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Optical properties of potential-inserted quantum wells in the near infrared and Terahertz ranges

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ABSTRACT

We propose an engineering of the optical properties of GaAs/AlGaAs quantum wells using AlAs and InAs monolayer insertions. A quantitative study of the effects of the monolayer position and the well thickness on the interband and intersubband transitions, based on the extended-basis $sp^3d^5s^*$ tight-binding model, is presented. The effect of insertion on the interband transitions is compared with existing experimental data. As for intersubband transitions, we show that in a GaAs/AlGaAs quantum well including two AlAs and one InAs insertions, a three level $\{e_1, e_2, e_3\}$ system where the transition energy $e_3 - e_2$ is lower and the transition energy $e_2 - e_1$ larger than the longitudinal optical phonon energy (36 meV) can be engineered together with a $e_3 - e_2$ transition energy widely tunable through the TeraHertz range.

1. Introduction

Semiconductor quantum wells (QW) are the building blocks of a large number of opto-electronic devices. Interband transitions in QWs have been used in devices such QW lasers, modulators and detectors while intersubband (ISB) transitions have allowed engineering of quantum cascade lasers and QW infrared photodetectors [1]. Due to unlimited choice in terms of width and material combinations, these structures can be used in opto-electronic applications covering a wide spectral range. Moreover, different techniques to tune the opto-electronic properties of QWs have been proposed such as strain engineering [2], doping [3,4], or monolayer insertion [5–7]. The latter have been used successfully for tailoring the interband transitions and their Stark shift in electro-absorption modulators [8] by simply changing the position of the insertion within the well.

More recently, strong effort has been devoted to extending the range of ISB applications to the terahertz (THz) range [9]. Although asymmetric semiconductor QW structures can be used as laser sources of controllable THz radiation, whatever the active region design, intrinsic non-radiative recombination processes are generally faster than the radiative lifetime of excited states, which hinders the population inversion between subbands [10]. QWs based on GaAs and AlAs are particularly interesting for intersubband applications thanks to the close lattice constants which guarantees small epitaxial stress and allows the thick epilayers needed in QCL devices. In existing THz QCLs, the lifetime of the lower laser state is determined by the tunneling electron extraction time into the collector/injector and do not display a strong temperature dependence. Conversely, the lifetime of the upper laser state strongly increases when increasing the temperature. This is a major limitation, preventing these QCLs from lasing at high temperature [11–14]. The design of new active region where the lifetime of both upper and lower laser states have the same temperature dependency would represent an important step toward THz laser device operating at room temperature.

For a quantitative modeling of such structures, different approaches may be considered. First principle calculations cannot be used, due to the large size of relevant systems (several hundred atom supercells) and their limited precision for excited states representation. Conversely, empirical-parameter models, such as the **k.p** or envelope-function theory (EFT)[15,16] or atomistic approaches like the empirical pseudopotential [17] and tight-

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binding (TB) methods, are suitable for this purpose. While EFT is still the most widely used technique, its applicability to the sub-nm scale (like monolayer insertions) is questionable. Conversely, atomistic approaches have no methodological limitation in handling the case of ultrathin layers and chemical discontinuities. In particular, the TB method and its extended basis $sp^3d^5s^*$ model have been shown to provide a description of the band structure with sub-meV precision throughout the Brillouin zone of the binary semiconductors as well as their heterostructures [18,19].

In this work, we present a quantitative study of the effects of an inserted AlAs monolayer on the interband and intersubband transitions in a GaAs/GaAlAs QW. The results for interband transitions are compared to existing experimental data. A large tunability of transition energies and dipole moments between electron subbands are demonstrated in the THz window as function of the insert position. We also show that a new functionality, the fast depopulation of intermediate state by LO-phonons in a 3-level scheme can be engineered. The paper is organized as follows: in Section 2, we describe the considered structure and the simulation model. In Sections III and IV, we present and discuss the effects of the insert position on the transition energies and the optical dipole momentum of the interband and intersubband transitions respectively, before we conclude in Section 5.

2. System of interest and methods

In the present study, we consider a (001)-oriented $(GaAs)_n/(AlGaAs)_m$ superlattice structure where n and m are the numbers of the molecular monolayers (ML) of GaAs and GaAlAs respectively. The basic unperturbed structure studied in this work consists in a GaAs well with ~15 nm width (52 ML), alternating with $Al_{0.3}Ga_{0.7}As$ barriers grown on a GaAs (001) substrate. The barrier is thick enough to ensure that the tunnel coupling between adjacent wells be negligible. The alloyed barrier is modeled using virtual crystal approximation (VCA) where the TB parameters of the virtual crystal are arithmetic means of the constituent material parameters weighted to their concentrations. The unperturbed system is characterized by the D_{2d} point group symmetry and interband transitions obey a parity selection rule with a largely dominant $\delta n = 0$ contribution. Unless perfectly centered, the AlAs monolayer insertion reduces the symmetry level to C_{2v} and breaks the parity selection rule. When the well contains an even number of monolayers, this holds for any position of the insert since the latter will always be surrounded by GaAs layers of slightly different thicknesses, e.g. at best 26 ML and 25 ML respectively for a 52 ML QW. Conversely, for a QW with odd ML number, the insert can be perfectly centered and in this particular case the potential inserted QW retains the D_{2d} point group symmetry. Finally, it is noteworthy that in addition to breaking the parity selection rule, C_{2v} symmetry allows for in-plane optical polarization anisotropy, that is particularly visible in the narrow spectral range between the e_1-hh_1 and e_1-lh_1 transitions [20,21].

The electronic structure of the superlattices is computed using the extended basis $sp^3d^5s^*$ TB model based on Jancu et al. parameters [18]. This parametrization has shown to allow excellent full-band representation of bulk semiconductors and a good transferability to quantum heterostructures [18,19]. The supercell is built by translating the standard cubic zinc-blende cell in the z direction. Each cubic cell contains two molecular ML. So, for a $(GaAs)_n/(AlGaAs)_m$ superlattice structure we have $(n+m)/2$ cubic cells containing eight atoms each. In the spds* TB model, each atom contributes with twenty orbitals, so the system is represented by a $80(n+m) \times 80(n+m)$ Hamiltonian matrix. For each atom, the 20×20 intra-atomic Hamiltonian matrix is an average of the intra-atomic Hamiltonians in the up to four bulk compounds it composes with its four nearest neighbors. The lattice mismatch between AlAs and GaAs is neglected. However, in the case of InAs insertions, a relaxation of the structure is performed using Keating valence force field (VFF) model [22]. Modeling of a single InAs ML in a GaAs matrix compares satisfactorily with experiments [23,24]. We used a GaAs/AlAs and InAs/GaAs valence band offsets (VBOs) of 0.56 eV and 0.4 eV respectively. In order to calculate the optical properties of the superlattices, we have coupled the TB Hamiltonian to an electromagnetic field, following the approach described in Refs. [25]. This coupling model produces bulk semiconductor dielectric function in good agreement with experimental results and accurately accounts for QW optical absorption spectra, in particular interface-induced optical anisotropy [26].

3. Interband transitions

We firstly focus on the interband transitions energies and the corresponding dipole matrix elements. Calculations of electronic band structure of the systems described in the previous section are performed with varying the AlAs monolayer position from the left barrier to the center of the well. Fig. 1 shows the optical transitions energies calculated using our tight binding model, compared with envelope function approximation (EFA) and experimental data [5,6] obtained from low temperature photoluminescence, excitation and photo-reflectance spectra. The transition energies were calculated at the center of the Brillouin zone (Γ-point) and labelled according to the dominant bulk-state component of initial and final states: conduction (e), heavy-hole (hh) and light-hole (lh). As can be seen from Fig. 1, the TB calculation agrees with experiment within experimental uncertainties. In particular, the predicted reduction of the hh1–lh1 splitting for an insert at the mid-well is clearly observed in PLE data of Ref. [5]. The EFA results [6] are also given in the figure for comparison. Despite the still reasonable agreement of these results with experience, one should keep in mind that there is no theoretical ground for modeling an AlAs ML insertion by 3 Å of bulk AlAs material, using standard EFT continuity relations. It can be observed that the blueshift of the e_1-hh_1 and e_1-lh_1 transitions is maximal when the ML is localized at mid-well (~7.5 nm or 26 MLs). In contrast, the maxima of the e_2-hh_2 and e_2-lh_2 transitions occur when the insert is located at about the quarter of the well (~3.75 nm). A qualitative explanation of these observations can be obtained from a first-order perturbation approach where the insert act as a delta-like repulsive perturbation on the original QW states. Indeed, as it can be seen on the Fig. 2(a), the largest amplitudes of the unperturbed e_1, lh_1 and hh_1 ground-state wave functions are located at the mid-well, whereas the maxima corresponding to e_2 and hh_2 are located at the quarter

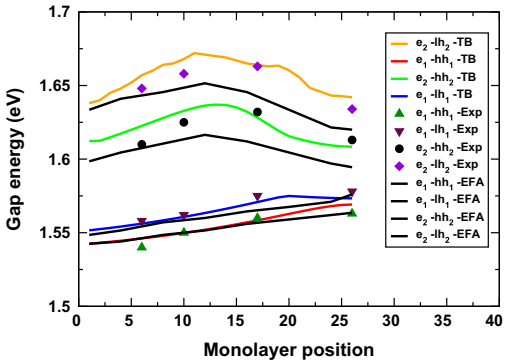

Fig. 1. (Color online) Interband energy transitions of a ~15 nm-thick GaAs/GaAlAs multiple quantum wells as a function of the position of the AlAs monolayer from the barrier (in MLs).