Optical anisotropy of (311) superlattices

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(Received 25 January 1994)

We report a calculation of the electronic properties of GaAs/AlAs (311) superlattices through the Brillouin zone using realistic values of the parameters in a tight-binding Hamiltonian. The nature and the localization of the lowest conduction bands for these low-symmetry structures is investigated and its origin is studied with respect to the layer number. A direct-gap–to–indirect-gap transition is evidenced for $L=3$ nm which is equal to the thickness for which the crossing of Γ-X states occurs in the (100) superlattices. The in-plane anisotropy of the optical transitions and the relative intensity is found to be dependent on both the layer number and the nature of the states involved in the transition. Comparison with available experimental data is quite satisfactory.

The GaAs-(Ga,Al)As superlattices are among the most widely studied microstructures because of their relatively easy growth means of molecular-beam epitaxy and also in view of their technological applications. These heterostructures exhibit two-dimensional confinement and have been used to realize high-performance optical devices. Most of these studies concern the (100)-oriented structures since high-quality epitaxial growth is usually achieved for this orientation. Some interest has been recently focused on the growth along other crystallographic directions and ($11N$)-oriented structures obtained by molecular-beam epitaxy have shown good crystallographic quality.[1] The optical properties of ($11N$) structures are anisotropic, except for (100)- and (111)-oriented quantum wells or superlattices. On the other hand, GaAs/AlAs superlattices are an interesting subject of investigation because of the nature of the lowest conduction band. For thin enough AlAs layers, the X-like states, mainly localized in AlAs, lie at lower energy than the states built from the Γ state of GaAs and type-II superlattice results.[2–7] Moreover, the state degeneracy at the X point is split by the anisotropy of the effective masses and the $X_z(X_{x,y})$ states associated with the longitudinal (transverse) effective mass are not contributing in the same manner to the formation of the superlattice conduction bands. Also, the bonding configuration at the interfaces of the (311) heterostructures is unique and presents interesting properties as compared with (100)- and (111)-oriented systems.[8] The interfaces are nonpolar and are the only one vicinal surfaces with an equal number of step and terrace atoms. Moreover, by using molecular-beam epitaxy at high enough substrate temperature, the flat (311) surfaces break up into facets with lower surface energy and lead to the formation of quantum wires by periodic lateral corrugation of interfaces.[9] Experimental studies on (311) quantum wells and superlattices are not as numerous as on (100) orientation and only some optical studies[10–13] have been carried out on these structures. On the theoretical side, the only study[14] of the electronic structure of (311) superlattices is limited to the zone center which cannot allow to determine the nature of the gap. Moreover, in this work, the parametrization of the Hamiltonian give greatly overestimated values of the Γ and X conduction-band effective masses and reduces the confinement of the superlattice electronic states. We present a quantitative study of the electronic structure of (311)-GaAs/AlAs superlattices over the whole Brillouin zone to investigate the nature of the lowest conduction band and determine whether the superlattices are indirect or direct band-gap materials. We also address the differences with (100) superlattices. The optical properties of these heterostructures are investigated and the oscillator strengths of more important transitions present an in-plane anisotropy.

To describe the bulk crystals, we use a tight-binding approach. The interest of this method lies in the microscopic description of the materials from the interactions between anions and cations which retains the full symmetry of the crystal. We use a sp^3s^* basis[15] including spin-orbit interactions. We have fitted the Hamiltonian matrix elements to get the best possible values for the energies and effective masses at Γ and X points in the manner described in Ref. 16. To obtain some dispersion for bulk electronic bands along the X-W symmetry line we have included second-nearest-neighbor interactions between the cation and anion p orbitals. Table I shows the band energies and effective masses determined from our tight-binding parameters. The valence-band discontinuity between GaAs and AlAs is taken to be 35% of the direct-band-gap difference. The effects of the small lattice mismatch between GaAs and AlAs are neglected because

TABLE I. Band energies (in eV) and effective masses (in unit of electron mass) calculated from our tight-binding parameters.

	GaAs	AlAs
Γ_{8v}	0.0	0.0
X_{7v}	−2.908	−2.543
Γ_{6c}	1.519	3.13
X_{6c}	1.986	2.229
$m_c(\Gamma)$	0.066	0.150
$m_{\mathrm{LH}}(\Gamma)$	0.080	0.133
$m_{\mathrm{HH}}(\Gamma)$	0.323	0.406
$m_l(X)$	1.21	1.31
$m_t(X)$	0.287	0.276

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they are not important for the considered superlattices. Figure 1 shows the electronic band structure near the gap for the $(GaAs)_{13}/(AlAs)_{13}$ (311) superlattice consisting of 2.2-nm-wide layers. The minimum of the conduction band occurs at the point $\bar{Y}$ which limits the Brillouin zone along the $[-2,3,3]$ direction. This point depends on N, it is not equivalent to a high-symmetry point of the fcc Brillouin zone but it lies near the point $X=(2\pi/a)(\bar{1}00)$ of this zone. The $\bar{Y}$ state is practically degenerate with the X minimum and has a lower energy than the Γ subband, leading to an indirect-gap superlattice with the extreme of the valence and the conduction bands situated at two different points of the superlattice Brillouin zone. The spin-orbit splitting due the lack of the inversion symmetry is not visible on the figure because of its small value and all the bands are quasidegenerate. The more important splitting arises at the $\bar{Y}$ point where the two spin components of the highest valence band are separated by 7 meV. The dispersion along the growth direction is small both for the conduction and the valence band. The valence bands present a large in-plane anisotropy and the dispersion along the two directions $[0,1,-1]\bar{\Gamma}-\bar{X}$ and $[-2,3,3]\bar{\Gamma}-\bar{Y}$ are very different.

Figure 2 shows the variation of the lowest energy states at the $\bar{\Gamma}$ and $\bar{Y}$ points with respect to the layer number. As expected, the two $\bar{\Gamma}$ conduction-state energies decrease when N increases but unlike the (100) superlattices, there are no crossing between the bands. These two states are confined within the GaAs layers. The $\bar{\Gamma}_{1c}$ state has no node and the $\bar{\Gamma}_{2c}$ state, which results from mixing of s and p Bloch functions allowed by the low symmetry of the (311) direction, has one node. To better understand the (311) electronic band structure, we have given

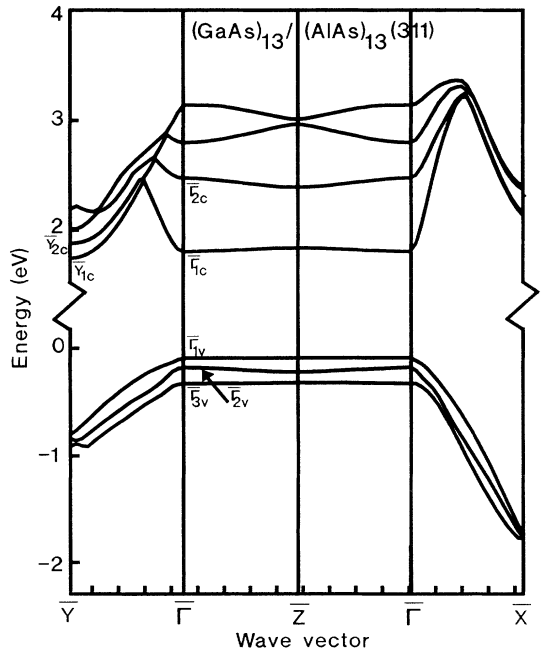

FIG. 1. Electronic band structure of $(GaAs_{13}/(AlAs)_{13}$ (311) superlattice along the directions $(01\bar{1})\bar{\Gamma}-\bar{X}$, $(233)\bar{\Gamma}-\bar{Y}$, and $(311)\bar{\Gamma}-\bar{Z}$.

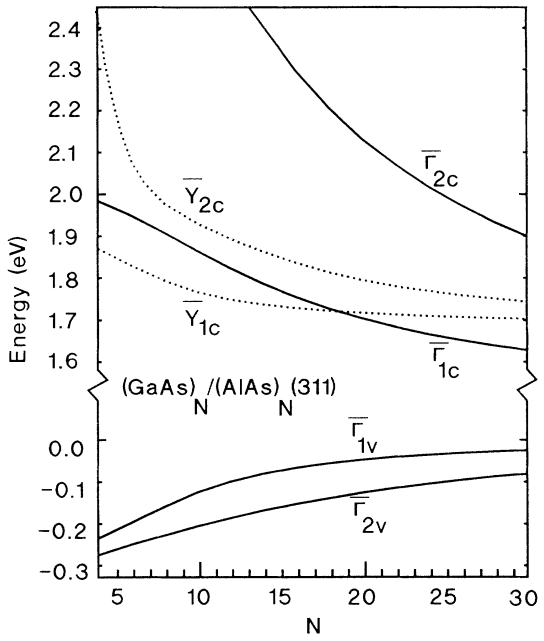

FIG. 2. Dependence of the two lowest-energy conduction states at $\bar{Y}$ and $\bar{\Gamma}$ points, upon the number of the layers N for $(GaAs)_N/(AlAs)_N$ (311) superlattices.

in Fig. 2, the variation with respect to the layer number of the two first conduction states at $\bar{Y}$ point. These states are localized in AlAs, the lowest state $\bar{Y}_{1c}$ is degenerate with $\bar{\Gamma}_{1c}$ for $N=18$ which corresponds to 3-nm-wide layers. For thicker layers, the (311) superlattice gap is direct in the **k** space and electrons and holes are localized in GaAs layers. This deeply changes the characteristics of the optical properties, in particular, a large increasing of the optical efficiency must be observed.

The thickness of each semiconductor slab in GaAs/AlAs (311) superlattices with N layers is the same as in GaAs/AlAs (100) superlattices with $N'=(2/\sqrt{11})N$ layers and it is interesting to compare the characteristics of the two systems in order to analyze the influence of the growth direction on the electronic properties of superlattices of same thicknesses. We have calculated the variation of the electronic states at Γ for $(GaAs)_N/(AlAs)_N$ (100) superlattices as a function of the layer number. The two lowest states are essentially X- and Γ-like and anticrosses at about $N=11$ (3 nm). This value is in excellent agreement with the expected thickness of a type-I–type-II superlattice transition[17,18] showing the ability of our parametrization to give an adequate description of the superlattices. This anticrossing arises to the same thickness as the indirect-direct transition of (311) superlattices and brings out some similarities between the two sorts of superlattices. For $L<3$ nm, the X-like state confined in AlAs layers lies lower than the Γ-like state localized in GaAs layers. For (311) superlattices, the gap is indirect while for (100) superlattices, the X-like state is folded on the center of the Brillouin zone of the superlattice, the gap is "pseudodirect," i.e., direct in **k** space between states localized in two different layers. For $L>3$

nm, the gap is direct whatever the growth direction of the superlattices. This situation leads to infer that the transition towards type-I superlattices is mainly dependent on the layer thickness regardless of the growth direction which only determines the nature pseudodirect or indirect of the superlattice gap below the transition. We have investigated the valence states at Γ point for $(GaAs)_{13}/(AlAs)_{13}$ (311) superlattices. The highest energy state $\bar{\Gamma}_{1v}$ has a predominant heavy-hole character, its energy is 18 meV higher than in the same thickness (100) superlattice. However, the difference is much less important than for the (111) direction where the mass anisotropy is maximum. The second state $\bar{\Gamma}_{2v}$ has a strong light-hole character and is not sensitive to the growth axis orientation because of the isotropy of the light-hole effective mass. There is only a difference of 4 meV between the $\bar{\Gamma}_{2v}$ state energies for the (311) and (110) directions.

We have calculated the optical properties of two superlattices with different thicknesses so that they have gaps of different sorts. The first one is the $(GaAs)_{13}/(AlAs)_{13}$ (311) superlattice which is a gap indirect superlattice with a $\bar{Y}$ state lower than the conduction band minima at Γ, the second is the $(GaAs)_{26}/(AlAs)_{26}$ (311) superlattice with a direct gap at the zone center. The interband transition probabilities when the light is polarized along the two directions $[-2,3,3]$ and $[0,1,01]$ are shown in Fig. 3. The three lowest transitions in energy appearing in the calculated spectra originate from the upper valence bands which have, respectively, a heavy-hole, light-hole, and split-off dominant character while the final state is always the lowest-lying Γ conduction band. The fourth transition takes place between the second heavy-hole-like state and the second conduction band, which both have an odd parity. The features of the two superlattices are similar. The relative intensity of the two main polarization orientations is defined by

$$\rho=\frac{I_{0\bar{1}1}}{I_{\bar{2}33}}\ .$$

We can observe that for one given transition, it is always the same polarization orientation which has the larger intensity. For the two transitions $\bar{\Gamma}_{1v}-\bar{\Gamma}_{1c}$ and $\bar{\Gamma}_{3v}-\bar{\Gamma}_{2c}$, which originate from the heavy-hole-like states, the transition probability for light polarized along the $[-2,3,3]$ direction is always larger than for the $[0,-1,1]$ one. The opposite situation occurs for the second and the third transitions for which the initial valence state is, respectively, light-hole- and split-off-like. The anisotropy of the optical absorption varies with respect to the layer number. Our results reveal an increase in the relative intensity for the transitions from the heavy-hole-like states when the layer thickness increases. For $N=13$, we get $\rho(\bar{\Gamma}_{1v}-\bar{\Gamma}_{1x})=0.82$ and $\rho(\bar{\Gamma}_{3v}-\bar{\Gamma}_{2c})=0.58$. For $N=26$, the relative intensity rises to 0.89 and 0.74 and the anisotropy is reduced. The relative intensity of the two polarizations for transitions involving the light-hole- and split-off-like states also depends on the layer thickness but its variation is in the opposite way the values decreasing from $\rho(\bar{\Gamma}_{2v}-\bar{\Gamma}_{1c})=1.34$ and $\rho(\bar{\Gamma}_{4v}-\bar{\Gamma}_{1c})=1.3$ for $N=13$ to $\rho(\bar{\Gamma}_{2v}-\bar{\Gamma}_{1c})=1.20$ and $\rho(\bar{\Gamma}_{6v}-\bar{\Gamma}_{1c})=0.99$ for $N=26$. The significant result is that the optical anisotropy is reduced when the superlattice layers become wider whatever the nature of the electronic states involved in the transitions. This effect is more pronounced for the high-energy transitions for which the optical anisotropy might be used as an indication of the thickness of the layers. Recently, piezoreflectance experiments have been performed on GaAs/AlAs (311) superlattices grown by atomic layer molecular-beam epitaxy.[13] These measurements of the in-plane optical anisotropy of transitions have been realized on long-period samples which are, in fact, quantum wells. They show that the transitions involving the heavy (light- and split-off) -like hole are more polarized along the $[-2,3,3]$ ($[0,-1,1]$) direction and that the relative intensity ρ increases (decreases) as the thickness of the GaAs layer decreases. Our results are in agreement with these experiments and show that this trend observed for long-period samples persists for smaller period superlattices when tunneling through the AlAs barriers is present.

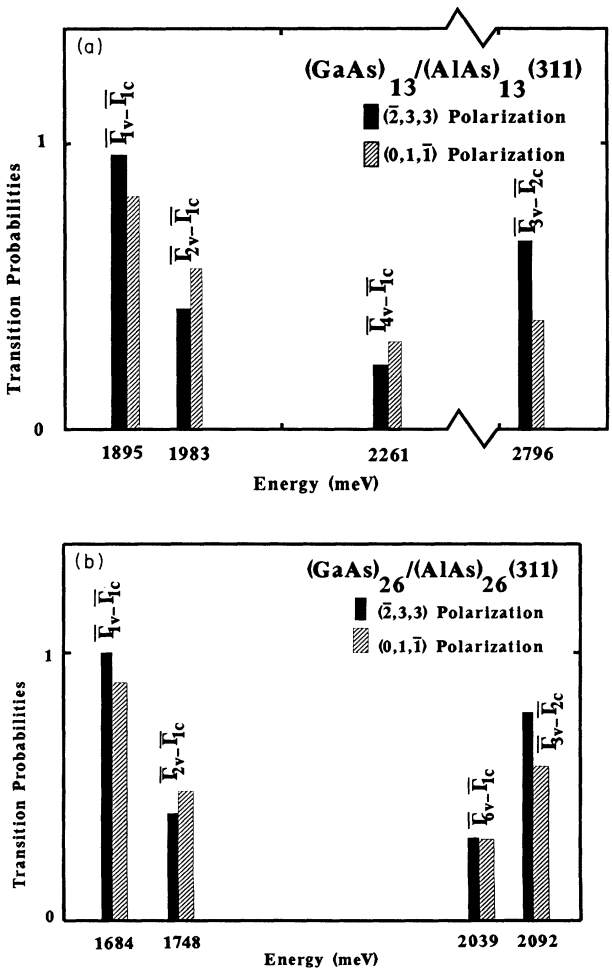

FIG. 3. Transition probabilities (in arbitrary units) between the valence states $\bar{\Gamma}_{1v}$ and the conduction states $\bar{\Gamma}_{jc}$ for two $(GaAs)_N/(AlAs)_N$ (311) superlattices (a) $N=13$ and (b) $N=26$ in the two polarization directions $[-2,3,3]$ and $[0-1,1]$.

In summary, we have studied the nature of the electronic band structure in GaAs/AlAs (311) superlattices using a tight-binding model with realistic parameters determined from the bulk bands. We have brought to fore that for $N < 18$, the (311) superlattices have an indirect gap in **k** space between the lowest conduction band situated at the zone boundary $\bar{Y}$ and $\bar{\Gamma}$ valence maximum which is mainly heavy-hole-like. These two states are localized in different layers, electrons in GaAs and holes in AlAs so that their overlap is weak. The gap is direct for $N > 18$. This change in the gap nature arises for the same layer thickness $L = 3$ nm than the type-I–type-II transition in (100) superlattices. The lower symmetry of the quantum confinement direction results in an optical transition in-plane polarization anisotropy which varies with the valence state involved in the transition and with the layer thickness. The calculated values of the relative intensity are in good agreement with the optical measurements of the anisotropy of large period samples.

The Group d'Etude des Semiconducteurs is "Unité Associée au Centre National de la Recherche Scientifique No. 357. We thank the "Centre de Compétences en Calcul Numérique Intensif de Centre National Universitaire Sud de Calcul de Montpellier" for financial support for the vector computation.

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