

## Interface-induced localization in AlSb/InAs heterostructures

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The existence of localized states at perfect InSb-like interfaces in AlSb/InAs superlattices is predicted from *ab initio* pseudopotential calculations. Localized states are predicted in both the valence and conduction bands, the former being identifiable with the interface states proposed by Kroemer, Nguyen, and Brar [J. Vac. Sci. Technol. **10**, 1769 (1990)]. The existence of these interface localized states is invoked to explain the reported experimental dependence of the band gap upon interface types in such superlattices.

One of the outstanding problems of solid-state physics is the question of a link between the microscopic properties of interfaces and spectroscopic data concerning localized states peculiar to the heterostructure in question. Although a number of studies have examined from first principles or experimentally the structural stability and the electronic structure of heterointerfaces, the link between structure and electrical and optical data that might refer to distinct localized effects peculiar to defect-free (perfect) interfaces has not been established. In this study we have identified what is, to the best of our knowledge, the first example of such a localized feature. We present *ab initio* pseudopotential calculations for AlSb/InAs superlattices, which demonstrate the formation of localized valence states at perfect InSb-like interfaces. These localized states are similar in nature to the so-called "Tamm states" invoked by Kroemer, Nguyen, and Brar<sup>1</sup> to explain experimentally observed carrier concentrations in AlSb/InAs/AlSb quantum wells. Subsequent studies have suggested that the interface states may not be the source of the carriers,<sup>2,3</sup> though the possibility of their existence is not excluded. Indeed, the calculations of Shen *et al.*<sup>4</sup> predict that such interface states do exist, but that an alternative mechanism is responsible for the excess carriers. In this paper we do not address the question of whether the microscopic origin of the localized states lies in the intrinsic interface dipoles,<sup>5</sup> or whether they are genuine Tamm states. Rather, for the stable structure studied, we are concerned with the prediction of the existence of such states, and their observable consequences. The formation of these states qualitatively explains the differences in band-gap energies for structures with various interface configurations, as reported from photoluminescence spectra by Spitzer *et al.*<sup>6</sup> Our study thus provides a clear link between specific microscopic interface features and experimental observations in AlSb/InAs superlattices.

The calculations presented are based upon the local-density approximation of density-functional theory and use the *ab initio* pseudopotentials of Bachelet, Hamann, and Schlüter.<sup>7</sup> We apply this formalism within the framework of large unit cells (supercells) containing 24, 32, and 128 atoms. The wave function is expanded in terms of Gaussian basis functions, made *s*- and *p*-type through multiplication by an appropriate spherical harmonic. A

total of 16 such functions are centered on each atom in the unit cell, giving 2048 functions in total for the 128-atom system. We find that this is easily sufficient to describe the *pseudo* valence states as these are smooth functions that do not oscillate rapidly near the core. An intermediate fit to the charge density that is also required by our formalism (see, for example, Jones<sup>8</sup>) uses six functions per atom. The 24- and 32-atom supercells consist of 12 and 16 ML of material, respectively, with only a single spiral of atoms perpendicular to the growth direction. This was described using a set of 12 special *k* points, chosen to be equivalent to the set of 10 *k* points frequently used in the primitive two-atom zinc-blende unit cell. The 128-atom supercell was derived from the 32-atom system described but had four spirals of atoms in the plane, and used an appropriately reduced set of special *k* points. The accuracy of our treatment is illustrated by the lattice constants of the four bulk materials related to the AlSb/InAs system studied here. These are given in Table I.<sup>9</sup> It is seen that the accuracy is similar to that obtained with conventional plane-wave-based treatments. Our principal concern is in the question of under what circumstances we expect interface localization to occur, rather than the precise energies of the minibands. Consequently, the absence of spin-orbit coupling in our calculations, which will affect the detailed band structure, should not affect the principal conclusions arrived at. Provided the heavy-hole band offset in our calculation (deduced from the positions of the states to be  $\approx 350$ – $400$  meV) is reasonable (compared, for example, with the 310 meV of Dandrea and Duke<sup>10</sup>), the neglect

TABLE I. Bulk lattice constants of the four bulk materials associated with AlSb/InAs structures, as calculated from our theory, and as measured experimentally [see *Semiconductors: Group IV Elements and III-V Compounds*, edited by O. Madelung, Data in Science and Technology (Springer-Verlag, Berlin, 1991)].

Bulk material	Lattice constant (atomic units)	
	Our theory	Experiment
AlSb	11.607	11.594
InAs	11.311	11.448
InSb	12.125	12.244
AlAs	10.722	10.695

of the spin-orbit interaction should not affect the qualitative description of the localized states.

Several AlSb/InAs superlattices were studied by relaxing the positions of all of the atoms to minimize the total energy. The approximate one-electron energies, and charge densities of the zone-center ( $\Gamma$ ) wave-function states were obtained. The first structure studied was a 4AlSb/4InAs superlattice (where 4AlSb refers to four lattice constants of AlSb), strained to an AlSb substrate. This structure had one of each type of interface, AlAs and InSb, in its unit cell. Full relaxations were performed with a four-spiral, 128-atom, unit cell to examine the possibility of interface reconstruction. Since no such reconstruction was observed the single-spiral unit cells were used to obtain the results presented below. Also, calculations were performed on a superlattice with two AlAs interfaces formed by replacing the interface In atom with Al, and a superlattice with two InSb interfaces with the As interface atom swapped with an Sb. Schematic diagrams of each of these structures are shown in Fig. 1, together with the charge densities (integrated over the plane parallel to the interfaces) of the uppermost valence state in each superlattice. Examination of Fig. 1 shows quite clearly the tendency for charge to localize in the vicinity of the InSb interfaces. Figure 1(c) shows the charge density of the structure with two AlAs interfaces, a typical heavy-hole ground-state envelope with charge concentrated in the center of the AlSb well. With one InSb interface [Fig. 1(a)] the charge is localized at the

side of the well with the InSb interface, while for the structure with two InSb interfaces the charge is drawn away from the well center in each direction to yield an almost flat charge distribution. We suggest that these states localized at InSb interfaces may be thought of like the “Tamm states” proposed by Kroemer, Nguyen, and Brar<sup>1</sup> to describe the high carrier concentrations in not-intentionally-doped AlSb/InAs/AlSb single quantum wells. These states ought then to be able to be understood qualitatively in terms of the simple bulk band-edge model discussed in Ref. 1, where the single InSb monolayer is regarded as presenting a bulklike InSb potential well. To verify this we consider our original structure with the As-In-Sb-Al interface sequence replaced by As-In-Sb-In-Sb-Al (and a reduction in the InAs layer width to maintain the same period). Since the effective width of the InSb layer has increased, it would be expected that the degree of localization would increase. Figure 2 shows the schematic diagram of the structure, together with the integrated charge density of the valence band-edge state (at  $\Gamma$ ). A clear increase in localization is seen. In addition to the localization of charge at the interfaces, the localized states are found to lie at higher energies, relative to the bulk band edges, than the nonlocalized heavy-hole state. As expected in the simple framework outlined above the localized state in the wide InSb interface lies at considerably higher energies than the corresponding single-monolayer states.

Let us now consider in more detail the implications of the different energies of the localized states. The presence of interface states at higher energies ought to man-

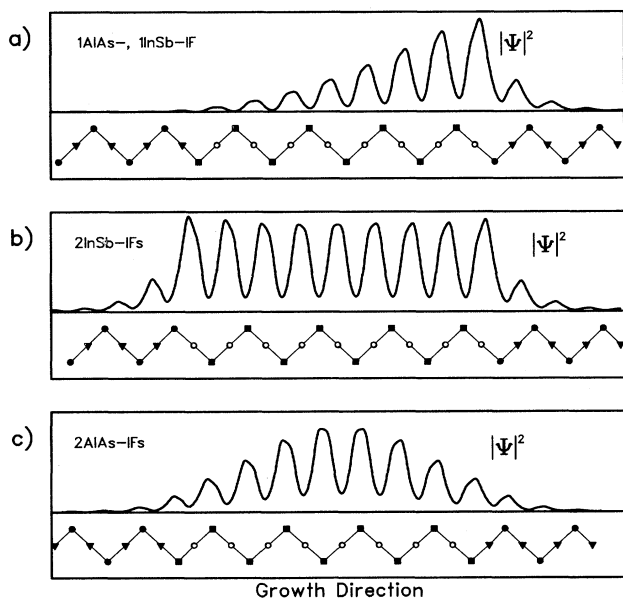


FIG. 1. Schematic diagrams of AlSb/InAs superlattices with (a) 1AlAs and 1InSb interface, (b) 2InSb interfaces, and (c) 2AlAs interfaces are shown. The In atoms are represented by solid circles, As by triangles, Al by squares, and Sb by open circles. The charge densities of the uppermost valence state in each structure (integrated over the plane perpendicular to the growth axis) are plotted (as arbitrary units) against distance along the growth direction. The positions of atoms are to scale in the growth direction.

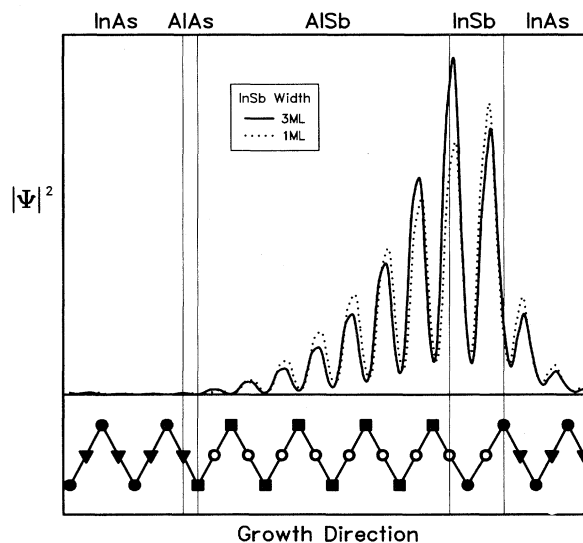


FIG. 2. A schematic diagram of the structure with 3 ML of InSb at one interface is shown (the symbols are as in the previous figure). The charge density of the uppermost valence state (integrated over the plane perpendicular to the growth axis) is plotted (as arbitrary units) against distance along the growth direction. The dotted line shows the charge density of the structure with a single 1-ML InSb interface for comparison. The vertical lines indicate the positions and approximate extent of the interfaces.

ifest itself experimentally as a change in the band gap of structures with different interface configurations. Of course, in changing the interface structure it is inevitable that the effective conduction and valence well widths are also altered. Consequently, the band-gap reduction associated with the interface localization appears in combination with the changes in confinement energies.<sup>11</sup> In Ref. 6 Spitzer *et al.* reported experimental studies of several AlSb/InAs superlattices, with widths changed slightly to create differing interfaces while keeping a period of six lattice constants. We have performed simulations of the structures they describe, and summarize the results in Table II, where the structures have been labeled (a) to (c). Although density-functional theory does not give absolute band gaps accurately, we have found that trends in the energies of one-electron states are given with reasonable quantitative accuracy. Therefore, in Table II we compare the changes in ground heavy-hole to conduction state separations calculated [relative to structure (c), the perfect 3AlSb/3InAs superlattice with one of each interface], with the differences in photoluminescence peak energies of Ref. 6. Where Ref. 6 presents results for more than one sample with nominally the same interface structure, we compare our results with the structure shown to exhibit the highest-quality growth. We have also performed calculations of other similar structures, (d) and (e), where the changes in interfaces are achieved by different layer width alterations. The fourth and fifth columns of Table II show the changes to the layer widths from the perfect 3AlSb/3InAs structure. A comparison of the local-density approximation (LDA) and experimental shifts in structures (a) and (b) shows a close agreement with experiment. The agreement is at least as good as might be expected from this technique. At this point it is worth bearing in mind that in comparing with the experimental result for structure (b), it is generally accepted that there is a large concentration of As defects in AlSb layers grown with a lower AlAs-like interface.<sup>6</sup> These defects are not included in our calculations.

Structures (a) and (c) have effectively the same conduction-band well width, since the potential barrier presented by the InSb layer encroaching into the well is small. The valence well width is, however, widened, and were the valence band-edge states conventional confined states we would expect (a) to have a reduced gap with respect to (c). No such change occurs, indicating that the valence states are fixed with respect to well width, consis-

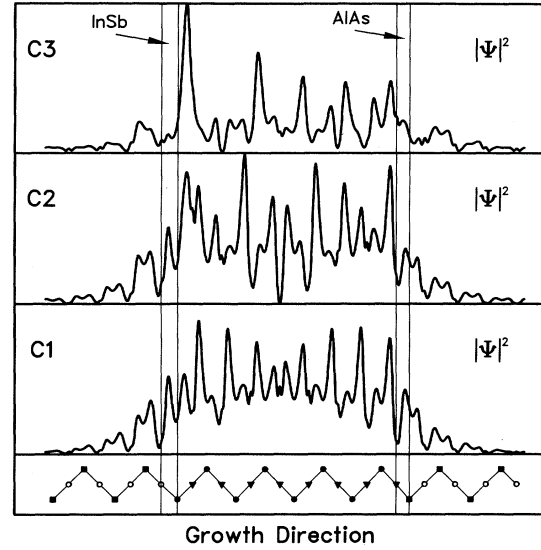


FIG. 3. The charge densities of the lowest three conduction states (integrated over the plane parallel to the interfaces) are plotted (in arbitrary units) against distance along the growth axis for a 4AlSb/4InAs superlattice, with one of each interface type. A schematic diagram of the structure is plotted with the growth direction atomic positions to scale (the symbols are as in the previous figures). Vertical lines are drawn to indicate the position of the interfaces.

tent with the view that these are localized InSb interface states lying at or above the AlSb band edge, such as those labeled “Tamm states” by Kroemer, Nguyen, and Brar.<sup>1</sup> Comparing structures (c) and (d), each possessing at least one InSb interface, we expect the energy of the valence states again to remain virtually unchanged, while the wider effective conduction well reduces the electron confinement energy. This results in the 103-meV reduction in the gap of (d) in Table II. Now, though, consider the change from (c) to (b), which has two AlAs-like interfaces. Again the conduction-band well width is effectively unchanged, but now there are no InSb-interface localized states. The confinement energy of the valence states increases the gap by 112 meV. Finally, structure (e), with the same interface structure as (b) but with wider valence and narrower conduction wells shows a further gap increase of 97 meV. This occurs because the conduction confinement energy increases more from (b) than the valence confinement decreases, due to the lighter electron

TABLE II. The interface types and structural properties of the superlattices studied are presented. The quantities  $\Delta w_{\text{InAs}}$  and  $\Delta w_{\text{AlSb}}$  represent the change in InAs and AlSb layer widths (in half-monolayers) from structure (c). Similarly, the energy gaps  $\Delta E_g^{\text{LDA}}$  and  $\Delta E_g^{\text{Expt}}$  are the calculated and experimental differences from the gap in structure (c).

Structure	Number (Ref. 6)	Interface types	$\Delta w_{\text{InAs}}$ ( $\frac{1}{2}\text{ML}$ )	$\Delta w_{\text{AlSb}}$ ( $\frac{1}{2}\text{ML}$ )	$\Delta E_g^{\text{LDA}}$ (meV)	$\Delta E_g^{\text{Expt}}$ (meV)
(a)	1	InSb + InSb	-1	+1	-2	+22
(b)	2	AlAs + AlAs	+1	-1	+112	+120
(c)	5	InSb + AlAs	0	0	0	0
(d)		InSb + InSb	+1	-1	-103	
(e)		AlAs + AlAs	-1	+1	+209	

effective mass. We note that the trends observed here, and the wave functions in Fig. 1, are in good agreement with those of Dandrea and Duke,<sup>10</sup> though the greater number of structures studied enables the role of localization to be isolated, to a degree, from the changes in effective layer widths.

So far, we have studied only the distributions of the charge densities in the valence band. Can localizations occur also in the conduction band? In Fig. 3 we show the integrated charge densities of the conduction minibands of the 4AlSb/4InAs superlattice. The form of the lowest conduction state is seen to resemble a simple ground-state envelope function, while the second conduction state can be identified as having a first-excited-state envelope. The third conduction state, however, is dominated by a charge localization close to the InSb-like interface. In fact, closer examination reveals the charge to be localized in the InAs layer immediately adjacent to the interface bonds. Clearly, the presence of the InSb interface bonds modifies the InAs bonding to the interface ion. Even for the case of the structure with wide InSb interfaces (studied previously), the charge localization oc-

curs on the InAs side of the interface. These conduction-band charge localizations are absent in structures with two AlAs-like interfaces. This brief examination of the conduction states indicates that significant interface localization effects may also occur in the conduction band, and suggests the need for more thorough future study.

In conclusion, we have predicted the existence of localized states at perfect InSb-like interfaces in AlSb/InAs superlattices. Such states are shown to occur in both the valence and conduction bands. We have shown that the existence of interface-localized valence states results in a model consistent with the reported experimental dependence of superlattice band gap on interface type. Finally, we predict the possibility of the presence of localized states in the conduction band.

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<sup>9</sup> The exponents of the Gaussian basis functions were chosen principally with the object of minimizing the total energy of the unit cells of the bulk materials. However, in the case of InAs, a number of basis sets were obtained that gave comparable total energies but gave rise to lattice constants that varied by 2%.

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