A Nonparabolicity Model compared to Tight Binding: The Case of rectangular Quantum Wires

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The assumption of parabolic bands always provides a good starting point for the quantum mechanical treatment of charge transport in electronic devices. However, the effective mass approximation (EMA) is intended for problems whose external perturbations are smooth compared to the periodicity of the underlying material. Thus, in semiconductor devices reaching the nanometer scale the validity of EMA becomes questionable. More advanced methods such as the tight-binding formalism **[1]** consider the atomistic nature of the material thus being more precise than the single band picture of the EMA. On the other hand, the gain in precision of an atomistic simulation goes at the expense of the simulation time which increases significantly.
The aim of this work is to elaborate a method which is capable to improve the results of EMA without loosing its time efficiency. Given a fixed device configuration and calculated quantities such as currents from an atomistic simulation, the method should reproduce these results by means of simple tuning parameters. For this purpose we consider a nonparabolicity model used by Trellakis *et. al.* **[2]**. This model turns out to be treatable within the same transport model as we use for EMA thus maintaining a reasonable time efficiency. The inclusion of the nonparabolicity is reflected in a change of the kinetic operator of the underlying Hamiltonian

$$\frac{\hbar^2}{2}\left(\frac{1}{m_x^*}\frac{\partial^2}{\partial x^2}+\frac{1}{m_y^*}\frac{\partial^2}{\partial y^2}+\frac{1}{m_z^*}\frac{\partial^2}{\partial z^2}\right)\longrightarrow\frac{\hbar^2}{2m_x^*}\frac{\partial^2}{\partial x^2}+\frac{1}{2\alpha}\left[\sqrt{1+4\alpha\frac{\hbar^2}{2}\left(\frac{1}{m_y^*}\frac{\partial^2}{\partial y^2}+\frac{1}{m_z^*}\frac{\partial^2}{\partial z^2}\right)}-1\right],$$

where the nonparabolicity coefficient α has the dimension of an inverse energy. We restrict our attention to the case of a rectangular quantum wire whose channel consists of silicon grown in the <100> direction being surrounded by a 1nm thick silicon oxide layer as depicted in **Figure 1**. The transport is restricted to the x-direction such that the nonparabolic part of the Hamiltonian merely affects the transverse modes by decreasing their eigenenergies. The resulting increase in the source-drain current can be therefore controlled via the nonparabolicity coefficient α.
We calculate source-drain currents as a function of the gate voltage (V_G) at a finite source-drain bias of 0.6 V for several channel diameters (d) ranging from 2nm to 5nm. The off currents (V_G = 0 V) for the case $\alpha = 0$ Ha^{-1} (parabolic) and $\alpha = 5$ Ha^{-1} as a function of d are plotted in **Figure 2** whereas the inset shows the averaged relative error in percent for the corresponding characteristics. In addition we have tight-binding data for three distinct diameters $d_{2.1}$ = 2.1nm, $d_{2.5}$ = 2.5nm, and $d_{2.9}$ = 2.9nm. The nonparabolic curve as well as the tight-binding data approach the parabolic curve for increasing diameters as expected. Furthermore, we minimize the error between the tight-binding currents and the nonparabolic ones for $d_{2.1}$, $d_{2.5}$, and $d_{2.9}$ by means of α as shown in **Figure 6** and obtain $\alpha_{2.1}$ = (4.00±0.25) Ha^{-1}, $\alpha_{2.5}$ = (4.50±0.25) Ha^{-1}, and $\alpha_{2.9}$ = (7.00±0.25) Ha^{-1}. Thus, for an increasing channel diameter d the coefficient α has to be increased too in order to keep up with tight-binding. For a detailed analysis of α as a function of d some more data from tight binding is needed. Finally, the currents for $d_{2.1}$, $d_{2.5}$, and $d_{2.9}$ are explicitly depicted in **Figures 3**, **4**, and **5** showing a good agreement between tight-binding and the nonparabolic characteristics.

References

[1] M. Luisier, A. Schenk, W. Fichtner, and G. Klimeck. "Atomistic simulation of nanowires in the $sp^3d^5s^*$ tight-binding formalism: From boundary conditions to strain calculations," *Phys. Rev. B*, vol. 74, no. 205323, November 2006. (Journal Article)

[2] A. Trellakis and U.Ravaioli. "Three-dimensional spectral solution of the Schrödinger equation for arbitrary band structures," *J. Appl. Phys.* vol. 92, no. 7, pp. 3711-3716, June 2002. (Journal Article)

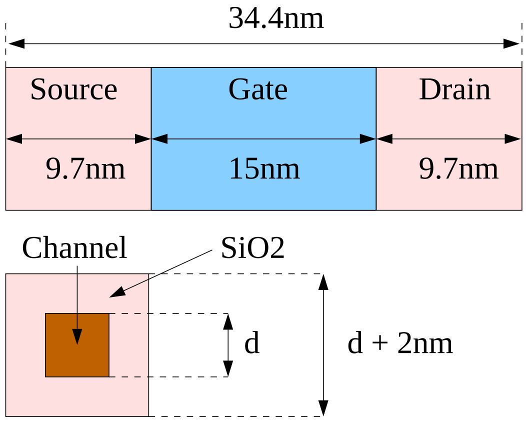

Figure 1: Schematic representation of the considered quantum wire. The channel is surrounded by a 1nm thick oxide layer whereas the source- and drainregion are n-doped with a concentration of 1e20 cm^{-3}.

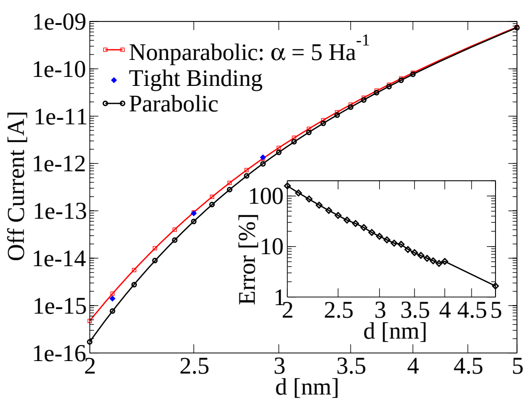

Figure 2: Off currents as a function of the channel diameter. The black curve shows the result for $\alpha = 0$ Ha^{-1} whereas the red curve is for $\alpha = 5$ Ha^{-1}. The blue points represent the tight binding result for three distinct diameters $d_{2.1} = 2.1$nm, $d_{2.5} = 2.5$nm, and $d_{2.9} = 2.9$nm. The inset shows the averaged relative error between the current caracteristics belonging to the red and black curve. For increasing d the nonparabolic curve as well as the tight-binding data approach the parabolic curve as expected.

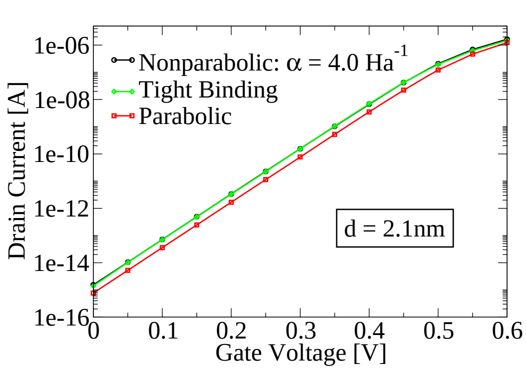

Figure 3: Current-Voltage characteristics at a source drain bias of 0.6 V (d = 2.1nm).

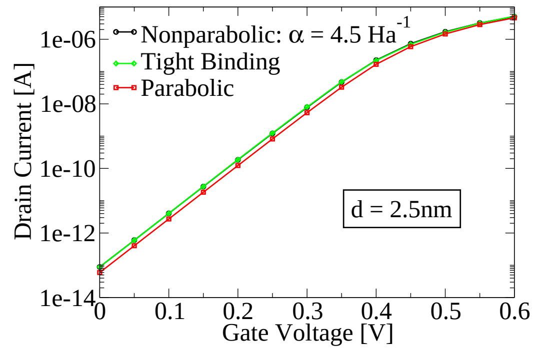

Figure 4: Current-Voltage characteristics at a source drain bias of 0.6 V (d = 2.5nm).

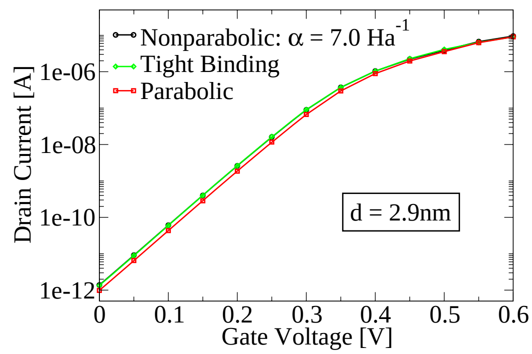

Figure 5: Current-Voltage characteristics at a source drain bias of 0.6 V (d = 2.9nm).

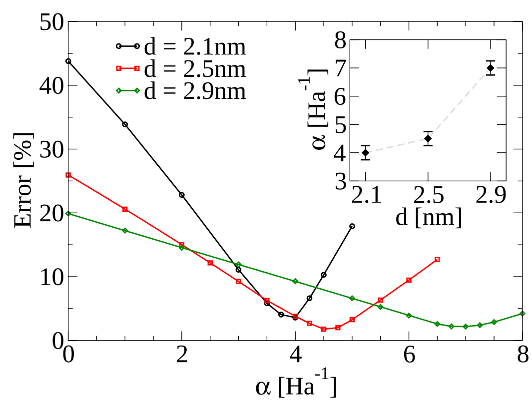

Figure 6: Averaged relative error between the tight-binding characteristic and the result obtained via the nonparabolicity model as a function of α. Plotted are the results for three diameters d=2.1nm, d=2.5nm, and d=2.9nm showing three distinct minima. The inset shows the nonparabolicity coefficient resulting from the minimization for the three diameters. The results are $\alpha_{2.1} = (4.00\pm0.25)$ Ha^{-1}, $\alpha_{2.5} = (4.50\pm0.25)$ Ha^{-1}, and $\alpha_{2.9} = (7.00\pm0.25)$ Ha^{-1}.