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InAs-GaSb superlattice energy structure and its semiconductor-semimetal transition

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We performed a band calculation, based on the LCAO (linear combination of atomic orbitals) method, for the InAs-GaSb superlattice. Of possible semiconductor combinations the InAs-GaSb is of special interest because of indications that at a heterojunction interface the bottom of the conduction band of InAs lies below the top of the valence band of GaSb. Our results show that the InAs-GaSb superlattice is a semiconductor when the layers of the constituent materials are thin, and becomes a semimetal when the layer thicknesses are increased. The critical InAs thickness for this transition is approximately 115 Å, over which the electrons from the valence band of GaSb "flood" the conduction band of InAs. For the thick-layer limit, we treat the problem in a Fermi-Thomas approximation.

I. INTRODUCTION

For a semiconductor superlattice in which the crystal structure is continuous across the interfaces that separate alternate layers of different semiconductors, there is no difficulty, in principle, in calculating the energy bands. Such a calculation for Ge-GaAs and AlAs-GaAs has in fact recently been completed by Pickett, Louie, and Cohen.[1] There are, however, two complications relative to the calculation for a homogeneous semiconductor. First is the computational complexity arising from the alternate structure which effectively increases the size of the primitive cell that must be considered. This is not serious even for traditional methods of band calculation (othogonal plane wave, augmented plane wave, etc.) and we will see that for the linear-combination-of-atomic-orbitals (LCAO) method we use it can be handled without problems. The second complication is in the determination of a self-consistent potential, or equivalently the parameters entering an LCAO calculcation. Superimposed atomic potentials are generally used as a starting approximation to the potential and in fact are usually a rather good approximation to a true self-consistent potential in a homogeneous semiconductor. However, one would worry that charge redistribution at the material interfaces would introduce dipole layers and important corrections to the potentials. Fortunately a more careful look[1-3] has indicated that these corrections are in fact less than 0.1 eV and of the order of experimental uncertainities in the band positions. Thus, it is not unreasonable to proceed to a calculation of the bands using the same parameters which are used for the homogeneous system.

We select for study what may be the most interesting combination of compounds, InAs-GaSb. A comparison of electron affinities of various semiconductors with compatible lattice distances indicates[4] that this combination has a conduction band edge on one side (InAs) lying lower in energy than the valence band edge on the other side (GaSb). This same special feature was noted also in the theoretical prediction of band positions for all possible combinations.[3] Recent measurements of I-V characteristics in experimental junctions, prepared by molecular-beam epitaxy (MBE), are consistent with such a crossing of the bands.[5] (The comparison of electron affinities shows that GaP-Si would also exhibit this feature but the theory[3] suggests that the result is erroneous due to application of electron-affinity arguments to a polar-homopolar junction. The experimental test has not been made.) The InAs-GaSb system then is the most extreme case having the greatest variety of behavior with interesting technical possibilities.[4] We proceed to a calculation of the energy bands, in the neighborhood of the fundamental gap, in alternate layers of N atomic planes (each layer has a thickness $\frac{1}{4}Na$) with a the unit-cube edge of InAs and N' atomic planes of GaSb, stacked in a [100] direction and will obtain the bands for various thicknesses.

II. LCAO BAND CALCULATION FOR THE HOMOGENEOUS SYSTEM

We begin with a minimal basis set (one s and three p states on each atom) LCAO calculation including only nearest-neighbor matrix elements. This is sufficient to give a reasonable description of the lowest conduction band at Γ as well as the valence bands for homogeneous semiconductors[6] and should be equally applicable to the heterogeneous case. A universal set of parameters is available[6] which would enable us to proceed directly to the calculation, but since the bands of both constituent semiconductors are quite well known it will be preferable to "tune" the parameters to the known band gaps and effective masses of the homogeneous materials.

We will perform the calculation for electrons propagating perpendicular to the heterojunction planes, in a direction which we will take to be the z axis, a [100] direction. The energy bands for the homogeneous semiconductor can be obtained in analytic form for our minimal basis set, nearest-neighbor LCAO description for propagation in this direction. They have been given by Chadi and Cohen,[7] with the neglect of spin-orbit coupling. The upper valence bands consist of a doubly degenerate heavy-hole band and a light-hole band, degenerate with it at the center of the Brillouin zone. Spin-orbit splitting drops one of the heavy-hole bands to lower energy. The lowest conduction band is nondegenerate, with a minimum energy at the zone center. Since we will only be interested in the bands nearest the gap we can reduce our basis set still further in the calculation of the conduction band and the light-hole band by discarding the p orbitals on the metallic atoms and the s orbitals on the nonmetallic atoms. Their energies are well removed from the region of interest and any effect they have can be absorbed in the parameters of the fit to the pure material. This step is not essential, but it simplifies the problem of the superlattice sufficiently to be worth doing. In fact, because the bands are describable in principle by as many Wannier functions as there are bands, this is not really an additional approximation in the description of the two bands, but a change in the importance of the neglect of more distant-neighbor interactions.

In this context, the energy of the nondegenerate bands can be written[7]

$$E=\tfrac{1}{2}(\epsilon_s+\epsilon_p)\pm(V_3^2+4V_2^2\sin^2\phi)^{1/2}. \qquad (1)$$

The wave number is related to ϕ by $\phi=\frac{1}{4}ka$, ϵ_s and ϵ_p are the s-state energy on the gallium and the p-state energy on the antimony in GaSb, for example. Their absolute values are not important since in the superlattice only the relative positions of the bands have significance, and we take the relative values in the two materials from the more complete calculation.[3] V_3 is a polar energy which could be estimated from the difference in these two atomic energies and the covalent energy; V_2 is a matrix element which can be estimated from the known internuclear distances.[6] However, we choose to fit these to the observed band gap and effective mass in order to more accurately describe the bands of the homogeneous material.

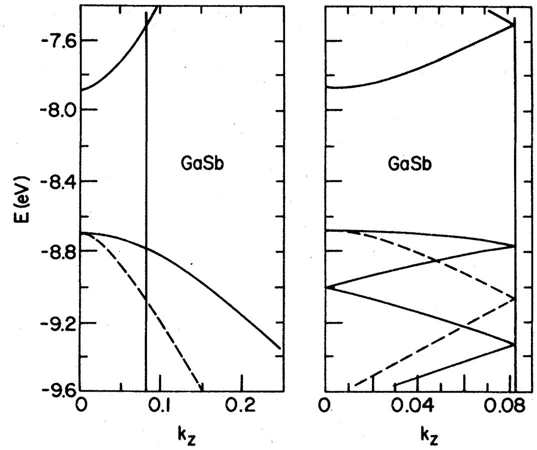

FIG. 1. Energy bands for GaSb. The electron and heavy-hole bands are shown as solid lines, the light-hole band as a dashed line. The wave vector is given in units of $2\pi/a$. In the left panel we use the usual zone where the edge is at $2\pi/a$. The vertical line indicates $\frac{1}{12}$th of the zone which is an artifical edge if the homogeneous material is regarded as a superlattice of successive layers, each 12 atomic planes thick. On the right-hand side the bands are shown with the artificially introduced superperiodicity of 12 atomic planes.

The heavy holes rigorously contain only p states on the two atom types but will show dispersion (in the nearest-neighbor approximation) if both are included. They then are formally very similar to the light-hole bands and are written

$$E=\bar{\epsilon}\pm(V_{3h}^2+4V_{2h}^2\sin^2\phi)^{1/2}. \qquad (2)$$

The relevant average energy $\bar{\epsilon}$ is the average of the atomic p-state energies and we know[6] them relative to the valence-band maximum of Eq. (1). Again, the V_{2h} and V_{3h} could be written in terms of the atomic-term-value differences and universal interatomic matrix elements but we instead fit them to obtain the correct band position and curvature. We then imagine the degeneracy lifted by spin-orbit splitting such that the bands given in Eq. (2) become nondegenerate.

The resulting bands, Eqs. (1) and (2), for GaSb are shown in the left-hand panel of Fig. 1, with the zero of the energy scale at the vacuum level.[8] This corresponds to a rather accurate energy-band calculation for a limited region of energy with parameters tuned to the experimental bands. The necessary parameters for both GaSb and InAs are listed in Table I. We will make the same band calculation for the superlattice bands using the same parameters.

Although these two equations give the band completely, we must note in detail where they came

TABLE I. Parameters of the band calculation. All values are in electron volts.

	GaSb	InAs
ϵ_p	−8.69	−9.21
ϵ_s	−7.88	−8.79
V_3	0.405	0.21
V_2	2.57	2.69
$\bar{\epsilon}$	−6.07	−6.3
V_{3h}	2.62	2.91
V_{2h}	2.55	2.42

from if we are to make the same calculation for the superlattice system. We show in Fig. 2 a projection of one of the lattices on a (010) plane. We have assumed that the wave function of the nondegenerate bands or the heavy-hole band can be written as a linear combination of atomic orbitals.

$$|\Psi\rangle = \sum_j u_j |\Psi_j\rangle , \tag{3}$$

with a single orbital (p state or s state) from each atom. The coefficients can be written in terms of the wave number k of the state, which we have taken to lie to the right. We have numbered the atomic planes by n, increasing to the right, and we see from the figure that all atoms in the odd-n planes are group-V atoms and are translationally equivalent to each other, and all atoms in even-n planes are group-III atoms, which again are translationally equivalent to each other. Thus the coefficients for every orbital in a given plane are the same. We may label the coefficient u_j of Eq. (3) by the plane index n. Now to show that this is an eigenstate and to obtain its energy E, we substitute Eq. (3) into the Schrödinger equation, $H|\Psi\rangle = E|\Psi\rangle$, multiply on the left by a particular atomic state in the nth plane (assumed orthogonal to all other atomic states), and integrate over all space:

$$\epsilon_n u_n + 2V_{n,n+1}u_{n+1} + 2V_{n-1,n}u_{n-1} = Eu_n . \tag{4}$$

ϵ_n is of course the energy $\langle\Psi_n|H|\Psi_n\rangle$ of the atomic state in the crystal. $V_{n,n+1}$ is the matrix element between nearest-neighbor atoms on the planes n and $n+1$. The factor of 2 arises from the two neighbors each atom has in the forward plane or the backward plane. All orbitals may be taken real so that $V_{n,n+1} = V_{n+1,n}$, but note from Fig. 2 that because the p state on the group V is odd, the matrix element with a group-III site to the right has the opposite sign from that with the state to the left. We write the magnitude of $2V_{n,n+1}$ as V_2 to accord with the notation of Eq. (1).

Now we may confirm that there is a solution of the form

$$\begin{aligned} u_n &= v_0 e^{in\phi} \quad \text{for } n \text{ even}, \\ u_n &= v_1 e^{in\phi} \quad \text{for } n \text{ odd}, \end{aligned} \tag{5}$$

with v_0 and v_1 parameters to be determined. (v's rather than u's were chosen since though $v_0 = u_0$, $v_1 = e^{-i\phi}u_1$.) We substitute this form into Eq. (4) for $n=0$ and for $n=1$ to obtain

$$\begin{aligned} &\epsilon_s v_0 - 2iV_2 \sin(\phi) v_1 = E v_0 , \\ &2iV_2 \sin(\phi) v_0 + \epsilon_p v_1 = E v_1 . \end{aligned} \tag{6}$$

The same equations are obtained, by translational symmetry, for all other even and odd n so if Eq. (6) is satisfied, all other equations are satisfied. The sign in the V_2 terms was chosen to accord with Fig. 2, but changing the sign in both equations does not affect the results. It is elementary algebra to solve for the energy E to obtain Eq. (1) with $V_3 = \frac{1}{2}(\epsilon_s - \epsilon_p)$.

We note that for real ϕ Eq. (1) has solutions only over one band of positive energy relative to $\frac{1}{2}(\epsilon_s + \epsilon_p)$ and one band of negative energy. However, continuing the equation to imaginary ϕ gives solutions at all energies in the gap and continuing it into the complex plane from $\frac{1}{2}\pi$ leads to solutions at high and low energies. The corresponding exponentially growing or decaying solutions may be ruled out in infinite homogeneous systems but they become important when there are surfaces and interfaces.

Before we leave the homogeneous system we may reinterpret Eqs. (5) and (6) in a different way which will be most useful for the superlattice system. We may say that these equations allow us to continue the solution at any energy from one part of the crystal to another. For example, given the

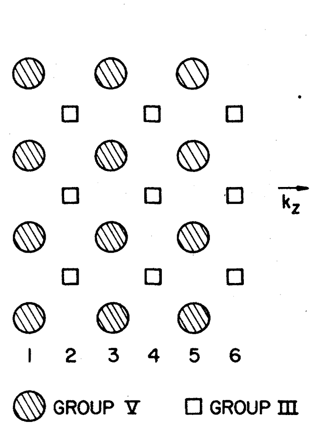

FIG. 2. Projection onto the (010) plane and the numbering of the atomic planes for the host materials.

values of u_0 and u_1 we may obtain u_n and u_{n+1}. This is, of course, done by writing the general solution as a linear combination of solutions propagating (or decaying) to the right and to the left, e.g.,

$$\begin{aligned} u_n &= A v_0^+ e^{in\phi} + B v_0^- e^{-in\phi} \quad \text{for } n \text{ even,} \\ u_n &= A v_1^+ e^{in\phi} + B v_1^- e^{-in\phi} \quad \text{for } n \text{ odd.} \end{aligned} \tag{7}$$

(Note v_0^+ need not be the same as v_0^-, etc.) A and B are picked to fit a given u_0 and u_1 and then u_n and u_{n+1} are obtained immediately.

III. CALCULATION OF THE BANDS FOR THE SUPERLATTICE

We turn next to the superlattice system. Atomic layers for $0 < n \leq N$ are imagined to be of one material; those for $N < n \leq N+N'$ are taken to be of another; those for $N+N' < n \leq 2N+N'$, the first, etc. (It is simpler to take N and N' always as even integers.) Translational periodicity told us that, in the homogeneous crystal, states could be constructed with the coefficient for translationally equivalent orbitals in planes n_2 and n_1 related by $e^{i(n_2-n_1)\phi}$, where ϕ was given in terms of the wave number. The reduced translational symmetry of the superlattice tells us that states can be constructed with coefficients for orbitals in planes with n_2 and n_1, differing by an integral multiple of $N+N'$ related by a phase factor $e^{ika(n_2-n_1)/4}$. The wave number k in the superlattice is again in the [100] direction but now is restricted to the smaller Brillouin zone $-4\pi/(N+N')a \leq k \leq 4\pi/(N+N')a$ and there are $N+N'$ times as many bands.

For the special case in which the two types of semiconductors are, in fact, the same, this gives a representation of the bands for the homogeneous system in the smaller Brillouin zone. This is illustrated for GaSb in the second panel in Fig. 1 for $N=N'=12$. Any measurable property of the system calculated in terms of this representation of the bands will be the same as for the usual representation. In the left-hand side of Fig. 3 we show the bands of InAs in this reduced zone; also note that the conduction band minimum in InAs lies below the valence band maximum of GaSb, as we indicated earlier.

A trick may be used to obtain the bands when the two types are different. A solution within a single layer is written in the form of Eq. (7), with n numbering the atoms within the layer, $0 < n \leq N$. This solution can be continued into the next layer by satisfying Eq. (4) with n corresponding to the last atomic plane of the first layer and the first atomic plane of the second layer. This leads to modified coefficient A' and B' in the second layer. The solution in that layer is given by Eq. (7) with A' and B', numbering atoms in the second layer $0 < n \leq N'$. (Note that we now number from one in each layer.) We similarly relate the coefficients A'' and B'' in the third layer to those in the second and, hence, also to those in the first. Thus we have constructed a transfer matrix which continues the solution through the superlattice:

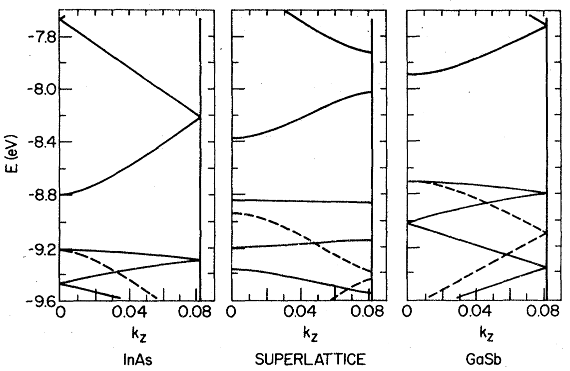

FIG. 3. Band structure for superlattices consisting of alternate layers each 12 atomic planes thick. On the side panels both host layers are of the same material, GaSb on the right and InAs on the left. These two are shown for comparison with the middle panel which is the InAs-GaSb superlattice. The energy scale is the same for all three panels. k is in units of $2\pi/a$. The light-hole bands again are shown as dashed lines.

$$\begin{pmatrix} A'' \\ B'' \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = e^{i(N+N')ka/4} \begin{pmatrix} A \\ B \end{pmatrix}. \tag{8}$$

The equality on the right-hand side results from the fact that A'' and B'' are coefficients of an atomic plane positioned exactly $N+N'$ planes to the right from the plane of coefficients A and B. To find a solution to the eigenvalue equation in (8) with real or imaginary k, corresponding to propagating or decaying states, the determinant of T has to be 1, and then the solution gives the superlattice wave vector such that $2\cos[(N+N')ak/4]$ is equal to the trace of T.

Note first the properties of this matrix for the special case in which all layers are identical, corresponding to homogeneous material. Then it is easy to see

$$T = \begin{pmatrix} e^{i(N+N')\Phi} & 0 \\ 0 & e^{-(N+N')\Phi} \end{pmatrix} . \tag{9}$$

T obviously has a determinant equal to 1. The trace is $2\cos[(N+N')\phi]$ if ϕ is real and $2\cosh[(N+N')|\phi|]$ if ϕ is imaginary, giving $k=4\phi/a$, which is just the definition of the wave vector for the homogeneous case. Similarly, when the two semiconductors differ we may distinguish solutions which propogate from those which decay by evaluating the trace of T; when it is less than 2 we obtain a propagating wave vector.

The procedure is now clear in principle, though somewhat complicated algebraically. We select an energy of interest and from Eq. (2) or (3), depending whether we are dealing with the nondegenerate or the degenerate bands, and obtain ϕ in each material which of course can be real or imaginary depending on the choice of the particular energy. To perform this step we have to know the relative energy scales in the hosts, that is, the lineup of the bands at the interfaces. As mentioned earlier, we take this parameter from the general calculation of band lineups at heterojunction interfaces,[3] which places the bottom of the conduction band in InAs 0.1 eV below the top of the valence band of GaSb. Next we solve Eq. (6) to obtain v_0 and v_1 for each of the ϕ's obtained. Using these in Eq. (7), we may satisfy Eq. (4) in the boundary layers to obtain transfer matrices from AB to $A'B'$ and from $A'B'$ to $A''B''$; multiplying these two matrices we get the T matrix. We then obtain the superlattice bands in the energy regions where propagating solutions for k exist, that is where the trace of T is less than 2. It is a straightforward, albeit lengthy, exercise in algebra to verify that the T matrix derived according to the procedure given above has a determinant of 1. Generally we carried out the procedures by numerical methods. A resulting plot is shown in the center panel of Fig. 3, along with the corresponding bands (see Fig. 1) for pure GaSb and InAs—all are for $N=N'=12$.

IV. DISCUSSION

We note immediately from Fig. 3 that for the selected thickness, despite the overlap between the InAs conduction band and the valence band of GaSb, the overall picture is similar to the GaAs-$Ga_{1-x}Al_xAs$ superlattice case. The InAs-GaSb superlattice is a semiconductor with a well-defined gap between the valence and conduction band states. At the zone edge, at $k_z = 4\pi/(N+N')a$, gaps are opening up and the dispersion in the z direction flattens out, indicating the tendency toward quasi-two-dimensional states. The degeneracy at $k=0$ of the light and heavy holes is lifted, with the light holes shifting to lower energies. This behavior can be understood in the same framework of electron confinement that was successfuly used in interpreting[9] GaAs-$Ga_{1-x}Al_xAs$ superlattices. The lowest conduction-band states are strongly concentrated in the InAs and become shifted in energy because of the confining effect of the GaSb. On the other hand, the valence band states are concentrated in the GaSb and the InAs acts as an effective potential barrier. It is not surprising that for the thin layers selected in Fig. 3 the InAs-GaSb superlattice is a semiconductor, since all combinations GaAs, GaSb, InAs, and InSb are semiconductors and any alloy might be expected to be, whether ordered or not. At the same time, we know that for thick layers the confinement effects become smaller and in that limit, just as for bulk materials, electrons must spill from the GaSb valence band to the InAs conduction band. Our calculation shows this trend toward a "metallic" state. The results are shown in Fig. 4, where we plotted the bands in a 300-meV energy region around the gap as a function layer thickness. The arrows on the figure indicate the progress of the bands between panels. As can be seen, the lowest conduction and highest valence bands approach until crossing occurs. Beyond layer thicknesses of ~115 Å the superlattice, although composed of two semiconductors, becomes semimetallic as a result of the ordered structure.

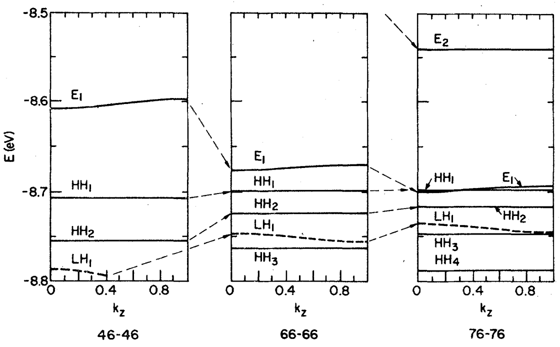

FIG. 4. Dependence of the superlattice bands on layer thickness. E_m, LH_m, and HH_m are the mth electron, light-hole, and heavy-hole bands, respectively. At the bottom of the panels the number of atomic planes is given for each host. Arrows indicate the motion of the bands with increasing layer thickness. In each panel k_z is in units of $4\pi/(N+N')a$. Note that for the 76-76 panel the first heavy-hole and electron bands have crossed.

V. BAND BENDING IN SEMIMETAL REGIME

Once the layers are thick enough that the system is no longer insulating, our neglect of charge redistribution at the interface becomes serious. The electrons which "flood" from the GaSb valence band to the InAs conduction band produce a strong dipole layer and a self-consistent calculation is required. This has not been carried through completely for such a system, but an approximate solution, in the thick layer limit, can be obtained rather simply using a self-consistent Fermi-Thomas approximation. The solution on each side of a heterojunction plane is exactly the same as the solution Keyes[10] gave for the Si surface. The band edge, measured from the Fermi energy which is constant throughout the system, is given by

$$E_b = \frac{E_b^0}{(1+z/z_0)^4}, \tag{10}$$

where z is the distance from the junction, E_b^0 is the band-edge position at the junction ($z=0$), and z_0 is a screening length given by

$$z_0 = (225\pi^2\hbar^6\epsilon^2/8m^{*3}e^4E_b^0)^{1/4}, \tag{11}$$

where e is the electron charge and ϵ the dielectric constant in the material. This assumes a single band of effective mass m^*; when two bands are flooded (heavy and light holes of masses m_h and m_l), m^* should be replaced by $(m_h^{3/2}+m_l^{3/2})^{2/3}$.

We estimate the band shapes in the superlattice by superimposing forms from each heterojunction plane. This is not strictly valid, even within the Fermi-Thomas approximation, but should be qualitatively correct. We first have to divide the band discontinuity (between the valence-band edge in GaSb and the conduction-band edge in InAs) between the two sides, that is, to determine the position of the Fermi energy at the junction. This is done by integrating the total electron charge [Eq. (10)] in the InAs side and equating it to the total hole charge on the GaSb side. Knowing E_b^0 for each side, the corresponding z_0 may be found from Eq. (11). Then all parameters in Eq. (10) are fixed and it may be plotted. We have illustrated the result in Fig. 5 for layer thicknesses of 500 Å. The approximations are appropriate for such thick layers; however, they become progressively less accurate as the layers are reduced toward the values at which the system becomes insulating. The strong asymmetry between the two sides, evident in Fig. 5, is caused by the large mass difference of the carriers between the GaSb side (where the heavy-hole mass dominates) and the InAs side. As the result of the small effective mass in InAs and the small overlap between the opposite bands in the junction plane, the electrons that flood from the GaSb to the InAs are relatively few. For the situation in Fig. 5 this number is $3.6\times10^{11}/\text{cm}^2$ for each junction, which corresponds to an electron density of $3.7\times10^{17}/\text{cm}^3$ at the interface on the InAs side, and $1.8\times10^{18}/\text{cm}^3$ on the GaSb side.

As the layer thicknesses further increase we approach the regime where the system cannot be regarded as a superlattice but rather as a succession of independent heterojunctions. The electronic structure is that of a set of conducting planes (the junctions) separated by insulating regions (the host materials). In estimating the width of the junction region, we have to deal with a well-known defect of the Fermi-Thomas approximation, namely, that it does not give a cutoff in the particle density. In our case it leads to an accumulated free-carrier concentration proportional to $(1+z/z_0)^{-6}$ which falls very rapidly away from the interface but remains finite everywhere. Consequently, we estimate that approximately twice the screening length gives the junction region. This means that free carriers penetrate ~1000 Å into the InAs and ~250 Å into the GaSb side of the interface. Finally, we note that the presence of large thermal carrier concentrations or of dopant impurities would significantly alter the profile of the junctions, but discussion of these effects is beyond the scope of the present paper.

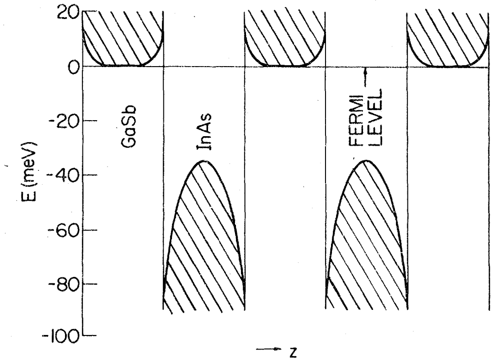

FIG. 5. Band edges of the superlattice hosts as a function of distance with each layer 500 Å thick. The shaded regions are gaps of the hosts. The region between the InAs shaded region and the Fermi level, for example, corresponds to occupied electronic states. As indicated by the position of the Fermi level the valence band of GaSb and the conduction band of InAs are only partly filled, showing semimetallic character.

VI. CONCLUSIONS

In a restricted energy region, around the fundamental gap, we have calculated by a simple procedure based on the LCAO method, the energy bands of InAs-GaSb superlattice for electron wave vectors perpendicular to the layers. Our calculation showed the existence of two distinct regimes in the superlattice band structure depending on the thickness of the layers. For thin layers confinement effects dominate just as in the familiar GaAs-$\text{Ga}_{1-x}\text{Al}_x\text{As}$ case. The superlattice in spite of the direct contact of filled and empty bands of the two host materials remains a semiconductor. The conduction-band states nearest to the gap are concentrated in the InAs and the corresponding states in the valence band are chiefly in the GaSb. The bands exhibit quasi-two-dimensional behavior as the layer thicknesses increase.[11] In the thick-layer limit, over ~115 Å for each host, the conduction and valence bands cross resulting in a semimetallic superlattice. We found that for the very thick layer limit a Fermi-Thomas approximation described the situation adequately.

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