Sensitivity of Carbon Nanotube Transistors to a Charged Dielectric Coating

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Abstract—This paper investigates the electronic properties of single-walled carbon nanotube field-effect transistors (SWCNT-FETs) in which the SWCNT element is coated with a charged dielectric. The presence of remote charge on the surface of the dielectric is considered to affect carrier transport in the nanotube as a result of both carrier-scattering and gate screening. Nanotube device characteristics are simulated using the multiband Boltzmann transport method incorporating scattering from both phonons and remote charges. This allows assessment of the sensitivity of a nanotube FET to the presence of a charged dielectric coating during room temperature operation. Results show remote charge scattering affects the diameter (d) dependence of the peak conductance and peak field-effect mobility of carbon nanotube devices. Under phonon-limited transport conditions, these peak values increase as \( \sim d \) and \( \sim d^2 \), respectively. When remote charge scattering is significant, peak values cease to vary with diameter once a critical diameter reached. Charges scattering is found to particularly degrade device current at gate voltages that allow carriers scattering into or out of a subband minimum. Furthermore, simulations show that intersubband scattering resulting from asymmetry in the circumferential remote charge density becomes increasingly important as the nanotube length decreases. The authors propose that remote charge scattering effects may be applicable in sensing devices allowing for the identification of the charge on a functionalized CNT coating.

Index Terms—Carbon nanotubes, phonon scattering, remote charge scattering, sensor devices.

I. INTRODUCTION

THE DEVELOPMENT of nanoscale materials in recent years is leading to many exciting possibilities for novel chemical and biological electronic sensors [1]–[6]. These devices have the potential to far exceed the sensitivity and detection speed of conventional sensors, and allow for low-power identification of very small concentrations of targeted molecules or microbes/viruses. Among enabling nano-materials of interest, single-walled carbon nanotubes (SWCNTs) offer a very large carrier mobility [7], [8] and, thus, the potential for high sensitivity and fast detection. When compared with other nanowire materials, nanotubes are expected to be very sensitive to the surrounding environment since the charge carrier states exist on the tube surface. As expected, excellent sensitivity to adsorbed chemicals has been demonstrated in experiments [9], [10]. The advantages of using carbon nanotubes in sensing devices are numerous. The nanoscale SWCNT diameter allows ultra-fast sensing to occur in a small volume. Arrays of nanotubes can be employed allowing for very large effective sensing areas [11]. Carbon nanotubes can be functionalized with sensing polymers or antigens which are immobilized on the nanotube surface with nanoscale spatial resolution [12], [13]. The large SWCNT aspect ratio and high mobility allow for low-power lightweight sensors. Although interest in the scientific and engineering communities is high, the physical mechanisms involved in nanotube-based electronic sensing are still largely undetermined. Chemical sensing may alter the transistor current by a number of mechanisms including variations in: charge transfer/doping, carrier scattering, screening and polarization, mechanical strain, and contact resistance/work function. In this work, we focus on an investigation of the importance of remote charges, which likely affect all of the above sensing modalities.

Theoretical studies have indicated that ions located nearby the nanotube surface alter the electronic and mechanical properties of carbon nanotubes [14]–[20]. These effects have found applications in high-performance actuators [14], [21], [22], pH sensors [23], [24], and chemical sensors. Remote ionic charge may change CNT device characteristics through classical electrostatic/mechanical strain effects and through quantum effects including band structure variations, scattering, and bond weakening mechanisms. In this work, we focus on an investigation of SWCNT carrier scattering with remote charges. Also considered in simulations is the SWCNT device threshold voltage shift due to the presence of remote charge. Since it is often desirable to desensitize or to selectively functionalize a nanotube device with respect to the environment, we investigate the sensitivity of a single-walled carbon nanotube field-effect transistor (SWCNT-FET) to an exterior coating of nonconducting charge separated from the SWCNT surface by a thin polymer or dielectric coating. We envision that the coating is functionalized so that the surface charge can be switched on and off by adsorbing bio(chemical) molecules or by environmental changes (e.g., pH).

To study the effect of remote charge on the device properties of SWCNT-FETs, we employ Boltzmann transport methods which have been successfully used to model phonon-scattering limited transport [8], [25]–[32], [51]. This allows investigation of charging affects alongside phonon scattering, the physical mechanisms that typically sets the intrinsic device behavior. Remote charges are assumed to be immobile, isolated from the CNT-FET by a thin encapsulating polymer or dielectric, as
shown in Fig. 1. In this work, such charges are considered to alter device characteristics by varying the SWCNT Fermi level and by enhancing carrier scattering. Variations in the thickness ($t_2$) and surface charge density (NC) of the dielectric coating are investigated. Results will show that the electronic properties of SWCNT-FETs depend on the nanotube length and diameter. The electronic properties of SWCNT-FETs are found to be sensitive to the transverse distribution of remote charge only when the tube length is small ($L < \mu$m). As the SWCNT diameter increases, phonon scattering is reduced allowing charge scattering effects to become increasingly prominent.

Results of this investigation are expected to lead to important insights into the sensitivity of SWCNT transistors to remote charges in the environment. Although only individual electrical charges are considered, results give a qualitative description of carrier scattering via higher electronic moments such as remote dipoles. The sensing of remote charge may be employed in sensing bio(chemical) molecules and environmental properties such as the pH. This will allow identification of device designs that successfully take advantage of the electronic and material properties of carbon nanotubes-polymer/dielectric device architectures.

II. PHYSICAL DEVICE MODELS

A. Phonon Scattering

If environmental influences are removed, the characteristics of a long defect-free CNT-FET should be determined by carrier transport through the pristine quasi-1D nanotube band structure under the influence of phonon scattering [8], [25]. Carrier subbands and phonon subbranches in a nanotube can be specified by a circumferential wavevector $\beta$, with $\beta = 2/3d$, $4/3d$, and $8/3d$ for the first three subbands [33], [34]. The carrier subband structure of a SWCNT is shown in Fig. 2. Wavevectors $k$ and $q$ along the tube axis further define the carrier and phonon eigenstates, respectively. Using Fermi’s golden rule, the phonon mediated scattering rate from initial carrier state $(k, \beta)$ to final carrier state $(k + q, \beta + \Delta \beta)$ is given by

$$W_{k,\beta \rightarrow k+q,\beta+\Delta\beta} = \frac{\hbar D^2}{\rho_{2D} E_P d} \cdot DOS(k + q, \beta + \Delta \beta) \frac{N_f(E_P) + \frac{1}{2}(\pm) \frac{1}{2}}{\rho_{2D} E_P d}$$

Here, $D$, $E_P$, and $N_f$ are the deformation potential per unit lattice displacement, phonon energy, and phonon number, respectively. $N_f$ is determined by the Bose–Einstein equilibrium distribution. Phonon energies, shown in Fig. 2, are determined by continuum modeling [35]. The mass density of the nanotube is $\rho_{2D} = 7.6\times10^{-4} \text{ kg/m}^2$. The density of carrier states is $DOS(k, \beta) = \xi / \hbar V G_k$, with $\xi = (1 + \beta^2 / 12)^{1/2}$ [33], [34] and $V G_k = 9 \times 10^5 \text{ m/s}$ is the Fermi velocity of graphene [26]. Here, $DOS(k + q, \beta + \Delta \beta)$ is equal to 1/4 of the total density of final carrier states at $k + q$ due to conservation of both spin and circumferential momentum in the interaction.

The diagonal ($D_1$) and off-diagonal ($D_2$) elements of the deformation potential are [25], [35], [36]

$$D_1 = g_1 \left[ \frac{2}{d} \frac{E_p^2(q = 0)}{E_P P} + 2 \frac{V^2}{V_L} \right]$$

$$D_{2S} = 2 \eta g_2 \frac{V^2}{V_L} \cos(3\phi_c), \quad D_{2T} = \eta g_2 \sin(3\phi_c)$$

Here, the longitudinal and transverse sound velocities in graphene are $V_L = 21.1 \text{ km/s}$ and $V_T = 15 \text{ km/s}$. Coupling constants are $g_1$ and $g_2$. $\phi_c$ is the chiral angle, and $E_P P$ is the energy of the breathing phonon mode [35], [37]. For intersubband scattering and intrasubband scattering by the breathing phonon mode, the carrier-phonon interaction is given by $D_1$. 
When the Fermi level is sufficiently close to the Fermi point of graphene in metallic carbon nanotubes, carriers couple with stretching (S) and twisting (T) phonons via the off-diagonal components $D_{2S}$ and $D_{2T}$, respectively. Otherwise, the deformation potential for the $S$ mode is $D_1$, whereas the deformation potential vanishes for the $T$ mode. In this work, we consider only semiconducting carbon nanotubes and, hence, use only the $D_1$ deformation potential and do not consider the suppression of backscattering expected in armchair nanotubes ($n = m$) and small bandgap nanotubes ($\pi \text{mod}(n - m, 3) = 0$) [35], where $n, m$ are fundamental nanotube indices.

We investigate carrier transport in single-walled semiconducting carbon nanotubes by solving the spatially homogenous multisubband Boltzmann equation [25]

$$\frac{eF}{h} \frac{\partial f_{k_i\beta}}{\partial k} = \sum_{q_{\Delta \beta}} \left[ f_{k + q_{\Delta \beta}}(1 - f_{k_{i\beta}}) \cdot W_{k + q_{\Delta \beta} - k_{i\beta}} - f_{k_{i\beta}}(1 - f_{k + q_{\Delta \beta}}) \cdot W_{k_{i\beta} - k + q_{\Delta \beta}} \right]$$

subject to a small external field ($F \ll k_B T$) directed along the tube axis. The distribution function ($f_{k_{i\beta}}$) is solved for a given Fermi energy through specification of the 1-D SWCNT charge density $N$. Considering a CNT-FET as in Fig. 1, application of a gate voltage is used to vary $N$. The multisubband conductance is then $G(N) = \sum_{\beta} G_{\beta} = eN_\beta \mu_{\beta}(N)/L$, where the sum rule is used to sum over each subband (defined by unique $\beta$). The mobility $\mu_{\beta}$ is found from the drift velocity ($V_{d\beta}$) and field according to

$$\mu_{\beta} = \frac{V_{d\beta}}{F} = \frac{V_G}{F} \cdot \frac{\sum_{k} f_{k}\frac{\partial}{\partial k} \cdot \text{sgn}(k)}{\sum_{k} f_{k\beta}} \cdot \frac{\partial (N_\beta \mu_{\beta})}{\partial N}.$$ 

Previous simulations of phonon-limited transport [8], [20], [25] based on the above formulism, compare well with experimental measurements in semiconducting SWCNTs [7], [38], where micron scale tube lengths allowed diffusive transport. As expected, only the zone center low-energy phonons in Fig. 3 contribute significantly to scattering under the experimental conditions: low source-drain bias when the finite temperature Fermi level lies within the nanotube bands (degenerate). Since nanowires have also found application as sensors [39], a comparison of phonon-limited transport is of interest. The large phonon-limited mobility of a carbon nanotube ($> 10^4$ cm$^2$/Vs for a 4 nm diameter tube) [7], [8], [25], [38] is larger than theoretical predictions for a corresponding width silicon nanowire (430 cm$^2$/Vs) [40]. This is likely a result of well defined transverse quantization of carriers and phonons in the nanotube when compared with a nanowire. Carrier scattering is typically increased in the nanowire as more final carrier states are available due to enhanced wavefunction overlap [40]. Material properties such as the effective mass, phonon spectrum, and deformation potential would also play a role. Experimental measurements on FETs where the channel material employs silicon nanowires with widths of 10–20 nm, have shown mobilities as large as 1350 cm$^2$/Vs [41] and 1000 cm$^2$/Vs [42]. Enhanced mobility was found by device annealing/passivation [41] and by the introduction of strain [42]. Semiconducting carbon nanotubes of similar diameter are not expected to form, yet such large mobilities in silicon nanowires should enable enhanced device performance.

### B. Remote Charge Scattering

To investigate the effects of remote charge scattering, the appropriate rate must be included in (3). For long nanotubes, appropriate in sensing applications, the remote charge scattering rate is developed from methods used to model scattering at extended heterostructure interfaces [43]. However, for the present system charge is distributed on the surface of a concentric cylindrical dielectric shell encapsulating the SWCNT. This is shown in Fig. 1. Previous studies by Petrov and Rotkin [18] considered scattering arising from charged impurities located on the surface of a planar substrate underlying a carbon nanotube. Results showed enhanced scattering for small momentum transfer as is typical of coulombic scattering, and conductance degradation via the onset of intersubband scattering. Our treatment...
of remote charge scattering in semiconducting SWCNTs is distinguished from these previous studies since we: 1) include a multisubband nonequilibrium transport study applicable to devices; 2) investigate charge scattering in the presence of phonon scattering; and 3) develop a theory for remote charge correlation effects using methods that have found success in 2-D systems. Screening theory will be based on the self-consistent method of Petrov and Rotkin [18], [19]. In the present work, the unscreened carrier scattering rate due to a linear remote charge density \( N_C^{1D} \) is

\[
W_{k_{\beta}q_{\beta}+\Delta \beta} = \frac{e^2\text{DOS}(k + q_{\beta} + \Delta \beta)}{2\pi^2\hbar^2L_x^2} |I(q_{\beta}, \Delta \beta)|^2 \times \left\langle \frac{\tilde{N}_C^{1D}(q_{\beta}, \Delta \beta)\tilde{N}_C^{1D*}(q_{\beta}, \Delta \beta)}{\text{avg}} \right\rangle.
\]

(5)

The \( \langle \rangle \) bracketed term is the density correlation function of the remote charge shell [20], [43], \( \varepsilon_0 \) is the vacuum static dielectric constant, while \( L \) is the length of both the nanotube and the surrounding charge shell. Also

\[
I(q_{\beta}, \Delta \beta) = \int_0^{2\pi} d\theta e^{-i\frac{q_{\beta}}{\varepsilon_0} \sin \left( \frac{\Delta \beta}{2} \right)} \sqrt{\left( \frac{d}{2} \right)^2 + \rho_a^2 - \rho_a d \cos(\theta)}
\]

(6)

where \( K_0 \) is the zero order modified Bessel function and \( \rho_a \) is the radius of the dielectric shell. The density correlation function is calculated assuming a finite length SWCNT

\[
\left\langle \frac{N_C^{1D}(q_{\beta}, \Delta \beta)\tilde{N}_C^{1D*}(q_{\beta}, \Delta \beta)}{\text{avg}} \right\rangle = \frac{N_C^{1D} \frac{1}{L} \left[ 1 + N_C^{1D}Lx(qL) \right]}{Y(\Delta \beta - \delta_{\Delta \beta,0}) - X(qL)Y(\Delta \beta)}
\]

(7)

where

\[
X(qL) = \begin{cases} 
1, & q = 0 \\
\left( \frac{2}{qL} \right)^3 \sin \left( \frac{qL}{2} \right), & q \neq 0
\end{cases}
\]

(8)

Here, we have considered a random distribution of uncorrelated remote charges. The azimuthal charge distribution enters through the term

\[
Y(\Delta \beta) = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} W(\theta, \theta') e^{i\Delta \beta \frac{2}{\varepsilon_0}(\theta - \theta')} \, d\theta \, d\theta'
\]

(9)

where \( W \) is the charge pair probability distribution function. The formulation for the remote charge density function is appropriate for SWCNT carrier scattering in this work as we consider semiclassical homogeneous transport along the tube axis (\( z \)). Scattering is formulated in terms of the average fluctuation in the remote charge distribution. This treatment is analogous to previous work in 2-D and 3-D systems [43]. A distinct circumferential distribution of remote charge \( F(\theta) \) may be considered and incorporated into the probability distribution function through (9). Specific \( F(\theta) \) distributions will be presented in the next section. Note that the specification of \( F(\theta) \) and the 2-D charge density on the surface of the coating dielectric \( N_C \), allows calculation of the linear remote charge density. In the case of a uniform distribution along \( \theta, N_C^{1D} = N_C \pi d \).

In the limit of an infinitely long SWCNT/dielectric shell, the density correlation function in (7) is \( N_C/L \), independent of both the momentum transfer \( (q_{\beta}, \Delta \beta) \) and the distribution of charges along the azimuthal direction (\( \theta \)). However, as the SWCNT length decreases these effects begin to influence the density function, particularly when the charge density is large. Since the second term in (7) vanishes for intrasubband scattering \( (Y = \delta_{\Delta \beta,0} = 1) \), azimuthal remote charge distributions \( F(\theta) \) will enhance intersubband scattering events. Note that even in the limit of infinite \( L \), the scattering rate will still depend on \( (q_{\beta}, \Delta \beta) \) through the term \( \left\langle |I(q_{\beta}, \Delta \beta)|^2 \right\rangle ^2 \) in (5) and (6).

Screening of the remote charge by the SWCNT and the surrounding medium must be considered in the scattering rate [(5)]. Following the theory in [18] and [19], for a long SWCNT the charge fluctuation is screened according to

\[
\tilde{N}_C^{1D}(q_{\beta}, \Delta \beta) \rightarrow \frac{1}{C_Q^{-1} + C_{g1}^{-1} + C_{g2}^{-1}} \left[ \varepsilon_2 + \varepsilon_3 \right].
\]

(10)

The first term multiplying the charge fluctuation on the right side of (8) accounts for screening by the SWCNT mobile carriers, the back gate, and the dielectric shell. The nanotube is assumed to be long enough so that screening by the contact region may be ignored [18], [19]. Capacitances per unit length appearing in (10) are the SWCNT quantum capacitance \( (C_Q) \), the geometric capacitance of the SWCNT/gate \( (C_{g1}) \), and the geometric capacitance of the SWCNT/dielectric coating \( (C_{g2}) \). The geometrical capacitances are \( C_{g1} = 2\pi\varepsilon_0/\ln(1 + 2L/d) \) and \( C_{g2} = 2\pi\varepsilon_0/\ln(1 + 2L/d) \), for the dielectric geometry in Fig. 1. The quantum capacitance of the SWCNT is \( C_Q = \varepsilon_0^2 \text{DOS} (E_F) \), the density of states at the SWCNT Fermi level \( E_F \) (chemical potential).

The second term multiplying the charge fluctuation in (10) accounts for image charge effects at the local interface region, where the remote charge resides [18]-[20]. As shown in Fig. 1, \( \varepsilon_2 \) and \( \varepsilon_3 \) are the static dielectric constants of the SWCNT coating material and the external surrounding material, respectively. If the device is in aqueous solution, \( \varepsilon_3 \approx 80 \), the image charge screening term would then be a method to account for hydration of the remote charge surface.

It is the fluctuation from the average remote charge distribution that scatters carriers in the encapsulated nanotube. The average charge density is expected to cause a shift in the finite temperature Fermi level \( E_F \) of the SWCNT. The corresponding threshold voltage shift can be approximated as

\[
\Delta V_{TH} = \frac{\varepsilon_0^2 \text{DOS}(E_F) \cdot (1/C_{g1} + 1/C_{g2})}{2\varepsilon_2 + \varepsilon_3}.
\]

Considering a p-type CNT-FET covered with a negative average charge density the turn-on gate voltage experiences a positive shift of

\[
\Delta V_{TH} = \left| \Delta V_{TH} \right|.
\]

It is important to discuss the range of validity for using 1st order perturbation theory to develop the carrier/remote charge scattering rate. This approximation requires that the interaction energy is small compared with the carrier band energy which may be taken as the finite temperature Fermi energy \( E_F \) [18]. Assuming \( I = 1 \) in (6) and the density correlation function is \( N_C^{1D}/L \), in (7), the perturbation scheme is then valid when

\[
E_F > 2\varepsilon_0 \sqrt{\frac{N_C^{1D}}{L}} \left[ \text{screened} \right].
\]

(11)
Here, the right side of the equation is screened as in (10). Using parameters $L = 100$ nm, $d = 4$ nm, and $E_F = 20$ eV [35] for graphic materials, we find (11) is satisfied ($E_F$ more than $10\times \text{larger}$) as long as $N_C < 2 \times 10^{17}$ m$^{-2}$. As we consider much smaller charge densities in this work, the first-order perturbation approximation in (5) should be valid.

III. SIMULATION RESULTS

To include the effects of remote charges on the device properties of a CNT-FET, we consider the charge distributions shown in Fig. 4. Three distributions around the circumferential direction ($\theta$) are investigated and are designated as $F\theta = 1$, 2, and 3. The $F\theta = 3$ distribution is the most asymmetric whereas the $F\theta = 1$ distribution is completely symmetrical in $\theta$. In all cases remote charge extends along the entire SWCNT axis $z$. As mentioned in the previous section, a random fluctuation of the remote charge density is considered. Analysis of carrier scattering and the effects on device characteristics will be studied as a function of the properties of the nanotube and the dielectric coating material.

In Fig. 5, results are shown indicating SWCNT-FET device conductance variations predicted to occur when a 2-nm-thick charged dielectric covers the SWCNT channel. The SWCNT length $L$ is set at a micron, while both the gate and SWCNT coating dielectrics are silica ($\varepsilon_1 = \varepsilon_2 = 3.9$). For the medium surrounding the device, results are shown for vacuum ($\varepsilon_3 = 1$), silica ($\varepsilon_3 = 3.9$), and salty water ($\varepsilon_3 = 80$). The density of charges on the dielectric surface is set at $N_C = 1 \times 10^{16}$ /m$^2$ and is uniform along $\theta (F\theta = 1)$. As we might expect, the density of surface oxygen atoms to occur at a density of $\sim 1$ per $\text{nm}^2$ in silica, $N_C$ corresponds to the case when about 1% of the surface oxygen atoms are charged. In the absence of remote charge, variations in the CNT-FET conductance with nanotube diameter, carrier density, and tube length have been shown to follow from phonon-limited transport [8], [25], [32]. These results showed that the conductance increased with increasing SWCNT tube diameter due to a reduction in phonon scattering and a decrease in carrier effective mass. Simulation results in Fig. 5 show that the effects of remote charge scattering are enhanced in larger diameter tubes. The SWCNT-FET is found to be more sensitive to charge scattering near the conductivity peaks which identify the onset of an additionally occupied subband. This agrees with experiments that report plateaus in the source to drain current of highly doped nanotubes [45], [46]. These results were attributed to interband scattering [45]. As shown in Fig. 6, when the Fermi level is close to a subband minima, Coulombic scattering via remote charge is enhanced since carriers can undergo transitions incurring a small momentum transfer. Reported current plateaus [45], [46] at gate voltages corresponding to the onset of a new transport subband mode may well result from Coulombic scattering of carriers with impurity charge. The effect of the medium surrounding the SWCNT-FET is found to be significant. For the simulated parameters in Fig. 5, we see significant conductance degradation in vacuum, yet minimal effects when the remote charges are in a salty water environment.

The sensitivity of the SWCNT-FET to the circumferential symmetry of surrounding remote charges is found to depend on the length of the nanotube. As seen in Fig. 7, for a 500 nm length SWCNT the ON conductance is reduced by a factor of 2 as the charge distribution varies from $F(\theta) = 1$ to $F(\theta) = 3$. 

![Circumferential charge distributions](image)

Fig. 4. Distributions of remote charge covering the surface of a dielectric coated SWCNT. Shown are three distributions around the nanotube circumference ($F\theta = 1, 2, 3$), corresponding to charge isolated to $2\pi$, $\pi$, and $\pi/2$ of the circumference, respectively.

![Simulated SWCNT conductance as a function of applied gate voltage](image)

Fig. 5. Simulated SWCNT conductance as a function of applied gate voltage. Two one micron length tubes with diameters of 2 and 4 nm are shown. Results are given for two cases: 1) without remote charge and 2) with a remote charge density of $N_C = -1 \times 10^{16}$ /m$^2$ of distribution $F\theta = 1$ located on the surface of a 2 nm thick SiO$_2$ dielectric coating the nanotube. For case 2), the dielectric constant of the surrounding medium is varied between $\varepsilon_3 = 1$ and $\varepsilon_3 = 80$ for vacuum and salty water, respectively.

![SWCNT valence band diagram showing cases when the Fermi level is at two levels $E_{F1}$ and $E_{F2}$](image)

Fig. 6. SWCNT valence band diagram showing cases when the Fermi level is at two levels $E_{F1}$ and $E_{F2}$. Since the carrier-remote charge Coulombic rate decreases sharply with momentum transfer, scattering is stronger when the Fermi level is near a subband minima.
When the tube length is increased to a micron, the conductance varies little as $F(\theta)$ varies. Note that we have scaled the density of charges ($N_C = -5 \times 10^{16} / \text{m}^2$ when $F(\theta) = 1$) in Fig. 7 so that the linear charge density $N_C^{1/2}$ is the same for all simulated charge distributions. The gate voltage shift is, therefore, the same in each case $\approx 2 \text{ V}$. The $LO$ dependence of the conductance is a result of variations in the remote charge scattering rate. As seen in (7) and (8), $X$ is strongly reduced as the tube length increases leading to a reduction in the $F(\theta)$-dependent terms in (7). As mentioned in the previous section, $\theta$ variations in the remote charge density will lead to enhanced intersubband scattering. This effect explains why the ON conductance, which occurs when multiple subbands are occupied, is reduced by $F(\theta)$ variations, whereas little $G$ degradation is seen in the TURN-ON region when only one subband is typically occupied.

So far, simulations have been for a $t_2 = 2 \text{ nm}$-thick dielectric material coating the SWCNT. In Fig. 8, the device conductance is shown as a function of varying $t_2$. Parameters are set to those in Fig. 5 for the case of a 4-nm diameter nanotube with vacuum as the surrounding medium. Results show that the device conductance is quite sensitive to the thickness of the dielectric coating. Note that there is more remote charge present when the dielectric is thicker since a fixed 2-D remote charge density is considered. For weak scattering, the conductance curves in Fig. 8 would rigidly shift due to variations in the threshold voltage. However, results show that there is a large increase in scattering as a function of $t_2$, particularly when the dielectric thickness drops below 2 nm. When $t_2 < 2 \text{ nm}$ the shape of the conductance profile is distorted due to enhanced scattering.

Simulations for the peak values of the field-effect mobility and conductance are shown in Fig. 9. Results are for $L = \mu m$, $N_C = -1 \times 10^{16} / \text{m}^2$ with silica used as the dielectric material. When only phonon scattering is considered, the mobility and conductance peaks are expected to increase with SWCNT diameter as $\sim d^2$ and $\sim d$, respectively (for degenerate transport) [25]. When remote charge scattering is included, the peak values are found to saturate at large diameters. This concurs with experiments where upon heavy doping a reduction in: 1) the sharpness of the nanotube turn-on current and 2) the current saturation level were both observed. [45] Here, theory predicts that the diameter for conductance (current) saturation onset increases with increasing thickness of the dielectric coating ($t_2$). The onset diameter is typically smaller for the peak mobility as compared with the peak conductance. In Fig. 9, the onset diameter is $\sim 2-2.5$ for the mobility and $\sim 3-3.5$ for the conductance. Variations with SWCNT diameter are found since: 1) phonon scattering dominates when $d$ is small, and 2) small momenta transferring intersubband scattering is enhanced as $d$ increases. Note that the saturation onset diameter
may be shifted by a variation in the dielectric coating or a variation in the density of remote charges.

IV. CONCLUSION

Simulations of the characteristics of carbon nanotube devices have been preformed incorporating scattering due to both phonons and remote charges within the nanotube environment. This study is based on the semiclassical Boltzmann treatment and is applicable to long nanotubes typically desired in sensing applications. For transport in short nanotubes where coherent effects are needed, the reader is directed to references [47]–[50]. Our results show that CNT device properties are sensitive to the density and proximity of external charges. Such devices are typically sensitive to variations in the circumferential symmetry of the remote charge density distribution only when the nanotube length is small ($L < \mu m$ for remote charge densities $\leq 10^{16} \text{m}^{-2}$). Contrary to the effects of phonons whereby scattering weakens with increasing tube diameter, remote charge scattering is enhanced as the tube diameter increases. The Coulombic nature of the interactions provides increased device sensitivity when the gate voltage is set to a level which allows small momentum transfer scattering. This effect may be intrasubband in nature at lower carrier densities, reducing the peak field-effect mobility, or an intersubband effect at higher CNT carrier densities. Both the peak field-effect mobility and the peak conductance are found to be strongly degraded by remote charge scattering for larger diameter tubes. Such an effect may be applicable in sensing devices allowing for the identification of the charge on a functionalized CNT coating.

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