A Multi-Scale Model for Localized and Mobile Electroluminescence in Carbon Nanotube Field-Effect Transistors

by

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Abstract

A multi-scale model of a carbon nanotube (CN) field-effect transistor (FET) has been developed that captures the novel electroluminescence (EL) behaviour observed in experimental devices. First, the electronic properties of the CN are derived from the nearest-neighbour tight-binding approximation. The electrostatics of a coaxially-gated CNFET are then rigorously established. In simulations, the open boundaries of this structure are closed by null-Neumann conditions. Based on an asymptotic analysis, limits of validity for the null-Neumann boundary condition are established, and it is shown that one may improve the accuracy of results by including a length of contact in the simulation domain. Next, charge transport is included in the model to address EL. Transport will be diffusive in the long CN channels ($\geq 10\mu m$) found in experimental devices, however quantum tunnelling currents will be present through the Schottky-barriers at the interface between the contacts and the CN. A solution to the 1D effective-mass Schrödinger wave equation determines the thermionic emission and tunnelling currents in a region near the CN-contact interface. These currents establish boundary conditions for the 1D drift-diffusion and continuity equations, which describe charge transport in the long channel, where a finite and field-dependent mobility is assumed. The charge and electrostatics are solved self-consistently to obtain carrier density distributions on the CN surface. When both electrons and holes are present in the CN, they are assumed to recombine with an empirically determined rate, resulting in photon emission. Simulations of this system exhibit four experimentally observed EL phenomena. First, a light-spot that is localized to $\sim 5\mu m$ may be positioned longitudinally on the CN surface by varying the gate bias, and this mobile light-spot increases in intensity as it approaches the CN-contact interface before decaying. When the height of the Schottky-barrier is reduced, a persistent, fixed-position light-spot appears at a CN-contact interface. Finally, when a charge defect is introduced on the CN surface, a fixed-position light-spot appears under certain bias conditions where the injection of one type of carrier is favoured. These EL effects are predicted by the proposed model without resorting to any further physical explanations.
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Statement of Co-Authorship

The research presented in the body of this thesis has been performed in conjunction with members of the UBC Nanoelectronics Group between 2004 and 2006. This statement serves to confirm that the author of this thesis was the primary person responsible for the research contained herein, and acknowledge the contribution of others involved. The work presented in this thesis uses code and methods based on the developments of David L. John and Leonardo C. Castro. The particular modifications made by the author are described in Chapters 2 and 3. The research contained in Chapters 1-3, including derivations, analysis, and conclusions is solely the work of the author of this thesis. Preparation of the two papers that have resulted from this work was, in both cases, a collaborative effort amongst the co-authors, and the author of this thesis assumed primary responsibility in the production of those publications. All data and figures presented in this thesis are the work of its author.
Chapter 1

Introduction

The carbon nanotube (CN) was first discovered by Sumio Iijima in 1991 [1], and in the following two years, the groups of Iijima et al. and Bethune et al. found that CNs could be grown with a single-atomic-layer shell [2, 3]. The CN is a molecule with exceptional mechanical and electronic properties, giving it great potential as the foundation of a new generation of devices, including nanoscale transistors. In 1992, Saito et al. proposed a simple tight-binding model to derive the energy band structure and electronic properties for CNs by rolling a sheet of graphene [4, 5]. CNs may be either metallic or semiconducting, depending on atomic arrangement, and as semiconductors, they have a diameter-dependent bandgap, which suggests the possibility of all-carbon, bandgap-engineered electronic systems. As semiconductors, CNs have demonstrated mobilities as high as 79,000 cm$^2$/V-s in long devices (> 100 μm) [6], ballistic transport in short devices (< 300 nm) [7], and the ability to carry currents over 60 μA in a single molecule [8].

The first CN field-effect transistor (CNFET) was reported in 1998 by Tans et al. [9]. Initially assumed to behave like a bulk-silicon MOSFET, where modulation of the conductance between source and drain contacts occurs in the channel [10], it soon became clear that CNFETs operated through modulation of a Schottky-barrier (SB) formed at the metallic contacts to the CN [11–13]. Early models addressing equilibrium CNFET electrostatics focused on coaxial geometries, in which insulator and gate fully surround the CN [14–16]. While all experimental devices produced up to the time of this writing have been planar in nature, coaxial structures reduce simulation time and complexity. This allows researchers to evaluate the optimal electrostatic structure [17], and obtain qualitative insight into the behavior of experimental CNFETs. The area of CNFET modeling has since evolved to evaluate the performance limits of the device under either DC [18–20] or AC [21, 22] operating conditions. Through self-consistent simulations, quantum-mechanically determined charge and Poisson electrostatics are combined to determine figures of merit. More recently, non-equilibrium Green’s functions have been employed to solve the Schrödinger wave equation (SWE) in atomistic
models of 3D CNFETs, such as planar devices [23–25].

Interestingly, Tans et al. remarked in their original publication describing the first CNFET that, despite the nanometre scale of the device, the semi-classical models for the electronic behaviour of traditional FETs seemed to apply [9]. This has in fact been the case, particularly in the modeling of electroluminescence in long devices. CNs are direct-bandgap semiconductors, therefore the emission of photons can be expected. In 2003, Misewich et al. observed infrared luminescence from a CNFET biased for the simultaneous injection of electrons and holes [26]. Following this initial report, Freitag et al. observed that the luminescence was localized longitudinally on the CN, and could be positioned through a variation in gate bias [27]. This novel effect could be predicted through the application of a finite-mobility model of diffusive charge transport [28, 29].

In this thesis, the author presents theoretical investigations of CNFET behaviour based on research performed between 2004 and 2006 with the UBC Nanoelectronics Group. The objectives of this research were two-fold: first, a study was made of a common modeling assumption, where open boundaries were closed with a null-Neumann condition, with the goal of establishing limits of validity; and second, a novel model was proposed to predict and describe the mobile and fixed electroluminescence observed experimentally [27, 30]. In the remainder of this chapter, relevant CN properties and justification for the assumptions underpinning the proposed CNFET models will be presented, followed by an outline of the thesis.

## 1.1 Carbon Nanotube Field-Effect Transistors

The CNFET is part of a greater family of nanowire and nanotube FETs. Common amongst these devices is the presence of a quasi-one dimensional semiconductor that forms a channel, analogous to that found in a traditional Si-MOSFET, which joins the source and drain contacts. Conductance between the two contacts is modulated by a third contact, the gate, which capacitively induces charge in channel. Therefore, the composition and interfaces between the metal contacts, the semiconductor CN, and the dielectric all play a critical role.

Three key differences exist between the nanotube FET and a traditional Si-MOSFET: first, the source and drain contacts are metallic, giving rise to Schottky-barriers at the CN-contact interface; second, the hollow tube is formed from a rolled sheet of 2D material, such as a sheet of boron-nitride or carbon (known as graphene), leaving no dangling bonds and reducing surface scattering; third, the
nanotube FET is inherently coaxial. The presence of the Schottky-barrier implies that conductance from source to drain will be modulated in one of two ways. In the case of a large barrier, due to choice of metallization, a tunnelling current may be enhanced or suppressed by thinning or widening the barrier, respectively. Alternately, that barrier height may be reduced for one type of carrier through choice of metallization [31], through applied electrostatics [32], or through chemical charge-transfer doping [33, 34]. By creating ohmic or near-ohmic contacts, conductance is modulated by varying the height of the electrostatic barrier within the channel, as in a traditional Si-MOSFET. As noted, nanotube FETs readily lend themselves to fully-surrounding gates that offer optimal control of the electric fields in the channel. This facilitates the operation of minimum-length devices by overcoming short-channel effects, such as drain-induced barrier lowering (DIBL). Traditional Si-MOSFETs have made progress in this area with double-gate (e.g., the FinFET [35]) and tri-gate devices [36]. Currently, all CNFET devices that have been fabricated are planar in nature, although coaxial structures are being vigorously pursued, and have already appeared for nanowire FETs [37]. Controlled growth and placement of CNs is still the primary barrier to the production of CNFETs.

As will be shown below, the CN is a direct-bandgap semiconductor, implying that photons may be emitted when there is recombination of an electron-hole pair (EHP). Further, the presence of Schottky-barriers at the contacts leads to the simultaneous injection of both electrons and holes, known as ambipolar conduction. This combination of properties has led to the development of a novel application for the CNFET: it can emit light from a position along the length of the CN channel that depends on the bias of the transistor [27, 30]. In order to model and evaluate these many aspects of the CNFET, details of the CNs electronic structure must be understood, as must the relation between the CN and the contact. Many of the underlying physical principles have been covered in detail elsewhere, e.g., [38, 39], but will be presented briefly here to clearly establish the theoretical basis for this work.

1.1.1 Carbon Nanotubes

A single atomic-layer sheet of carbon in a hexagonal arrangement is known as graphene, which is a 2D system, forming a lattice with a basis (there are two atoms per unit cell). A nearest-neighbour
tight-binding calculation employing the Slater-Koster approximation gives a dispersion relation

\[ E_{2D}(k_x, k_y) = \pm \gamma_0 \left[ 1 + 4 \cos \left( \frac{\sqrt{3}k_x a}{2} \right) \cos \left( \frac{k_y a}{2} \right) + 4 \cos^2 \left( \frac{k_y a}{2} \right) \right]^{1/2} , \] (1.1)

where \( a = 2.49 \, \text{Å} \) is the lattice constant and \( \gamma_0 \) is the nearest-neighbour hopping or transfer integral [4]. To form the CN, a point in the graphene lattice (A) is rolled back to the origin (O), as shown in figure 1.1. The chiral vector \( \mathbf{C}_h \) is a linear combination of unit vectors \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \) for the graphene lattice,

\[ \mathbf{C}_h = n\mathbf{a}_1 + m\mathbf{a}_2 , \] (1.2)

where \( n, m \in \mathbb{Z} \) and \( 0 \leq |m| \leq n \). Chiralities can be written as an ordered pair \((n, m)\) ranging from \((n, 0)\) (zigzag) to \((n, n)\) (armchair), and have a corresponding chiral angle \( \theta \) which ranges from \( 0^\circ \leq \theta \leq 30^\circ \) without redundancy. Clearly, the CN diameter may be obtained from the chirality:

\[ d_{cn} = \frac{\|\mathbf{C}_h\|}{\pi} = \frac{a}{\pi} \sqrt{n^2 + m^2 + nm} . \] (1.3)

The translational vector \( \mathbf{T} \), satisfying \( \mathbf{T} \cdot \mathbf{C}_h = 0 \), can also be written as a linear combination of the lattice unit vectors,

\[ \mathbf{T} = t_1\mathbf{a}_1 + t_2\mathbf{a}_2 , \] (1.4)

where \( t_1, t_2 \in \mathbb{Z}, t_1, t_2 \geq 0 \), and \( \text{gcf}(t_1, t_2) = 1 \).

The chiral vector and the translational vector form a rectangle \(\text{OAB'B} \) (figure 1.1) bounding the CN unit cell. The unit cell is composed of \(2N\) carbon atoms, and \(N\) unit cells of graphene, from which the dispersion relation was derived. The reciprocal lattice vectors for the CN in \( k \)-space are \( \mathbf{K}_1 \) and \( \mathbf{K}_2 \), corresponding to \( \mathbf{C}_h \) and \( \mathbf{T} \) respectively,

\[ \mathbf{K}_1 = \frac{1}{N}(-t_2\mathbf{b}_1 + t_1\mathbf{b}_2) \quad \mathbf{K}_2 = \frac{1}{N}(m\mathbf{b}_1 - n\mathbf{b}_2) , \] (1.5)

where \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \) are the unit vectors in \( k \)-space. If the CN is assumed to be infinite in length, then its dispersion relation will be continuous in the longitudinal direction. As a result, the first Brillouin zone will be a one-dimensional line segment with length \( 2\pi/T \), directed along \( \mathbf{K}_2 \). By rolling the sheet of graphene, a periodic boundary condition is introduced, which discretizes the dispersion relation in the transverse direction, and is known as zone-folding. Noting that \( N\mathbf{K}_1 = -t_2\mathbf{b}_1 + t_1\mathbf{b}_2 \),
Figure 1.1: The chiral vector $\mathbf{C}_h = \overrightarrow{OA}$ joins the point (A) and the origin (O) as the sheet of graphene is rolled to form a CN. The rectangle OAB'B formed by the translational vector $\mathbf{T}$, which is normal to $\mathbf{C}_h$, completes the unit cell of the CN. $\theta$ is the chiral angle, measured from the “armchair” orientation of $\mathbf{C}_h$. 

is a reciprocal lattice vector in $k$-space, then two vectors differing by $N \mathbf{K}_1$ will be equivalent. This implies that there are $N$ distinct wave vectors $q \mathbf{K}_1$, $q = 0, \ldots, N - 1$ arising from the periodic boundary condition, such that the 1D dispersion relation for the CN comes from “slices” of the 2D dispersion of graphene.

Graphene is a semi-metal, as the gap in the dispersion relation $E_{2D}(k)$ closes at singular points. Therefore, the spacing between Brillouin zones in the transverse direction is critical in determining the electronic properties of the CN. Defining $k \in \mathbb{R}$ to include all values in the 1D first Brillouin zone of the CN, i.e., $-\pi/T \leq k \leq \pi/T$, the dispersion relation for a CN becomes

$$E_q(k) = E_{2D} \left( k \frac{K_2}{K_1} + q \mathbf{K}_1 \right) \quad q = 0, \ldots, N - 1,$$

yielding $N$ curves, which may in some cases be degenerate. An example is shown in figure 1.2 for a (10, 0) CN. Analysis of the location of the distinct Brillouin zones shows that the condition for a
Figure 1.2: Dispersion relation for a (10, 0) CN derived from the zone-folding method applied to the graphene dispersion relation from the nearest-neighbour tight-binding approximation. Only bands above the Fermi level are shown, as the result is symmetric in energy. Note the bandgap at $k = 0$ is $E_g = 0.948 \text{eV}$ using an overlap energy of $\gamma_0 = -2.7 \text{eV}$ [40]. The lowest-energy conduction band in the CN is doubly-degenerate, and the effective mass of an electron near the bottom of the band is $0.093 m_0$ for this particular CN.

For semiconducting CNs, i.e., those not meeting the conditions of (1.7), the dispersion relation provides bandgap and effective mass information. Note that the dispersion relation of (1.6) obtained from the zone-folding method holds only for CNs with diameters above $\sim 7 \text{Å}$ [41], e.g., corresponding to a (8, 0) CN. Below this diameter, the strong bending of the bond angles reduces the validity of the tight-binding approach.
1.2 Modeling Coaxial CNFETs

Based on the experimental and theoretical evidence compiled earlier in this chapter, it has been the goal of the UBC Nanoelectronics Group to develop models that predict and further explain the behaviour of the CNFET. Work by group members D. John and L. Castro has led to the development of a self-consistent Schrödinger-Poisson solver, upon which this author’s work is based [19]. In the remainder of this section, a framework will be established for the research presented in this thesis. In particular, the boundary conditions employed in the simulation of partially-gated CNFETs will be discussed in relation to the electrostatics. Further, the extension of the quantum-mechanical Schrödinger-Poisson model to a multi-scale model, integrating quantum and semi-classical approaches, will be discussed in relation to the simulation of electroluminescence in CNFETs.

The model 3D device that will be referred to in the following sections is shown in figure 1.3. Again, while the devices studied here are coaxial, the simulated results have consistently been shown to be in agreement with the electronic behaviour of planar experimental devices [42].

![Figure 1.3: 3D CNFET geometry.](image-url)
1.2.1 Electrostatics

Since the model CNFET of figure 1.3 possesses axial symmetry, a reduction of dimension is possible, yielding the simulation domain shown in figure 1.4. Within the domain $F$ (see figure 1.4), the Poisson equation in cylindrical coordinates is solved,

$$\frac{1}{r} \frac{\partial V}{\partial r} + \frac{\partial^2 V}{\partial r^2} + \frac{\partial^2 V}{\partial z^2} = -\frac{1}{\epsilon} Q \quad z, \ r \in F, \quad (1.8)$$

where $V(r, z)$ is the electrostatic potential, $\epsilon$ is the permittivity, and $Q$ is the charge density. At a dielectric interface, electric flux must be preserved in relation to the surface charge, according to

$$\hat{n} \cdot (D_1 - D_2) = \rho_S, \quad (1.9)$$

where $\hat{n}$ is the unit normal directed away from region 1, $D_i = \epsilon_i E$ is the electric flux density at the interface in region $i$, and $\rho_S$ is the surface charge density. In the CNs studied, the relative permittivity $\kappa_{cn}$ is taken to be unity [43]. Since there are no incomplete bonds on the surface of the CN, lattice matching to reduce surface scattering does not restrict the choice of dielectric used in CNFET fabrication. In the literature, various high-$\kappa$ dielectrics have been proposed, including hafnium oxide $\kappa \simeq 16$ and zirconium oxide $\kappa \simeq 25$ [44], in addition to the more usual silicon dioxide.

Figure 1.4: 2D Simulation domain of the CNFET $F$ (indicated by the outer boundary $\partial F$), including sub-domains for the metallic contacts $G, S, D$, for the dielectric $K$, and for the CN $C$ (indicated by its surface $\partial C$). Axes $z$ and $r$ are also shown.
κ = 3.9, e.g., as in [26]. These values were used in simulations representative of the experimental devices.

Two approaches are used to solve the Poisson equation numerically for partially-gated CNFETs: the finite-difference (FD) approach using null-Neumann boundaries (see figure 1.4) to close the simulation space, as in [19], and the finite-element (FE) approach using a conformal mapping to include all space in a finite set, as in [16]. The key difference between these two approaches lies not in the numerical approximation used (FD or FE), but in the closure of open boundaries: the FD approach uses a non-physical boundary to terminate the simulation space. This has the effect of reducing the set of required space, and is justified by the fact that the components of interest are well contained, as long as certain conditions are met. These conditions will be addressed below, and are the subject of the following chapter. It must be noted that the conformal mapping of space outside the device is only applicable to 2D geometries, and cannot be extended when simulating non-symmetric devices in 3D. Therefore it is important to address the limitations of validity in the truncated-space approach.

In both cases, Dirichlet boundary conditions are used to define the potential on the surface of the source, drain, and gate terminals,

\[
V_S = -\phi_S \quad z, \ r \in \partial S \tag{1.10}
\]
\[
V_D = V_{DS} - \phi_D \quad z, \ r \in \partial D \tag{1.11}
\]
\[
V_G = V_{GS} - \phi_G \quad z, \ r \in \partial G \tag{1.12}
\]

where \( \phi \) represents the work function of the contact metal, expressed in electron volts (eV). At equilibrium, the alignment of the Fermi-levels between the metal contacts and the CN results in the formation of Schottky-barriers. The metal-semiconductor Schottky-barrier height for electrons, in an unpinned system [45], will be given by

\[
\phi_B = \phi_M - \chi_S \, , \tag{1.13}
\]

where \( \chi_S = \phi_S - (E_c - E_F) \) is the electron affinity of the semiconductor, and \( \phi_M \) is the metal work-function. Here, the CN is assumed to be intrinsic, as implied by the symmetric band-structure from the tight-binding approach presented in the previous section, such that the electron and hole effective masses will be the same and the Fermi-level \( E_F \) will be exactly at mid-gap. While many transistors in reported in the literature appear as p-type, this is likely caused by oxygen adsorption
near the contacts that modifies the barriers there [46]. This process is reversible, and the oxygen can be driven off by annealing in a vacuum, causing the device to transition from p-type to ambipolar and then to n-type [39]. Further, when titanium contacts are patterned over the CN and annealed in a vacuum, a TiC interface forms that has nearly symmetrical barriers, indicating that the Fermi level lies near the middle of the bandgap as expected from an intrinsic device [11].

The computation of $V(r, z)$ from Poisson’s equation (1.8) gives the electrostatic potential for the entire simulation space (figure 1.4), however it is the 1D potential $V_{CS}(z)$ along the surface of the CN $\partial C$ that is of primary interest. The valence and conduction bands of the CN are assumed to rigidly shift with the local potential, such that $E_c$ and $E_v$ are pinned to $V_{CS}$. This is appropriate for an electric field that varies slowly over the distances associated with the wavelength of an electron wave-packet, such that it appears approximately uniform [47]. However, in larger diameter CNs, the validity of this assumption comes into question as electrons are significantly de-localized. Evidence of this can be seen in the effect of transverse (radially-directed) electric fields on the bandgap: while the bandgap of a (17, 0) CN with radius $r_{cn} = 0.67$ nm remains stable for electric fields $E_r \lesssim 1$ V/nm, the bandgap of a (40, 0) CN ($r_{cn} = 1.5$ nm) begins to close for $E_r \gtrsim 0.1$ V/nm [48].

Since the conduction and valence bands are fixed at the locations of the contact-CN interfaces by the Schottky-barriers, the local electrostatic potential rigidly shifts the vacuum potential, such that $E_{vac}(z) = -qV_{CS}(z)$ on the CN surface, and from this, the conduction and valence band energies are defined as

$$E_c(z) = E_{vac}(z) + \chi \quad (1.14) \quad E_v(z) = E_c(z) - E_g \quad (1.15)$$

Clearly, the electric fields near the CN surface are responsible for modulation of the valence and conduction bands. Near the contacts, the SB shape (width) will be modulated, influencing the current through the CNFET. Therefore, it is critically important to obtain accurate electrostatics near the contact-CN interface.

Because CNs exist in a metallic form, it may be possible to construct a continuous CN structure that encompasses the source and drain contacts as well as the semiconductor channel. In this case, the radii of the source and drain contacts are equal to the radius of the semiconductor CN in the channel ($r_{cn} = r_{sd}$), and are known as “needle” contacts. This geometry is illustrated in figure 1.5, including a region very close to the surface of the CN, at the contact interface. Intuitively, the
electric field will bend around the corner of the metallic contact, and intersect the domain boundary ∂F (see figure 1.5). If a null-Neumann boundary is specified along ∂F, then the electric field normal to ∂F must be zero:

\[ \hat{n}_{\partial F} \cdot \nabla V = 0 \quad z, \; r \in \partial F. \]  

(1.16)

An analysis of the region near the contact-CN interface is required to determine if this null-Neumann boundary condition is valid.

Figure 1.5: The interface between needle-contacts and the CN, and associated regions defined for asymptotic analysis. Domain boundary ∂F indicates the possible location of a Neumann boundary.

As presented in Chapter 2, asymptotic analysis of the CN-contact interface region shows that the Cartesian Laplacian equation will apply when \( r/r_{cn} \approx 1 \). Further, it can be shown that at the location of the CN-contact interface \( z = z_0 \), the electric field normal to the domain boundary ∂F will decay proportional to \( (r - r_{cn})^{K-1} \), where \( K < 1 \) (see appendix A). Therefore, a null-Neumann boundary condition is invalid for narrow-radius contacts, and the distortion of the electrostatic potential will significantly alter the tunnelling current. By comparing the results of simulations using the FE approach against those using the FD approach with a null-Neumann boundary condition, this source of error was confirmed.

Two solutions are possible to maintain the integrity of the simulation. First, the Neumann
boundary may be adapted such that the electric field normal to the boundary decays inversely to the radius. This reduces the size of the simulation space, but is complicated by the singularity as \( r \to r_{cn} \) and relies on a parameter \( K \) that is impractical to determine from analysis. The second, and most commonly used solution, is to extend the simulation domain \( F \) to include a portion of the contact. Two simulations are shown in figure 1.6 comparing the case where 0.1 nm of contact is included (such that null-Neumann boundary is effectively at the contact-CN interface), with the case where 30 nm of contact is included.

![Figure 1.6: Comparison of lines of equipotential between the case where (a) the null-Neumann boundary is placed at \( z = -0.1 \) nm, and (b) the null-Neumann boundary is placed at \( z = -30 \) nm. Note that in (a) the non-physical boundary significantly alters the potential near the CN-contact interface (\( z = 0 \) nm). \( V_{GS} = 0.5 \) V, \( V_{DS} = 0.7 \) V, \( r_{sd} = r_{cn} \), (10, 0) CN.](image)

As the position \( z \) varies away from the CN-contact interface along the contact surface, the electric field normal to the boundary decreases proportional to \( x^{K-1} \). This is intuitively satisfying from the perspective of an infinite length of rod: the lines of equipotential will be parallel to the rod’s surface. As mentioned previously, the conformal transformation of [16] is valid only in 2D; however, the methods proposed here for improving the accuracy of Neumann boundary conditions may apply equally well in 3D, assuming that certain conditions on the azimuthally varying potential are met.
1.2.2 Charge Transport

To evaluate non-equilibrium conditions, charge transport must be incorporated into the simulations of the CNFET. In the model upon which the work presented in this document is based, John et al. combined a 1D Schrödinger wave equation (SWE) solution for the charge on the CN surface with Poisson’s equation to establish a self-consistent relation between the potential and charge within the CNFET domain. Charge transport is then determined from the Landauer equation. Their methods are described in [19], however a brief overview will be provided here for the convenience of the reader.

To initialize the system, the Laplace solution for the potential is computed in the CNFET domain $F$ (see figure 1.4), subject to the electrostatic boundary conditions described previously. From this solution, a 1D potential $V_{CS}(z)$ along the CN surface $\partial C$ is obtained, which defines the conduction and valence bands for the semiconductor CN as in (1.14) and (1.15). These energies are then used in the SWE to obtain information about the charge density and transmission probability. In the metal contacts, a Fermi distribution is assumed, with the Fermi-level positioned 5.5 eV above the bottom of the band. The effective mass of the electron is held to be the same in the metal contact as in the CN. In the CN, only the first doubly-degenerate band is considered, i.e., a single effective mass from the parabolic band approximation defines the carriers in the CN. The SWE is solved using the scattering-matrix method [49], approximating the potential energy as piecewise-constant. The normalization condition is specified through conservation of the flux [50]. Thus, a Landauer current may be obtained from the transmission probability and the Fermi distributions in the source and drain contacts. Transmission is assumed to be coherent and ballistic, and the charge distribution is determined by integrating the complete wave function solution in energy. Both source and drain injection are considered simultaneously at all energies. Metal-induced-gap-states (MIGS) are included by accounting for the evanescent waves in the bandgap near the contact; in the model of John et al., these contribute to the charge in the channel, and as a result, the band-bending [19]. This 1D charge is then included in Poisson’s equation, and a new electrostatic potential is determined. This process continues iteratively using a Picard scheme until convergence is obtained.

While this method is effective in the simulation of short-channel devices, where ballistic transport is present and a full quantum treatment is appropriate, it is cumbersome and unnecessary for longer devices where charge transport is diffusive. The acoustic phonon mean-free-path (mfp) in a CN has been shown to be on the order of 300 nm [8], such that treatment of carriers as thermalized in devices
where $l_{cn} > 1 \mu m$ is reasonable. In devices with lengths of $l_{cn} \sim 50 \mu m$, this assumption has proved correct, as the observed mobile electroluminescence [27] can be attributed to drift current in the presence of finite mobility in a diffusive system [28]. To address this, a multi-scale model based on the work of [29] was proposed.

Recognizing that Schottky-barriers will still be present at the interface between the metallic contacts and the CN, quantum-mechanical tunnelling will contribute to the current in the device. Therefore, the 1D effective-mass SWE solver of [19] is adapted to evaluate SB tunnelling between the contact and the CN. First, the Laplace solution for the electrostatic potential is computed, and $V_{CS}(z)$ is extracted. A length of the CN is then chosen at each contact to define a quantum region, where the SWE is solved to find the transmission probability $T(E)$. The lengths of these regions are determined by the location where the electric field reaches a fraction of the maximum electric field, typically 0.001, such that the region extends 100 – 400 nm into the CN. While the distance where tunnelling is appreciable is on the order of 10 nm, this choice allows for the inclusion of interband tunnelling in situations where severe band-bending is present. A schematic band-diagram illustrating this process is shown in figure 1.7.

Carrier injection is assumed to be unidirectional for the bias conditions leading to ambipolar conduction. Under those biases, reverse injection is limited by large barriers ($> 20kT$), and the absence of tunnelling (the barriers formed by the bands allow only for thermionic emission). At the source, electron injection dominates for positive biases, and energies above $E_c$ at the CN-edge of the quantum region are considered (see shaded region, figure 1.7). Using this approach, boundary condition information for charge transport is obtained in the form of thermionic emission and tunnelling currents. In contrast to the method of [29], where the WKB approximation was used to estimate the tunnelling current below the Schottky-barrier, and unity transmission was assumed above it, a complete SWE solution addresses non-unity transmission for the thermionic emission current, and allows interband tunnelling to contribute.

To evaluate charge transport in the long channel, the semi-classical drift-diffusion equations (DDEs) are used in conjunction with the continuity equations to account for recombination. Through a substitution of variables and scaling to remove units (see appendix B), a system of three equations
Figure 1.7: Schottky-barrier tunnelling and thermionic emission for electrons at the source. Carriers are assumed to have a Fermi distributions \( f_S(E) \) in the contact and \( f_{\phi n}(E) \) in the CN, where the quasi-Fermi level \( \phi_n \) in the CN is obtained self-consistently, and the difference between the source Fermi-level \( \mu_S \) and the conduction band edge \( E_c \) at the contact-CN interface is determined by the SB height.

can be established in terms of carrier charge densities \( u \) and \( v \) and electrostatic potential \( V \),

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial V}{\partial r} \right) + \frac{\partial^2 V}{\partial z^2} = u e^V - v e^{-V} \quad z, \ r \in F \tag{1.17}
\]

\[
- \frac{d}{dz} \left( D_n \frac{du}{dz} e^V \right) + Buv = B - G_n \quad z, \ r \in \partial C \tag{1.18}
\]

\[
- \frac{d}{dz} \left( D_p \frac{dv}{dz} e^{-V} \right) + Buv = B - G_p \quad z, \ r \in \partial C , \tag{1.19}
\]

where \( D_n \) and \( D_p \) are the field-dependent diffusivities of the electrons and holes, respectively; \( B \) is the direct radiative recombination velocity, which will be addressed in the following section; and \( G_n \) and \( G_p \) are the generation rates of electrons and holes, respectively, which are addressed in Chapter 3. Equation (1.17) is simply the 2D Poisson equation as in (1.8), with a substitution made
for the charge. Note that (1.18) and (1.19) are 1D, and that $u$ and $v$ are defined only on the CN surface $\partial C$. The boundary conditions for (1.17) have been described in the previous section. The boundary conditions for (1.18) and (1.19) are established from the thermionic emission and tunnelling currents at the injecting contact. The thermionic emission current is used as a Neumann boundary condition, and the tunnelling current is transformed to a generation rate $G_{TUN}(z)$, as described in [51]. Further details are provided in Chapter 3. At the opposite end of the channel, an infinite recombination velocity is assumed, such that the intrinsic charge concentration $n_i$ is imposed as a Dirichlet boundary condition. The intrinsic charge is computed numerically assuming a single doubly-degenerate band and a constant effective mass, consistent with the approach applied to the system as a whole. Note that charge information from the SWE solution is discarded, and that the semi-classical solution is used to define the charge over the complete length the CN. While some information is lost through the neglect of quantum phenomena (e.g., MIGS), there is still strong agreement with experimentally observed electroluminescence results, which have their basis in semi-classical diffusive transport.

The charges $u$ and $v$ in (1.18) and (1.19) are coupled by the recombination term in the continuity equation. Thus, to solve for one charge, an estimate of the other is required. This estimate is obtained from a previous iteration, or when one does not exist, the intrinsic charge is used. Due to the exponential nature of the DDE and the charge coupling, oscillations tend to destabilize the numerical simulation. To combat this, memory is employed to damp the charge estimate used in the current iteration. Once updated charges are computed, a linearized Poisson’s equation is solved to update the electrostatic potential for the CNFET. This procedure is repeated iteratively until charge and voltage convergences have been obtained (see appendix B).

1.2.3 Electroluminescence

Having established a multi-scale model for charge transport in long Schottky-barrier CNFETs, it is now possible to examine the mechanisms leading to the various electroluminescence (EL) effects observed experimentally [27,30]. In this model, the work of Guo et al. [29] has been extended through the inclusion of a full quantum treatment of the Schottky-barriers, as well as a field-dependent mobility. EL is assumed to result from the direct band-to-band recombination of electron-hole pairs (EHPs). The steady-state continuity equations, which are incorporated into (1.18) and (1.19), are
\[
\frac{1}{q} \frac{dJ_n}{dz} = R, \quad \text{and} \quad \frac{1}{q} \frac{dJ_p}{dz} = -R,
\]

(1.20) \quad (1.21)

where \( R \) is the net rate of recombination. First considering the net direct band-to-band recombination \( R^{bb} = R^{optbb} - G^{bball} \),

\[
R^{optbb} = B^{bb}_{ec} np \quad (1.22) \quad G^{bball} = B^{bb}_{ee}
\]

(1.23)

where \( B^{bb}_{ec} \) is the EHP capture rate, and \( B^{bb}_{ee} \) is the EHP generation rate. Again, recombination \( R^{optbb} \) results in photon emission, while it is assumed that \( G^{bball} \) is a thermal process in the absence of illumination. At equilibrium,

\[
R^{optbb} = G^{bball} \rightarrow B^{bb}_{ec} n_i^2 = B^{bb}_{ee} \rightarrow R^{bb} = B(np - n_i^2),
\]

(1.24)

and replacing \( B^{bb}_{ee} \) with \( B \), the direct radiative recombination velocity, the familiar expression for recombination is obtained. This value is determined empirically, as shown in Chapter 3. In the absence of uniformly distributed trapping sites, as would appear in a doped semiconductor, Shockley-Read-Hall (SRH) recombination is assumed to be negligible.

Significant investigations have been made into the impact of excitons on EL [52–54]. These studies probed the energy structure of the CN and continue to provoke debate on the actual path of photon emission. Excitonic EL is a high-field, electron-electron (e-e) interaction process that is not directly considered by (1.24). A recombination rate relating exciton formation to EL would follow from the model of an Auger emission process, which also captures the microscopic behaviour of impact excitation [55]. However, Auger emission assumes that a conduction band electron (or a valence band hole) is generated through an e-e scattering event, whereas the formation of an exciton necessitates that no electron enters the conduction band of the CN: the generation rate would be zero. The complementary process, Auger recombination, would result in the emission of a photon through an e-e interaction in the conduction band, and has the form

\[
R^A = (B^A_n n + B^A_p p)(np - n_i^2).
\]

(1.25)

The model proposed here assumes that electron-phonon interaction is the dominant scattering mechanism leading to recombination, and neglects Auger recombination. Therefore, it is possible that not all excitonic photon emission will be captured. An investigation comparing the recombination
process used in this model to e-e scattering may yield further insight into the actual mechanism of impact excitation, but is outside the scope of this work.

As demonstrated in Chapter 3, the proposed multi-scale model qualitatively captures important aspects of EL in CNFETs, while remaining able to handle long devices. In the original publication of mobile EL results by Freitag et al., the authors suggested that hot-electrons injected from the source and drain were responsible for the increase in luminescence intensity as the light spot approached the contacts [27]. Modeling charge transport through the semi-classical DDE, it can be shown, without resorting to any further physics, that this property of the EL is inherent to an ambipolar biased device where the mobility is finite. In later experiments, Freitag et al. observed fixed EL localized to defects and to the contact-CN interface, and proposed that excitonic relaxation following excitation in the strong fields near both features was the likely source [30]. While exciton effects have not been directly included in the DDE-centric model, the EL simulated corresponds well with the observed phenomena, including the more unipolar nature of operation.

1.3 Thesis Outline

In the following chapters, two manuscripts produced over the course of researching CNFETs are presented, followed by a conclusion summarizing the key achievements and addressing future work. Chapter 2 details the investigation of error introduced by terminating the simulation space with null-Neumann boundaries. Chapter 3 presents the multi-scale model describing electroluminescence in long CNFETs, and offers comparison between simulated and experimentally observed phenomena.

1.4 Specific Contributions

The work presented in this thesis has contributed to the understanding of the means by which the CNFET operates through improvements to numerical models and modeling techniques. Specific limits of validity were formulated for the common practice of closing open boundaries with a null-Neumann condition. In addition, a careful analysis of novel optical properties recently observed in CNFETs has shed light on the underlying principles of operation. The model developed here was constructed in close relation to experimental results, combining both quantum and semi-classical behaviour, and is found to closely replicate the phenomena observed in actual devices.
References


Chapter 2

Error Analysis of Boundary Condition Approximations in the Modeling of Coaxially-Gated Carbon Nanotube Field-Effect Transistors

2.1 Introduction

The modeling of carbon nanotube field-effect transistors (CNFETs) is an active area of research, one of the present goals of which is to evaluate the performance limits of devices as regards operation under conditions of either DC [1,2], or AC [3]. The majority of modeling work thus far has concentrated on coaxial transistors with wrap-around gates, as such a structure offers the ultimate gate control over the nanotube surface potential [4]. Fabrication of such structures is difficult, but is being vigorously pursued [5,6]. In the numerical modeling of semiconductor devices it is customary to use a null Neumann boundary condition, in which the normal component of the electric field set to zero, to terminate the open boundaries of the model space. In nanoscale devices, this practice is widely followed [3,7,8], although strict null Neumann boundaries are not typically found a priori. In this study, an asymptotic analysis examining the electric field near the carbon nanotube (CN)-contact interface reveals that a Cartesian formulation of Poisson’s equation is applicable in the local region and demonstrates that a null Neumann boundary is not physically correct.

When the symmetry of the device allows a reduction in dimension to 2-D, a conformal transfor-
formation yields an exact solution for the potential in all regions [9]. We use this method as a benchmark, solving the cylindrical Poisson equation in all space, and compare against results obtained from imposing a null Neumann condition at open boundaries in Schottky-barrier (SB) CNFETs. We consider the error introduced in the DC ON-current, extending the earlier work of Ref. [9], in which only the equilibrium case was considered. We continue to evaluate a coaxial structure as a benchmark device in terms of scale and performance, although the device dimensions are based on a state-of-the-art planar device [10], with short CN length, high-permittivity gate dielectric, and thin source/drain contacts. We consider the effect of several geometry modifications on the accuracy of the results, including reductions to the radius of the source/drain contacts, changes to the gate dielectric thickness and material, and changes to the spacing between the source/drain electrodes and the edge of the gate electrode.

2.2 Modeling Procedures

Fig. 2.1 illustrates the coaxial structure simulated in this work: the 2-D Poisson equation is solved using a standard finite-element software package\(^1\), and the effective-mass Schrödinger equation is solved self-consistently in 1-D to compute the charge distribution [11]. The current is computed using the Landauer equation [12]. In one instance, null Neumann boundary conditions are used at the open boundaries (see Fig. 2.1 (b), dashed line); in the benchmark case, the conformal transformation method described in Ref. [9] is used. Solving the conformally mapped problem numerically, error sources are restricted to the convergence tolerance and the element size.

As discussed in the following section, we observed the largest error when using “needle” contacts, i.e. \(r_{sd} = r_{cn}\). Therefore, we performed an asymptotic analysis of the potential at the CN-contact interface near the CN surface to understand how this error may be reduced. This analysis follows the method presented in Ref. [13, pp. 75-79], and extends it by including both a dielectric and a surface charge. The surface charge \(Q\) is assumed to be constant in the region of interest.

We begin by establishing that sufficiently close to the contact, where \(r/r_{cn} \approx 1\), a Cartesian formulation of Poisson’s equation is valid. The situation is illustrated in the inset of Fig. 2.1 (b).

\(^1\)FEMLAB, see http://www.comsol.com
Figure 2.1: Geometry overview showing (a) the cylindrical device and (b) the radial cross-section including key device parameters. The dashed line indicates the location of the null Neumann condition used to close the open boundaries. A non-zero $l_{sd}$ is illustrated although typically, $l_{sd} = 0$. The inset shows the important region at the contact/nanotube interface and the regional numbering scheme used in the text.

Defining local coordinates

$$x = \frac{z - z_0}{\delta} \quad \text{and} \quad y = \frac{r - r_{cn}}{\delta},$$  

(2.1)

where $\delta \ll r_{cn}$ and $z_0$ is the location of the CN-contact interface, Poisson’s equation (for potential $\phi(z, r)$) in cylindrical coordinates becomes

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\delta}{\delta y + r_{cn}} \frac{\partial \phi}{\partial y} = \delta^2 \frac{Q}{\epsilon}.$$  

(2.2)

As $r/r_{cn} \to 1$, $\delta y \ll r_{cn}$ and the coefficient of the first partial derivative is $O(\delta)$. For a small $\delta$, we conclude that the cylindrical Poisson equation can be locally approximated by the Cartesian Laplacian.

Based on this conclusion, we proceed by transforming the Cartesian Laplacian into polar coordinates and solving for the potential $\phi(\sigma, \theta)$. Separation of variables is used to break the problem
into a radial equation and an angular equation with a well-known series solution [13], which can be written in terms of one arbitrary constant \( K \), which is related to the dielectric constant \( \kappa_{\text{ins}} \), boundary layer charge \( Q \) (see inset, Fig. 2.1 b) and boundary conditions as \( \sigma \to \infty \). In this analysis, no attempt is made to join the inner and outer regions, leaving the boundary conditions where \( \sigma \to \infty \) undefined. Therefore, \( K \) may be treated as a geometry-dependent parameter chosen to account for the influence of structures in the outer region, e.g. the gate, on the electric field. Assuming that \( \sigma \ll 1 \), and that \( K_j \) increases monotonically with \( j \), the series index, we approximate the general solution by the first solution in the series, yielding

\[
\phi(\sigma, \theta) \approx a_0 + a_i f_i(K) \sigma^K \left[ g_i(K) \cos(K \theta) + \sin(K \theta) \right], \tag{2.3}
\]

where \( i \) is a domain index. \( f_i(K) \) and \( g_i(K) \) represent the replacement of other constants in terms of \( K \), and may depend on \( \kappa_{\text{ins}} \) and \( Q \). This provides a means for including the iteratively computed charge in the approximation to the electric field at a selected boundary.

This analysis provides two methods for reducing error introduced by the null Neumann boundary. Taking the derivative of Eq. 2.3 normal to the Neumann boundary at the location of the CN-contact interface,

\[
\left. \frac{\partial \phi}{\partial x} \right|_i = a_i y K f_i(K) \left[ g_i(K) \sin \left( K \tan^{-1} \frac{y}{x} \right) - \cos \left( K \tan^{-1} \frac{y}{x} \right) \right] \left( x^2 + y^2 \right)^{K/2 - 1} - 2 x f_i(K) \left[ g_i(K) \cos \left( K \tan^{-1} \frac{y}{x} \right) + \sin \left( K \tan^{-1} \frac{y}{x} \right) \right] \left( x^2 + y^2 \right)^{K/2}. \tag{2.4}
\]

At the CN-contact interface of a needle-contacted device, \( x = 0 \), and Eq. 2.4 implies that the normal gradient of the potential will decay proportional to \( y^{K-1} \), where \( K \) is chosen based on the geometry and it is implicit that \( K < 1 \). Therefore, replacing the null Neumann boundary with a normal gradient that varies as \((r-r_{\text{cn}})^{K-1}\) will better approximate the physical boundary conditions, locally.

Alternately, we observe that by extending the simulation space to include a portion of the contact \( (l_{sd} > 0) \), the error can be reduced. Near the surface of the CN and, equivalently, the surface of the contact in region I, \( y \ll 1 \), and \( \theta = \tan^{-1}(x/y) \approx 0 \). As \( x \) is increased, such that \( x \gg y \), Eq. 2.4 can be simplified to

\[
\left. \frac{\partial \phi}{\partial x} \right|_1 \approx -a_i K f_1(K) x^{K-1}. \tag{2.5}
\]
in the valid range of the local approximation. With $K < 1$, Eq. 2.5 suggests that as $x$ is increased near the surface of the contact, the gradient of the potential in the direction normal to the boundary approaches zero.

### 2.3 Results and Discussion

Results are presented for the five SB-CNFETs listed in Table 2.1. Note that all devices except

Table 2.1: Device Properties. In all cases $l_{cn} = 50$ nm, and the CN work function is 4.73 eV [14].

Devices 1 and 2 have Pd end contacts with barrier heights obtained from Ref. [15], while devices 3-5 have (9,0) metallic CN contacts. Geometry dimensions are referenced to Fig. 2.1 (b), $E_g$ is the CN bandgap, and $\Phi_B$ is the SB height for holes.

<table>
<thead>
<tr>
<th>Device</th>
<th>$r_{cn}$ (nm)</th>
<th>$r_{sd}$ (nm)</th>
<th>$t_{ins}$ (nm)</th>
<th>$l_{gap}$ (nm)</th>
<th>$n_{ins}$</th>
<th>Chirality</th>
<th>$E_g$ (eV)</th>
<th>$\Phi_B$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 [10]</td>
<td>0.85</td>
<td>6.15*</td>
<td>8.00</td>
<td>8.00</td>
<td>16</td>
<td>(22,0)</td>
<td>0.46</td>
<td>-0.04</td>
</tr>
<tr>
<td>2</td>
<td>0.39</td>
<td>5.69**</td>
<td>8.00</td>
<td>8.00</td>
<td>16</td>
<td>(10,0)</td>
<td>0.98</td>
<td>+0.30</td>
</tr>
<tr>
<td>3</td>
<td>0.39</td>
<td>0.39</td>
<td>8.00</td>
<td>8.00</td>
<td>16</td>
<td>(10,0)</td>
<td>0.98</td>
<td>+0.49</td>
</tr>
<tr>
<td>4</td>
<td>0.39</td>
<td>0.39</td>
<td>2.00</td>
<td>12.0</td>
<td>16</td>
<td>(10,0)</td>
<td>0.98</td>
<td>+0.49</td>
</tr>
<tr>
<td>5</td>
<td>0.39</td>
<td>0.39</td>
<td>8.00</td>
<td>8.00</td>
<td>25</td>
<td>(10,0)</td>
<td>0.98</td>
<td>+0.49</td>
</tr>
</tbody>
</table>

* Chosen to give $r_{sd} + r_{cn} = 7$ nm [10]  ** Chosen to keep $r_{sd} - r_{cn} = 5.3$ nm, as in device 1

for device 1 use a (10,0) CN. These latter devices have larger bandgaps, resulting in FETs with significantly improved ON/OFF-current ratios [1]. The errors in the potential and drain current, evaluated with respect to the results obtained using the conformal transformation are summarized in Table 2.2. The maximum error in the potential was computed by taking the infinity norm of the relative error at all positions on the CN surface. In all cases, the greatest deviation between potentials occurred close to the source. The valence band diagrams in the vicinity of the source for each of devices 1-4 are shown in Fig. 2.2.

For devices 1 (circle) and 2 (square), there is no discernible difference in potential, however the relative ON-current error in device 2 is higher because tunneling dominates in this positive-barrier device, and is exponentially dependent on the shape of the barrier. Devices 3 (triangle) and 4 (diamond) illustrate the significant error that arises from non-physical boundaries near needle
Table 2.2: Error in potential and drain current for bias conditions of $V_{GS} = V_{DS} = -0.5V$

<table>
<thead>
<tr>
<th>Device</th>
<th>Max. V Error (%)</th>
<th>$I_D$ Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.24</td>
<td>0.62</td>
</tr>
<tr>
<td>2</td>
<td>0.36</td>
<td>4.13</td>
</tr>
<tr>
<td>3</td>
<td>26.6</td>
<td>62.7</td>
</tr>
<tr>
<td>4</td>
<td>42.2</td>
<td>435</td>
</tr>
<tr>
<td>5</td>
<td>21.2</td>
<td>43.4</td>
</tr>
</tbody>
</table>

Figure 2.2: Valence band diagrams for devices 1 to 4 near the source contact, referenced to the Fermi level. Conformal mapped case: solid line. Null Neumann bounded: $l_{sd} = 0$ nm, dashed line. Device 1: ◦, device 2: □, device 3: ▽, device 4: ◆

contacts. In the case of the aspect ratio of the gate and source/drain contact gap to the dielectric thickness, comparing devices 3 and 4, we note that by reducing $l_{gap}$ or increasing $t_{ins}$, the electric field between the gate and the source/drain contact is oriented in a more radial direction, reducing the component normal to boundary. This makes the null Neumann boundary a better approximation, reducing error. From the flux continuity condition, it is clear that greater refraction will exist when a high-$\kappa$ gate dielectric is present, reducing the normal component of the potential gradient. In device 5, a 56% increase in $\kappa$ with respect to device 3 led to a 44% decrease in relative ON-current.
error.

To illustrate how the large error associated with needle contacts can be reduced, we refer to the asymptotic analysis. With $K < 1$, Eq. 2.5 suggests that as $x$ is increased near the surface of the contact, the gradient of the potential in the direction normal to the boundary will approach zero. This coincides with the intuitive picture that a flat plate behaves like an infinite plane when observed at a position far from the corners: the equipotential lines are parallel to the plate’s surface. By including a portion of the contact in the simulation, and imposing the null Neumann boundary condition further from the CN-contact interface, the error from the non-physical boundary will be reduced. To support this hypothesis, simulations were performed for device 4 (the one with the largest error), with $l_{sd}$ extended beyond the value 0 nm used in the previous simulations. Results are shown in Fig. 2.3 (a). In Fig. 2.3 (b), we demonstrate the validity of the asymptotic analysis in the prediction of the local electric field. Extending the simulation space, we note that a limit in the reduction of error is reached at $\approx 2.5\%$. Based on the predictions of the asymptotic analysis and the simulation results, we conclude that for contacts with the same radius as the CN, the boundary should be extended to include $l_{sd} \geq 10r_{cn}$ of the contact to reduce the relative ON-current error below 10% or $l_{sd} \geq 20r_{cn}$ to ensure that the error remains below 5%. These metrics are arrived at for the worst case CN-contact interface geometry and will apply conservatively for contacts with $r_{sd} > r_{cn}$.

### 2.4 Conclusions

From this error analysis of methods used to compute the potential in co-axial SB-CNFETs, we conclude that caution must be exercised when employing non-physical boundaries in cases where narrow-radius contacts are present. The error can be significantly reduced, without unduly compromising the simulation efficiency, by extending the simulation space to include a length of contact.
Figure 2.3: Asymptotic analysis results for device 4. (a) Simulated relative ON-current error as $l_{sd}$ is increased, which decays as an exponential $\propto l_{sd}^{K-1}$, $K = 0.15$ (see Eq. 2.5). It is assumed that as the electric field at the boundary approaches zero, the error will decrease proportionally. (b) Comparison of $\frac{d\phi}{dz}$ (circles) as computed at the CN-contact interface (needle contacts) to the asymptotic approximation (solid) with $K = 0.15$. Away from the contact, the local approximation is less valid. In the far field, we find it convenient to use $\frac{d\phi}{dz} \propto r^{-1}$ as in an infinite rod to describe the electric field.
References


Chapter 3

A Multi-Scale Model for Mobile and Localized Electroluminescence in Carbon Nanotube Field-Effect Transistors

3.1 Introduction

Electroluminescence (EL) from carbon nanotube field-effect transistors (CNFETs) has recently been demonstrated [1–5]. Initial reports on EL were of a mobile light spot with a width of ≈ 5μm that could be positioned longitudinally along the CN by varying the gate bias [1, 2]. The intensity of this mobile luminescence increased as the spot neared the contacts [2]. Most recently, localized luminescence at a contact and at defect sites has been reported [3]. Both free-carrier recombination and exciton relaxation have been proposed as possible radiation mechanisms. In this paper, we present a multi-scale model in which only free-carrier, band-to-band recombination is considered, but which is able to predict all of the experimentally observed EL phenomena in non-looping CNs.

Light spot mobility in long-channel devices under ambipolar bias conditions has been modeled by Tersoff et al. using a simple analytic drift-current expression that assumes a negligible recombination length [6]. That model captures the movement of the emission spot but fails to account for the peaking in intensity of the mobile emission near the contacts. Guo et al. solved the drift-diffusion, continuity and Poisson equations self-consistently, but did not investigate many of the observed EL effects [7]. The model presented in this work improves on other models in that it does not assume a negligible recombination length [6]; it uses a full quantum mechanical treatment for carrier injection.

rather than a WKB approximation for tunneling and thermionic emission [7]; and it uses a field-dependent mobility, rather than an arbitrary, constant mobility [7]. By using a Schottky barrier height for the source and drain contacts that is more appropriate to the palladium contacts used experimentally [2,3], localized emission at one contact can be predicted. Introduction of a charged defect in the tube, which obviously will affect the electrostatics [8], is also shown to create a site of localized emission, as reported in [3].

3.2 Model

Although the experimental devices are planar [2,3], we follow the approach of Guo et al. and evaluate co-axial structures [7], due to their relative ease of simulation [9]. The simulation space is shown below in figure 3.1 and is closed by null-Neumann boundaries. The length of the contacts \( l_{sd} \) is chosen to be sufficiently large as to minimize the error introduced by these non-physical boundary conditions [10].

A multi-scale model is required because the transport of interest is both quantum mechanical and classical in nature. At the SB source and drain contacts, quantum mechanical tunneling and reflection occurs, while transport in the long CN channel (\( l_{cn} \geq 10 \mu m \)) is diffusive in nature. Further, the acoustical phonon mean free path is on the order of 300nm, which suggests that approximating the carriers involved in long-range transport as being thermalized is appropriate [11]. Therefore,
the model presented in this paper combines a Schrödinger wave equation (SWE) solution, defining a transmission probability where quantum mechanical tunneling and thermionic emission are significant, with the drift-diffusion equations, describing charge transport along the full length of the channel. The net rate of recombination \( R \) of electron-hole pairs (EHPs) is incorporated in the steady-state continuity equations,

\[
\frac{1}{q} \nabla \cdot \mathbf{J}_n = R - G_{\text{TUN},n} \quad \frac{1}{q} \nabla \cdot \mathbf{J}_p = -R + G_{\text{TUN},p},
\]  

(3.1)

where \( R \) is the sum of band-to-band, radiative recombination and band-to-band generation,

\[
R = B (n p - n_i^2),
\]  

(3.2)

and the generation terms \( G_{\text{TUN}} \) are a representation of the electron and hole tunneling currents at the source and drain contacts, respectively, as described later in this section. In 3.2, \( B \) is the direct radiative recombination velocity. As described in the Results section, we ascribe a value to \( B \) based on a fit to experimental data. We do not attempt to explicitly model other recombination mechanisms, such as Auger [12] or exciton relaxation [4,13], that may be operative.

Charge transport is restricted to the CN surface, such that the drift-diffusion and continuity equations are solved in one dimension. Transport is assumed to be unidirectional in the case of each carrier (i.e., source-injected electrons and drain-injected holes). At the injecting contact, the thermionic emission (TE) current is used as a Neumann boundary condition. The transmission probability above the barrier is significantly less than unity (see figure 3.2), therefore the TE current is computed from the Landauer equation for the case of a single, doubly-degenerate band (e.g. electrons at the source),

\[
I_{\text{TE}} = -\frac{4q}{h} \int_{E_c(0)}^{E_{\text{max}}} T(E) (f_{\mu_S}(E) - f_{\phi_N}(E)) \, dE
\]  

(3.3)

where \( T(E) \) is the transmission coefficient derived from the SWE solution for the bands near the contact, \( \mu_S \) refers to the source Fermi level, and \( \phi_N \) is the electron quasi-Fermi level, which is obtained self-consistently from our solver. The tunneling current can be conveniently incorporated into our multi-scale model by representing it as a generation rate, as described in [14] and adapted as follows (the electron case is given as an example here, however only minor modifications are necessary to treat holes): transforming the continuity equation,

\[
G_{\text{TUN},n}(z) = -\frac{1}{q} \nabla \cdot J_{\text{TUN},n} = \frac{dJ_{\text{TUN},n}}{dE} \cdot \nabla \psi,
\]  

(3.4)

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the generation rate $G_{\text{TUN, n}}$ can be expressed in terms of the gradient of the tunneling current with respect to energy $E = -q\psi$ and the gradient of the potential on the CN surface $\nabla \psi$. Using the Landauer equation for the tunneling current, we obtain an expression for the generation rate that depends on the transmission coefficient $T(E)$ obtained from the SWE solution,

$$G_{\text{TUN, n}}(z) = -\frac{4q}{h} T(E_c(z)) \left[ f_{\mu_0} (E_c(z)) - f_{\phi_n} (E_c(z)) \right] \frac{d\psi}{dz},$$

(3.5)

where conduction band energy $E_c(z)$ links energy and position. At the collecting contact, an infinite recombination velocity is assumed. This implies that a Dirichlet boundary is set by the intrinsic carrier concentration $n_i$, for which we ascribe a value using an effective-mass density of states [15]. The relation between the various components in the multi-scale model is illustrated in figure 3.2.

Figure 3.2: Top graph: Schottky barrier at the contact-CN interface ($z = 0$ nm). The large wavevector discontinuity leads to $T(E) < 1$, even above the barrier ($T(E)$ in blue on a rotated axis). The quantum mechanical region is bounded (dashed grey line) at $z \approx 380$ nm; at this point, the electric field is less than a minimum tolerance. Bottom graph: $G_{\text{TUN}}(z)$ as computed from the transmission probability $T(E)$ [14]. At the source, only electrons are generated (as opposed to EHPs).

As there is a significant variation in the electric field along the length of the CN, it is important
to include that dependence in the electron and hole mobilities $\mu(E)$. Under low-field conditions, CNs are expected to demonstrate near-ballistic behaviour [16]. Under the influence of larger fields, carrier behaviour is less well understood. Theoretical predictions suggest negative differential mobility may arise from electron transfer between subbands [17, 18], and that optical phonons, whose mean-free-path is in the range of 10-100 nm, may be excited [19]. Experimentally, mobilities have been reported between 10 cm$^2$/V-s and 100,000 cm$^2$/V-s [16,20]. An analysis based on electrons scattering by longitudinal acoustic (LA) phonons found low-field mobilities in reasonable agreement with the experimental results [17]. This theoretical result is used to describe the mobility of the electrons and holes in the CN channel in this paper. Under the bias conditions used in our simulations, the electric field strength ranges from 0.01-100 kV/cm and mobilities vary from 20,000-20 cm$^2$/V-s.

3.3 Simulation Method

A damped iterative method is used to seek a convergent numerical solution to the system of equations given in the previous section. The equations are approximated by the finite difference method on a variably-spaced mesh. The Laplace solution is used to initialize the simulation along with an estimate of carrier concentration distributions from a previously converged simulation when available (otherwise, intrinsic carrier concentrations are used). Due to the exponential nature of the equations and their interdependence, convergence is difficult to obtain, and large oscillations in charge tend to destabilize the simulation. To overcome this difficulty, memory was incorporated into the charge estimates $n_k$ and $p_k$ such that

\begin{align}
  n_k &= wn_{k-1} + (1-w)n_{k-2} \\
  p_k &= wp_{k-1} + (1-w)p_{k-2},
\end{align}

where $w$ is a weighting factor (typically, $w = 0.5$) and $k$ is the iteration index. This technique dramatically improves convergence over a wide range of cases without significantly impacting the simulation time. Once the charge residual has reached an intermediate tolerance, e.g., a factor of $10^2$ larger than the final tolerance, the weighting can be shifted to favour the nearest charge estimate to improve convergence rates. Updates to the electrostatic potential are obtained by linearizing the potential and computing the difference based on the latest charge estimate. Convergence is obtained when voltage and charge residuals meet specified absolute tolerances. Charge tolerances
must be tight enough such that the location where the net charge is zero, \( Q_{\text{net}} = p - n = 0 \), stabilizes.

### 3.4 Results and Discussion

Results are reported that relate to three features of EL observed recently in experimental devices and not described by previous models [6,7], namely variations in intensity of the mobile luminescence [2], localized light emission at one of the contacts [3], and localized EL at space-charge regions induced by charge defects in the oxide [3]. The dimensions of the device shown in figure 3.1 are chosen to capture the critical characteristics of the experimental devices in [2, 3]; these parameters are listed in table 3.1. In the presentation of these results, the photon emission rate is attributed to the recombination rate \( R \) obtained from self-consistent simulation: we normalize \( R \) to the bandgap energy \( E_g = 0.4eV \) (i.e., the emission spectrum), and assume a photon emission efficiency of \( 10^{-4} \) as in an excitonic process [4]. A constant drain current (0.2\( \mu \)A in our simulations) was maintained while \( V_{DS} \) and \( V_{GS} \) were varied, consistent with the biasing scheme of the experimental work [2]. \( B \) was determined by fitting the width of the simulated luminescence peak to the experimental result at the half-power level as shown in figure 3.3.
Figure 3.3: Comparison of the simulated emission peak $R$ (solid) with the measured rate (red circles) of [2]. Measured emission is in arbitrary units and its height is scaled so that both peaks have the same value. $B$ is then determined by matching the width of both peaks at half-power (dashed bars).

3.4.1 Mobile Electroluminescence

We begin by noting that the recombination term $R$ (see 3.2) depends on the charge product $np$. Luminescence intensity measurements reported in the work of Freitag et al. indicate a peaking of emission as the light spot approaches the contact [2]. In their work, the authors suggest that this may be from injected carriers at higher energies that scatter and emit photons at energies greater than the bandgap. Simulations using our multi-scale model demonstrate that this peaking, as shown in figure 3.4, can result solely from the consideration of ambipolar transport. While the shift in the bias (lowering $V_{GS}$ relative to $V_{DS}$) increases the population of holes relative to the populations of electrons, the low mobility in the high-field region near the contact, coupled with the continued presence of electrons, leads to a peaking in the intensity of the light spot. Freitag et al. report that the intensity of mobile luminescence is approximately 20% higher near the contact than at mid-tube [2]. In our simulations, the intensity increases by 14%. Looking at the recombination profile in figure 3.4, the peak intensity remains constant once the peak location moves more than $\approx 8\mu m$ from the contact. In this middle length of the CN, the electric field is low, and the mobility typically
reaches its peak value. This is in contrast to the experiments, which relied on much higher biases, and would therefore expect lower mobilities. It is important to note that the simulated recombination rate $R$ is approximately six orders larger than the experimentally observed result for the actual light intensity [2]. When normalized to the bandgap energy and scaled by emission efficiency, the peak simulated emission rate at the mid-channel bias point compares well to the experimental result: it is a factor of four smaller than reported in [2].

![Graph of photon emission rate vs. position](image)

Figure 3.4: Simulated photon emission rate under varying bias, constant current ($I_D = 0.2\mu A$) for device 1 (see table 3.1). Emission efficiency is assumed to be $10^{-4}$ [4] and the result is normalized to the bandgap energy $E_g = 0.4\text{eV}$. Central bias point (peak #1 at $z = 25\mu m$) $V_{DS} = 2V_{GS} = 2.3\text{V}$. Second and third highlighted curves (near $z = 5\mu m$) illustrate emission peaking (peak #5, $V_{DS} = 2.183V_{GS} = 2.286\text{V}$) and decay as device operation become more unipolar (peak #7, $V_{DS} = 2.703V_{GS} = 2.141\text{V}$).

### 3.4.2 Fixed Bright Spot at Contact

To consider the effects of the contacts on the luminescence profiles, we vary the SB height at the contacts to make the device more unipolar in operation (as in device 2, table 3.1), such that the CNFET operates as a p-type device, with $\phi_{Bp} = 0.05\text{eV}$. Our simulations show a localized luminescence with high intensity that develops at the drain contact, as shown in figure 3.5. Injection of holes at the drain forms a large positive charge that pulls the bands down sharply. This creates
an electric field that retards the exit of electrons from the device at the drain. The pile up of both types of carriers enhances recombination, resulting in a strong emission peak. A representative band diagram and charge profile are shown in figure 3.6. This contact-related phenomenon is very strong, and persists even when more gate control of the electrostatics is introduced by thinning the oxide (device 2, table 3.1). It is important to note that as the bias is varied, we continue to observe the motion of the mobile light spot in the manner outlined previously. The intensity of the mobile light spot remains similar to that previously reported, while the bright spot at the contact is approximately a factor of six larger in intensity.

Figure 3.5: Bright, fixed-location emission peak at the drain contact for a p-type device ($\phi_B = 0.05\text{eV}$ for holes). Constant current $I_D = 0.2\mu\text{A}$, $V_{DS} = 2V_{GS} = 0.665\text{V}$ at the bias point 1. Recombination profile shows the varying position of the mobile light spot ($z = 0 - 5\mu\text{m}$) as well as the persistent bright emission at the drain ($z = 10\mu\text{m}$).

Varying results on localized luminescence at a contact have been reported, including the absence of such a persistent bright-spot [2]. We did not observe persistent EL at a contact when representing the SB with a barrier height equal to half the bandgap [7]. Our observance of contact-localized EL with a lower $\phi_{Bp}$ suggests that the phenomenological modeling of the contact as a simple barrier may need improvement. Such SB models have proven adequate at capturing a broad range of electronic effects, and have proved valuable in device modelling when exploring the performance limits of proposed devices [9,21,22]. However, the strength of the contact-localized EL observed in
Figure 3.6: Energy bands (a) and carrier density (b) for bias point 1 (figure 3.5, \( V_{DS} = 2V_{GS} = 0.665 \text{V} \)). Energy bands (a) show strong band bending at drain, creating a barrier to electrons exiting the CN (see inset, (a)), causing pile-up. The low barrier to holes (\( \phi_{BP} = 0.05 \text{eV} \)) leads to significant hole injection and a large recombination rate. Corresponding carrier density profile (b) showing electrons (blue, left) and holes (green, right).

This model depends strongly on the SB height, and this may offer a means to better characterize the contact-CN interface.

In comparison with the experimental devices of Freitag et al., we note that both palladium and palladium with a titanium adhesion layer were used as contacts [2, 3]. Titanium contacts would form a small positive barrier to holes, similar to the \( \phi_B \) used in these simulations, while palladium on its own would induce a negative barrier to holes, enhancing the observed effect [23]. Previous experimental work suggested that the barrier heights to both electrons and holes were significantly reduced when titanium contacts were used due to barrier thinning from strong electric fields [24]. Further simulations at a range of barrier heights indicate that, under the bias conditions used, a fixed bright peak is present for \( \phi_B \lesssim 0.1 \text{eV} \). This of course is dependent upon the magnitude of the gate-induced electric field and the separation between the gate and source/drain contacts, which, in turn, influence the thickness of the tunnelling barrier.
3.4.3 Fixed Bright Spot at Defects

A fixed-point defect was simulated by introducing a charge of $+0.2e$ on the surface of the CN at distance of 6 $\mu$m from the source contact (device 3, table 3.1). The EL results are shown in figure 3.7a, from which it is clear that, in addition to the usual mobile EL, fixed EL appears at the defect site once certain bias conditions are met. In our simulations of defect-localized EL, the Zener effect is not considered as a possible means for electron excitation, neither is impact excitation of excitons from the strong field, as was proposed in [3]. Here, the p-type defect creates an electron trap (figure 3.7c), therefore we would expect that a hole-dominant bias would be required to induce defect-localized EL. As clearly shown in figure 3.7b, a majority population of holes is required at the defect to observe localized EL. This confirms the requirement of polarity from [3], however, in our model, the EL is solely a by-product of radiative free-carrier band-to-band recombination in a diffusive system.

On the surface of the CN, the charge defect causes band-bending, which acts as a trap for carriers. From the plot of the carrier distribution (figure 3.7b), we observe a strong peak in the electron density at the defect due to carrier trapping, as expected. With the mobile light spot beginning at the drain end ($z = 20\mu$m, figure 3.7a - bias point 1), electrons are the dominant carrier, and few holes are present in the CN. In this situation, there is no emission at the defect location. As hole injection increases, the mobile light spot moves towards the defect (see bias points 2 to 6, figure 3.7a), but with no presence of holes near the defect, no stationary, localized EL develops. As the bias is changed to further favour hole injection (green arrow, figure 3.7d), holes are blocked by the electric field barrier that results from defect-induced band-bending. This forms a region of further positive charge located next to the defect, which then pulls the bands down (black arrow, figure 3.7d). As the mobile light spot approaches the defect location, electrons trapped at the p-type defect and injected electrons recombine with the growing population of injected holes, leading to the formation of a defect-localized bright spot (see bias points 7 and 8, figure 3.7a). This localized EL persists as the mobile spot moves past the defect towards the source (see bias points 9-13, figure 3.7a) due to the strong hole injection and continued presence of electrons at the defect location.
Figure 3.7: The presence of a charge defect (positive charge trapped in oxide at CN surface, 6μm from the source) gives rise to a fixed peak in the recombination rate (a) as the bias varies. The carrier charge profile (b) clearly shows the presence of the defect and the conditions leading to localized EL while the holes are the dominant carriers. Bias points 1 (dot), 8 (solid), and 12 (dash) are shown for electrons (left, blue) and holes (right, green). The band diagram (c) for bias point 12 highlights the effect of the defect on the band-bending, which is shown schematically in (d).

3.5 Conclusion

From this simulation study of EL from CNFETs using a multi-scale modeling approach, it can be concluded that the experimental observations of mobile EL, the variation in intensity of the mobile
EL, fixed EL at one of the contacts, and localized EL at the site of the charge defects can all be described by attributing the EL to the direct recombination of free electrons and holes. The model combines a quantum mechanical approach to compute tunneling and thermion emission currents at the contacts with a semi-classical formulation to solve long devices operating under diffusive conditions. Evaluating the effect of SB height on contact-localized EL, we conclude that a strong dependence exists, and that the EL appears when the SB height is reduced to less than 0.1eV. In all simulations, the presence of a mobile peak in EL was observed. Through an understanding of EL behaviour in CNFETs, we are better positioned to investigate the CN-contact interface and the sensitivity of the device to charge defects through its optical properties, which may lead to novel methods for device evaluation and categorization.

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References


Chapter 4

Conclusions

The primary goal of device modeling research is the establishment of robust and predictive instruments that capture, explain, and extend the behaviour of those devices. In the preceding chapters, a multi-scale model, demonstrating the fixed and mobile electroluminescence (EL) in carbon nanotube field-effect transistors (CNFETs), was presented. This model was able to explain the intensity peaking of the mobile EL as the light spot approached the CN-contact interface solely through the application of a semi-classical framework for charge transport. Further, simulations showing fixed EL at the CN-contact interface and at a charge defect on the CN surface were achieved through the use of that same multi-scale model. Based on the theoretical structure developed in the Introduction and the modeling techniques developed in Chapter 2, this work provides a new and capable set of tools to evaluate the novel EL found in CNFETs.

In Chapter 2, limitations on the validity of the null-Neumann boundary used to close the simulation space were established through an asymptotic analysis of the electric fields near the CN-contact interface. This investigation was performed on a set of CNFETs chosen to represent both the state-of-the-art fabrication present at the time of the study and devices with optimal DC characteristics. The Schottky-barrier CNFETs were highly sensitive to the electric field near the CN-contact interface. Changes in the electrostatic potential are reflected in the shape of the Schottky-barrier, whose width modulates conductance between the source and drain. It was clearly demonstrated in the analysis of narrow-contact-radius CNFETs that the application of a null-Neumann boundary condition at the CN-contact interface would incur significant error in both the electrostatic and current calculations. The domains closed by null-Neumann boundaries were compared against an open domain, where a conformal transformation mapped the infinite space outside the CNFET to a finite space. The domain using the conformal transformation acted as a benchmark simulation, where no assumptions were required for the boundary conditions. However, that method resulted in a significant increase in the simulation space, and was not extensible to higher dimensions. Based on
the asymptotic analysis, it was possible to replace the null-Neumann boundary with an analytical expression for the electric field normal to the boundary. That method was determined to be impractical to implement, as it depended on the CNFET geometry. In the proposed solution, a portion of the contact was included in the simulation space: away from the CN-contact interface, the “infinite-rod” approximation, and as a result, the null-Neumann boundary condition, was more applicable. This was simple to implement, and did not significantly increase the size of the simulation space. In addition, the method of extending the simulation space may be transferable to non-symmetric CNFET geometries where no reduction of dimension is possible.

Having established limits for a valid simulation domain, a multi-scale model was implemented to investigate EL in CNFETs. In Chapter 3, it was shown that this model captures the mobility of the light-spot under ambipolar biases, similar to previously proposed models. Due to the presence of the Schottky-barrier at the CN-contact interface, CNFETs allow simultaneous injection of electrons and holes into the channel, which may radiatively recombine. The proposed multi-scale model combines a quantum mechanics treatment of the Schottky-barrier tunneling current with a diffusive model in the long-channel regime, where a finite, field-dependent mobility regulates charge transport. Without resorting to any further physical explanations, three other key aspects of EL in CNFETs are observed: the intensity-peaking of the mobile EL as the light-spot approaches a contact, fixed-location EL at a CN-contact interface when a near-ohmic barrier is present, and fixed-location EL at a charge defect. In the high-field regime near the CN-contact interface, the mobility is reduced to approximately 10 cm$^2$/V-s. When the CNFET is biased towards unipolar operation, and the mobile EL moves towards a contact, there is an increase in the rate of recombination. Both types of carriers accumulate near the contact, resulting in a peaking of the mobile EL intensity. This is in contrast to the presence of a persistent, bright peak in EL at a contact when the barrier height is reduced. In the case presented in Chapter 3, the barrier to holes was reduced, such that it was near-ohmic and representative of the experimental devices described in the literature. Under positive, ambipolar biases, a bright spot formed at the drain contact, and the mobile EL continued to be present in the device. While this result corresponds well with the experimental observations of the same phenomenon, it is not present in all reported EL studies, which suggests that the understanding of the CN-contact interface is still incomplete. Finally, when a charge defect was introduced on the CN surface, a fixed-location bright-spot appeared for near-unipolar bias conditions that favoured the carrier type whose charge was the same as that of the defect. This observation was
in excellent agreement with the experimental studies, although the proposed mechanism is markedly different. It was suggested that the band-bending at the defect might produce an electric field with sufficient strength to form an exciton through impact excitation; however, using fractional charges, the proposed multi-scale model indicated the presence of the defect-localized EL in the absence of strong fields. Thus, it appears that, despite the nanometre scale of the CNFET, the semi-classical models for charge transport are still relevant to the understanding of these new devices.

As established in the early models of CNFETs, the interface between the contact and the CN plays an important role in the device operation. While the original intention of this research was not to directly investigate the CN-contact interface, continuing study of the device has illustrated the need for further understanding in this area. With a lack of consistent and repeatable data from experimental devices, it is difficult to draw conclusions as regards the pertinent details of a particular phenomenon. Without a reliable fabrication technique, such as the one for silicon-based devices, CN diameter is poorly controlled, as is placement. Studies of the CN-contact interface are further hindered by the wide variety of parameters involved, and the general lack of consistency from one set of results to the next. However, as demonstrated in this research, many novel effects specific to the CNFET can still be qualitatively captured through carefully prepared models. There is significant opportunity in the future to exploit the CNFET EL as a tool for the study of the device. Due to the specific and bias-dependent behaviour of the EL at the site of a charge defect, further study of this phenomenon may lead to a better means of process characterization, which would help to improve fabrication techniques. Based on the similar contact-localized EL, new and independent methods to explore the contact influence may be possible. By refining the model proposed in this research, a comparison could be made between electronic and optical properties both theoretically and experimentally, further advancing research in this field.
Appendix A

Asymptotic Analysis of CN-Contact Interface and Surrounding Oxide

In this appendix, the asymptotic analysis of the electrostatic potential near the surface of the carbon nanotube (CN) at the CN-contact interface is detailed. The objective is to demonstrate that the electric field normal to the CN-contact interface and extending above the CN surface is not well described by a null constant, as would be the case with a null-Neumann boundary condition. First, it must be established that the Cartesian Laplacian is a good approximation to the cylindrical Poisson equation in the region of interest. Next, the derivation of an electric field near a sharp corner, as presented in [1, pp. 75-79], is extended to include a region of dielectric and a line of surface charge. The domain under consideration is shown in Chapter 1, figure 1.5.

A.1 Cartesian Laplacian

Poisson’s equation, in cylindrical coordinates and in the presence of axial symmetry, is

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial V}{\partial r} \right) + \frac{\partial^2 V}{\partial z^2} = \frac{1}{\epsilon} Q, \tag{A.1}
\]

where once again, \( V(r, z) \) is the electrostatic potential, \( \epsilon \) is the permittivity, and \( Q \) is the charge. Defining local variables near the CN-contact interface,

\[
x = \frac{z - z_0}{\delta} \quad \text{and} \quad y = \frac{r - r_{cn}}{\delta}, \tag{A.2}
\]

where \( z_0 \) is the location of the CN-contact interface, \( r_{cn} \) is the CN radius, and \( \delta \ll r_{cn} \) is the scaling parameter that defines the asymptotic region. Substituting for \( r \) and \( z \) in (A.1),

\[
\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\delta}{\delta y + r_{cn} \partial y} = \delta^2 \frac{Q}{\epsilon}, \tag{A.4}
\]
where $\phi(x, y)$ is the potential in the asymptotic region, equivalent to $V(z, r)$ with scaled variables $x$ and $y$. As $r/r_{cn} \to 1$, $\delta y \ll r_{cn}$, such that 

$$
\frac{\delta}{\delta y + r_{cn}} \to \frac{\delta}{r_{cn}},
$$

which is $O(\delta)$. Eliminating all terms that are $O(\delta)$ and smaller, (A.4) simplifies to the 2D Cartesian Laplacian,

$$
\Delta \phi(x, y) = 0.
$$

### A.2 Solving the Potential

Having established that the Cartesian Laplacian describes the electrostatic potential near the CN-contact interface at $r = r_{cn}$ in the limit of small $\delta$, (A.6) is transformed into polar coordinates, and separation of variables is used to seek a general solution. In polar coordinates, (A.6) is

$$
\frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial \phi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \phi}{\partial \theta^2} = 0.
$$

(A.7)

Assuming that $\phi(\rho, \theta)$ is separable,

$$
\phi(\rho, \theta) = R(\rho)\Psi(\theta),
$$

yielding a radial equation

$$
\rho \frac{d}{d\rho} \left( \rho \frac{dR}{d\rho} \right) = K^2 R,
$$

(A.9)

with the solution

$$
R(\rho) = \begin{cases} 
  a\rho^K + b\rho^{-K} & K \neq 0 \\
  a_0 + b_0 \ln \rho & K = 0 
\end{cases},
$$

(A.10)

and an angular equation

$$
\frac{d^2 \Psi}{d\theta^2} = -K^2 \Psi,
$$

(A.11)

with the solution

$$
\Psi(\theta) = \begin{cases} 
  A \cos(K\theta) + B \sin(K\theta) & K \neq 0 \\
  A_0 + B_0 \theta & K = 0 
\end{cases}.
$$

(A.12)
Next, coefficients in (A.10) and (A.12) are simplified through consideration of the boundary conditions. From figure 1.5 (Chapter 1), the solution must be sought in each of the three subdomains I, II, and III, such that the dielectric boundary condition,
\[ \hat{n}_i \cdot (\epsilon_i E^- - \epsilon_j E^+) = Q_s, \]  
(A.13)
is satisfied at the boundary of each subdomain, where \( i \) and \( j \) correspond to two neighbouring subdomains and \( Q_s \) is the surface charge on the boundary. Since \( \Psi(\theta) \) will describe the component of the potential normal to each of the subdomain boundaries in the model domain, (A.13) simplifies to
\[ -\epsilon_i \frac{d\Psi}{d\theta} \bigg|_{\theta=\theta_i^-} + \epsilon_j \frac{d\Psi}{d\theta} \bigg|_{\theta=\theta_j^+} = \frac{Q_i}{\epsilon_0}, \]  
(A.14)
where \( \epsilon \) is the relative permittivity, \( \epsilon_0 \) is the permittivity of free-space, and \( Q_i \) is the charge on the boundary.

In all domains, coefficients \( b \) and \( b_0 \) may be set to zero since the electrostatic potential must remain finite. From (A.10), it can be seen that as \( \rho \to 0 \), \( \ln \rho \to \infty \). Restricting the solution to the set of \( K > 0 \), \( \rho^{-K} \to \infty \) as \( \rho \to 0 \) as well, justifying the choice of \( b = 0 \). Further, the electrostatic potential on the contact is a constant \( V_0 \), which can be assumed to be zero without a loss of generality.

### A.2.1 Subdomain I

Here, the solution is subject to two boundary conditions. First, for \( K \neq 0 \),
\[ \Psi(0) = 0 \to A_1 = 0, \text{ and } \Psi_1(\theta) = B_1 \sin(K\theta). \]  
(A.15)
Next, at the dielectric boundary (where no charge is present)
\[ -\frac{d\Psi}{d\theta} \bigg|_{\theta=\pi/2^-} + \epsilon_r \frac{d\Psi}{d\theta} \bigg|_{\theta=\pi/2^+} = 0, \]  
(A.16)
yielding a relation to subdomain II,
\[ K_1 B_1 \cos \left( K_1 \frac{\pi}{2} \right) = \epsilon_r K_2 \left[ B_2 \cos \left( K_2 \frac{\pi}{2} \right) - A_2 \sin \left( K_2 \frac{\pi}{2} \right) \right]. \]  
(A.17)
As well, \( \Psi_1(\pi/2) = \Psi_2(\pi/2) \), giving
\[ B_1 \sin \left( K_1 \frac{\pi}{2} \right) = A_2 \cos \left( K_2 \frac{\pi}{2} \right) + B_2 \sin \left( K_2 \frac{\pi}{2} \right). \]  
(A.18)
A.2.2 Subdomain II

At $\theta = \pi/2$, the boundary condition is the same as (A.16), which has already been accounted for. At $\theta = \pi$, the boundary condition

$$-\epsilon_r \frac{d\Psi}{d\theta} \bigg|_{\theta=\pi^-} + \frac{d\Psi}{d\theta} \bigg|_{\theta=\pi^+} = \frac{Q}{\epsilon_0} \tag{A.19}$$

yields the relation to the angular equation in subdomain III,

$$-\epsilon r K_2 [B_2 \cos(K_2\pi) - A_2 \sin (K_2\pi)] = \frac{Q}{\epsilon_0} - K_3 [B_3 \cos(K_3\pi) - A_3 \sin (K_3\pi)] \tag{A.20}$$

Further, as in the first subdomain, $\Psi_2(\pi) = \Psi_3(\pi)$, giving

$$A_2 \cos(K_2\pi) + B_2 \sin(K_2\pi) = A_3 \cos(K_3\pi) + B_3 \cos(K_3\pi). \tag{A.21}$$

A.2.3 Subdomain III

Finally, at the CN-contact interface in subdomain III,

$$A_3 \cos \left( K_3 \frac{3\pi}{2} \right) + B_3 \sin \left( K_3 \frac{3\pi}{2} \right) = 0, \tag{A.22}$$

yielding the final boundary condition for the angular equation.

Considering the radial equation under the assumption that $\phi(\rho, \theta)$ is separable, it is clear that $R_i(\rho) = R_j(\rho)$ along each of the subdomain boundaries. From this, it can be concluded that the constant $K_i$ is the same in each subdomain, such that $K_1 = K_2 = K_3 = K$. Collecting (A.17), (A.18), (A.20), (A.21), and (A.22), a system of equations is obtained, which can be simplified. Combining (A.17) and (A.18) gives

$$B_2 = \frac{B_1}{\epsilon_r} \left[ \frac{1 + \epsilon_r \tan^2 \left( \frac{K\pi}{2} \right)}{1 + \tan^2 \left( \frac{K\pi}{2} \right)} \right] \tag{A.23}$$

Next, combining (A.20), (A.21), and (A.22), the following relation is obtained

$$\epsilon_r (B_3 - B_2) \tan(K\pi) + (B_3 - \epsilon_r B_2) \cot(K\pi) + B_3(1 - \epsilon_r) \tan \left( \frac{3K\pi}{2} \right) = \frac{Q}{K\epsilon_0} \csc(K\pi). \tag{A.24}$$

At this point, it is convenient to note that if $\epsilon_r \to 1$ and $Q \to 0$, then the electrostatic potential at a metal corner in free space is obtained [1, pp. 75-79]. In (A.23), taking $\epsilon_r \to 1$ yields $B_2 = B_1$, 56
which in turn implies that $A_2 = 0$. In (A.24), taking $\epsilon_r \to 1$ and $Q \to 0$,

$$(B_3 - B_2) [\tan(K\pi) + \cot(K\pi)] = \frac{B_3 - B_2}{\sin(K\pi) \cos(K\pi)} = 0,$$

(A.25)

which implies $B_2 = B_3$, and $A_3 = 0$. Therefore, from (A.22),

$$A_3 = -B_3 \tan\left(\frac{3K\pi}{2}\right) = 0,$$

(A.26)

which then implies

$$K = \frac{2m}{3} \quad m = 1, 2, \ldots.$$

(A.27)

Note that in equations (A.17)-(A.22), there are nine unknowns ($A_1$-$A_3$, $B_1$-$B_3$, and $K_1$-$K_3$), but only eight constraints (two Dirichlet boundaries at the contacts, and six matching conditions). A boundary condition is required at the outside of the asymptotic region (i.e., at the boundary with normal space) to completely specify the solution. Because such a boundary condition would depend on the geometry of the CNFET, it is impractical to specify one. Each system would have to be solved in full, negating any gains that could be achieved by closing the simulation space with an analytically derived boundary condition.

Therefore, the derivation proceeds with the goal of obtaining general information regarding the electric field near the CN-contact interface. In the limit of a low-permittivity dielectric $\epsilon_r$ and small CN surface charge $Q$, it is assumed that the potential will be similar in form to the series solution for a metal corner,

$$\phi(\rho, \theta) = V_0 + \sum_{m=1}^{\infty} a_m \rho^{2m/3} \sin \left(\frac{2m}{2} \theta \right),$$

(A.28)

where coefficient $a_m$ is related to the far-field boundary condition, and the value of $K$ from (A.27) is used. In this case, it is the $m = 1$ term that dominates as $\rho \to 0$. Therefore, a general solution to $\phi(\rho, \theta)$, where $0 < K < 1$, is considered. At the Neumann boundary imposed at the location of the CN-contact interface, a comparison is made to the gradient of the potential normal to that boundary, equivalently,

$$\left. \frac{\partial \phi}{\partial x} \right|_{x=0} = \frac{\partial}{\partial x} \left\{ A \cos \left( K \tan^{-1} \frac{y}{x} \right) + B \sin \left( K \tan^{-1} \frac{y}{x} \right) \right\} \left( y^2 + x^2 \right)^{K/2},$$

(A.29)
where substitutions for $\rho = \sqrt{x^2 + y^2}$ and $\theta = \tan^{-1} y/x$ have been made. Evaluation of (A.29) yields

\[
\frac{\partial \phi}{\partial x} \bigg|_{x=0} = yK \left[ A \sin \left( K \tan^{-1} \frac{y}{x} \right) - B \cos \left( K \tan^{-1} \frac{y}{x} \right) \right] (x^2 + y^2)^{K/2-1} \\
+ 2x \left[ A \cos \left( K \tan^{-1} \frac{y}{x} \right) + B \sin \left( K \tan^{-1} \frac{y}{x} \right) \right] (y^2 + x^2)^{K/2-1} \\
= K \left[ A \sin \left( \frac{K\pi}{2} \right) - B \cos \left( \frac{K\pi}{2} \right) \right] y^{K-1},
\]

which is valid for the region where $r/r_{cn} \sim 1$. Knowing that $A$, $B$, and $K$ are constants, it can be conclude that

\[
\mathbf{n}_{ins} \cdot \nabla V \propto (r - r_{cn})^{K-1},
\]

at the location $z = z_0$ and under the constraints $r/r_{cn} \sim 1$ and $0 < K < 1$, which is clearly not zero. Therefore, the null-Neumann boundary condition is invalid when placed at the CN-contact interface.

Approached from a different aspect, (A.30) can yield valuable insight regarding the placement of a null-Neumann boundary. Rather than evaluating the derivative at $x = 0$ in the asymptotic space, $x$ can be allowed to vary in the positive direction away from the CN-contact interface, while $y$ remains small. In this limit, $\tan^{-1} y/x \to 0$, and

\[
\frac{\partial \phi}{\partial x} \bigg|_{y=0} \approx -2Ax^{K-1}.
\]

As $x$ is increased along the length of the contact, the electric field becomes more normal to a boundary extending radially from the contact surface, and as a result, the null-Neumann boundary condition becomes a better approximation.
References

Appendix B

Formulation of the Drift-Diffusion and Continuity Equations

In this appendix, details are presented for the multi-scale model used in the simulation of electroluminescence (EL) in carbon nanotube field-effect transistors (CNFETs), as described in Chapter 3. The multi-scale model combines a quantum mechanics solution for transmission through a tunneling Schottky-barrier (SB) with the semi-classical drift-diffusion equation (DDE) and continuity equation (CE) for charge transport in CNFETs with long channel lengths ($\geq 10 \mu$m). The electrostatic potential is determined from Poisson’s equation, which is solved self-consistently in conjunction with the charge equations.

This formulation begins with the development of a system of equations for charge and electrostatic potential suitable for the finite-difference (FD) numerical approximation, including variable substitution and scaling. This derivation is adapted from [1]. Next, boundary conditions on the charge equations are established from the SWE solution to the tunneling probability through the SBs. Finally, the procedure for obtaining a self-consistent solution is presented.

The model CNFET is coaxial in nature, and comprised of a CN surrounded by a metallic gate contact, which is separated from the CN by a layer of dielectric material. The ends of the CN are joined to metallic source and drain contacts, forming a three-terminal device with axial symmetry. An illustration of this geometry is shown in figure 1.3 (Chapter 1). The dielectric has a relative permittivity $\epsilon_r$, which corresponds to the choice of material used in the device. Each contact metal has a work function $\phi$, determined by the material used, which influences the alignment of the Fermi-levels between CN and contact, as described in the preceding chapters. In this system, charge appears on the surface of the CN, both from injected carriers and from localized defects. It is assumed that no other charge is present, although the model presented here does not explicitly require that assumption.
In the CNFET domain, shown in figure 1.4 (Chapter 1), the relation between charge and the electrostatic potential is determined from Poisson’s equation, given here in general form for cylindrical coordinates,

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial V}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 V}{\partial \theta^2} + \frac{\partial^2 V}{\partial z^2} = -\frac{Q}{\epsilon}, \tag{B.1} \]

where \( V(r, z, \theta) \) is the electrostatic potential, \( \epsilon \) is the permittivity, and \( Q \) is the charge per unit volume. Due to the axial symmetry of the model CNFET, a reduction in dimension can be performed, and the domain of interest can be simplified to two dimensions, as in figure 1.4. Assuming an equal charge distribution in the azimuthal angle \( \theta \), there will be no variation in \( V \) with respect to \( \theta \), and (B.1) reduces to,

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial V}{\partial r} \right) + \frac{\partial^2 V}{\partial z^2} = -\frac{Q}{\epsilon} \delta(\theta_0), \tag{B.2} \]

where \( V(r, z) \) is the new 2D electrostatic potential, \( Q \) is a charge per unit area, and the necessary units of length are carried by the \( \delta \)-function.

In this reduced-dimension domain, the CNFET surface appears as a 1D conductor. Charge in the CN is found through the solution to the DDE for both electrons and holes, where the current density \( J \) is defined as

\[ J_n = q\mu_n n E + qD_n \nabla n \]
\[ J_p = q\mu_p p E - qD_p \nabla p, \tag{B.3} \tag{B.4} \]

where \( n \) and \( p \) are the electron and hole concentrations, respectively; \( \mu_n \) and \( \mu_p \) are the electron and hole mobilities, respectively; \( E \) is the electric field; and \( D_n \) and \( D_p \) are the electron and hole diffusivities, which are related to mobility through the Einstein relation

\[ \frac{D}{\mu} = \frac{k_B T}{q}, \tag{B.5} \]

in which \( k_B \) is the Boltzmann constant and \( T \) is temperature. Finally, charge recombination is described by the continuity equations,

\[ \frac{1}{q} \nabla \cdot J_n = R \]
\[ -\frac{1}{q} \nabla \cdot J_p = R, \tag{B.6} \tag{B.7} \]
where \( R \) is the net rate of recombination and steady-state is assumed. Both the DDEs and CEs appear in this system in 1D form, where carrier concentration, mobility, electric field, and current density vary longitudinally along the CN surface. Recombination is assumed to be direct band-to-band and radiative, and is described by

\[
R^{bb} = B(np - n_i^2),
\]

(B.8)

where \( B \) is the direct radiative recombination velocity in 1D. The net rate of recombination \( R \) also includes a generation term related to the tunneling current, such that \( R = R^{bb} - G_{TUN} \).

### B.1 System of Equations

Before attempting to solve the system of equations presented in the previous section, variables are scaled to remove units. The scaling used here is adapted from that proposed by De Mari [2], and summarized in table B.1. Due to the exponential nature of the carrier densities \( n \) and \( p \), numerical approximations to the DDE and CE are often unstable. To combat this, a change of variables is made, replacing \( n \) and \( p \) with \( u \) and \( v \), respectively, according to

\[
u = \tilde{n}e^{-\tilde{\psi}} \]

(B.9)

\[
v = \tilde{p}e^{\tilde{\psi}},
\]

(B.10)

where \( \psi \) refers to the electrostatic potential on the CN surface, \( i.e. \psi(z) = V_{CS}(z) = V(r_{cn}, z) \), and the variables \( \tilde{n}, \tilde{p} \), and \( \tilde{\psi} \) have been scaled to remove their units. Throughout the remainder of this

<table>
<thead>
<tr>
<th>Variable</th>
<th>Units</th>
<th>Scaling</th>
</tr>
</thead>
<tbody>
<tr>
<td>( z, r )</td>
<td>m</td>
<td>( l_d = 2\pi r_{cn} \epsilon k_B T/(q^2 n_i) )</td>
</tr>
<tr>
<td>( V )</td>
<td>V</td>
<td>( V_{th} = k_B T/q )</td>
</tr>
<tr>
<td>( n, p )</td>
<td>m(^{-1})</td>
<td>( n_i )</td>
</tr>
<tr>
<td>( D_n, D_p )</td>
<td>m(^2)s(^{-1})</td>
<td>( D_0 = 1) m(^2)s(^{-1})</td>
</tr>
<tr>
<td>( B )</td>
<td>m/s</td>
<td>( B_0 = D_0/l_d^2 n_i )</td>
</tr>
<tr>
<td>( J )</td>
<td>C/s</td>
<td>( J_0 = qD_0 n_i / l_d )</td>
</tr>
</tbody>
</table>

Table B.1: De Mari scaling factors for the DDE and CE. For example, \( \tilde{n} = n/n_i \), where \( \tilde{n} \) is the scaled (unitless) variable.
appendix, the cumbersome “∼” notation referring to the scaled (unitless) variables will be omitted, and the reader may assume that, unless otherwise noted, scaled variables are in use.

It is now the objective to obtain a simplified set of equations in the variables \{u, v, \psi\}. Beginning with (B.3) in its 1D form, which is also scaled to remove units,

\[
J_n = D_n \left( \frac{dn}{dz} - n \frac{d\psi}{dz} \right),
\]

and noting that, from (B.9),

\[
\frac{du}{dz} = \frac{dn}{dz} e^{-\psi} + n \frac{d}{dz} (e^{-\psi}) = \left( \frac{dn}{dz} - n \frac{d\psi}{dz} \right) e^{-\psi}
\]

the following expression for electron current density is obtained,

\[
J_n = D_n \frac{du}{dz} e^{\psi}.
\]

Cast in terms of \(u\) and \(v\), (B.6), in its 1D, scaled form is

\[
\frac{dJ_n}{dz} = B(uv - 1) - G_{TN,n},
\]

and combining (B.13) and (B.14) yields

\[
-\frac{d}{dz} \left( D_n \frac{du}{dz} e^{\psi} \right) + Buv = B - G_{TN,n}.
\]

Similarly, an equation in terms of \(v\) can be derived from the hole current density and CE, giving

\[
-\frac{d}{dz} \left( D_p \frac{dv}{dz} e^{-\psi} \right) + Buv = B - G_{TN,p}.
\]

To solve Poisson’s equation (B.2), first note that the charge \(Q\) will be determined by the carrier concentrations \(n\) and \(p\) and any defect charges present on the CN surface, such that

\[
Q = \left[q(p - n) + Q_d\right] \delta(r_{cn}),
\]

where the \(\delta\)-function limits the charge to the CN surface. The potential \(V\) is linearized around an approximate solution \(\hat{V}\), such that \(V = \hat{V} + \gamma\),

\[
\left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} \right) (V + \gamma) = ve^{-\hat{\psi} - \gamma} - ue^{\hat{\psi} + \gamma} + \frac{Q_d}{qn_i}
\]

\[
\rightarrow \mathcal{L}V + \mathcal{L}\gamma = ve^{-\hat{\psi}}(1 - \gamma + \cdots) - ue^{\hat{\psi}}(1 + \gamma + \cdots) + \frac{Q_d}{qn_i}
\]

\[
\rightarrow \mathcal{L}\gamma + \left(ve^{-\hat{\psi}} + ue^{\hat{\psi}}\right) \gamma = -\mathcal{L}V + ve^{-\hat{\psi}} - ue^{\hat{\psi}} + \frac{Q_d}{qn_i},
\]

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where the expansion of the exponential is used under the assumption of a sufficiently small \( \gamma \). Note that both the 2D electrostatic potential \( V \) and the 1D electrostatic potential on the CN surface \( \psi \) are shown in (B.17) to clearly differentiate between the two, and emphasize that the charge is present only on the CN surface. In addition, it is important to recognize that in (B.15), \( v \) and \( \psi \) are estimates that are held fixed when solving for \( u \), and similarly in (B.16), where \( u \) and \( \psi \) are estimates when solving for \( v \). In (B.17), \( u \), \( v \), and \( V \) are each estimates obtained prior to evaluation of the equation for \( \gamma \). From (B.15)-(B.17), the system of three equations has been established in the set of variables \( \{ u, v, \psi \} \) that completely define the solution, subject to the necessary boundary conditions, in the domain of interest.

### B.2 Discretizing the System of Equations

A FD approximation is used to obtain a numerical solution to the system of equations described above. In the domain of interest, the space is discretized as a variably-spaced mesh. First, mesh spacing variables \( h \) and \( k \) are defined as,

\[
\begin{align*}
  h_i &= z_{i+1} - z_i & i &= 1, \ldots, N_z - 1 \\
  k_j &= r_{j+1} - r_j & j &= 1, \ldots, N_r - 1 
\end{align*}
\]

where \( N_z \) and \( N_r \) are the total number of mesh points in the longitudinal and radial directions, respectively, and indices \( i \) and \( j \) refer to the position of the mesh point.

Having established a system of equations and a discrete mesh, the next step is to approximate that system of equations by finite differences. The following is adopted from [3] and is presented here for the convenience of the reader. First, observe that both (B.15) and (B.16) are of the same form, namely,

\[
-(\alpha y')' + \beta y = f ,
\]

where \( \alpha \) and \( \beta \) are constants and \( f \) is independent of \( y \). Here, it has been assumed that \( D_n \) and \( \psi \) vary slowly with position, such that they are encapsulated in the constant \( \alpha \). The expression \( \alpha y' \)
can be approximated on two neighbouring intervals as

\[ \alpha y' \simeq \left( \frac{\alpha_i + \alpha_i-1}{2} \right) \left( \frac{y_i - y_{i-1}}{h_{i-1}} \right) \quad \text{on } [z_{i-1}, z_i] \]  
\[ \text{(B.21)} \]

\[ \alpha y' \simeq \left( \frac{\alpha_i+1 + \alpha_i}{2} \right) \left( \frac{y_{i+1} - y_i}{h_i} \right) \quad \text{on } [z_i, z_{i+1}] . \]  
\[ \text{(B.22)} \]

Defining

\[ \chi_i = \frac{\alpha_i+1 + \alpha_i}{h_i}, \]

and combining (B.21) and (B.22),

\[ (\alpha y')' \simeq \frac{\chi_i (y_{i+1} - y_i) - \chi_{i-1} (y_i - y_{i-1})}{h_i + h_{i-1}} = \frac{\chi_i y_{i+1} - (\chi_i + \chi_{i-1}) y_i + \chi_{i-1} y_{i-1}}{h_i + h_{i-1}} . \]  
\[ \text{(B.23)} \]

Therefore, (B.20) can be expressed as

\[ - \left( \frac{\chi_i}{h_i + h_{i-1}} \right) y_{i+1} + \left( \frac{\chi_i + \chi_{i-1}}{h_i + h_{i-1}} + \beta \right) y_i - \left( \frac{\chi_i y_{i+1} - (\chi_i + \chi_{i-1}) y_i + \chi_{i-1} y_{i-1}}{h_i + h_{i-1}} \right) y_{i-1} = f_i , \]  
\[ \text{(B.24)} \]

which is convenient for numerical evaluation.

Next, the standard FD procedures [1] are employed to discretize the 2D Poisson equation given in (B.17). To simplify the notation, \( V_{i,j} \) will be used to represent \( V(r_j, z_i) \).

\[ \frac{1}{r_j} \left( \frac{V_{i,j+1} - V_{i,j-1}}{k_j + k_{j-1}} \right) + \frac{2}{k_j + k_{j-1}} \left( \frac{V_{i,j+1} - V_{i,j}}{k_j} - \frac{V_{i,j} - V_{i,j-1}}{k_{j-1}} \right) \]
\[ + \frac{2}{h_i + h_{i-1}} \left( \frac{V_{i+1,j} - V_{i,j}}{h_i} - \frac{V_{i,j} - V_{i-1,j}}{h_{i-1}} \right) = \frac{Q_{i,j}}{\epsilon} \]  
\[ \text{(B.25)} \]

A template can be defined, as shown in figure B.1, to enumerate the coefficients as they apply to each of the locations surrounding mesh point \((i, j)\). The coefficients associated with each location on the template are given in table B.2. The preceding finite difference approximation to the system of equations (B.15)-(B.17) is a general formulation that does not yet take into account the influence of both internal and external boundary conditions. However, these equations are appropriate to a numerical treatment of the system, as they are readily adapted to a matrix operator form.

### B.3 Boundary Conditions

In order to completely specify a solution to the system, boundary conditions must be established. These conditions bound the simulation domain and relate the tunneling current through the SB to the carrier density on the CN surface.
![Finite difference mesh template](image)

Figure B.1: Finite difference mesh template, showing neighbouring sites and mesh spacing.

Table B.2: Poisson operator matrix coefficients by location on the template

<table>
<thead>
<tr>
<th>Location</th>
<th>Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i, j + 1$</td>
<td>$\frac{1}{k_j + k_{j-1}} \left( \frac{1}{r_j} + \frac{2}{k_j} \right)$</td>
</tr>
<tr>
<td>$i, j - 1$</td>
<td>$\frac{1}{k_j + k_{j-1}} \left( -\frac{1}{r_j} + \frac{2}{k_{j-1}} \right)$</td>
</tr>
<tr>
<td>$i - 1, j$</td>
<td>$\frac{1}{h_i + h_{i-1}} \frac{2}{h_{i-1}}$</td>
</tr>
<tr>
<td>$i + 1, j$</td>
<td>$\frac{1}{h_i + h_{i-1}} \frac{2}{h_i}$</td>
</tr>
<tr>
<td>$i, j$</td>
<td>$-2 \left( \frac{1}{h_i h_{i-1}} + \frac{1}{k_j k_{j-1}} \right)$</td>
</tr>
</tbody>
</table>
Three classes of boundary condition exist

1. Dirichlet boundary conditions: the electrostatic potentials at the source, drain and gate contacts are fixed constants, as is the carrier density at the collecting contact.

2. Neumann boundary conditions: null-Neumann conditions are applied to the electrostatic potential at open boundaries and at the central axis of the CN, and a Neumann current boundary condition is applied to the charge equations.

3. Internal dielectric boundary conditions: electric flux density is conserved with surface charge at the CN surface, which is in contact with the dielectric.

The Dirichlet boundary conditions are straightforward to apply, and simply force the electrostatic potential or carrier density to a fixed constant value as described in introductory chapter.

Along the CN surface exists a dielectric boundary with an associated surface charge. The defining equation at this interface is

$$\frac{\epsilon_{\text{ins}}}{\epsilon_0} \left( V_{i,j} + 1 - V_{i,j} \right) - \frac{\epsilon_{\text{cn}}}{\epsilon_0} \left( V_{i,j} - V_{i,j-1} \right) = -\frac{q}{\epsilon_0} (p_{i,j} - n_{i,j}) \quad \text{(B.26)}$$

where $\epsilon_{\text{ins}}$ and $\epsilon_{\text{cn}}$ are the relative permittivities of the dielectric and CN, respectively, and $Q_s = q(p - n) + Q_d$ is the surface charge. This equation can be readily discretized along the set of mesh points located at the CN surface, yielding

$$\epsilon_{\text{ins}} \left( \frac{V_{i,j+1} - V_{i,j}}{k_j} \right) - \epsilon_{\text{cn}} \left( \frac{V_{i,j} - V_{i,j-1}}{k_{j-1}} \right) = -\frac{q}{\epsilon_0} (p_{i,j} - n_{i,j}) \quad \text{(B.27)}$$

This equation replaces the Poisson equation for points on the CN surface.

Finally, the Neumann condition boundaries are considered. At $r = 0$, the term $r^{-1} \frac{\partial V}{\partial r}$ appears singular. Using L'Hôpital’s rule, this singularity can be removed [4],

$$\lim_{r \to 0} r^{-1} \frac{\partial V}{\partial r} = \lim_{r \to 0} \frac{\partial}{\partial r} \left( \frac{\partial V}{\partial r} \right) \left[ \frac{\partial}{\partial r} (r) \right]^{-1} = \lim_{r \to 0} \frac{\partial^2 V}{\partial r^2} (1) = \frac{\partial^2 V}{\partial r^2} \quad \text{(B.28)}$$

which reduces the Poisson equation at $r = 0$ to

$$2 \frac{\partial^2 V}{\partial r^2} + \frac{\partial^2 V}{\partial z^2} = -\frac{Q}{\epsilon} \quad \text{(B.29)}$$

This equation can also be readily discretized, similar to (B.25), and becomes the defining relation along the mesh at $r = 0$. 
For all open boundaries, including the axis at \( r = 0 \), a null-Neumann condition is specified, such that
\[ \mathbf{n} \cdot \nabla V = 0, \]
where \( \mathbf{n} \) is the outward normal. Under the finite difference approximation, the virtual point outside the simulation space is simply taken to be identical to the mirroring point inside, such that their coefficients are summed.

While the boundary conditions discussed above have pertained largely to the electrostatic potential, perhaps the most critical condition is that defining the current at the injecting contact for each of the carriers. At the CN-contact interface, the thermionic emission current is imposed as a Neumann boundary condition for the charge equations (B.15) and (B.16). For (B.15), (B.13) is discretized, and the 1D current density is set equal to the source thermionic emission current \( I_{TE,S} \),
\[ J_{n,1} = I_{TE,S} = D_n \frac{u_2 - u_1}{h_1} e^{\psi_{3/2}} \]
\[ \rightarrow -u_1 + u_2 = h_1 D_n^{-1} e^{-\psi_{3/2}} I_{TE,S}, \]
where \( \psi_{3/2} = \frac{1}{2}(\psi_1 + \psi_2) \), such that an equation is obtained for \( u \) at the first two mesh points. A similar approach can be employed to set a Neumann boundary condition for (B.16) at the drain contact in terms of hole thermionic emission current.

Coupled with the Dirichlet boundary at the collecting contact, the Neumann boundary condition from the thermionic emission current completely specifies a solution to (B.15) and (B.16). However, this approach fails to incorporate the tunneling current through the SB. To include the tunneling current, the approach of [5] is used, and a summary of the method is presented here for the convenience of the reader. First, the tunneling current is introduced into the CE (the example shown here will describe electrons, but can be easily adapted to the hole case),
\[ \frac{1}{q} \frac{dJ_{TUN}}{dz} = -G_{TUN}(z). \]
No recombination is present in the tunneling process, as it is assumed to be coherent without scattering. The generation rate \( G_{TUN}(z) \) is associated with carriers that have tunneled through the barrier to appear at location \( z \) and energy \( E_c(z) \). The generation rate can be related to the energy distribution of carriers in the contact by re-arranging (B.32),
\[ G_{TUN}(z) = -\frac{1}{q} \frac{dJ_{TUN}}{dz} = \frac{dJ_{TUN}}{dE} \frac{dE}{dz}. \]
where $E = -q\psi$ relates the energy to the electrostatic potential $\psi$ along the CN surface. If the 1D tunneling current density is treated as a Landauer current (for a doubly-degenerate band in the case of a CN), then an expression for $\frac{dJ_{TUN}}{dE}$ may be readily obtained,

$$
\frac{dJ_{TUN}}{dE} = -\frac{d}{dE} \left[ \frac{4q}{h} \int_{E_c(z_{qs})}^{E_c(0)} T(\varepsilon) \left[ f_{\mu S}(\varepsilon) - f_{\phi n}(\varepsilon) \right] d\varepsilon \right] = -\frac{4q}{h} T(E) \left[ f_{\mu S}(E) - f_{\phi n}(E) \right] \bigg|_{E_c(z_{qs})}.
$$

where $z_{qs}$ is the length of the tunneling region as measured from the source contact, $\mu_S$ is the source Fermi level, $\phi_n$ is the electron quasi-Fermi level at $z_{qs}$, and $T(E)$ is the transmission probability. Therefore, the generation rate due to tunneling is

$$
G_{TUN}(z) = -\frac{4q}{h} T(E_c(z)) \left[ f_{\mu S}(E_c(z)) - f_{\phi n}(E_c(z)) \right] \frac{d\psi}{dz}.
$$

Here, the relation $E_c(z)$ is used to relate the energy of the carriers in the contact to the position at which they appear in the CN after tunneling through the SB. This is illustrated in [5].

### B.4 Algorithm

Having established a system of equations (B.15)-(B.17), and discretized them as appropriate to a FD approximation, an algorithm is now presented to solve for $\{u, v, \psi\}$ self-consistently. The simulation flow is illustrated in figure B.2. Because the system is non-linear, a damped iterative scheme is used. The system is initialized by solving (B.17) in the absence of charge, i.e. the Laplacian. This estimate of the electrostatic potential is then used to obtain a transmission probability from a SWE solution to the SB near the contact, establishing the thermionic emission and tunneling current boundary conditions. As well, the estimate is used by (B.15) and (B.16). Because (B.15) and (B.16) are coupled, each requires an estimate of the charge from the other. These estimates for $u$ and $v$ are obtained from a previous iteration, and when no previous iteration exists, intrinsic charge is assumed.

Due to the exponential nature of the DDE, convergence can be difficult to obtain, as oscillations tend to manifest themselves in the charge, destabilizing the system. To combat this, memory is introduced in the charge estimate, as shown in figure B.2. The charge estimate used in the current step of the iteration $k + 1$ is determined from a weighted sum of the charges in the previous two
iterations, such that

\[ n_{k+1} = wn_k + (1-w)n_{k-1} \quad (B.36) \]

\[ p_{k+1} = wp_k + (1-w)p_{k-1} \quad, \quad (B.37) \]

where \( w \) is a weighting factor, \( 0 < w < 1 \), and typically \( w = 0.5 \).

Having obtained new estimates for the charges, (B.17) is solved for \( \gamma \). If \( ||\gamma||_\infty \) reaches a specified tolerance, then the simulation has converged, otherwise, the updated electrostatic potential becomes the new estimate, and the loop repeats. In order to converge, tolerance on current density and charge must also be reached. Oscillations in the charge distributions tend to vanish once the difference in
charge between iterations approaches $n_i$, however the coupling of electrons and holes through the CE means that this is an insufficient criteria. The location where the electron and hole densities intersect stabilizes very slowly, requiring a much tighter tolerance on charge; a value of 0.05$n_i$ is typically used.

In summary, the system of equations describing the electrostatic potential and charge distribution in the CNFET has been established through a reduction in dimension, scaling to remove units, and variable substitution. These equations were then discretized as appropriate to a finite difference numerical approximation. Boundary conditions were established for the electrostatic potential, the carrier densities, and the electric flux at a dielectric interface. Finally, combining these components, a self-consistent algorithm was presented for the numerical solution of the system of equations.
References


