Simulation of the Rashba Effect in a Multiband Quantum Structure

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Introduction

Devices containing asymmetric quantum wells where quantized states are spin-split by the Rashba effect have been proposed. In this work we introduce a multiband model derived within the Bloch-Wannier formalism, which gives a full description of the coupling between the conduction and the valence band, including the effect of the degenerate bands and the spin-orbit coupling. In particular, we present the six-band version of our model and some numerical results related to an asymmetric resonant interband tunneling diode.

Multiband envelope function model

We consider an electron of mass m_0 moving in a periodic potential V_L and subject to an additional external potential U which is treated as a perturbation. The Hamiltonian which governs the motion of the electron is given by

$$\mathcal{H} = \mathcal{H}_0 + U(\mathbf{r}) - i\zeta\left(\nabla U(\mathbf{r}) \wedge \nabla\right) \cdot \boldsymbol{\sigma}$$
$$\mathcal{H}_0 = -\frac{\hbar^2}{2m_0}\nabla^2 + V_L(\mathbf{r}) - i\zeta\left(\nabla V_L(\mathbf{r}) \wedge \nabla\right) \cdot \boldsymbol{\sigma},$$

where $\zeta = \hbar^2/(4m_0^2c^2)$, and $\boldsymbol{\sigma}$ is a vector whose components are the Pauli spin matrices. The evolution of the electron wave function $\Psi(\mathbf{r}, t)$ is determined by the Schrödinger equation with the perturbed Hamiltonian $\mathcal{H}$. The Bloch basis $\psi_n^\alpha(\mathbf{k}, \sigma, \mathbf{r})$ provides a set of functions for the expansion of the wave function

$$\Psi(\mathbf{r}, t) = \sum_{n,\alpha,\sigma} \int_B \varphi_n^\alpha(\mathbf{k}, \sigma)\, \psi_n^\alpha(\mathbf{k}, \sigma, \mathbf{r}, t)\, \mathrm{d}\mathbf{k},$$

Here B indicates the first Brillouin zone, the index n denotes the bands and α runs over the possible n_α degenerate states related to the eigenvalue E_n. Finally, the index σ labels the spin of the electron.
The aim of the "kp" approach is to separate the fast oscillating contributions to the Hamiltonian, due to the periodic potential V_L, from the slower contributions, due to the external potential U. This is achieved by expanding the equation of motion with respect to $|\mathbf{k}|$ and by taking the Fourier transform of the resulting system. To the first order we obtain

$$i\hbar\frac{\partial \varphi_n^\alpha(\mathbf{r}, \sigma)}{\partial t} = E_n^\sigma(-i\hbar\nabla)\, \varphi_n^\alpha(\mathbf{r}, \sigma) + \frac{\hbar}{m_0} \sum_{\substack{n' \neq n,\\ \alpha', \sigma'}} \int_B \nabla U(\mathbf{r}) \cdot \mathbf{Q}\, \varphi_{n'}^{\alpha'}(\mathbf{r}, \sigma')\, \mathrm{d}\mathbf{k},$$

$$\mathbf{Q} = \frac{\boldsymbol{\pi}_{n,n'}^{\alpha,\alpha'}(\sigma, \sigma')}{E_n^\sigma - E_{n'}^{\sigma'}} + \left\langle u_n^{\alpha,\sigma} \middle| \boldsymbol{\sigma} \middle| u_{n'}^{\alpha',\sigma'} \right\rangle \wedge \nabla - \zeta \left\langle u_n^{\alpha,\sigma} \middle| \boldsymbol{\sigma} \wedge \nabla \middle| u_{n'}^{\alpha',\sigma'} \right\rangle,$$
$$\boldsymbol{\pi} = \left\langle u_n^{\alpha,\sigma} \middle| \frac{\hbar}{4m_0c^2}\left(\boldsymbol{\sigma} \wedge \nabla V_L\right) - i\hbar\nabla \middle| u_{n'}^{\alpha',\sigma'} \right\rangle$$

Six-band model

The symmetry properties of the crystal lattice considerably reduce the number of independent parameters in the previous expressions. In particular, we consider the six-band model, which includes the conduction and the light and heavy holes valence bands.
By taking the y coordinate along the growth axis, we have $\boldsymbol{\varphi}(\mathbf{r}) = \boldsymbol{\varphi}(y)e^{ik_\perp \cdot \mathbf{r}}$, where $k_\perp$ is the transverse momentum, which is conserved. The equations for $\boldsymbol{\varphi}(y)$ are

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} \boldsymbol{\varphi}_c \\ \boldsymbol{\varphi}_h \end{pmatrix} = \begin{pmatrix} \mathbf{H}_{cc} & \mathbf{H}_{cv} \\ \mathbf{H}_{cv}^\dagger & \mathbf{H}_{vv} \end{pmatrix} \begin{pmatrix} \boldsymbol{\varphi}_c \\ \boldsymbol{\varphi}_h \end{pmatrix}$$

$$\boldsymbol{\varphi}_h(\mathbf{r}) = \left(\varphi_h^{3/2}\,,\, \varphi_h^{1/2}\,,\, \varphi_h^{-1/2}\,,\, \varphi_h^{-3/2}\right)^T$$
$$\boldsymbol{\varphi}_c(\mathbf{r}) = \left(\varphi_c^{+}\,,\, \varphi_c^{-}\right)^T$$

where with $\mathbf{I}_{n\times n}$ we indicate the $n \times n$ unit matrix, and

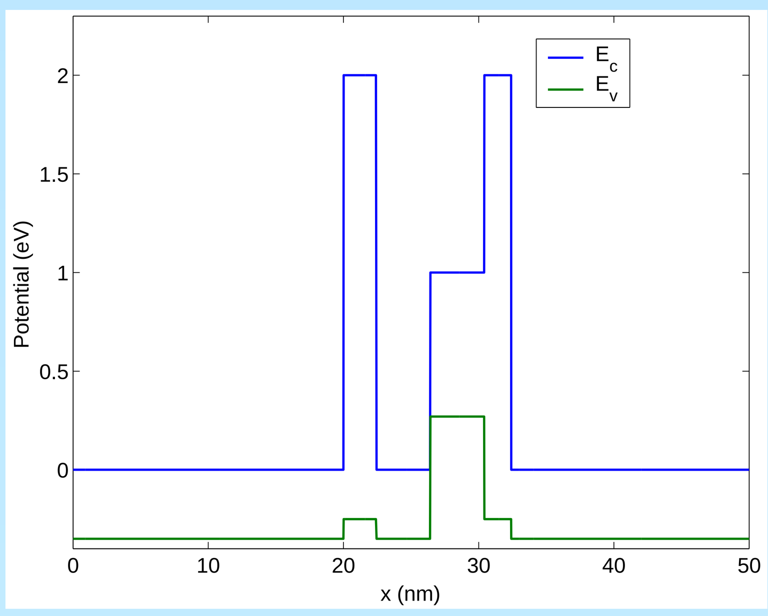
$$\mathbf{H}_{cc} = \mathbf{I}_{2\times 2}\left(E_c - E + U - \frac{\hbar^2}{2m_c}\frac{\mathrm{d}^2}{\mathrm{d}y^2}\right) + \zeta k_\perp \frac{\partial U}{\partial y}\boldsymbol{\sigma}_z$$
$$\mathbf{H}_{vv} = \mathbf{I}_{6\times 6}\left(E_v - E + U\right) + \mathbf{I}_h\frac{\hbar^2}{2}\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{k_\perp\zeta}{3}\frac{\partial U}{\partial y}\mathbf{J}_z^{3/2}$$
$$\mathbf{H}_{cv} = \overline{\lambda}\frac{\partial U}{\partial y}\mathbf{T}_y$$
$$\mathbf{I}_h = \mathrm{diag}\left(\frac{1}{m_{hh}},\ \frac{1}{m_{lh}},\ \frac{1}{m_{lh}},\ \frac{1}{m_{hh}}\right)$$
$$\mathbf{J}_z^{3/2} = \mathrm{diag}\left(3,\ 1,\ -1,\ -3\right)$$
$$\mathbf{T}_y = -\frac{i}{3\sqrt{2}}\begin{pmatrix} \sqrt{3} & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{3} \end{pmatrix}$$

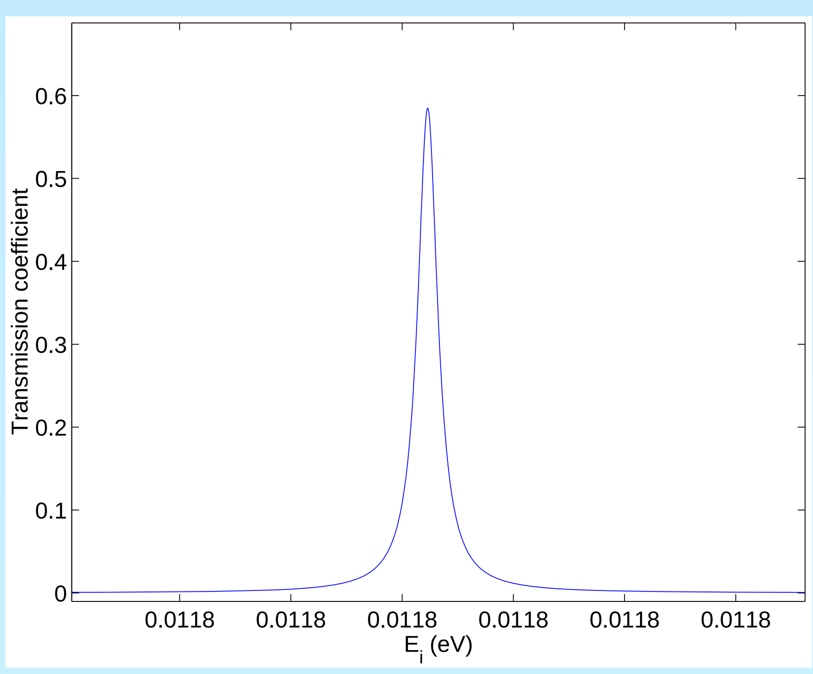
The other parameters are defined in the Table

Symbol	Physical Meaning
m_c	Effective mass in conduction band
m_{lh}, m_{hh}	Light and heavy holes effective masses
$u_n^{\alpha,\sigma}$	Periodic part of Bloch function related to $\mathbf{k} = 0$
$\lambda = \zeta\frac{\sqrt{3}}{\hbar}P + \frac{\hbar}{m_0}\pi^K$	Interband coupling coefficient
$\pi^K = \frac{3}{\sqrt{2}}\mathbf{e}_z \cdot \boldsymbol{\pi}_{c,h}^{+,1/2}$	Kane momentum
$P = -i\frac{\hbar^2}{m_0}\left\langle \psi_S \middle| \frac{\partial}{\partial_z} \middle| \psi_Z \right\rangle$	Kane momentum without spin

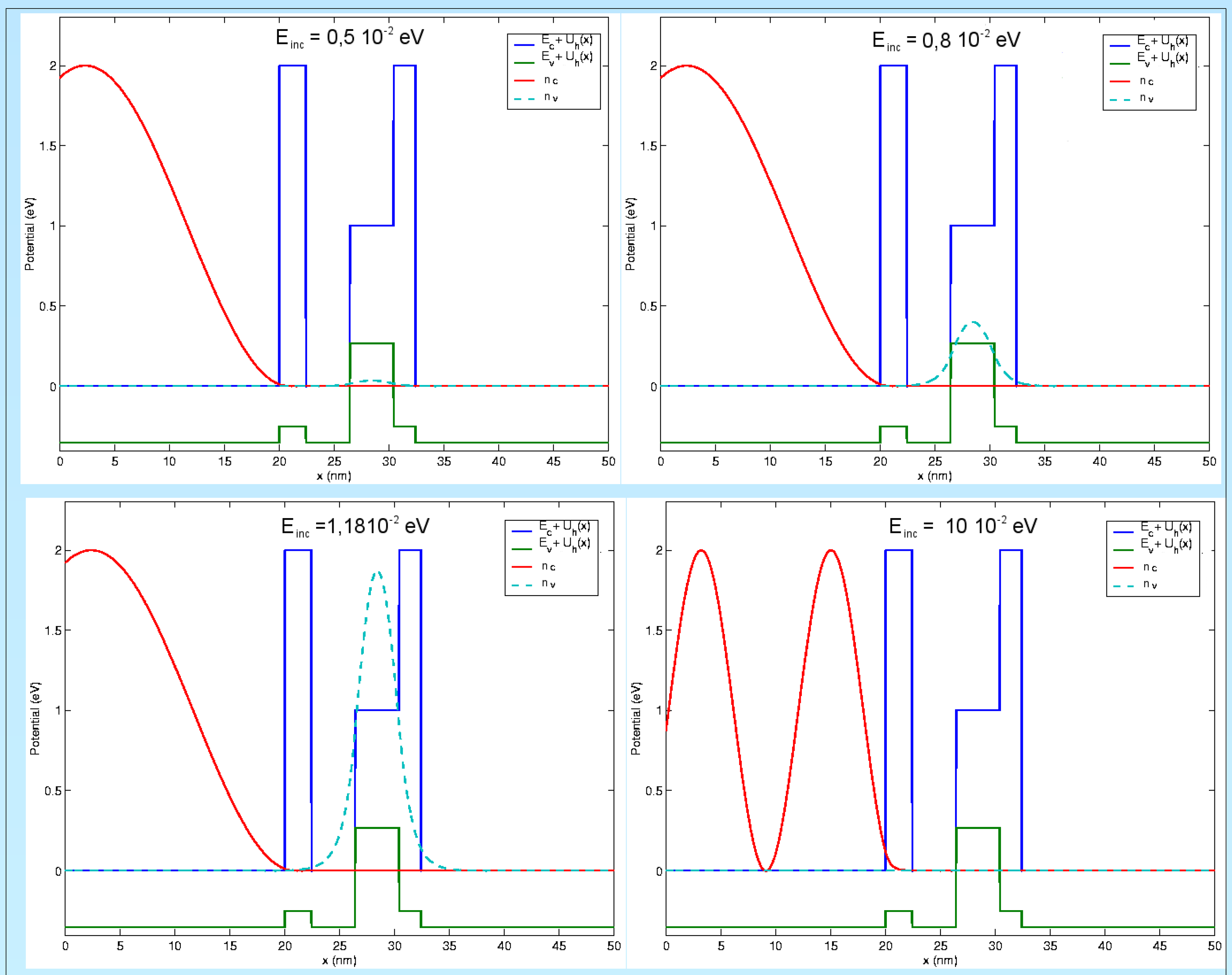
Numerical results

Band alignments of the $InAs/AlSb/GaSb/AlSb/InAs$ double barrier structure used in the simulation. Transport through this system involves resonant tunneling of electrons from the $InAs$ emitter, through unoccupied electron states in the subbands of the $GaSb$ well, and subsequently back into the conduction band of the collector.





Calculated transmission coefficient for the resonant diode for the six band system. The in-plane wave vector is $k_\perp = \frac{2\pi}{a}(0.03,\,0,\,0)$ where a is the lattice constant. The resonant peak is related only to the spin-up conduction electrons, and it disappears completely for the spin-down states. In this way, the device is able to select electrons both from the energy and form the spin direction.



By using a Runge-Kutta scheme, we calculate the envelope function solution for incremental values of the electron beam energy for both directions of the spin. The figures show the electron density in the valence bands $n_v(y) = \sum_{j=\pm 1/2, \pm 3/2} |\varphi_h^j|^2$ and in the conduction band $n_v(y) = \sum_{j=\pm} |\varphi_c^j|^2$ for of spin up electron.
When the electron energy approaches the resonant level, charge cumulates in the valence quantum well. On the other hand, no resonance effects are present for spin down electron.