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HAL Id: jpa-00249043
https://hal.archives-ouvertes.fr/jpa-00249043
Submitted on 1 Jan 1993

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Electronic properties of strained heterostructures

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(Received 10 November 1992, revised 11 February 1993, accepted 25 February 1993)

Résumé. — Dans cette communication, nous présentons une approche théorique des propriétés électroniques des hétérostructures composées d’une couche semiconductrice contrainte en sandwich entre deux semiconducteurs identiques. Notre calcul est basé sur la théorie des fonctions-réponse d’interface et sur un modèle à deux bandes permettant de décrire convenablement la structure électronique de volume des matériaux « hôtes ». Nous présentons des applications aux systèmes suivants : AlSb/GaSb/AlSb, InAs/GaSb/InAs et GaSb/InAs/GaSb. Les contraintes interfaciales dont nous tenons compte sont dues au désaccord de maille qui existe entre ces matériaux. Nous comparons la structure électronique calculée en présence de la contrainte interfaciale avec celle sans contrainte. Nous étudions par ailleurs l’effet de la variation de l’épaisseur de la couche intercalée sur les états électroniques de l’hétérostructure.

Abstract. — We present a theoretical study of the electronic properties of heterostructures composed of strained layers sandwiched between two identical semiconductors. The electronic structure is calculated by using the theory of interface response functions within the frame of a two band model which provides a reasonable description of the bulk electronic structure of the host materials. This theory is then applied to the heterostructures AlSb/GaSb/AlSb, InAs/GaSb/InAs and GaSb/InAs/GaSb. In our model, the strains are due to weakly-lattice mismatched materials. The evolution of the electronic structure is examined in function of the interfacial strains and of the sandwiched layer thickness.

1. Introduction.

Heterostructures are man-made systems in which a cleaver association of different semiconductors (host materials) aims to produce specific electronic features required for a particular application in electronics and optoelectronics. The fabrication of semiconductor heterostructures presenting a high degree of integration and high speed elementary operations relies on the reduction of their size. As far as the dimension perpendicular to the layer (growth axis) is concerned, this task may be achieved by modern growth techniques like molecular beam
epitaxy (MBE), metalorganic chemical vapor deposition (MOCVD), chemical beam epitaxy (CBE) and gaz source molecular beam epitaxy (GSMBE). It is then possible to fabricate, for example, very well controlled-quality heterostructures made of a semiconductor thin layer (e.g. GaAs well) sandwiched between two semiconductor layers (e.g. GaAlAs barriers). This heterostructure is in fact aimed to provide more efficient electronic and optoelectronic devices. In conventional devices, such that silicon-based homostructures, conduction electrons are introduced by impurity donor atoms. When ionized, these latter transform into ions and constitute scattering centers which may present a high scattering rate for collisions with electrons. This is especially true in heavily doped homostructures in order to obtain high conductivity systems. Such conductivity limitations due to impurity scattering do not exist in heterostructure-based devices. This latter feature can be understood on the following basis. When a contact is made between two semiconductors, there exists a band discontinuity between their electronic structures (band offsets). New electronic possibilities are then created by the spatial localization of the electrons injected by donor atoms in one of the two semiconductors (e.g. medium 1). The issue relies on the choice of the host materials and consequently on the relative position of the bands. If for example, the energy of the conduction electrons in semiconductor 2 is lower than the donor levels in semiconductor 1, an energy favorable situation triggers the electron localization in medium 2, while the interfacial barrier insures their localization, far enough from the highly doped region to avoid impurity scattering.

Depending on the relative positions of bandedges energies of the host materials, several types of heterostructures may be produced. In this article, we consider two types of heterostructure : (i) the first one, AlSb/GaSb/AlSb, belongs to the type I, where the bandgap of GaSb is completely embedded within that of AlSb ; (ii) the second example involves the host materials GaSb and InAs and provides a type II misaligned heterostructure, as the top of the valence band in GaSb is higher than the bottom of the conduction band in InAs. This band configuration triggers a flow of electrons from the topmost valence band of GaSb to the lowest conduction band in InAs. So we have electron accumulation in InAs and hole accumulation in GaSb. Two configurations are considered, depending on the nature of the sandwiched layers (GaSb or InAs), i.e. GaSb/InAs/GaSb and InAs/GaSb/InAs. For thin sandwiched layers, discrete levels may be created which add to the valence and conduction band continuum : this corresponds to the quantum well regime in which carriers have a bi-dimensional behaviour corresponding to well defined quantum states. At large thicknesses, carrier confinement is less effective and three-dimensional features establish.

In the next section, the formalism and the interaction model will be briefly recalled. In section 3, the results of the electronic structure calculation for the selected heterostructures will be presented and the effect of strains and of the sandwiched layer thickness will be studied.

2. Formalism and interaction model.

2.1 Formalism. — Our heterostructure model (see Fig. 1) involves a semiconductor layer (medium 2) sandwiched between two semi-infinite semiconductors : mediums 1 and 3. We then deal with two interfaces respectively between materials $1 \Rightarrow 2$ and $2 \Rightarrow 3$. The chosen heterostructures correspond to material-symmetrical configurations as the semiconductors 1 and 3 are identical. However, by assuming that the two semi-infinite semiconductors are terminated in polar surfaces, comprising respectively anions and cations, a kind of interfacial asymmetry is then introduced.

The method we use to calculate the heterostructure electronic spectrum is based on the interface response theory (see Ref. [1] for more details). In this approach, we start off with the bulk Green’s functions (reference functions) which are used to calculate the bulk electronic
structure of the host semiconductors 1, 2 and 3. All what we have to do is to calculate the interface response operator from which the heterostructure electronic states will be extracted. The latter spectral operator involves the perturbative interactions which are introduced in building up the heterostructure as explained below:

(i) out of the infinite semiconductor 2, a slab of thickness $L$ is created by removing all interactions between the principal layers $l = 0$ and 1 on one hand and $l = L$ and $L + 1$ on the other.

(ii) out of the infinite semiconductors 1 and 3, two semi-infinite crystals are created.

This procedure is represented by «cleavage» operator $V_S$.

(iii) then the slab 2 is inserted between these latter semi-infinite crystals by introducing interfacial interactions $\tilde{\gamma}$. These interactions are represented by the interface coupling operator $V_1$ which binds the free-surface slabs together.

The complete interface response operator $A'$ is then defined by the following relationship:

$$A' = V_S G_K + V_1 G$$

where $G$ is the bulk response function, giving all electronic bulk properties of the heterostructure material. This quantity $G$ is indeed the reference quantity in the theory and $G_K$ is the bulk response function for each semiconductor. The final energy spectrum associated with the heterostructure originates from the modified spectrum of $G$.

The elements of the heterostructure response function $g$ can be calculated by using the general relationship [1]

$$(I + A') \cdot g = G.$$  

$I$ is the unit matrix.

Once this response function is known, one can calculate the electronic spectrum associated with the heterostructure.

The general expressions of the different operators, have been given elsewhere [1].
2.2 Interaction Model. — A two-band model is used to describe the electronic structures of host semiconductors. The main features of the two-band model used in this work should first be brought to mind. It is possible to reasonably describe the lowest conduction band near the Brillouin-zone center and the valence bands for homogeneous and heterogeneous semiconductors. This is done by using a tight-binding Hamiltonian restricted by nearest-neighbor interactions and represented in a minimal basis consisting of one s- and three p-electron states, namely sp³ orbitals localized on each lattice site [2]. While the lowest conduction band is nondegenerate and has a minimum energy at the zone center, the upper valence band is doubly degenerate, consisting of heavy- and light-hole branches with a degeneracy occurring at the center of the Brillouin zone. Spin-orbit splitting drops one of the heavy-hole bands to lower energies. If one is interested in electron states falling in the neighborhood of the gap, it is possible to make further approximations by disregarding the s orbitals on the nonmetallic atoms in the compound and the p orbitals on the metallic atoms. This is true because their associated energies are situated outside the relevant energy domain, contributing slightly to the corresponding electron states.

The interaction parameters relevant to this model [3] include (i) two orbital self-energies, \( E_1 \) and \( E_2 \) associated with anions and cations constituting each semiconductor, and (ii) the hopping integrals \( \gamma_K \) characterizing the nearest-neighbor interactions. The Hamiltonian \( H_K \) associated with this model has the following expression:

\[
H_K(\ell \beta ; \ell' \beta') = \langle \ell \beta | H_K | \ell' \beta' \rangle
\]

with nonzero elements

\[
\langle \ell \beta | H_K | \ell \beta \rangle = E_\beta \quad \beta = 1, 2
\]

and nearest-neighbor off-diagonal elements (hopping integrals)

\[
\langle \ell 1 | H_K | \ell 2 \rangle = \gamma_K \quad K = 1-3
\]

with

\[
\langle \ell \beta | \ell' \beta' \rangle = \delta_{\ell \ell'} \delta_{\beta \beta'}
\]

where \( (\ell \beta) \) represents the position of the \( \beta \)-th-type basis atom in the \( \ell \)-th unit cell of the crystal; \( \beta = 1 \) or 2 for the two types of atoms in the unit cell.

The bulk electronic states of material of type (K) are then obtained in the form of the energy spectrum of the bulk response function \( G_K \) given by the following relationship:

\[
H_K G_K = I.
\]

The following dispersion relations are then obtained:

\[
E_K = \left( \frac{E_1 K + E_2 K}{2} \right) \pm \left( \left( E_1 K - E_2 K \right)/2 \right)^2 + \frac{1}{4} \left( \int \gamma_K \prod_{k=1}^{3} \cos^2 (k_i a_0/2) \right)^{1/2}
\]

where \( k_j = (k_1, k_2, k_3) \) is the wave vector. For (001) direction, we can use the wave-vector representation \([k_1 (k_1, k_2)]\) parallel to the (001) plane (Fourier transformation). The analytic expressions of the elements of \( G_K \) referring to type-1 and -2 atoms are [3]

\[
G_K(k_1, \ell 1 ; \ell' 1 ; E) = a_K t_{k}^{\ell - \ell' + 1} \left[ f_{k}^2 (t_K^2 - 1) \right],
\]

\[
G_K(k_1, \ell 2 ; \ell' 2 ; E) = - d_K t_{k}^{\ell - \ell' + 1} \left[ f_{k}^2 (t_K^2 - 1) \right].
\]
\[ G_K(k_1, t_1' ; t_2' ; E) = -\chi (t^f_k t^{-f \prime}_j + t^f_j t^{-f \prime}_k) \gamma [f^2_k t^2_k - 1] \]

\[ G_K(k_1, t_2 ; t_1' ; E) = -\chi (t^f_k t^{-f \prime}_j + t^f_j t^{-f \prime}_k) \gamma [f^2_k t^2_k - 1] \]

where

\[ a_K = E - E_{2K} \]
\[ d_K = E - E_{1K} \]
\[ \chi = e^{\mu L_1 + k v^2} \]
\[ f_K = 4 \gamma_K \cos (k_1 a/2) \cos (k_2 a/2) \]

\[ t_K = \begin{cases} 
\xi_K - (\xi^2_K - 1)^{1/2}, & \xi_K > 1, \\
\xi_K + i(1 - \xi^2_K)^{1/2}, & -1 < \xi_K < 1, \\
\xi_K + (\xi^2_K - 1)^{1/2}, & \xi_K < -1,
\end{cases} \]

with

\[ \xi_K(k_1, E) = -1 + a_K d_K/2 f^2_K. \]

In order to take account of the effect of strains resulting from the lattice mismatch, these parameters are appropriately modified according (i) to the values of the energy band offsets in presence of interfacial strains and (ii) to the strain matched interfacial lattice parameters.

A simple approach is used to the calculation of valence-band offsets at strained heterojunctions [4]. This method combines a fully strain-dependent version of the optimized tight-binding model with Tersoff's quantum-dipole heterojunction model. Offsets calculated using this combined approach are shown to agree with experimental data better than either strain-dependent natural tight-binding offsets or offsets calculated directly from Tersoff's model.

3. Results.

In what follows, the results for three heterostructures, based on antimonide compounds and InAs will be given. These are analysed in function of strains and of the thickness \( L \) of the sandwiched layer.

3.1 InAs/GaSb/InAs and GaSb/InAs/GaSb Heterostructures. — With regards to the relative positions of band edges (valence and conduction) of the host materials GaSb and InAs, different carrier confinements may be obtained:

(i) The InAs/GaSb/InAs heterostructure may provide a well for heavy and light holes.
(ii) The GaSb/InAs/GaSb heterostructure may provide a well for electrons.

The results concerning the former heterostructure are represented in figures 2 respectively for unstrained (2a) and strained (2b) interfaces.

Here we deal with a GaSb thin layer uniformly compressed in the layer plane to match the lattice constant of InAs. As we can see, the effect of strains on the bulk electronic structure is to lift off the degeneracy between the bulk heavy- \( \left(E_{hh}\right) \) and light-hole \( \left(E_{lh}\right) \) levels in GaSb. The valence band offsets in presence of strains are equal to 0.48 eV and 0.43 eV respectively for heavy- and light-hole levels. These values are in agreement with other estimations [5-9].

The comparison with the unstrained bulk band edges (Fig. 2a) shows that the strains shift these levels downward by an amount respectively equal to 20 meV \( \left(E_{hh}\right) \) and 80 meV \( \left(E_{lh}\right) \). However, as \( E_{hh} \) and \( E_{lh} \) are above the level \( E_c \) in InAs, the strained heterostructure remains of type-II misaligned for both heavy and light holes. The net effect is an increase of the bandgap of GaSb by an amount equal to 85 meV. This effect may be understood on the basis
that a lattice compression induces effects analogous to those due to a temperature decrease. The other effect is that the shift of $E_{\text{LH}}$ is larger than that of $E_{\text{HH}}$. This association of host materials provides a type II-misaligned heterostructure with a completely broken-gap band alignment and an overlapping between the GaSb valence band (the heavy-hole band edge) and the InAs conduction band approximately equal to 0.13 eV. This may allow interband transport. This kind of broken-gap heterostructure has led to several novel devices [10, 11].

The figure 3 shows several discrete heavy and light holes levels falling within the bulk valence band of GaSb. It is some of these states which may be relevant to resonant interband tunneling or coupling processes, especially those positioned at an energy comparable to the Fermi energy in the InAs conduction band. Moreover, because of their much wider energy distribution, light-hole resonances show stronger coupling with InAs conduction-band states than do GaSb-heavy-hole states [12]. Consequently, light-hole states may be more relevant to the transport mechanisms, and especially the first $E_{\text{LH}}$ level.

The next heterostructure we consider is GaSb/InAs/GaSb. This provides a well for electrons. Recently, this system has been applied to the hot-electron transistors, and room temperature operation has been realized [13, 14]. In this case, the lattice of the thin InAs layer is uniformly

Fig. 2. — Electronic structure of InAs/GaSb/InAs heterostructures for unstrained (2a) and strained (2b) interfaces. The thickness of the GaSb sandwiched layer is 10 monolayers (= 30 Å).

Fig. 3. — The same as the figure 2b with 30 monolayers (= 90 Å) width of GaSb slab. The resonance states appear between GaSb valence band and InAs conduction band.
extended in the layer plane to match the larger lattice constant of GaSb. The comparison of figures 4a and 4b reveals that the effect of strains on the bulk electronic structure is to lift off the degeneracy between the heavy- \((E_{\text{HH}})\) and the light-hole \((E_{\text{LH}})\) levels in InAs. Contrarily to the previous case, the fundamental gap transforms into an electron-light-hole gap. It seems that this situation is not specific of the particular choice of host materials but involves the fact that the InAs sandwiched layer is in extension after its contact with the surrounding lattices of GaSb. A such tendency to form a fundamental light-hole to conduction electron band gap has been demonstrated for GaSb/AlSb superlattices where the GaSb layers are much thinner than

Fig. 4. — Electronic structure of GaSb/InAs/GaSb heterostructure for unstrained (4a) and strained (4b) interfaces. The thickness of the InAs sandwiched layer is 10 monolayers (= 30 Å). A resonant level \(E_1\) appears between InAs conduction band and GaSb valence band.

Fig. 5. — Electronic structure of AlSb/GaSb/AlSb heterostructure for unstrained (5a) and strained (5b) interfaces. The thickness of the GaSb sandwiched layer is 10 monolayers (= 30 Å). Both electron- and hole-states are confined in GaSb layer.
AlSb layers and consequently more strained (lattice in extension) than AlSb layers [15]. Our calculation is also in agreement with the measured ground quantum level and the calculated one based on envelope function method [16].

The results are depicted in figures 4 respectively for unstrained (4a) and strained (4b) heterostructures. The calculated electronic structure shows several InAs confined states, and a state $E_1$ resonant with the GaSb valence band in agreement with other results [17].

3.2 AlSb/GaSb/AlSb HETEROSTRUCTURE. — This heterostructure provides a well for electrons and holes. This system corresponds to a configuration in which the GaSb lattice is in extension. The results are represented in figure 5 respectively for unstrained (5a) and strained (5b) layers. We find again that the effect of strains is : (i) to lift off the degeneracy between the bulk heavy- ($E_{\text{HH}}$) and light-hole ($E_{\text{LH}}$) levels in GaSb, and (ii) to produce a fundamental light-hole to conduction electron band gap, in agreement with other results [15]. The calculated electronic structure shows several states which may be relevant to transport processes. The figure 6 shows the evolution of the first levels $E_1$, $E_{\text{HH}}$, and $E_{\text{LH}}$ in function of the thickness $L$ of the GaSb layer. As $L$ increases a crossover between the levels $E_{\text{LH}}$ and $E_{\text{HH}}$ occurs. This effect is well understood on the basis of photoluminescence and electroreflectance experiments.

![Diagram](attachment:image.png)

Fig. 6. — The evolution of the electronic structure of AlSb/GaSb/AlSb in function of the sandwiched layer thickness. A crossing occurs between the levels $E_{\text{LH}}$ and $E_{\text{HH}}$ when the thickness of GaSb layer is 16 monolayers.
In our heterostructure model, this crossover occurs because of the introduction of interfacial strain in taking up the lattice mismatch. Accordingly, it is shown in reference [15] that in such heterosystem, the effect of in-layer strain is to transform the band structure in such a way that the first light hole level is the ground QW valence state. This shows that our simple model reproduces such fundamental aspect of the strain-induced modification of the QW valence band structure.

4. Conclusion.

In this article, the electronic structure of several heterostructures are calculated, within the framework of a two band model and by using the interface response theory. The effects of strain and of the layer thickness are analysed. Our study reveals several striking features as:
(i) the occurrence of resonant and confined quantum well states;
(ii) the crossover of light-hole and heavy-hole states;
(iii) the formation of fundamental light-hole to conduction electron band gap.

References

