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Ballistic modeling of InAs nanowire transistors

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ABSTRACT

In this work, the intrinsic performance of InAs nanowire transistors is evaluated in the ballistic limit. A self-consistent Schrödinger–Poisson solver is utilized in the cylindrical geometry, while accounting for conduction band non-parabolicity. The transistor characteristics are derived from simulations of ballistic transport within the nanowire. Using this approach, the performance is calculated for a continuous range of nanowire diameters and the transport properties are mapped. A transconductance exceeding 4 S/mm is predicted at a gate overdrive of 0.5 V and it is shown that the performance is improved with scaling.

Furthermore, the influence from including self-consistency and non-parabolicity in the band structure simulations is quantified. It is demonstrated that the effective mass approximation underestimates the transistor performance due to the highly non-parabolic conduction band in InAs. Neglecting self-consistency severely overestimates the device performance, especially for thick nanowires. The error introduced by both of these approximations gets increasingly worse under high bias conditions.

1. Introduction

Nanowire transistors are developed to extend the performance scaling of conventional transistors [1–4]. Combining the high mobility of III–V materials with the excellent gate control provided by a gate-all-around architecture, the performance of these devices has been predicted to reach the THz regime [5,6]. A cutoff frequency of 2.7 THz has been estimated for an optimized nanowire MOSFET with a realistic footprint [7].

The transport properties of highly scaled nanowires has been extensively studied using various approaches [8–16]. A common approach is to use a tight-binding model to simulate the band structure [17–21]. However, the use of a tight-binding model is very computationally expensive, especially for thick nanowires with many subbands. This limits a reasonable analysis to a small number of data points with thin nanowires. In order to reduce simulation time, self-consistency between the band structure and the electrostatic potential is occasionally disregarded [18]. Others have utilized $k{\cdot}p$ perturbation theory or resorted to the basic effective mass approximation, which is a relatively rough approximation, especially under high bias conditions [22–24]. Although this approximation may be reasonable for Si, the highly non-parabolic conduction band in InAs introduces a significant error [25].

In this work, the intrinsic performance of an InAs nanowire transistor structure is studied, following the approach previously used in [25], where the intrinsic properties of an InAs nanowire capacitor was determined by the development of a Schrödinger–Poisson solver adapted to InAs nanowire structures [26–28]. This solution method is customized for the cylindrical geometry and is fully self-consistent, while accounting for the non-parabolic conduction band in InAs. Furthermore, the simulations are repeated using the effective mass approximation, as well as for a constant electrostatic potential, in order to quantify the effect of these approximations.

The calculated band structure is used to derive the transistor characteristics, using a conventional ballistic transistor model [29,30]. The ballistic transport is modeled self-consistently with regard to the indirect control of the gate barrier height, including the influence of the quantum capacitance [29]. The model is sufficiently fast to simulate even relatively thick nanowires on a standard laptop. This allows an analysis to be performed for a continuous range of nanowire diameters between 5 nm and 35 nm. Furthermore, this work provides a complete insight into the transport properties of differently scaled nanowires, by mapping the location of the carrier concentration and velocities within the nanowire. The model is designed for the ballistic limit and does not incorporate any scattering due to impurities or the nanowire surface, which may degrade the transistor performance for longer gate lengths.

2. Structure and materials

The transistor structure considered in this study consists of a single InAs nanowire, covered by a high-κ dielectric with an assumed permittivity of 15, roughly corresponding to HfO_2. The

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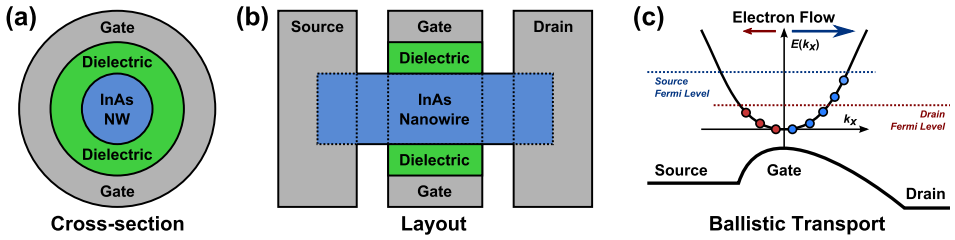

Fig. 1. A schematic illustration of (a) the cross-section, (b) the layout of a generalized nanowire MOSFET in a gate-all-around configuration, (c) illustration of the ballistic transport within the nanowire.

thickness of the gate dielectric is scaled as one tenth of the nanowire diameter, although no thinner than one nanometer. The gate is aligned in a gate-all-around configuration, in order to maximize the control of the electrostatic potential. A schematic illustration of a generic nanowire transistor structure is presented in Fig. 1. This transistor structure is similar to the nanowire transistors fabricated in [31–34]. The modeled transistor structure, however, is scaled to thinner nanowire diameters and shorter gate lengths than in the fabricated devices. The results in this work are relevant for both vertical and lateral transistor architectures.

Nanowire diameters from 5 nm to 35 nm are simulated, with emphasis on 12 nm and 22 nm. The gate length is short enough to suppress most short channel effects and is related to the natural length of the transistor as described by [18]. This corresponds to 16.1 nm and 29.6 nm for a diameter of 12 nm and 22 nm, respectively. In this work, no parasitic elements are considered, as the focus is on the ultimate intrinsic performance of the transistor structure. An overview of the influence of the parasitic capacitances and resistances is presented in [7].

3. Band structure simulations

In order to calculate the electrostatic potential within the nanowire, $V(r)$, Poisson's equation is solved for the 2-D nanowire geometry in Fig. 1(a). This is performed in polar coordinates along the radial dimension, r, with the surface potential as boundary condition at the nanowire surface:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)V(r)=-\frac{q(N_d-n(r))}{\varepsilon_s\varepsilon_0}, \tag{1}$$

where N_d is the doping concentration, $n(r)$ the carrier concentration, and ε_s the permittivity of InAs.

The resulting electrostatic potential is used as input to the Schrödinger-like solver, which calculates the corresponding eigenvalues, $E_{n,v}$, and eigenfunctions, $\psi_{n,v}(r)$, for each subband in the nanowire [27,28,25]. Due to the cylindrical geometry, there are two quantum numbers associated to each eigenvalue: one radial, r, and one azimuthal, v. In order to account for non-parabolicity, the parameter α is introduced and the solver is repeated for each wave vector, K [25]:

$$(1+\alpha E_{n,v}(K))E_{n,v}(K)\mid\psi_{n,v}(r)\rangle=\left[-\frac{\hbar^2}{2m^*}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}-\frac{v^2}{r^2}-K^2\right)\right.$$
$$\left.+(1+2\alpha E_{n,v}(K))V(r)-\alpha\langle\psi_{n,v}(r)\mid V(r)^2\mid\psi_{n,v}(r)\rangle\right]\mid\psi_{n,v}(r)\rangle. \tag{2}$$

This eigenvalue problem is solved by employing the shooting method with a discretization of 100 steps in the radial dimension. Due to axial symmetry, the wave function must be continuous within the center of the nanowire. This is used to intelligently test different eigenvalues, e.g. by interval bisection, until the boundary condition is matched at the nanowire surface. In this work, no penetration of the wavefunction inside the gate dielectric is allowed, which means that the boundary condition, and thus the carrier concentration, is zero at nanowire surface. A threshold of 0.5 eV above the Fermi level is used to exclude high-energy subbands with an insignificant contribution the carrier concentration.

By adding the contribution of all subbands, the carrier distribution within the nanowire may be determined from the density of states, $g(E)$, and the Fermi–Dirac distribution, $f(E)$:

$$n(r)=\sum_{n,v}\left|\psi_{n,v}(r)\right|^2\int_{E_{n,v}(0)}^{\infty}f(E)g(E)\,\mathrm{d}E. \tag{3}$$

$$\left[g(E)=\frac{2}{\pi}\left(\frac{\mathrm{d}E}{\mathrm{d}K}\right)^{-1},\ f(E)=\frac{1}{1+e^{E/kT}}\right] \tag{4}$$

Consistency is ensured between the electrostatic potential and the band structure by solving the Schrödinger-like equation together with Poisson's equation self-consistently in an iterative loop until convergence.

In this work, the model has been extended to calculate the carrier velocities required for the ballistic transistor simulations. The velocity, $v(E)$, may be calculated by considering the kinetic energy of the carriers, which is dependent on the occupied states in the band structure. The velocity is proportional to the slope of the energy dispersion relation:

$$v(E)=\frac{1}{\hbar}\left(\frac{\mathrm{d}E}{\mathrm{d}K}\right). \tag{5}$$

In the effective mass approximation, the bands are fully parabolic, which means that the effective mass of the carriers is constant. Thus higher energy states will have increasingly higher velocities. When considering the non-parabolicity of the conduction band, the shape of the dispersion relation is no longer completely parabolic and is approaching a linear slope of 1.4 eV^{-1} for InAs [35,36]. This results in an increasingly higher effective mass for high energy carriers and the velocity saturates at a constant value. In order to quantify the influence of the non-parabolicity, simulations have also been performed using the simple effective mass approximation. Simulations have also been performed without self-consistency, by solving the Schrödinger-like equation in a constant potential well.

The resulting band structure is presented in Fig. 2, where the energy at the bottom of each subband is shown. It is evident that there are a lot more subbands in thicker nanowires and that the non-parabolicity causes a significant shift in the subband energy levels. Furthermore, if self-consistency is ensured, the charge from the carriers within the nanowire deforms the electrostatic potential, thereby pushing the subbands to higher energies. This effect is more prominent for high surface potentials, due to the increased number of carriers and thus charge within the nanowire. As more carriers fit inside non-parabolic bands, this effect is larger than in the effective mass approximation. It is also more severe in thick