18^{th} **International Conference on Transport Theory (18ICTT)**

Rio de Janeiro (Brazil)

20-25 July 2003

Numerical results for the Wigner-Kane model

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INTRODUCTION

Heterojunction resonant interband tunneling diodes (RITD) make use of interband resonant tunneling through potential barriers. When computing the current flowing through these devices, the multi-band structure has to be taken into account in the transport model [1][4].

A simple multi-band model was introduced by Kane in the early 60's; it describes the behaviour of the charge carriers in a system with two allowed energy bands separated by a forbidden region. It provides the simplest framework for including one conduction band and one valence band (light hole) in each material of a heterogeneous structure.

A new two-band formulation of the Kane model, based on the Wigner-function approach, was recently introduced. Here, we outline the model and show some numerical results concerning the two-band thermal equilibrium for a sample heterostructure.

THE TWO-BAND KANE MODEL

The two-band Schrödinger-Kane system, in the framework of the $k \cdot P$ theory [2], is given by

$$\begin{cases} i\hbar \dfrac{\partial \Psi_1}{\partial t} = -\dfrac{\hbar^2}{2m}\triangle\Psi_1 + (E_c + V)\Psi_1 - \dfrac{P\hbar}{m}\nabla\Psi_2 \\ i\hbar \dfrac{\partial \Psi_2}{\partial t} = -\dfrac{\hbar^2}{2m}\triangle\Psi_1 + (E_v + V)\Psi_1 + \dfrac{P\hbar}{m}\nabla\Psi_1 \end{cases}$$

where Ψ_1 and Ψ_2 are the Luttinger-Kohn envelope functions of the two bands (e.g., valence and conduction bands), defined by

$$\Psi_n(x) = \int \mathrm{d}k \sum_m a_m(k) C_{m,n}(k) e^{ikx} \tag{1}$$

with $a_m(k) =< \psi_m(k), \psi >$ $\quad C_{m,n}(k) =< u_m(0), u_n(k) >$.
Here, $\psi(x)$ is the single-electron wave function, $\psi_n(k,x) = u_n(k,x)e^{ikx}$ is the Bloch function of the $n-$th band and $u_n(0,x) \equiv u_n(x)$ are the Luttinger-Kohn eigenfunctions. The scalar product is defined by

$$< f, g >= \int_{u-cell} f(x)g(x)\mathrm{d}x \quad .$$

In matrix form:

$$\mathcal{H} = \begin{pmatrix} -\dfrac{\hbar^2}{2m}\nabla^2 + V_c & -\dfrac{P\hbar}{m}\nabla \\ \dfrac{P\hbar}{m}\nabla & -\dfrac{\hbar^2}{2m}\nabla^2 + V_v \end{pmatrix}$$

where $P = \hbar \int_{-\pi/a}^{\pi/a} u_c(x) \frac{\partial u_c(x)}{\partial x} dx.$ is the Kane momentum.

PHYSICAL MEANING OF ENVELOPE FUNCTION

The Schrödinger wave function can be written in the form (called envelope functions expansion):

$$\psi(x) = \Psi_1(x)u_1(x) + \Psi_2(x)u_2(x)\,. \tag{2}$$

The **electronic density** is $n(x) = |\psi(x)|^2$. If we integrate (2) over a unit cell, we have:

$$< n(x) >= |\Psi_1(x)|^2 + |\Psi_2(x)|^2 \equiv n_1(x) + n_2(x)$$

where $< n >$ is the average of the electronic density over a unit cell.

The **electronic current** inside the device is:

$$\mathcal{J} = \frac{\hbar}{m}\Im\left(\overline{\psi}\frac{\partial\psi}{\partial x}\right)$$

After integration over the unit cell,

$$< \mathcal{J} >= \mathcal{J}_{1,1} + \mathcal{J}_{2,2} + 2\frac{P}{m}\Im(\overline{\Psi_1}\Psi_2)\,,$$

where

$$\mathcal{J}_{i,i} \equiv \frac{\hbar}{m}\Im\left(\overline{\Psi_i}\frac{\partial\Psi_i}{\partial x}\right)\,. \tag{3}$$

Finally,

$$\frac{\partial}{\partial t}(n_1 + n_2) = -\nabla\left(\mathcal{J}_{1,1} + \mathcal{J}_{2,2} + 2\frac{P}{m}\Im(\overline{\Psi_1}\Psi_2)\right)\,. \tag{4}$$

is the envelope function version of the **continuity equation**.

ENERGY BAND STRUCTURE OF THE KANE MODEL

The diagonalization of the Kane-Hamiltonian gives the Kane approximation to the energy bands and to the Bloch eigenfunctions near $k = 0$. The dispersion relation for the energy bands is given by

$$E_{c,v}(k) = E_c + \frac{E_g}{2} + \frac{\hbar^2 k^2}{2m} \pm \frac{\sqrt{\eta}}{2} \tag{5}$$

where E_c is the edge of the conduction band, E_g is the energy gap, $\eta = E_g^2 + 4\frac{\hbar^2 k^2 P^2}{m^2}$ and the upper sign refers to the conduction band and the lower to the valence band.

This gives for the effective masses at the band edge:

$$\frac{1}{m_c} = \frac{2P^2}{m^2 E_g} + \frac{1}{m}; \quad \frac{1}{m_v} = \frac{2P^2}{m^2 E_g} - \frac{1}{m}.$$

and the Kane momentum P can be expressed in terms of $m_{c,v}$:

$$P = \frac{m}{2}\sqrt{\frac{m_c + m_v}{2 m_c m_v}}$$

The eigenfunctions which diagonalize the Kane Hamiltonian are given by

$$\underline{\Psi}_c = \begin{pmatrix} A(k) \\ B(k) \end{pmatrix} \quad \underline{\Psi}_v = \begin{pmatrix} B(k) \\ -A(k) \end{pmatrix}$$

where $A(k)$, $B(k)$ are given by

$$A(k) = \Theta(k)\sqrt{\frac{\sqrt{\eta}+E_g}{2\sqrt{\eta}}} - \Theta(-k)\sqrt{\frac{\sqrt{\eta}+E_g}{2\sqrt{\eta}}}$$
$$B(k) = \Theta(k)\sqrt{\frac{\sqrt{\eta}-E_g}{2\sqrt{\eta}}} - \Theta(-k)\sqrt{\frac{\sqrt{\eta}-E_g}{2\sqrt{\eta}}}$$

$\underline{\Psi}_c$ and $\underline{\Psi}_v$ are the envelope functions of an electron belonging to the conduction or the valence band, respectively.

It is easy to verify that the electron current related to the eigenfunction is:

$$< \mathcal{J} >= \mathcal{J}_{1,1} + \mathcal{J}_{2,2} + 2\frac{P}{m}\Im(\overline{\Psi_1}\Psi_2) =$$

$$\frac{\hbar}{m}\Im\left(\overline{\Psi_1}\frac{\partial\Psi_1}{\partial x}\right) + \frac{\hbar}{m}\Im\left(\overline{\Psi_2}\frac{\partial\Psi_2}{\partial x}\right) + 2\frac{P}{m}\Im(\overline{\Psi_1}\Psi_2) = \frac{\hbar k}{m} + 2\frac{P}{m}AB$$

which is equal to

$$< \mathcal{J}_c >= \left.\frac{1}{\hbar}\frac{\partial E}{\partial k}\right|_{k\in cond.band} \quad , \quad < \mathcal{J}_v >= \left.\frac{1}{\hbar}\frac{\partial E}{\partial k}\right|_{k\in val.band}$$

DIRECT INTERBAND TUNNELING, PHYSICAL PICTURE

We can outline an intuitive picture of interband tunneling according to the Kane model. The following argument follows a semiclassical reasoning, very similar to the WKB method, and remains valid for weak external fields.

From the dispersion curve, we see that the solutions of the system imply imaginary values for k in the forbidden gap and real values in the allowed energy bands. We deduce that

- in the allowed bands the wave function is a travelling wave, written as the sum of two waves which propagate along the x axis with oppisite wave numbers;

- in the forbidden bands the solution suffers exponential decay.

If we consider an electron in the conduction band, with energy E_A (Figure 1) and we add to the flat bands a constant electric field, according to the WKB approximation the electron energy decreases during its propagation $E = E_0 - Fx$ and the electron will move towards point C on the curve. between point A and point C, all values of k are real, and thus correspond to propagating modes. When the electron reaches A, it is eitherreflected or it enters the forbidden region, thus making and indirect interband transition. In this case, the transition is from the lower edge of the conduction band to the upper edge of the valence band, with the wave number becoming imaginary. The electron thus reaches the upper edge of the valence band in point V, and then continues propagating into the valence band. The situation is illustrated in Figure 2, where the 3-d dispersion diagrams are shown.

THE WIGNER-KANE MODEL

The Wigner function is defined as:

$$f_w(x,v,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \rho\left(x + \frac{\hbar}{2m}\eta, x - \frac{\hbar}{2m}\eta\right) e^{i\,v\eta}\mathrm{d}\eta$$

where $\rho(x,x')$ is the density matrix in the space representation.

In the Kane model, the Wigner transformation is carried out separately on each combination of the envelope functions, thus defining four Wigner-like functions [4]:

$$f_{1,1}(x,v,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \overline{\Psi}_1\left(x + \frac{\hbar}{2m}\eta\right)\Psi_1\left(x - \frac{\hbar}{2m}\eta\right) e^{i\,v\eta}\mathrm{d}\eta \quad (6)$$

$$f_{2,2}(x,v,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \overline{\Psi}_2\left(x + \frac{\hbar}{2m}\eta\right)\Psi_2\left(x - \frac{\hbar}{2m}\eta\right) e^{i\,v\eta}\mathrm{d}\eta \quad (7)$$

$$f_{1,2}(x,v,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \overline{\Psi}_1\left(x + \frac{\hbar}{2m}\eta\right)\Psi_2\left(x - \frac{\hbar}{2m}\eta\right) e^{i\,v\eta}\mathrm{d}\eta \quad (8)$$

$$f_{2,1}(x,v,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \overline{\Psi}_2\left(x + \frac{\hbar}{2m}\eta\right)\Psi_1\left(x - \frac{\hbar}{2m}\eta\right) e^{i\,v\eta}\mathrm{d}\eta \quad (9)$$

with $f_{2,1} = \overline{f}_{1,2}$.

By using the evolution equations for the envelope functions given by the Kane model, we obtain the evolution equations for the four Wigner-Kane functions introduced above [3]:

$$\frac{\partial f_{1,1}}{\partial t} = -v\frac{\partial f_{1,1}}{\partial x} + i\theta_{c,c} f_{1,1} - \frac{P\hbar}{m}\nabla_x \Im(f_{1,2}) - v\frac{2P}{\hbar}\Re(f_{1,2})$$
$$\frac{\partial f_{2,2}}{\partial t} = -v\frac{\partial f_{2,2}}{\partial x} + i\theta_{v,v} f_{2,2} - \frac{P\hbar}{m}\nabla_x \Im(f_{1,2}) + v\frac{2P}{\hbar}\Re(f_{1,2})$$
$$\frac{\partial f_{1,2}}{\partial t} = -v\frac{\partial f_{1,2}}{\partial x} + i\theta_{c,v} f_{1,2} + \frac{iP}{2m}\left(\nabla_x f_{2,2} + \frac{1}{2}\nabla_x f_{1,1}\right) + \frac{P}{\hbar}v\left(f_{1,1} - f_{2,2}\right)$$
$$\frac{\partial f_{2,1}}{\partial t} = -v\frac{\partial f_{2,1}}{\partial x} + i\theta_{v,c} f_{2,1} - \frac{iP}{2m}\left(\nabla_x f_{2,2} + \frac{1}{2}\nabla_x f_{1,1}\right) + \frac{P}{\hbar}v\left(f_{1,1} - f_{2,2}\right)$$

where

$$\theta_{i,j} = \frac{1}{2\pi}\int_\eta\int_{v'} \frac{V_i\left(x + \frac{\hbar}{2m}\eta\right) - V_j\left(x - \frac{\hbar}{2m}\eta\right)}{\hbar} e^{i(v-v')\eta} f(x,v')\mathrm{d}v'\mathrm{d}\eta$$

is the usual pseudo-differential operator.

The densities and currents defined in the usual way by the integrals of the Wigner-Kane functions over the momentum space,

$$n_{1,1} = \int_{-\infty}^{\infty} f_{1,1}\mathrm{d}v \qquad n_{2,2} = \int_{-\infty}^{\infty} f_{2,2}\mathrm{d}v$$
$$n_{1,2} = \int_{-\infty}^{\infty} f_{1,2}\mathrm{d}v \qquad n_{2,1} = \int_{-\infty}^{\infty} f_{2,1}\mathrm{d}v = \overline{n}_{1,2}$$
$$\mathcal{J}_{1,1} = \frac{1}{m}\int_{-\infty}^{\infty} f_{1,1} v\mathrm{d}v \qquad \mathcal{J}_{2,2} = \frac{1}{m}\int_{-\infty}^{\infty} f_{1,1} v\mathrm{d}v$$

are the averages over the unit cell of the true densities and currents.

A PARTICULAR SOLUTION OF THE STATIONARY WIGNER-KANE SYSTEM

We have obtained a steady-state solution of the Wigner-Kane system for the particular case of flat band edges, i.e. no external potential and no doping are presentand therefore $V_c(x) = V_c$ and $V_v(x) = V_c + E_g$. In this case we have for the the pseudodifferential operators: $\theta_{cc} f = \theta_{vv} f = 0$ and $\theta_{vc} f = -\theta_{cv} f = E_g f$ and the steady-state Wigner-Kane system becomes

$$\begin{cases} 0 = -v\dfrac{\partial f_{1,1}}{\partial x} - \dfrac{P\hbar}{m}\nabla_x \Im(f_{1,2}) - v\dfrac{2P}{\hbar}\Re(f_{1,2}) \\ 0 = -v\dfrac{\partial f_{2,2}}{\partial x} - \dfrac{P\hbar}{m}\nabla_x \Im(f_{1,2}) + v\dfrac{2P}{\hbar}\Re(f_{1,2}) \\ 0 = -v\dfrac{\partial f_{1,2}}{\partial x} - iE_g f_{1,2} + \dfrac{iP}{2m}\left(\nabla_x f_{2,2} + \dfrac{1}{2}\nabla_x f_{1,1}\right) + \dfrac{P}{\hbar}v\left(f_{1,1} - f_{2,2}\right) \\ 0 = -v\dfrac{\partial f_{2,1}}{\partial x} + iE_g f_{2,1} - \dfrac{iP}{2m}\left(\nabla_x f_{2,2} + \dfrac{1}{2}\nabla_x f_{1,1}\right) + \dfrac{P}{\hbar}v\left(f_{1,1} - f_{2,2}\right) \end{cases}$$

By using the traslational symmetry of the problem, we obtain space homogeneous solutions:

$$f_{1,1} = \frac{\sqrt{\eta(k)} + E_g}{2\sqrt{\eta(k)}}\,\delta(p/\hbar - k)$$

$$f_{2,2} = \frac{\sqrt{\eta(k)} - E_g}{2\sqrt{\eta(k)}}\,\delta(p/\hbar - k)$$

$$f_{1,2} = -i\frac{k^2 P}{\sqrt{\eta(k)}}\,\delta(p/\hbar - k)$$

These solutions represent momentum eigenstates in the single-electron Wigner picture.

BLOCH EQUATION AND BOUNDARY CONDITIONS

For the numerical simulation of real devices we have to impose suitable boundary conditions.

Such conditions can be built thinking the anion and the cation of IRTD diodes in thermal contact with a reservoir. In the Wigner formalism this boundary conditions are easily inserted with the inflow conditions in the phase plane.

To obtain the Wigner distribution function of the thermal equilibrium we have to solve the following Bloch-Kane system [5].

$$
\begin{aligned}
\frac{\partial f_{1,1}}{\partial \beta} &= \frac{\hbar^2}{8m}\frac{\partial^2 f_{1,1}}{\partial x^2} - \frac{p^2}{2m} f_{1,1} - \theta^+_{1,1} f_{1,1} + P\frac{\hbar}{m} p \Im(f_{1,2}) + \frac{\hbar^2}{2m} P \nabla_x \Re(f_{1,2}) \\
\frac{\partial f_{2,2}}{\partial \beta} &= \frac{\hbar^2}{8m}\frac{\partial^2 f_{2,2}}{\partial x^2} - \frac{p^2}{2m} f_{2,2} - \theta^+_{2,2} f_{2,2} + P\frac{\hbar}{m} p \Im(f_{1,2}) - \frac{\hbar^2}{2m} P \nabla_x \Re(f_{1,2}) \\
\frac{\partial f_{1,2}}{\partial \beta} &= \frac{\hbar^2}{8m}\frac{\partial^2 f_{1,2}}{\partial x^2} - \frac{p^2}{2m} f_{1,2} - \theta^+_{1,2} f_{1,2} - P\hbar\left(\frac{\hbar}{4m}\nabla - \frac{ip}{2m}\right) f_{1,1} + \\
&\quad + P\hbar\left(\frac{\hbar}{4m}\nabla + \frac{ip}{2m}\right) f_{2,2}
\end{aligned}
$$

where

$$
\theta^+_\hbar[f] = -\frac{1}{2\pi\hbar}\int_r\int_{p'} \frac{V\left(x+\frac{r}{2}\right) + V\left(x-\frac{r}{2}\right)}{2} e^{i(p-p')\frac{r}{\hbar}} f(x,p') \quad \mathrm{d}p'\mathrm{d}r \qquad (10)
$$

Here we report the thermal equilibrium Wigner funtion for the device under test.

NUMERICAL TECHNIQUE OF SOLUTION

To solve the Wigner-Kane system we discretize the simulation domain and, accordingly, the equations. The simulation domain is discretized as follows:

$$
\begin{array}{lll}
x_i = i\triangle_x & \text{con} & i = 1, 2, \ldots, N_x \\
v_j = \frac{\pi}{\triangle_x m}\left[-\frac{(j-1/2)}{N_v} + \frac{1}{2}\right] & \text{con} & j = 1, 2, \cdots, N_v
\end{array}
$$

Using a second-order upwind differential scheme to discrete the position derivative, we can define the following "Translation operator"

$$
(\mathcal{T} f_w)_{i,j} = -\frac{v_j}{\triangle_x} \times \begin{cases} +\frac{1}{2}\left[-3f_i + 4f_{i+1} - f_{i+2}\right] & v_j < 0 \\ -\frac{1}{2}\left[-3f_i + 4f_{i-1} - f_{i-2}\right] & v_j > 0 \end{cases}
$$

and the "Gradient operator"

$$
(\mathcal{G} f_w)_{i,j} = -\frac{P\hbar}{\triangle_x} \times \begin{cases} +\frac{1}{2}\left[-3f_i + 4f_{i+1} - f_{i+2}\right] & v_j < 0 \\ -\frac{1}{2}\left[-3f_i + 4f_{i-1} - f_{i-2}\right] & v_j > 0 \end{cases}
$$

Then we define the "Potential operator"

$$
(\mathcal{P} f)_{i,j} = -\frac{1}{\hbar}\sum_{j'=1}^{N_v} U_{i,j-j'} f_{i,j'}
$$

$$
U_{i,j} = \frac{2}{N_v}\sum_{i'=1}^{N_x/2} \sin\left(\frac{2j\triangle_v i'\triangle_x}{\hbar}\right)\left(V_{i+i'} - V_{i-i'}\right)
$$

and $f_{i,j}$ the real column vector of $N_x \times N_v$ components. Now we can write the Wigner-Kane system in the following matrix form:

$$\begin{cases} (\mathbf{T} + \mathbf{P}_{1,1} - \mathbf{I}\frac{2}{\triangle_t})F_{1,1} = -\mathbf{G}\Im(f_{1,2}) - \mathbf{M}\Re(f_{1,2}) \\ (\mathbf{T} + \mathbf{P}_{2,2} - \mathbf{I}\frac{2}{\triangle_t})F_{1,1} = -\mathbf{G}\Im(f_{1,2}) + \mathbf{M}\Re(f_{1,2}) \\ (\mathbf{T} + \mathbf{P}_{1,2} - \mathbf{I}\frac{2}{\triangle_t})F_{1,2} = -\frac{i}{2}\mathbf{G}(f_{1,1} + f_{2,2}) + \mathbf{M}(f_{1,1} - f_{2,2}) \end{cases}$$

We consider the following cases:

Transient solution: We use the Cayley discretization scheme for the time derivative:

$$F_{i,j} = f_{i,j}^{n+1} + f_{i,j}^{n};$$

$f_{i,j}^{n}$ is the Wigner function to n-ieme temporal step.

Stationary solution: We use

$$F_{i,j} = 2f_{i,j}\,.$$

Numerical aspects of realistic semiconductor devices will be object of a future work.

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