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Study of valence intersubband absorption in tensile strained Si/SiGe quantum wells*

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The hole subband structures and effective masses of tensile strained $Si/Si_{1-y}Ge_y$ quantum wells are calculated by using the 6×6 $\boldsymbol{k}\cdot\boldsymbol{p}$ method. The results show that when the tensile strain is induced in the quantum well, the light-hole state becomes the ground state, and the light hole effective masses in the growth direction are strongly reduced while the in-plane effective masses are considerable. Quantitative calculation of the valence intersubband transition between two light hole states in a 7nm tensile strained $Si/Si_{0.55}Ge_{0.45}$ quantum well grown on a relaxed $Si_{0.5}Ge_{0.5}$ (100) substrates shows a large absorption coefficient of 8400 cm^{-1}.

Keywords: Si/SiGe, tensile strain, effective mass, valence intersubband transition
PACC: 7360F, 7320D, 0762

1. Introduction

In the last few years, considerable attention has been directed towards the quantum well infrared photodetectors (QWIPs) for the application in tactical and space based surveillance, imaging, ranging and tracking. P-type Si/SiGe QWIPs are of particular interest because valence intersubband transitions are able to couple normally incident radiation without grating couplers, detect all incident IR radiation polarizations and have lower dark currents.[1] Moreover, the epitaxial growth and processing of Si/SiGe heterostructures is compatible with Si microelectronics technology including on-chip integration of SiGe focal-plane arrays with Si readout circuits.[2−4]

Many experimental investigations were recently performed on Si/SiGe quantum wells in order to study the valence intersubband transitions. These experiments have demonstrated the existence of the photoinduced intersubband absorption in doped or undoped wells.[5−7] Furthermore, a large variety of methods for studying the pertinent experiments have been reported in the literature, such as the pseudopotential method[8] and the computation of the dispersion in the valence band taking into account the coupling between the three valence band, heavy holes, light holes, and spin orbit.[9,10] However, among all of these works regarding the valence intersubband transitions in compressive strained Si/SiGe quantum wells, reported study concerning the optical properties of material under biaxial tension has been limited. The rapid advance of epitaxial growth techniques have opened the possibility for the development of high quality tensile strain $Si/Si_{1-y}Ge_y$ layers grown on relaxed $Si_{1-x}Ge_x$ (001) virtual substrate ($y < x$).[11] When tensile strain is applied in the quantum wells, the ground hole is then a light hole state. Since the absorption coefficient is inversely proportional to the effective mass of the carriers,[12] the valence-band configuration that arises from biaxial tensile strain should be particularly well suited for devices that involve optical absorption.[13]

This paper investigates the energy band structures and effective masses of holes in tensile strain Si/SiGe quantum wells. The intersubband transitions between the first two light hole subbands and the absorption coefficient in this system are quantitative examined.

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2. Valence-subband structures

The problem under consideration is that of a $Si/Si_{1-y}Ge_y$ quantum well grown on $Si_{1-x}Ge_x$ (100) virtual substrate ($y < x$), in which the Si barriers and the $Si_{1-y}Ge_y$ wells are tensile strained. In order to understand the valence intersubband transitions in Si/SiGe quantum wells, knowledge of the hole states and subband structure is essential. We work in the envelope function approximation and the full 6×6 Luttinger–Kohn Hamiltonian including the heavy hole, the light hole and the split-off hole valence bands. The energies and wavefunctions of valence subbands then are obtained by solving the multiband effective mass equation.

Based on the theory of Luttinger–Kohn,[14,15] the 6×6 Hamiltonian which includes heavy-hole, light-hole, and split-off bands reads[16]

$$H = -\begin{pmatrix} P+Q & -S & R & 0 & -\sqrt{1/2}S & \sqrt{2}R \\ -S^\dagger & P-Q & 0 & R & -\sqrt{2}Q & \sqrt{3/2}S \\ R^\dagger & 0 & P-Q & S & \sqrt{3/2}S^\dagger & \sqrt{2}Q \\ 0 & R^\dagger & S^\dagger & P+Q & -\sqrt{2}R^\dagger & -\sqrt{1/2}S^\dagger \\ -\sqrt{1/2}S^\dagger & -\sqrt{2}Q & \sqrt{3/2}S & -\sqrt{2}R & P+\Delta & 0 \\ \sqrt{2}R^\dagger & \sqrt{3/2}S^\dagger & \sqrt{2}Q & -\sqrt{1/2}S & 0 & P+\Delta \end{pmatrix} \begin{matrix} |3/2,3/2\rangle \\ |3/2,1/2\rangle \\ |3/2,-1/2\rangle \\ |3/2,-3/2\rangle \\ |1/2,1/2\rangle \\ |1/2,-1/2\rangle \end{matrix}, \tag{1}$$

where

$$\begin{aligned} &P = P_k + P_\varepsilon, \quad Q = Q_k + Q_\varepsilon, \\ &R = R_k + R_\varepsilon, \quad S = S_k + S_\varepsilon, \\ &P_k = (\hbar^2/2m_0)\gamma_1(k_x^2 + k_y^2 + k_z^2), \\ &Q_k = (\hbar^2/2m_0)\gamma_2(k_x^2 + k_y^2 - 2k_z^2), \\ &R_k = (\hbar^2/2m_0)\sqrt{3}[-\gamma_2(k_x^2 - k_y^2) + 2\mathrm{i}\gamma_3 k_x k_y)], \\ &S_k = (\hbar^2/2m_0)2\sqrt{3}\gamma_3(k_x - \mathrm{i}k_y)k_z, \\ &P_\varepsilon = -a_\mathrm{v}(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}), \\ &Q_\varepsilon = -b(\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz})/2, \\ &R_\varepsilon = \sqrt{3}b(\varepsilon_{xx} - \varepsilon_{yy})/2 - \mathrm{i}d\varepsilon_{xy}, \\ &S_\varepsilon = -d(\varepsilon_{zx} - \mathrm{i}\varepsilon_{yz}). \end{aligned} \tag{2}$$

Here $\varepsilon_{xx} = \varepsilon_{yy} = (a_{\mathrm{substrate}} - a_{\mathrm{layer}})/a_{\mathrm{layer}}$, $\varepsilon_{zz} = -2\varepsilon_{xx}C_{12}/C_{11}$, $\varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{zx} = 0$, and γ_1, γ_2, γ_3 are the Luttinger parameters. In a one-dimensional-modulation, the quantities γ_1, γ_2, γ_3 all vary along the z axis, and the position-dependent valence-band edge is added to the diagonal terms. This may include the valence-band offset, the external field bias, and the self-consistent potential as well. In $Si_{1-x}Ge_x$ (001)-grown $Si/Si_{1-y}Ge_y$ structures there exists a biaxial strain. The P and Q terms in Eq.(1) are then amended with strain-dependent terms P_ε and Q_ε as shown in Eq.(2), a_v and b in terms P_ε and Q_ε are the hydrostatic and shear deformation potentials. And for the case of a biaxial strain, $R_\varepsilon = S_\varepsilon = 0$. Material parameters used for calculation in this paper can be found in our earlier work.[17]

Figure 1(a) shows our 6×6 $\boldsymbol{k}\cdot\boldsymbol{p}$ calculation of the valence-subband structure in a $Si/Si_{0.55}Ge_{0.45}$ tensile strained quantum well grown on a relaxed $Si_{0.5}Ge_{0.5}$ buffer layer. The widths of the well and barrier are assumed to be 7nm and 10nm, respectively. Eigenvalue having light (heavy) hole character is marked with LH (HH) according to its characteristic at the band edge, and the hole wavefunctions (squared) are plotted. As we can see from Fig.1(a), the tensile strain pushes the light hole states upwards as the populated ground state. Figure 1(b) shows the four lowest energy levels and LH band offset for tensile strained $Si/Si_{0.55}Ge_{0.45}$ quantum well grown upon a relaxed $Si_{0.5}Ge_{0.5}$ buffer layer as a function of well width. The possible bound-to-quasi-bound transitions are pointed out using the dashed vertical arrows from the populated ground state (LH1) to the top of the well (HH1, HH2 or LH2).

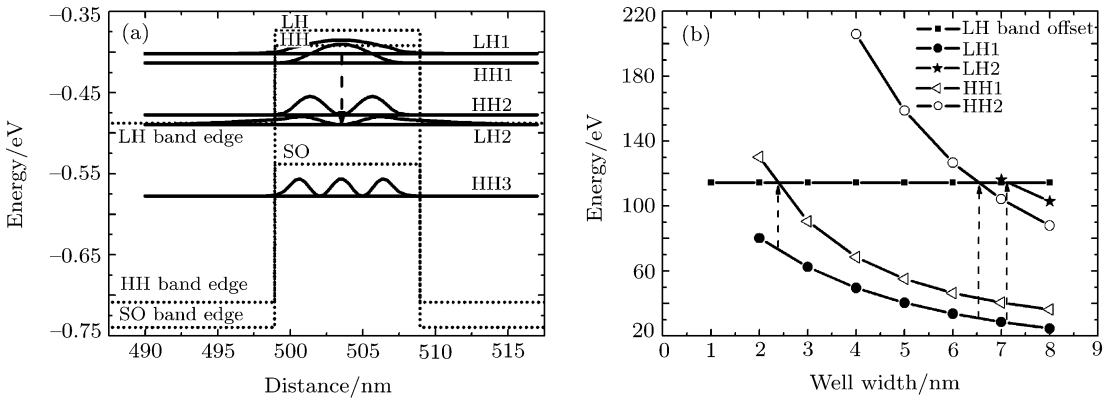


Fig.1. (a) Valence-subband structure of a 7nm tensile strained $Si/Si_{0.55}Ge_{0.45}$ quantum well. (b) The four lowest subband energies and LH band offset versus well width in tensile strained $Si/Si_{0.55}Ge_{0.45}$ quantum well grown upon a relaxed $Si_{0.5}Ge_{0.5}$ buffer layer. The dashed vertical arrows show possible bound-to-quasi-bound transitions in the quantum well.

3. Hole effective mass

Hole effective masses are among the important parameters needed to properly characterize any particular device. Using the light-hole state as the heavily doped ground state has the benefits of smaller effective mass, which translates into larger absorption coefficients and better transport characteristics.

In order to calculate the effective masses at $k = 0$, the series expansion of $E - k$ relation determined by the full 6×6 Luttinger–Kohn Hamiltonian up to the second order of k are,

$$\begin{aligned}
E_{\mathrm{HH}}(k) &\approx E_{\mathrm{HH}}(0) - (\hbar^2/2m_0)[(\gamma_1+\gamma_2)k_{\parallel}^2 + (\gamma_1-2\gamma_2)k_{\perp}^2],\\
E_{\mathrm{LH}}(k) &\approx E_{\mathrm{LH}}(0) - (\hbar^2/2m_0)[(\gamma_1-f_+\gamma_2)k_{\parallel}^2 + (\gamma_1+2f_+\gamma_2)k_{\perp}^2],\\
E_{\mathrm{SO}}(k) &\approx E_{\mathrm{SO}}(0) - (\hbar^2/2m_0)[(\gamma_1-f_-\gamma_2)k_{\parallel}^2 + (\gamma_1+2f_-\gamma_2)k_{\perp}^2],
\end{aligned} \tag{3}$$

where $f_{\pm}$ is a dimensionless, stain-dependent factor

$$f_{\pm} = \frac{2x\left[1+\frac{3}{2}(x-1\pm\sqrt{1+2x+9x^2})\right]+6x^2}{\frac{3}{4}(x-1\pm\sqrt{1+2x+9x^2})+x-1\pm\sqrt{1+2x+9x^2}-3x^2}, x = \frac{2Q_{\varepsilon}}{\Delta}. \tag{4}$$

From Eq.(3), we obtain the effective masses

$$\begin{aligned}
\frac{m^*_{\mathrm{HH},\perp}}{m_0} &= \frac{1}{\gamma_1-2\gamma_2}, \quad \frac{m^*_{\mathrm{HH},\parallel}}{m_0} = \frac{1}{\gamma_1+\gamma_2},\\
\frac{m^*_{\mathrm{LH},\perp}}{m_0} &= \frac{1}{\gamma_1+2f_+\gamma_2}, \quad \frac{m^*_{\mathrm{LH},\parallel}}{m_0} = \frac{1}{\gamma_1-f_+\gamma_2},\\
\frac{m^*_{\mathrm{SO},\perp}}{m_0} &= \frac{1}{\gamma_1+2f_-\gamma_2}, \quad \frac{m^*_{\mathrm{SO},\parallel}}{m_0} = \frac{1}{\gamma_1-f_-\gamma_2}.
\end{aligned} \tag{5}$$

The top most valence band effective mass of compressive and tensile strained SiGe layers are shown in Fig.2(a) and Fig.2(b), respectively. They are given in the units of the free electron mass, m_0. Note that the heavy hole has a large effective mass along the z direction ($m_{\perp}$) and a smaller effective mass along the x and y directions ($m_{\parallel}$), and vice versa for the light hole. The ground hole state (LH1) effective masses in the z direction show strong reduction for all tensile strained SiGe alloys. The light-hole band also has a considerable in-plane effective mass, therefore, a large density of states which also increases absorption can be expected.

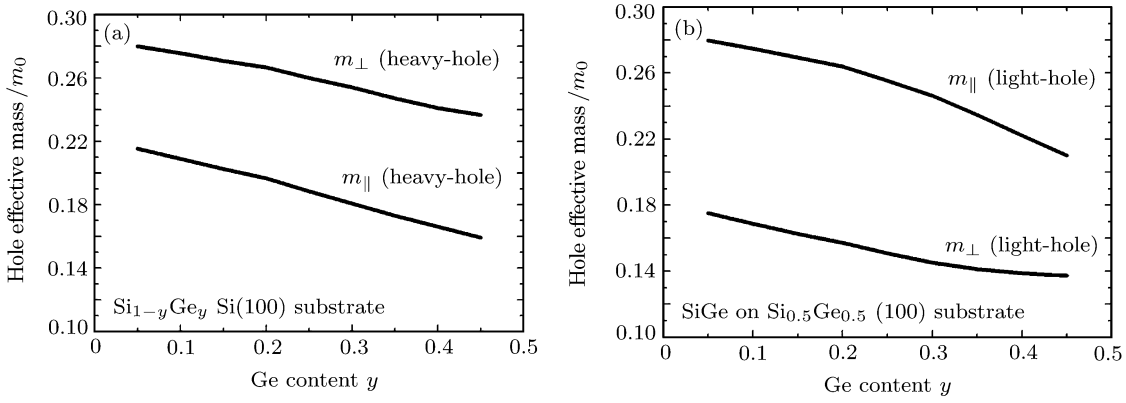


Fig.2. (a) Calculated hole effective masses for the top most valence band versus Ge content y in $Si_{1-y}Ge_y$ alloys grown upon Si (100) substrates, and (b) $Si_{1-y}Ge_y$ alloys grown upon a relaxed $Si_{0.5}Ge_{0.5}$ (100) substrates, the in-plane ($\parallel$) and the growth direction ($\perp$) conductivity masses are shown.

4. Optical transitions between two light hole states

For the analysis of optical absorption of intersubband transition between two light hole states, it is a good approximation by considering intersubband transition in the limit of infinitely large potential barriers surrounding the quantum well and in the limit of small mixing of the light and heavy hole states. The approximation of the above boundary condition gives the calculated absorption coefficient within a factor of two of experimental data.[18] So is the oscillator strength, as expected. In the limit of small hole in-plane wave vector, the light hole envelope function reads

$$f_n(z) = \sqrt{\frac{2}{L_{\rm W}}} \sin\left(\frac{n\pi z}{L_{\rm W}}\right). \tag{6}$$

Thus, the optical dipole describing the absorption of TM polarized radiation has the well-known form,

$$\begin{aligned} f_{mn} =& \frac{2}{m_\perp^* \hbar\omega_{mn}} \left\{\langle f_n(z)| p_z |f_m(z)\rangle\right\}^2 \\ =& \frac{64}{\pi^2} \frac{m^2 n^2}{(m^2-n^2)^3} \\ & (\text{for} \quad m-n \quad \text{odd}). \end{aligned} \tag{7}$$

The oscillator strength is used to calculate the absorption coefficient, which is simply proportional to the product of the oscillator strength and the two-dimensional density of states.

The absorption coefficient for intersubband transition between the subband m and the subband n is given by

$$\begin{aligned} \alpha(\omega) =& \frac{\hbar\omega \times \text{energy absorbed per unit volume and time}}{\text{incident energy flux}} \\ =& \frac{\pi e^2 \hbar c \mu_0}{2 m_\perp^* n_{\rm r}} \times f_{mn} \times \Delta N \times g(\omega), \end{aligned} \tag{8}$$

where μ_0 is the permeability, c is the speed of light and $n_{\rm r}$ is the index of refraction. N is the population difference between two states, and $g(\omega)$ is the Lorentzian line shape function,

$$N = \frac{m_\parallel^*}{\pi\hbar^2 L} kT \ln \frac{1+{\rm e}^{-(e_m-E_{\rm f})/kT}}{1+{\rm e}^{-(e_n-E_{\rm f})/kT}}, \tag{9}$$

$$g(\omega) = \frac{\Gamma/2\pi}{(\varepsilon_m - \varepsilon_n - \hbar\omega)^2 + (\Gamma/2)^2}, \tag{10}$$

where $\varepsilon_m(\varepsilon_n)$ is subband energy, L is well thickness, $E_{\rm f}$ is Fermi level and $\Gamma/2$ is the full width at half maximum (FWHM), and can be experimentally determined from the width of the absorption spectrum.

Now we evaluate the absorption coefficient for the intersubband transition between LH1 and LH2 in a 7 nm tensile strained $Si/Si_{0.55}Ge_{0.45}/Si$ quantum well at 300 K. As showed in Fig.1(a), $\varepsilon_{\rm LH2}$=–0.490 eV, $\varepsilon_{\rm LH1}$=–0.402 eV, in a case that boron doping two-dimensional density of holes is 1×10^{12} cm^{-2}. Assume for simplicity that only valence subbands LH1 and HH1 are occupied, the Fermi energy level is –0.421 eV. The LH1 effective masses obtained from Fig.2(b)

gives $m_\perp$=0.137m_0, $m_\parallel$=0.21m_0. And we use the FWHM $\Gamma/2$ of 75 meV obtained from Ref.[19]. Using the above parameters, we obtain the peak absorption coefficient of 8400 cm^{-1} at 14 μm. Karunasiri, Park and Wang[5] has presented their experimental results on two heavy hole transition in heavily doped $Si/Si_{0.85}Ge_{0.15}$ multiple quantum wells, and obtained the peak absorption of about 3000 cm^{-1}. The $Si_{0.85}Ge_{0.15}$ quantum well used in their experiment are of 3nm-thick and doped to $\sim 1\times10^{19}$ cm^{-3}, which gives the two-dimensional density of 3×10^{12} cm^{-2}, and only HH1 is occupied. The HH1 effective masses obtained from Fig.2(a) gives $m_\perp$=0.27m_0, $m_\parallel$=0.2m_0, and the FWHM obtained from the measured absorption spectrum at 300K is about 80 meV.[5] Using these parameters we obtained the peak absorption coefficient of 4400 cm^{-1}. The calculated absorption coefficient is a bit larger than that of experiment because the two heavy holes in calculating were assumed to be bounded in the well. As we mentioned above, the approximation gives the calculated absorption coefficient within a factor of two of experimental data.[18] We believe that the infrared absorption in tensile strained Si/SiGe quantum well is greatly enhanced due to their large ratio of in-plane/growth direction effective masses $m_\parallel/m_\perp$. As we can deduce from Eq.(8) and Eq.(9), the infrared absorption is proportional to the ratio of in-plane/growth direction effective masses $m_\parallel/m_\perp$, and the values of $m_\parallel/m_\perp$ obtained from Fig.2 for tensile strained $Si/Si_{0.55}Ge_{0.45}$ quantum wells and compressive strained $Si/Si_{0.85}Ge_{0.15}$ are 1.533 and 0.74, respectively. Moreover, as we can see from Fig.1(a), HH1 is close to the ground state LH1 and is occupied when the well is heavily doped. Thus, valence intersubband absorption between HH1 and LH2 is possible and will be responsible for the observed normal incident detection. The effects of subband nonparabolicity, valence-band anisotropy and heavily doped hole distribution on the photoresponse have been discussed in Refs.[19] and [20].

5. Conclusions

We have presented the basic theory for valence intersubband transitions and calculated the valence subband hole effective masses for tensile strained Si/SiGe quantum wells. Our calculation clearly shows that tensile strain in the Si/SiGe quantum wells push up the light hole state as the ground hole, and the ground hole state effective masses in the growth direction showed a strong reduction compared to the compressive strain quantum wells, which translates into larger absorption coefficients. The light-hole band also has a considerable in-plane effective mass, therefore, a large density of states which also increases absorption can be expected. This study demonstrates that highly doped tensile strained Si/SiGe quantum wells can be used in improving high performance quantum well infrared photodetectors.

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