Proceedings of the XXVI International School of Semiconducting Compounds, Jaszowiec 1997

INFRARED ABSORPTION IN Si–$Si_{1-x}Ge_x$–Si QUANTUM WELLS

G. FISHMAN

Laboratoire de Spectrométrie Physique, UMR 5588, UJF Grenoble 1-CNRS, BP87
38402 Saint Martin d'Hères Cedex, France

AND R. OSZWAŁDOWSKI

Institute of Physics UMK, Grudziądzka 5, 87-100 Toruń, Poland

We use the eight-band $k\cdot p$ model to describe the infrared inter-subband absorption in Si–$Si_{1-x}Ge_x$–Si quantum wells, which takes explicitly into account the $\Gamma'_{25}(\Gamma_8^+ + \Gamma_7^+$ in the double group) valence band and the second conduction band $\Gamma'_2(\Gamma_7^-)$. We then obtain an accurate description of mixing of the S wave function with the valence band functions.

PACS numbers: 73.20.Dx, 78.66.–w, 85.30.Vw

1. Introduction

Up to now the admixture of the Γ'_2 S function, (for a non zero in-plane wave vector $k_\parallel$), into the Γ'_{25} hole function has been taken into account in perturbative ways [1, 2] in Si–$Si_{1-x}Ge_x$–Si quantum wells. This admixture is needed to understand the absorption of light polarized parallel to the plane of the quantum well (the so-called x-polarization). Our aim is to find the transition matrix elements between pairs of quantum well hole states as a function of $k_\parallel$ length, taking into account the conduction band (CB) in an exact (i.e. non-perturbative) manner.

2. Theory

We use an eight-band $k\cdot p$ model to write down an effective Hamiltonian in which the CB (point $\Gamma'_2(\Gamma_7^-)$) is taken into account on an equal footing with the valence band (VB). Parameters describing the CB are poorly determined, especially as functions of mole fraction x, but as it is not our goal to describe interband transitions but only the intersubband (VB) ones, linear interpolation (between $x = 0$ and 1) will be sufficiently accurate.

The upper left (UL) part of our Hamiltonian $\mathcal{H}$ ($\hbar = m_0 = 1$) is

$$\begin{bmatrix} E_g + \frac{\widetilde{\gamma}'_0}{2}k^2 & \frac{-1}{\sqrt{2}}\bar{\omega}k_x & \frac{1}{\sqrt{6}}\bar{\omega}\left(-k_x + 2\partial_z\right) & \frac{1}{\sqrt{3}}\bar{\omega}\left(k_x + \partial_z\right) \\ \text{c.c.} & -\frac{1}{2}\left[k_x^2\widetilde{\gamma}_+ - \partial_z^2\widetilde{\gamma}_{2-}\right] & \frac{\sqrt{3}}{2}\left(-\widetilde{\gamma}_R k_x^2 + 2a\right) & \frac{-\sqrt{6}}{2}\left(\widetilde{\gamma}'_R k_x^2 + 2a'\right) \\ \text{c.c.} & \text{c.c.} & -\frac{1}{2}\left[k_x^2\widetilde{\gamma}_- - \partial_z^2\widetilde{\gamma}_{2+}\right] & \frac{1}{\sqrt{2}}[\widetilde{\gamma}'_2(k_x^2 + 2\partial_z^2) + 3a'] \\ \text{c.c.} & \text{c.c.} & \text{c.c.} & -\frac{1}{2}\widetilde{\gamma}'_1(k_x^2 - \partial_z^2) + \Delta \end{bmatrix}$$

where $\bar{\omega} = \langle S|\, p_x \,|iX\rangle$ is real, $a = \tilde{\gamma}_3 k_x \partial_z, a' = \tilde{\gamma}'_3 k_x \partial_z, k^2 = k_x^2 - \partial_z^2, \tilde{\gamma}_- = \tilde{\gamma}_1 - \tilde{\gamma}_2, \tilde{\gamma}_+ = \tilde{\gamma}_1 + \tilde{\gamma}_2, \tilde{\gamma}_{2-} = \tilde{\gamma}_1 - 2\tilde{\gamma}_2, \tilde{\gamma}_{2+} = \tilde{\gamma}_1 + 2\tilde{\gamma}_2, \tilde{\gamma}_R = (\tilde{\gamma}_2 + \tilde{\gamma}_3)/2, \tilde{\gamma}'_R = (\tilde{\gamma}'_2 + \tilde{\gamma}'_3)/2$. The growth direction is [001] parallel to the quantization axis. The lower right block (LR) of the 8×8 Hamiltonian has the same form, and the other two 4×4 blocks are zero. The constants $\tilde{\gamma}_i, \tilde{\gamma}'_i$ are Pidgeon–Brown like and differ from those used in the Luttinger (Γ_8^+) Hamiltonian — $\gamma_i, i = 1, 2, 3$. The so-called renormalization formulas are: $\tilde{\gamma}_1 = \gamma_1 - E_p/3E_g, \tilde{\gamma}_{2,3} = \gamma_{2,3} - E_p/6E_g$. It is readily seen that $\tilde{\gamma}'_i \simeq \tilde{\gamma}_i$ and $\tilde{\gamma}'_0 = \gamma_0 - \frac{E_p}{3}[2/E_g + 1/(E_g + \Delta)]$, where $E_p = 2\bar{\omega}^2/m_0$. Our parameters are as follows:

	E_g[meV]	Δ [meV]	γ_0	γ_1	γ_2	γ_3	E_p [eV]
Si	4185	−44	25	4.26	0.38	1.56	26
Ge	850	−290	25	13.38	4.25	5.69	26

The optical transition matrix elements of eigenfunctions of the UL can be conveniently expressed as $\left|\langle f_1|\,\widehat{M}\,|f_2\rangle\right|^2$ with the following notation: $\langle f_{1,2}| \rightarrow (\chi^c_{1,2}\ \chi^h_{1,2}\ \chi^l_{1,2}\ \chi^{so}_{1,2})$ and $\widehat{M} = \eta_x \widehat{M}_x + \eta_z \widehat{M}_z$ (η is the polarization vector);

$$\widehat{M}_x = \bar{\omega} \begin{bmatrix} 0 & \frac{-1}{\sqrt{2}} & \frac{-1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ \frac{-1}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{-1}{\sqrt{6}} & 0 & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & 0 & 0 \end{bmatrix}, \quad \widehat{M}_z = - \begin{bmatrix} i\hbar\partial_z & 0 & \text{c.c.} & \text{c.c.} \\ 0 & i\hbar\partial_z & 0 & 0 \\ i\bar{\omega}\sqrt{\frac{2}{3}} & 0 & i\hbar\partial_z & 0 \\ i\bar{\omega}\frac{1}{\sqrt{3}} & 0 & 0 & i\hbar\partial_z \end{bmatrix},$$

where $\chi_i = \chi_i(z)$ are the (real) envelope functions. From the form of the matrix operator $\widehat{M}_x$ we see that the x-polarization absorption is going to be zero if both the initial and final state have a zero χ^c component, but if this component is nonzero in one of the states, the normal incidence absorption becomes possible. If $\mathcal{H}$ described only the VB, $\widehat{M}_x$ would simply be a zero 3×3 matrix. The non-diagonal terms $\widehat{M}_z$ suggest that also the results for z-polarization absorption might differ from those obtained without taking into account the CB.

3. Method and results

Our method of determining the energy levels and wave functions of either the CB or the VB has been described elsewhere [3]. Here we use it for an 8×8 Hamiltonian. It is not easy to say a priori whether the variational method will work for an operator with spectrum without lower bound. We found out that some spurious solutions appear with energies within the forbidden gap, but their wave functions and their behaviour with respect to changes of variational parameters make them easy to recognize and reject.

In our calculation we have taken linear interpolation of all the parameters. The mole fraction x equals 0.2, the heavy (light) hole well "bottom" is 240 (200) meV above the Si VB (i.e. barrier) and the spin–orbit splitting is measured down from the average of heavy and light hole bands. The well width is 30 Å.

Figure 1 shows the dispersion curves of VB calculated within the 6 × 6 model ("without CB") and the 8 × 8 one ("with CB"). As one can see there is no point in using the 8 × 8 model if one is interested only in the energies and not in the envelope functions. Figure 2 shows admixtures of the $|c\rangle = \alpha\,|S\uparrow\rangle + \alpha^*\,|S\downarrow\rangle$ component to VB wave functions ($\alpha = \exp(3i\pi/4)$), where the admixture is defined as $\int |\chi^c(z)|^2\,dz$. Figure 3 presents the ratio of sums of matrix elements

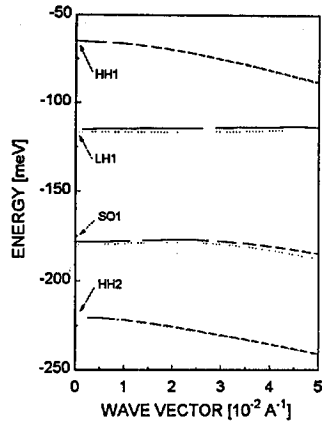

Fig. 1. Dispersion curves of the valence band. The well is 3 nm of $Si_{0.8}Ge_{0.2}$, barriers are pure silicon. Dotted lines signify calculation without the conduction band. Solid lines correspond to calculation with the conduction band.

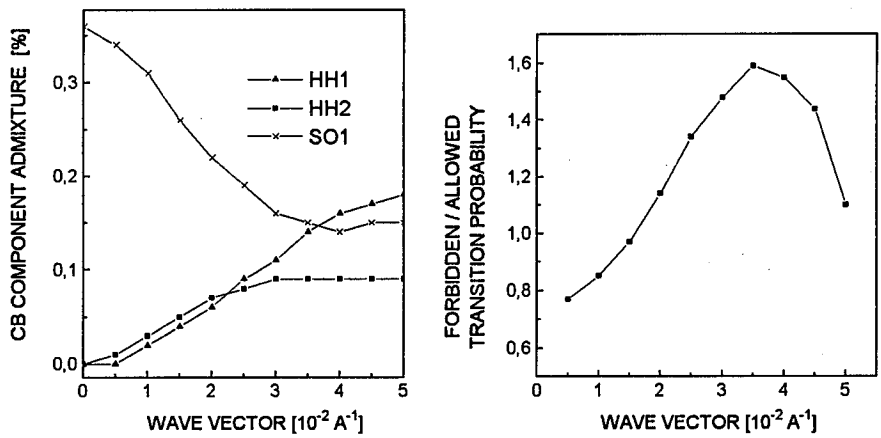

Fig. 2. Conduction band wave functions admixtures (i.e. integrals of squared $|c\rangle$ components of envelope functions) to heavy holes ground and first excited levels (HH1 and HH2) and the "spin–orbit" band level SO1, in function of the in-lane vector $k_\parallel$.

Fig. 3. Ratio of optical transition matrix elements "x" to "z" polarization in function of the in-plane wave vector $k_\parallel$, HH1–SO1 transition.

for x- and z-polarizations $\left[2\left|\langle f_1|M_x|f_2\rangle\right|^2 / \left(\left|\langle f_1'|M_z|f_2'\rangle\right|^2 + \left|\langle f_1|M_z|f_2\rangle\right|^2\right)\right]$ for the transition HH1–SO1 (primed functions correspond to the LR block). As one can see absorption of x-polarized light could actually be stronger than that of z-polarized beam if only some of HH1 states for $|k_\parallel| > 0.02$ Å^{-1} were empty.

Acknowledgments

One of us (R.O.) thanks TEMPUS (JEP 08343-94) for financing his stay in Grenoble during his doctoral studies and the Committee for Scientific Research (Poland) (project No. 2 PO3B 156 10) for support.

References

[1] Y.C. Chang, R.B. James, *Phys. Rev. B* **39**, 12672 (1989).

[2] R. People, J.C. Bean, S.K. Putz, C.G. Bethea, L.J. Peticolas, *Thin Solid Films* **222**, 120 (1992).

[3] G. Fishman, *Phys. Rev. B* **52**, 11132 (1995).