3D Modeling of Direct Band-to-Band Tunneling in Nanowire TFETs

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1 Abstract

Nanowire tunneling field-effect transistors have garnered much attention recently. They provide a steep subthreshold swing, making them viable candidates for ultra low power switching applications. An appropriate description of band-to-band (BTB) tunneling in realistic devices necessitates a 3D approach. We present a simple but effective model for 3D BTB tunneling in direct semiconductor devices. By defining an effective tunneling barrier the computation simplifies from a BTB tunneling to a single barrier problem yielding wave functions and transmission.

2 Band-to-Band Tunneling Model

Band-to-band (BTB) tunneling is a complex mechanism and challenging to model accurately. Recently, we presented a 1D model for BTB tunneling in direct semiconductors [1]. We determined an effective tunneling barrier from the conduction and valence band energies. Using this potential, the wave functions, transmission coefficient and current are computed by applying the quantum transmitting boundary method (QTBM) [2]. In this paper, we extend this approach to 3D tunneling systems.

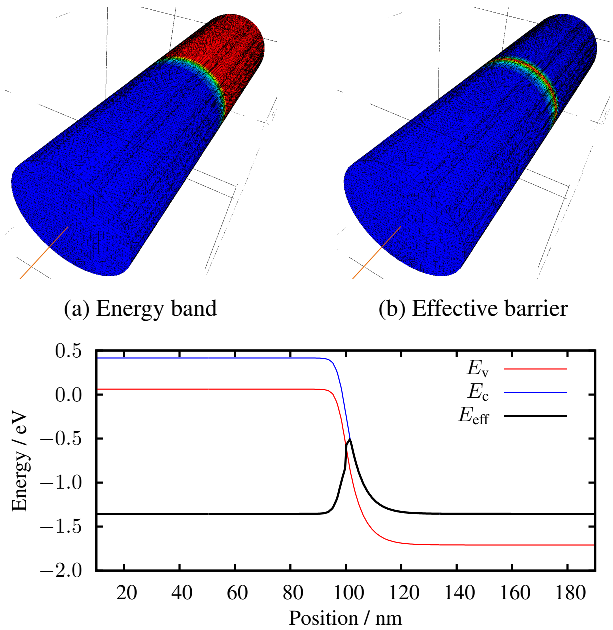
The developed method enables the calculation of the wave function using a single barrier of arbitrary shape with varying effective mass. Throughout the following model description we will use an InAs nanowire (see Fig. 1a) with 50 nm diameter and a symmetric p-n junction (N_D=N_A=$3 \times 10^{19}\,\mathrm{cm}^{-3}$) to demonstrate the methods and concepts.

2.1 Extraction of Effective Barriers

In order to obtain the tunneling potential barrier the conduction and valence bands need to be computed. This is performed using a self-consistent Schrödinger-Poisson model that is part of the Vienna Schrödinger-Poisson (VSP) solver framework [3]. A finite volume spatial discretization is applied to solve the Schrödinger equation and calculate the potentials [4]. Figure 1a shows the band edges of the 3D simulation of a nanowire pn junction.

In our band-to-band tunneling model an effective single tunneling barrier is determined. The potential barrier exhibits valence band properties in some parts of the device, and conduction band properties in others. The locations of these transitions are calculated for a specific energy E by comparing the momenta of valence and conduction band:

$$M_\mathrm{v}^2 = m_\mathrm{v}\,(E - E_\mathrm{v}) \quad \text{and} \quad M_\mathrm{c}^2 = m_\mathrm{c}\,(E_\mathrm{c} - E)\,.$$



(a) Energy band (b) Effective barrier

(c) 1D Effective barrier

Fig. 1: (a) Self-consistently calculated energy bands of a nanowire p-n junction; (b) Effective tunneling potential barrier from (a); (c) 1D cut through (a) and (b)

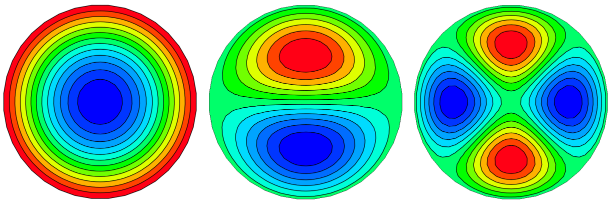
The effective barrier potential and tunneling mass are then set according to the following rules

$$E_\mathrm{eff} = \begin{cases} 2E - E_\mathrm{v}, \\ E_\mathrm{c}, \end{cases} \quad \text{and} \quad m_\mathrm{eff} = \begin{cases} m_\mathrm{v}, & M_\mathrm{v} \le M_\mathrm{c} \\ m_\mathrm{c}, & M_\mathrm{v} > M_\mathrm{c}. \end{cases}$$

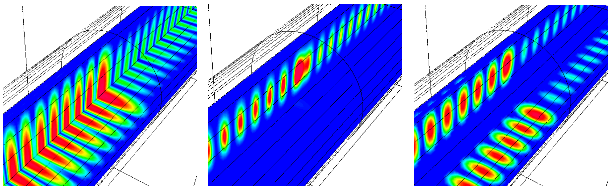
The resulting effective potential barrier for the exemple nanowire is shown in Fig. 1b.

2.2 Computation of Wave Functions

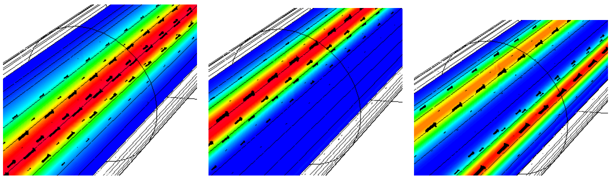
In [2], QTBM was introduced to calculate wave functions and transmission in 2D devices. For our model we implemented a 3D QTBM solver using the finite volume discretization scheme of VSP. The computation of the wave function in the device is divided into two problems. First we calculate the injecting contact eigenmodes. Then we propagate the wave through the device for each mode. The boundaries of the system are defined by 2D surfaces. For each contact the eigenmodes are determined by numerically solving the closed boundary effective mass Schrödinger equation. As an example, the contact modes of the InAs nanowire are shown in Fig. 2a.



(a) Contact modes



(b) Wave functions from contact modes in (a)



(c) Current contribution from contact modes in (a)

Fig. 2: Propagating wave functions through a p-n NW junction for different contact modes at a single energy, E

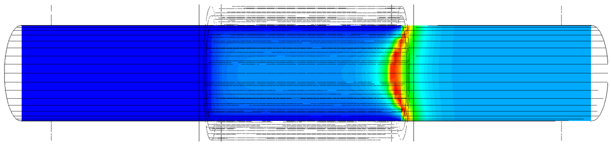
Once the wave functions in the contacts are found, the propagating waves through the 3D device can be calculated for each mode. The wave function in the device is obtained by solving the QTBM-like Schrödinger equation

$$\left[\frac{-\hbar^2}{2m_{\text{eff}}}\nabla^2 + V + E\right]\Psi_\lambda = \Psi_\text{n},$$

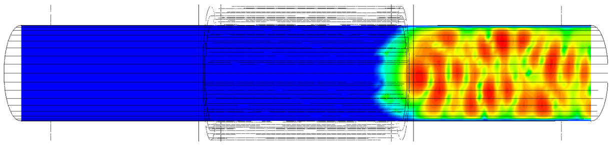
where V contains the self-consistent Hartree potential and the extracted effective potential barrier E_eff. Ψ_n are the eigenmodes injecting from the contacts and Ψ_λ the resulting wave functions in the device (see Fig. 2b). The tunneling current is obtained by summing over all energies E and contact modes n.

3 Results and Discussion

To demonstrate the ability of the presented method, a realistic device structure is simulated. We investigate an InAs gate-all-around NW TFET with 50 nm diameter doped at N_A=$3\times10^{19}\,\text{cm}^{-3}$, N_D=$7\times10^{18}\,\text{cm}^{-3}$. Applying a gate bias of -5 V, allows for tunneling to occur between the channel and drain. The 3D effective tunneling barrier and a sample tunneling wave are shown in Fig. 3. Alternatively, applying a positive bias of 5 V, creates tunneling from the source. The effective barrier shape and location change accordingly (Fig. 4). The tunneling barrier computation automatically responds to changes in device geometry, material parameters and applied bias.

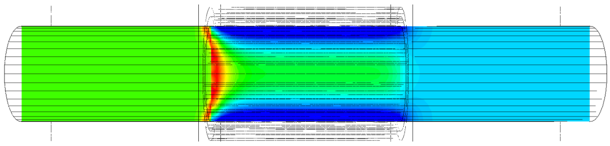


(a) Effective tunneling barrier

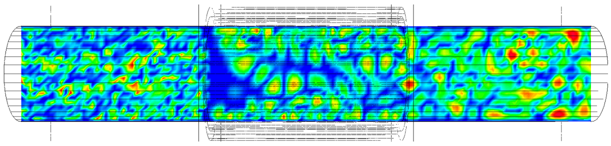


(b) Wave function from first contact mode in Fig. 2a

Fig. 3: Effective tunneling barrier of a InAs TFET at an applied gate voltage of -5 V and a single energy, E



(a) Effective tunneling barrier



(b) Wave function from first contact mode in Fig. 2a

Fig. 4: Effective tunneling barrier of a InAs TFET at an applied gate voltage of 5 V and a single energy, E

4 Conclusion

We developed a simple but effective model to describe direct band-to-band tunneling in 3D devices of arbitrary shape. Our novel method is based on the QTBM approach and yields the self-consistent wave functions in the entire device. As demonstrated using a GAA NW TFET, the computation of the tunneling barrier considers the 3D device geometry, material properties and bias, allowing for a diverse application of the presented model. Transmission coefficents and tunneling currents are obtained naturally.

Acknowledgment

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