Selection rules for intersubband transitions in valley split [001]-Ge quantum wells

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Abstract—**By a $sp^3d^5s^*$ tight-binding model we have investigated intervalley splitting of the fundamental and first excited confined subbands in strained Germanium quantum wells (QWs). Intervalley interaction splits each subband into a doublet; we report numerical results for inter-doublets optical transitions and interpret them exploiting the peculiar spatial symmetry of the doublet states involved.**

BACKGROUND

In the past, intervalley splitting has been observed experimentally in Silicon QW systems [1] and addressed theoretically in terms of interference effects between degenerate bulk states related to the Δ valleys [2]. Valley splitting interaction is also expected in Germanium QW systems because of the presence of eight equivalent half-valley in the conduction band which are located at the bulk crystal Brillouin boundary (L points). Furthermore, because these valleys are along the [111] crystallographic axis, non-vanishing off-diagonal terms in the mass tensor are present and intersubband transitions in [001]-Ge QW systems can be induced also by a radiating field polarized in the QW plane, i.e. by normal incident light [3].

Here we exploit previous results on band-offsets for strained SiGe heterostructures to choose alloy compositions of the substrate and of the barrier regions of a symmetric Ge-QW so to obtain strain compensation and confinement of electrons in the Germanium region. A first-neighbor $sp^3d^5s^*$ tight-binding Hamiltonian [4] is exploited to describe the electronic and optical properties of the QW system. Valley splitting of the ground and first excited subband are studied as function of the well width and superimposed electric fields. We also study optical transitions between the valley split doublets induced by parallel and normal incident radiation. We find numerically selection rules for parallel and normal incidence light which are explained by the parity character of the involved states.

RESULTS

We have evaluated the valley splitting for the ground and first excited subbands as a function of the number of monoatomic layers in the well region (see Fig.1). Results are given both for unbiased QWs and for QW systems with a uniform electric field superimposed along the growth direction. As for Silicon QWs, we find that the splitting magnitude is an oscillating function of the well width with power law decay. Period and phase of the oscillations for the ground and first excited doublets are the same and are governed by the position of the conduction minima in the Brillouin zone of bulk Ge. Our results indicate that the valley splitting magnitude is greater as compared to Silicon systems, probably due to the Germanium lighter conduction masses.

At zero electric field the QW systems are symmetric for mirror reflection with respect to the center of the well and subband states are non degenerate because of intervalley splitting. Therefore doublet levels must have definite parity. Since the envelope function of states belonging to a given doublet is the same, in order to preserve orthogonality their parity have to be opposite. This fact is demonstrated in Fig.2 where we report the wavefunction amplitude of the two levels belonging to the ground doublet ($E_0^{(1)}$, $E_0^{(2)}$) and indicate the contributions from orbitals which are even or odd under the $z \rightarrow -z$ transformation.

Intersubband absorption spectra have been evaluated sampling the QW *k*-space in a neighbor of the conduction minima. Results at zero electric field for a 37 (38) monolayers QW system, corresponding to a maximum (minimum) in the valley splitting magnitude are shown in Fig.4 (see also Fig.3 for levels diagram and subbands dispersion). As reported in the inset of Fig.3, for $E_f > E_0^{(2)}$ four transitions are possible. For the 37 monolayers QW system these transitions occur at different energies while become degenerate for the 38 monolayers system. Nevertheless, only two peaks for normal incident light are present in the calculated spectra of the 37 monolayers QW, the remaining two transitions being strongly suppressed (Fig.4, top panel, solid lines). For parallel incident light, the suppressed and allowed transitions are now interchanged (Fig.4, top panel, dashed lines).

These selection rules can be understood considering that the dipole operator with polarization vector in the QW plane (normal incident radiation) is even for $z \rightarrow -z$. Then only states with the same parity can be optically coupled and therefore the $E_0^{(1)} \rightarrow E_1^{(1)}$ and the $E_0^{(2)} \rightarrow E_1^{(2)}$ transitions are not allowed. Vice versa, for polarization vector along the growth direction, the dipole operator is odd for $z \rightarrow -z$ and optical coupling is possible only between states with opposite parity i.e. the forbidden transitions are now $E_0^{(2)} \rightarrow E_1^{(1)}$ and $E_0^{(1)} \rightarrow E_1^{(2)}$.

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REFERENCES

[1] A. B. Fowler, F. F. Fang, W. E. Howard, and P. J. Stiles, "Magneto-Oscillatory Conductance in Silicon Surfaces", Phys. Rev. Lett., vol. 16, pp. 901-903, 1966.

[2] Boykin, G. Klimeck, M. Friesen, S. N. Coppersmith, P. von Allmen, F. Oyafuso, and S. Lee, "Valley splitting in low-density quantum-confined heterostructures studied using tight-binding models", Phys. Rev. B, vol. 70, pp. 165325-165337, 2004 and references therein.

[3] M. Virgilio and G. Grosso, "Conduction intersubband transitions at normal incidence in $Si_{1-x}Ge_x$ quantum well devices", Nanotechnology, vol. 18, pp. 075402-075407, 2007.

[4] J.-M. Jancu, R. Scholz, F. Beltram, and F. Bassani, "Empirical *spds*[*] tight-binding calculation for cubic semiconductors: General method and material parameters", Phys. Rev. B, vol. 57, pp. 6493-6593, 1998.

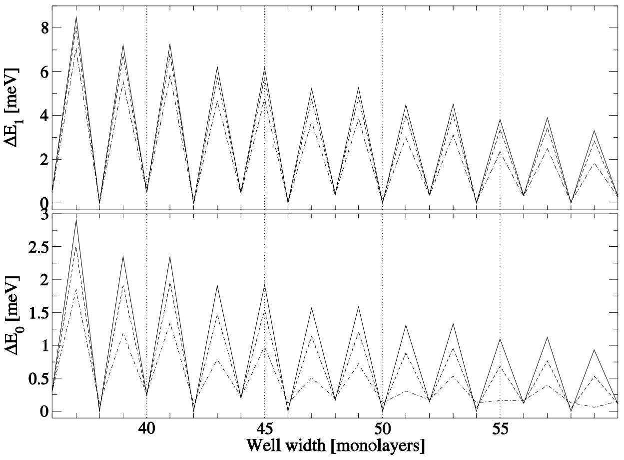

Fig.1: Valley splitting magnitude versus well width for the ground (bottom panel) and for the first excited (top panel) subbands of the QW system discussed in the text. Valley splitting for biased QW with field strength of 0.5 and 1.5 meV/Å are represented by dashed and dot-dashed lines, respectively. Solid lines refer to the zero electric field case.

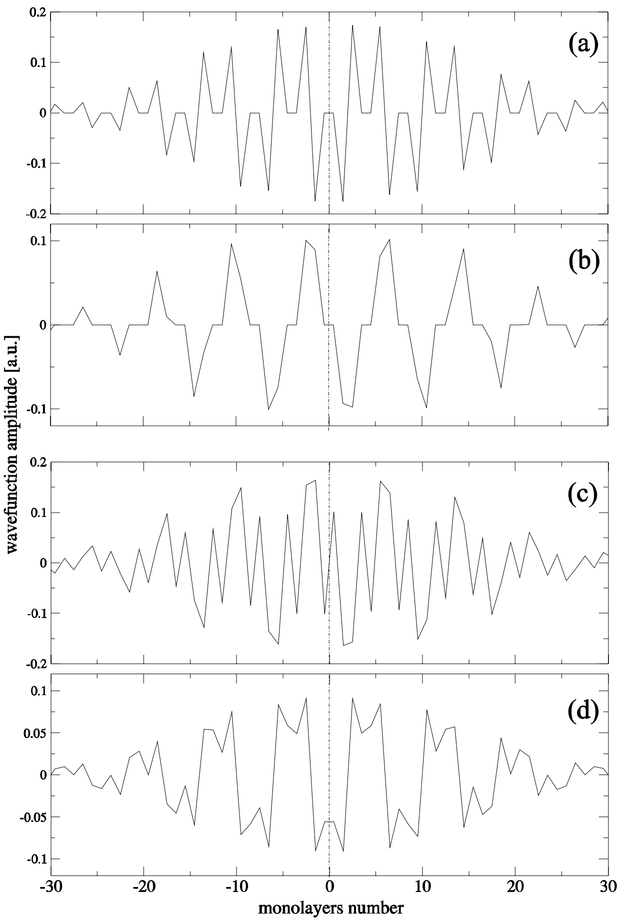

Fig.2: Wavefunction amplitude at zero electric field of the even ($E_0^{(1)}$) and of the odd ($E_0^{(2)}$) state, belonging to the ground doublet of the Ge QW system. Well thickness is 37 monoatomic layers, corresponding to a maximum in the valley splitting amplitude. Plots (a) and (b) represent the contribution to the wavefunction amplitude of the $E_0^{(1)}$ state obtained from orbitals which are even and odd under the $z \to -z$ transformation, respectively. Plots (c) and (d) refer to the even and odd orbital contributions to the $E_0^{(2)}$ wavefunction, respectively.

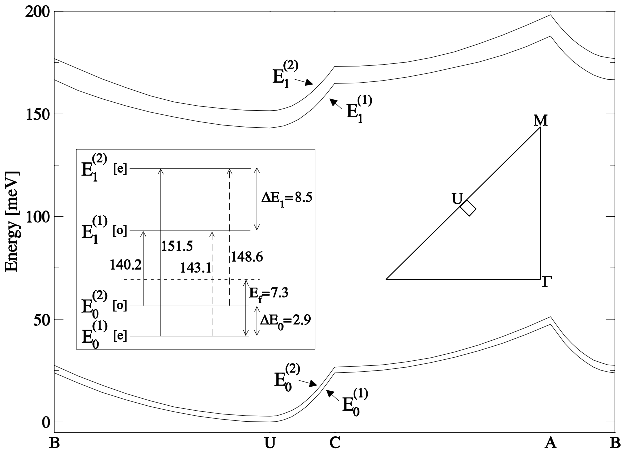

Fig.3: Band structure for the E_0 and E_1 QW subbands, evaluated at zero electric field for the Ge-QW of 37 monolayers. B,C,A points are chosen along rectangle around the U point sketched in the right inset. The U point of the tetragonal Brillouin zone corresponds to the conduction minimum (L point) of the Ge crystal. Energy separations at the U point, Fermi energy, parity of the states and allowed transitions for normal (solid arrows) and parallel (dashed arrows) incident light are reported in the left inset (not in scale).

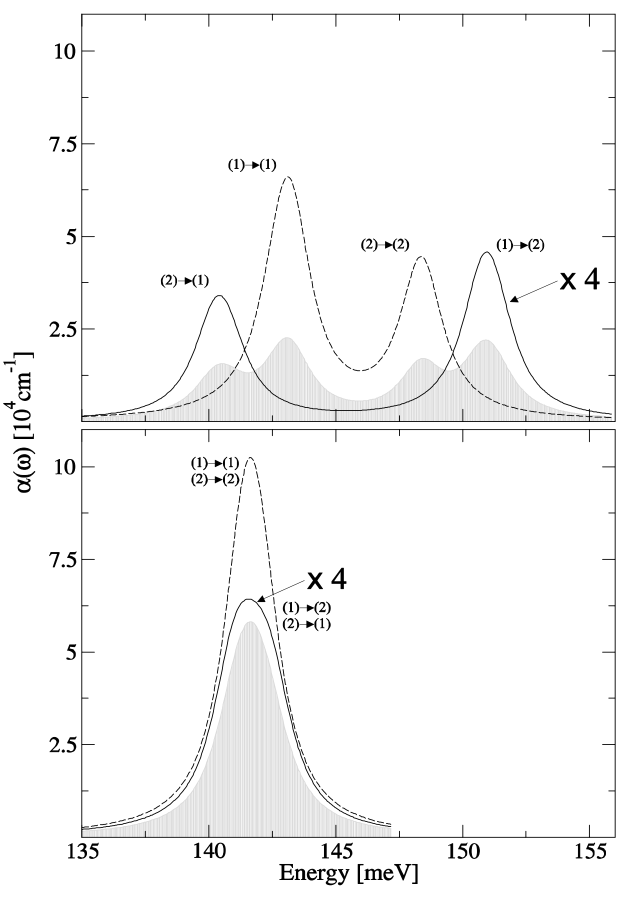

Fig.4: Intersubband absorption spectra for the Ge-QW system. Top (bottom) panel refer to well width of 37 (38) monolayers, corresponding to a maximum (minimum) in the valley splitting amplitude. Carrier concentration in the well region is $8 \cdot 10^{12}$ cm^{-2} per layer. Solid and dashed lines refer to normal and parallel incident light, respectively. Normal absorption is reported magnified by a factor 4. The grey shaded features represent the joint density of states.