An Improved Evaluation of the DC Performance of Carbon Nanotube Field-Effect Transistors

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Abstract. A self-consistent Schrödinger-Poisson solver is used to improve upon a recent evaluation of the attainable DC performance of coaxial carbon nanotube field-effect transistors. The earlier evaluation, which was based on the predictions of a compact model, is shown to be optimistic because of the model's inadequate treatment of quantum-mechanical reflection of thermionically injected carriers. This deficiency of the compact model is remedied, to a large extent, by incorporating a new, short expression for quantum-mechanical reflection under phase-incoherent conditions.

1. Introduction

In a recent evaluation of carbon nanotube field-effect transistors (CNFETs), devices were specified that yielded simulated drain currents and transconductances approaching the ultimate limits of a one-dimensional (1-D) ballistic transistor [1]. These devices were coaxial in geometry and had a thin, high-permittivity, gate dielectric. The source and drain metallizations to the ends of the nanotube imposed negative Schottky barriers to electron flow, and as such, were predicted to perform much better than CNFETs with positive-barrier end contacts. The designation of barriers as either negative or positive is used here with respect to electrons. With appropriate changes in work functions it applies equally to holes, which are the dominant carrier in recent experimental devices [2, 3].

The compact non-equilibrium model, from which the results were obtained, allows for quantum-mechanical tunneling of electrons and holes at appropriate interfaces, using a simplified expression obtained from the JWKB approximation. Consideration of tunneling is important for studying positive-barrier devices, as in the original presentation of the model [4], but, in negative-barrier devices, attention must be paid to thermionic emission of electrons, and to their quantum-mechanical reflection at energies above the barrier height. By assigning a transmission probability of unity to all carriers of energy above the barrier, the original compact model (CM1) is likely to severely overestimate the current.

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In this paper, the need for a more detailed treatment of quantum-mechanical reflection by the compact model is confirmed by examining the correspondence of the latter's method of computing the nanotube charge with that of a solution from Schrödinger's Wave Equation. Then, we present a derivation of a tractable expression for quantum-mechanical reflection that is incorporated into a new version, CM2, of the compact model. The predictions of the latter for the ON/OFF current ratio, ON current, and transconductance, match more closely the results from a recently developed self-consistent Schrödinger-Poisson solver (SP) [5], and indicate that Schottky-barrier CNFETs are likely to operate further from the ultimate limit than previously thought.

2. Correspondence of the Compact and Quantum Models

In this work, SP is used not only to obtain a better evaluation of the performance of CNFETs, but also to indicate how CM1 may be improved to achieve the same end. To accomplish the latter, it is first necessary to establish that the quantum and compact models correspond at a fundamental level. The basic premise is that there exists a region in the mid-length of the tube in which the potential energy, E_{mid}, is relatively flat, and serves to connect the regions of rapidly varying potential energy near to the end contacts. This condition is primarily dependent on device length, insulator thickness and contact geometries [6]. The decay length for the end potential is of the order of the gate radius [7], which is about 3 nm in the example used here. A constant E_{mid} is commensurate with a constant charge in the mid-length region of the nanotube, and it is under these conditions that we seek to prove the correspondence of the CM and SP approaches. It is also assumed that ballistic transport applies, which should not be unreasonable for the tubes of length 20 nm that are considered here [8].

In our compact models, the mid-length charge is estimated from a calculation of E_{mid} via a simple capacitance expression, thereby obviating the use of Poisson's equation. Self-consistency is achieved by reconciling the resulting mid-length charge with that computed from the fluxes of electrons and holes through and over the interfacial barriers. Transport is taken to be phase-incoherent, and back-scattering at the interfaces is allowed, leading to a composite transmission probability, $T^{\star}$, which is a function of both the source and drain transmission probabilities, $T_{\mathrm{S,D}}$. The mid-length charge is given by

$$n_{\mathrm{mid}} = \int_{E_{\mathrm{mid}}}^{\infty} g_{\mathrm{1D}} T^{\star} \left[\frac{f_{\mathrm{S}}}{2} \left(\frac{2}{T_{\mathrm{D}}} - 1 \right) + \frac{f_{\mathrm{D}}}{2} \left(\frac{2}{T_{\mathrm{S}}} - 1 \right) \right] \mathrm{d}E, \qquad (1)$$

where g_{1D} is the 1-D nanotube density-of-states, numerically computed from a tight-binding method, f is the Fermi-Dirac distribution (as is relevant for carriers in the metallized regions), and the subscripts S and D refer, respectively, to source and drain injection. The two terms in the square brackets can be viewed as the components of n_{mid} arising from electrons injected from the source (first term) and the drain (second term).

If we now consider just the lowest band, which is doubly degenerate, and introduce into Eq. (1) the effective-mass approximation via

$$g_{\mathrm{1D}}(E) = \frac{4}{\pi}\frac{\mathrm{d}k}{\mathrm{d}E} \approx \frac{2}{\pi\hbar}\sqrt{\frac{2m}{E-E_{\mathrm{mid}}}},$$

and consider, for brevity, just the component originating at the source, we obtain

$$n_{\mathrm{S,mid}} = \frac{\sqrt{2m}}{\pi\hbar}\int_{E_{\mathrm{mid}}}^{\infty}\frac{1}{\sqrt{E-E_{\mathrm{mid}}}} f_{\mathrm{S}}\left[\frac{T_{\mathrm{S}}(2-T_{\mathrm{D}})}{T_{\mathrm{S}}+T_{\mathrm{D}}-T_{\mathrm{S}}T_{\mathrm{D}}}\right]\mathrm{d}E. \quad (2)$$

Now, from a quantum-mechanical perspective, let the amplitude of a unity-input wavefunction immediately after crossing the source barrier region be given by P. Then, under phase-incoherent transport conditions, and allowing for multiple reflections of these carriers between the source and drain barriers, the total probability density in the mid-length region of the channel due to source injection, $|\Psi_{\mathrm{S,mid}}|^2$, can be found from the infinite geometric series relation, and is given by

$$|\Psi_{\mathrm{S,mid}}|^2 = \frac{|P|^2+|P|^2(1-T_D)}{T_{\mathrm{S}}+T_{\mathrm{D}}-T_{\mathrm{S}}T_{\mathrm{D}}}\,. \quad (3)$$

However, the source transmission probability can also be written as

$$T_{\mathrm{S}} \equiv \frac{j_{\mathrm{trans}}}{j_{\mathrm{inc}}} = \frac{k_{\mathrm{mid}}}{k_{\mathrm{S}}}|P|^2 = \sqrt{\frac{E-E_{\mathrm{mid}}}{E-E_{\mathrm{S}}}}|P|^2,$$

where the j's are probability density currents, the k's are wavevectors, and E_{S} is the energy of the conduction band edge of the source metal. Therefore, from Eq. (3),

$$\frac{T_{\mathrm{S}}(2-T_{\mathrm{D}})}{T_{\mathrm{S}}+T_{\mathrm{D}}-T_{\mathrm{S}}T_{\mathrm{D}}} = \frac{\sqrt{E-E_{\mathrm{mid}}}}{\sqrt{E-E_{\mathrm{S}}}}|\Psi_{\mathrm{S,mid}}|^2\,. \quad (4)$$

Substituting into Eq. (2), and including the analogous term for injection from the drain, we get

$$n_{\mathrm{mid}} = \frac{\sqrt{2m}}{\pi\hbar}\int_{E_{\mathrm{mid}}}^{\infty}\left(\frac{f_{\mathrm{S}}|\Psi_{\mathrm{S,mid}}|^2}{\sqrt{E-E_{\mathrm{S}}}}+\frac{f_{\mathrm{D}}|\Psi_{\mathrm{D,mid}}|^2}{\sqrt{E-E_{\mathrm{D}}}}\right)\mathrm{d}E\,. \quad (5)$$

This is precisely the expression for the electron contribution to the mid-length charge that results from a self-consistent Schrödinger-Poisson solution under the conditions of: a single, doubly degenerate band; a constant effective mass for both nanotube and end-contact metallization; a nanotube length that is sufficient for the contribution to the charge at mid-length due to evanescent states to be neglected, and for the transport to be considered phase-incoherent; and a normalization of the carrier density using the Landauer Equation, as in Ref. [5]. The effective-mass representation of the band structure is employed in CM2; thus, the correspondence of Eqns. (2) and (5) proves the fundamental equivalence of CM2 and SP under the stated assumptions.

As regards the actual numerical equivalence of SP and CM2, it can now be appreciated that this will depend totally on how the transmission probabilities are estimated. Concerning the numerical equivalence of SP and CM1, this will depend also on the agreement between the effective-mass- and density-of-states-representations of the band structure. The agreement is sufficiently good for the single-band case considered here that the numerical difference between SP and CM1 is due almost entirely to the difference in estimating the transmission probability, T. In CM1 and CM2, the T's are computed for phase-incoherent transport using the JWKB approximation in the case of tunneling, and, in CM1, are set equal to unity in the case of thermionic emission. In SP, a full Schrödinger calculation, under phase-coherent transport conditions, yields exact values for the T's at all energies. It is not reasonable to expect that there is a compact expression for T in the phase-coherent case, but one may well exist for phase-incoherent transport of thermionically emitted carriers, in which case it's incorporation into the compact model should yield a significant improvement. Such an expression, which is derived in the next section, is incorporated into CM2.

3. An Analytical Expression for Quantum-Mechanical Reflection for the Thermionic Case

Typically, the JWKB approximation is used to compute the tunneling probability for carriers through a barrier, however, it may also be used to compute the reflection of carriers above the barrier. For this thermionic current component, we assume the usual JWKB form for the wavefunction in three regions:

$$\Psi(z) = \begin{cases} A\mathrm{e}^{\mathrm{i}k_{\mathrm{M}}z} + B\mathrm{e}^{-\mathrm{i}k_{\mathrm{M}}z} & , \quad z < 0\,, \\ \frac{1}{\sqrt{k_{\mathrm{B}}(z)}}\left(C\mathrm{e}^{\mathrm{i}z\int_0^z k_{\mathrm{B}}(\hat{z})\mathrm{d}\hat{z}} + D\mathrm{e}^{-\mathrm{i}z\int_0^z k_{\mathrm{B}}(\hat{z})\mathrm{d}\hat{z}}\right) & , \quad 0 < z < w\,, \\ F\mathrm{e}^{\mathrm{i}k_{\mathrm{mid}}(z-w)} + G\mathrm{e}^{-\mathrm{i}k_{\mathrm{mid}}(z-w)} & , \quad z > w\,, \end{cases} \tag{6}$$

where A through G are constants, w is the barrier width, and k_{M}, $k_{\mathrm{B}}(z)$, and k_{mid} are the wavevectors in the contact, in the region of the nanotube close to the contact where the potential may change significantly, and in the mid-length region of the nanotube where the potential is relatively constant, respectively. Note that only k_{B} is a function of z. Taking source injection as an example, we set $G = 0$, and assume an abrupt change in the band edge when crossing from the source metal into the nanotube. This permits the usual continuity condition for Ψ and its derivative.

For phase-incoherent transport, we can compute the transmission through the regions close to the source and drain contacts separately. If we consider the source barrier, for example, we note that $k_{\mathrm{B}}(w) = k_{\mathrm{mid}}$ and $k'_{\mathrm{B}}(w) = 0$, where the primed notation denotes a derivative with respect to z. This provides a compact expression for the source transmission probability,

$$T_{\mathrm{S}} = \frac{16k_{\mathrm{M}}k_{\mathrm{B0}}^3}{(k'_{\mathrm{B0}})^2 + 4(k_{\mathrm{B0}}^2 + k_{\mathrm{M}}k_{\mathrm{B0}})^2}\,, \tag{7}$$

where the zero subscript indicates that the quantity is evaluated at $z = 0$.

An analogous expression holds for the drain transmission probability T_{D}, and the composite transmission probability for phase-incoherent transport is given by

$$T^{\star} = \frac{T_{\mathrm{S}}T_{\mathrm{D}}}{T_{\mathrm{S}} + T_{\mathrm{D}} - T_{\mathrm{S}}T_{\mathrm{D}}}\,. \tag{8}$$

The new compact model (CM2) incorporates Eqns. (7) and (8), whereas, in the original compact model (CM1), $T^{\star}$=1.

4. Results and Discussion

We model the coaxial geometry CNFET illustrated in Fig. 1. The device consists of a semiconducting carbon nanotube surrounded by insulating material of relative permittivity ϵ_{ins}, and a cylindrical, wrap-around gate contact. The source and drain contacts terminate the ends of the device. The device dimensions of note are the device length, L_{t}, the gate radius, R_{g}, and the nanotube radius, R_{t}. Here we take $R_{\mathrm{g}}/R_{\mathrm{t}} = 5$, and we consider a (16,0) tube with $R_{\mathrm{t}} = 0.63\,\mathrm{nm}$ and $L_{\mathrm{t}} = 20\,\mathrm{nm}$. For the relative permittivities, $\epsilon_{\mathrm{ins}} = 25$, and ϵ_{t}, which is not relevant to CM1 and CM2, is set to unity in SP [9]. For the work functions, 4.5 eV is taken for the nanotube and the gate, and 3.9 eV is taken for the source and drain. This arrangement leads to a negative barrier height of approximately one-half of the bandgap, as used elsewhere in simulations of high-performance CNFETs [1, 10]. All simulations are performed for a temperature of 300 K.

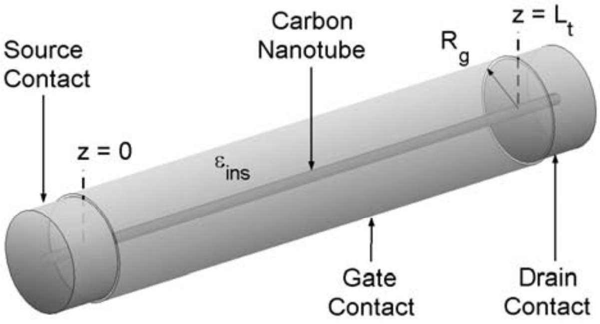

Figure 1. Coaxial CNFET model geometry.

The gate characteristics are shown in Fig. 2. It can be seen that the improved models do not alter the previous conclusion of Ref. [1] that ON/OFF ratios of around 10^3 appear possible. Higher values could result from operating at lower V_{DS} [10]. This is because, with a saturating I_{D}-V_{DS} characteristic, selection of V_{DS} at the onset of saturation ensures the highest ON current, yet the low value of V_{DS} delays the onset of hole conduction when V_{GS} is reduced, thus allowing a lower OFF current to be attained. In practical circuitry it would be desirable to use a single power supply, so it is to be hoped that metals of suitable work function exist to give a flat-band voltage such that the minimum in drain current can be engineered to occur at a gate bias of V_{GS}=0 [1, 10].

The results for the ON current and transconductance are shown in Fig. 3. The dotted lines are for the ultimate limit, as defined previously [1, 11]. The shortfall predicted by CM1 is an indication of how far below this limit CNFETs would perform,

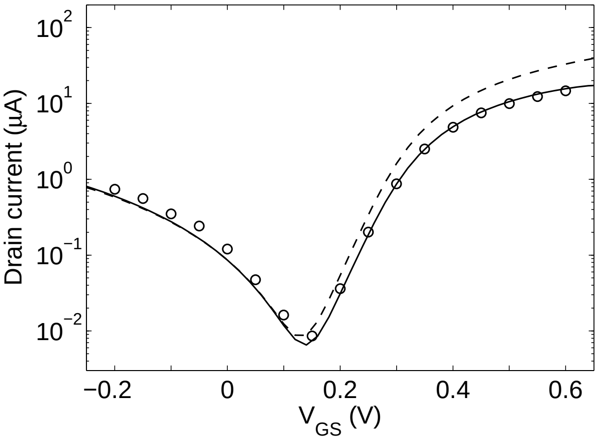

Figure 2. Drain current versus gate-source voltage at $V_{\mathrm{DS}} = 0.4\,\mathrm{V}$ for the various models: SP (circles), CM1 (dashed), and CM2 (solid).

even if the transmission probability for all thermionically injected carriers were unity. The further reduction in performance predicted by SP is due mainly to a more realistic representation of this transmission probability, $T^\star(E)$. The effect is severe and suggests that CNFETs, even with negative barrier heights as extreme as one-half of the bandgap, are unlikely to come close to performing at the ultimate limit.

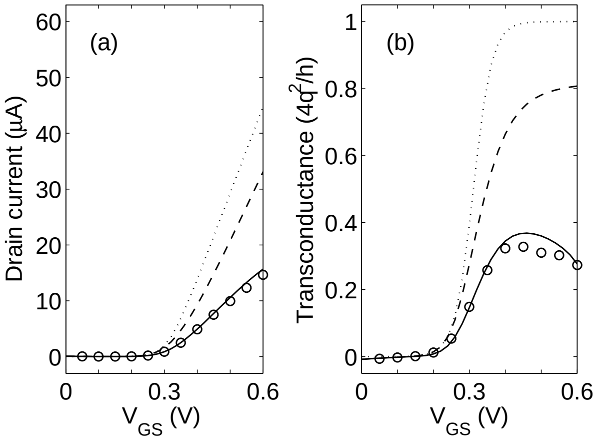

Figure 3. (a) Drain current and (b) transconductance, as a function of gate-source voltage at V_{DS}=0.4V. The dotted lines are for the ultimate limit (see text). Other curves illustrate SP (circles), CM1 (dashed), and CM2 (solid).

Another revelation of the improved models used in this work is their prediction of a decline in the transconductance, g_m, at high gate bias. This is due to the complicated interaction of the charge and V_{GS} with E_{mid} [12]. In fact, we have since found that CM1 also predicts a similar decline, but at a much higher gate bias due to its overestimation of the charge on the nanotube.

The actual form of $T^\star(E)$ is illustrated in Fig. 4. Obviously, CM1 does not capture the interference phenomena exhibited in the results of SP by virtue of the latter's consideration of phase-coherent transport. Equally clear is that, unless all the carriers are grouped together at an energy for which $T^{\star}(E)$ shows a peak close to unity, then CM1's employment of an energy-independent value of $T^{\star}$=1 will lead to a substantial overestimate of the charge and the current. Evidently, this is happening in the results shown in Fig. 3. The employment in CM2 of Eq. (7), and its analogue for drain injection, should lead to some improvement because, even though the expression is derived for phase-incoherent transport, it does allow for $T^{\star}(E)$ to take on values of less than unity. The ensuing, greatly improved correspondence in the predictions of the current between the compact model and SP is demonstrated in Figs. 2, 3 and 5. It may appear unreasonable to expect that the still-large difference in $T^{\star}(E)$ between CM2 and SP should allow such an improved concordance in current. However, as quantities of

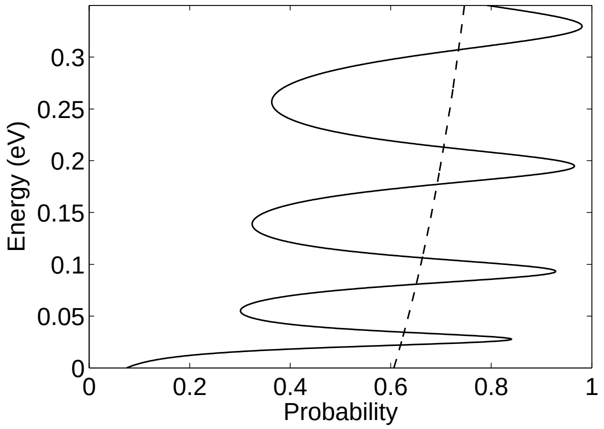

Figure 4. Transmission probabilities, above E_{mid}, of source-injected electrons for the SP (solid) and CM2 (dashed) models, at $V_{\text{GS}} = 0.4\,\text{V}$ and $V_{\text{DS}} = 0.4\,\text{V}$.

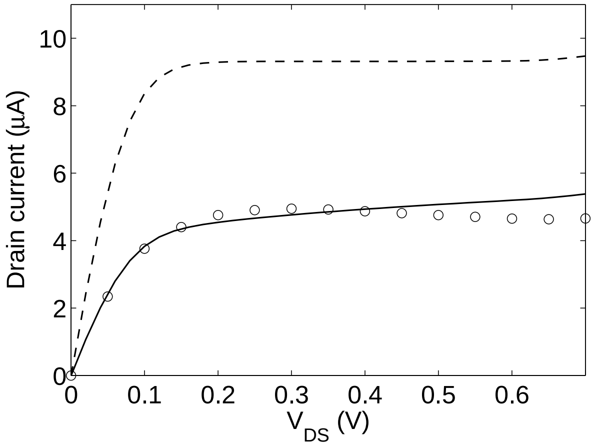

Figure 5. Drain current versus drain-source voltage for various CNFET models at $V_{\text{GS}} = 0.4\,\text{V}$: SP (circles), CM1 (dashed), and CM2 (solid).

interest, such as the charge and the current, are computed by performing an integral over energy, some averaging occurs, and, evidently, leads to a mean value for the SP case that is close to that predicted by the phase-incoherent analysis. The structure in the SP results for $T^\star(E)$ is due to phase coherence, which will become less important for longer devices, so we would expect the new compact model to give even better results for tubes with $L_\mathrm{t} > 20\,\mathrm{nm}$. The converse applies to shorter tubes, when, additionally, issues due to evanescent charge and direct tunneling between source and drain will need to be considered. Operation at lower gate bias may also lead to the appearance of larger phase-coherence effects, due to the increase in height of the potential barriers at the end contacts. These phenomena will need to be taken into account in further compact modeling of CNFETs.

5. Conclusions

From this re-evaluation of the DC performance of coaxial carbon nanotube field-effect transistors with negative-barrier contacts, it can be concluded that:

(i) ascribing a value of unity to the transmission probability of thermionically injected carriers leads to a significant overestimate of the current and transconductance;

(ii) inclusion of a short expression for quantum-mechanical reflection into a compact model yields much-improved predictions for the current and transconductance, inasmuch as they are in excellent agreement with results from a comprehensive Schrödinger-Poisson solver;

(iii) accounting for quantum-mechanical reflection indicates that these transistors with metallized end contacts may not be capable of operating as close to the ultimate limit as previously thought.

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