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Coupling between Γ- and X-type envelope functions at GaAs/Al(Ga)As interfaces

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Connection rules for envelope functions related to the Γ- and X-point conduction-band valleys in GaAs/Al(Ga)As systems are formulated in terms of a transfer matrix. The transfer-matrix elements are calculated using a method in which wave functions, which are obtained using empirical pseudopotentials, are matched at the interface. The nonzero transfer-matrix elements appear to depend weakly on energy which enables us to give a simple prescription for connection rules for envelope functions in which Γ-X coupling is incorporated.

One of the most intensively studied semiconductor-heterostructure systems is the GaAs/$Al_xGa_{1-x}As$ based heterostructure, which is largely motivated by its important application in the field of device technology. In the field of fundamental research GaAs/$Al_xGa_{1-x}As$ heterostructures have, e.g., offered the possibility to produce high-quality low-dimensional electron systems. Most of the GaAs/$Al_xGa_{1-x}As$ heterostructures are designed with Al concentrations below 40% since for higher Al concentrations $Al_xGa_{1-x}As$ has an indirect band gap resulting in a so-called type-II band lineup. For a type-II system like a single indirect AlAs layer in between two GaAs layers, the AlAs layer forms a barrier for Γ-valley conduction-band electrons but a quantum well for X-valley electrons. It has theoretically been shown[1–4] that tunneling through a single AlAs layer is largely dominated by X-valley assisted resonant tunneling. The coupling between the discrete states formed in the X-valley quantum well and the continuum of tunneling states through the Γ-valley barrier gives rise to so-called Fano resonances in the transmission spectrum such that the transmission may even drop to zero.[5] There are indeed various experiments which show evidence for tunneling through indirect-gap states,[6–8] most clearly when pressure is applied in order to shift the X minima with respect to the Γ-point minima.[9]

In describing the electronic states in type-I GaAs/AlAs heterostructures use is often made of the relatively simple envelope-function approach, although its success is somewhat surprising regarding the problem of matching the envelope functions at heterostructure interfaces.[10,11] The envelope-function approach can in principle be used to describe the Γ- and X-valley electronic states separately, but this neglects the coupling between Γ-point and X-point electronic states at the interface completely. It is the purpose of this paper to devise connection rules for envelope functions which account for this coupling. We succeed in constructing a transfer matrix connecting both Γ- and X-type envelope functions and their first derivatives, based on our method (Ref. 3) in which (pseudo) wave functions are properly matched at the GaAs/AlAs interface. There have been earlier attempts to do so, e.g., the one given by Akera, Wakahara, and Ando[1] (see also Ref. 12). In Ref. 1 the mixing between Γ- and X-type envelope functions at GaAs/Al(Ga)As interfaces is calculated using either empirical tight-binding or empirical pseudopotential schemes. Although at first sight it seems that our approach is quite analogous, there are in fact important differences between their method and ours. For instance, Akera, Wakahara, and Ando suppose *a priori* that the unit-cell averaged current density as given in the effective-mass approximation is continuous at heterostructure interfaces. In previous work[11] we have shown that this is not true for GaAs/AlAs interfaces due to a breakdown of the validity of the effective-mass approximation. A more or less phenomenological model for Γ-X mixing is put forward by Pulsford *et al.*[13] who introduce an adjustable coupling parameter in the interface transfer matrix for Γ- and X-type envelope functions. Their simple model is not based on a microscopic theory and, as we will see later on, cannot be justified by our calculations. More recently, Aversa and Sipe[14] have presented a method to deal with Γ-X coupling in the envelope-function formalism, not presenting, however, transfer-matrix elements which are ready to be used in an envelope-function calculation. Furthermore, in their theory the current density is only approximately continuous which is a serious drawback. Here, we calculate the connection rules for envelope functions starting from (pseudo) wave functions and their first derivatives which are matched *exactly* at the heterostructure interface. As a result the charge density and the flux will be continuous *by construction.*

We assume that the material layers are entirely bulklike in which case the general wave function in a material j can be written as a linear combination of Bloch and evanescent waves belonging to material j which may exist at a particular energy E and parallel wave vector $\mathbf{k}_\parallel$,

$$\psi^j_{E,\mathbf{k}_\parallel}(\mathbf{r}) = \sum_s \alpha^{js} \psi^{js}_{E,\mathbf{k}_\parallel}(\mathbf{r}). \tag{1}$$

The coefficients α^{js} follow from the matching procedure outlined in Ref. 3 which was formulated in terms of an empirical pseudopotential approach. As is shown in Ref. 15 each Bloch or evanescent wave $\psi^{js}_{E,\mathbf{k}_\parallel}(\mathbf{r})$ with wave vector $(\mathbf{k}_\parallel, k_z^{js})$ can be expanded in z-dependent envelope functions:

$$\psi^{js}_{E,\mathbf{k}_\parallel}(\mathbf{r}) = e^{(\mathbf{k}_\parallel - \mathbf{k}_{0\parallel})\cdot\mathbf{r}_\parallel} \sum_n f^{js}_{n;\mathbf{k}_0}(z) \psi^j_{n;\mathbf{k}_0}(\mathbf{r}), \tag{2}$$

in which $\psi^j_{n;\mathbf{k}_0}(\mathbf{r})$ are the Bloch eigenfunctions of the unperturbed bulk crystal of material j with band index n at $\mathbf{k} = \mathbf{k}_0$. The vector $\mathbf{k}_0$ should preferably be taken such that the wave vector $(\mathbf{k}_\parallel, k_z^{js})$ is close to $\mathbf{k}_0$. The related envelope functions $f^{js}_{n;\mathbf{k}_0}(z)$ are then slowly varying and there will be a few relevant band-indexed terms only contributing in (2). In this paper we will focus our attention on GaAs/Al(Ga)As heterostructures in which the interface planes are perpendicular to the [001] direction. Electron energies are at the conduction-band minimum of GaAs and above. Furthermore we restrict $\mathbf{k}_\parallel$ to a zone close to $\mathbf{0}$. A natural choice for $\mathbf{k}_0$ is then either $\mathbf{k}_\Gamma = (0,0,0)$, i.e., the Γ point, or $\mathbf{k}_{X_z} = (0,0,2\pi/a)$, i.e., the X_z point. We therefore proceed by dividing Eq. (1) into two parts and substituting (2)

$$\begin{aligned}\psi^j_{E,\mathbf{k}_\parallel}(\mathbf{r}) &= \sum_s^{\Gamma} \alpha^{js}\psi^{js}_{E,\mathbf{k}_\parallel}(\mathbf{r}) + \sum_s^{X} \alpha^{js}\psi^{js}_{E,\mathbf{k}_\parallel}(\mathbf{r}) \\ &= e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel}\left(\sum_n \mathcal{F}^{j\Gamma}_n(z)\psi^j_{n;\mathbf{k}_\Gamma}(\mathbf{r}) \right. \\ &\quad \left. + \sum_n \mathcal{F}^{jX}_n(z)\psi^j_{n;\mathbf{k}_X}(\mathbf{r})\right) \qquad (3)\end{aligned}$$

in which the superscript Γ/X means restriction to states with wave vectors whose real part is closest to $\mathbf{k}_\Gamma/\mathbf{k}_{X_z}$ and where the envelope functions $\mathcal{F}^{j,\Gamma/X}_n$ are given by

$$\mathcal{F}^{j,\Gamma}_n(z) = \sum_s^{\Gamma} \alpha^{js} f^{js}_{n;\mathbf{k}_\Gamma}(z), \qquad (4a)$$

$$\mathcal{F}^{j,X}_n(z) = \sum_s^{X} \alpha^{js} f^{js}_{n;\mathbf{k}_X}(z). \qquad (4b)$$

Note that there is an important difference at this point between this work and the work of Ando, Wakahara, and Akera who use both X- and Γ-type channels in the calculation of Γ-type envelope functions.[12] The boundary conditions for Γ- and X-type conduction-band valley envelope functions and their first derivatives are generally expressed as

$$\begin{pmatrix} \boldsymbol{\mathcal{F}}^{j+1,\Gamma} \\ \boldsymbol{\mathcal{F}}^{j+1,X} \\ a\,\frac{\partial \boldsymbol{\mathcal{F}}^{j+1,\Gamma}}{\partial z} \\ a\,\frac{\partial \boldsymbol{\mathcal{F}}^{j+1,X}}{\partial z} \end{pmatrix} = T \begin{pmatrix} \boldsymbol{\mathcal{F}}^{j,\Gamma} \\ \boldsymbol{\mathcal{F}}^{j,X} \\ a\,\frac{\partial \boldsymbol{\mathcal{F}}^{j,\Gamma}}{\partial z} \\ a\,\frac{\partial \boldsymbol{\mathcal{F}}^{j,X}}{\partial z} \end{pmatrix}, \qquad (5)$$

in which a is the lattice constant and where the vector $\boldsymbol{\mathcal{F}}^{j,\Gamma} = [\mathcal{F}^{j,\Gamma}_{c1}(z_0)]$ and $\boldsymbol{\mathcal{F}}^{j,X} = [\mathcal{F}^{j,X}_{c1}(z_0), \mathcal{F}^{j,X}_{c2}(z_0)]$ with $c1$ the band index of the lowest conduction band, $c2$ the band index of the second conduction band, and z_0 the interface position. So T becomes a 6×6 matrix with dimensionless elements. The interface position z_0 is chosen to lie on the As plane for which choice the deviations between the actual heterostructure potential and the bulk potential of a material layer are shown to be smallest.[3]

For a particular incoming electron, being either a Γ- or one of the two X-type electrons traveling (or decaying if the wave functions are evanescent) towards the interface from either the GaAs side or the AlAs side we are able to calculate, using the scattering-matrix method, the coefficients α^{js} of all outgoing channels (see Ref. 3). Furthermore we are able to calculate the envelope functions $f^{js}_{n;\mathbf{k}_0}(z_0)$ and their first derivatives corresponding to each Bloch and evanescent wave which gives us the necessary ingredients to calculate the general envelope functions $\mathcal{F}^{j,\Gamma}_{n_i}(z_0)$ and $\mathcal{F}^{j,X}_{n_i}(z_0)$ and their first derivatives. Applying this procedure for all six possible choices for incoming channels we obtain the precise number of Eqs. (5) which are required to fix the T-matrix elements.

We use the pseudopotential form factors given by Baldereschi *et al.*[16] in which we have lowered the antisymmetric form factor $v^a(4)$ for GaAs from 0.06 Ry to 0.0511 Ry. The latter value leaves the direct energy gap unchanged but reduces the energy distance between the X-point minima of the two lowest conduction bands from 0.6 eV to 0.35 eV, which is in much better agreement with experiment,[17] and gives rise to a camel's back structure[18,19] in the lowest conduction band of GaAs at the X point. For AlAs we do not observe a camel's back structure, but it should be noted that a slight decrease of $v^a(3)$ and/or $v^a(4)$ already gives rise to a camel's back structure.

For $\mathbf{k}_\parallel = \mathbf{0}$ the scattering-matrix calculation reveals that for incoming channels which are Γ- or X-type the only outgoing channels which play a non-negligible role in (3) are indeed the two channels making up the Γ-point conduction band and the four channels connected with the X-point minima of the first two conduction bands.[3] The Γ-point envelope functions are therefore constructed according to Eq. (4a), where s runs over the two Γ-type conduction-band channels[11] only. The X-type envelope functions are constructed similarly [Eq. (4b)] taking into account the four channels connected with the X_z minima of the first two conduction bands. The values of the diagonal transfer-matrix elements T_{nn} are plotted in Fig. 1. The phase of $\psi^j_{n;\mathbf{k}_0}(\mathbf{r})$ has been chosen such that it is real valued at $\mathbf{r} = (0,0,z_0)$. Then the diagonal elements all are real valued and positive. It is of interest to note that the diagonal elements appear to be almost constant, except T_{44} and T_{66} which show approximately a linear dependence on energy. The diagonal elements connecting

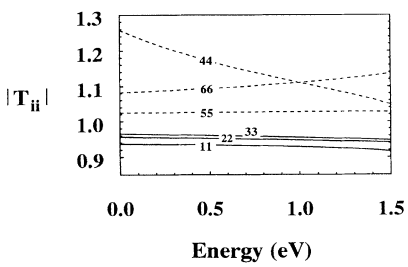

FIG. 1. The absolute value of the diagonal elements T_{ii} for a GaAs/AlAs interface at $\mathbf{k}_\parallel = \mathbf{0}$. The energy range runs from the bottom of the conduction band of GaAs at 0 eV to 1.5 eV which is approximately 0.5 eV above the Γ-point conduction-band edge of AlAs.

the envelope functions are close to unity, but, except for the 55 element, the elements connecting the first derivatives of the envelope functions happen to deviate from unity. This is, however, not related to effective-mass ratios in contradiction to the starting point of Akera, Wakahara, and Ando. The ratio of the effective masses of the Γ-point conduction-band minimum of AlAs and GaAs as obtained using empirical pseudopotentials equals 1.8; the ratios of the effective masses of the X-point conduction-band minima of AlAs and GaAs are equal to -0.1 and 0.834 for the first and second conduction band, respectively. Note that the camel's back in GaAs gives rise to a *negative* effective mass at $\mathbf{k}_X$. The effective mass of GaAs at $\mathbf{k}_X$ depends strongly on the value of the form factors $v^a(3)$ and $v^a(4)$. For instance, if we take the antisymmetric form factor $v^a(4)$ of GaAs to be 0.06 Ry the camel's back disappears and the effective mass of the lowest conduction band at the X-point changes sign. The value of the diagonal elements, however, is almost independent of the value of $v^a(4)$ which provides further evidence that the ratio of the effective masses and the the transfer-matrix element connecting first derivatives of the envelope functions are unrelated. The use of effective-mass ratios instead of our results may introduce substantial errors: For instance, using $T_{44} = 1.8$ introduces an error of approximately 35 meV in the bound state energy in a 28.3-Å wide AlAs/GaAs/AlAs Γ-band quantum well.[11] For a 56.5-Å wide $GaAs/Al_{0.3}Ga_{0.7}As/GaAs$ single barrier calculations have shown that this value for T_{44} produced an error of the order of 10% in the tunneling current.

In Fig. 2 the absolute value of the largest off-diagonal elements are plotted against energy. All other off-diagonal elements have absolute values smaller than 0.01. The elements T_{12}, T_{21}, T_{34}, and T_{62} are real and negative; the elements T_{43}, T_{53}, T_{54}, and T_{61} are real and positive. Also the off-diagonal elements depend only weakly on energy (the phases are energy independent), so that simple connection rules for envelope functions including Γ-X mixing can be used over a large energy interval. The coupling from X-type to Γ-type envelope functions is almost an order of magnitude smaller than vice versa. This asymmetry is in clear contradiction with the model used in Ref. 13. The absolute values of the off-diagonal elements are rather sensitive to changes in the value of $v^a(4)$. It is therefore important to use accurate values for the pseudopotential form factors for a quantitative analysis. The energy difference between the two conduction bands at the X point and the direct energy gap are sensitive tools to adjust the important parameters $v^a(3)$ and $v^a(4)$.

For the AlAs/GaAs interface the diagonal elements of the transfer matrix have the reciprocal values of the ones depicted in Fig. 1. The off-diagonal elements which differ appreciably from zero are the same ones as those for the GaAs/AlAs interface and have similar values, but they have opposite sign. In order to test our programs we have multiplied the full transfer matrix for the AlAs/GaAs interface with the transfer-matrix for the GaAs/AlAs interface which indeed gives the unit matrix in accordance with time-reversal symmetry.

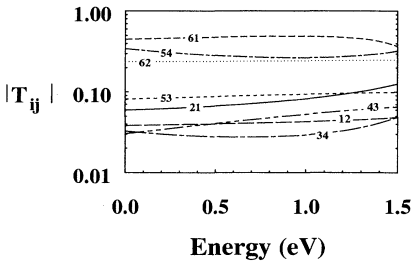

FIG. 2. As Fig. 1, but now the off-diagonal elements which are larger than 0.01 are given. Note the logarithmic y axis.

For $GaAs/Al_xGa_{1-x}As$ interfaces with $0 < x < 1$ we suggest that, as a first approximation, a transfer matrix should be used obtained by linear interpolation between the transfer matrix for $x = 0$ (which is a unit matrix) and $x = 1$, in line with the well-known virtual crystal approximation. Deviations from this simple linear approximation are expected to be of minor importance. A slightly more drastic but possibly very useful approximation could be the neglect of the energy dependence of the involved transfer-matrix elements entirely, such that the connection rules for $GaAs/Al_xGa_{1-x}As$ interfaces are governed by the transfer matrix $I+x\bar{T}$, where the overbar indicates averaging with respect to energy and I is the unit matrix. The diagonal elements of $\bar{T}$, where we have averaged over the important energy interval from 0 to 1 eV, are given by $\bar{T}_{11} = -0.07$, $\bar{T}_{22} = -0.05$, $\bar{T}_{33} = -0.04$, $\bar{T}_{44} = 0.18$, $\bar{T}_{55} = 0.03$, and $\bar{T}_{66} = 0.1$. The nonzero off-diagonal elements are given by $\bar{T}_{21} = -0.07$, $\bar{T}_{61} = 0.48$, $\bar{T}_{62} = -0.24$, $\bar{T}_{54} = 0.29$, $\bar{T}_{53} = 0.09$, $\bar{T}_{12} = -0.04$, $\bar{T}_{43} = 0.05$, and $\bar{T}_{34} = -0.03$.

In conclusion, we have presented results for a transfer matrix between envelope functions at a GaAs/Al(Ga)As heterostructure interface, which includes the coupling between Γ- and X-type envelope functions. Our calculation is based on an exact matching of (pseudo) wave functions and their first derivatives at the interfaces, such that the flux is continuous by construction at the interface. All nonzero transfer-matrix elements depend only weakly on energy such that simple connection rules for envelope functions at interfaces can indeed be given. These connection rules are ready to be used in combination with separate envelope-function descriptions for Γ- and X-valley conduction-band states. We find no evidence at all for effective-mass ratios governing the connection rules for the first derivatives. The pseudopotential form factors have considerable influence on the off-diagonal transfer-matrix elements and should therefore be chosen carefully. A more detailed (experimental) analysis of the conduction-band structure at the X point should provide a basis for a correct choice for these values.

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