(InAs)$_n$/(GaSb)$_m$ superlattices: Band gaps and band edges

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The band edges and band gaps of InAs$_n$/GaSb$_m$ $n,m=1,20$ superlattices have been theoretically studied through the plane-wave empirical pseudopotential method for different situations: i different substrates, GaSb and InAs; ii different point group symmetries, C_{2v} and D_{2d}; and iii different growth directions, 001 and 110. We find that a the band gaps for the 001 C_{2v} superlattices on a GaSb substrate exhibit a nonmonotonic behavior as a function of the GaSb barrier thickness when the number of InAs 001 $C2$

~150 meV below the GaSb valence band maximum.[2] For short-period $InAs_n/GaSb_m$ superlattices, quantum confinement pushes up the electron level,

computational cost. In these methods, the wave functions of the system are expanded in a basis set built from only Γ-like Bloch functions of the parent bulk materials.[34,35] If the basis set is complete all bands the method would be in principle exact provided that interface related features are correctly taken into account .[36] In practice . ·¸ EFA calculations employ a small basis set, with the most common approximations involving just the bands at the top of the valence band the 6×6 . ·¸ model , or including additionally the states at the bottom of the conduction band the 8×8 model . The incompleteness of the truncated basis set is then mitigated by adjusting the model parameters to match the available experimental data. This procedu0ooductam00Gk-359.4(rweltam00G4efo.8(TD[)49(w3(m00G4efo.8(TDIesntal)359.-49(w93djuw)49(w93djuqu

atomic pseudopotentials are described through a strain-dependent continuous analytic function of momentum , whose parameters are adjusted to reproduce calculated and measured[58] properties of the four binaries InAs, InSb, GaAs, and GaSb and their possible ternary or pseudobinary compounds.[1,23] The target properties are the band gaps; the eigenvalues at the L, X, and Γ points; the effective masses; the deformation potentials; the spin-orbit splitting; and the valence band offsets. The multiplying factor β in Eq. 1 is a scaling parameter for the kinetic energy that recovers, to a first order approximation, the contributions due to the self-energy.[59] The expression of the strain-dependent screened atomic pseudopotential is given by[45]

$$v_\alpha\, q,\epsilon\, = v_\alpha\, q,0\, 1 + \gamma_\alpha\, \mathrm{Tr}\, \epsilon\, , \qquad 4$$

where γ_α is a strain related parameter and Tr ϵ is the trace of the strain tensor, ϵ, calculated through the VFF method.

The wave functions ψ_i in Eq. 2 are expanded in terms of plane waves, with a cutoff energy of 5 Ry determined at the stage when the pseudopotential V_{ps} is generated . The diagonalization of the Hamiltonian in Eq. 1 is performed via the folded spectrum method,[60] in which the Schrödinger equation is transformed into a quadratic form, according to

$$\hat{H} - \epsilon_{ref}\,^2 \psi_i = \epsilon - \epsilon_{ref}\,^2 \psi_i, \qquad 5$$

and the problem is solved for a chosen number of eigenvalues that are the closest, in absolute values, to the given reference energy, ϵ_{ref}. Thus, once one is interested in the eigen-

barrier layers is smaller than the corresponding CBM variation for thin InAs$_n$ $n<5$ layers. Consequently, the variation of the band gap is governed by the variation in the CBM, which increases monotonically for increasing number of GaSb layers. This blueshift has already been observed experimentally[11] and is in agreement with previous theoretical calculations.[22,24]

ii *Isolated holes: Thick InAs layers*. In this case the gap shows a decreasing behavior for thin

the increasing thickness of the InAs wells reduces the interaction between hole levels in neighboring barriers. For narrow GaSb layers, the confinement effect on the hole levels is larger. When the number of GaSb layers increases, the confinement effect reduces its intensity and the hole levels show an upshift. This VBM upshift is larger than the CBM upshift for the same variation of the barrier thickness, which leads to a reduction of the gap value.

2 *Toward an isolated QW regime: Thick GaSb layers*

Figure 3 e shows the following.

i Blueshift of the band gap for increasing GaSb layers. The hole level is practically pinned at the energy of the substrate VBM, since the barrier widths are wide enough. The variation of the gap then follows the CBM variation, and the gap increases with increasing number of GaSb layers, due to the reduction of the electron level repulsion.

ii Redshift of the band gap for increasing InAs layers. The reduction of the confinement effect on the electron levels pushes down the superlattice CBM, reducing the band gap value.

The absolute value of the changes in the CBM and VBM energies as a function of the number of GaSb layers is shown in Fig. 4

GaSb layers, tending to the CBM of the pure strained GaSb bulk material.

ii For thick InAs and thin GaSb layers, the superlattice CBM is lower in energy than the VBM of the strained GaSb bulk: This occurs because of the level repulsion between the electron levels in adjacent wells that shifts down the CBM energy. Also, the VBM of the GaSb strained bulk, on an InAs substrate, increases in energy by 36 meV relatively to the VBM of the freestanding GaSb bulk. These two factors contribute to the superlattice CBM being lower in energy than the VBM of the strained GaSb bulk.

iii For thick GaSb layers, the superlattice VBM tends to the VBM of the strained GaSb bulk: Since the effective mass of the hole levels is relatively higher than the electron effective mass which reduces the changes in the hole level energy due to confinement effects , and since the hole levels are mainly localized in the GaSb barrier region, the increase in the number of GaSb layers leads to the pinning of the superlattice VBM energy at the VBM level of the strained GaSb bulk.

The characteristic behavior of the superlattice's CBM and VBM for these short-period InAs $_n$/ GaSb $_m$ superlattices on InAs and GaSb substrates shows similarities but the eigenvalues are certainly not identical. The differences in the superlattice's CBM and VBM energies, due a/F71T2368.7(he)TJl.3(ue)0.5

of the InAs bulk, being higher in energy on the InAs −5.16 eV than on the GaSb −5.20 eV substrates. By calculating the difference between the CBM level in the InAs bulk and the VBM level in the GaSb bulk materials on both substrates, the band gap in the limit of thick InAs and GaSb layers can be determined. These band gaps are 0.18 and 0.14 eV difference of 0.04 eV for GaSb and InAs substrates, respectively. The same difference calculated for the $\mathrm{InAs}_{20}/\mathrm{GaSb}_{20}$ superlattice gives 0.018 eV, with the GaSb band gap being higher in energy. Hence, as both InAs and GaSb layers in the superlattices turn thicker, larger will be the difference between the band gaps on InAs and GaSb substrates, with the last case presenting larger band gap values.

As seen from Fig. 5 c , the change in the energetic ordering between the band gaps for $\mathrm{InAs}_n/\mathrm{GaSb}_m$ superlattices on the InAs and GaSb substrates occurs at different GaSb thicknesses, for each number of InAs layers. The crossing point changes from $m \simeq 14$ at $n=5$ to $m \simeq 4$ to $n=20$. For $n<5$, the band gaps of the superlattices on an InAs substrate are always higher than those for a GaSb substrate.

T T T C_{2v} D_{2d}

The 001 superlattices with C_{2v} symmetry all have integer numbers of InAs and GaSb monolayers each monolayer consisting of one cation plus one anion atomic layers in the 001 direction In this way, the atomic bonds at adjacent interfaces will alter from In-Sb to Ga-As. On the other hand, $\mathrm{InAs}_n/\mathrm{GaSb}_m$ 001 superlattices with D_{2d} symmetry require that both the InAs and GaSb layers have a half-integer number of monolayers to fulfill the symmetry constraints. For example, a typical D_{2d} 001 superlattice with In-Sb bonds at the interfaces will have the following sequence of atomic planes:

$$\cdots \text{–In-As-In-As-In-Sb-Ga-Sb-Ga-Sb-In-As-In-As-In}\cdots$$

where an odd number of atomic planes is required in each InAs or GaSb layers. A similar pattern would be required for 001 superlattices with D_{2d} point group symmetry and Ga-As bonds at the interfaces.

A.

Figures 6 a –6 f compare the calculated CBM and VBM eigenvalues for $\mathrm{InAs}_n/\mathrm{GaSb}_m$ superlattices grown in the 001 direction with different point group symmetries, D_{2d} and C_{2v}. For the superlattices with D_{2d} symmetry, the bonds at the interfaces are exclusively either In-Sb D_{2d}/In-Sb or Ga-As D_{2d}/Ga-As . A comparison of these figures shows the following.

i The D_{2d} superlattice, with In-Sb bonds at the interfaces, shows a reduced spread in energy of the CBM levels as a function of the InAs thickness, as compared to the C_2

C

the electron and hole levels, the gap not being zero due to the underlying symmetry of the superlattice.

(001) (110)

The characteristic feature of the 110 superlattices is that, differently from the cases discussed so far, their interfaces are nonpolar, presenting both cations and anions in equal proportion at each abrupt interface. All interfaces will show both In-Sb and Ga-As bonds. The interfaces at each side of a given layer can be symmetry related through a mirror plane reflection or by the inversion symmetry operator. When the InAs and GaSb layers are composed by an odd number of atomic planes, the mirror symmetry is fulfilled. On the other hand, for an even number of atomic planes in both InAs and GaSb layers, the inversion symmetry is observed.

The CBM and VBM levels for the 110 InAs $_n$/ GaSb $_m$ superlattices with mirror symmetry, as a function of the number of GaSb layers, are shown on Figs. 3 b and 3 d , respectively, for each InAs $_n$ well width $n=1,20$. The CBM and VBM levels for the 110 InAs $_n$/ GaSb $_m$ superlattices with inversion symmetry are very similar to those shown in Figs. 3 b and 3 d and are not explicitly shown here. However, when differences between the two types of 110 superlattices occur, they are presented in the following discussion. An analysis of these figures reveals the following aspects.

A.

From Figs. 3 b and 3 d , the following is seen.

i The CBM eigenvalues

and 100%, as is the case for the ordered superlattices, where the In/As composition ratio is 1.

In general, the higher band gaps in random alloys, as compared to ordered superlattices, can be traced to the different folding of k points in the irreducible Brillouin zone. The random alloys will have many folded k points, with a weak repulsion among the folded levels. However, the ordered superlattices will have comparatively few folded k

23.1 meV for the $InAs_{26}/GaSb_{15}$ and 4.4 meV for $InAs_{26}/GaSb_{27}$ superlattices. Since the atomic segrega-

GaSb barriers and the InAs wells. For thin InAs $_n$ layers $n<5$, the band gap presents a blueshift with increasing number of GaSb layers. For thick InAs $_n$ $n\geqslant 6$ layers, the band gaps show a nonmonotonic behavior, as a function of the GaSb thickness. For thin GaSb layers the band gaps show a blueshift as a function of the InAs layers. As the GaSb layer thickness is progressively increased, the band gap shows a redshift, passing through a minimum value >0 and finally a blueshift.

The band gap behavior of the 001 C_{2v} superlattices on different substrates, InAs, and GaSb, will depend on the degree of localization of the electron level conduction band maximum . For thin InAs wells, the electron levels will be mostly delocalized along the superlattice, and the influence of the different strain fields on the band gaps will be determined mostly by the behavior of the GaSb layers on strain. The superlattices with thin InAs will present larger band gaps on InAs substrates. As the InAs wells turn thicker, the VBM and CBM levels from the superlattices follow the behavior of the corresponding levels in their parent bulk on strain, leading gradually to smaller band gaps on InAs substrate.

The band gaps of 001 D_{2d} superlattices present different behaviors depending on the type of atomic bonds at the interfaces. The superlattices with In-Sb bonds at the interfaces show reduced band gap values, as compared to the 001 C_{2v} case, due to the pinning of the band edge states by the In-Sb bonds. On the other hand, the D_{2d} superlattices with Ga-As bonds at the interfaces present larger band gaps than both C_{2v} and D_{2d}/In-Sb superlattices.

The superlattices with 110 layer orientation show a reduced variation of the band edge states as a function of both the InAs and GaSb thicknesses, as compared to the 001 C_{2v} case. The band gaps for the 110 superlattices are also smaller than the corresponding values for 001 C_{2v}. An anticrossing between the light and heavy-hole levels occurs for thin GaSb and thick InAs layers.

The comparison of the band edges and band gaps between the superlattices grown on a GaSb substrate and the random alloys lattice matched to a GaSb substrate, with the same In composition, show that the band gaps and CBM VBM values of the random are almost always higher lower than the corresponding values in the superlattices. It gives a direct quantitative indication of the influence of the superlattice's ordering and period on the band gap and band edges. Also, it allows us to compare the degree of localization of the band edge states among the superlattices and between the superlattices and the random alloys.

A comparison between the calculated band gaps for the superlattices with abrupt and interdiffused interfaces with some available experimental data shows that the atomic interdiffusion in the layers close to the interfaces tends to increase the band gap values, with greater influence on superlattices with the shortest periods.

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