MULTIBAND ANALYSIS OF QUANTUM TRANSPORT – A NUMERICALLY EFFICIENT AND STABLE APPROACH

D. Z.-Y. Ting and T. C. McGill
Thomas J. Watson, Sr. Laboratory of Applied Physics
California Institute of Technology
Pasadena, California 91125

Abstract

We describe a numerically stable and efficient method for computing transmission coefficients in semiconductor heterostructures using multiband tight-binding band structure models. This method can be used to investigate band structure effects such as valley mixing and band mixing. We use a GaAs/AlAs double barrier heterostructure and an InAs/GaSb/AlSb interband tunnel device to illustrate the application of this method.

INTRODUCTION

The inclusion of band-mixing and valley-mixing effects in quantum transport studies of semiconductor heterostructure tunnel devices is essential in treating a number of important physical phenomena such as intervalley scattering, hole mixing, and interband tunneling. The proper treatment of these effects require the use of realistic multiband band structure models. However, progress in multiband quantum transport calculations had been hampered by the lack of numerically stable algorithms for calculating transmission coefficients. It is well known that the transfer matrix method[1]-[2], a standard method for computing transmission coefficients, is numerically unstable for treating device structures with active regions larger than a few tens of Å when used in conjunction with realistic multi-band band structure models. Recently, we have developed a new method of computing transmission coefficients for multi-band tight-binding band structure models[3]. We calculate the transmission probability by solving a system of linear equations representing the tight-binding form of the Schrödinger equation over a finite region of interest, with specially formulated boundary and inhomogeneous terms to account for the effects of the incoming and outgoing plane-wave states. Our formulation of the boundary conditions is similar to the approach taken by Frensley[4] and Lent[5] in their works with single-band models. Compared to the transfer matrix method, our method is equal in numerical efficiency, and superior in numerical stability and ease of implementation.

METHOD

A detailed description of our method has been published elsewhere[3]. Here we briefly outline the essential features of our method. We wish to compute transmission coefficients for a heterostructure with a central region of interest consisting of N monolayers labeled $\sigma = 1, 2, \ldots, N$. We assume flat-band conditions exist in the incoming and outgoing electrodes outside the central region. Let M be the number of orbitals per unit cell in the tight-binding basis set. The Schrödinger equation

$(H - E)|\psi\rangle \equiv \bar{H}|\psi\rangle = 0$ in the tight-binding planar orbital basis is

$$\mathbf{H}_{\sigma,\sigma-1}\mathbf{C}_{\sigma-1} + \bar{\mathbf{H}}_{\sigma,\sigma}\mathbf{C}_{\sigma} + \mathbf{H}_{\sigma,\sigma+1}\mathbf{C}_{\sigma+1} = 0, \tag{1}$$

where $\mathbf{C}_\sigma$ is a vector of length M corresponding to the coefficients of the tight-binding orbitals at plane σ, and $\mathbf{H}_{\sigma,\sigma'}$ and $\bar{\mathbf{H}}_{\sigma,\sigma}$ are $M \times M$ matrices containing tight-binding matrix elements. To impose open boundary conditions on the central region, we let $\mathbf{I}$, $\mathbf{r}$ and $\mathbf{t}$ be the coefficient of the incoming, reflected, and transmitted plane-wave states. They can be related to the tight-binding coefficients at the boundaries of the central regions by a basis transformation :

$$\begin{bmatrix} \mathbf{C}_1 \\ \mathbf{C}_2 \end{bmatrix} = \mathbf{D}^L \begin{bmatrix} \mathbf{I} \\ \mathbf{r} \end{bmatrix} = \begin{bmatrix} \mathbf{D}^L_{11} & \mathbf{D}^L_{12} \\ \mathbf{D}^L_{21} & \mathbf{D}^L_{22} \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{r} \end{bmatrix}, \tag{2}$$

$$\begin{bmatrix} \mathbf{C}_{N-1} \\ \mathbf{C}_N \end{bmatrix} = \mathbf{D}^R \begin{bmatrix} \mathbf{t} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{D}^R_{11} & \mathbf{D}^R_{12} \\ \mathbf{D}^R_{21} & \mathbf{D}^R_{22} \end{bmatrix} \begin{bmatrix} \mathbf{t} \\ \mathbf{0} \end{bmatrix}. \tag{3}$$

$\mathbf{D}^L$ and $\mathbf{D}^R$ are $2M \times 2M$ matrices whose column vectors are the eigenvectors obtained by diagonalizing the bulk transfer matrices in the left ($\sigma = 1$) and right ($\sigma = N$) electrodes. Eliminating $\mathbf{r}$ and $\mathbf{t}$ from Eqs. (2) and (3), we obtain

$$\mathbf{C}_1 - \mathbf{D}^L_{12}{\mathbf{D}^L_{22}}^{-1}\mathbf{C}_2 = \mathbf{D}^L_{11}\mathbf{I} - \mathbf{D}^L_{12}{\mathbf{D}^L_{22}}^{-1}\mathbf{D}^L_{21}\mathbf{I}, \tag{4}$$

and

$$-\mathbf{D}^R_{21}{\mathbf{D}^R_{11}}^{-1}\mathbf{C}_{N-1} + \mathbf{C}_N = 0. \tag{5}$$

The above equations, together with Eq. (1) taken at $\sigma = 2, 3, \ldots, N-1$, constitute a system of MN linear equations. Solving the system of equations yields the tight-binding coefficients, and, from Eq. (3), the coefficients of the transmitted plane-wave states are then given by

$$\mathbf{t} = {\mathbf{D}^R_{21}}^{-1}\mathbf{C}_N. \tag{6}$$

The amplitudes of the transmitted states $\mathbf{t}$, in turn, can be used to compute the transmission coefficient :

$$T(E,\mathbf{k}_{||}) = \sum_{j=1}^{M} |t_j(E,\mathbf{k}_{||})|^2 \frac{|v_j(E,\mathbf{k}_{||};R)|}{|v_I(E,\mathbf{k}_{||};L)|}, \tag{7}$$

where $v_I(E,\mathbf{k}_{||};L)$, and $v_j(E,\mathbf{k}_{||};R)$ are the group velocities of the incident and the transmitted bulk pane-wave states, respectively.

RESULTS AND DISCUSSION

Figure 1 shows the electron transmission spectra for a GaAs/AlAs double barrier structure calculated with our method for an eight-band second-neighbor sp^3 tight-binding model[6]. To illustrate the importance of using realistic band structure models, we have also included the results calculated using a simple two-band model which only correctly describes the Γ-valley band structure of the lowest conduction band and the light-hole band. Note that while the two-band model shows only a single resonance due to the lowest quasi-bound state in the GaAs quantum well, the eight-band result reveals a set of additional resonances due the X-point quantum wells in the AlAs layers.

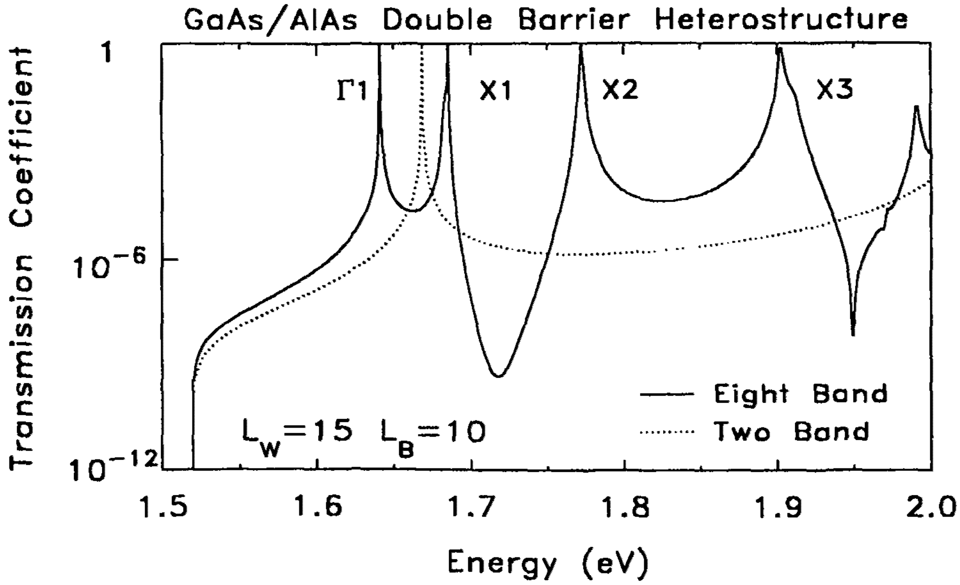

Figure 1: Transmission coefficients for a (001) GaAs/AlAs double barrier structure calculated using an eight-band tight-binding model and a simple two-band model.

Since the transmission coefficient represents the transmission probabilities for a Γ-valley electron in the GaAs electrode, the presence of the X-point resonances in the transmission spectrum indicates strong coupling between the GaAs Γ-valley states and the AlAs X-valley states. The structure used in this calculation exceeds 100 Å in length; numerical instabilities would have made it impossible to obtain the eight-band model transmission coefficients with the transfer matrix method.

In the second example we are concerned with the InAs-GaSb-AlSb-GaSb interband tunnel device, which consists of an n-type InAs electrode and a p-type GaSb electrode, with the active region being a GaSb quantum well sandwiched between the InAs electrode and a AlSb barrier. In the range of operation, we are primarily interested in electrons tunneling from the conduction band of the InAs electrode, via quantized valence states in the GaSb well, into heavy-hole or light-hole states in the GaSb electrode. Figure 2 shows the transmission coefficients for this interband device structure calculated using the eight-band effective bond orbital model[7] and a simple two-band model. While the two-band model result shows a single light-hole resonance, the effective bond orbital model shows both heavy-hole and light-hole resonances. A careful examination of the wavefunctions of the transmitting states in the multiband model reveals that the resonances seen in the transmission spectrum include those which are associated with quasibound states of mixed heavy- and light-hole characteristics. As is clearly seen in this figure, band structure effects such as hole mixing can produce features which are impossible to predict with simple band structure models.

The examples which we discussed demonstrated the importance of band structure effects such as band mixing and valley mixing in quantum transport. We have presented an approach to multiband analysis of quantum transport which is numerically stable, efficient, and simple to implement.

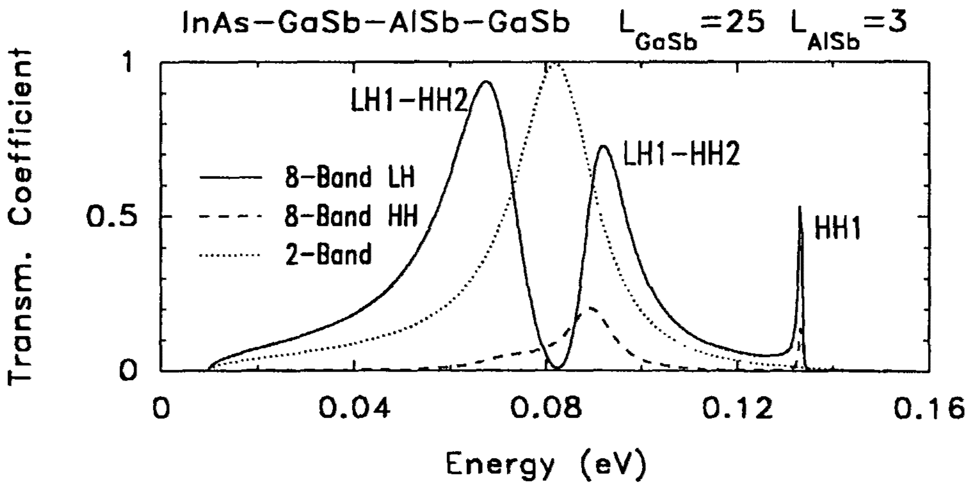

Figure 2: Transmission coefficients for a (001) InAs-GaSb-AlSb-GaSb interband tunnel device calculated using the eight-band effective bond orbital model and a simple two-band model. The incoming electron in InAs has $\mathbf{k}_{||} = (0.0075, 0, 0)2\pi/a$, and is transmitted into heavy-hole and light-hole states in GaSb.

We have successfully used this method to study a variety of quantum transport phenomena in semiconductor tunnel structures, including the role of heavy-hole states in InAs/GaSb/AlSb-based interband tunnel structures[3], the reduction of hole tunneling times in GaAs/AlAs double barrier structures[8], and Γ-X valley mixing induced interference effects on electron tunneling times in GaAs/AlAs double barrier structures[9].

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