11th International Workshop on Computational Electronics
TU Wien, 25-27 May 2006

Simulation of the Rashba Effect in a Multiband Quantum Structure

O. Morandi, L. Demeio*
Dipartimento di Elettronica e Telecomunicazioni, Università degli Studi di Firenze
Via S. Marta 3, I-50139 Firenze, Italy, e-mail: omar.morandi@unifi.it
*Dipartimento di Scienze Matematiche, Università Politecnica delle Marche

THE MULTI-BAND ENVELOPE FUNCTION MODEL

The aim of this work is to present an application of the "kp" multiband model, derived in [1], to some spin-sensitive devices. In recent years, much interest has been devoted to the investigation of spin phenomena in semiconductors with the aim of controlling not only the spatial degrees of freedom of the electrons, but also the spin. Various devices have already been proposed. These devices contain asymmetric quantum wells where quantized states are spin-split by the Rashba effect, and achieve spin filtering by exploiting the phenomenon that the spin of a resonantly transmitted electron aligns with that of the quasibound state traversed.

Several models have been proposed in order to analyze the properties of such devices from a theoretical point of view [2], [3]. The mixing of valence and conduction bands at the interfaces makes a many-band treatment necessary and, in particular, the investigation of the bands for k parallel to the layers requires a realistic description of the degenerate valence-band edge; furthermore, the occurrence of charge transfer requires self-consistent calculations. The envelope-function method, which is based on an expansion of the full wave function in a suitable othonormal and complete L^2 basis, is the most popular method for calculating the properties of electrons in semiconductor heterostructures.

In this work we propose a new model derived within the usual Bloch-Wannier formalism by a k-expansion. The effective-mass equations are based on an invariant expansion of the valence-band Hamiltonian, which is intimately related to the symmetry of the diamond lattice (point group $\mathcal{O}_h$) [4]. The equations are restricted to the manifold of the uppermost ($j = 3/2$) valence-band states, coupled with the split-off and the conduction states. They are formulated in terms of a set of coupled equations for the electron envelope functions. Our approach allows us to obtain a very simple and direct interpretation of the phenomena involved in the electronic motion in heterostructure devices. The initial formalism is equivalent to the one-electron Schrödinger equation; approximations suitable to treat heterostructure devices are then introduced.

In this contribution, we present the eight-band version of our model which gives a full description of the coupling between the conduction and the valence band for the most common semiconductors.

NUMERICAL RESULTS

Here, we apply our multiband envelope function model to an asymmetric resonant interband tunneling diode (a-RITD), and we present some numerical results showing the ability of our model to reproduce the spin-orbit splitting arising from the Rashba effect.

Figure 1 shows the band alignments of the $InAs/AlSb/GaSb/AlSb/InAs$ double barrier structure (p-type-well resonant interband tunneling diode at room temperature) used in the simulation. The band offset between $InAs$ and $GaSb$ is such that the conduction-band edge of $InAs$ lies $0.15\,eV$ below the energy of the valence-band edge of $GaSb$. 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.

Figure 2 shows the calculated transmission coefficient for the resonant diode. The in-plane wave vector is $k_{\|} = \frac{2\pi}{a}(0.03, 0, 0)$ where a is the lattice constant. The resonant peak is related only to

ISBN 3-901578-16-1

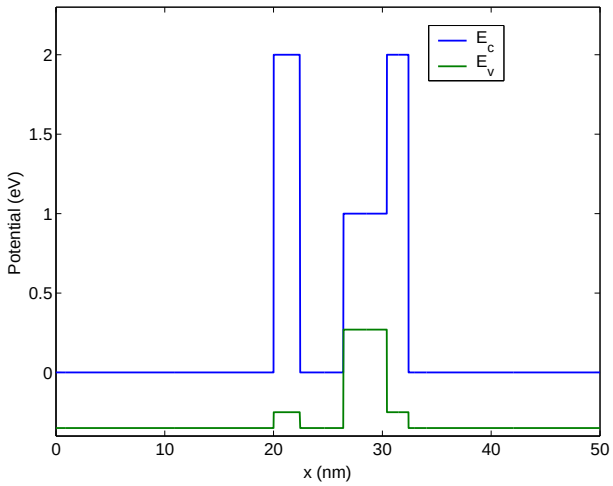

Fig. 1. Band alignments of the double barrier structure used in the simulations.

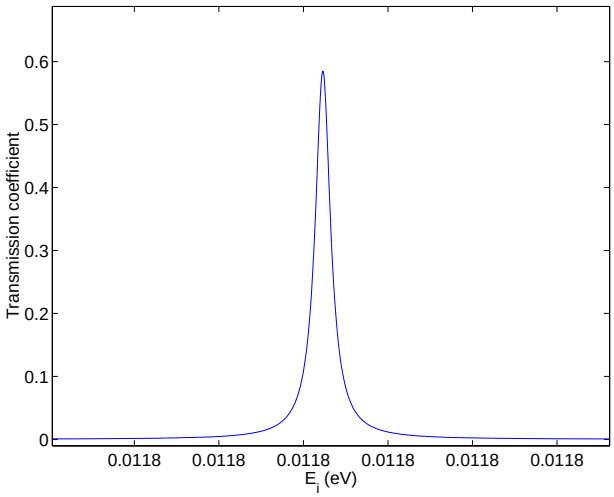

Fig. 2. Transmission coefficient spectra for the $InAs/GaSb/AlSb$ diode of Fig. 1 related to the spin up conduction electrons.

the spin-up conduction electrons, and it disappears completely for the spin-down states. In this way, only conduction electrons injected into the device with resonant energy and with spin parallel to the direction of motion can travel from the emitter to the collector lead; electrons with anti-parallel spin are reflected.

Finally, in Figures 3 and 4 we show the conduction and valence envelope functions, for the spin-up and spin-down case respectively, in the two band approximation, calculated in the resonant energy case.

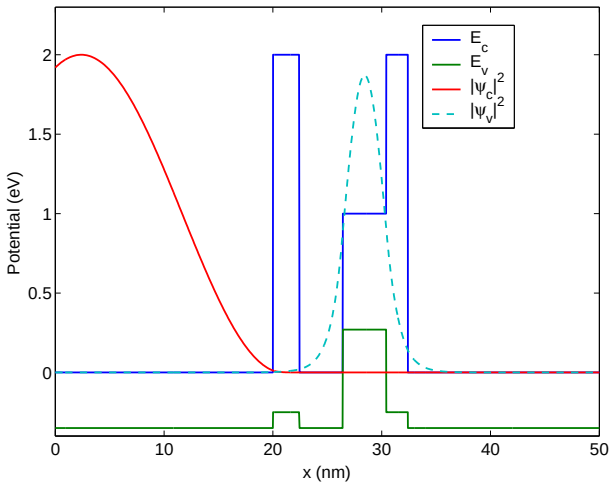

Fig. 3. Conduction and valence envelope functions, ψ_c and ψ_v, related to the resonant energy $E = 1.18\ eV$ for the spin-up case.

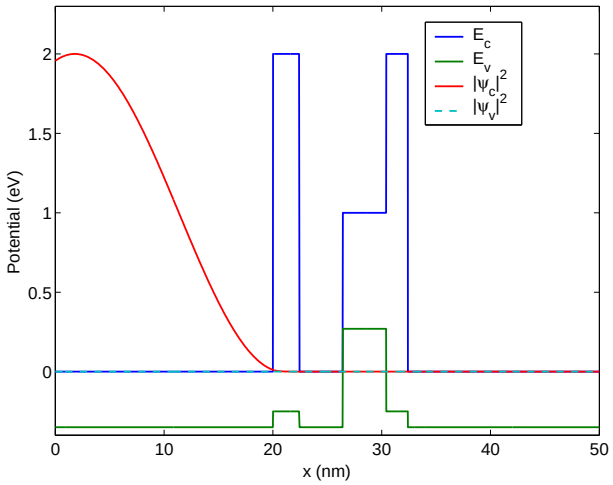

Fig. 4. Conduction and valence envelope functions, ψ_c and ψ_v, related to the resonant energy $E = 1.18\ eV$ for the spin-down case.

REFERENCES

[1] O. Morandi and M. Modugno, A multiband envelope function model for quantum transport in a tunneling diode, Phys. Rev. B **71**, 235331 (2005).

[2] M. Altarelli, Electronic structure and semiconductor-semimetal transition in InAs GaSb superlattices, *Phys. Rev. B* **28**, 842-845 (1983).

[3] D. Z. Y. Ting, E. T. Yu, and T. C. McGill, Multiband treatment of quantum transport in interband tunnel devices, *Phys. Rev. B* **45**, 3583-3592 (1992).

[4] H. R. Trebin, U. Rössler and R. Ranvaud, Quantum resonances in the valence bands of zinc-blende semiconductors. I. Theoretical aspects *Phys. Rev. B* **20**, 686-700 (1979).