Intrinsic interface states in InAs–AlSb heterostructures

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Abstract

We examine the formation of intrinsic interface states bound to the plane of In–Sb chemical bonds at InAs–AlSb interfaces. Careful parameterization of the bulk materials in the frame of the extended-basis $sp^d$s tight-binding model and recent progress in predictions of band offsets severely limit the span of tight-binding parameters describing this system. We find that a heavy-hole-like interface state bound to the plane of In–Sb bonds exists for a large range of values of the InSb–InAs band offset.

Keywords: interface states, tight-binding, quantum well

(Some figures may appear in colour only in the online journal)

1. Introduction

Ever since the seminal paper (Tamm 1933), the possible existence of intrinsic surface or interface states in semiconductors has been a hotly debated issue, and the emerging topic of topological insulators has recently renewed interest in this field (Hasan and Kane 2010), in connection with predicted ‘quantum immunity’ of edge-state currents against scattering. In the early 1980s, the first type of interface state was predicted to occur in HgTe–CdTe heterostructures (Bastard 1982, Chang et al 1985, Schulman and Chang 1986), due to the boundary conditions between the inverted band structure of HgTe and the normal band structure of CdTe. In this case, the existence of interface states is primarily due to anomalous properties of one of the bulk constituents.

Much more recently, attention was drawn to the original situation of interfaces between materials sharing no common atom (NCA), such as InAs–GaSb, InAs–AlSb, BeTe–ZnSe and (InGa)As–InP. In these materials, interfaces involve chemical bonds that do not exist in the host materials, for instance In–Sb or Ga–As in the first example. Such interface bonds can, in principle, act as a local potential well that may capture the carriers. This second type of interface state, if it exists, relies mainly on local interface properties and proper modeling requires detailed atomic-scale information that is normally missed by the standard envelope-function approximation (Bastard 1981, 1988). The existence of interface states in the InAs–AlSb system was first suggested heuristically by Kroemer et al (1992) as a possible explanation for the heavy n-type doping observed in nominally undoped superlattices, but it was soon argued that possible values of band offsets would not allow for an interface state resonant with the conduction band (Dandrea and Duke 1993). Later, this question was revisited using ab initio methods by Shaw et al (1995), Shaw (1998), who found localization of the hole ground state near the plane of In–Sb bonds. However, in the bare density functional theory (DFT) without spin–orbit interaction used in these calculations, InAs and InSb are metals rather than semiconductors (Kim et al 2010), and this makes comparison to experimental results difficult. InAs–AlSb has a type II band line-up with ground electrons (holes) in the InAs (AlSb) layers, and reported values of valence band offset (VBO) in the 100–200 meV range (Kroemer 2001, Vurgaftman et al 2001). In recent years, the InAs–AlSb system has proved its technological importance with the emergence of high performance optoelectronic devices based on intersubband transitions,
Figure 1. Sketch of the arrangement of chemical bonds at a C₁A₁ – C₂A₂ interface grown along the [0 0 1] direction. C and A stand for cation and anion species, respectively.

such as quantum cascade lasers (Teissier et al 2004) in the mid-infrared. A need to better analyze and control interface composition was evidenced (Nicolai et al 2014), as a large strain can accumulate and lead to plastic relaxation when preferential formation of Al–As interface bonds prevails. In addition to recent progress in electron microscopy that allow for chemical and strain analysis with sub-nanometer resolution (Colliex 2011, Nicolai et al 2014), it has become possible to observe directly the wavefunctions of quantum states using scanning tunneling microscopy (Fain et al 2012). Thus, advances in fine material characterization offer a unique opportunity to obtain conclusive experimental proof of the existence of intrinsic interface states. On the modeling side, progress in computing would now allow for ab initio studies combining full atomic relaxation and a realistic electronic structure of narrow gap semiconductors, but there is also room for computationally easier, yet predictive calculations based on empirical-parameter atomistic theories such as advanced empirical tight-binding (ETB) (Jancu et al 1998) or atomistic empirical pseudo-potentials (AEPP) schemes (Zunger 1996, Bester 2009). A sp³ ETB model with first and second neighbor interactions was first used by Theodorou and Tsengas (2000). Later, modeling of InAs–AlSb and ZnSe–BeTe within the sp³ s* tight-binding model was discussed by Ivchenko and Nestoklon (2004). In this early work, in addition to the intrinsic limitation of the sp³ s* model for precision modeling, the effects of a large strain of the interface bonds were not discussed, and simply ‘renormalized’ in the interfacial s–p two-center integrals considered as adjustable parameters. Proper consideration and full modeling of elastic relaxation actually reduces the number of adjustable parameters to a few band offset parameters. The purpose of this paper is to re-examine the particular case of InAs–AlSb quantum wells (QWs) using an advanced tight-binding scheme, integrating recent methodological progress in the treatment of strain, and to delineate the range of parameters for which intrinsic interface states would exist in this system.

In the case of the standard [0 0 1] growth axis, the mere presence of an interface between materials C₁A₁ and C₂A₂ (where A and C stand for anion and cation species) breaks not only the translational invariance but also a rotational degree of freedom, as the four-fold roto-inversion (or S₄) symmetry of the T₄ point group is no longer allowed. The atomic arrangement in the interface cell is shown in figure 1 and shows that at the interface the C₁A₁ bonds lie in the (1 1 0) plane while the A₄C₂ bonds lie in the (1 1 0) plane.

The corresponding point group symmetry is C₄v. For a symmetric QW with equivalent interfaces, an S₄ symmetry operation centered on an atom in the central layer exists and transforms one interface into the other, upgrading overall symmetry to D₄d. Although these features were clearly stated in early publications on tight-binding calculations (Schulman and Chang 1981, 1983, Chang and Schulman 1985, Smith and Mailhiot 1990), it was only in the mid 1990s that the resulting consequences in terms of polarization anisotropy of the optical properties were clearly observed and understood. In particular, methods for curing the native over-symmetry of the classical envelope-function approach have been proposed, following more or less explicitly the theory of invariants (Aleiner and Ivchenko 1992, Krebs and Voisin 1996, Ivchenko et al 1998, Ivchenko and Nestoklon 2004). These methods introduce at least one new interface parameter whose value is in general not provided within the same theory and must be fixed by comparison with experiment or more elaborate calculations, therefore their predictability is limited. From this point of view, NCA interfaces are particularly problematic, because specific interface bonds exist in a single direction, either (1 1 0) or (1 1 0), and generally undergo considerable strain. For instance, in an InAs–AlSb QW, the host materials are nearly lattice matched, but the nominal interfaces, respectively, involve In–Sb bonds that are 6.3% too long, and Al–As bonds that are 7.3% too short. Hence, one has to cope with very large, sharply localized strain, the modeling of which requires special attention. Finally, it is worth mentioning that desired or undesired atom exchange during growth can affect the composition of the interfacial layer, so that NCA QWs can exist with either nominal C₂v symmetry, or with same bonding at both interfaces and D₄d symmetry, or in many intermediate, non-ideal configurations.

2. Model

Since atomic positions are an input of ETB models, the first problem to be solved is the relaxation of atomic positions under the effect of local interface strain. A zeroth order approach consists in extrapolating classical elasticity down to the single layer of chemical bonds, or the molecular layer. Obviously, in order to go beyond this crude approximation, one must use atomistic elasticity such as the valence force field (VFF) model (Keating 1966, Martin 1970). In this model the bond stretching (α) and bond bending (β) force constants are determined from the elastic constants (c₁₁ and c₁₂) as follows:

\[
\begin{align*}
c₁₁ &= (\alpha + 3\beta)a \\
c₁₂ &= (\alpha - \beta)a
\end{align*}
\]  

where a is the lattice constant. Here we use the elastic constants of Vurgaftman et al (2001). For the sake of simplicity, we shall consider that the heterostructure is strained as a whole to maintain an epitaxial relation to a GaSb substrate, but adaptation to the case of a ‘free-standing’ superlattice is straightforward. The VFF model is known to provide atomic positions
in good agreement with experiments for small or intermediate strain values (Steiger et al. 2011), but its validity for the extreme strain situation of InSb and AlAs bonds in InAs–AlSb heterostructures is not completely guaranteed. To check this, we have performed DFT calculations of atomic relaxation using the VASP (Kresse and Furthmüller 1996) and Quantum Espresso (Giannozzi et al. 2009) codes, and found excellent agreement with the present VFF results, within the numerical and methodological limitations of DFT within the local density approximation (LDA). In the classical elasticity limit the distance between atomic planes \( i \) and \( i + 1 \) is given, for each molecular layer, by \( d_{i,i+1} = d_{i,i+1}^{(0)} (1 + 2c_{12}/c_{11}(a_{i+1} - a_i)/a_i) \) where \( a_{i,i+1} \) is the lattice parameter of the pseudo-binary compound corresponding to atomic planes \( i \) and \( i + 1 \) and \( a_i \) is the substrate parameter. \( c_{12} \) and \( c_{11} \) are the corresponding elastic constants. This result is obviously incorrect for an interface sequence such as Sb = In–As since In atom would have two highly strained ‘backward’ bonds Sb = In, and two essentially unstrained ‘forward’ bonds In–As.

Next we need to include equilibrium atomic positions and the related strain effect in the extended-basis spds’ tight-binding formalism (Jancu et al. 1998). For bulk materials, it is widely accepted (Jancu and Voisin 2007, Zielińska 2012) that, in addition to changes in phase factors and power-law scaling of two-center transfer integrals with interatomic distances, one should consider that the on-site orbitals (in particular, the quasi-free electron orbitals \( d \) and \( s' \) ) feel the ‘geometry’ of the deformed crystal, and their energies must therefore be shifted and possibly split according to the symmetry of the deformation. It was proved that this approach leads to a satisfactory fit of bulk deformation potentials. Here we use a generalization of this scheme to the situation of an atom surrounded by arbitrarily chosen partners. Say we consider a cation \( C \) surrounded by four different anions \( A_i, i = 1 - 4 \), located at arbitrary positions, and need to define a local strain acting on the cation. Nominal anion positions \( \{ n_i \}_i = 1 - 4 \) are first defined, using bond lengths corresponding to the \( \text{CA} \) bulk lattice parameter and \( \{ 1 1 1 \} \) bond orientations. After relaxation, this nominal, unstrained tetrahedron transforms to the actual one with atoms at positions \( \{ r \}_i = 1 - 4 \). The shapes of these tetrahedrons can be characterized using three arbitrarily chosen vectors \( \{ R \}_i = 1 - 3 \). We choose them as: \( R_1 = r_2 - r_1, R_3 = r_3 - r_1, \) and \( R_2 = 1/2(r_1 + r_2 - r_3 - r_4) \). It is then easy to find the matrix \( T \) connecting the nominal and strained sets: \( TR_{ij} = R_i \). The local strain tensor \( \varepsilon \) acting on on-site orbitals is defined by the polar decomposition \( \varepsilon = (1 + \varepsilon) R \), where \( R \) is the orthogonal matrix which rotates the ‘nominal’ tetrahedron to the strained one. One may note that \( \varepsilon \) does not fully describe the local atomic configuration: it is uniquely defined by the relative coordinates of four anions surrounding a given cation (or vice versa) and the change of cation position does not affect the local strain tensor. To account for the cation position we introduce an additional internal strain vector \( u \) defined as the (scaled to unstrained interatomic distance) displacement of the cation from the center of the sphere which touches the surrounding anions. Note that in a bulk material, strain and internal displacement are proportional and related by the Kleinman parameter \( \zeta \), which is not the case for atomic positions in a situation of arbitrary chemical surroundings. As carried out implicitly in Jancu and Voisin (2007), we assume that the effect of the internal strain on the tight-binding Hamiltonian is the same as that of the strain tensor part which transforms as a vector. In summary, the local strain Hamiltonian acting on the \( p \) orbitals \( (p_x, p_y, p_z) \) and \( d \) orbitals with the symmetry \( \Gamma_{15} \) \((d_{xz}, d_{yz}, d_{xy})\) on-site orbitals is written as:

\[
\delta H = \begin{pmatrix}
\lambda_1(\sqrt{3}(\varepsilon_1 - \varepsilon_2) - \lambda_2(\varepsilon_{xy} + \xi u_x) & \lambda_3(\varepsilon_{xx} + \xi u_x) \\
\lambda_2(\varepsilon_{xy} + \xi u_y) & -\lambda_4(\sqrt{3}(\varepsilon_1 + \varepsilon_2)) & \lambda_5(\varepsilon_{xy} + \xi u_z) \\
\lambda_3(\varepsilon_{xx} + \xi u_y) & \lambda_2(\varepsilon_{xy} + \xi u_y) & 2\lambda_6\varepsilon_2
\end{pmatrix}
\]

(2)

where we use \( \varepsilon_1 = \sqrt{3}(\varepsilon_{xx} - \varepsilon_{yy}), \varepsilon_2 = 2\varepsilon_{zz} - \varepsilon_{xx} - \varepsilon_{yy} \). In the notation of Jancu and Voisin (2007), for \( p \)-orbitals \( \lambda_1 = \frac{1}{2}E_p\delta_{000}, \lambda_2 = \frac{8}{3}E_p\delta_{111} \) and for \( d \)-orbitals \( \lambda_4 = \frac{1}{2}E_d\delta_{000}, \lambda_5 = \frac{8}{3}E_d\delta_{111} \). The parameter \( \xi \) is equal to \( +1 \) for cations and to \(-1 \) for anions. Note that in principle, the \( \pi \) and \( \delta \) parameters may have different values for anions and cations. Here, this difference is handled by the scaling to orbital energy, which limits the number of adjustable strain parameters. These prescriptions give the same result as in Jancu and Voisin (2007) for strained bulk semiconductors.

However, an obvious difficulty with this general frame is the large number of parameters that need to be determined: it is clear that the sole consideration of deformation potentials at the zone center (that are reasonably well documented) does not provide enough information. On the other hand, even the most sophisticated \emph{ab initio} schemes still encounter difficulties with conduction band dispersions, and blind fitting may lead to unsatisfactory parameterization. For current purposes, one can rely on any parameterization that gives sound values of \( d_{xx}, b, \) and \( d \). Here, we reworked the strain parameters using an optimization algorithm and looking for a set of strain parameters close to the one of Jancu et al. (1998) and which reproduces the recommended values of deformation potentials in the center of the Brillouin zone given in Vurgaftman et al. (2001). For simplicity, since \( \pi \) and \( \delta \) parameters have the same effects on deformation potentials in the \( \Gamma \) point, the \( \delta \) parameters were set to zero and thus renormalized in the \( \pi \) parameters. Strain parameters used in the present calculations and resulting zone-center deformation potentials are listed in tables 1 and 2.

3. Results and discussion

The approach outlined in the previous section is similar to that introduced by Pryor et al. (1998) and used by Magri et al. for the AEP approach (Magri and Zunger 2001, Piquini et al. 2008), or to that used by Zielińska (2012) for EPTB. It differs however on a very important point, which is the unambiguous definition of the internal displacement vector that is mandatory for a proper account of trigonal deformations (Jancu and Voisin 2007). Yet, to the best of our knowledge, these
atomistic models were not validated by a crucial comparison with a well-established experimental result. A possible test case is an In monolayer inserted in a GaAs matrix. The experimental gap is well documented with a low temperature value of 1.434 eV from the optical properties of samples containing a slight sub-monolayer amount of In giving rise to large, anomalously large band gaps.

Next we come to InAs–AlSb superlattices. In table 3, we compare the atomic distances in the interface regions of a 8/8 InAs–AlSb superlattice, obtained in the ‘classical’ and ‘atomistic’ elasticity models. For the latter, we use the parameters of Keating (1966). To find minimum energy and corresponding atomic positions in VFF, we use conjugate gradient minimization. It can be observed that in the VFF calculations, interface strain perturbs the atomic positions on typically one monolayer (3 Å) on both sides of the ‘anomalous’ interface bond, with an oscillatory behavior before the interplane distances stabilize to the classical elasticity value.

In table 4, we show the local strain tensor associated with the different atomic sites in a 8/8 InAs–AlSb superlattice, using the VFF atomic positions. A remarkable, perhaps counterintuitive feature is the existence of a trigonal (shear) component ε_{xy} for atoms that have asymmetrical chemical surroundings. The bulk material parameters used in this work are listed in table 5. The calculation also requires band offset values. For the well-documented offsets for the nearly unstrained heteropairs InAs–GaSb, InAs–AlSb, and GaSb–AlSb we take, respectively, 570, 200, and 350 meV (Yu et al 2014). The experimental values agree with ab initio calculations. Unfortunately, the situation for InSb–InAs is not as clear, with no direct experimental result and a strong dispersion of theoretical predictions from 400 meV (Wei and Zunger 1987) to 700 meV (Van de Walle and Neugebauer 2003).

The molecular layer of InSb certainly act as a potential well in the valence band, but uncertainty in VBO implies that the depth of this trap is unknown, and we shall consider it as the only free parameter in the calculations. Conversely, the AlAs bonds act as a potential barrier whose height is also not so well documented, but the impact of this uncertainty on our results is actually negligible. When epitaxial strain is taken into account, the AlSb heavy-hole band extremum lies at 208.7 meV above the arbitrary reference level of the unstrained InAs valence band maximum (VBM). The heavy-hole confinement in a regular 12.2 nm-thick (40 monolayer) QW is 6.4 meV. Hence, one reasonably expects a hole ground state at 202.3 meV. Figure 2 shows the evolution of the actual hole ground state energy in a 20/40 InAs–AlSb superlattice as a function of InSb band offset, for the three ideal situations: C_{2v} (AIAs and InSb interfaces), D_{2h} (2AIAs) and D_{2d} (2InSb). In the C_{2v} case for an InAs–InSb VBO larger than 600 meV, the ground state is above the AlSb VBM, hence it is clearly trapped by the

| Table 1. The strain parameters used in calculations and the resulting zone-center deformation potentials. Notations from Jancu and Voisin (2007). |
|---|---|---|---|
| n_s | n_p | n_d | n_s' |
| 1.7520 | 0.1500 | 1.8270 | 2.0000 |
| 1.7970 | 0.8400 | 0.9630 | 2.0000 |
| 0.5160 | 0.7230 | 1.7280 | 2.0000 |
| 1.2960 | 0.0330 | 1.2360 | |
| n_s^* | n_s'e | n_s'd | n_s'd' |
| 1.9600 | 3.4760 | 3.1360 | 0.0000 |
| 2.7000 | 2.6940 | 2.4640 | 0.0000 |
| 1.8440 | 2.9880 | 3.0260 | 0.0000 |
| 4.7500 | 3.4860 | 2.1600 | 0.0000 |
| n_s'' | n_s'& | n_s'd& | n_s'd'' |
| 0.3410 | 0.4830 | 0.5890 | 0.0000 |
| 0.4830 | 0.3940 | 0.5890 | 0.0000 |
| 0.5890 | 2.9460 | 3.0800 | 0.0000 |
| 0.3260 | 0.0000 | 3.8060 | 0.0000 |
| n_s^*e | n_s'e& | n_s'd&e | n_s'd''e |
| 3.1360 | 0.0000 | 0.0000 | 0.0000 |
| 2.4640 | 0.0000 | 0.0000 | 0.0000 |
| 3.0260 | 0.0000 | 0.0000 | 0.0000 |
| 2.1600 | 0.0000 | 0.0000 | 0.0000 |

| Table 2. Tight-binding deformation potentials of bulk materials. The fitted values are identical to the target values taken from Vurgaftman et al (2001), except that we use the sign convention for \( \varepsilon_{xy} \) for atoms that have asymmetrical chemical surroundings. |
|---|---|---|
| AlAs | InAs | AlSb |
| \( a_e \) | \( a_e \) | \( a_e \) |
| \( -5.64 \) | \( -5.08 \) | \( -4.50 \) |
| \( -4.90 \) | \( -6.94 \) | |
| \( a_t \) | \( 4.27 \) | \( 1.00 \) |
| \( 1.40 \) | \( 0.36 \) | |
| \( b \) | \( -2.30 \) | \( -1.80 \) |
| \( -1.35 \) | \( -2.00 \) | |
| \( d \) | \( -3.40 \) | \( -3.60 \) |
| \( -4.30 \) | \( -4.70 \) | |

| Table 3. Interplane distances in the vicinity of interfaces. VFF calculations are made for a several period 8/8 InAs–AlSb superlattice grown on a GaSb substrate. |
|---|---|---|
| Al–Sb | n Bulk | h Classical | h VFF |
| Al–Sb | 1.5339 | 1.5437 | 1.5436 |
| Sb–Al | 1.5339 | 1.5437 | 1.5441 |
| Al–Sb | 1.5339 | 1.5437 | 1.5367 |
| Sb–In | 1.6198 | 1.7234 | 1.7233 |
| In–As | 1.5146 | 1.5041 | 1.4962 |
| As–In | 1.5146 | 1.5041 | 1.5046 |
| In–As | 1.5146 | 1.5041 | 1.5041 |
| Al–Sb | 1.5339 | 1.5437 | 1.5428 |
| Sb–Al | 1.5339 | 1.5437 | 1.5436 |

Interplane distances in the vicinity of interfaces. VFF calculations are made for a several period 8/8 InAs–AlSb superlattice grown on a GaSb substrate.
Table 4. Local strain tensor acting on the atomic orbitals’ on-site energies for a 8/8 InAs–AlSb superlattice grown lattice-matched to a GaSb substrate.

|          | εxx(%) | εyy(%) | εzz(%) | εxy(%) | εxz(%) | εyz(%) | u(%) |
|----------|--------|--------|--------|--------|--------|--------|------|
| In       | −2.647 | −2.647 | 3.005  | 0.     | 0.     | 3.272  | 4.349|
| As       | 0.626  | 0.626  | −0.930 | 0.     | 0.     | −0.160 |      |
| In       | 0.626  | 0.626  | −0.669 | 0.     | 0.     | −0.010 |      |
| As       | 0.626  | 0.626  | −0.686 | 0.     | 0.     | 0.     |      |
| In       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| In       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| In       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| In       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| In       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| In       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| In       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| In       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| In       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| In       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |
| As       | 0.626  | 0.626  | −0.685 | 0.     | 0.     | 0.     |      |

InSb bond. For smaller offsets, the ground state lies between the AlSb VBM and 204 meV: the situation is better described as a regular QW with an attractive perturbation at one interface, that decreases the confinement energy and polarizes the wavefunction. As shown in figure 3(a), in all cases the wavefunction is strongly asymmetrical with respect to the center of the AlSb layer: as long as the AlSb thickness remains finite, it is difficult to define a rigorous criterion for the existence of an interface state. By exploring numerically larger layer thicknesses, we find that 500 meV is a practical threshold offset value for the existence of an interface state at an InSb interface between InAs and AlSb.

The D2h case with two AlAs interfaces (see figures 2 and 3(b)) corresponds to the regular QW case. The D2d, 2InSb configuration is more interesting, because the interface states may exist at both interfaces, and combine into symmetric (bonding) or antisymmetric (antibonding) states, with a splitting depending strongly on AlSb layer thickness. Due to this interaction, the ground state energy remains nearly constant when decreasing the AlSb thickness. This result is illustrated in figure 4. A similar trend is also valid for interface state coupling through the InAs layer, but to a much smaller extent due to the fast decay of the interface state into InAs. Note, however, that this remark holds only in as much as the unavoidable difference between the two interface state energies is smaller than their mutual coupling. Results displayed in figure 3 are qualitatively similar to those obtained from LDA calculations by Shaw et al (1995), but the decay of the interface state in AlSb is much slower in our calculations. It is worth noting that calculations of Shaw et al (1995) do not include spin-orbit interaction and, therefore, the effective valence band QWs differ. Finally, it is interesting to examine the effect of a change in InAs–AlSb VBO, within the experimental uncertainty range 150 ± 50 meV: the smaller this offset is, the easier it is for the interface trap to capture the valence ground state. For vanishing InAs–AlSb VBO, any value of InSb VBO would lead to an interface state, whose decay in both layers would become almost symmetrical. In figure 5, we show the dependencies on InSb–InAs offset for an InAs–AlSb offset of 100 meV. It is seen that in this case, the interface state exists as soon as the InSb–InAs offset exceeds 314 meV.
So far, we have discussed interface potential in terms of a ‘diagonal’ or scalar contribution. However, as mentioned in the introduction, the interface also breaks a rotational invariance and the corresponding Hamiltonian admixes heavy and light holes, which results in the linear polarization of optical spectra when the system has $C_{2v}$ symmetry (Krebs and Voi
tin 1996, Ivchenko et al 1998, Theodorou and Tsegas 2000). Here, valence states are confined in the AlSb layer, and ground state peaks close to the InSb bonds. They undergo the strong spin–orbit coupling of Sb. Since spin–orbit interaction tends to force total angular momentum eigenstates, weak polarization anisotropy is expected. This anisotropy is confirmed by the calculations: for the 20/40 InAs–AlSb superlattice, we obtain a degree of linear polarization of the ground optical transition (with the principal axis along the [1 1 0] and [−1 1 0] directions) equal to 6%.

4. Conclusion

We have used extended-basis tight-binding to model the no common atom system of InAs–AlSb with the highest possible accuracy. We find that for a large range of the natural band offset of InSb, there exists an intrinsic interface state ‘trapped’ by the plane of interfacial InSb bonds. The existence of such a state is important for valence band physics in this system, but also plays an important role in the material characterization using interband optics. Spectrally resolved scanning tunneling microscopy is expected to allow for direct experimental evidence of the localization of valence band ground states near the InSb interface bond.

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