Energy levels of Ge quantum wells embedded in Si: A tight-binding approach

G. Grosso
Dipartimento di Fisica and Istituto Nazionale di Fisica della Materia, Piazza Torricelli 2, I-56126 Pisa, Italy

G. Pastori Parravicini
Dipartimento di Fisica and Istituto Nazionale di Fisica della Materia, Via A. Bassi 6, I-27100 Pavia, Italy

C. Piermarocchi*
Institut de Physique Théorique, Ecole Polytechnique Fédérale, CH-1015 Lausanne, Switzerland
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We calculate the energy levels of Ge quantum wells embedded in Si and grown on an arbitrary Si_xGe_{1-x} substrate. The calculations are carried out using the tight-binding-renormalization approach and reliable Slater-Köster parameters including interactions up to second neighbors. The substrate affects the positions of the Si and Ge atoms, and the Slater-Köster parameters are modified consistently using scaling laws beyond the d^{-2} Harrison rule. Our results provide theoretical support to the observed photoluminescence lines within the Ge quantum wells. We study the effect of substrate alloy composition on the position of these lines and find that the two main energy transitions in the Ge quantum wells approach when the Ge concentration in the substrate increases.

In this paper we investigate theoretically the electronic structure of thin Ge quantum wells embedded in thick slabs of Si grown along the (001) direction on a Si_xGe_{1-x} substrate. We have considered quantum wells of 2, 4, and 6 ML of germanium, for which luminescence experiments exist in the literature.[1,2] The condition of *isolated* quantum wells is realized by constructing an ideal periodic superlattice where the primitive cell in the growth direction is made by a tiny Ge quantum well followed by a thick region of Si multilayers. The presence of this ideal periodicity allows us to use the tight-binding-renormalization approach that can efficiently treat superlattices of arbitrary length.[3,4] The calculations performed on such long-period superlattices simultaneously provide the energy levels confined in the quantum well and the levels in the continuum. We have presented elsewhere the details of this method, which decimates and renormalizes the whole cell along the (001) direction and represents the bulk Hamiltonian $H(\mathbf{k})$ on the basis of ''two-dimensional Bloch sums'' made by ''layer orbitals.''[3,4] By means of standard iterative decimation techniques,[5] one can reduce the whole superlattice cell to a couple of interacting effective layers where the Green's function can be conveniently evaluated. From the matrix elements of the Green's function we can then deduce all the relevant physical information on the system; in particular we are interested in the electronic band structure and in the spatial localization of electron and hole density.

We start from a localized basis representation of the Hamiltonian $H(\mathbf{k})$ for bulk silicon and germanium. Our Slater-Köster[6] tight-binding parametrization[7] of $H(\mathbf{k})$ takes its origin from an orthogonal basis of *s* and *p* atomiclike orbitals with nearest neighbors and few selected second neighbor interactions. Spin-orbit coupling is included, and effective masses of bulk crystals around the fundamental gap are well reproduced. Scaling laws for these parameters, for different separation between atomic orbitals have also been calculated,[7] with values that are more accurate with respect to the d^{-2} Harrison rule. From them, deformation potentials of Si and Ge under hydrostatic and uniaxial pressure have been obtained[7] in good agreement with experimental and other theoretical results. The knowledge of these scaling laws are essential to study Si/Ge heterostructures; due to

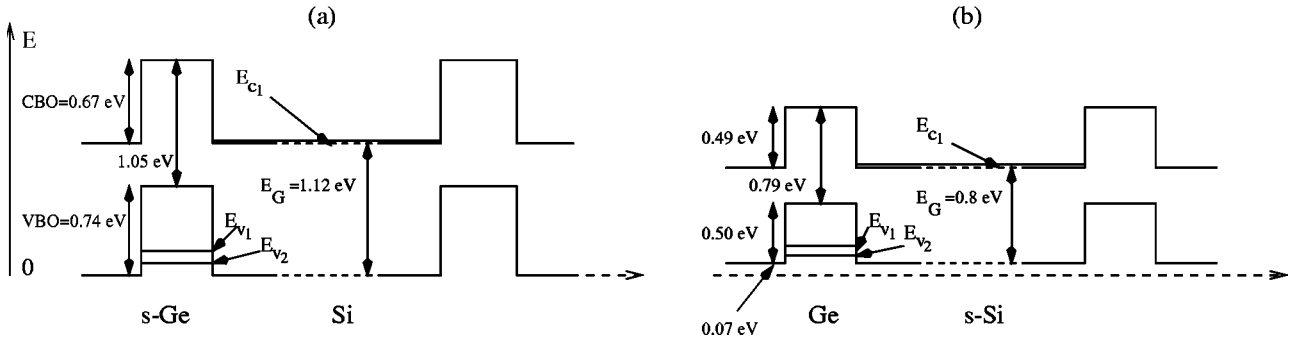

FIG. 1. Schematic band-structure potential of the Ge/Si superlattice, (a) The buffer is pure Si, (b) the buffer is pure Ge. The reference energy zero is the top of the Si valence band of the case (a). For both cases the superlattice is composed of 4 ML of Ge separated by 220 ML of Si.

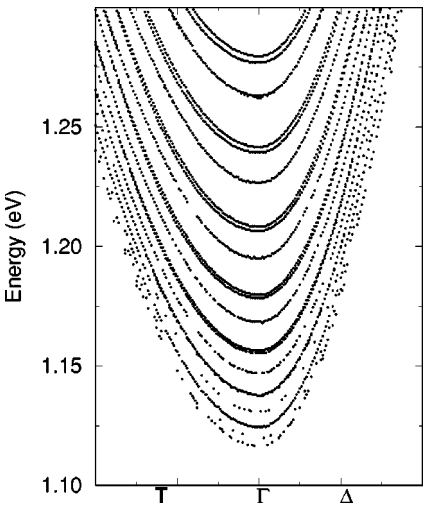

FIG. 2. Conduction-band structure of the germanium/silicon superlattice around the two-dimensional Brillouin zone center, for the case shown in Fig. 1(a).

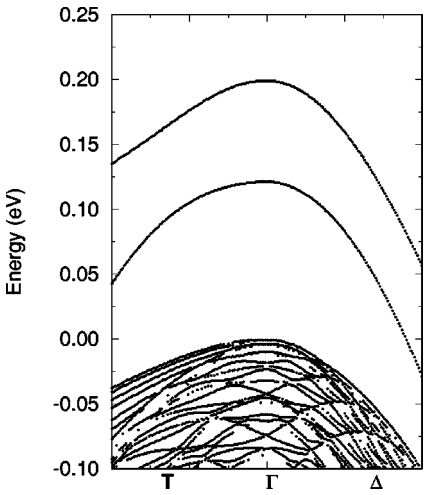

FIG. 3. Valence-band structure of the germanium/silicon superlattice around the two-dimensional Brillouin zone center, for the case shown in Fig. 1(a).

their lattice mismatch, the lattice constants are in fact $a_{Si}=5.431$ Å and $a_{Ge}=5.657$ Å. For a given alloy concentration in the substrate the in-plane lattice constant $a_{\parallel}$ is constant throughout the sample, while the macroscopic lattice constant $a_{\perp}$ is determined by the elasticity theory[8] and is different for each material.

We give in Fig. 1 the schematic profile of the potential experienced by the carriers at the Γ point of the two-dimensional Brillouin zone. The two limit cases when the superlattice is grown on a pure Si buffer (a), and on a pure Ge buffer (b), are shown. The values of the energy gaps of 1.12 eV for the Si slab in (a) and of 0.79 eV for Ge in (b) correspond to the unstrained bulk values. The 0.8 eV for Si in (b) and 1.05 eV for Ge in (a) are instead determined taking into account the effects of the strain on the whole structure. We remark that in our procedure only one parameter in the bands alignment has been fixed (the value of 0.74 eV for the valence-band offset of Ge on Si,[9] from experimental measurements). All the other energies in the profile of the bands result from the corresponding calculation of the energy levels of bulk Si grown on Ge and vice versa using the tight-binding parametrizations and scaling laws of Ref. 7. The valence-band offset at the interface between pure Si and pure Ge grown on a substrate made by Si_xGe_{1-x} alloy has been investigated in the literature;[8,10] we exploit these results to take qualitatively into account the effect of charge redistribution at the interface. In the figure the relevant confined levels in the Ge region are also reported.

We have first investigated pseudomorphic Ge quantum wells grown on a pure Si (001) substrate. This has been motivated by measurements of luminescence lines from monolayer-thick Ge quantum wells embedded in silicon. We have considered 4 ML of Ge separated by 220 ML of Si. For such thick Si regions we have verified that the energy levels in the Ge quantum wells are not affected by the ideal periodicity of the superlattice introduced in the renormalization procedure. The energy separation obtained between the states c_1 and v_1 in the case of Fig. 1(a) is $E_{c_1-v_1}=0.920$ eV (which compares well with the experimental values of the electroluminescence emission $E_{c_1-v_1}=0.918-0.935$ eV obtained by Olajos *et al.*[2] for Ge quantum well separated by 17 Si monolayers) and $E_{c_1-v_1}=0.735$ eV in the case of Fig. 1(b).

Figure 2 shows the conduction electronic structure of the superlattice with the lowest c_1 level confined in the Si region at $E_{c_1}\approx 1.12$ eV (see Fig. 1 for the reference zero of the energy). Figure 3 shows the valence electronic structure of the superlattice with the heavy hole v_1 and the light hole v_2 confined in the Ge region. We have, moreover, confirmed the experimental finding that increasing the width of the Ge quantum wells, with 2, 4, and 6 ML, makes a redshift of the luminescence appear: this is simply due to the increasing of the confinement for the holes in the larger wells. As suggested in Ref. 8 and Ref. 10, one can tune the lattice parameters and thus the position of the confined levels in the Ge quantum well by growing the superlattice on substrates of different lattice constants. We have thus varied the composition of the Si_xGe_{1-x} alloy buffer on which the superlattice is

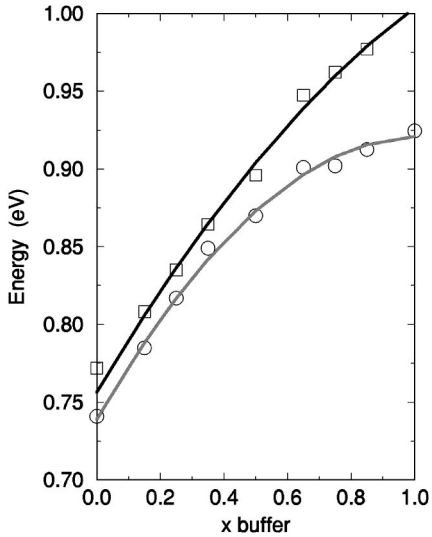

FIG. 4. Energies of the transitions $E_{c_1-v_1}$ (circles) and $E_{c_1-v_2}$ (squares) versus the buffer alloy concentration, in superlattices composed of 4 ML of Ge separated by 220 ML of Si.

grown, from pure Ge to pure Si. The results are summarized in Fig. 4, where the gaps $E_{c_1-v_1}$ and $E_{c_1-v_2}$ versus the alloy concentration are shown. From the figure it is evident that the values of these gaps, and thus the positions of the corresponding luminescence lines, approach when the Ge concentration in the substrate increases. Moreover, one can notice that the uniaxial expansion increases with x and further lifts the separation of the heavy-hole and light-hole band edges due to the superlattice confinement; this is in qualitative agreement with resonant tunneling measurements in strained Si-SiGe nanostructures.[11]

In conclusion, we have investigated theoretically the electronic structure of thin strained Ge quantum wells embedded on Si slabs, considering also the role of the buffer on which the multilayer structure is grown. We have found good agreement with the experimental photoluminescence experiments on pure Si-strained Ge structures and have shown that the photoluminescence lines can be shifted by controlling the concentration of the Si_xGe_{1-x} alloy buffer.

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*Present address: Department of Physics, University of California San Diego, La Jolla, CA 92093-0319.

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