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Confined electron states in corrugated GaAs/AlAs superlattices

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ABSTRACT: The electronic and optical properties of GaAs/AlAs superlattices grown in the [311] direction are investigated in the framework of an empirical tight-binding model which includes second-neighbor interactions. The [311] superlattices are of great interest because of their non-flat interfaces and because the periodic corrugation which appears gives rise to a lateral confinement. This results in the formation of quantum wires which present a pronounced degree of optical anisotropy. The characteristics and the energy gap value of these wires are studied as functions of the layer thickness and the differences with [001]-grown superlattices are discussed. The calculated cross-over of \( \Gamma \)- and \( X \)-like levels is in good agreement with the experimental observations. The nature of the lowest conduction states is explained in terms of the symmetry of the superlattice.

The GaAs/AlAs system is now often used in the fabrication of artificially layered semiconductor crystals and the improvement of the epitaxial growth techniques allows the achievement of high-quality superlattices with very short periods. These superlattices have been studied extensively mainly for [100] growth orientation. More recently, synthesis of superlattices grown by molecular beam epitaxy on unusual orientations like [311] have been achieved. Such superlattices are of great interest because, for high enough substrate temperature, the flat (311) surfaces break up into {311} facets with lower surface energy and give rise to lateral confinement leading to the formation of quantum wires for thin semiconductor layers[1]. The existence of double periodicity in the superlattice growth direction [311] as well in the lateral direction [011] leads complex mixing of all the bulk electronic states which are mapped onto the same point of the superlattice Brillouin zone. Further, this configuration must be studied carefully because in GaAl/AlAs superlattices the confinement effect can lower the states originating from the X valleys in AlAs under the \( \Gamma \) states in GaAs when the layer thicknesses become sufficiently small.

In this paper, we determine the electronic structure of corrugated GaAl/AlAs superlattices. We estimate the effects of the lateral confinement on the electronic states and we clarify the origin of the observed optical transitions. For our calculation, we employ a tight-binding approach. The interest of this method lies in the microscopic description of the materials from the atomic interactions between anions.
and cations. It retains the full symmetry of the crystal and avoids preliminary hypothesis on the origin of the superlattice electronic states. The schematic structure of a corrugated superlattice is shown in figure 1.

**Figure 1:** Structure of [311]-grown corrugated superlattice.

We use a sp$^3$ basis including spin-orbit interaction. As we are mainly interested in the lowest conduction states of the corrugated superlattice, it is important to fit the lowest conduction states of the bulk materials at high symmetry points in the Brillouin zone, e.g. $\Gamma$, $X$ and $L$ conduction edges and their associated effective masses. For this, we have included second-neighbor interactions because neglecting them yields an infinite transverse effective mass in $X$. The valence-band offset has been taken equal to 35% of the direct band gap difference between AlAs and GaAs. The tight-binding parameters are affected near the interfaces and various geometrical situations occur in corrugated superlattices. These different configurations have been taken into account by the utilisation of mean values of the two bulk parameters. As the very short-period superlattices are not concerned by this work, the electronic band structure is not sensitive to this hypothesis. The slight mismatch (0.16 %) between the lattice constant of AlAs and GaAs is neglected. The unit cell of corrugated superlattices is two-dimensional and the tight-binding basis is very large containing 320N local orbitals for a superlattice of N layers along the growth direction [311]. The electronic energies are computed by direct diagonalization or by alternative methods as the orthogonalized-moment method which are more adapted to handle large dimensional matrices. Figure 2 shows the two lowest conduction states at the center of the Brillouin zone of the superlattice $\Gamma$ as a function of the number N of layers of each semiconductor in (GaAs)$_N$(AlAs)$_N$ corrugated superlattices. The solid line denotes the state having mainly a $\Gamma$-like character and the dashed line the state having a $X$-like character. The identification of these states results from the examination of their wavefunctions. The $\Gamma$ state is mainly formed by the contribution of the s atomic orbitals of the cation in GaAs layers and is identified as coming from the $\Gamma$ GaAs bulk eigenstate. On the other part, the major contribution to $X$ state is due to the p orbitals of cations in the AlAs layers. The weight of px and py orbitals is insignificant and this state corresponds to the $X$, valley of AlAs. This analysis is confirmed by the behaviour of these states as a function of the layer number.
Figure 2: Energy variation of the two lowest conduction bands as a function of the number of layers N for (GaAs)$_N$(AlAs)$_N$ corrugated superlattices. The energies are measured from the top of the valence band in bulk GaAs.

As the $\Gamma$ effective mass is smaller than the longitudinal effective mass at X, the $\Gamma$ level decreases in energy more rapidly than the X level as N increases. $\Gamma$-X crossing occurs for $N=19$ which corresponds to GaAs and AlAs layer thicknesses of about 32 Å. Moreover it can be noted that the space group of [311] superlattices $C_s$ has two irreducible representations. This allows the mixing of bulk states and each superlattice eigenstate is formed by some bulk eigenstates. However, this mixing is generally weak and the levels retain the greatest part of their primitive character except near quasi-degeneracy domains. The two upper valence states are localized in the GaAs layers and their localization is similar to that obtained in [100] superlattices taking into account the anisotropy of the hole effective masses. However, they result from a strong mixing of the bulk states and show a pronounced degree of in-plane anisotropy.

This situation can be analysed in the framework of the envelope function approximation. The strong anisotropy of the effective mass tensor at X leads to a splitting of the energy levels associated with these minima. The confinement energy must be calculated using the masses along the directions where the periodicity exists. The $X_y$ and $X_z$ valleys have a transverse character both in the two [311] and [011] directions. They give rise to energy states higher in energy than the $X_x$ valley which is pure transverse in [011] and in greatest part longitudinal in [311] direction.

It is interesting to compare our results on corrugated superlattices with data on superlattices grown in other directions. The most common direction is the [100] direction. There are many similarities between these two orientations. In [100]-grown structures, for widths less than about 35 Å, the lowest $\Gamma$ state is localized in GaAs and lies at an energy above the X state localized in AlAs. This X state originates from the longitudinal part of the $X_x$ valley like in corrugated superlattices. A type-II superlattice results. However the corresponding levels are less sensitive to the superlattice period because of the larger effective mass in [100] direction than in [311] one.

Photoluminescence and photoluminescence excitation measurements have been performed on some [311] corrugated superlattices[1]. For short period superlattices with
layer thicknesses less than 25 Å, the photoluminescence spectra reveal a strong phonon line and phonon sidebands. These features are characteristic of the conduction band minimum originating from the $X_X$ valley in AlAs layers. High-pressure measurements on several superlattices confirm the nature of the conduction states\textsuperscript{[4]}. The $\Gamma$ state exhibits a large blue-shift to be compared to a weaker red-shift for states related to the AlAs $X$ point. Samples with widths above 43 Å corresponding to $N \geq 25$ show a type-I band structure. Our tight-binding results give the type I to type II transition at 32 Å in good agreement with these experimental results.

Strong modifications of the excitonic properties have been observed in [311] corrugated superlattices\textsuperscript{[5]}. This can be explained by the large in-plane anisotropy of the corresponding valence band states which modifies the strengths of the optical transitions and by the lateral confinement which plays an important role in determining the optical properties.

From our tight-binding calculation, we make the following predictions for corrugated superlattices. For short period superlattices with $N < 19$, the lowest conduction state originates from the $X_X$ valleys and electrons in this ground state are localized in AlAs while the holes are in the GaAs layers. Electrons and holes are then separated in real space and the corresponding optical transition will be only weakly allowed. For $N > 19$, electrons and holes are localized in GaAs and the corrugated superlattices are of the type I. At the opposite of the [100] superlattices, an in-plane anisotropy of the hole states exists which explains the optical anisotropy.

References: