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Electron and light-hole energy oscillations and band overlapping in semiconductor superlattices

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We have discovered that, in type-II misaligned-band semiconductor superlattices, electron and light-hole bands experience periodic anticrossing oscillations when we increase the layer thickness. These oscillations are induced by an overlapping of conduction and valence states which occur in these heterosystems. When the oscillations are damped by introducing interfacial strains, they may be restored by incorporating interlayer charge transfer. Our results reveal the existence of a stable energy level E_0 related to the valence- and conduction-band edges which shows a pinning behavior.

Because of the development of such modern growth techniques as molecular-beam epitaxy, metalorganic chemical vapor deposition, etc., a plethora of new classes of heterostructures which exhibit striking electronic properties has been fabricated. These systems are generally made of a stack of different host materials. The ensuing multilayered geometry is generated by a periodic repetition of a superunit cell larger than either of the unit cells of the host materials from which the heterosystem is built up. An optimized choice of an ensemble of host materials requires that the final heterostructure presents interfaces free of extended defects. However, the number of lattice-matched semiconductors, and consequently, the range of the device wavelengths which may be produced, is small. In order to overcome this difficulty, one may use lattice-mismatched materials. For layer thickness less than a critical thickness, the lattice mismatch may be accommodated by interfacial strains. These strains may modify the band structure of the heterosystem. We invoke here the effect of the inversion of the relative positions of the energy of heavy-hole (HH) and light-hole (LH) states at a certain layer thickness, leading to $E_{\rm LH}>E_{\rm HH}$. This, for example, is the case in an AlSb/GaSb/AlSb heterostructure.

In conventional homostructure-based devices, carriers are generally introduced by impurity donor atoms. When ionized, the latter transform into ions and constitute scattering centers which limit electron mobility. If one considers a heterostructure such as the broken-gap one (e.g., GaSb/InAs) the conduction-band edge E_C of InAs is lower than the valence-band edge E_V of GaSb. In a superlattice (SL) made of GaSb and InAs, this latter host material band feature may be recovered from the SL minibands by increasing the layer thickness L. While in each semiconductor, valence and conduction bands are separated by a band gap; in an SL, an overlapping exists between conduction and valence bands. This may result in intrinsic carrier confinement.

In this work, we study the semiconductor SL electronic features arising from the overlapping of SL minibands and we analyze the effect of interfacial strains on these features. As an application, we consider the cases of GaSb/InAs and GaSb/AlSb/InAs SL's.

Two models are used to calculate the electronic band structure of each host material (K) and of the SL.

(i) The two-band model[1] enables us to carry out analytical calculations within the framework of a method based on the use of the Green's functions to obtain the SL electronic structure. In this method, the electronic spectrum of each host material can be computed by using the corresponding bulk Green's function,

$$G_K(E)=\lim_{\varepsilon\to 0}[(E+i\varepsilon)I-H_K]^{-1}, \quad (1)$$

where E represents the energy, I is the identity matrix, and ε is an infinitesimal number. An SL reference response function G is then defined as a block diagonal matrix formed out of the set of $\{G_K\}$.

The Hamiltonian H_K has the general expression

$$H_K=\sum_S E_K(S)C^\dagger(S)C(S) - \sum_{S,\delta} \gamma_K(S,S+\delta)C^\dagger(S+\delta)C(S). \quad (2)$$

We then end up[1,2] with a three-parameter band model: conduction- (E_{CK}) and valence- (E_{VK}) band edges are represented by two orbital self-energies, respectively, associated with cations and anions constituting each semiconductor; γ_K is a hopping integral characterizing the nearest-neighbor interactions. In Eq. (2), $C^\dagger(S)$ and $C(S)$ are, respectively, the creation and annihilation operators for electronic excitations defined at the site S.

The next step in building up the SL is to produce from each infinite semiconductor K a slab of thickness L_K, keeping translational invariance parallel to the slab plane. This is done by removing all interactions between two adjacent principal layers $S=0$ and 1 on one hand and $S=L_K$ and L_K+1 on the other: this defines the surface creation operator V_K. The slab atomic planes are assumed to be polar, i.e., formed out of anions or cations.

Eventually, we couple all these slabs ($K=1,2,\ldots,N$) arranged in the configuration we choose, in order to create an SL unit cell, which repeated periodically along the growth axis, generates the SL lattice. The associated Hamiltonian is

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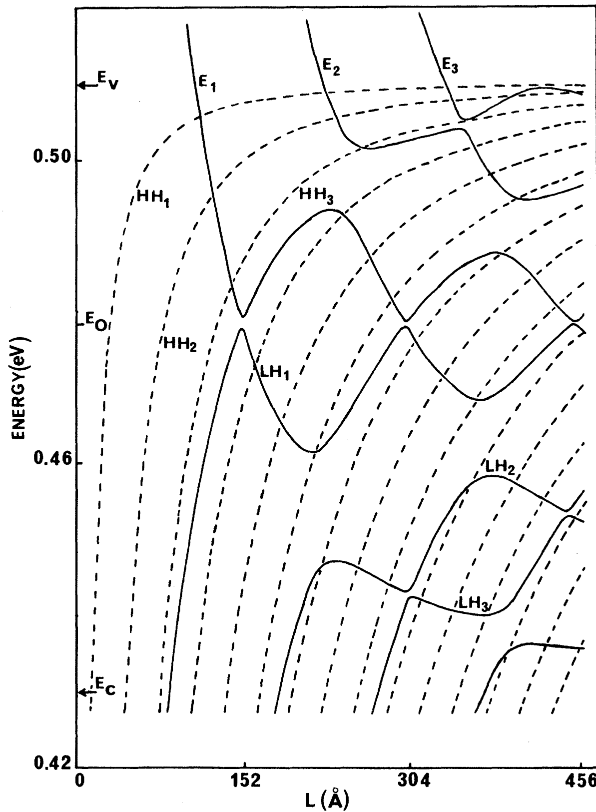

FIG. 1. Energy of lower conduction-band levels (E_i) and upper heavy-hole (HH_i) and light-hole (LH_i) valence-band levels, at the zone center, of GaSb/InAs SL as a function of the layer thickness L. These levels are calculated by using an sp^3s^* model. The tight-binding parameters do not take into account the spin-orbit interaction. The origin of energy is taken at the top of the valence band of bulk InAs. The valence-band offset is equal to 0.51 eV and the InAs band gap is equal to 0.43 eV.

$$H_I(nK;n'K')=\sum_{S,S'} V_I(nKS;n'K'S')C^\dagger(S')C(S), \quad (3)$$

where V_I represents the interface coupling operator which binds the free-surface slabs together.

The SL response function g can be calculated by using the general relationship

$$(I+A)g=G, \quad (4)$$

where A resumes all perturbations introduced to produce the SL. Once g is known, one can calculate the SL electronic structure.

(ii) In the sp^3s^* model, within the framework of tight-binding method, the bulk band structure of each material is described by the sp^3s^* hybrids.[3] Two sets of parameters are used, depending on whether we incorporate the spin-orbit interaction in the associated Hamiltonian[4] or not. Respectively, we deal with 20 and 10 bulk states per material for each value of the wave vector. The SL electronic structure is then computed by standard diagonalization of the SL Hamiltonian.

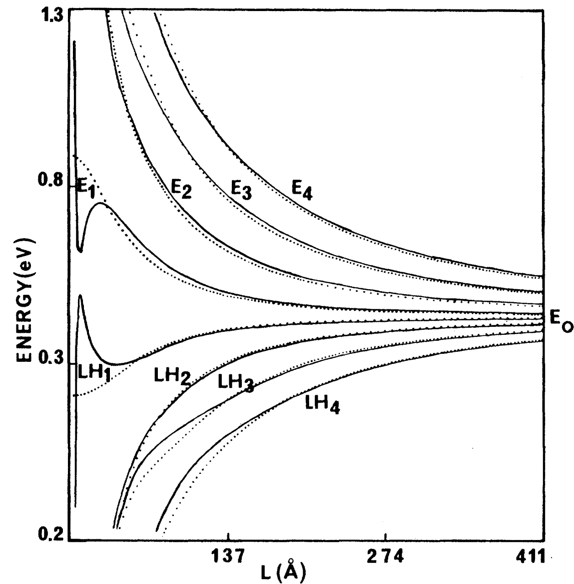

FIG. 2. Same as Fig. 1 but for a two-band model. Here, we take account of strains induced by lattice mismatch. The dotted curves represent the non-self-consistent solution. Solid lines show the bands when we incorporate charge transfer, limited to the first plane on both sides of each interface. Now the valence-band offset is equal to 0.43 eV and the band edges E_V(GaSb) and E_C(InAs) are very close, leading to a very narrow energy range of conduction- and valence-band overlapping.

In the response function method, the layer thickness appears as an explicit parameter, while in the diagonalization method, one must increase the size of the Hamiltonian matrix when the layer thickness increases, so the numerical calculations become heavier.

The GaSb/InAs SL is chosen to represent the type-II misaligned band SL family: GaSb and InAs present a small lattice mismatch, as their lattice parameters are, respectively, equal to 6.095 and 6.058 Å at room temperature. The interface geometry is such that two interfaces, namely, Ga-As and In-Sb, must be parametrized. This is done by using bulk GaSb and InSb tight-binding parameters. In this work, we give the results at the zone center. In order to simulate the SL conduction-band–valence-band overlapping, we calculate the energy of the corresponding states as a function of the host material layer thickness L, for the symmetric case, i.e., $L=L_1=L_2$. The results obtained by disregarding the spin-orbit interaction (sp^3s^* model) and the effect of interface strains are represented in Fig. 1. Two main effects must attract our attention: (i) The first one is the familiar crossover of the lowest conduction (E_1) and highest heavy-hole (HH_1) states at a critical layer thickness $L_C \cong 112$ Å. This may result in a semiconductor-semimetal transition,[5] which produces a confinement of intrinsic carriers periodically repeated throughout the SL, along its growth axis: electrons flow from the GaSb valence band to the InAs conduction band, leaving holes in the GaSb layers. (ii) If we increase the layer thickness beyond L_C, our results show that the energy of HH_1 states converges towards E_V, the GaSb valence-band maximum. This is the familiar host material regime.

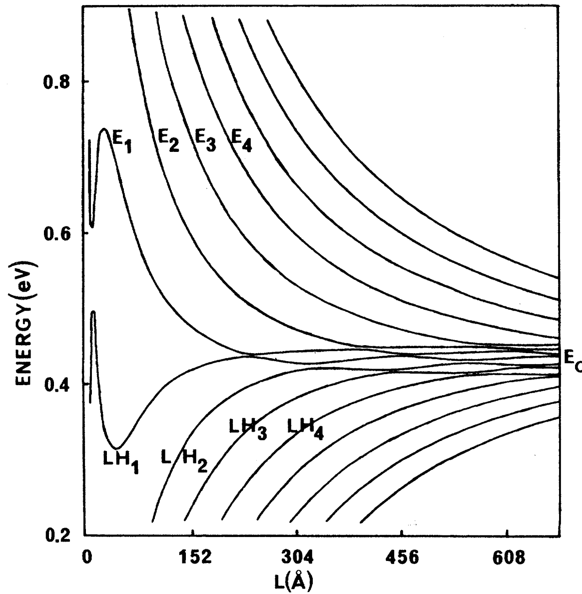

FIG. 3. Same as Fig. 2 but we now extend the charge transfer to several planes inside each host material.

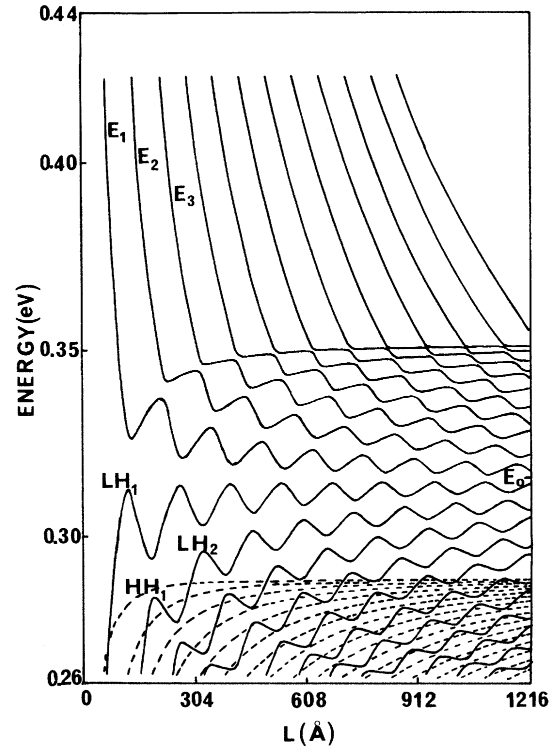

FIG. 4. Energy of lower conduction-band levels (E_i) and upper heavy-hole (HH_i) and light-hole (LH_i) valence-band levels, at the zone center, of a polytype GaSb/AlSb/InAs strained SL as a function of the thickness L of GaSb and InAs layers. We use a two-band model. E_V(GaSb)=0.351 eV, E_C(InAs)=0.255 eV. L_2=15 Å and the origin of energy is taken at the top of the valence band of bulk AlSb.

More striking is the behavior of the lowest E_1 state and the highest light-hole state (LH_1). We discover that E_1 and LH_1 show periodic and damped oscillations as functions of L, starting at $L \cong 150$ Å with a period equal to 150 Å. Eventually the oscillating levels collapse on an energy level E_0 calculated by using a simple rule:

$$E_0 = \tfrac{2}{3} E_V(\text{GaSb}) + \tfrac{1}{3} E_C(\text{InAs}). \tag{5}$$

We obtain, for $E_V = 0.51$ eV and $E_C = 0.43$ eV, $E_0 = 0.48$ eV, in agreement with the numerical value.

It is worth noting that our results are independent of the SL model and of the method of calculation. Indeed, if we include the spin-orbit interaction, the oscillations of E_1 and LH_1 are still present starting at a layer thickness and an energy level close to the latter values. We notice that $E_2, E_3, \ldots$ and $LH_2, LH_3, \ldots$ also show an oscillatory regime. However, the corresponding anticrossing energy levels are unstable and tend towards E_0.

Figure 2 shows the results obtained with a two-band model and a method based on the use of the Green's functions. The parameters take account of interface strains due to the host material lattice mismatch. Because of interface strains, the oscillatory regime has not yet been established for layer thickness up to 411 Å for the non-self-consistent solution (Fig. 2, dotted curves).

Let us give the physical meaning of the pinning level E_0. The bulk bands of the host material K are characterized by the energy and wave-vector-dependent parameter[6] $\zeta_K = -1 + (E - E_{CK})(E - E_{VK})/2f_K^2$, where f_K, defined in Ref. 6, is a function of the wave vector. At band edges E_{CK} and E_{VK}, $\zeta_K = -1$. For type-II SL's, when we vary the energy from E_{C2} to E_{V1}, with $E_{V1} > E_{C2}$, ζ_2, starting at -1, increases while ζ_1 approaches -1 by values greater than -1 until a crossover occurs ($\zeta_1 = \zeta_2$) at an energy exactly equal to E_0. Then E_0 appears as an energy level where host material bulk-band features align.

Let us now consider a self-consistent approach. To do so, we must allow for charge transfer across the interface and then introduce self-consistent potentials which arise from charge redistribution across the interface. We ensure that the charge neutrality condition is satisfied. The self-consistent results are represented in Fig. 2 (solid curves) for strained SL when the charge transfer is limited to the first plane on both sides of each interface. One can note the strong repulsive effect of the self-consistent potential on E_1 and LH_1 at a small layer thickness. This repulsive effect competes with the effect of increasing layer thickness L to produce one oscillation, followed by an asymptotic approach of the non-self-consistent solution at large L. When the charge transfer extends to several atomic planes, we discover that the oscillations are restored in the strained SL (Fig. 3).

We consider the case of a polytype SL $(\text{GaSb})_L/(\text{AlSb})_{L_2}/(\text{InAs})_L$ which adds to the latter the effect of the barrier AlSb, a material suitable for heteroepitaxy with GaSb and InAs ($a = 6.136$ Å). The considered geometry involves a three-layer configuration in each SL period where GaSb and InAs are separated by a barrier (AlSb) layer on one side of the InAs layer, while on the other side a direct AsIn/SbGa interface connects two adjacent SL unit cells. For

small L_2, the anticrossing E_1 and LH_1 levels are very close even at the beginning of the oscillation process for $L \cong 152$ Å. By increasing L_2, the separation between these latter levels increases and saturates at $L_2 \cong 15$ Å. For unstrained layers, we obtain $E_0 \cong 0.373$ eV in agreement with the above $(\frac{2}{3};\frac{1}{3})$ rule. For a strained SL (Fig. 4), we obtain an inversion of the HH_1 and LH_1 states: $E(LH_1) > E(HH_1)$. This is a well-known feature in structures where the active layer is under tension. The calculated anticrossing level E_0 is equal to 0.315 eV in agreement with the value obtained with the $(\frac{2}{3};\frac{1}{3})$ rule.

Comparing Figs. 2 (dotted E_1 and LH_1 curves) and 4, we note that the oscillatory behavior is strongly damped when we remove the barrier in the strained SL. As we have shown, E_0 depends on the relative positions of the band edges E_V(GaSb) and E_C(InAs). Although Fig. 4 corresponds to well-separated E_V and E_C levels, these levels are very close in the case of Fig. 2: this latter situation leads to a damping of the oscillation amplitudes and the oscillatory regime transforms into an asymptoticlike evolution of E_1 and LH_1 towards E_0. This is a straight result of the very small conduction- and valence-band overlapping which prevails for strained GaSb/InAs SL's where GaSb is under compression and InAs under tension. However, GaSb and InAs are both under tension because of the presence of the barrier layer in GaSb/AlSb/InAs: this results in an increase of the energy range of band overlapping, i.e., $E_V(\text{GaSb}) - E_C(\text{InAs})$.

In conclusion, we have shown that in type-II misaligned band SL, due to the overlapping of conduction and valence bands, periodic oscillations of the allowed electron and light-hole states' energy, as a function of layer thickness, are established. It is essential to understand that the oscillations of E_1 and LH_1 are triggered by an overlapping of valence and conduction bands of host materials: this can be seen in Fig. 2 where the oscillations are damped because of weak overlapping (dotted curves) and then resorted when a charge transfer takes place (solid lines). This means that charge transfer and band overlapping have similar effects on the behavior of E_1 and LH_1. Once the oscillations of E_1 and LH_1 are established, the oscillations of E_i and LH_i $(i>1)$ can be naturally explained in terms of interacting levels (E_j, E_{j+1}) and (LH_j, LH_{j+1}) with $j \geq 1$. Although the anticrossing behavior between E_1 and LH_1 for GaSb/InAs SL has been mentioned in Ref. 7, its oscillatory and periodic aspect has never been discussed. In Ref. 8, an anticrossing feature between electron and heavy-hole levels has been reported for the same SL for wave vectors in the plane of the layers. In Ref. 9, an anticrossing mechanism between $(HH_1 - HH_2)$ and $(E_1 - HH_2)$ levels has been reported for $Hg_xZn_{1-x}Te$/CdTe SL. In Ref. 10, a theoretical study of the interference effect between conduction-band levels in two multivalley SL's has been presented. The mechanism involved in these systems is basically different from the band overlapping mechanism invoked in this work. In a polytype GaSb/AlSb/InAs SL, we have shown that the periodic oscillations are still present even in the strained SL.

We demonstrate that our results are independent of the interaction model and of the method of calculation. We discover that the anticrossing level E_0, emerging as a result of conduction- and valence-band overlapping, shows a pinning behavior and we emphasize the relevance of E_0 to SL-based devices. We demonstrate that E_0 is an energy level where host material bulk band parameters align. Although the band oscillations may be damped in strained GaSb/InAs SL, they are restored by incorporating, in the model, charge transfer between the constituent host materials.

[1] M. D. Rahmani, P. Masri, and L. Dobrzynski, J. Phys. C **21**, 4761 (1988).
[2] G. A. Sai-Halasz, L. Esaki, and W. A. Harrison, Phys. Rev. B **18**, 2812 (1978).
[3] P. Vogl, H. P. Hjalmarson, and J. D. Dow, J. Phys. Chem. Solids **44**, 365 (1983).
[4] J. N. Schulman and Yia-Chung Chang, Phys. Rev. B **31**, 2056 (1985).
[5] L. L. Chang, N. Kaway, G. A. Sai-Halasz, R. Ludeke, and L. Esaki, Appl. Phys. Lett. **35**, 939 (1979).
[6] P. Masri, L. Dobrzynski, B. Djafari-Rouhani, and J. O. A. Idiodi, Surf. Sci. **166**, 301 (1986).
[7] G. Bastard, Phys. Rev. B **24**, 5693 (1981).
[8] M. Altarelli, Phys. Rev. B **28**, 892 (1983).
[9] Y. Guldner, J. Manasses, J. P. Vieren, M. Voos, and J. P. Faurie, Surf. Sci. **263**, 541 (1992).
[10] Yia-Chung Chang and D. Z.-Y. Ting, J. Vac. Sci. Technol. B **1**, 435 (1983).