Diameter-dependent analytical model for light spot movement in carbon nanotube array transistors

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We present a rigorous analytical model for the movement of light spot emitted in single-wall nanotube transistors (SWNTs) including the dependence of this movement on tube diameter. Since the rate of change of light spot movement with gate bias is a sensitive function of the tube diameter, the model can be used as an in situ nondestructive tool to probe the electrically relevant diameter distribution in SWNT arrays and thereby could complement traditional indirect techniques like Raman spectroscopy and atomic force microscopy. Establishing such a diameter distribution has broad implications regarding the performance/integration of SWNT for potential applications in emerging carbon electronics. © 2011 American Institute of Physics. [doi:10.1063/1.3549769]

The remarkable electrical, optical, and mechanical properties of single-walled carbon nanotubes (CNTs) make them attractive candidates for many electronic and optoelectronic applications such as high performance transistors,1 sensor systems,2 memory and logic devices, and flexible electronics.3 Grouping of single-wall nanotube transistors (SWNTs) in the form of aligned arrays [Fig. 1(a)] provides a scalable way to exploit the excellent properties of individual tubes1 while avoiding the low current outputs, small active areas, and large device-to-device performance variations.4

Since many crucial properties of SWNT such as the band gap energy, Schottky barrier (SB) at contacts, mobility, and threshold behavior depend strongly on its diameter, the behavior of SWNT arrays are substantially affected by the distribution of diameters of their tubes.6 Consequently, it is critical to characterize the diameters of SWNT arrays and to include its effect in their device and circuit models.5 Various ex situ experimental methods such as optical absorption spectroscopy, Raman spectroscopy, transmission electron microscope imaging, and atomic force microscopy6 have been used to characterize the diameter distribution of CNTs.7 In this letter, we propose an in situ characterization technique based on the principle of light spot movement to determine the diameter distribution of CNT array transistors.

Transport in short (<100 nm) carbon nanotube field effect transistors (CNFETs) have been previously studied either by sophisticated (but numerically intensive) nonequilibrium Green’s function approach8 using a simpler modeling methodology based on ballistic transport assumption.9,10 For devices longer than a few mean-free-paths, the transport is essentially diffusive and thus more efficiently simulated using drift-diffusion (DD) transport11 in the channel, coupled with quantum tunneling through SB near the tube/metal contacts9,10,12-14 [see Fig. 1(b)]. The goal of the paper is to use this DD/Tunneling formulation to develop an analytical model for localized light emission in SWNT as a function of gate bias and to show that the spatial movement of the light spot is a sensitive probe for tube diameter variation. The model is explained as follows.

SWNT arrays can emit an electronically positioned light spot, which moves along the tube with applied bias.12,15,16 The detailed physics of light emission is complex and has been elegantly discussed in various publications such as in Ref. 17. Here, we will follow the argument suggested by Tersoff et al.,15 that, in a long device, the potential in the tube is determined by the gate voltage and the local charge,

\[ V = V_G + \frac{\rho}{C_{ox}}, \]

where \( V_G \) is the gate voltage, \( \rho \) is the linear charge density, \( \rho = -q(n+p) \), and \( C_{ox} \) is the nanotube capacitance per unit length. In the channel of a long device, and away from the contacts (region 2 in Fig. 1), DD transport is assumed, so that the steady state current is given by

\[ I = q\mu(n+p)E + qV_T\mu \left( \frac{dn}{dx} - \frac{dp}{dx} \right), \]

where \( q \) is the electronic charge; \( \mu \) is the mobility (the same for both carriers); \( n \) and \( p \) are the linear densities of electrons and holes, respectively; \( E \) is the electric field; and \( x \) is the distance along the length of the tube. At any \( V_G \) gate bias, the channel is naturally partitioned into two regions—each dominated by either electrons or holes15 injected from the respective contacts. The boundary of the two regions at \( x_0 \) defines the position of maximum recombination rate accom-

![FIG. 1. (Color online) (a) Schematic diagram of array of SWNTs. (b) Energy band diagram of a SWNT device showing the injection of both electrons (from source) and holes (from drain) at ambipolar bias conditions resulting in enhanced recombination rate accompanied by light emission.](image-url)
panied by light spot emission. Equation (2) can therefore be simplified for the left or the right region as

$$I = q \mu E \pm qV T \mu \frac{d\eta}{dx}, \quad (3)$$

where \(\eta\) is the linear carrier density \(n\) or \(p\), and + is for electrons and − is for holes. Unlike Tersoff et al.,\textsuperscript{15} however, we need to retain the diffusion term and assume that \(E = \text{const.}\) for most of the channel.\textsuperscript{14} Solving Eq. (3) for the carrier density \(\eta\) gives

$$\eta = \frac{1}{q \mu E} \left[ 1 - e^{E(x_0 - x)/V T} \right]. \quad (4)$$

Substitution from Eq. (4) into Eq. (1) and given that \(\rho = \mp q \eta\),

$$V = V_G \mp \frac{l}{\mu E C_{ox}} \left[ 1 - e^{E(x_0 - x)/V T} \right], \quad (5)$$

where the upper sign is for electrons and the lower sign is for holes.

To solve Eq. (5) explicitly, we now need the boundary conditions for potential for the diffusion-dominated region, which are readily obtained by recognizing the continuity between quantum tunneling dominated transport region near the contact and the DD-transport region. Assuming the tunneling distance of \(\delta\) for both contacts, the boundary conditions are \(V(\delta) = V_S\) for the case of electrons (source side) and \(V(L - \delta) = V_D\) for the case of holes (drain side), we get two equations in \(I\) and \(x_0\) from Eq. (5). The solution yields

$$x_0 = \frac{V_I}{E} \left[ \frac{V_D + V_S - 2V_G}{2(V_D - V_G)} \right] e^{E(V_D - V_S)/V T}$$

$$= \frac{1}{2} \sqrt{\left( \frac{V_D + V_S - 2V_G}{V_D - V_G} \right)^2 e^{2E(V_D - V_S)/V T} + 4 e^{E(V_D - V_S)/V T} \left( \frac{V_G - V_S}{V_D - V_G} \right)}, \quad (6)$$

which has two unknown parameters \(E\) (linear drop in the channel region) and \(\delta\) (SB tunneling distance into the channel) and is valid for the range 0 < \(V_G < V_D\). It can be verified that Eq. (6) satisfies the condition \(x_0 = L/2\) at \(V_G = V_D/2\) and that \(x_0\) increases (light spot translates toward drain end) with increasing \(V_G\) relative to \(V_D\). The electric field \(E\) depends on the ratio \(V_D/L\), i.e.,

$$E = \alpha(V_D/L), \quad (7)$$

where \(\alpha\) is a fitting parameter. The tunneling distance \(\delta\) is modeled using

$$\delta = \frac{\beta e^{-d\lambda}}{(V_D/L)}, \quad (8)$$

where \(d\) is the tube diameter, and \(\beta\) and \(\lambda\) are fitting parameters. Note that it is through the parameter \(\delta\) that the light spot location \(x_0\) becomes sensitive to the diameter of CNT. The fitting parameters are readily obtained by comparing the analytical results with those extracted using a self-consistent numerical simulator.\textsuperscript{14} It is found that the optimum values for \(\alpha, \beta,\) and \(\lambda\) are 0.09, 3, and 0.425 for broad range of diameters and bias conditions. From Eq. (6), we can now extract the sensitivity of light spot movement, \(S_0\), with the change in the gate bias \(V_G\) at the middle of the channel (at \(V_G = V_D/2\)):

$$S_0 = \frac{dx_0}{dV_G} \big|_{V_G = V_D/2} = \frac{2V_T}{E V_D} \left( 1 - e^{-E(L - 2\delta)/2V_T} \right). \quad (9)$$

Since \(S_0\) is exponentially sensitive to the tube diameter (through the parameter \(\delta\)) and it is also easily measured,\textsuperscript{16} we demonstrate the use of this quantity as a probe to characterize the diameter distribution in SWNT arrays.

Figure 2 shows the variation of the position of the light spot \(x_0\) (relative to the channel length \(L\)) along the tube with gate bias \(V_G\), calculated both using Eqs. (6)–(8) and using self-consistent numerical simulation,\textsuperscript{14} for \(V_D = 1.5\) V [Fig. 2(a)] and \(V_D = 2.5\) V [Fig. 2(b)]. It is noted that at the ambipolar bias condition (\(V_G = V_D/2\)), the light spot is at the middle of the channel (\(x_0 = L/0.5\)). Decreasing \(V_G\) below this point pulls the energy bands up [see Fig. 1(b)] and, thus, reduces the electron injection from the source while enhances the hole injection from the drain. This moves the high recombination point (light spot) toward the source end. The opposite happens when increasing \(V_G\) above \(V_G = V_D/2\). It is also noted in Fig. 2 that the maximum rate of movement is attained at the ambipolar point. These effects are consistent with the measured electroluminescent characteristics found by Tersoff et al.\textsuperscript{15} and Zaumseil et al.\textsuperscript{16} Moreover, Fig. 2 demonstrates the exponential dependence of the light spot movement on the tube diameter, as anticipated by Eq. (9). This can be attributed to the dependence of the band gap energy on the tube diameter. Increasing the diameter \(d\) leads to smaller band gap energy \(E_G = (E_G - 1/d)\) and thus to higher concentration of injected carriers from both contacts (electrons injected from the source and holes injected from the drain). This leads to larger concentration gradients and more sensitivity of light spot position to the variation of gate bias. Moreover, it is noted from Fig. 2 that emission does not

\[\text{FIG. 2. (Color online) The position of the light spot emitted vs the applied gate bias at (a) } V_D = 1.5 \text{ V and (b) } V_D = 2.5 \text{ V for a channel length of 10 } \mu\text{m and for two tube diameters of 0.626 and 1.27 nm. Black lines represent the self-consistent simulation results while blue lines represent results of proposed model.}\]

\[\text{Simulation} \quad \text{Analytical Model} \quad \text{Simulation} \quad \text{Analytical Model}\]

\[d = 0.626 \text{ nm} \quad d = 1.72 \text{ nm} \quad d = 0.626 \text{ nm} \quad d = 1.72 \text{ nm}\]

\[V_D = 1.5 \text{ V} \quad V_D = 2.5 \text{ V} \quad V_D = 1.5 \text{ V} \quad V_D = 2.5 \text{ V}\]

\[x_0/L = 0 \quad x_0/L = 1 \]

\[x_0/L = 1 \quad x_0/L = 0 \]

\[S_0 = \frac{dx_0}{dV_G} \big|_{V_G = V_D/2} = \frac{2V_T}{E V_D} \left( 1 - e^{-E(L - 2\delta)/2V_T} \right). \quad (9)\]
extend all the way across the channel but is confined to part of the channel. The same effect was observed in experimental measurements, but was attributed there to reasons other than diameter dependence. This diameter dependence of light spot movement is further illustrated in Fig. 3 by showing the average sensitivity of movement of the light spot position near the middle of the channel with the change of tube diameter for the typical range 0.6–1.8 nm. The figure clearly shows that $S_{av}$ increases with increasing tube diameter, as expected. This result suggests that, if one follows the spatial location of the light spot in fully processed CNT, we can characterize in situ the relevant diameter distribution of the array transistor. Such a variation in light spot movement can be used to back extract diameter distribution from those transistors.

In order to use the dependency of $S_{av}(V_D)$ as a probe for the diameter distribution in SWNTs, some parameters such as the drain bias used and the thickness of the oxide should be carefully chosen to maximize this sensitivity with the tube diameter. We define $\Delta S$ as the change in sensitivity of movement when the diameter changes from the smallest diameter of 0.63 nm to the largest one, 1.72 nm—the typical range of diameters for both chemical-vapor deposition processed and HiPico CNTs. $\Delta S$ is plotted against the drain bias used, $V_D$, for different oxide thicknesses as shown in Fig. 3(b). For small drain bias $V_D$, the carrier injection rates are controlled by the band gap energy which depends on the tube diameter. On the other hand, for high $V_D$, the injection of carriers is supported by $V_D$, while the band gap (or the tube diameter) becomes less effective. This explains the decrease with increasing $V_D$ shown in Fig. 3(b). Regarding the effect of the oxide thickness $T_{ox}$, while increasing $T_{ox}$ decreases the sensitivity of light spot movement with gate bias due to the decrease of gate coupling to the channel, increasing $T_{ox}$ has the positive effect that it increases the sensitivity to diameter variation—the key characterization goal. Small drain biases and large oxide thicknesses should therefore be used for getting larger $\Delta S$.

In this letter, we have provided an in situ protocol for electrical characterization of diameter distribution of CNTs—a parameter that is of broad interest for CNT-based device optimization. We found that the position of the light spot due to electron-hole recombination is an exponentially sensitive function of tube diameter and could be used as a sensitive probe of diameter distribution. This characterization methodology therefore complements the existing characterization approaches such as Raman spectroscopy and atomic force microscopy and therefore could have broad implications for nanotube electronics.

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