Electronic structure of a Si δ-layer embedded in Ge (001)

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Abstract. Using the Green function formalism with layer orbitals we studied the electronic structure of a Si δ-layer in germanium. We found two-dimensional parabolic subbands near the band edges. This approach is extended to treat the electronic structure of a single quantum well without invoking the periodically repeating models.

The incorporation of an extremely sharp and high-density doping profile consisting of a few atomic layers during the growth of semiconductors is denoted as δ-doping. Such a doping can modify the electronic properties of a semiconductor heterostructure [1, 2]. In fact, Capasso and his coworkers [3] showed that the band offset of an $Al_xGa_{1-x}As/GaAs$ heterojunction is modified by a δ-doping. A new type of non-alloyed Ohmic contact with GaAs is achieved by placing a high-density donor sheet a few layers away from the metal–semiconductor interface [2]. Zeindl et al [4] have incorporated a sheet of Sb into Si(001) with a density of $\sim 1.6 \times 10^3$ Sb cm^{-2}. The diffusion of dopants seems to be the major difficulty in producing a sharp doping profile during the growth of the superlattice. Of course the ultimate goal is to incorporate a stable and defect-free atomic plane made from impurity atoms. This way one can fabricate superlattices consisting of repeating 2D metals and insulators or polarizable crystals. Recently, such a superlattice $(YBCO)_m/(PrBCO)_n$ has been grown [5], whereby important properties related to the theory of high T_c superconductivity have been deduced [6]. Similarly, hole and electron δ-layers separated by dielectric media can be an interesting system in which to examine the possibility of hole–electron pair formation and a BCS-like transition [7, 8].

In this paper, we study the electronic properties of a Si δ-layer embedded in an infinitely large Ge(001) crystal by using the Green function method with layer orbitals. The same method is extended to study a single quantum well without invoking a supercell having an artifical periodicity. In this respect, the method is rather convenient in studying the electronic structure of a single δ-layer without the artifacts of the periodically repeating models.

We can treat this type of problem as a defect problem within a perturbative approach [9, 10]. The Hamiltonian of the perturbed system can be written in two parts:

$$H = H_0 + V \tag{1}$$

H_0 is the perfect crystal Hamiltonian of a periodic lattice with eigenvalues E_{nk} and eigenstates Ψ_{nk}. V denotes the deviation from the perfect potential due to the defect, such as δ-layers. Let the Schrödinger equation of the perturbed crystal be

$$H\Psi = (H_0 + V)\Psi = E\Psi. \tag{2}$$

The solutions of (2) can be classified into two groups depending on whether the eigenvalue E coincides with the spectrum of H_0. These are bound states and resonances or antiresonances. If the eigenvalue E does not coincide with the spectrum of H_0, (say it is in the band gaps of the unperturbed crystal), the corresponding states are bound states localized around the perturbing potential. In this case (2) is transformed to a system of linear algebraic equations by expanding the wavefunction Ψ in terms of a suitable basis set ϕ_α ($\Psi = \sum_\alpha C_\alpha \phi_\alpha$). Hence, within the band gaps the Schrödinger equation becomes

$$\sum_{\alpha'}\left(\delta_{\alpha\alpha'} - \sum_{\alpha''}G_0^{\alpha\alpha''}(E)V_{\alpha''\alpha'}\right)C_{\alpha'} = 0 \tag{3}$$

where

$$G_0^{\alpha\alpha'}(E) = \sum_{nk}\frac{\langle\alpha|nk\rangle\langle nk|\alpha'\rangle}{E - E_{nk}} \tag{4}$$

are the Green matrix elements of the unperturbed system. For the non-trivial solution of a bound state the determinant of $Q(E) = 1 - G_0(E)V$ vanishes,

$$\det \|Q(E)\| = 0. \tag{5}$$

If the eigenvalue E coincides with the energy spectrum

of H_0 (within the bands of the unperturbed crystal), solutions always exist with the bands of a perfect crystal. The wavefunctions, of course, are not Ψ_{nk} but are given by the Lippman–Schwinger equation. The density of states

$$N(E) = -\frac{1}{\pi}\text{Im}\,[\text{Tr}G(E)] \qquad (6)$$

is changed in the vicinity of the defect. Here $G(E)$ is the Green function for the perturbed system and it can be calculated from Dyson's equation. In this range of energy the Green function is defined by analytic continuation. The change in density of states is obtained from the following equation:

$$\Delta N(E) = -\frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}E}\arctan\left(\frac{\text{Im det}\,\|\,Q\,\|}{\text{Re det}\,\|\,Q\,\|}\right). \qquad (7)$$

A peak in $\Delta N(E)$ is called a resonance while a dip is called an antiresonance.

We apply this approach to the case of the δ-doping by taking the δ-layer as a planar perturbation. Since the system preserves the two-dimensional periodicity, the basis set is taken as layer orbitals which are simply Bloch sums in two dimensions [11].

$$\Phi_q^{m\alpha\mu}(r) = \frac{1}{\sqrt{N_1N_2}}\sum_l e^{iq\cdot(\rho_l+\lambda_\mu^m)}\varphi_\alpha(r-\rho_l-\lambda_\mu^m) \qquad (8)$$

where ρ_l are the lattice vectors of the two-dimensional lattice, λ_μ^m are the position vectors of the atoms in the two-dimensional unit cell and they can be decomposed into two parts as the surface parallel component, σ_μ^m, and perpendicular component, κ^μ. The index m labels the layer while μ labels different atoms in the same plane. $\{\rho_l,\lambda_\mu^m\}$ span the entire bulk lattice, and α labels the orbitals. N_1N_2 is the number of lattice points in the 2D lattice. Similarly the Bloch wavevector k is decomposed as

$$k = q + g + k_\perp \qquad (9)$$

where q is a two-dimensional wavevector, g is the reciprocal lattice vector of the two-dimensional lattice and $k_\perp$ is the perpendicular component.

States of the perturbed system are then expanded in terms of the layer orbital [11]

$$\Psi_{sq}(r) = \sum_j A_{sq}^j\Phi_q^j(r) \qquad (10)$$

where $j = m\alpha\mu$ is a composite index for the layer orbitals and s labels the states. Then the Green function becomes [11]

$$G_{jj'}^0(q,E) = \frac{1}{N_3}\sum_{k_\perp}\sum_g{}'e^{ik_\perp\cdot(\kappa^m-\kappa^{m'})}e^{iq\cdot(\sigma_\mu^m-\sigma_{\mu'}^{m'})}$$
$$\times\sum_n\frac{C_l^n(q+g,k_\perp)C_{l'}^{n\star}(q+g,k_\perp)}{E^+-E_n(q+g,k_\perp)} \qquad (11)$$

where C_l^n and E_n are the eigenfunction and eigenvalue of the entire bulk lattice. The energy, E^+, is given as

$E+i\epsilon$ where ϵ is a very small quantity for the energies within the bands of the unperturbed system. N_3 is the number of lattice points in the perpendicular direction. The prime over the summation indicates g vectors corresponding to k which lie inside the first Brillouin zone according to (9). Note that these bulk states are calculated once and for all in an appropriate cell and used for defects (or δ-dopings) having perturbative potentials of similar range. The element of the potential matrix is

$$\langle j,q|V|j',q\rangle = \langle j,q|H|j',q\rangle - \langle j,q|H_0|j',q\rangle. \qquad (12)$$

For a localized perturbation, the potential matrix will have blocks with all zeros. Thus, depending on the chosen basis set and the range of the perturbation, the size of the matrices with non-zero elements can be rather small.

Having presented a brief summary of the method, we now turn to the theoretical study of the electronic energy structure of a Si δ-layer in a Ge(001) crystal. Since Si layers are pseudomorphically grown on the Ge (001) surface, in-plane lattice constants are restricted to the lattice constant of Ge (5.65 Å). Therefore, while the Ge layers preserve the cubic symmetry, Si layers are distorted tetragonally, i.e. $a_{\|Si} = 5.65$ Å, $a_{\perp Si} = 5.26$ Å. The lattice parameters are obtained from self-consistent field pseudopotential calculations [12]. The interlayer spacing at the Ge–Si interface is taken to be the average of the interlayer spacings in the Ge and Si layers. We used the energy parameters of Li and Chung [13] for construction of the empirical tight-binding Hamiltonian. Since the Si–Ge and Si–Si interatomic distances deviate from their ideal bulk values owing to the strain imposed by the lattice mismatch, the energy parameters are scaled by the d^{-2} scaling [14]. Another critical parameter in our calculation is the band offset, ΔE_V. We used the value (0.3 eV) calculated by Van de Walle et al [12] for the Si–Ge superlattice grown on the Ge(001) surface. In all calculations we neglect the spin-orbit splitting.

The electronic structure of the Si_n–Ge (001) ($n = 1, 2, 3, 4$) δ-doping structure is calculated by using the Green function formalism to investigate the electronic structure of a single quantum well in the Ge crystal. The energy band structure of bound states of the Si_4–Ge (001) δ-doping structure is calculated by solving (5), and is shown with the projected bands of Ge (001) in figure 1. Since the Si–Ge heterojunction shows a type-II behaviour, the electrons are confined in the Si sublattice, while the holes are in the Ge sublattice. As seen in figure 1(a), near the conduction band edge, the energy band of the bound state shows a parabolic dispersion which is characteristic of a 2D electron system treated in the effective mass approximation. The total contribution of the Si orbitals is 90%. This indicates strong confinement of electrons in the quantum well occurring in the Si δ-layers. For the value of the band offset, $\Delta E_V = 0.3$ eV, bound states appear also near the conduction band edge between M and X points, but they merge in the conduction band of Ge (001) and become
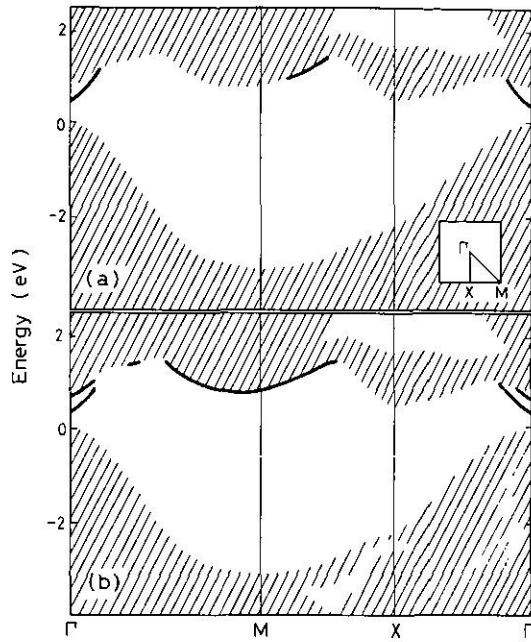
Figure 1. Energy band structure of Si_4–Ge (001). Bound states are shown by full curves, and the projected bands of Ge(001) are hatched. The band offset values are (a) $\Delta E_v = 0.3$ eV and (b) $\Delta E_v = 0.5$ eV.
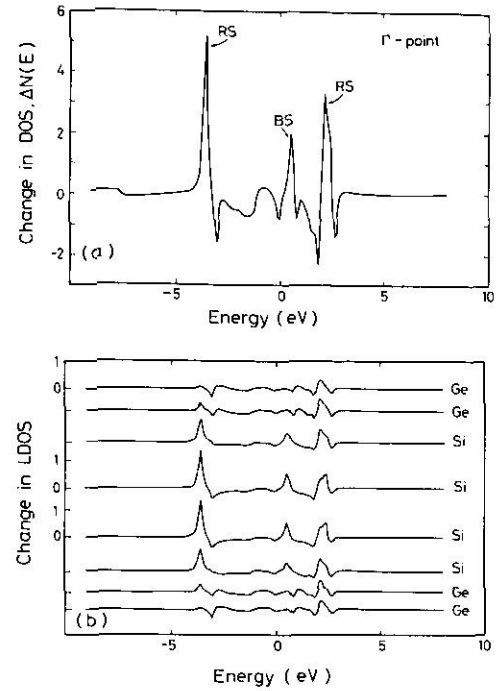
Figure 2. $\Delta N(E)$, the change in the density of states (in units of states/eV unit cell) at the Γ point. (a) Total change in density of states. (b) Layer-resolved change in density of states. (Energies are broadened by 0.1 eV in the calculation of the Green function.)
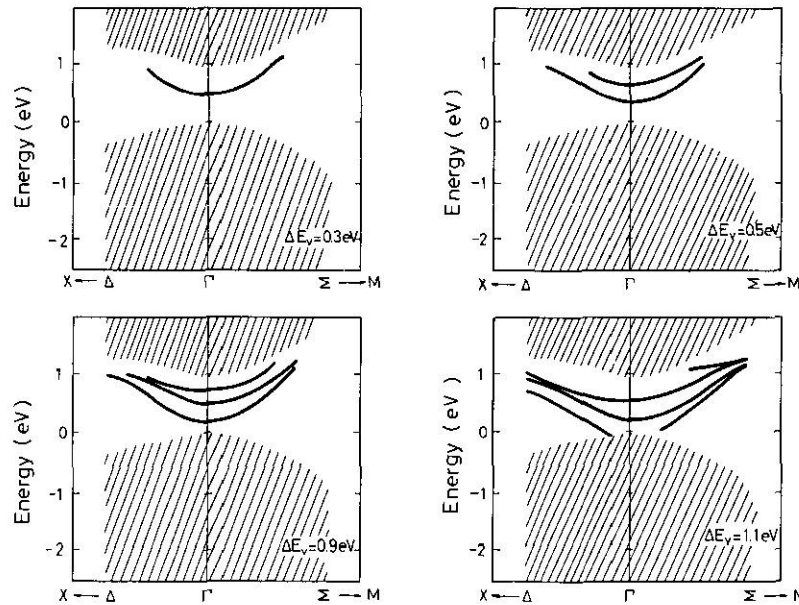
Figure 3. Energy band structure of Si_4–Ge (001) for different band offset values ΔE_v. (Δ and Σ points are such that $|\Gamma\Sigma| = 0.15 |\Gamma M|$ and $|\Gamma\Delta| = 0.13 |\Gamma X|$.)

resonances. As seen in figure 1(b), increasing the value of band offset causes these resonance states to shift down in energy towards the band gap and to become bound states. Changes in density of states are calculated at the Γ point by using (6) and (7) and are shown in figure 2. The peak at 0.5 eV corresponds to the bound state originating from Si δ-layers while the dip near 0 eV is due to the antiresonance state. Note that dips in the continuum of projected bands are antiresonance states and simply mean a charge transfer from these states to

the bound states or to the resonance states. The nature of these states is revealed in the layer-resolved change in density of states. While the peak is just the addition of change in density of states in Si layers, all layers contribute to the dip as seen in figure 2(b). In addition to these states, there are other bound states within the gaps in the projected valence and conduction bands of Ge (001). For $n = 1, 2$ and 3, we observed the same trends in the energy band diagram. The 2D parabolic band around the Γ point and bands near the conduction

band edge along the ΓM and MX directions are found for all n values ($1 \leqslant n \leqslant 4$). However, the dispersion of the parabolic bands decreases with decreasing n. For a single δ-layer ($n = 1$) it becomes a shallow level 30 meV below the band edge. Note that the subbands calculated within the effective mass approximation having a free electron behaviour in the plane of the epilayer display equivalent dispersion.

Finally, to explore the effect of the band offset on the subband structure the electronic structure of the Si$_4$–Ge (001) quantum well is calculated for different band offset values (ΔE_V), i.e. for different depths of quantum wells. The calculated energy bands near the Γ point are presented for different ΔE_V values in figure 3. As ΔE_V increases, the bands of bound states are shifted down in energy (since the tops of the valence and conduction bands of Ge are raised) and new parabolic bands emerge in the band gap of Ge. For example, the number of parabolic bands is found to be two and three for $\Delta E_V = 0.5$ and 0.7 eV, respectively, since the deeper quantum wells support larger numbers of subbands. Upon further increase of ΔE_V the lowest subband overlaps with the valence band continuum of Ge. As soon as the energy of the lowest subband coincides with the maximum of the valence band, the charge starts to transfer from Ge to the Si δ-layer.

In conclusion, the electronic structure of a single quantum well is treated by using the Green function method. States of the parabolic bands in the fundamental band gap of the host Ge are confined in the δ-layer. As the band offset and thus the depth of the quantum well increases, the number of subbands increases. We have shown that the electronic structure of the quantum well or δ-doping can be handled by using the Green function method. Another aspect to note is that the Green function is calculated once and for all to treat different problems in the same host lattice (such as different doping concentrations, different doping atoms, etc). We believe that the theoretical method exemplified in this paper is convenient to treat the electronic

structure of a δ-layer, in particular a metal δ-layer, by using the self-consistent field tight-binding method (with a Gaussian orbital basis set or without any specific form of orbitals).

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