Effects of Non Parabolicity in Si Quantum Wires

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INTRODUCTION

Semiconductor nanostructures such as quantum wells, quantum wires and quantum dots have interesting properties which could be used for the future development of nanodevices. Since the quantum confinement in these structures removes the subband edges several tenths of meV from the bulk band edges, a good model of the bands should be used to investigate the subband structures. This model will determine not only the energy of the subband edges but also the shape of the dispersion relations. In this work we present a method for solving the Schrödinger equation in quantum wires, considering a general isotropic and a non-parabolic band. We apply it to calculate the subband structure in a squared Si 10 nm×10 nm quantum wire. We examine the curvatures of the subband edges and comment on the results.

THEORETICAL TREATMENT

Any isotropic and non-parabolic dispersion relation, $\varepsilon(\vec{k})$ could be expanded in power series on k^2 in the following manner:

$$\varepsilon(\vec{k}) = \sum_{n=0}^{\infty} b_n k^{2n} \tag{1}$$

The b_n terms can be calculated using the Taylor theorem. The n=0 term appears for bands where there is a certain energy for $k = 0$, i.e. the split-off band in the valence band. Following the Effective Mass Theorem, we performed the substitution $\vec{k} \rightarrow -i\nabla$ in Eq.(1) and obtained the operator $\varepsilon(-i\nabla)$

$$\varepsilon(-i\nabla) = \sum_{n=0}^{\infty}\left[b_n \times \left(-\nabla^2\right)^n\right] \tag{2}$$

Thus, the effective mass Schrödinger equation of the problem can be written as

$$\left[\sum_{n=0}^{\infty}\left[b_n \times \left(-\nabla^2\right)^n\right] + V(x,z)\right]\psi(\vec{r}) = E\psi(\vec{r}) \tag{3}$$

where y is considered as the transport direction in the wire. In the case of a constant potential inside the wire, $V(x,z) = V_0$, the envelope functions of the hole states are known to be

$$\psi(\vec{r}) = e^{ik_y y}\sin(k_x x)\sin(k_z z) \tag{4}$$

where $k_x = n_x\pi / L_x$, $k_z = n_z\pi / L_z$. Combining Eq. (3) and (4) we obtained

$$\varepsilon(k_x^2 + k_y^2 + k_z^2) = E - V_0 \tag{5}$$

Using the valence band model presented in a previous work [1], the condition of Eq. (5) is fulfilled when

$$\begin{aligned}\frac{E - V_0}{\chi_{H,L}(E - V_0)} &= \frac{\hbar^2}{2m_{H,L}}\left[\frac{n_x^2\pi^2}{L_x^2} + \frac{n_z^2\pi^2}{L_z^2} + k_y^2\right] \\ \frac{E - V_0 - \Delta_{so}}{\chi_S(E - V_0 - \Delta_{so})} &= \frac{\hbar^2}{2m_{so}}\left[\frac{n_x^2\pi^2}{L_x^2} + \frac{n_z^2\pi^2}{L_z^2} + k_y^2\right]\end{aligned} \tag{6}$$

Where $m_{H,L,so}$ and $\chi_{H,L,S}(\varepsilon)$ are the effective mass values and the functions that describe the non-parabolicity of the band for the heavy, light and split-off holes respectively, and Δ_{so} is the split-off energy. Varying the value of k_y it is possible to obtain the $E(k_y)$ relation of each subband.

RESULTS AND CONCLUSIONS

The results in Fig. 1 indicate the effective mass value at the edge of each subband obtained by using both a non-parabolic and a parabolic band model. In conclusion, our work suggests that non- parabolicity plays a very important role in the determination of the hole subband structure in quantum wires. In addition, the method demonstrated could be a good tool to carry out investigations on these devices.

REFERENCES

[1] S. Rodríguez-Bolívar, F. M. Gómez Campos, J. E. Carceller, *Simple analytical valence band structure including warping and non-parabolicity to investigate hole transport in Si and Ge*, Semiconductor Science and Technology, **20**, 16 (2005).

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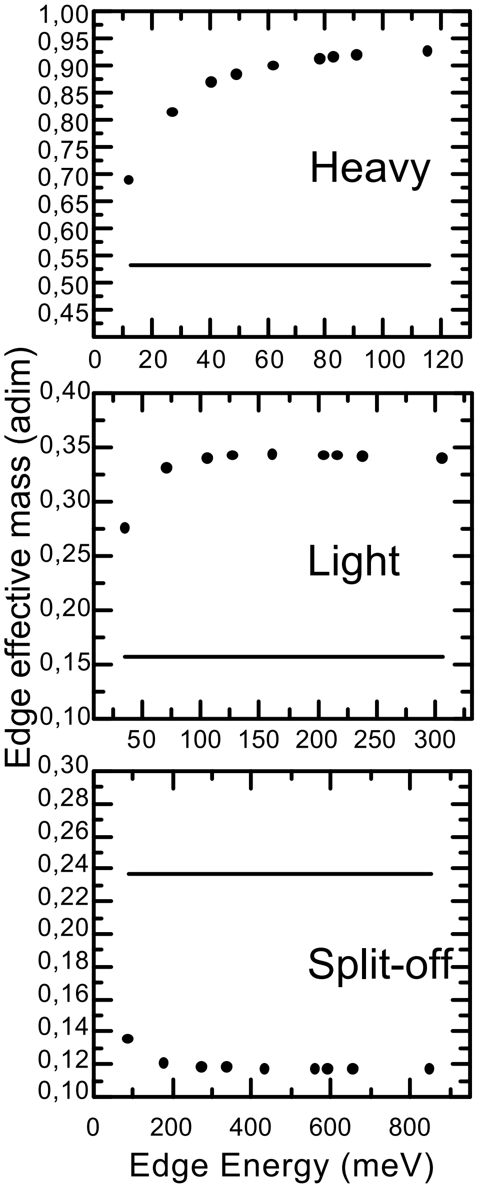

Fig. 1. Effective masses at the edges of the nine lowest subbands of heavy (a), light (b) and split-off (c) holes in a Si 10 nm×10 nm quantum wire obtained by means of the method shown in this work (points) and by means of a parabolic model (solid line). The effective masses at the subband edges increase for higher subbands in heavy and light hole subbands, and decrease for higher subbands in split-off hole subbands. Important differences between our results and the parabolic model are observed.