Silicon-Germanium heterostructures for optoelectronic devices

Silicon and Germanium semiconductors are well known for electronic applications. However Si, Ge and their alloys were not been considered attractive as active materials in light emitting devices due to the indirect nature of fundamental interband transitions. The advent of epitaxial growth techniques, has encouraged many attempts to convert the indirect band gap into a direct band gap exploiting nanostructures engineering by means of control of growth conditions, system geometry, chemical composition, strain, bands alignment and external fields.

For this aim, the preliminary theoretical understanding and design of the complete structure is a key requirement.

We have investigated the electronic and optical properties of Si/SiGe and Ge/SiGe strained-layer multiple quantum wells grown on SiGe substrates with arbitrary alloy composition and strain. The good agreement with the experimental results demonstrates the effectiveness of the adopted theoretical approach based on the tight binding model, and its potential as precious tool to design realistic three dimensional heterostructures with desired electronic and optical properties.

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Understanding of the electronic properties of semiconductor quantum-confined structures is a key requirement for the development of their potential applications in electronic and photonic devices. This is particularly relevant for heterostructures based on the SiGe system, in view of their compatibility with Si technology.

In particular, Ge has been playing an important role in Si-based photonics. Ge is a material largely compatible with Si processing, it is an indirect gap material but with the 0.8 eV direct transition at the Γ point not far above the indirect fundamental gap at 0.66 eV. This fact, together with the miscibility of Si and Ge over the whole concentration range, has led to a number of proposals for Si compatible Ge-based photonic device applications. Photo detectors made from epitaxial Ge layers on Si substrates, optical modulators based on the Franz-Keldysh effect, and most recently, optical modulators based on the quantum-confined Stark effect in strained Ge wells have been demonstrated. These results have motivated our objective to find a route toward an optoelectronics platform based on Si CMOS and Ge quantum wells. A $sp^3d^5s^*$ tight-binding model has been adopted to evaluate the electronic properties and the interband and intraband optical transitions of a variety of low- and rich- content Ge quantum wells between SiGe alloys barriers, grown along the [001] direction, under strain conditions imposed by a relaxed SiGe buffer alloy.

As first item we have investigated the possibility of achieving conduction intersubband transitions induced by normal incidence radiation in a n-type SiGe-based quantum well (QW) structure coherently grown on a SiGe substrate along the [001] direction [1]. The quest of normal incidence geometry, i.e. incident electric field polarized along the growth plane (TE polarization), is motivated by the technical simplifications it allows in fabrication of planar large array of infrared detectors for imaging applications. In fact quantum mechanical selection rules forbid coupling of radiation with electrons degree of freedom if the incident electric field has no component along the growth direction. In p-type QWs, due to the mixing of heavy hole, light hole and split off subbands, valence intersubband transitions are possible for whatever polarization of the incident radiation. In n-type QWs, we have to distinguish the case of isotropic conduction band minimum at the Γ point in direct gap structures and the case of indirect gap structures but with effective mass tensor diagonal with respect to the growth axis (Si-rich QW grown along the [001] direction), from the case of conduction band ellipsoid minimum tilted with respect to the QW growth direction (Ge-rich QW grown along the [001] direction). We have demonstrated numerically that for the former class of structures normal incidence intersubband transitions are forbidden while they are allowed for the latter one [2, -4].

We have then analyzed the energy profile of the lowest conduction bands in Si and Ge QWs under different strain conditions [2, 4]. In particular we have investigated how the degeneracy of equivalent valleys in the bulk materials is resolved by uniaxial stress or other perturbations along the [001] axis, and how valley splitting depends from the well width or superimposed electric fields (see Fig.1).

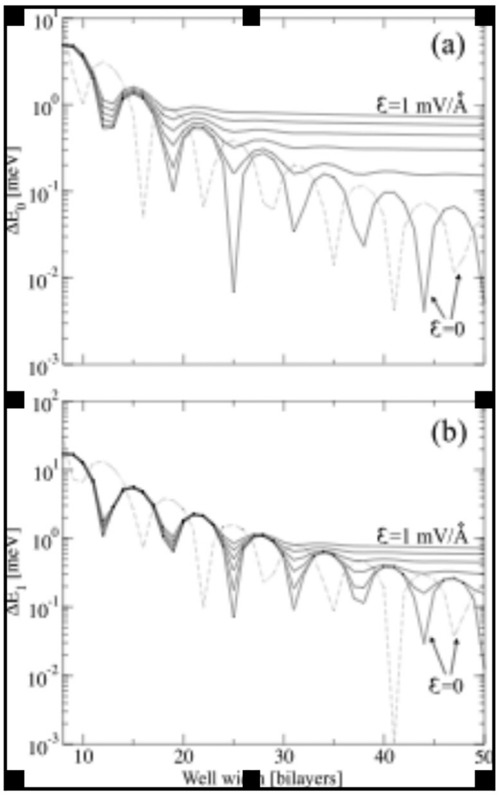

Fig. 1
Valley splitting magnitude versus well width for the ground (E_0 level), and first excited (E_1 level) QW subbands. Solid lines refer to the finite QW for electric field strengths ranging from 0 to 1 mV/Å. The dotted line represents the valley splitting for the hard wall system in the absence of electric field.

As second item we have studied interband optical transitions in Ge/SiGe MQWs with Ge-rich barriers [5,6]. Strain effects in the structure have been taken into account by means of elasticity theory and scaling the tight-binding hopping parameters according to the modified interatomic distances. Alloying in the barrier region was described by the virtual-crystal approximation.

To interpret the near-gap absorption, we show in the inset of Fig. 2 the band-edge profiles at the Γ and *L* points and the confined states obtained from the diagonalization of the multilayer Hamiltonian. The arrows in Fig. 2 indicate the calculated transition energies between QW states at Γ, without excitonic effects. The peaks in the transmission spectra can thus be attributed to dipole allowed HH*n*-cΓ*n*, LH*n*-cΓ*n*, and SO*n*-cΓ*n* transitions. Here, HH*n*, LH*n*, and SO*n* indicate heavy- and light-hole and split-off valence states at Γ, respectively, and cΓ*n* indicate conduction states at Γ. All of them are confined in the Ge region with a type-I band-edge profile. In the transmission spectra, no clear evidence was found of the expected indirect transitions at lower energies between confined hole states at Γ and conduction-band states at the *L* point.

We have also performed numerical investigations of the confined Stark effect in strained Ge quantum wells separated by Si $_{0.15}$ Ge $_{0.85}$ barriers [7]. Our simulations (see Fig. 3) support the experimental results of Kuo *et al.* (Nature 437, 1334 (2005)) that this effect is robust even in group IV heterostructures involving Ge QWs provided that direct transitions at Γ are exploited. Excitonic effects below and above the interband threshold are also included in our calculations.

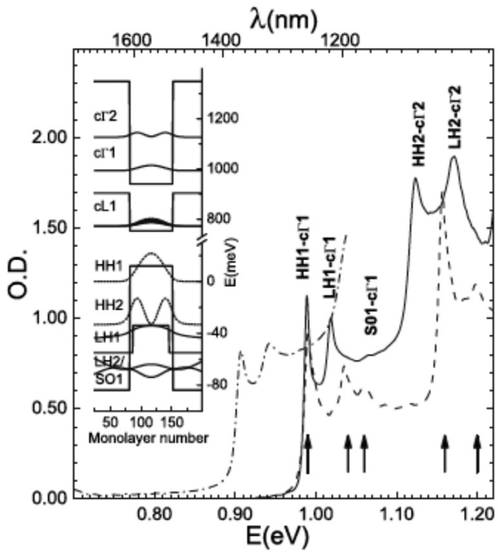

Fig. 2
Transmission spectra of Ge/ Si0.18Ge0.82 200 period MQW sample measured at 300 K (dashed-dotted line) and at 2 K (full line). The dashed line is the calculated low-temperature absorption spectrum. The arrows indicate the calculated transition energy between the QW states. In the inset the conduction and valence edge profiles and the square modulus of the wave functions of the electron- and hole-confined states are shown.

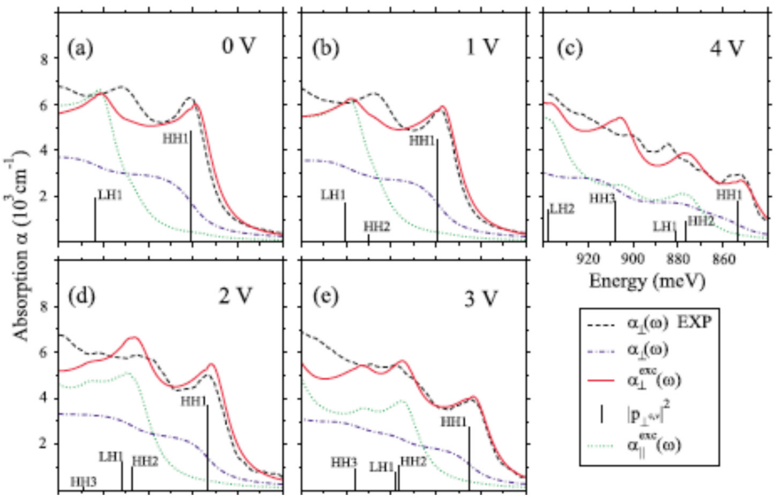

Fig. 3.
Experimental and theoretical near gap absorption spectra at room temperature under different bias voltages. For normal incidence, we report experimental data (black dashed lines), numerical absorption evaluated with (red solid line) and without (blue dot-dashed line) excitonic contributions, and square modulus of the optical matrix elements (vertical bars). The label on the vertical bars indicates the starting state of the transition; the final state is cΓ1. The absorption excitonic spectrum evaluated for parallel incident radiation is also reported (green dotted line).

References

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