Light Emitter in Si – Ge Double Barrier Structures at Room Temperature

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Abstract:

Full - scale microscopic calculations reveal that the allowed transitions across the superlattice band gap arise not from zone-folding but in fact are due to the presence of the heterointerfaces. In accord with this finding we have demonstrated that the band gap is highly sensitive to the degree of disorder at the interface. We proposed a structure in which the superlattice periodicity is absent, but the calculated transition strength is comparable with that for an optimum short period Si-Ge superlattice. The aim of this paper is to provide a mechanism to explain how these selection rules are broken, thereby, allowing no-phonon transition to the minima in the interface plane.

Introduction:

There have been many reports of luminescence from short period Si-Ge superlattice, it is evident that the strength and line widths of these spectra do not correlate with the theoretical predictions(1). Indeed, similar spectra have been observed from SiGe alloy layers and multiple quantum well system where the zone-folding argument does not apply. The formation of a quasi-direct gap in Si-Ge superlattices is generally attributed to a zone-folding mechanism in which the periodicity of the superlattice causes the conduction minima near the bulk X point along the superlattice axis to be folded into the Brillouin zone centre(2).

In recent experiments performed on proposed thin layer structure both electroluminescence and photoluminescence measurements have confirmed that no-phonon transitions occur in these systems(3,4). Furthermore of these experiments deserves farther theoretical investigation(5). Hydrostatic pressure measurements have shown that the conduction states which gives rise to the luminescence are derived from bulk like minima which are orientated parallel to the interface plane. This is puzzling because in an ideal structure the only new allowed transition should be to the two minima which are aligned along the superlattice axis – no-phonon transitions to the other four minima should remain forbidden(6,7).

Method, Discussion and Results:

We proposed a structure consists of two thin Ge layers separated by a wider layer of Si, the whole structure being contained within a Si matrix (Figure 1). The presence of the large confining barriers means that luminescence should be observable at relatively high temperatures. Therefore to provide a mechanism to explain how these selection rules are broken, thereby allowing no-phonon transitions to the minima in the interface plane.

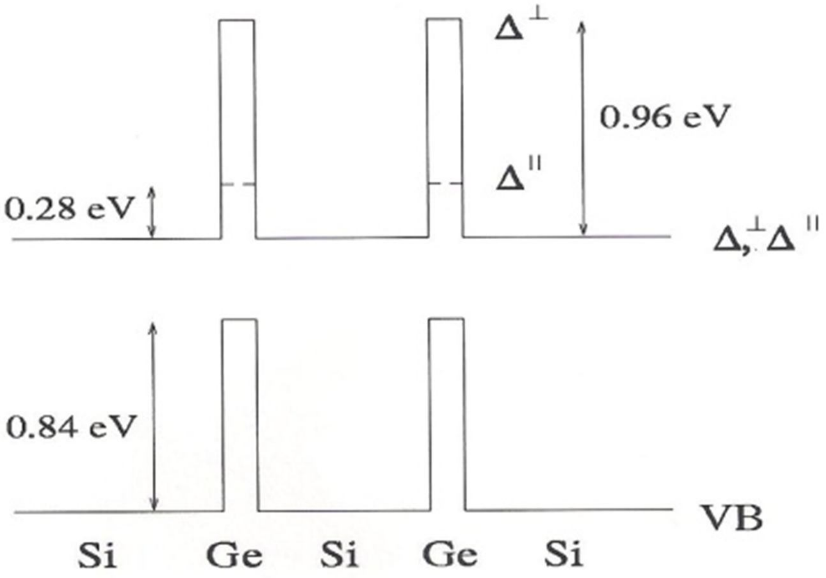

Figure 1: shows the band offsets for the proposed Ge double barrier strcture. Offsets for the in-plane minima, $\Delta^{||}$ are shown by dashed lines.

We have performed full-scale pseudopotential calculations on these structures using a 3-D supercell wavefunction, ψ, in terms of a complete set of eigenfunctions, $\emptyset_{nk}$, corresponding to a suitable host material, thus

$$\sum_{nk} \mathrm{A}_{\mathrm{nk}} \, \emptyset_{nk} = \psi$$

Where:

$$\emptyset_{nk} = \sum_{G} a_{nk} \, (\mathrm{G}) e^{i(K+G).r}$$

Here n represents the band index, k the wavevector and G the reciprocal lattice vectors.

Eigenvalues, E, of the supercell are then given by

$$(\hat{H}_0 + \hat{V} - E)\, \psi = 0$$

Where $\hat{H}_0$, is the Hamiltonian of the host material and $\hat{V}$ represents the difference in potential between the supercell and the host. This gives rise to a secular equation of the form

$$A_{nk}\,(E_{nk} - E\,)\,\delta_{nn'}\,\delta_{kk'}$$

$$+ \sum_{nk} A_{nk} \frac{1}{\Omega} (k' + G'|\hat{V}|k + G) = 0$$

Which is solved numerically by direct diagonalization of the matrix. The matrix elements $\Omega^{-1}\,(k' + G'|\hat{V}|k + G)$ can be written as(8)

$$\frac{1}{\Omega_{sc}} \sum_{GG'} a *_{n'k'}(G')a_{nk}(G)\langle v_{Si}(g) \sum_{\tau_{Si}} e^{ig.\tau_{Si}} + v_{Ge}(g) \sum_{\tau_{Ge}} e^{ig.\tau_{Ge}} + v_0(g) \sum_{\tau_0} e^{ig.\tau_0} \rangle$$

Where Ω_{sc} is the volume of the supercell, v_{Si}, v_{Ge}, v_0 and $\tau_{Si,}\tau_{Ge}, \tau_0$ represent the potentials and atomic positions of the *Si, Ge* and host atom respectively, and g is the superlattice reciprocal lattice vector

$$g = k' - k + G' - G.$$

In this way one can perform the supercell calculation using only those bulk bands that contribute to the state of interest, i.e. those around the band gap. We will discuss first the ideal case and then consider to what extent imperfections in the structure alter the selection rules.

I- Ideal thin Ge Double Barrier Structures :

Consider firstly the case in which the structure is grown on a Si substrate. From figure 1, it is obvious that the conduction ground state in this case lies in the continuum of states in the Si substrate. Since the offsets for the in-plane minima, $\Delta^{||}$, are small, these states are unconfined and lie just above the conduction band edge. Confined states which are associated with the minima along the superlattice axis, $\Delta^{\boxed{?}}$, occur in the Si well between the two Ge barriers (Figure 2). These are resonance states.

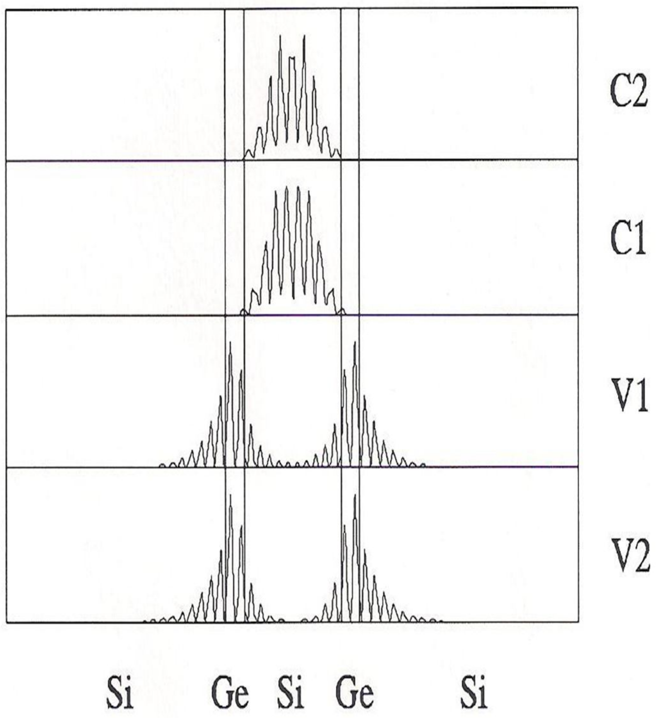

Figure 2: Shows charge densities for the uppermost valence states, V1 and V2, and the confined conduction states, C1 and C2, for the double barrier structure strained to a Si substrate. It should be noted that states C1 and C2 are not the lowest lying states in the conduction band.

The above comments describe the results obtained for a calculation in which no doping is present, but of course any real system contains dopant atoms. Assuming uniform doping with acceptors, the concentration of holes in the Ge layers results in a band bending potential (Figure 3).Although the magnitude of the band bending effects is small, it is expected to have a significant effect on any electrons localized in the Si well.

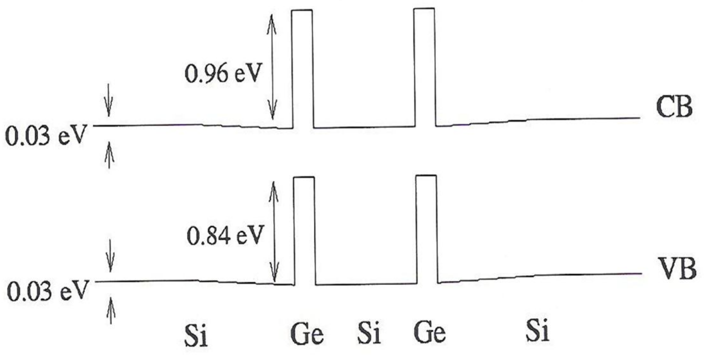

Figure 3: Shows the band edges for the structure in Figure 1, subject to uniform acceptor doping of $10^{18}\ cm^{-3}$

Consequently, the bound states C1 and C2 shown in Figure 2 are expected to move down in energy relative to the continuum band edge as the doping concentration is increased. Including the band bending potential in our calculations we predict that an acceptor doping of about 2×10^{18} cm^{-3} is sufficient to move the bound state below the continuum band edge. However, this is still not the conduction ground state in the system because the , $\Delta^{||}$, minima are also moved down in energy as a result of this band bending (Figure 4).

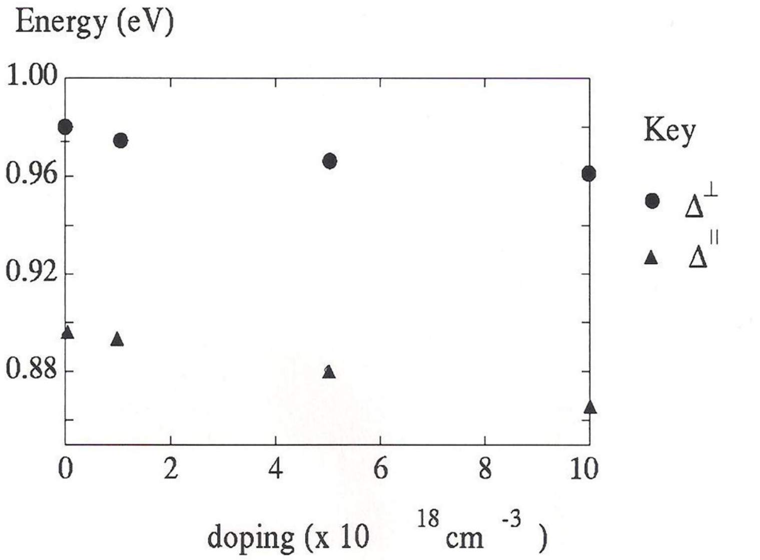

Figure 4: Shows variation in transition energy to the in-plane conduction minima $\Delta^{||}$ (triangles) and the $\Delta^{\perp}$ minima (circles) as a function of acceptor doping concentration.

II- Interface Disorder Effects:

The presence of disordered interfaces can account for the experiment results(9), but a large degree of disorder is required to produce the transitions from the $\Delta^{||}$ minima which are comparable in strength to those from the $\Delta^{\perp}$ minima(10). A perturbation in the planes parallel to the interfaces can produce allowed transitions to the in-plane minima. In this disordered interface model we quantify the degree of disorder by a parameter D given by

$$D = 2\times \frac{number\ of\ misplaced\ atoms}{total\ number\ of\ atoms\ in\ supercell}$$

A value of zero describes the ideal situation of a perfectly abrupt interface whereas a disorder parameter of 1.0 characterizes a random alloy.

Conclusions:

In conclusion, we provide a mechanism to explain how these selection rules are broken, thereby allowing no-phonon transitions to the minima in the interface plane. And to demonstrate the importance of the interfaces, we proposed a structure in which the superlattice periodicity is absent, but the calculated transition strength is comparable with that for an optimum short period Si-Ge superlattice.

The presence of the large confining barriers means that luminescence should be observable at relatively high temperatures. In accord with this finding we have demonstrated that the predicted transition probability across the band gap is highly sensitive to the degree of disorder at the interface.

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