Universal description of channel conductivity for nanotube and nanowire transistors

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A theory of drift-diffusion transport in a low-dimensional field-effect transistor is developed. Two cases of a semiconductor nanowire and a single-wall nanotube are considered using self-consistent electrostatics to obtain a general expression for the transconductance. This quantum-wire channel device description is shown to differ from a classical device theory because of the specific nanowire charge density distribution. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1604462]

In the present work we consider the carrier distribution in a quantum-wire channel, which may be a semiconductor nanowire or a carbon nanotube, placed between two metal electrodes over a gate electrode. This calculation yields the current–voltage characteristic (CVC) and transconductance of a quantum-wire field-effect transistor (FET). This type of FET is comprised of a fully constrained one-dimensional (1D) electron gas in the quantum-wire channel. The 1D electron system is described both classically (i.e., for the semiconductor nanowire) and quantum mechanically (i.e., for the nanotube). The electrostatic characteristics of the device and the transistor properties depend on the geometry of the source/drain and gate electrodes and are discussed.

In this letter, we focus on analytical rather than numerical simulations. Numerical results on the transport properties of nanotube-FETs have been published recently.[1–3] Here we concentrate on a universal analytical solution for the transport equations under the drift-diffusion approximation in 1D–FETs, which has not been considered previously. In particular, we present analytical expressions for conductance in a 1D–FET at zero drain bias, the cutoff gate voltage and subthreshold CVC (near the cutoff). Finally, numerical solutions for the nonlinear part of the CVC (at nonzero bias) are given when analytical expressions are not available.

The 1D–FET includes source and drain electrodes (in our model they are assumed to be identical) connected by a nanowire/nanotube $-L/2<x<L/2$, and a gate electrode separated by a thin dielectric layer of the thickness d. We assume the quantum-wire channel to be uniformly doped with 1D charge density $N=\mathrm{const}(x)$. In pristine nanotubes, $N=0$, though charge injection due to the work function difference between the channel and electrodes can occur and determines the equilibrium carrier density profile. When the structure is in operation, the source-drain voltage V_d causes a current j along the channel and a redistribution of the carrier concentration. A voltage V_g is applied to the gate and changes the concentration in the channel, which controls the FET transport. We employ the drift-diffusion model in this letter and assume that the scattering rate in the channel is sufficiently high to support a local charge equilibrium. This is likely valid the most nanowire FETs and, at least, for some of nanotube devices. In the opposite (ballistic) limit, the channel conductance has less influence on the CVC. The ballistic model[1] is not considered in this work.

We measure the bias from the middle point in the wire ($x=0$) so that the source and drain potentials are $\pm V_d/2$. In this case, the potentials along the wire and concentration changes caused by V_g, the contact potentials, and V_d are, respectively, symmetric and antisymmetric functions of x and denoted by subscripts s and a: $\phi_{s,a}(x)$ and $n_{s,a}(x)$.

The potentials $\phi_{s,a}(x)$ can be divided into two parts: the components $\phi^0_{s,a}(x)$ created by the electrodes (including the work function difference if not zero), which should be found from the Laplace equation containing no channel charge density and the components $\phi^1_{s,a}(x)$, caused by the electron charge in the channel $-en_{s,a}(x)$. We assume that the characteristic length $l=\min\{L,2d\}$ determining the potential and density distribution along the channel, exceed noticeably the nanowire/nanotube radius a. In this case, the relationship between $\phi^1_{s,a}(x)$ and $n_{s,a}(x)$ is approximately linear[4–7] and for a nanowire with nondegenerate carriers, the current j can be written as

$$\frac{j}{e\mu}=n(x)\frac{d\phi^0}{dx}-\left[\frac{2e}{\varepsilon}\ln\left(\frac{l}{a}\right)n(x)+\frac{kT}{e}\right]\frac{dn}{dx}, \tag{1}$$

where $n=n_s+n_a$, $\phi^0=\phi^0_s+\phi^0_a$, ε is the ambient dielectric permittivity, μ is the carrier mobility. The second term describes the drift in the self-consistent field $-\nabla\phi^1_{s,a}(x)$ and the last term corresponds to the diffusion current, which in 1D transport cannot be neglected in comparison with the drift current. For a nanotube with degenerate carriers, the thermal energy kT should be replaced by the Fermi energy and Eq. (1) reads as

$$\frac{j}{e\mu}=n(x)\frac{d\phi^0}{dx}-eC_t^{-1}n(x)\frac{dn}{dx}, \tag{2}$$

where $C_t^{-1}=C_g^{-1}+C_Q^{-1}$ is the inverse capacitance of the nanotube derived in Refs. 6 and 7 and containing both the logarithmic geometrical capacitance, $C_g^{-1}\sim\log(l/a)$, similar

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to Eq. (1) and the quantum capacitance of the 1D electron gas, $C_Q = 1/(e^2\nu) \simeq 0.31$ for one degenerate subband of a single wall nanotube.

The boundary conditions $n(\pm L/2) = n_c$ assume that the source and drain contacts support a constant concentration at the contacts, independent of the applied voltage. The condition $n_c = N$ corresponds to an ideal Ohmic contact not disturbing the electrical properties of the wire. $n_c < N$ corresponds to a Schottky contact and $n_c > N$ describes the situation where the carriers are provided by electrodes, which is often the case for nanotubes. We are aware of importance of Schottky barriers (SB), often forming at the contacts, for transport in a nanotube SB–FET.[13,14] Our theory can be generalized in a straightforward manner for this case.

For $n_c = N$, in the absence of current we have the trivial answer for the equilibrium concentration profile $n_0 = N = \mathrm{const}(x)$. For $n_c \neq N$ in the close vicinity of the contacts there exists a finite charge density $e(N - n_c)$ in the channel and its image charge $-e(N - n_c)$ beyond the metallic contacts. But this means a discontinuity in the charge density at $x = \pm L/2$ and brings into question the adequacy of the continuum approach, which assumes smooth charge and potential variations. To avoid this difficulty, we measure n_0 from n_c by assuming $n_0(x) = n_c + \Delta n_0(x)$. Then $\phi_c(x)$ represents the potential for a wire with uniform charge $e(N - n_c)$ between metallic contacts $x = \pm L/2$ as calculated in Ref. 5. This is just the charge which, together with its images, has discontinuities at the contacts. Its potential (taking into account its image in the gate electrode) can be calculated exactly for each contact geometry.

Direct integration of the drift-diffusion equation [Eq. (1)] transforms it into an algebraic equation for $\Delta n_0(x)$ determining it for a given $\phi_c(x)$. For a degenerate nanotube [or for $(2e^2 N/\varepsilon kT)\log(l/a) \gg 1$], the equation reduces to the direct proportionality: $\Delta n_0(x) = C_t \phi_c(x)$.

Now we can find the analytical expressions for Δn_s and n_a and j if we restrict ourselves to the linear case by assuming V_d to be sufficiently small. In the zeroth order approximation, there is no current and both $\phi^0(x)$ and $n(x)$ contain only a symmetric component: $n(x) = n_c + \Delta n_s(x)$. $\Delta n_s(x)$ should be found from the same equation as $\Delta n_0(x)$, with $\phi_c(x)$ replaced by $\phi_s^0(x) = \phi_c(x) + \phi_g(x)$ where $\phi_g(x)$ is the potential created by the bias V_g at the gate electrode.

When $n_s(x)$ is found, Eq. (1) can be linearized in n_a and solved under the condition $n_a(0) = n_a(L/2) = 0$. This gives the concentration profile and the current j, which for a single-wall nanotube reduces to Kirchhoff's law

$$j = \frac{V_d}{R}, \quad R = \frac{2}{e\mu}\int_0^{L/2} \frac{dx}{[n_c + \Delta n_s(x)]}. \tag{3}$$

The resulting j depends on the gate voltage V_g through the functions $\phi_s^0(x)$ and $\Delta n_s(x)$, which allows us to calculate the transistor transconductance $G = dj/dV_g$.

The potential profile $\phi^0(x)$ and, hence, all the results depend noticeably on the geometry of the structure, in particular, on the type of source and drain contacts. We consider in detail bulk contacts representing metallic or heavily doped semiconductor regions with all three dimensions considerably exceeding the characteristic lengths a, d, L as well as the screening length in the contact material and thus assumed to be infinite.

For the linear case, in the limit $A \gg 1$ when the expression Eq. (3) is applicable, the dimensionless current $i = jL/(n_0 e\mu V_d)$ has an explicit form

$$i = \left[2\int_0^{1/2} \frac{dt}{1 + g\Psi(t)}\right]^{-1}, \tag{4}$$

where $g = 2\varepsilon V_g/[\pi e n_0 \ln(l/a)]$ is the dimensionless gate voltage and for $n_c = n_0$: $\Psi(t) = \Sigma_0^\infty (-1)^n/(2n+1)\cos[\pi t(2n+1)]\exp[-\pi d(2n+1)/L$. The channel conductivity near the cutoff is determined by the point of minimal concentration, which in a symmetric structure is at $x = 0$, and hence, is determined by the properties of $\Psi(t)$ at small t. Expansion of $\Psi(t)$ allows us to integrate Eq. (4) and obtain

$$i = \frac{\sqrt{(g - g_0)\sinh\left(\frac{\pi d}{L}\right)}}{\sqrt{2}\cosh\left(\frac{\pi d}{L}\right)},$$

$$g_0 = \left\{\frac{\pi}{2} - \arctan[\exp(-\pi d/L)]\right\}^{-1}. \tag{5}$$

Thus, the transconductance di/dg increases in the vicinity of cutoff as $\sim (g - g_0)^{-1/2}$.

So far we have assumed that the source and drain contacts are bulk. However, there also exist structures with 2D and even quasi-1D contacts (nanowires) where potential profiles ϕ_c, ϕ_g, and ϕ_a will have essentially different x dependence with singularities near the contacts.[5] The resulting modified FET characteristics have been also calculated and will be published elsewhere. The quantitative difference is in a particular profile of the $\Psi(t)$ function. Its expansion near the maximum is, of course, also quadratic, and hence, results in the same qualitative result $di/dg = A(g - g_0)^{-1/2}$ near cutoff, with particular values of the cutoff voltage g_0 and the coefficient A different from the case of bulk contacts.

The simplified expressions Eqs. (2) and (4) neglected diffusion effects, which is equivalent to the limit $T = 0$. The formula $\Delta n_0(x) = C_t \phi_c(x)$ does not take into account activation processes and simply gives $n_s = 0$ for all points where $\phi_s^0(x) < -C_t^{-1} n_c$. Thus, in the linear approximation, the cutoff voltage g_0 corresponds to the condition $\phi_s^0(0) = -C_t^{-1} n_c$ and at lower $g(V_g)$ the current is exactly zero. It is evident that at $T > 0$, the current at $g < g_0$ will have an activated character: $j \sim \exp(-\Delta/kT)$, where $\Delta = e[-C_t^{-1} n_c - \phi_s^0(0)]$. Since $\phi_s^0(0)$ depends linearly on V_g, the activation energy Δ is directly proportional to $g_0 - g$.

Now we consider the case of arbitrary V_d voltage when the linear approach fails. The problem requires a solution of the general nonlinear Eq. (1) [or Eq. (2)] and the potential consists of three parts: $\phi^0(x) = \phi_c(x) + \phi_g(x) + \phi_a(x)$ describing, respectively, the influence of contact work function, gate voltage, and source-drain voltage calculated earlier. Two boundary conditions: $n(\pm L/2) = n_c$ determine the integration constant and the so far unknown value of j. Since $\phi_g(x)$ is proportional to V_g and $\phi_a(x)$ is proportional to V_d, the resulting solution gives us the CVC of a nanowire $j(V_d)$ for various gate voltages.

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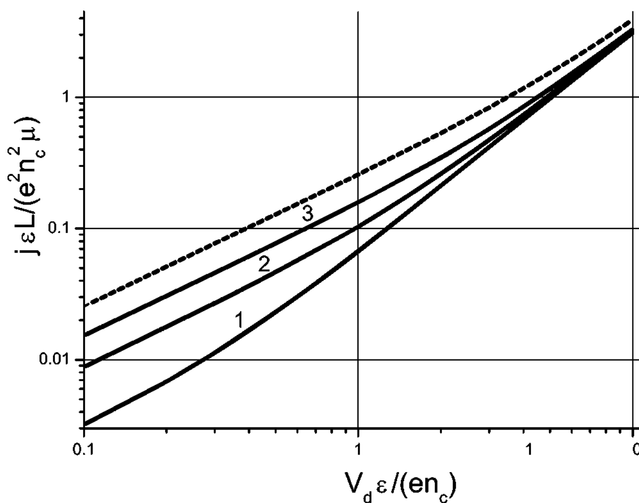

FIG. 1. Current–voltage characteristic of a nanowire with bulk contacts and $d/L=0.3$ at two gate voltages $g=-2.5$ in units $\pi e n_c \ln(l/a)/(2\varepsilon)$ (dashed line) and $g=-2.8$ (solid lines) for the dimensionless temperatures: $\tau=\varepsilon kT/(e^2 n_c)=0.05$ (1); 0.1 (2), and 0.2 (3).

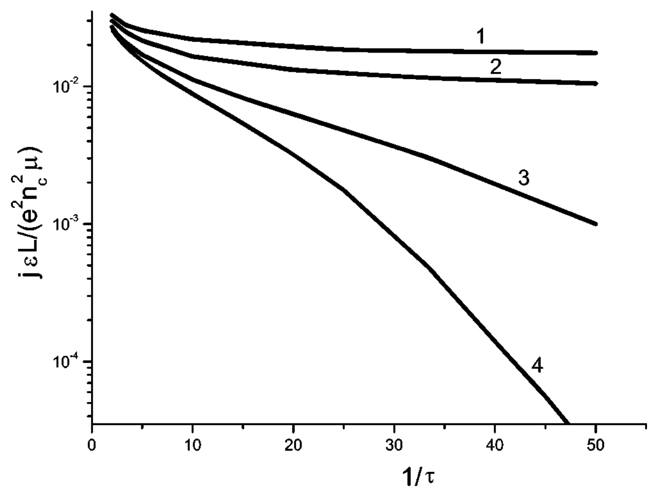

FIG. 2. Dimensionless current vs dimensionless temperature at different dimensionless gate voltages: $g=-2.5$ (1); -2.6 (2); -2.7 (3); and -2.8 (4).

To calculate it quantitatively, we choose particular values $\ln(l/a)=3$ and $d/L=0.3$ and assume a bulk geometry and Ohmic character for the contact with $n_c=N$, where the dimensionless threshold estimated with Eq. (5) (that is, in the limit of low temperatures) $g_0=-2.7$. Figure 1 shows CVC at $g=-2.8$ (below the threshold) and $g=-2.5$ (above the threshold). All characteristics have a superlinear character, which has a simple explanation. High driving voltage V_d tends to distribute carriers uniformly along the channel. In our conditions when powerful contact reservoirs fix the concentration n at the points where it is maximal, such a redistribution will increase the minimal value n in the center of channel, and hence, increase conductivity of the latter. Such superlinear behavior experimentally observed in nanowire-based transistors[8–11] differs noticeably from a sublinear dependence typical for both bulk FETs and ballistic nanotube[12–14] structures. We assume that the mechanism of the CVC saturation is due to the contact resistance (not presented here). When the channel resistance becomes much less than the contact resistance, $R \ll R_c$, almost all the bias drops at the contacts.

Figure 1 presents also information on temperature dependence of the channel conductivity. Above the threshold this dependence is practically absent. The CVC curves for $g=-2.5$ at different temperatures do not deviate from the dashed line corresponding to $\varepsilon kT/(e^2 n_c)=0.2$ more than by 10% and for this reason are not shown in the figure. For V_g below threshold and for not very high V_d, Fig. 1 demonstrates a strong temperature dependence of the current, shown in more detail in Fig. 2 calculated for low V_d ($V_d=0.02$), corresponding to the linear (zero bias) part of CVC. While the two upper curves, corresponding to the earlier-threshold V_g, have no noticeable temperature dependence, the two lower curves demonstrate such a dependence with the activation energy growing with $|V_g|$, in accordance with our predictions. At high V_d, where contact injection and electric field tend to create uniform carrier concentration equal to n_c, different CVC curves approach each other and temperature dependence collapses.

In conclusion, an analytical theory of a drift-diffusion transport in a field effect device with a 1D channel is presented. The model gives a universal description for nanowire and nanotube (nonballistic) FETs. An essential difference for the 1D–FET model as compared with textbook models for planar FET is due to poor screening at the low dimensions. Thus, the zero-bias resistance of the channel, which is shown to depend on the self-consistent equilibrium charge density in the channel, can be more effectively controlled by a gate voltage. Although, the operation principle of the 1D–FET is similar to the planar device, different electrostatics for the 1D channel results in different behavior, and in different device characteristics. For example, the transconductance at the threshold is $G \propto 1/\sqrt{V_g - V_{\rm th}}$ in contrast to the textbook result ($G \propto$ const). With a lower (leakage) OFF currents observed recently in 1D–FETs, this makes these devices very attractive for electronic applications.

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