Electronic structure of [110] PbTe nanowires

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Abstract. An envelope-function model for the electronic structure of [110] square PbTe quantum wires, with simple analytical solutions, is presented based on the 4-band Dimmock kp model for the bulk. The subband structure of states for the confined electrons is obtained including band nonparabolicity and anisotropy effects. Results for the subband dependent effective mass, for the total density of states (added over the non equivalent valleys) and for the Fermi energy are shown and discussed, as a function of the PbTe band-gap parameters and of the wire width L.

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INTRODUCTION

PbTe semiconductor nanostructures are attracting an increasing attention due the recently observed enhanced thermoelectric power in PbTe quantum wells and wires[1,2]. However, available model calculations of their electronic properties are mostly based on simple one-band parabolic models, in part to simplify the calculation of the transport coefficients[1,2]. A nonprabolic multi-band kp model for the electronic structure of PbTe quantum wells[3], based on the 4(or 2 without spin)-band Dimmock kp model for the PbTe bulk, is here extended to the quantum wire problem. The model has been successfully applied to calculate different properties of PbTe/PbEuTE thin quantum wells[4,5]. We show that within this model, the electronic structure of [110] PbTe square quantum wires can be solved analytically, in the limit of strong confinement. The 1D subband structure of [110] PbTe quantum wires is calculated in the independent valley approximation.

MODEL

We start from a PbTe quantum well grown along the [001] (// z) direction, as on a NaCl substrate. Then, the four equivalent valleys along the [111] directions are projected into the 2D plane, and seen to separate into two valleys with the main axis parallel and two with it perpendicular to [110]; which we call longitudinal and transverse valleys, respectively. Then, we consider an extra confinement perpendicular to [110], so that the electrons are free to move only along x // [110]. The effective Hamiltonian for the quantized subbands from each valley reads [3]:

$$H_{eff.} = \frac{\hbar^2 k_x^2}{2m_1(E)} - \frac{\hbar^2}{2m_2(E)}\frac{d^2}{dy^2} - \frac{\hbar^2}{2m_3(E)}\frac{d^2}{dz^2} + V(y,z) \quad (1)$$

with, in the infinite barrier approximation,

$$V(y,z) = \begin{cases} \infty \ ; |y| \geq L_y/2 \ \ or \ \ |z| \geq L_z/2 \\ 0 \ , otherwise \end{cases} \quad (2)$$

where L_y and L_z give the wire width and, for each kind of valley, $m_i = m_{i,0}(E+E_g)/E_g$, i=1,2,3, corresponding to the two-band nonparabolic effective mass along the main axes of the projected ellipsoids. The band edge values $m_{i,0}$ are listed in Table 1, and the zero of energy is placed at the conduction band edge. The same model applies to holes with the corresponding masses. The general solution of (1) is:

$$\psi = A \sin\left(\frac{n\pi}{L_y} y\right) \sin\left(\frac{m\pi}{L_z} z\right) e^{ik_x x} \quad (3)$$

with n,m=1,2,3…; and for the dispersion relation we get:

$$E = -\frac{E_g}{2} + \frac{1}{2}\sqrt{E_g^2 + 4\left(k_{nm}^2 + k_x^{\ 2}\right)} \quad (4)$$

with

$$k_{nm}^2 = \gamma_2\left(\frac{n\pi^2}{L_y}\right) + \gamma_3\left(\frac{n\pi^2}{L_z}\right) \quad (5)$$

where for each valley, the mass ratios γ_2 and γ_3, are listed in Table 1. The density of states from each set of valleys, transverse and longitudinal, each with valley degeneracy n_v=2, is then given by:

$$D_{nm}(E) = \frac{n_v}{\pi} \frac{(2E+E_g)/E_g}{\sqrt{E(E_g+E)/E_g - k_{nm}^2}} \quad (6)$$

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TABLE 1. Effective masses for the transverse and longitudinal valleys in a [110] PbTe quantum wire, in units of free electron mass (m_e) and using the bulk masses given in Ref. 3.

valley	x[110]	y[-110]	z[001]	γ_2	γ_3
transverse	0.034	0.168	0.024	0.204	1.43
longitudinal	0.168	0.034	0.024	4.90	7.00

Now we add the states from the different valleys, and for each carrier density, we integrate and find the Fermi energy. The contribution from each kind of valley, to the total number of states (or carrier concentration) as a function of the Fermi energy is then given by:

$$N(E_F) = \frac{4}{\pi}\sqrt{\frac{E_F\left(E_F + E_g\right)}{E_g} - k_{nm}^2} \qquad (7)$$

And finally, from Eq.(4), in the small k_x limit, we obtain the following subband dependent effective mass for electrons moving along the wire:

$$m_{nm}^* = m_{1,0}\frac{\sqrt{E_g\left(E_g + 4k_{nm}^2\right)}}{E_g}. \qquad (8)$$

As expected, these results reduce to the well known single-band approximation when the energy correction to the effective mass in Eq. (1) is neglected.

RESULTS

In Fig.1, for the first subband of a PbTe square quantum wire with L=10nm, we compare the obtained dispersion relation with the parabolic approximation,

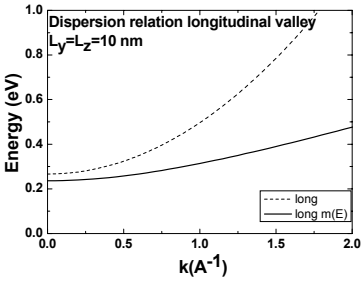

FIGURE 1. Dispersion relation for the first subband from the longitudinal valley, in a PbTe square quantum wire, compared with the one-band or parabolic approximation.

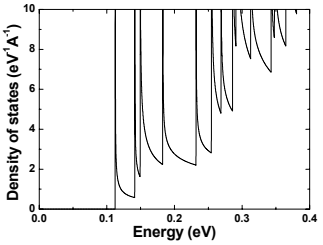

FIGURE 2. The total density of states for the same PbTe square quantum wire as in Fig. 1.

and see a considerable reduction in the confined energy due to nonparabolicity. The total density of state, i.e. added over the different valleys, and the total number of occupied states at T=0 as a function of the Fermi energy, are shown in Figures 2 and 3, respectively.

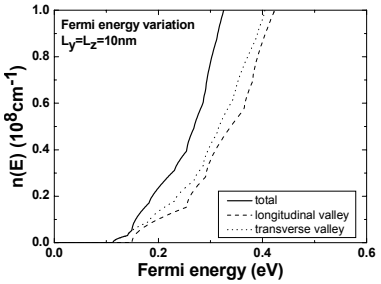

FIGURE 3. The Fermi energy of the PbTe square wire 1DEG, as a function of the electron density, with the contributions from the transverse and longitudinal valleys.

CONCLUSIONS

The present solution for the electronic structure of PbTe quantum wires, within the multi-band envelope-function approximation, shows that different band effects can be easily incorporated in a simple analytical model. The results for a [110] square quantum well in particular, indicate that both kinds of valleys play a similar role and must be considered together. The simple expression for the subband dependent electron effective mass, Eq. (8), can help the modeling of diffusive electronic transport in such wires. To conclude, the model presented is seen to have simple analytical solutions which can be useful in particular in the study and calculation of the corresponding thermal and charge transport phenomena in these important nanostructures.

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