In-plane dispersion relations of InAs/AlSb/GaSb/AlSb/InAs interband resonant-tunneling diodes

J. Genoe*

*Laboratoire des Champs Magnétiques Intenses, Centre National de la Recherche Scientifique, Boîte Postale 166,
F-38042 Grenoble CEDEX 9, France*

K. Fobelets

Physics Department, Trinity College Dublin, Dublin 3, Ireland

C. Van Hoof and G. Borghs

IMEC vzw, Kapeldreef 75, B-3001 Leuven, Belgium

(Received 14 April 1995; revised manuscript received 2 August 1995)

We report on a flexible eight-band model, derived from a modified Kane base, generating a transfer-matrix formalism to calculate the transmission probability of carriers through, and the in-plane dispersion relations of, stratified media. We apply this model to study InAs/AlSb/GaSb/AlSb/InAs interband resonant-tunneling diodes. We show that the boundary-condition sets deduced from current continuity and the boundary-condition sets deduced from a Hermitian Hamiltonian defined across the interface are equal. A simplified triple-band model is found to be a good approximation to calculate the deep light-hole energy levels in a resonant interband tunneling diode. However, these simplified triple-band approximations are no longer valid when the carriers have an in-plane momentum.

I. INTRODUCTION

In recent years tremendous experimental and theoretical investigations have been done on intraband¹ and interband² tunneling diodes, not only due to their promising features for high speed applications³ and new optoelectronic devices,⁴ but also because of the huge range of components⁵ they generate. These devices are appealing to study experimentally and theoretically because of the more fundamental parameters of the quantum processes which are involved in these structures.

Intraband resonant-tunneling diodes (RTD's) are normally grown by molecular-beam epitaxy in III-V materials, typical GaAs/AlAs materials. In resonant interband tunneling diodes (RIT's), the material system is typically InAs/AlSb/GaSb, where AlSb forms the potential barriers. InAs (GaSb) can be used as an *n*- (*p*)-type contact material with a GaSb (InAs) quantum well. The transport process of carriers in these structures is interband, as in the Esaki diodes. The special feature of RIT's is that the contact and quantum-well material form a broken band gap because the bottom of the conduction band of InAs is lower than the top of the valence band in GaSb. A schematic band diagram of the RIT studied in this paper is given in Fig. 1.

The theoretical description of the tunneling process can be done in two ways. One can assume that the transport is sequential or coherent. In this work the coherent tunneling approach is applied in a transfer matrix formalism to calculate the transmission probability of carriers through the multilayer structure.

The coherent tunneling process through unipolar RTD's has already been extensively studied using a single-band model,⁶ when tunneling in the conduction band is considered, and a four-band⁷⁻¹¹ model when tun-

neling in the valence band is considered. However, when RIT's are studied both the conduction and valence bands have to be taken into account for it is an interband tunneling process. Three-band models, valid for the case where the wave vectors perpendicular to the propagation direction of the carriers are zero, have been developed.^{12,13} Multiple band models have also been used to calculate the band structure and dispersion relations of type-I (Ref. 14) and -II superlattices.¹⁵

The models to calculate the transmission probability through multilayer structures based on the envelope-function approximation (EFA) are determined by the boundary conditions between the different layers. The exact definition of these boundary conditions is the cause

FIG. 1. Band structure of the interband tunneling structure under investigation. The band gap is indicated by the grayed area. The conduction, light-hole, heavy-hole, and spin-split-off bands are given in the Γ minimum. The zero point for the energy scale is chosen to be the bottom of the conduction band of GaAs.

of some confusion. This confusion is mainly due to the fact that the Hamiltonian operator has to be Hermitian for varying material constants across the interface. Two equivalent methods can be found to define the boundary conditions, namely the use of border conditions deduced from the current continuity condition, and border conditions deduced from the integration of the Hermitian Hamiltonian across the interface. We show in this work that both approaches to determine the boundary conditions give the same transfer matrices.

Due to the difficulties of numerical accuracy, a transfer-matrix method beyond four bands has not yet been implemented to calculate the tunneling probability. In this work, however, we present a transfer matrix formalism for eight bands: conduction, light hole, heavy hole, and spin-split-off band for both spin orientations. The influence of the remote bands on the carriers in the structure is also taken into account. The transfer-matrix method developed can be applied to arbitrary stratified media, although the calculation time grows with the amount of layers in the structure. This paper is organized as follows. In Sec. II the theory for the eight-band effective-mass equation is developed based upon the framework of the $\mathbf{k}\cdot\mathbf{p}$ model that is used in the theory of the electronic band structure of bulk materials. However, we start from a slightly modified Luttinger-Kohn basis¹⁶ which makes calculations and physical interpretation more straightforward. The Hamiltonian is given explicitly. The method to determine the transfer matrices is based upon the current continuity conditions. In Sec. III we show that the current continuity conditions and the integration of the Hermitian Hamiltonian across the interface generate the same transfer matrices. In Sec. IV we discuss the influence of the in-plane dispersion rela-

tion on the transmission probability in the case of an InAs/AlSb/GaSb resonant interband tunneling diode. In Sec. V we demonstrate the simplified triple-band model. We compare the full eight-band method to the better known single- and double-band transfer-matrix methods. In Sec. VI the conclusions are summarized.

II. THEORY

The theory of the envelope-function approximation (EFA) is normally used to calculate multilayer tunneling in one band, but can be extended to incorporate the effects of multiple bands. The eight-band Hamiltonian for bulk materials has already been the subject of many papers and textbooks. To use this description in stratified media the same requirements on the lattice-periodicity conservation in the structure must be imposed as in the single-band model, such that Bloch's theorem will be valid.

In this section, we incorporate the effect of the electron, light-hole, heavy-hole, and spin-split-off bands for both spin orientations in the EFA. We used the Luttinger-Kohn model,^{16,17} similar to Ram-Mohan,¹⁴ to construct the multiband Hamiltonian. However, we made a different choice of the Kane basis¹⁸ to construct the periodic parts of the Bloch functions for a (100) substrate orientation. We permuted the Kane basis functions $|2\rangle$, $|3\rangle$, and $|6\rangle$, in a cyclic way and interchanged $|4\rangle$ and $|8\rangle$ to obtain eigenvectors (at $k_{\perp}=0$) that consist of either a dominant spin-up or a dominant spin-down part. The choice of this basis has more intrinsic logic, and also results in better numerical procedures to obtain the eigenvectors. The following basis functions are used to construct the multiband Hamiltonian:

$$\begin{aligned} |1\rangle &= |\tfrac{1}{2}, \tfrac{1}{2}\rangle = |iS\uparrow\rangle, \text{ conduction band (C)}, \\ |2\rangle &= |\tfrac{3}{2}, \tfrac{1}{2}\rangle = -\sqrt{\tfrac{3}{2}}|Z\uparrow\rangle + \sqrt{\tfrac{1}{6}}|(X+iY)\downarrow\rangle, \text{ light-hole band (LH)}, \\ |3\rangle &= |\tfrac{3}{2}, \tfrac{3}{2}\rangle = \sqrt{\tfrac{1}{2}}|(X+iY)\uparrow\rangle, \text{ heavy-hole band (HH)}, \\ |4\rangle &= |\tfrac{1}{2}, \tfrac{1}{2}\rangle = \sqrt{\tfrac{1}{3}}|Z\uparrow\rangle + \sqrt{\tfrac{1}{3}}|(X+iY)\downarrow\rangle, \text{ spin-split-off band (SSO)}, \\ |5\rangle &= |\tfrac{1}{2}, -\tfrac{1}{2}\rangle = |iS\downarrow\rangle, \text{ conduction band (C)}, \\ |6\rangle &= |\tfrac{3}{2}, -\tfrac{1}{2}\rangle = -\sqrt{\tfrac{2}{3}}|Z\downarrow\rangle - \sqrt{\tfrac{1}{6}}|(X-iY)\uparrow\rangle, \text{ light-hole band (LH)}, \\ |7\rangle &= |\tfrac{3}{2}, -\tfrac{3}{2}\rangle = \sqrt{\tfrac{1}{2}}|(X-iY)\downarrow\rangle, \text{ heavy-hole band (HH)}, \\ |8\rangle &= |\tfrac{1}{2}, -\tfrac{1}{2}\rangle = \sqrt{\tfrac{1}{3}}|Z\downarrow\rangle - \sqrt{\tfrac{1}{3}}|(X-iY)\uparrow\rangle, \text{ spin-split-off band (SSO)}. \end{aligned}$$

The functions $|S\rangle$, $|X\rangle$, $|Y\rangle$, and $|Z\rangle$ have the following symmetry properties: $|S\rangle$ is symmetric in x , y , and z ; $|X\rangle$ is antisymmetric in x but symmetric in y and z and analogous for $|Y\rangle$ and $|Z\rangle$. $\uparrow$ and $\downarrow$ are spin functions corresponding, respectively, to up and down.

The solutions associated with the first (last) four basis functions have a dominant spin-up (-down) behavior. In the calculations we take the z direction as the propagation direction. The x - y plane is parallel to the layer structure.

The 8×8 effective Hamiltonian of this system can be written in a simplified way as

$$H = \begin{bmatrix} HA & HB \\ HC & HD \end{bmatrix} + V(z), \quad (1)$$

where $V(z)$ is the potential variation through the structure, and

$$\begin{aligned}
HA &= \frac{\hbar^2}{m_0} \begin{bmatrix} (F + \frac{1}{2})k^2 & -\sqrt{\frac{2}{3}}Pk_z & Pk^+ & \frac{1}{\sqrt{3}}Pk_z \\ -\sqrt{\frac{2}{3}}Pk_z & -\frac{1}{2}\gamma_1 k^2 - F_3^1 & \sqrt{3}F_4^+ & \sqrt{2}F_3^1 \\ Pk^- & \sqrt{3}F_4^- & -\frac{1}{2}\gamma_1 k^2 + F_3^1 & -\sqrt{\frac{3}{2}}F_4^- \\ \frac{1}{\sqrt{3}}Pk_z & \sqrt{2}F_3^1 & -\frac{3}{2}F_4^+ & -\frac{1}{2}\gamma_1 k^2 \end{bmatrix} + \begin{bmatrix} E_c & 0 & 0 & 0 \\ 0 & E_v & 0 & 0 \\ 0 & 0 & E_v & 0 \\ 0 & 0 & 0 & E_s \end{bmatrix}, \\
HB &= \frac{\hbar^2}{m_0} \begin{bmatrix} 0 & -\frac{1}{\sqrt{3}}Pk^- & 0 & -\sqrt{\frac{2}{3}}Pk^- \\ \frac{1}{\sqrt{3}}Pk^- & 0 & F_3^2 - iF_4^z & -\frac{3}{\sqrt{2}}F_4^- \\ 0 & -F_3^2 + iF_4^z & 0 & -\sqrt{2}(F_3^2 - iF_4^z) \\ \sqrt{\frac{2}{3}}Pk^- & \frac{3}{\sqrt{2}}F_4^- & \sqrt{2}(F_3^2 - iF_4^z) & 0 \end{bmatrix}, \\
HC &= \frac{\hbar^2}{m_0} \begin{bmatrix} 0 & \frac{1}{\sqrt{3}}Pk^+ & 0 & \sqrt{\frac{3}{2}}Pk^+ \\ -\frac{1}{\sqrt{3}}Pk^+ & 0 & -F_3^2 - iF_4^z & \frac{3}{\sqrt{2}}F_4^+ \\ 0 & F_3^2 + iF_4^z & 0 & \sqrt{2}(F_3^2 + iF_4^z) \\ -\sqrt{\frac{2}{3}}Pk^+ & -\frac{3}{\sqrt{2}}F_4^+ & -\sqrt{2}(F_3^2 + iF_4^z) & 0 \end{bmatrix}, \\
HD &= \frac{\hbar^2}{m_0} \begin{bmatrix} (F + \frac{1}{2})k^2 & -\sqrt{\frac{2}{3}}Pk_z & Pk^- & \frac{1}{\sqrt{3}}Pk_z \\ -\sqrt{\frac{2}{3}}Pk_z & -\frac{1}{2}\gamma_1 k^2 - F_3^1 & \sqrt{3}F_4^- & \sqrt{2}F_3^1 \\ Pk^+ & \sqrt{3}F_4^+ & -\frac{1}{2}\gamma_1 k^2 + F_3^1 & -\sqrt{\frac{3}{2}}F_4^+ \\ \frac{1}{\sqrt{3}}Pk_z & \sqrt{2}F_3^1 & -\sqrt{\frac{3}{2}}F_4^- & -\frac{1}{2}\gamma_1 k^2 \end{bmatrix} + \begin{bmatrix} E_c & 0 & 0 & 0 \\ 0 & E_v & 0 & 0 \\ 0 & 0 & E_v & 0 \\ 0 & 0 & 0 & E_s \end{bmatrix},
\end{aligned}$$

with

$$P = \sqrt{m_0 E_p / 2\hbar^2},$$

$$k^2 = k_x^2 + k_y^2 + k_z^2,$$

$$k^\pm = \frac{1}{\sqrt{2}}(k_x \pm ik_y), \quad \gamma_1 = \gamma_1^L - \frac{E_p}{3E_g},$$

$$F_3^1 = \frac{1}{2}\gamma_2(2k_z^2 - k_x^2 - k_y^2), \quad \gamma_2 = \gamma_2^L - \frac{E_p}{6E_g},$$

$$F_3^2 = \frac{\sqrt{3}}{2}\gamma_2(k_x^2 - k_y^2),$$

$$F_4^\pm = \gamma_3 k_z(k_x \pm ik_y), \quad \gamma_3 = \gamma_3^L - \frac{E_p}{6E_g},$$

$$F_4^z = \sqrt{3}\gamma_3 k_x k_y.$$

k is the total wave vector. P gives the coupling between the different bands which are taken into account in the Hamiltonian. F is the parameter introduced to describe the effect on the electrons of the remote bands which are not included in the Hamiltonian. The Luttinger parameters (γ^L) correct the effective mass in the calculation for the neglect of the other bands. It is therefore straightfor-

ward that these correction terms will be dependent on the number of bands which are taken into account. The γ terms used in the calculations are the modified Luttinger parameters for the eight-band model.¹⁹ The material parameters F , γ_i^L (with $i=1, \dots, 3$), and E_p can be found in literature²⁰ for the different materials. E_c , E_v , and E_s , respectively, are the bottom of the conduction band, the top of the valence band, and the top of the spin-split-off band at $k=0$. $\hbar$ is the reduced Planck constant, and m_0 is the free-electron mass. The influence of a magnetic field is not introduced in this Hamiltonian. It can, however, be added to the model according to Ref. 14.

The Hamiltonian H is Hermitian. The elements in the matrix give the coupling with the different bands as follows: columns 1-8 and rows 1-8 correspond at $k=0$ with the $C\uparrow$ band, the $LH\uparrow$ band, the $HH\uparrow$ band, the $SSO\uparrow$ band, the $C\downarrow$ band, the $LH\downarrow$ band, the $HH\downarrow$ band, and the $SSO\downarrow$ band, respectively. As we can see from the shape of the matrix, the chosen basis results in a Hamiltonian which can be divided into four matrices with a specific physical meaning. Matrices HA and HD , respectively, give the Hamiltonian of the four bands without coupling between the two opposite spin directions, but with coupling of the different bands of the same spin. We see that the elements of one matrix are the complex con-

jugate of the corresponding elements of the other matrix. These small matrices are also Hermitian. The matrices HB and HC give the coupling between states with dominant spin-up and states with dominant spin-down. The elements of these matrices are also the complex conjugates of each other multiplied by -1 , which is a result of the hermiticity of the Hamiltonian H . It is easy to see that with the in-plane momenta k_x and k_y at zero, these matrices are zero, and both spin orientations are uncoupled. Therefore, to construct the Hamiltonian with the chosen basis, it is sufficient to construct matrices HA and HB .

To calculate the transmission probability of a carrier with a given energy E and a given in-plane momentum (k_x, k_y) through the total structure, we need first to solve the eigenvalue-eigenvector relation $H\Psi = E\Psi$ for each layer. In every layer, four k_z values are obtained, which are all twice degenerate. Eight eigenvectors are obtained, corresponding to each state. When there is no in-plane momentum ($k_x = k_y = 0$), the complexity of the calculations will be strongly reduced because both HB and HC are zero matrices and HA equals HD . The order of the system then becomes 4, and the spin-up and spin-down states are uncoupled. Moreover, the heavy-hole solution is in this case independent of the other solutions. This reduces the order further, respectively, to 3 (coupling between conduction, light-hole and split-off bands) and 1 (the heavy-hole band). Several authors have already published calculations of the tunneling probability through interband devices without the incorporation of the in-plane momentum.^{13,21}

To construct a transfer matrix which couples the solutions in the different layers across the interface, we used the continuity of the wave functions and the current-conserving boundary conditions between the different layers in which symmetry and hermiticity were fulfilled, as has been indicated in Ref. 12. In Sec. III we will show that these conditions give identical results as the integration of the Hermitian Hamiltonian across the interface.

The eigenvectors and the transfer matrix are determined numerically because of their complexity. In Sec. V we will give in more detail the shape of the eigenvectors and the continuity conditions in the discussion of the model for the triple-band effective-mass equation.

The eight-band model has been implemented in a transfer-matrix algorithm using the MATHEMATICA (Ref. 22) program. This programming environment allows to do the calculations with arbitrary high precision, which makes these calculations possible. For each interface in the structure a 16×16 transfer matrix is obtained, and the global transfer matrix of the structure is the product of the matrices across all interfaces.

In order to calculate the transmission probability through stratified media, we have to consider one incident wave and all transmitted and reflected waves. This means that, e.g., when spin-up electrons are injected into the structure, different types of carriers can occur in the input layer through reflection at the interface, and that there also exists a finite probability to find different carrier types in the collector layer. This transforms the global transfer matrix of the structure into a set of 16 cou-

pled equations. By solving this set of equations, the solution for the tunneling probability can be found.

During the calculations, fast rising and decaying exponential terms occur which are generated by states that are too far in a forbidden energy range and that do not contribute. For reasons of accuracy and calculation time these terms have to be restricted. This has been done as follows. When we restrict the maximum imaginary k vector to $k_{\max}$ the required working precision w to obtain a final given accuracy a , is

$$w = a + \frac{l_{\text{tot}} \times k_{\max}}{\ln(10)} \quad (2)$$

where l_{tot} is the total length.

In this work we restrict $k_{\max}$ to 6 nm^{-1} ; i.e., we do not allow wave functions to decay or increase faster than a factor 20 in one unit cell of the crystal. This requires a working precision of ~ 60 digits. Reducing the maximum imaginary k vector further will reduce the required working precision further, and can shorten the required calculation time, but the resonant enhancement of the wave functions amplitude in the quantum well is also reduced in this way. The reduction of the resonant enhancement in the quantum well reduces the height of the peaks in the tunneling probability. Because of the different matrix and vector manipulations in this calculation, the Gram-Schmidt orthogonalization procedure is used to construct a set of orthogonal eigenvectors, belonging to each momentum vector.

It is important to note that to calculate the tunneling probability of one carrier through the structure, a set of equations determined by the obtained transfer matrix has to be solved. The accuracy of this set of equations is determined by the least accurate equation, which will quite often correspond to a remote band. The calculation of the eigenstates in stratified structures is usually not so stringent on the accuracy of the transfer matrix.

III. BOUNDARY CONDITIONS

To determine the boundary conditions, the wave functions are taken as continuous across the interface. Later, however, some confusion has arisen as to the technique to determine the boundary conditions for the derivatives. Two equivalent methods exist: the integration of the Hamiltonian,^{23,24} and the probability-current continuity condition¹⁵ across the interface. The integration technique (integration of the bulk Hamiltonian) is not straightforward due to varying Luttinger parameters and momenta P in the layers. Overlooking these variations gives a non-Hermitian Hamiltonian.

In what follows, we deduce the Hermitian shape of the Hamiltonian across the interface, determine the boundary conditions by integration, and compare these with the current continuity. We show that the latter method allows some freedom in the boundary conditions, which corresponds to a δ -function potential in the Hamiltonian.

The integration method consists of two steps: the construction of a Hermitian Hamiltonian operator for varying material constants, and the derivation of the boundary conditions.

For varying P , neglecting the fact that this implies that the Bloch functions are not continuous across the interface, the Hamiltonian is

$$H = \left[\frac{\partial}{\partial z} A \frac{\partial}{\partial z} + \frac{1}{2} \left[\frac{\partial}{\partial z} B + B \frac{\partial}{\partial z} \right] + C \right], \quad (3)$$

with matrices $A(\gamma_1, \gamma_2)$, $B(P, \gamma_3)$, and $C(V, \dots)$.

At $z = z_0$ a discontinuity in the matrices A and B exists:

$$A(z) = A_L + \theta(z - z_0)(A_R - A_L),$$

$$B(z) = B_L + \theta(z - z_0)(B_R - B_L),$$

with $\theta(z)$ the step function.

To determine the boundary conditions, we integrate the eigenvalue-eigenvector equation around $z = z_0$. H is the Hamiltonian operator given by Eq. (3), ψ is an eigenfunction with eigenvalue E , and ε and η are small positive numbers:

$$\begin{aligned} \int_{z_0 - \varepsilon}^{z_0 + \eta} (H\psi - E\psi) = & \left[A \frac{\partial \psi}{\partial z} \right]_{z_0 - \varepsilon}^{z_0 + \eta} + \frac{1}{2} (B\psi) \Big|_{z_0 - \varepsilon}^{z_0 + \eta} \\ & + \int_{z_0 - \varepsilon}^{z_0 + \eta} \left[\frac{1}{2} B \frac{\partial \psi}{\partial z} + (C - E)\psi \right] = 0. \end{aligned}$$

Taking the limit $\varepsilon \rightarrow 0$ and $\eta \rightarrow 0$, and supposing finite discontinuities of the integrand at the interface, gives

$$\left[A \frac{\partial \psi}{\partial z} \right]_L^R + \frac{1}{2} (B\psi) \Big|_L^R = 0. \quad (4)$$

The indices L and R , respectively, describe the left-hand-side and the right-hand-side values. When the momentum P and δ_3 are constant, the boundary conditions reduce to the first term in (4).^{23,24}

We now compare these conditions to the current continuity, using Eq. (3):

$$\begin{aligned} \frac{\partial \psi^+ \psi}{\partial t} &= \psi^+ (H\psi) - (H\psi)^+ \psi \\ &= \text{div} \left[\psi^+ A \frac{\partial \psi}{\partial z} - \frac{\partial \psi^+}{\partial z} A \psi + \psi^+ B \psi \right] = \text{div}(J). \end{aligned}$$

The current can then be written as

$$J \approx \psi^+ \left[A \frac{\partial \psi}{\partial z} + \frac{1}{2} B \psi \right] - \left[A \frac{\partial \psi}{\partial z} + \frac{1}{2} B \psi \right]^+ \psi. \quad (5)$$

The current conservation condition ($J_L = J_R$) gives

$$\left[A \frac{\partial \psi}{\partial z} + \frac{1}{2} B \psi \right] \Big|_L = \left[A \frac{\partial \psi}{\partial z} + \frac{1}{2} B \psi \right] \Big|_R + Z\psi, \quad (6)$$

with Z an arbitrary Hermitian matrix.

When comparing the boundary conditions (4) with (6), we notice an additional term $Z\psi$. This term also arises in the first method if we modify the Hamiltonian (3) by adding a term $Z\delta(z - z_0)$. This modification does not change

the expression for the current (5). Since no δ functions appear in the Hamiltonian, we take $Z = 0$ in Eq. (6); then the boundary conditions (4) and (6) are equal. Note that imposing current continuity does not completely determine the boundary conditions, while the integration method uses all the information available in the Hamiltonian. We conclude this section by observing that using boundary conditions derived for constant P , while taking a different value of P in each layer, can generate nonphysical results. However, if we compare the numerical results derived with boundary conditions for constant and varying P , similar results (within ± 5 meV) are obtained.

IV. IN-PLANE DISPERSION RELATIONS OF AN INTERBAND DOUBLE-BARRIER TUNNELING DIODE

To illustrate the eight-band model, the tunneling probability through an interband resonant-tunneling diode is calculated. Interband tunneling diodes were introduced by Söderström in 1989.² The structure we study consists of an InAs emitter and collector layer, two 3-nm AlSb barriers, and a 10-nm GaSb quantum well. The structure has been grown on a (100)-oriented substrate, and we consider an in-plane momentum in the [010] direction. The schematic band structure of this layer is shown in Fig. 1. We see that InAs forms a broken band gap with GaSb such that the bottom of the conduction band in the InAs layer is lower than the top of the valence band in the GaSb layer. The values of the band alignment in the calculations are taken from Ref. 25.

In Fig. 2, we show the logarithm of the transmission probability of electrons (spin-up) from the InAs emitter layer through the RIT as a function of the energy for different values of the parallel wave vector. It is clear from Fig. 2 that there is no tunneling through the energy levels that can be associated with the heavy holes if there is no in-plane momentum ($k_x = 0$), since in this case the heavy-hole part of the Hamiltonian is decoupled from the other bands. As soon as there is an in-plane momentum, three additional peaks associated with heavy holes appear in the transmission characteristics. However, their linewidth is so small that they do not contribute significantly to the tunneling current. When the in-plane momentum increases, especially the peak associated with the second heavy-hole level gains linewidth while the first light-hole peak loses linewidth. In actual tunneling devices, the in-plane momentum will always exist due to scattering processes which occur during the transport of carriers through the structure. The energy levels no longer have a pure light- or heavy-hole nature as soon as an in-plane momentum is present. This is also observed in the extracted dispersion relations (Fig. 3). In these dispersion relations we have drawn the energy position of the different peaks as a function of the in-plane momentum. The first light-hole level initially even has an inverse curvature. The broken lines in this figure indicate the conduction-band onset of bulk InAs, and the valence-band onsets of bulk GaSb (both light hole and heavy hole), and border as such the region in which tunneling can occur.

FIG. 2. Logarithm (base 10) of the transmission probability T through the inter-band tunneling structure of Fig. 1 for electrons as a function of their energy calculated with the eight-band model. k_x is the in-plane momentum along the [010] crystal axes.

We also note the existence of energies having a transmission probability going to zero ($-\infty$ on a logarithmic scale). At these energies destructive interferences occurs between the different waves occurring in the quantum well. Analogous total reflection energies can be found in the calculation of the transmission probability of holes in traditional RTD's⁸ or in the calculation of Γ -X coupling in resonant-tunneling diodes.²⁶

The in-plane mass of the second light-hole level, that can be extracted from the dispersion relation (LH2) in Fig. 3 ($0.054m_0$), corresponds rather well to the theoretical light-hole in-plane mass of a single GaSb quantum well $m_0/(\gamma_1 + \gamma_2)$: $0.056m_0$.²⁷ The overall correspon-

dence with calculations using only the heavy- and light-hole bands²⁸ is also very good.

V. SIMPLIFIED TRIPLE-BAND EFFECTIVE-MASS EQUATION

To simplify the calculations and to optimize the calculation time, one can in many cases only use three bands (conduction, light-hole valence, and spin-split-off bands) for carriers without in-plane momentum. An additional simplification is to abbreviate the wave functions to the single-band wave functions and with these solve the multiple-band Hamiltonian. In this section we will there-

FIG. 2. (Continued).

FIG. 3. The dispersion relations extracted from the calculations shown in Fig. 2 (plain line). The bulk dispersion relations for InAs (long dashes) and for GaSb (dotted for heavy holes and short dashed for light holes) border the area in which transmission is allowed.

fore first compare the results of the triple-band model with the simplified single-band wave functions to the solutions with the wave functions derived from the eigenvectors of the Hamiltonian.

In Ref. 13 the triple-band effective-mass equation was derived based on a transfer-matrix formalism, and using wave functions for each band which are the solution of the corresponding single-band effective-mass equations. Using these eigenvectors implies that the different tunneling channels are uncoupled. The use of these eigenvectors, however, greatly simplifies the transfer matrices and therefore decreases the computation time.

In Ref. 13 the following simplified eigenvectors are used:

$$\Psi_c(z) = A_c \exp(ik_c z) + B_c \exp(-ik_c z),$$

$$\Psi_l(z) = A_l \exp(ik_l z) + B_l \exp(-ik_l z), \quad (7)$$

$$\Psi_s(z) = A_s \exp(ik_s z) + B_s \exp(-ik_s z).$$

However, the correct expressions of the envelope functions Ψ_i ($i=c, l$, and s) are a linear combination of the eigenvectors of the effective-mass equation: $H\Psi = E\Psi$.

We have six wave vectors k for each eigenvalue E . The

eigenvector for each k has the shape of

$$\begin{bmatrix} 1 \\ \alpha(k) \\ \beta(k) \end{bmatrix} \exp(ikz) .$$

The first element in the eigenvector is normalized to 1 and is the amplitude of the conduction-band wave function, the second term is of the light hole, and the third term of the spin-split-off wave function. Thus the wave functions have to be written as

$$\begin{aligned} \Psi_c(z) &= A_c \exp(ik_c z) + B_c \exp(-ik_c z) + A_l \exp(ik_l z) + B_l \exp(-ik_l z) + A_s \exp(ik_s z) + B_s \exp(-ik_s z) , \\ \Psi_l(z) &= \alpha(k_c) A_c \exp(ik_c z) + \alpha(-k_c) B_c \exp(-ik_c z) + \alpha(k_l) A_l \exp(ik_l z) + \alpha(-k_l) B_l \exp(-ik_l z) \\ &\quad + \alpha(k_s) A_s \exp(ik_s z) + \alpha(-k_s) B_s \exp(-ik_s z) , \\ \Psi_s(z) &= \beta(k_c) A_c \exp(ik_c z) + \beta(-k_c) B_c \exp(-ik_c z) + \beta(k_l) A_l \exp(ik_l z) + \beta(-k_l) B_l \exp(-ik_l z) \\ &\quad + \beta(k_s) A_s \exp(ik_s z) + \beta(-k_s) B_s \exp(-ik_s z) . \end{aligned} \quad (8)$$

The first wave function $\Psi_c(z)$ gives the probability that the carrier is in the conduction band, while the second and third wave functions, respectively, give the probability of the state of the light-hole and spin-split-off bands. The correct wave functions consist of six terms. These wave functions are dependent on the wave vectors of all the bands which are taken into account.

The shape of the eigenvectors as a function of the material parameters is rather complicated. The material-dependent constant P_1 is defined in order to simplify:

$$P_1 = \sqrt{\frac{1}{3}} \hbar \frac{P}{m_0} .$$

The denominator of the expressions is

$$\begin{aligned} N &= E^2 - E(E_{l0} - E_{s0}) + E_{l0}E_{s0} \\ &\quad + \left[\frac{E - E_{s0}}{m_{0l}} + \frac{E - E_{l0}}{m_{0s}} \right] \frac{\hbar^2 k^2}{m_0} + \frac{\hbar^2 k^4}{m_{0l}m_{0s}m_0^2} . \end{aligned}$$

Then the elements of the eigenvectors are

$$\begin{aligned} \alpha(k) &= ik \frac{(E - E_{s0})\sqrt{2}P_1 + \frac{\sqrt{2}\hbar}{m_{0s}m_0}P_1k^2}{N} , \\ \beta(k) &= k \frac{(E - E_{l0})P_1 + \frac{\hbar}{m_{0l}m_0}P_1k^2}{N} . \end{aligned}$$

In the approximated case (7), we assume that each wave function can be described by the wave vector of the corresponding band alone, such that they consist of only two terms. In Fig. 4 we give the results of the calculation of the position of the first energy level in a RIT as a function of the thickness for the quantum well, with both expressions for the wave functions. We can conclude that the results with the approximated wave functions are a good approximation in the case of wide quantum wells. The calculation with the approximated wave functions gives results which differ more from the single-band model than in the case when the correct wave functions are used.

We also compared the results of the eight-band model

to the simplified Kane's two-band model. This two-band model also uses the correct two-band dispersion relationship but does not consider the real eigenvectors of the Hamiltonian. For energies in the conduction band (valence band), only the electronlike (light-hole-like) behavior is considered. We observe that the tunneling probability as a function of the energy is significantly different in this configuration, since multiple paths to tunnel are present in the eight-band model and each of them has a different wave vector in the barrier.

Table I compares the results of the different simulations. The heavy-hole level positions in this table for the eight-band model are the zero in-plane momentum extrapolations of the positions with an in-plane momentum, since no tunneling peak is obtained at the position of the heavy-hole level for carriers with zero in-plane momentum. The difference in position of the energy levels between the different models is larger when the levels are

FIG. 4. The obtained position of the light-hole energy level as a function of the GaSb quantum-well width. No in-plane momentum is considered. The solution using the correct eigenvector (+) is compared with the solution where only the dominant element of the eigenvector is considered (X). A significant difference is observed when the carriers are more confined in the GaSb quantum well (narrow GaSb quantum wells).

TABLE I. Comparison of the energy levels (in eV) obtained from the different simulations.

Eight-band model electron transmission	Kane's two-band model electron transmission	Single-band model light holes	Single-band model heavy holes
-0.9429(1HH)			-0.9408(1HH)
-0.9692(1LH)	-0.9702(1LH)	-0.9693(1LH)	
-0.9789(2HH)			-0.9673(2HH)
-1.0395(3HH)			-1.0127(3HH)
-1.0778(2LH)	-1.0752(2LH)	-1.0906(2LH)	
			-1.0776(4HH)

further away from the GaSb valence band. This is caused by larger nonparabolicity effects at higher energies.

VI. CONCLUSIONS

In this paper we have shown that the calculation of the coherent tunneling probability is still the most accessible tool to determine the position and the linewidth of the energy levels in the most prominent interband and intraband tunneling devices in III-V materials. However, scattering mechanisms need to be included, especially when studying time-dependent effects and charging phenomena. In that case a sequential tunneling approach would be more appropriate.

We have used a permutation of the functions of the Kane basis to reduce the complexity of the eigenvectors drastically. Using this modified basis we constructed the eight-band Hamiltonian. The conduction, light- and heavy-hole valence and spin-split-off bands are taken into account for both spin directions. The calculations take the in-plane momentum into account. A 16×16 transfer-matrix formalism has been constructed to couple the solutions in different layers of a multiple layered structure.

The transmission probability of the electrons through a resonant interband tunneling diode was calculated for different values of the in-plane momentum. These calculations show that the heavy-hole contribution to the tun-

neling current increases with increasing in-plane momentum. The in-plane dispersion relations show the coupling between the light- and heavy-hole band such that an exchange of linewidths between light and heavy holes becomes evident. This exchange can only exist in the case when the in-plane momentum is nonzero.

Since the eight-band model requires quite a large calculation time, simplifications are studied in order to speed up the calculations to determine the position of the energy levels in the quantum structures. Comparing the calculations of the eight-band model and Kane's two-band model gives significantly different results for the transmission probability because in the two-band model only one tunneling channel is foreseen. A better approximation can be made using a three-band model. We have shown in this paper that simplifying the eigenvectors in the three-band model, as is done in Ref. 13, gives results which are in good agreement with the complete three-band model. The simplification, however, reduces the complexity of the equations and the computation time drastically.

In this paper we have also cleared the confusion about the calculation of boundary conditions. It is proved that the boundary conditions deduced from the current continuity and the integration of the Hermitian Hamiltonian across the interface give the same results. It is the variation of the coupling momentum P across the interface which is generally overlooked in the definition of the Hermitian Hamiltonian. The MATHEMATICA package to calculate the in-plane dispersion relations and the transmission probability through stratified media using the eight-band formalism is available and can be requested from the author.

ACKNOWLEDGMENTS

We like to thank K. Thielemans from the Theoretical Physics Group, Imperial College in London for valuable discussions. J.G. and K.F. acknowledge the Human Capital and Mobility program of the European Community for financial support.

*Electronic address: genoe@polycnrs-gre.fr

¹L. L. Chang, L. Esaki, and R. Tsu, *Appl. Phys. Lett.* **24**, 593 (1974).

²J. R. Söderström, D. H. Chow, and T. C. McGill, *Appl. Phys. Lett.* **55**, 1094 (1989).

³T. C. L. G. Sollner, P. E. Tannenwald, D. D. Peck, and W. D. Goodhue, *Appl. Phys. Lett.* **45**, 1319 (1984).

⁴H. Ohno, L. Esaki, and E. E. Mendez, *Appl. Phys. Lett.* **60**, 3153 (1992).

⁵L. Yang, J. F. Chen, and A. Y. Cho, *J. Appl. Phys.* **68**, 2997 (1990).

⁶R. Tsu and L. Esaki, *Appl. Phys. Lett.* **22**, 562 (1973).

⁷J.-B. Xia, *Phys. Rev. B* **38**, 8365 (1988).

⁸C. Y.-P. Chao and S. L. Chuang, *Phys. Rev. B* **43**, 7027 (1991).

⁹R. Wessel and M. Altarelli, *Phys. Rev. B* **39**, 12 802 (1989).

¹⁰M. P. Houn, Y. H. Wang, and H. H. Chen, *J. Appl. Phys.* **74**, 7379 (1993).

¹¹L. C. Andreani, A. Pasquarello, and F. Bassani, *Phys. Rev. B* **36**, 5887 (1987).

¹²B. Chen, M. Lazzouni, and L. R. Ram-Mohan, *Phys. Rev. B* **45**, 1204 (1992).

¹³K. Fobelets, R. Vounckx, and G. Borghs, *Semicond. Sci. Technol.* **8**, 1815 (1993).

¹⁴L. R. Ram-Mohan, K. H. Yoo, and R. L. Aggarwal, *Phys. Rev. B* **38**, 6151 (1988).

¹⁵M. Altarelli, *Phys. Rev. B* **28**, 842 (1983).

- ¹⁶J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).
¹⁷J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).
¹⁸E. O. Kane, J. Phys. Chem. Solids **1**, 249 (1957).
¹⁹C. R. Pidgeon and R. N. Brown, Phys. Rev. **146**, 575 (1966).
²⁰*Semiconductors, Physics of Group IV Elements and III-V Compounds*, edited by K.-H. Hellwege and O. Madelung, Landolt-Bornstein, New Series, Group III, Vol. 17, Pt. a (Springer-Verlag, Berlin, 1982).
²¹H. M. Liu, Y. H. Wang, and M. P. Houng, J. Appl. Phys. **75**, 2699 (1994).
²²S. Wolfram, *Mathematica, A System for Doing Mathematics by Computer*, 2nd ed. (Addison-Wesley, Redwood City, CA, 1991).
²³G. Bastard, Phys. Rev. B **24**, 5693 (1981).
²⁴G. Bastard, Phys. Rev. B **25**, 7584 (1982).
²⁵S. Tiwari and D. J. Frank, Appl. Phys. Lett. **60**, 630 (1992).
²⁶K. Fobelets, Ph.D. thesis, Free University of Brussels (VUB), 1994.
²⁷G. Bastard and J. A. Brum, IEEE J. Quantum Electron. **QE-22**, 1625 (1986).
²⁸A. Nogaret, Ph.D. thesis, INSA Toulouse, 1994.