Elastic constant $c_{11}$ (Mbar)	1.675 <sup>b</sup>	1.315 <sup>b</sup>
Elastic constant $c_{12}$ (Mbar)	0.65 <sup>b</sup>	0.494 <sup>b</sup>
Luttinger parameter $\gamma_1$	4.22 <sup>c</sup>	13.4 <sup>c</sup>
Luttinger parameter $\gamma_2$	0.39 <sup>c</sup>	4.25 <sup>c</sup>
Luttinger parameter $\gamma_3$	1.44 <sup>c</sup>	5.69 <sup>c</sup>
Longitudinal mass $m_l^*(m_0)$	0.9163 <sup>d</sup>	0.7991 <sup>e</sup>
Transverse mass $m_t^*(m_0)$	0.1905 <sup>d</sup>	0.2 <sup>e</sup>

<sup>a</sup>Reference 13.<sup>b</sup>Reference 16.<sup>c</sup>Reference 3.<sup>d</sup>Reference 17.<sup>e</sup>Reference 18.

reveals that the increase of  $2Q_\varepsilon(x')$  (47.8 meV) is much slower than the reduction of  $E_{\text{hh}}^s(x')$  (110.3 meV) in the well region. The similar observation applies to the case in the barrier region. The conduction band offset  $\Delta E_c(x')$  is given by

$$\Delta E_c(x') = \Delta E_g(x') - \Delta E_v(x'), \quad (6)$$

where  $\Delta E_g(x')$  is the energy gap difference between the well and the barrier layer, and  $\Delta E_v(x')$  presents the valence band offset. All the terms have been taken into account the influence of strain effect. As discussed above, the alignment of the  $\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Si}$  QW is of type II, which means that  $\Delta E_g(x')$  is smaller than  $\Delta E_v(x')$ . It gives rise to a negative  $\Delta E_c(x')$ , i.e., the profile of CB, as shown in Fig. 2(a).

Considering the interdiffusion effect, the dependence of transition energy (C1-HH1) on diffusion lengths for the  $\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Si}$  QW structure calculated by the 6+2-band  $k \cdot p$  method is shown in Fig. 3(a). As  $L_d$  increases, a blueshift can be observed. Subsequently, the calculated transition energy shift  $\Delta E$  as a function of  $L_d$  is shown in Fig. 3(b). The experimental data are fitted with the theoretically calculated ones, as shown in Fig. 3(b). The corresponding diffusion

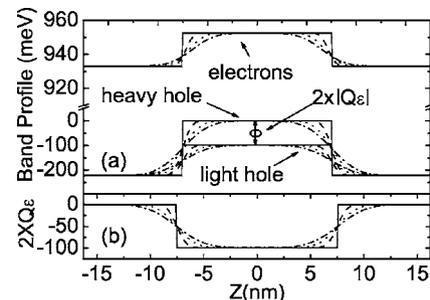


FIG. 2. Dependence of (a) electron, heavy hole, and light hole confinement potentials and (b)  $2Q_\varepsilon$  profile for  $\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Si}$  QW on diffusion lengths:  $L_d=0$  nm (solid line),  $L_d=0.5$  nm (dashed line),  $L_d=1$  nm (dotted line), and  $L_d=1.5$  nm (dashed dotted line), with well center at  $z=0$ .

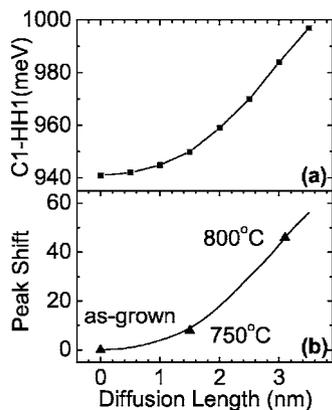


FIG. 3. Dependence of (a) C1-HH1 transition energy and (b) calculated PL-peak shifts for  $\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Si}$  QW on diffusion length:  $L_d=0-3.5$  nm.

lengths are 1.5 and 3.1 nm for the temperatures of 750 and 800 °C, respectively. According to the equation of diffusion coefficient given by

$$D = D_0 \exp\left(-\frac{E_a}{KT}\right), \quad (7)$$

where  $D$  is the diffusion coefficient and  $D_0$  is a constant, we derive the activation energy  $E_a$  of 2.75 eV, which lies in the range of those of Sunamura *et al.* and Boucaud *et al.* To further clarify the reliability of our method, we utilize our computational method to compare with the experimental results by Boucaud *et al.* (20 Å  $\text{Si}_{0.7}\text{Ge}_{0.3}/170$  Å Si), as illustrated in Fig. 4. The calculated fundamental PL peak of 1.199  $\mu\text{m}$  (1034 meV) is in agreement with the experimental 1.22  $\mu\text{m}$  (1016 meV). A smaller diffusion length of 1.1 nm than the simulated Boucaud *et al.* of 1.5 nm is derived, when the blueshift is as large as 70 meV. An  $E_a$  equals to 2.6 eV is obtained, which agrees well with the reported 2.42 eV by Boucaud *et al.* It justifies the reliability of our method in

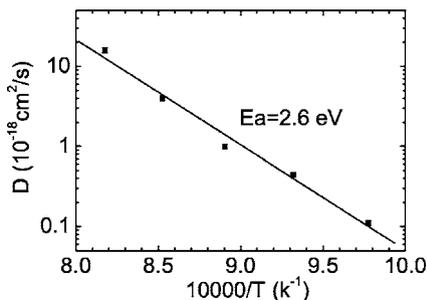


FIG. 4. Estimated diffusion coefficients  $D$  as a function of inverse temperature and activation energy  $E_a$  of  $\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Si}$  QW, obtained from the experimental data in Ref. 6.

calculating the band structure and interdiffusion mechanism of  $\text{SiGe}/\text{Si}$  QW structure.

In summary, the effect of annealing on the optical properties of  $\text{Si}_{0.7}\text{Ge}_{0.3}/\text{Si}$  QW structure is investigated by low-temperature PL measurements. A maximum PL blueshift (46 meV) under 800 °C for 100 s annealing is observed, which is modeled by Si-Ge atomic interdiffusion in our study. The ground state transition energy of the as-grown structure calculated by the 6+2-band  $k\cdot p$  method of 941 meV agrees with the measured 933 meV. As  $L_d$  increases to 3.1 nm, a blueshift of 46 meV can be derived which agrees with our PL results under the highest annealing temperature. Finally, an  $E_a$  equals to 2.75 eV is obtained, which supports that  $E_a$  lies in the 2–3 eV range derived by Sunamura *et al.* and Boucaud *et al.* Overall, experiments and simulations were performed to prove that the 6+2-band  $k\cdot p$  formalism can be utilized well to calculate the band structure and interdiffusion mechanism of  $\text{SiGe}/\text{Si}$  QW at  $\Delta$  valley.

## ACKNOWLEDGMENTS

One of the authors (W.J.F.) would like to acknowledge the part support for this work from A\* star (Grant No. 0421010077) and NTU Nano Cluster Programme Research Seed Fund.

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