The Luminescence in Si-Ge Quantum Wells
at Room Temperature

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Abstract:

We present the results of a computational study to investigate the Photoluminescence from an effectively isolated $Ge_m - Si_n - Ge_m$ structure. This structure has been demonstrated at room temperature(1). Experimental measurements have shown that this luminescence is associated with the four-fold degenerate conduction minima which lie in the plane of the interface. This paper shows that the observed luminescence cannot be explained by the popular alloy scattering interpretation, or by what is commonly called the zone-folding model. We propose an alternative mechanism which links the luminescence to anomalous localization at the heterointerfaces.

Introduction:

During the last years there have been many reports of Photoluminescence and electroluminescence from short period *Si-Ge* superlattices(2,3). These processes are usually attributed to the so called zone-folding mechanism in which the long rang atomic ordering in the superlattice causes the bulk conduction minima to be mapped onto the Brillouin zone centre(4,5), it is actually the rapid change of the microscopic potential at the interface which breaks the bulk nodal structure of the wavefunction. Alters the selection rule and so creates an allowed transition across the band gap. Nevertheless, the periodicity of the superlattice is also important. Theory predicts that the transition energy and oscillator strength are strongly dependent on the superlattice period. In particular, it has been shown that the optimum structure has a period of ten monolayers(5,6).

Results of the experiment shows a little evidence to suggest that the observed luminescence is related to the presence of the long range superlattice potential. Furthermore, the observed luminescence displays similar characteristics to that obtained from bulk *SiGe* alloys(6) or *SiGe* quantum wells(9), it is only observable at low temperatures and is highly sensitive to external fields. This suggests that the origin of the observed spectra is due mainly to alloy scattering. This is a short range effect which arises from the difference in potential between the *Si* and *Ge* atoms which are randomly distributed in the alloy. In short period *Si-Ge* superlattices alloy scattering is assumed to arise due to roughness and interdiffusion at the interfaces. This is confirmed by calculation, if disorder extends only ±1 monolayer from each interface in a ten- monolayer period *Si-Ge* superlattice, then alloy scattering becomes the dominant mechanism(10,11).

Method and Discussion:

We propose a structure consisting of two ultra-thin (4-monolayer) *Ge* layers separated by a wider (20- monolayer) *Si* well. The structure was assumed to be placed within a *Si* matrix of arbitrary thickness. The zone-folding mechanism, which relies on the periodicity of the structure. Nevertheless, full-scale pseudopotential calculations reveal that the presence of the interfaces gives rise to a transition which is comparable in strength with that predicted for an ideal ten-monolayer period Si-Ge superlattice. The transitions are to states which are localized in the Si well. In an undoped system these are resonant states, the ground conduction state lying in the continuum of the thick Si matrix. The structures are heavily doped with acceptors $(P{\sim}10^{18}\ cm^{-3})$. Which we will refer to as the symmetric case, a 10 nm thick $Si_{0.85}\ Ge_{0.15}$ alloy layer is grown either side of the structure. The second, or a symmetric, structure is grown directly onto Si and has a 10 nm alloy layer on one side only. In each of these cases a thick ($\sim$ 50 nm) Si layer is grown between each structure. 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

$$\sum_{nk} A_{nk}\ \emptyset_{nk} = \psi$$

Where:

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

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 (Morrison *et al 1987)*

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

$$\sum_{\tau_0} e^{ig.\tau_0})$$

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 the supercell calculation Can be Perfumed using only those bulk bands that contribute to the state of interest, i.e. those around the bandgap.

In this approach we are able to model the microscopic effects produced by rearrangement of the atoms at the interface. In particular, it is possible to study the changes in the optical transition probabilities as a function of disorder at the interface. The effects of doping are included in our calculation by adding a 1-D potential representing the coulomb interaction between the holes and the ionized acceptors.

We will first address the idealized case, i.e. in which the interface between the *Si* and *Ge* layers is assumed to be perfectly. The conduction

band edge profiles for structures grown directly onto a *Si* substrate and grown onto a thin $Si_{0.85}\ Ge_{0.15}$ alloy layer are drawn to scale in Fig 1.$\Delta^{||}$ denotes the four-fold degenerate conduction minima aligned in the plane of the interface and $\Delta^{\perp}$ refers to the conduction minima along the growth direction. We note that there is some uncertainty regarding the sign of the offset for the $\Delta^{||}$ minima between *Si* and low concentration *Ge* alloys. However, since this offset is very small it will not have any noticeable effect on states confined in the *Si* well, nor will it give rise to any new localized states.
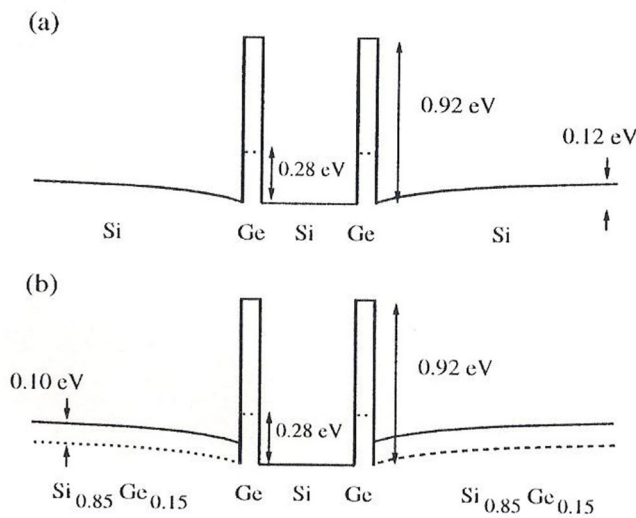
Fig(1) Shows the conduction band edge profiles (drawn to scale) for the Ge_m- Si_n- Ge_m structures grown (a) directly onto a Si substrate and (b) onto a thin $Si_{0.85}\ Ge_{0.15}$ alloy layer which is strained to Si . A solid line denotes the $\Delta^{\perp}$ band edge for minima aligned along the growth direction and a dashed line indicates the position of the four-fold $\Delta^{||}$ band edge where this is split by strain from the $\Delta^{\perp}$ state. The band bending is appropriate for a doping concentration of $10^{18}\ cm^{-3}$ assuming a 2-D hole concentration of $5\times10^{12}\ cm^{-2}$ in the Ge layers.

The large confining potentials for both the $\Delta^{\perp}$ and $\Delta^{||}$ minima give rise to sets of bound states in the *Si* well. The charge density of the ground

associated with each minimum is shown in Fig 2. The $\Delta^{\perp}$ state is strongly confined in the *Si* well, whereas the $\Delta^{\parallel}$ state exhibits some leakage into the surrounding regions.
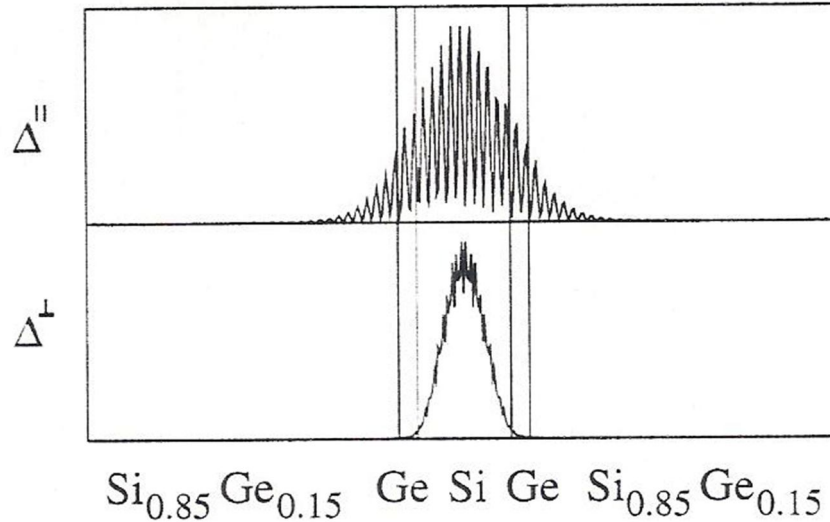

Fig (2) Shows charge densities of the lowest confined conduction states for the structure shown in Fig 1(b). (The change densities for the structure in Fig 1(a) are very similar to these.)

This difference can be understood intuitively on the basis that in the latter case the offsets are smaller and the mass is lighter. In an undoped system these are resonance states which lie above the continuum band edge. Uniform doping with acceptors produces a band bending potential which acts to lower the energy of the states confined in the *Si* well, as shown in Fig 1. In these figures the acceptor doping concentration is 10^{18} cm^{-3} and the 2-D carrier density in the *Ge* layers is 5×10^{12} cm^{-2} . The effect of doping on the states near to the conduction band edge is shown in Fig 3.
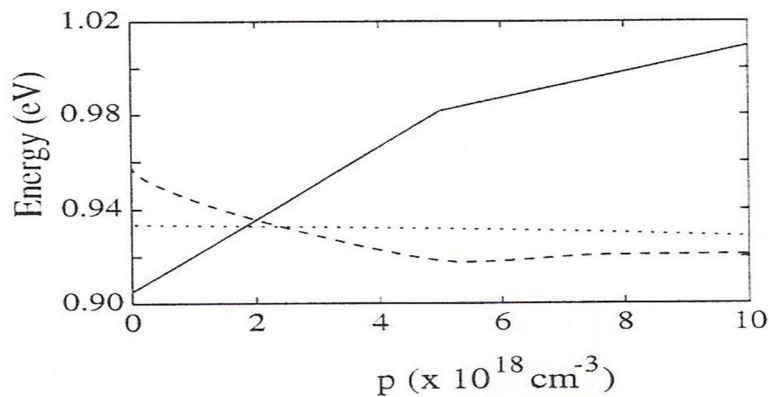
Fig (3) Shows movement of the conduction band edge states as a function of acceptor doping concentration *p*. The solid line represents the continuum band edge. The dashed line shows the confined $\Delta^{\parallel}$ state and the dotted line indicates the confined $\Delta^{\perp}$ state.

The continuum states are pushed up in energy, as expected, where the in-plane $\Delta^{\parallel}$ minima move down in energy with respect to the $\Delta^{\perp}$ states. Comparing these results with the experimental data of Gail et al(1) it is seen that the energies are in good agreement. The stability of the observed spectra at room temperature can be explained by the presence of the large confining potentials.

The selection rule to the $\Delta^{\parallel}$ minima can be broken if the potential in the direction parallel to the interfaces is perturbed. However, in this structure the optical behavior of the system is far less susceptible to the character of the interface. We have performed 3-D supercell calculations on the structure shown in Fig 1(a) incorporating various models of disorder such as (i) a random alloy occupying ±1 monolayer at each interface, (ii) a graded interface, and (iii) island of various sizes at an interface. The maximum transition strength to the $\Delta^{\parallel}$ minima obtained in any of these

cases is still 6 order of magnitude weaker than the allowed transition. This is illustrated in Fig 4 where the transition strength for the structure in case (i) are plotted against those for a Si_5- Ge_5 superlattice with a similar disorder.
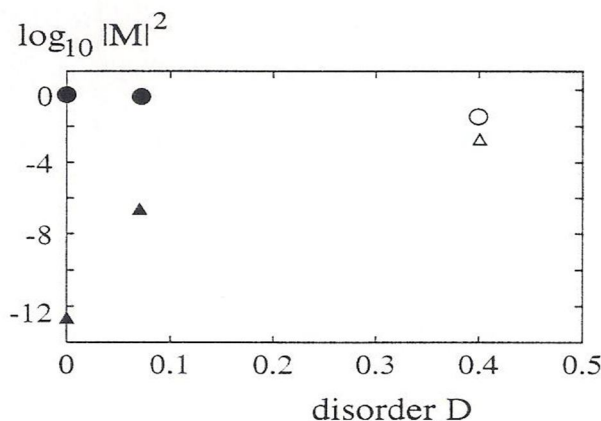

Fig (4) Shows a comparison of the cross gap transition probability to the $\Delta^{\perp}$ minima (circles) and the $\Delta^{\parallel}$ minima (triangles) as a function of the proportion of misplaced atoms. The disorder parameter is defined such that *D=0* for an ideal structure and *D=1* for a random alloy (. Solid markers indicate points for the structure in Fig 1(a) and open markers correspond to a Si_5-Ge_5 superlattice strained to a Si substrate. The transition strength has been normalized so that $|M|^2$ is equal to 0.1 for the ideal structure. In the imperfect cases there is a 2 monolayer random alloy at each interface.

In the ten monolayer period superlattice the interface region accounts for 40% of the total volume of the superlattice, whereas, in the structure described above it constitutes a much smaller percentage of the active region. For the same reason, similar results are obtained when the disorder is described by cases (ii) or (iii). We conclude from these results that, unless the grown structures are grossly distorted from the ideal configuration, this mechanism cannot account for the observed luminescence.

Another possibility is that emission is due to alloy scattering occurring in the 10 nm alloy layers cladding the structures. Although this would explain the existence of a no-phonon transition from the $\Delta^{||}$ minima, there are several arguments to suggest that this is not the origin of luminescence in this instance.

Firstly, luminescence from *SiGe* alloys has only previously been observed at temperatures less than 50K, some other source of localization must be invoked in order to explain the existence of room temperature luminescence. Secondly, it should be noticed that room temperature luminescence is observed only in the a symmetric structure (which has an alloy layer on one side) and is not observed in the symmetric structure (which has alloy layers on both sides). Finally, it is clear from Fig 2 that the bound states do not sample a significant portion of the alloy region.

Conclusions:

The key features are that the spectra is stable at room temperature, suggesting that both the electrons and holes strongly localized, and that the transitions are from states associated with the four-fold $\Delta^{||}$ minima, suggesting that the origin of this effect is a perturbation in the interface plane. One way these results can be explained is to assume that the spectra is dominated by anomalous localization at the interface. When no island is present we obtain the intuitive result that an electron bound to an impurity at the centre of the well has a larger binding energy than an electron bound to an impurity at the interface. However, our calculations predict that for island one monolayer high and greater than 3 lattice constants in extent, the ground state is formed by excitons which are bound to the interface. We have demonstrated in this paper that the origin of the observed spectra cannot be explained without some interface related electron localization.

This is an important step towards better understanding of this system and one which offers scope for fresh experimentation and modeling.

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