INELASTIC TRANSPORT IN CARBON NANOTUBE ELECTRONIC AND OPTOELECTRONIC DEVICES

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by
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To my ever loving parents…
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ABSTRACT


Discovered in the early 1990’s, carbon nanotubes (CNTs) are found to have exceptional physical characteristics compared to conventional semiconductor materials, with much potential for devices surpassing the performance of present-day electronics. Semiconducting CNTs have large carrier mobilities and a direct electronic bandgap, resulting in enhanced band-to-band tunneling (BTBT) as well as optical properties that could lead to novel electronic and optoelectronic applications. Therefore, detailed modeling and simulation of electronic transport in CNTs is required for a comprehensive understanding of the operation of CNT based devices. We have used the nonequilibrium Green’s function (NEGF) formalism for dissipative quantum transport simulation of CNT field-effect transistors. Previous experiments have shown that BTBT in CNT-MOSFETs can lead to subthreshold swings below the 60mV/decade conventional limit, which makes these devices promising candidates for low-power applications. Our simulations indeed confirm this observation, and further show that this regime of operation is dominated by phonon-assisted tunneling which degrades desirable device behavior. A detailed investigation of a CNT based $p-i-n$ tunneling transistor (TFET) geometry that has much favorable device characteristics is also presented. We observe less than 60mV/decade subthreshold swing for this geometry that leads to smaller off-state leakage and standby power dissipation compared to the conventional MOSFET operation. Under on-state performance, the drive current and the switching speed of $p-i-n$ TFETs are dominated by the tunneling barrier properties. Interestingly, the switching energy of the $p-i-n$ TFET is observed to be fundamentally smaller than that for the MOSFET at the quantum
capacitance limit of operation. Finally, a study on the modeling and simulation of inelastic transport in a CNT based optoelectronic device using the semiclassical Boltzmann transport equation is presented. The optical emission in these devices is attributed to an excitonic process. Localized exciton generation under high-field conditions is explored, and detailed device optimization schemes are discussed. These devices have the potential for ultra-bright light emission, among many other optoelectronic applications.
1. INTRODUCTION

With continual scaling of the CMOS transistor, first demonstrated in the early 1960’s, the semiconductor electronics industry is reaching a crossroads. The scaling has allowed exponential improvements in circuit performance over the decades and the device dimensions are soon reaching the atomic scales (Figure 1.1) [1]. The exponential enhancements, however, have come with a concomitant increase in circuit power dissipation. The present day microchips dissipate about 100W of power which is at the limit of economically feasible heat sinking technologies (Figure 1.2 (a)). Therefore, the continued scaling and the increase in transistor densities have led to power-performance tradeoffs, resulting in modern architectural solutions as multicore processors. Recent introduction of high-k oxides into semiconductor technology has alleviated the problem of gate leakage and allowed further scaling of device dimensions [2].

![Figure 1.1. Scaling of the physical dimensions of CMOS transistors [1].](image-url)
operational principles of thermal MOSFETs, however, have imposed fundamental limits on power dissipation in conventional CMOS technology that would be aggravated with continual increase in device densities. From a historical point of view, it is interesting to note that the semiconductor industry has indeed gone through technological “revolutions” due to power dissipation constraints, such as the move from bipolar devices to CMOS itself (Figure 1.2 (b)). Therefore, it is quite likely that the performance evolutions of the CMOS transistor might be coming to a roadblock, and a new technological “revolution” is called for.

Carbon nanotubes (CNTs), first discovered in the early 1990’s [3, 4], have proved to possess exceptional physical properties compared to all conventional semiconducting materials [5]. They have carrier mobilities of $10^4$–$10^5$ cm$^2$/Vs [6, 7] so high-performance electronic devices are possible. The conduction and the valence band effective masses in CNTs are small and they are the same; their band dispersions are approximately symmetric (they are exactly symmetric according to nearest-neighbor tight-binding calculations) [8]. This symmetry leads to equal performance for n-type and p-type transistors, which is a technologically desirable property. Semiconducting CNTs also
possess a direct electronic bandgap so they have increased band-to-band tunneling (BTBT) properties, as well as enhanced optical activity [9-12], that could lead to novel electronic and optoelectronic applications [5]. High-performance CNT transistors operating close to the ballistic limit have already been experimentally demonstrated [13-16]. Therefore, CNTs have been extensively investigated due to their aforementioned attractive properties that might be employed in solving some of the pressing challenges of the 21st century.

Nevertheless, phonon scattering in CNTs can influence their ballistic performance, and can be important for devices with channel lengths of a few 10’s of nanometers or more [17-19]. Therefore, computational simulations rigorously treating both quantum and incoherent effects are imperative for a comprehensive understanding of the operation, and the deterministic modeling, of these devices. The nonequilibrium Green’s function (NEGF) formalism has provided a universal framework in treating dissipative quantum transport in nanoscale devices [20-23]. In NEGF formalism the electronic structure of the device can be described by simpler models such as the effective-mass Hamiltonian, or, more accurate models such as atomistic tight-binding or \textit{ab initio} descriptions. Important quantum mechanical effects such as BTBT and level-broadening can also be rigorously treated.

The NEGF formalism can be contrasted with the popular semiclassical transport formalism, Boltzmann transport equation (BTE), that has been extensively used in Monte Carlo simulation of nano devices [24-26]. In BTE the electronic band-structure of the material system is calculated \textit{a priori} so any device and bias related modifications to the electronic structure are not rigorously captured (even though quantum corrections can be made for confinement effects). Furthermore, important effects such as BTBT need to be introduced separately. One of the major advantages of the BTE method, however, is that it can treat larger device dimensions compared to the atomistic models used in NEGF that can become computationally very expensive. More importantly, the treatment of carrier
scattering in realistic devices has been well studied in the case of Monte Carlo based simulations [25, 26]. On the other hand, microscopic treatment of dissipative quantum transport in realistic devices with the NEGF formalism still remains a challenge. It has been accomplished, along with some simplifying assumptions, in the case of silicon transistors [27, 28] using an effective-mass Hamiltonian for mode space transport, as well as for resonant tunneling devices (RTDs) with effective-mass [29] and atomistic tight-binding [22] Hamiltonians. As a consequence of this computational complexity a phenomenological model based on Buttiker probes for treating incoherent transport in NEGF has been utilized [30, 31].

In this thesis we describe the detailed modeling and simulation of inelastic carrier transport in CNT based electronic and optoelectronic devices. One major contribution of this work is the development of NEGF based simulator for dissipative carrier transport in CNT transistors. CNT electronic structure is described with the atomistic $p_z$ tight-binding Hamiltonian [8] so important non-parabolic effects beyond the effective-mass models are captured. The mode-space formalism is used for carrier transport in the lowest conduction and highest valence band in CNTs [32] which is valid for technologically important tubes with smaller diameters (larger bandgaps) that have considerable subband energy separation. More importantly, electron-phonon scattering is treated microscopically, within the deformation potential theory, along with detailed phonon dispersion calculations performed using force-constant methods [33]. The NEGF simulator is then used to explore the effects of phonon scattering on CNT transistor characteristics in two main regimes of device operation: (1) conventional operation of CNT transistors with doped source/drain regions (hereafter called CNT-MOSFETs) that operate by thermionic emission of carriers over the channel barrier [34, 35], (2) BTBT based transistors that could deliver less than 60mV/decade subthreshold swing [36-40]. Two device geometries are studied that utilizes BTBT operation. First, it is shown that BTBT in CNT-MOSFETs can produce less than 60mV/decade subthreshold swing [36, 38] as experimentally observed in [41, 42], even though BTBT in these devices is dominated by phonon
assisted tunneling. Then, we explore sub-60mV/decade operation in a gated \( p-i-n \) tunnel transistor geometry (hereafter called the \( p-i-n \) TFET) that has much favorable device characteristics even with phonon scattering \([37, 39, 40]\). One main challenge for BTBT based transistors is their limited current drive due to the presence of the tunneling barrier. Therefore, it is quite possible that there would be an initial performance penalty by moving to tunneling based transistors for general purpose computing. Nevertheless, this transition could potentially mitigate the power dissipation problems considerably, and increase the overall IC performance in the long run due to increased integration densities (e.g: multicore chips with more cores, or, 3D integration). The semiconductor industry has already witnessed a similar technological realignment due to power dissipation constraints in moving from bipolar to CMOS technology (Figure 1.2 (b)).

Finally, we describe modeling and simulation of a CNT based optoelectronic device \([43, 44]\) using a numerical solution of the BTE \([45]\) that treats phonon scattering and impact excitation of excitons under high-field transport. Optical emission in CNTs has received a lot of attention due to its potential for many technologically important applications such as fully integrable optical nano-switches for inter/intra chip communication \([9-12]\). Early experiments on CNT electroluminescence were based on Schottky-barrier transistors (hereafter called SB-CNTFETs) where the devices were fabricated on an oxidized silicon substrate \([9, 46]\). A recent experiment using a novel device structure with a partially suspended CNT \([10]\), however, reported an enhancement of optical emission intensity by a factor of 100~1000X compared to earlier results. The optical emission process was attributed to excitonic recombination, and was different from the free carrier recombination seen in earlier work. We have performed computational simulations on this particular device geometry, considering the exciton emission process, and found results that directly corroborate the experimental observations. This work is done in collaboration with Dr. Phaedon Avouris’ group at IBM T. J. Watson Research Center, which is a premier experimental group investigating the optoelectronic applications for CNTs \([9, 10, 12, 46]\). Present device simulations are
performed using the BTE for electron transport in the first conduction band. The BTE model is chosen because the experimental devices are in the micrometer length scale, and a quantum simulation based on the atomistic tight-binding Hamiltonian is computationally prohibitive.

At this point it is important to note that it is extremely difficult to predict the future directions of nanoelectronics device development. One thing, however, is certain to happen: devices will continue to get smaller, reaching the deep nanoscale. Thus, at a conceptual level, the device simulation techniques employed in this study, and device physics elucidated in turn, could potentially be applied to many of these future nanoscale devices, irrespective of the particular material system.

A brief outline of the rest of the thesis is as follows. Chapter 2 describes the simulation procedure for ballistic transport in CNT based transistors in detail. The treatment of self-consistent electrostatics with the Poisson’s equation is also discussed. This chapter is based on our publication [35]. Chapter 3 then describes the NEGF treatment of phonon scattering in CNT transistors. Here, electron-phonon coupling is treated microscopically and realistic phonon modes in CNTs have been distinguished [33]. Both optical and acoustic phonon modes are considered. The chapter also includes a description of the numerical procedures used in simulating phonon scattering in CNT based transistors. This chapter too is adapted from [35].

Chapter 4 presents the simulation results for dissipative transport in CNT-MOSFETs. Two main operational regimes are considered. Section 4.1 discusses the effect of phonon scattering on the conventional (over-the-barrier) operation of CNT-MOSFETs. It investigates the relative importance of optical vs. acoustic phonon scattering mechanisms on transistor performance. We also consider the diameter dependence of the relative influence of phonon scattering by studying CNTs with diameters in the range of 1.2nm ~ 1.8nm, an experimentally important class of tubes,
beyond which the bandgaps are too small for electronic applications, and below which the contact properties are poor. These results are adapted from [35]. Section 4.2 discusses the CNT-MOSFET operation in the BTBT regime. We show that these devices can produce sub-60 mV/decade subthreshold operation, confirming the recently reported experimental observations [41, 42]. It is found that the BTBT operation, however, is dominated by phonon-assisted inelastic tunneling, and results in a degradation of the desirable subthreshold properties. It is further shown that multiphonon scattering might also become important at large device biases. This section is adapted from [38].

Chapter 5 studies the operation of CNT based $p-i-n$ TFETs for sub-60mV/decade device applications. First, the device operation is explored using ballistic transport simulations. Then, the influence of phonon scattering is investigated. It is observed that, unlike in the case of BTBT in CNT-MOSFETs, the desirable device characteristics of the $p-i-n$ TFET are preserved even in the presence of phonon scattering. In the above-threshold regime the effect of phonon scattering on device performance is similar to that in the conventional operation of CNT-MOSFETs showing a distinct gate bias dependence of ballisticity. Under off-state conditions, however, phonon absorption assisted transport becomes important and subthreshold swing becomes temperature dependent, degrading at higher temperatures. Nevertheless, less than 60mV/decade subthreshold swing is consistently observed at room temperature. This section is adapted from [37, 39, 40].

Chapter 6 addresses the important task of a comprehensive comparison of device performance between the conventional $n-i-n$ MOSFET operation and the $p-i-n$ TFET geometry. Here, we use identical simulation conditions based on CNTs as the model channel material by changing the dopant type for source doping for each device, respectively. We observe that the $p-i-n$ TFET can indeed reduce off-state leakage leading to smaller standby power dissipation. Phonon absorption assisted transport, however, limits the desirable device characteristics that could have been achieved under ballistic transport. On-current and intrinsic device delay metric of the $p-i-n$ TFET are mainly
determined by the tunneling barrier properties. On the other hand, the switching energy of $p$-$i$-$n$ TFETs is observed to be fundamentally smaller compared to $n$-$i$-$n$ MOSFETs at the quantum capacitance limit of operation. The origin of these important differences for the two geometries will be elucidated. This chapter is adapted from [40].

Chapter 7 describes modeling and simulation of CNT based optoelectronic devices using a numerical solution of the BTE. The chapter first discusses the importance of excitonic processes in CNTs due to the enhancement of Coulomb interaction in these quasi-1D structures. Then, it summarizes the numerical procedure in solving the BTE for 1D transport employed here based on the original method described in [45]. The treatment of Schottky barrier tunneling in semiclassical BTE at source/drain contacts of a SB-CNTFET is elaborated. The electrostatic solution of the model device structure based on finite difference discretization of the Poisson equation is described next, including the non-linear scheme in solving the transport equations self-consistently with electrostatics. This chapter is adapted from [43, 44].

Chapter 8 presents the detailed simulation results for the partially suspended CNT optical emitter reported in [10]. We have modeled devices with both CNT-MOSFET and SB-CNTFET geometries. Note that the experimentally reported devices use Pd metal Schottky contacts similar to the latter geometry. It is observed that inside (and near) the trench region both these devices behave very similarly. Localized exciton generation at the trench-substrate junction near the drain side that would lead to localized optical emission seen in the experiment is confirmed. Furthermore, an exponential increase in exciton generation rate with a linear increase in gate bias dependent device current ($I_{DS} - V_{GS}$) is observed. This corroborates with the experimentally observed bias dependant device characteristics for optical emission intensities. The chapter also provides detailed insight into device operation, and proposes performance optimization schemes; deeper trench geometry is expected to increase exciton generation efficiency, and high-k substrate oxides could lead to even larger improvements. Exciton generation rate
increases for larger diameter (smaller bandgap) CNTs due to the reduction in impact excitation energy threshold, but this will also change the optical emission wavelength (will become larger for larger diameters). This chapter is also adapted from [43, 44].

Finally, chapter 9 presents the conclusions drawn from this work. It further discusses possible directions for future studies based on the finding of this thesis work.
2. NEGF TREATMENT OF BALLISTIC TRANSPORT IN CNT TRANSISTORS

Ballistic transport in CNTs has been experimentally demonstrated for low-bias conditions at low temperatures [47, 48]. High-performance CNT transistors operating close to the ballistic limit at room temperature have also been reported [13-16]. The experimentally obtained carrier mobilities are of the orders $10^4 \sim 10^5$ cm$^2$/Vs [6, 7] so exceptional device characteristics can indeed be expected. Current transport in long metallic CNTs, however, is found to saturate at $\sim 25$ µA at high biases, and the saturation mechanism is attributed to phonon scattering [17]. On the other hand, for short length metallic tubes, the current is found not to saturate but to increase well beyond the above limit [18, 19]. Nevertheless, carrier transport in these shorter tubes is still influenced by phonon scattering, and warrants a detailed physical understanding of the scattering mechanisms due to its implications on device characteristics for both metallic as well as semiconducting CNTs. This chapter describes the simulation procedure for ballistic transport in CNTFETs. The treatment of dissipative transport is presented in the next chapter. Note that this chapter is adapted from our publication [35].

2.1 NEGF Treatment of Transport

A detailed description of the NEGF modeling of ballistic transport in CNTFETs is described in [32]. Here we present a brief overview of that device model for the sake of completeness. The device Hamiltonian used in this study is based on the atomistic nearest-neighbor $p_z$-orbital tight-binding approximation [8]. The device geometry, shown in Figure 2.1(a), is a CNT MOSFET with doped source and drain regions ($L_{SD}$) and a
cylindrical wrap-around metallic gate electrode over the intrinsic channel region ($L_{ch}$). The gate oxide with thickness $t_{ox}$ covers the full length of the tube. We employ artificial heavily doped extension regions, $L_{ext}$. They do not influence the transport in the working part of the transistor, but are useful for better numerical convergence purposes when phonon scattering is present (however are not necessary for ballistic simulations). The cylindrical geometry of this device ensures symmetry in the angular direction thus drastically simplifying the mode-space treatment of electron transport [32, 49]. It also permits the treatment of self-consistent electrostatics using 2D finite difference method.

Figure 2.1. (a) Device structure with wrap-around gate, (b) NEGF model with coupling to the phonon bath, and (c) mode-space Hamiltonian.
The source and drain electrodes are treated as quasi-continuum reservoirs in thermal equilibrium and are modeled by the contact self-energy functions as in [32].

The NEGF model of the CNTFET used for transport simulations is shown in Figure 2.1(b). Here, $H_{pc}$ is the device Hamiltonian and the self-energy functions $\Sigma_{s/d}$ represent the semi-infinite ideal source/drain contacts. $\Sigma_{\text{scat}}$ is the self-energy for e-ph interaction, and one sets $\Sigma_{\text{scat}} = 0$ for the ballistic approximation. A detailed specification of $\Sigma_{\text{scat}}$ is presented later in section 3.2. Finally, the retarded Green’s function for the device in the matrix form is given by [21],

$$G(E) = \left[ \left( E + i\eta^+ \right) I - H_{pc} - \Sigma(E) \right]^{-1}$$

where $\eta^+$ is an infinitesimal positive value, and $I$ the identity matrix [21]. The self energy contains the contributions from all mechanisms of relaxation; the source and drain electrodes, and from scattering [21],

$$\Sigma(E) = \Sigma_s(E) + \Sigma_d(E) + \Sigma_{\text{scat}}(E)$$

Note that in Eq. (2.2) the self-energy functions are, in general, energy dependent.

In the mode-space treatment of an $(n,0)$ zigzag CNT, the dependence of the electronic state on the angle along the tube’s circumference, $\varphi$, is expanded in a set of circular harmonics $\exp(im\varphi)$ with the angular quantum number, $m$. It spans the integer values of 1 to $2n$, or, equivalently, $-n+1$ to $n$. Integer values on $m$ outside this range would produce equivalent harmonics at the crystal lattice sites. The total Hamiltonian splits into independent matrices for subbands associated with each value of $m$ [32], giving rise to a 1D Hamiltonian with two-site unit cell, as schematically shown in Figure 2.1(c), where each site corresponds to one of two non-equivalent real-space carbon rings, A or B. The
period of the zigzag tube in the longitudinal direction contains 4 such rings, ABAB, and has length $3a_{cc}$ [8], where $a_{cc} = 0.142nm$ is the carbon-carbon bond length in graphene. Therefore the average distance between rings is,

$$\Delta z = \frac{3a_{cc}}{4}.$$  \hspace{1cm} (2.3)

The diameter of the zigzag nanotube is [8],

$$d_i = \frac{n\sqrt{3}a_{cc}}{\pi}.$$ \hspace{1cm} (2.4)

The mode-space transformation procedure of the real-space atomistic tight-binding Hamiltonian is well described in [32], and is not repeated here. The two-site unit cell, as expected, gives rise to two subbands corresponding to the conduction and the valence band. The Hamiltonian matrix for the subbands with angular quantum number $m$ in an $(n,0)$ zigzag CNT is then given by [32],

$$H_{pc} = \begin{bmatrix}
U_1 & b_{2m} & & & \\
b_{2m} & U_2 & t & 0 & \\
t & U_3 & b_{2m} & & \\
0 & t & \cdots & & \\
& & & b_{2m} & U_{N-1} \end{bmatrix}_{N\times N} \hspace{1cm} \text{(2.5)}$$

where $b_{2m} = 2t \cos(\pi m/n)$, $t = 3eV$ is the nearest neighbor hopping parameter, and $N$ is the total number of carbon rings along the device. Here, the diagonal elements $U_j$ correspond to the on-site electrostatic potential along the tube surface. All electronic subbands in a CNT are four-fold degenerate: due to two spin states and the valley degeneracy of two [8]. The valley degeneracy comes from the two subbands with the
same energy dispersion, but different $m$-values. Each subband can be represented as a cut of the graphene 2D Brillouin zone by a line with a constant momentum $k_y$. In this paper we equate momentum with wavevector, having the dimension of inverse length. The cuts closest to the K-points of graphene correspond to lowest-energy conduction subbands as well as highest-energy valence subbands, and correspond in zigzag tubes to angular momenta $m_{L1} = \text{round}(2n/3)$ and $m_{L2} = \text{round}(4n/3)$.

Level broadening is defined as follows and can be shown [21] to be,

$$
\Gamma(E) = i \left[ \Sigma(E) - \Sigma^*(E) \right] = \Sigma^{\text{in}}(E) + \Sigma^{\text{out}}(E),
$$

(2.6)

where $\Sigma^*$ represents the Hermitean conjugate of $\Sigma$ matrix defined by Eq. (2.2). Here, $\Sigma^{\text{in/out}}$ are the in/out-scattering functions (see below). The same relations apply separately to each mechanism of relaxation. For a layered structure like the carbon nanotube, the source self-energy function $\Sigma_{\text{source}}$ has all its entries zero except for the (1,1) element. That is [32],

$$
\Sigma_S(i \neq 1, j \neq 1) = 0
$$

(2.7)

and,

$$
\Sigma_S(1,1) = \alpha_{\text{source}} - \sqrt{\alpha_{\text{source}}^2 - t^2}, \quad \alpha_{\text{source}} = \frac{(E - U_i)^2 + t^2 - b_{2m}^2}{2(E - U_i)}
$$

(2.8)

Similarly, $\Sigma_D$ has only its $(N,N)$ element non-zero and it is given by equations similar to (2.7) and (2.8) with $U_i$ replaced by $U_N$. As mentioned earlier, $\Sigma_{S/D}$ self-energies rigorously capture the effect of semi-infinite contacts on the device. With this we can define the in- and out-scattering functions for contact coupling,

$$
\Sigma_{S/D}^{\text{in}}(E) = \Gamma_{S/D}(E) f(E - E_{S/D}^F)
$$

(2.9)
\[ \Sigma_{S/D}^{\text{out}}(E) = \Gamma_{S/D}(E) \left[ 1 - f \left( E - E_{S/D}^F \right) \right] \] (2.10)

where \( f(E) \) is the Fermi distribution, and \( E_{S/D}^F \) are the source and drain Fermi energies, respectively. The electron and hole correlation functions are then given by [21],

\[ G^n = G \left[ \Sigma^n_S + \Sigma^n_D + \Sigma^n_{\text{scat}} \right] G^\dagger \] (2.11)

\[ G^p = G \left[ \Sigma^p_S + \Sigma^p_D + \Sigma^p_{\text{scat}} \right] G^\dagger \] (2.12)

where the energy dependence of the Green’s function and in/out-scattering functions is suppressed for clarity. The in/out-scattering functions for e-ph interaction, \( \Sigma^{\text{in/out}}_{\text{scat}} \), are discussed later in section 3.2. It is seen that, under ballistic conditions (i.e. \( \Sigma^{\text{in/out}}_{\text{scat}} = 0 \)), the electron/hole distribution throughout the device is determined by the occupation of the respective local density of states, LDOS\( _{S,D} \), by the corresponding reservoir Fermi functions, \( f_{S,D} \). The spectral function is [21],

\[ A(E) \equiv i \left( G(E) - G^\dagger(E) \right) = G^n(E) + G^p(E) \] (2.13)

Under ballistic conditions the spectral function can be separated into its source and drain contributions, respectively [21];

\[ A_{S,D} = G \Gamma_{S,D} G^\dagger \] (2.14)

where the diagonal elements of \( A_{S,D} \) are related to the local density of states (LDOS\( _{S,D} \)) evolving from the corresponding contact [21]. Note that the electron and hole correlation functions, \( G_{i,j}^{n/p}(E,m) \), are matrices defined in the basis set of ring numbers \( i,j \) and subbands \( m \) (we will imply the last index in the rest of the paper). Thus the diagonal
elements, \( G_{i,j}^{n,p}(E,m) \), correspond to the energy density of carrier occupation at those basis sites (single carbon ring, A or B, in a specific subband) with a given energy \( E \). So the total electron/hole density (per unit length) at a site \( z_j \) is given by,

\[
n(z_j) = \sum_{m,s} \frac{1}{\Delta z} \int_{-\infty}^{+\infty} G_{i,j}^{n}(E,m) \frac{dE}{2\pi}
\]

(2.15)

\[
p(z_j) = \sum_{m,s} \frac{1}{\Delta z} \int_{-\infty}^{+\infty} G_{i,j}^{p}(E,m) \frac{dE}{2\pi}
\]

(2.16)

where summation is performed over the spin and subband variables, and produces the degeneracy factor of 4 (for each non-equivalent subband). In the view of Eq. (2.13) one recognizes that the spectral function is proportional to the density of states which is traditionally defined [24] to include the spin summation, but is taken separately for each subband

\[
g_{1D}(E,z_j) = \frac{A_{i,j}(E,m)}{\pi \Delta z}
\]

(2.17)

Finally, the current flow from site \( z_j \) to \( z_{j+1} \) in the nearest-neighbor tight-binding scheme can be determined from [22, 23],

\[
I_{j\rightarrow j+1} = \sum_{m,s} \frac{i e}{\hbar} \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \left[ H_{j,j+1}(m) G_{j+1,j}^{n}(E,m) - H_{j+1,j}(m) G_{j,j+1}^{n}(E,m) \right]
\]

(2.18)

wherein the non-diagonal terms of the Hamiltonian Eq. (2.5) contain only contributions of hopping. The above equation is a general relationship, in that it is valid even under dissipative transport. Under ballistic conditions, however, Eq. (2.18) further simplifies (for each non-equivalent subband) to,
\[ I = \frac{4e}{\hbar} \int_{-\infty}^{\infty} dE T(E) \left[ f(E - E_g^+) - f(E - E_g^-) \right] \quad (2.19) \]

with the transmission coefficient, \( T(E) \), given by,

\[ T(E) = \text{Trace} \left[ \Gamma_s(E)G(E)\Gamma_p(E)G^+(E) \right] \quad (2.20) \]

Eq. (2.19) is the famous Landauer equation widely used in mesoscopic transport [21].

One can better understand the bandstructure of carbon nanotubes in by solving for the eigenvalues of the Hamiltonian (2.5) for zero external potential, and thereby obtaining [32] the energy dispersion relations, \( E(k_z) \), versus the momentum along the length of the tube, for each subband. For the lowest conduction and the highest valence subbands, close to the K-points the graphene band edge is approximately conic, thus [50],

\[ \left( \frac{2E}{E_g} \right)^2 = 1 + \left( \frac{k_z}{\Delta k} \right)^2 \quad (2.21) \]

with the bandgap [50],

\[ E_g = 2v_c \hbar \Delta k \quad (2.22) \]

and the distance to the K-point of [50],

\[ \Delta k = \frac{2}{3d_t} \quad (2.23) \]

The velocity of carriers in the band is [50],

\[ v = \frac{dE}{\hbar k_z} \quad (2.24) \]

Far enough from the band edge, the velocity tends to the constant value [50],

\[ v_f = \frac{3v_c}{2} t = 10^6 \text{ m/s} \quad (2.25) \]
The 1D density of states including spin summation but only one subband (valley) can thus be expressed as [50],

\[ g_{11}(E) = \frac{2}{\pi \hbar v(E)}. \]  

(2.26)

or, in other terms [50],

\[ g_{11}(E) = \frac{2}{\pi \hbar v_f} \cdot \frac{|E|}{\sqrt{E^2 - \left( E_g / 2 \right)^2}}. \]  

(2.27)

### 2.2 Poisson’s Equation

This section summarizes the implementation of self-consistent electrostatics in our simulation. The diagonal entries of the Hamiltonian in Eq. (2.5) contain the electrostatic potential on the tube surface, which thereby enters the NEGF calculation of charge distribution in Eqs. (2.15) and (2.16). On the other hand, the electrostatic potential and the charge distribution are coupled through the Poisson’s equation as well, leading to

![Figure 2.2. Self-consistency requirement between NEGF and Poisson solutions.](image-url)
the Poisson-NEGF self-consistency requirement shown in Figure 2.2. The 2D Poisson equation for the cylindrical transistor geometry in Figure 2.1(a) is,

$$ \nabla^2 U(r,z) = -\frac{\rho(r,z)}{\varepsilon}. \quad (2.28) $$

Here, $\rho(r,z)$ is the net charge density distribution which includes dopant density as well. At this point, it should be noted that even though Eqs. (2.15) and (2.16) give the total carrier densities distributed throughout the whole energy range, what we really need for determining the self-consistent potential on the tube surface, $U_j = U(r = r_{CNT}, z_j)$, is the induced charge density ($r_{CNT} = CNT$ radius). This can be determined by performing the integrals in Eqs. (2.15) and (2.16) in a limited energy range defined with respect to the local charge neutrality energy, $E_N$ [32, 51]. In a semiconducting CNT, due to the symmetry of the conduction and valence bands, $E_N$ is expected to be at the mid-gap energy. Finally, the induced charge density at site $z_j$ can be calculated from [32],

$$ Q_{ind}(z_j) = \frac{4}{\Delta z} \left[ (-e) \int_{E_N(j)}^{\infty} \frac{G_{j,j}^e(E)}{2\pi} dE + (+e) \int_{-\infty}^{E_N(j)} \frac{G_{j,j}^p(E)}{2\pi} dE \right] \quad (2.29) $$

where the first and second terms correspond to the induced electron and hole densities, respectively, with charge of the electron $e$.

Knowing the induced charge $Q_{ind}$, the net charge distribution $\rho(r,z)$ is given by,

$$ \rho(r = r_{CNT}, z_j) = Q_{ind}(z_j) + N_D^+ - N_A^- \quad (2.30) $$

$$ \rho(r \neq r_{CNT}, z_j) = 0 \quad (2.31) $$
where, $N_D^+$ and $N_A^-$ are ionized donor and acceptor concentrations, respectively. Here, it is assumed that the induced charge and the dopants are uniformly distributed over the CNT surface. Finally, Eq. (2.28) is solved to determine the self-consistent electrostatic potential $U_j$ along the tube surface. The finite difference solution scheme for the 2D Poisson equation is further described in section 7.2.2. The calculated potential, $U_j^{new}$, gives rise to a modified Hamiltonian (Eq. (2.5)), eventually leading to the self-consistent loop between electrostatics and quantum transport (Figure 2.2).

Even though the self-consistent procedure we have just outlined appears conceptually straightforward, it has poor convergence properties. Therefore, a non-linear treatment of the Poisson solution is used in practice, as explained in [22, 52], in order to expedite the electrostatic convergence. The convergence criterion used in this process is to monitor the maximum change in the potential profile between consecutive iterations, i.e.: 

$$\max \left| U_j^{old} - U_j^{new} \right| \leq U^{tol},$$

where the tolerance value $U^{tol}$ is normally taken to be 1meV.
3. NEGF TREATMENT OF DISSIPATIVE TRANSPORT IN CNT TRANSISTORS

There have been many theoretical studies on the calculation of carrier scattering rates and mobilities in CNTs using semiclassical transport simulation based on the Boltzmann equation [53-59]. Similarly, phonon mode calculations for CNTs are also performed with varying degrees of complexity: continuum and force-constant models [8, 60, 61] to first-principles based methods [62-64]. The determination of electron-phonon (e-ph) coupling strength is performed using tight-binding calculations [65-67] as well as first-principles techniques [68]. It has been shown, however, that the influence of phonon scattering on device performance depends not only on the phonon modes and e-ph coupling, but also on the device geometry [34, 69]. Therefore, in order to ascertain the impact of phonon scattering on the device performance, aforementioned calculations should be done in the context of specific device geometry. To that end, phonon scattering in CNT transistors has been treated using the semiclassical Boltzmann transport to determine its effects on device characteristics [69, 70]. Semiclassical transport, however, can fail to rigorously treat important quantum mechanical effects, such as band-to-band tunneling, that have been deemed important in these devices [36, 38, 39], as well as the self-consistent treatment of lifetime broadening due to scattering. Therefore, a device simulator based on dissipative quantum transport that rigorously treats the effects of phonon scattering will be essential for the proper assessment of CNT transistor characteristics, and to gain a deeper understanding of carrier transport at nanoscale. Treatment of phonon scattering in Schottky-barrier CNT transistors is described in [71, 72] where e-ph coupling is treated phenomenologically. This chapter describes the detailed treatment of phonon scattering in CNT-MOSFETs using the NEGF formalism, as
well as, rigorous determination of phonon modes and their e-ph coupling in CNTs using force-constant methods [33]. Note that this chapter is adapted from our publication [35].

3.1 Phonon Modes in a CNT

The parameters of the phonons are obviously determined by the structure of the nanotube lattice. The one-dimensional mass density of an \((n,0)\) nanotube is,

\[
\rho_{1D} = \frac{m_c n}{\Delta z}.
\]  

(3.1)

where \(m_c\) the mass of a carbon atom, \(\Delta z\) the average ring distance defined in Eq. (2.3). The energy of a phonon of momentum \(q\) (in the unconfined dimension) is \(\hbar \omega_q\). The index of the phonon subband \(l\) is implicitly combined with the momentum index here. The half-amplitude of vibration for one phonon in a tube of length \(L\) is [24],

\[
a_q = \sqrt{\frac{\hbar}{2 \rho_{1D} L \omega_q}}.
\]  

(3.2)

For the reservoir in a thermal equilibrium at temperature \(T\), the occupation of modes is given by the Bose-Einstein distribution,

\[
n_q = \left(\exp\left(\frac{\hbar \omega_q}{k_BT}\right) - 1\right)^{-1}.
\]  

(3.3)

As discussed earlier, the electron states in semiconducting CNTs have two-fold valley degeneracy with the lowest-energy subbands having angular quantum numbers \(m_{L1}\) and \(m_{L2}\). Electron-phonon scattering is governed by energy and momentum conservation rules. Thus, as shown in Figure 3.1(a) electrons can be scattered within the same subband.
(intra-valley) where they do not change their angular momentum, and, such scattering is facilitated by zone-center phonons having zero angular momentum ($l = 0$). As shown in Figure 3.1(b), it is also possible to have inter-valley scattering mediated by zone-boundary phonons having angular quantum number $l = |m_{L1} - m_{L2}|$. There can also be scattering to higher energy subbands assisted by phonon modes with $l \neq 0$ and $l \neq |m_{L1} - m_{L2}|$ [42, 46], however, we do not discuss results for such processes in this paper.

We have performed phonon dispersion calculations using the force-constant methods described in [8, 33]. As a result of this analysis, the matrix element for the electron-phonon interaction is expressed via the deformation potential, $J_i = 6eV/\AA$, and the dimensionless matrix element as follows: $\left| K_q \right| = \left| J_i \right| \left| M_q \right|$. Zone-center and zone-boundary phonon dispersions for a (16,0) zigzag CNT are shown in Figure 3.2(a) and Figure 3.2(b), respectively. It is seen that the representation of phonon modes according to fundamental polarizations, such as longitudinal (L), transverse (T), and radial (R), can only be done for zone-center modes as indicated in Figure 3.2(a). On the other hand, zone-boundary modes tend to be comprised of a mixture of such fundamental polarizations, as the $\sim 180\text{meV}$ mode highlighted in Figure 3.2(b), which is mainly a combination of longitudinal optical (LO) and transverse acoustic (TA) polarizations. It
should also be noted that the frequency of the radial breathing mode (RBM) calculated here is in very good agreement with the relationship derived from *ab initio* calculations,

\[
\hbar \omega_{\text{RBM}} = 28 \text{meV} / d, \tag{3.4}
\]

where \(d\) is the CNT diameter in nanometers [62, 63, 73]. The Hamiltonian of electron-phonon interaction in a general form is [24],

---

**Figure 3.2.** Energy dispersion for phonon modes in a (16,0) CNT: (a) zone-center phonons that allow intra-valley scattering and, (b) zone-boundary phonons that allow inter-valley scattering. Modes that effectively couple to the electrons are indicated by dashed circles. Zone-boundary phonons are composed of a mixture of fundamental polarizations.
\[ V = \sum_q K_q a_q \left( b_q e^{-i (q \cdot r)} + b_q^\dagger e^{i (q \cdot r)} \right) \]  

(3.5)

where \( b_q^\dagger, b_q \) are the creation and annihilation operators for phonons in the mode \( q \). The summation over momenta is generally defined via an integral over the momentum space,

\[ \sum_q = \left( \frac{L}{2\pi} \right)^D \int d^D q . \]  

(3.6)

where \( D \) is the number of unconfined dimensions. For carbon nanotubes \( D = 1 \) and the limits of the integral are \( \pm \infty \).

Electron-phonon (e-ph) coupling calculations have also been carried out, as described in [65], in conjunction with the dispersion calculations in order to account for the mode polarization effect on e-ph coupling value [33]. We find that only a few phonon modes that effectively couple to the electrons. As highlighted in Figure 3.2(a), out of zone-center modes only the LO (190meV), LA, and radial breathing mode (RBM) have sufficient coupling, whereas, from zone-boundary modes only the 180meV LO/TA mode has significant coupling. Even though we have shown phonon dispersions for a large section of the 1D Brillouin zone, only the ones close to the zone center (i.e.: \( q \approx 0 \)) are involved in electron transport [55]. Within that region of the Brillouin zone all the optical modes are found to have constant energy dispersion while the acoustic mode has a linear dispersion. Thus, in this study all the relevant optical modes for electron transport are considered dispersionless with constant energy, \( \hbar \omega_{op} \), and the zone-center LA mode is taken to be linear with, \( \omega_{Ap} = v_a q \), relationship where \( v_a \) is the sound velocity of that mode. The matrix element of interaction for acoustic phonons is approximated by a linear function \( |K_q| = \bar{K}_a(l)q \). In this paper, we take the matrix elements as inputs and describe
the general method of treatment of electron-phonon interaction in nanotubes for both optical and acoustic phonon modes.

3.2 Electron-Phonon Scattering

The e-ph scattering is treated within the self-consistent Born approximation (SCBA) [20], in that, the Green’s function $G(E)$ in eq. (2.1) and the scattering self-energy $\Sigma_{\text{scat}}(E)$ in eq. (2.2) have to be determined self-consistently. NEGF formulation of carrier scattering due to optical and acoustic phonons is described in this section. Section 3.3 discusses the numerical implementation of the SCBA approach. The in/out-scattering functions for optical phonon scattering of electrons in a ring $i$ from subband $m'$ to subband $m$ are [21],

$$
\Sigma_{\text{scat}}^{\text{in}}(i,i,m,E) = D_0(n_{m'} + 1)G^0(i,i,m',E + \hbar \omega) + D_0n_{m'}G^0(i,i,m',E - \hbar \omega) \quad (3.7)
$$

$$
\Sigma_{\text{scat}}^{\text{out}}(i,i,m,E) = D_0(n_{m'} + 1)G^p(i,i,m',E - \hbar \omega) + D_0n_{m'}G^p(i,i,m',E + \hbar \omega). \quad (3.8)
$$

Here, we have used the local interaction approximation in writing the in/out-scattering functions by assuming them to be diagonal [22]. In eqs. (3.7) and (3.8) the first term on the right hand side corresponds to phonon emission mediated processes while the second term to that of phonon absorption. The imaginary part of the self-energy, related to the level broadening is now given by [21],

$$
\Sigma_{\text{scat}}^i(E) = -\frac{i}{2} \Gamma_{\text{scat}}(E) = -\frac{i}{2} \left[ \Sigma_{\text{scat}}^{\text{in}}(E) + \Sigma_{\text{scat}}^{\text{out}}(E) \right]. \quad (3.9)
$$

The real part of self-energy is manifested as a shift of energy levels and is computed by using the Hilbert transform [21],

$$
\Sigma_{\text{scat}}(E) = \Sigma_{\text{scat}}^i(E) - \Sigma_{\text{scat}}^r(E).
$$
\[
\Sigma'_{\text{scat}} = \frac{dE'}{2\pi} \frac{\Gamma_{\text{scat}}(E')}{E - E'} \cdot (3.10)
\]

In this work we neglect the real part of e-ph self-energy in order to simplify the computations and because the estimates suggest small influence of the real part. For optical phonon scattering, the coupling constant \(D_0\) is [33],

\[
D_0 = \frac{\hbar |K_0|^2}{2\rho_{\alpha}\omega_0\Delta z}. \cdot (3.11)
\]

For elastic scattering, i.e. in case it is possible to neglect the energy of a phonon, the in/out-scattering functions are [21],

\[
\Sigma_{\text{scat}}^{\text{in}}(i,i,m,E) = D_{el} G^\eta(i,i,m',E) \cdot (3.12)
\]

\[
\Sigma_{\text{scat}}^{\text{out}}(i,i,m,E) = D_{el} G^\rho(i,i,m',E) \cdot (3.13)
\]

In this case there is no need to neglect the real part of self-energy, and its complete expression is,

\[
\Sigma_{\text{scat}}(i,i,m,E) = D_{el} G(i,i,m',E) \cdot (3.14)
\]

For acoustic phonon scattering, the coupling constant is [33],

\[
D_{el} = \frac{K_s^2 k_B T}{\rho_{1D} v_s^2 \Delta z} \cdot (3.15)
\]
3.3 Numerical Treatment of Dissipative Transport

Here, we summarize the overall simulation procedure used in this study. Throughout this work we encounter many energy integrals such as Eqs. (2.18) and (2.29). The use of a uniform energy grid becomes prohibitive when sharp features such as quantized energy states need to be accurately resolved. Therefore, an adaptive technique for energy integrations is used based on the `quad.m` subroutine of Matlab® programming language. The treatment of phonon scattering is performed using the self-consistent Born approximation [22, 23]. In that, we need to treat the interdependence of the device Green’s function, Eq. (2.1), and the scattering self-energy, Eq. (2.2), self-consistently. The treatment of OP scattering is presented first, followed by that for AP scattering.

3.3.1 Treatment of optical phonon scattering

The determination of in/out-scattering functions, Eqs. (3.7) and (3.8), for OP scattering requires the knowledge of the electron and hole correlation functions; specifically, the energy-resolved diagonal elements of these functions, \( G^{n/p}_{j,j} (E) \). It should be noted that only the diagonal elements are needed since we take the scattering self-energy functions to be diagonal in the local interaction approximation [22, 23]. With that, we use the following procedure to determine \( G(E) \) and \( \Sigma_{\text{scatt}}(E) \) self-consistently.

1) Start with known energy-resolved \( G^{n/p}_{j,j} \) distributions. Ballistic distributions are used as the starting point.
2) Determine \( \Sigma_{\text{in}}(E) \), \( \Sigma_{\text{out}}(E) \), and \( \Sigma_{\text{scatt}}(E) \) using Eqs. (3.7), (3.8), and (3.9), respectively, at a given energy \( E \).
3) Determine new \( G(E) \) using Eq. (2.1).
4) Now, determine new \( G'(E) \) and \( G''(E) \) from Eqs. (2.11) and (2.12), respectively.
5) Repeat steps 2 through 4 for all energies and build new \( G^{n/p}_{j,j} \) distributions.
6) Repeat steps 1 through 5 until convergence criterion is satisfied. We use the convergence of the induced carrier density, Eq. (2.29), as the criterion.

In the above calculations, there is a repetitive need for the inversion of a large matrix, Eq. (2.1), which can be a computationally prohibitive task. However, we only need a few diagonals of the eventual solution such as the main diagonal of $G^{n/p}$ for the calculation of scattering and carrier densities, and the upper/lower diagonals of $G^n$ for the calculation of current in Eq. (2.18). The determination of these specific diagonals, in the nearest-neighbor tight-binding scheme, can be performed using the efficient algorithms given in [74]. A Matlab® implementation of these algorithms can be found at https://www.nanohub.org/resources/1983/. Finally, it should be noted that the overall accuracy of the Born convergence procedure described above is confirmed at the end by observing the current continuity throughout the device, Eq. (2.18).

### 3.3.2 Treatment of acoustic phonon scattering

Similar to the above method, AP scattering is treated using the following procedure,

1) Start with known energy-resolved $G^{n/p}_{j,j}$ distributions. Ballistic distributions are used as the starting point.
2) Determine $\Sigma_{\text{scat}}^{\text{in}}(E)$, $\Sigma_{\text{scat}}^{\text{out}}(E)$, and $\Sigma_{\text{scat}}^{\text{us}}(E)$ using Eqs. (3.12), (3.13), and (3.9), respectively, at a given energy $E$.
3) Determine new $G(E)$ using Eq. (2.1).
4) Now, determine new $G'(E)$ and $G''(E)$ at energy $E$ from Eqs. (2.11) and (2.12), respectively.
5) Repeat steps 2 through 4 until convergence criterion is satisfied. Here, we use the convergence of $G^n(E)$.
6) Repeat steps 2 thru 5 for all energies and build new $G^{n/p}_{j,j}$ distributions.
7) Repeat steps 1 through 6 until convergence criterion is satisfied. We use the convergence of the induced carrier density, Eq. (2.29), as the criterion.

For the case of AP scattering we have introduced an additional convergence loop (step 5 above) since, unlike in inelastic scattering, here the self-consistent Born calculation at a given energy is decoupled from that at all other energy values. Similar to OP scattering, we use the efficient algorithms of [74] for numerical calculations, and confirm the overall accuracy of the convergence procedure by monitoring current continuity throughout the device.
4. EFFECT OF PHONON SCATTERING IN CNT-MOSFETS

This chapter presents the simulation results for transport in CNTFETs using the NEGF formalism described in the earlier chapters. Here, we explore two specific examples: 1) the conventional operation of a CNT-MOSFET wherein the carrier transport is due to thermionic injection over the channel barrier, 2) Band-to-band tunneling transport in a CNT-MOSFET where conduction is mainly due to carrier tunneling through the quantized conduction band states in a p-type MOSFET at large positive gate biases. It should be noted that section 4.1 is adapted from our publication [35], and, section 4.2 is adapted from [38].

4.1 Effect of Phonon Scattering on Conventional Operation of CNT-MOSFETs

Dissipative transport simulations are carried out as explained in the previous chapters, and the results are compared to that with ballistic transport. Here, we first study the effects of phonon scattering on CNTFET characteristics using a (16,0) tube as a representative case. Then, we compare the diameter dependence using (16,0), (19,0) and (22,0) tubes, that belong to the mod(n-m,3) = 1 family. The device parameters (Figure 2.1 (a)) used for the simulation of OP scattering are as follows: $L_{ch} = 20\text{nm}$, $L_{SD} = 30\text{nm}$, $L_{ext} = 0$, $t_{ox} = 2\text{nm}$ (HfO$_2$ with $\kappa = 16$), and the source/drain doping $N_{SD} = 1.5/\text{nm}$. This doping concentration should be compared with the carbon atom density of $(4n/3a_{cc})$ in an (n,0) zigzag CNT, which is $\sim 150/\text{nm}$ in a (16,0) tube. For the simulation of AP scattering, a heavy doped extension region is used for better convergence of the self-consistent electrostatic solution. In this case, $L_{SD} = 20\text{nm}$, $L_{ext} = 15\text{nm}$, $N_{SD} = 1.5/\text{nm}$, and the extension doping, $N_{ext} = 1.8/\text{nm}$ are used; and all the other parameters are same as for the
previous case. Except for assisting in the convergence procedure, the effect of the heavy doped extensions on the device characteristics is negligible. It should be noted that under OP scattering we consider the impact of intra-LO, intra-RBM, and inter-LO/TA phonon modes all together simultaneously (Table 4-1). The intra-LA mode is treated under AP scattering separately.

Table 4-1. Phonon energy and e-ph coupling parameters for the CNTs used in this study

<table>
<thead>
<tr>
<th>Phonon mode</th>
<th>(16,0)</th>
<th>(19,0)</th>
<th>(22,0)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>d = 1.25nm, E_G =0.67eV</td>
<td>d = 1.50nm, E_G =0.56eV</td>
<td>d = 1.70nm, E_G =0.49eV</td>
</tr>
<tr>
<td>Intra LO</td>
<td>9.80x10^{-3} eV²</td>
<td>8.19x10^{-3} eV²</td>
<td>7.00x10^{-3} eV²</td>
</tr>
<tr>
<td>(190meV)²</td>
<td>(21meV)</td>
<td>(18meV)</td>
<td>(16meV)</td>
</tr>
<tr>
<td>Intra RBM</td>
<td>0.54x10^{-3} eV²</td>
<td>0.36x10^{-3} eV²</td>
<td>0.25x10^{-3} eV²</td>
</tr>
<tr>
<td>a,b &amp; (18meV)²</td>
<td></td>
<td>(18meV)</td>
<td>(16meV)</td>
</tr>
<tr>
<td>Inter LO/TA</td>
<td>19.30x10^{-3} eV²</td>
<td>16.26x10^{-3} eV²</td>
<td>14.13x10^{-3} eV²</td>
</tr>
<tr>
<td>(180meV)²</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Intra LA</td>
<td>2.38x10^{-3} eV²</td>
<td>2.00x10^{-3} eV²</td>
<td>1.73x10^{-3} eV²</td>
</tr>
<tr>
<td>c</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

a) e-ph coupling for optical phonons is determined according to Eq (3.11);
b) RBM energy is diameter dependent, and shown in the parentheses;
c) e-ph coupling for acoustic phonons is determined according to Eq. (3.15).
Figure 4.1 compares the $I_{DS}$-$V_{DS}$ results for the (16,0) CNTFET under ballistic transport and that with OP and AP scattering. It is seen that phonon scattering can indeed have an appreciable effect on the device ON-current: at $V_{GS} = 0.6$ V the ON-current is reduced by $\sim 9\%$ and $\sim 7\%$ due to OP and AP scattering, respectively. The relative importance of the two scattering mechanisms also shows an interesting behavior. Up to moderate gate biases the effect of AP scattering is stronger ($V_{GS} \leq 0.5$ V). At large gate biases OP scattering becomes the more important process ($V_{GS} \geq 0.6$ V). This relative behavior can be better observed in the $I_{DS}$-$V_{GS}$ results shown in Figure 4.2. Here, it is seen that up to moderate gate biases AP scattering causes a larger reduction in the device current compared to OP scattering. Furthermore, the current reduction seen in this case for OP scattering is mainly due to the low-energy RBM mode [34]. At large gate biases, however, the effect of OP scattering becomes stronger, reducing the current by $\sim 16\%$ from the ballistic level at $V_{GS} = 0.7$ V. Previous studies have shown that the strong current degradation at larger gate biases is due to high-energy OP scattering processes becoming
effective (mainly inter-LO/TA and intra-LO modes) [58, 59]. Nevertheless, the importance of AP and low-energy RBM scattering should be appreciated since these might be the relevant scattering mechanisms under typical biasing conditions of a nanoscale transistor [75].

The relative behavior of OP and AP scattering can be understood by studying Figure 4.3. It shows the energy-position resolved current spectrum, which is essentially the integrand of Eq. (2.18), under ballistic transport and OP scattering. In Figure 4.3(a), it is seen that under ballistic conditions, carriers injected from the source reaches the drain without losing energy inside the device region. There exists a finite density of current below the conduction band edge ($E_C$) which is due to quantum mechanical tunneling. In the presence of OP scattering, however, it is seen that the carriers near the drain end relaxes to low energy states by emitting phonons (Figure 4.3(b)). Nevertheless, up to moderate gate biases high-energy OP scattering does not affect the device current due to the following reason. For such biasing conditions the energy difference between the

![Figure 4.2](image.png)

Figure 4.2. $I_{DS}-V_{GS}$ for the (16,0) CNTFET at $V_{DS} = 0.3V$ under ballistic transport, OP scattering (all modes together), and AP scattering. The inset shows that acoustic phonons are more detrimental up to moderate gate biases.
source Fermi level and the top of the channel barrier, $\eta_{FS}$, is smaller than the optical phonon energy: $\eta_{FS} \ll \hbar \omega_{OP}$. Therefore, a majority of the positive going carriers (source $\rightarrow$ drain) in the channel region does not experience high-energy OP scattering, except for a minute portion in the high-energy tail of the source Fermi distribution.

On the other hand, when these carriers reach the drain end there are empty low-lying states that they scatter to. After emitting a high-energy OP, however, these carriers
do not have enough energy to surmount the channel barrier and reach the source region again. Thus, the effect of high-energy OP scattering on the device current is suppressed until backscattering becomes effective at larger gate biases for $\eta_{FS} \geq \hbar \omega_{OP}$. On the other hand, low-energy RBM phonons and acoustic phonons can effectively backscatter at all gate biases. They are the dominant scattering mechanism until high-energy OP becomes important at large biases [34, 69].

Figure 4.4 shows the energy-position resolved electron density spectrum, which is essentially the integrand of Eq. (2.15). Examining Figure 4.4(a), one can see that electrons are filled up to the respective Fermi levels in the two contact regions. In these regions, a characteristic interference pattern in the distribution function is observed due to quantum mechanical inference of positive and negative going states [32]. Quantized valence band states in the channel region are due to the longitudinal confinement in this effective potential well [32]. In the presence of OP scattering, a few interesting features are observed in Figure 4.4(b). The interference pattern seen in the contact regions are smeared due to the broadening of energy states by incoherent OP scattering. The electrons near the drain end relax down to low lying empty states, even though they are less discernible in the linear color scale employed here. More interestingly, now we observe a multitude of quantized valence band states in the channel region. Such states with energies below the conduction band edge of the drain region are observed here due to their additional broadening by coupling to the phonon bath. They were unobservable in the ballistic case since they lied inside the bandgap regions of the contact reservoirs that led to zero contact broadening, $\Gamma_{S,D} = 0$. The additional low-intensity states observed are the phonon induced side-bands of the main quantized levels originating from the variety of OP modes considered here. Carrier transport through these quantized states is indeed possible under appropriate biasing conditions, and lead to many interesting properties such as, less than 60mV/decade subthreshold operation and, phonon-assisted inelastic tunneling [36, 38]. This regime of device operation will be discussed in the next section.
Figure 4.5 explores the diameter dependence of the impact of phonon scattering in CNTFETs. As mentioned earlier, we consider the $\text{mod}(n-m,3) = 1$ type of tubes. Similar trends in the behavior can be expected for the $\text{mod}(n-m,3) = 2$ family as well [66, 67].

Here we compare the ballisticity of tubes, defined as the ratio between current under scattering and the ballistic current ($I_{\text{scatt}}/I_{\text{ballist}}$), vs. $\eta_{FS}$, defined in Figure 4.3(b). Positive
$\eta_{FS}$ corresponds to the on-state of the device at large positive gate biases, and negative $\eta_{FS}$ is for the off-state. The characteristic roll-off of ballisticity under OP scattering is seen in Figure 4.5(a) [34]. In that, the roll-off is due to high-energy OP scattering becoming effective at large gate biases. The ballisticity reduction at small gate biases is due to the low-energy RBM scattering [34].

In Figure 4.5(a) it is seen that the impact of high-energy OP scattering decreases

![Figure 4.5: Ballisticity ($I_{\text{scat}}/I_{\text{ballist}}$) vs. $\eta_{FS}$ for (16,0), (19,0) and (22,0) CNTFETs, (a) with all OP modes together, (b) with AP scattering. $\eta_{FS}$ is defined as the energy difference between the source Fermi level and the channel barrier (see Figure 4.3(b)).](image-url)
for larger diameter tubes. This can be easily understood by noting that the e-ph coupling parameter for these modes (intra-LO and inter-LO/TA) monotonically decreases with increasing diameter (Table 4-1). On the other hand, the impact of the RBM mode at low gate biases seems to be nearly diameter independent for the tubes considered here, even though there is a similar decrease in e-ph coupling for larger diameter tubes (Table 4-1). This behavior is due to the concomitant reduction of energy of the RBM mode at larger diameters that leads to an increased amount of scattering events, which ultimately cancels out the overall impact on device current.

Diameter dependence of AP scattering is shown in Figure 4.5(b). The ballisticity for larger tubes is higher due to the corresponding reduction of the e-ph coupling parameter shown in Table 4-1. They all show a slight increase in the ballisticity at larger gate biases due to majority of the positive going carriers occupying states well above the channel conduction band edge [34]. The backscattering rate is a maximum near the band edge due to increased 1D density of states and decays at larger energies [53, 55, 57]. It is seen that for all the tubes on Figure 4.5, the impact of AP scattering is stronger compared to OP scattering until the high-energy modes become effective. Under typical biasing conditions for nanoscale transistor operation, \( \eta_{FS} \) will be limited (\( \eta_{FS} \leq 0.15 \text{eV} \)) and the transport will be dominated by AP and low-energy RBM scattering [75].

### 4.2 Phonon-Assisted Inelastic Tunneling in CNT-MOSFETs

Device power dissipation has become a major challenge for the continued scaling of integrated circuits [1, 76]. One important factor contributing to the overall power dissipation is poor sub-threshold (off-state) properties of modern transistors. This has led to large sub-threshold leakage currents, and it has limited the ability to scale the power supply voltage (\( V_{DD} \)), which has been the preferred way to decrease power dissipation in modern integrated circuits [76]. The sub-threshold swing (\( S \)) for conventional transistors, which determines how effectively the transistor can be turned off by changing the gate
voltage ($I_{DS}$ vs. $V_{GS}$), has a fundamental limit of $S = 2.3 \times k_B T / q \text{ mV/decade} \approx 60 \text{mV/dec}$ at room temperature, where $k_B$ is the Boltzmann constant, $T$ the temperature, and $q$ the electron charge [77]. The need to maintain a certain ratio of on-current to off-current limits scaling of the power supply voltage, aggravating heat dissipation problems in modern high-performance circuits.

The aforementioned limitations on the off-state performance of conventional transistors equally apply to those based on carbon nanotubes (CNTs): both Schottky-barrier transistors (SB-CNTFETs) and metal-oxide-semiconductor field-effect transistors (CNT-MOSFETs) with doped source/drain contacts [78-81]. It has been experimentally observed that carrier transport in CNTs can be nearly ballistic [47, 48, 82]. High-performance CNT transistors operating close to the ballistic limit have also been demonstrated [13-15]. Recently, p-type CNT-MOSFETs with near ideal gate control and sub-threshold operation close to the fundamental limit of $S \approx 60 \text{mV/dec}$ at negative gate voltages ($V_{GS}$) have been reported [41, 42]. At positive voltages, these CNT-MOSFETs begin to turn on again with a swing of 40~50mV/dec which is smaller than the conventional limit of 60mV/dec. This regime of operation is attributed to band-to-band tunneling (BTBT) [36, 41], and should be distinguished from the ambipolar operation in SB-CNTFETs where the ambipolar branch is due to opposite type of carrier injection (electrons in the case of p-type FETs) from the drain Schottky contact [80, 83]. Specialized device geometries including that based on BTBT have been actively investigated to obtain improved sub-threshold performance in CNT-MOSFET transistors [37, 84]. Here we present detailed theoretical simulations for the BTBT operation of CNT-MOSFETs using the NEGF formalism described earlier for both ballistic and dissipative quantum transport. Comparing these results with the recently reported data in Ref. [42], we provide compelling evidence that the BTBT operation of CNT-MOSFETs is strongly affected by phonon-assisted tunneling.
The idealized device structure used in this study, shown in Figure 2.1 (a), is a p-type CNT-MOSFET with wrap-around high-k (HfO$_2$ $\sim$ $\kappa$ = 25) gate dielectric with thickness $t_{OX}$ = 2nm, p-doped source/drain regions ($N_{S/D}$ = 0.6/nm) with $L_{SD}$ = 40nm, $L_{ext}$ = 0, and an intrinsic channel length of $L_{ch}$ = 30nm. A zigzag (16,0) CNT with diameter $\sim$ 1.2nm and bandgap $\sim$ 0.7eV is considered. The CNT-metal contacts at the ends of source/drain regions are assumed to be Ohmic, with perfect transparency for carrier transport. In experimental devices the Ohmic contacts with electrostatically induced doping is achieved through a back-gated geometry [41, 42, 85]. Although the device structure is idealized, the device parameters are in agreement with those in Ref. [42]. Our simulations are performed for p-type CNT-MOSFETs in correspondence with experiments [42]. Due to the symmetry of conduction and valence bands in CNTs [8], the simulated $I$-$V$ curves for n-type and p-type transistors are expected to coincide after reversing the polarity of voltages; and indeed we have verified this equivalence.

The NEGF calculations for dissipative transport are performed self-consistently with electrostatic simulations as described in previous chapters. We use the nearest neighbor $p_z$ tight-binding Hamiltonian ($H_{p_z,TB}$) to describe the CNT electronic structure [8, 21]. The simulations are carried out in the mode-space, considering transport through the first conduction and valence subbands ($E_{C1}$ and $E_{V1}$), respectively [49]. The difference of energy to the next highest subbands, i.e. $|E_{C2}-E_{C1}| = |E_{V2}-E_{V1}|$, is about 370meV so the transport through higher subbands can be neglected for typical biasing conditions.

In this study we include both one-phonon and two-phonon scattering processes in our simulation. For the (16,0) CNT and the longitudinal optical (LO) phonon mode considered in here, $\hbar\omega_{LO}$ = 195meV and $R_{OP}$ = 0.01eV$^2$, respectively (Table 4-1). Two-phonon scattering is included similarly, with the phonon energy replaced by $\hbar\omega_{2-ph}$ = 360meV, corresponding to 180meV zone-boundary optical phonons, and the coupling parameter related to that of the one-phonon transition via [86],
\[ R_{e-2ph}(E) = R_{OP} \frac{2\Gamma_{OP}}{\Gamma_{tot}(E \pm h\omega_{2ph}/2)}, \]  

where \( \Gamma_{OP} \) is the one-phonon broadening and \( \Gamma_{tot} \) is the total broadening due to scattering and the source/drain reservoirs defined in Eqs. (2.6) and (3.9).

We have performed self-consistent NEGF calculations for both ballistic (\( \Sigma_{scat} = 0 \)) and dissipative (\( \Sigma_{scat} \neq 0 \)) transport using the efficient numerical algorithms reported in Ref. [74]. The simulation results are compared against the data reported in Ref. [42]; the relevant experimental \( I_{DS}-V_{GS} \) plot is reproduced in Figure 4.6 for the sake of completeness. In examining Figure 4.6 we can observe a few important features of the p-type CNT-MOSFET operation: 1) near ideal (\( S \approx 60 \text{mV/dec} \)) sub-threshold behavior under conventional MOSFET operation for negative \( V_{GS} \) biases, 2) larger on-currents for the conventional operation compared to BTBT regime, 3) \( S \approx 50 \text{mV/dec} \) (\(< 60 \text{mV/dec conventional limit}) is observed for BTBT transport at \( V_{DS} = -0.01 \text{V} \). The BTBT sub-threshold swing, however, degrades with increasing \( V_{DS} \) biases. 4) The onset of BTBT occurs at a smaller \( V_{GS} \) with increasing \( V_{DS} \), i.e., the onset \( V_{GS} \) bias point moves left on

![Graph](image.png)

Figure 4.6. Experimental \( I_{DS}-V_{GS} \) data at different \( V_{DS} \) biases for the p-type CNT-MOSFET; reproduced from Ref. [42].
Figure 4.6 with increasing $V_{DS}$. Similar experimental characteristics for BTBT operation in p-type CNT-MOSFETs have also been observed by J. Appenzeller et al. at IBM T. J. Watson Research Center (personal communication). These experimental device characteristics will be compared against our computational results in order to elucidate the transport mechanisms.

Ref. [36] presents a detailed study of the BTBT operation in a CNT-MOSFET, and here we summarize the transport mechanism responsible for it. Figure 4.7 (a) and (b) depict the two main mechanisms for BTBT transport in p-type CNT-MOSFETs with sufficiently short channel lengths. For such devices, due to longitudinal confinement

![Figure 4.7](image)

Figure 4.7. BTBT operation in a p-type CNT-MOSFET: (a) For large positive $V_{GS}$, direct tunneling of electrons from drain to source through the quantized conduction band states in the channel region, (b) For moderately positive $V_{GS}$ direct tunneling is prohibited, but inelastic tunneling is possible in the presence of optical phonons (dashed arrows), (c) NEGF simulation results for energy-position resolved current density spectrum (logarithmic scale) under 195meV LO phonon scattering at $V_{GS} = 0.4V$, $V_{DS} = -0.3V$. 
inside the channel region, we observe quantized states in the conduction band. As shown in Figure 4.7(a), at sufficiently large positive gate biases these quantized states align with filled states of the valence band in the drain region, and direct (resonant) tunneling to the source region becomes possible. This alignment has a sharp onset, thus leading to steep sub-threshold slopes in $I_{DS}-V_{GS}$ characteristics [36]. This can be further understood by observing the hole Fermi distribution in the source region, noting that carrier conduction is equally explained through hole transport from source to drain. Here, bottom of the hole Fermi distribution in the source is cut off by the valence band edge, and the top is cut off by the conduction band edge in the channel. The result is a cooler current-carrying distribution, which leads to a smaller subthreshold swing. For moderate gate biases, as shown in Figure 4.7(b), direct tunneling through the conduction band states is prohibited, and the current will be dominated by thermionic emission of holes under the channel barrier in the valence band.

If we take into consideration high-energy optical phonon scattering, another transport channel is possible via phonon-induced virtual states as shown by the dashed arrows in Figure 4.7(b). In this case, for BTBT to occur, only the phonon virtual state needs to align with the empty valence band states in the source, and the drain bias should be large enough to allow the quantized conduction band states to be filled by the drain. The existence of the two transport channels is inferred from energy-position resolved current density spectrum in Figure 4.7(c). Thus, it can be expected that in the presence of optical phonons the onset of BTBT transport will begin at a smaller gate bias, and the device $I$-$V$ characteristics will be different from those expected in the ballistic case [36].
Figure 4.8 (a) shows the simulated $I_{DS}$-$V_{GS}$ characteristics under ballistic transport for the p-type CNT-MOSFET studied here. It is seen that the sub-threshold swing for regular MOSFET operation (negative $V_{GS}$ for p-type devices) is indeed at the theoretical limit of 60mV/dec, which is not surprising given the wrap-around gate geometry we have employed in our simulations. The on-current for regular operation is also larger than that for the BTBT operation. The overall device currents observed in our simulator, however, are larger than the experimental ones, which can be attributed to contact resistance in the experiment. The simulated sub-threshold swing in the BTBT regime is $S \approx 20$mV/dec at $V_{DS} = -0.01$V. Under ballistic transport, the steep slope for BTBT regime does not degrade for large $V_{DS}$, contrary to the experimental results in Figure 4.6. More
importantly, the onset of BTBT transport moves to more positive gate voltages with increasing \( V_{DS} \), i.e. to the right, as shown in Figure 4.8 (a). This behavior under ballistic transport is well understood and is attributed to the “charge pile-up”, or, “floating body” effect [70, 76]. As shown in Figure 4.7(b), under ballistic conditions at large \( V_{DS} \) and moderate \( V_{GS} \), the conduction band states are not aligned with the empty source states but are aligned with filled states in the drain. Carriers can tunnel into these states, resulting in a pile-up of electrons. Their potential causes the bands in the channel to move up, thus requiring an even larger positive gate bias before the onset of BTBT. As a result, the onset point in Figure 4.8(a) moves right to larger gate voltages with increasing \( V_{DS} \) in complete disagreement with the experimental observations.

Figure 4.8 (b) shows the simulated \( I_{DS}-V_{GS} \) results for the model p-type CNT-MOSFET in the presence of phonon scattering. The sub-threshold swing at \( V_{DS} = -0.01V \) for the steepest section of the BTBT transport is \( S \approx 35\text{mV/dec} \), which is poorer compared to the ballistic case [36]. It is also observed to further degrade with increasing \( V_{DS} \), in agreement with the experimental observations in Figure 4.6. Also, the onset of BTBT transport occurs at more negative \( V_{GS} \) (moves to the left) with increasing \( V_{DS} \), which is also in agreement with the experimental data. This shift in the onset of BTBT to lower voltages is due to phonon-assisted transport starting at more negative gate biases for larger \( V_{DS} \). It is also important to note that in the presence of optical phonons, the charge pile-up effect discussed earlier is suppressed since the conduction band states are constantly emptied into the source due to inelastic tunneling (see Figure 4.7(b)). At this point, by comparing the experimental data with ballistic \( I-V \) results versus that with optical phonon scattering, it is clear that the former completely fails to explain the observed BTBT features, while the inelastic transport simulation seems to be essential for the correct description. The value for the on-current in BTBT operation (at \( V_{GS} = 0.6V \)) with and without scattering, however, is very similar since at large positive gate biases the device current is mainly determine by the direct tunneling component. Thus, it is apparent that the BTBT operation of CNT-MOSFETs is governed by phonon-assisted transport,
and dominates the sub-threshold characteristics in this regime. At this point it should be noted that elastic scattering due to acoustic phonons is not expected to affect the BTBT sub-threshold swing which is mainly determined by the inelastic tunneling due to optical phonons. The saturation current in the BTBT regime, however, can be reduced by acoustic phonon back-scattering when such events become allowed by energy conservation. It should also be pointed out that our simulations show slight reduction of the BTBT on-current at large gate biases, $V_{GS} > 0.6$V. This reduction is, however, smaller than that seen in Figure 4.6 at low drain biases.

The device operation under large drain biases is discussed next. The solid-triangle curve of Figure 4.9 shows the $I_{DS}$-$V_{GS}$ relationship for the model p-type CNT-MOSFET at $V_{DS} = -0.6$V under 195meV LO phonon scattering. It is seen that, due to the charge pile-up effect at such a high drain bias, the onset of BTBT is pushed to larger positive voltages (right). On the other hand, Figure 4.6 indicates that the experimentally observed onset of BTBT does not show such effects at large drain biases, and may move further left to smaller gate voltages. Examining Figure 4.7 (b), it is clear that the onset of BTBT can be

Figure 4.9. Simulated $I_{DS}$-$V_{GS}$ with only one-phonon scattering due to 195meV zone center LO mode (solid lines) and, also including two-phonon scattering due to 2 x 180meV zone-boundary mode (dashed lines). Red-star, blue-circle, and green-square curves are at the same voltages as in Figure 4.8 (b), magenta-triangle curves are at $V_{DS} = -0.6$V.
moved left to smaller gate biases if there are higher energy optical phonons that could allow inelastic tunneling. The highest energy optical phonons available in CNTs, however, are the ~195meV LO mode. On the other hand, Raman scattering experiments on CNTs report strong evidence for multi-phonon mediated processes (overtones) [87, 88]. For example, the $G'$-band, attributed to two-phonon Raman scattering involving the zone-boundary optical phonons, is observed to have similar intensities compared to the $G$-band arising from the zone-center LO phonons [87, 88]. The $I_{DS}-V_{GS}$ results obtained with inclusion of two-phonon scattering are shown by the dashed curves in Figure 4.9. One can see that at small drain biases, it produces a negligible difference due to Pauli blocking of the two-phonon scattering mechanism. At larger drain biases (exceeding the energy of two phonons), this mechanism becomes effective. For such drain biases the device current near the onset of BTBT is dominated by two-phonon assisted tunneling due to one-phonon process being energetically inactive, and, the relatively strong e-ph coupling for multi-phonon mediated processes in CNTs, a fact observed in Raman experiments [87]. In Figure 4.9 the onset of BTBT is indeed moved to lower voltages (i.e. moves left) compared to the one-phonon case, and the overall $I-V$ characteristics look even closer to the experimental data. Thus, it can be concluded that at large drain biases multi-phonon assisted inelastic tunneling might also become important for BTBT transport in CNT-MOSFETs.

In summary, we have performed detailed simulations for BTBT operation of CNT-MOSFETs using both ballistic as well as dissipative quantum transport. By comparing the simulation results with the experimental data, we conclude that the BTBT regime is dominated by optical phonon-assisted inelastic transport. It also appears that under large biasing conditions, multi-phonon scattering may also become important. The strong effect of optical-phonons on BTBT transport should be contrasted with conventional CNT-MOSFET operation, where their influence is found to be marginal up to moderate biases [34, 69]. It is observed that BTBT operation can indeed produce sub-threshold swings below the conventional limit of 60mV/dec, which makes these devices
attractive for low-power applications. The sub-threshold properties, however, are found to severely degrade under typical biasing conditions, and sensitively depend on phonon energies, device geometry, source/drain doping, etc [36].
5. INFLUENCE OF PHONON SCATTERING IN CNT P-I-N TUNNEL TRANSISTORS

Field-effect transistors based on the band-to-band tunneling (BTBT) mechanism have recently gained a lot of interest due to their potential to reduce power dissipation. In the previous chapter (section 4.2) we observed that BTBT in CNT-MOSFETs can lead to less than 60mV/dec subthreshold swing, but the device characteristics severely degrade due to phonon assisted inelastic tunneling. This chapter presents a BTBT FET based on a different device structure; gated p-i-n geometry. Section 5.1 elaborates on the motivation for this device geometry. Section 5.2 discusses ballistic operation of this device, followed by the influence of phonon scattering on device characteristics for on-state operation (section 5.3) as well as subthreshold operation (section 5.4). This chapter is adapted from our publications [37, 39, 40].

5.1 Background on p-i-n Tunnel Transistors

With the continual miniaturization of the MOSFET transistors power dissipation in integrated circuits has become a major roadblock to performance scaling [1]. For more than 30 years numerous breakthroughs in device and material design have sustained an exponential increase in system performance [89]. Recent introduction of high-k gate oxides into semiconductor technology has also allowed much needed reduction in gate leakage, and improved the scalability of future devices [2]. Nevertheless, the physical operational principles of conventional MOSFETs, based on the thermionic emission of carriers over a channel barrier, have imposed fundamental limits on voltage scaling and the reduction of energy dissipation [89]. The subthreshold swing (S) of a conventional MOSFET, which determines the ability to turn off the transistor with the gate voltage
(VGS), has a fundamental limit of $2.3 * (k_BT/q)$ where $k_B$, $T$, and $q$ are the Boltzmann constant, temperature, and the elementary charge, respectively ($S = 60$ mV/decade at room temperature) [77]. Therefore, the requirement of achieving a large on-state current ($I_{ON}$), while maintaining a small off-state leakage ($I_{OFF}$), has hindered the scaling of the power supply voltage ($V_{DD}$) in recent years [1]. Consequently, a device with $S$ below the aforementioned conventional limit is desirable for continued voltage scaling, and thereby reducing power dissipation in circuits.

In this regard, field-effect transistors based on the band-to-band tunneling (BTBT) phenomenon have been actively investigated due to their potential for low standby leakage [90-97]. It has been predicted through detailed device simulations that BTBT FETs could produce subthreshold swings below the thermal limit in conventional semiconductor materials such as silicon [98-101], as well as in carbon nanotube (CNT) based transistors [36, 37, 84, 102, 103]. Indeed, this has been experimentally demonstrated in CNTs [41, 42, 104], and more recently, with a silicon based BTBT FET [105]. At this point it should be noted that there are two main device structures used in BTBT transistors; a popular $p$-$i$-$n$ geometry reported in [37, 84, 90-94, 96, 98, 100-105] (hereafter called the TFET), and the MOSFET geometry used in [36, 41, 42, 97]. In the case of CNT-MOSFETs [41, 42] it has been established that BTBT is dominated by phonon assisted inelastic tunneling that severely deteriorates the device characteristics [36, 38]. On the other hand, phonon scattering has a much moderated effect on TFETs, and useful device properties are preserved under practical biasing conditions [37, 39].

The objective of this chapter is to identify the physical mechanisms that limit the performance of a BTBT FET; specifically, the maximum on-state current, off-state current, and the steepness of the on-off transition. The next chapter addresses the important task of a comprehensive comparison of device performance between the $p$-$i$-$n$ TFET and the conventional $n$-$i$-$n$ MOSFET geometries. Here, we use CNTs as the model channel material due to many benefits of that system as summarized below. CNTs allow
1-dimensional carrier transport without depletion capacitance effects, and high performance transistors that operate near the ballistic limit have already been demonstrated [13-15]. They also have a direct energy bandgap and small carrier effective masses that are conducive to BTBT devices [8]. Furthermore, a detailed simulation framework has been developed for modeling carrier transport through CNT transistors [35, 71, 72, 106], and benchmarked against experiments [14, 38, 72]. Therefore, p-i-n TFET operation can be comprehensively explored using CNTs as the channel material, realistically treating effects such as phonon scattering. Although we use the CNT as a model channel material, the general conclusions are expected to be broadly applicable to this class of devices fabricated in different materials.

### 5.2 Ballistic Operation of p-i-n TFETs

Section 4.2 described the BTBT operation in CNT-MOSFETs, wherein it was

![Figure 5.1. (a) Gated CNT p-i-n Tunnel FET with wrapped around high-k cylindrical gate geometry, (b) Equilibrium band diagram for the p-i-n Tunnel FET. A (13,0) zigzag CNT with $E_G \approx 0.8$eV is being used.](image)
found that phonon-assisted inelastic tunneling dominated the device characteristics. That led to a severe degradation of the desirable subthreshold properties such as the steep subthreshold slope. The BTBT device described in section 4.2 suffers from two additional geometrical properties that limit its performance: 1) presence of two tunneling barriers, 2) longitudinal quantization of the electronic states in the channel region that reduces the density of states for carrier conduction. Both these properties detrimentally affect the device current, thus limiting its performance. These limitations imposed by the CNT-MOSFET structure can be circumvented by using a p-i-n based device geometry ([37] and references therein, [84]).

The CNT p-i-n Tunnel FET shown in Figure 5.1 (a) has a wrapped-around high-k gate oxide and, doped source (p-type) and drain (n-type) regions. The equilibrium band diagram is shown in Figure 5.1 (b). Ballistic NEGF simulations have been performed as described in Chapter 2. Figure 5.2 shows some specific results for the p-i-n device under on-state biasing conditions. Figure 5.2 (a) is the energy-position resolved electron density, which is essentially the integrand of Eq. (2.15). It clearly shows that electrons in the p-type source region are filled up to the Fermi level ($E_{F1}$) which is below the valence band edge. Similarly, electrons in the n-type drain are filled up to $E_{F2}$ which is above the

![Figure 5.2.](image)

Figure 5.2. (a) Energy-position resolved electron density distribution, (b) Energy-position resolved current density distribution (log scale).
conduction band edge. Under the on-state biasing conditions, we apply a positive drain bias and a positive gate bias which pushes down the bands in the channel region. As seen in Figure 5.2 (a), a tunneling barrier opens up near the source-channel junction and a net device current flows. This can be clearly seen in Figure 5.2 (b) which is an energy-position resolved current density distribution, i.e: the integrand of Eq. (2.18). At this point, comparing Figure 5.2 (b) and Figure 4.7 (c), the benefits of the p-i-n Tunnel FET geometry are evident. Unlike in the CNT-MOSFET, the new geometry has only one tunneling barrier. Furthermore, the electronic states in the channel region are not quantized in the latter geometry, resulting in an increased density of states. Both these features are expected to improve the device current compared to BTBT in the CNT-MOSFET geometry, thus increasing performance. It is important to note that the p-i-n Tunnel FET geometry can lead to ambipolar transport characteristics. This can be easily understood by observing Figure 5.2 for the case of a negative gate bias, in the direction of turning off the device. Under such biasing conditions the bands in the channel will be pulled up, and a tunneling barrier will appear at the drain-channel junction. Carriers will tunnel through this junction giving rise to an ambipolar current. In this regard, the CNT p-i-n Tunnel FET has similar behavior compared to the Schottky-barrier CNTFET operation [83].
5.3 Influence of Phonon Scattering on Above-Threshold Operation

The modeled CNT $p-i-n$ TFET structure with wrap-around gate used for this study is similar to that in Figure 5.1 (a). A (16,0) zigzag CNT with high-k HfO$_2$ ($k = 16$, $t_{ox} = 2$nm) gate oxide, intrinsic channel ($L_{ch} = 20$nm), doped source (p-type, $N_S = 0.75$/nm, $L_S = 35$nm) and drain (n-type, $N_D = 0.75$/nm, $L_D = 35$nm) have been used with $L_{cut} = 0$nm.
Source/drain doping levels can be compared to the carbon atom density in a (16,0) CNT of 150.2/nm. OP scattering by 190meV longitudinal optical (LO) mode, 180meV zone-boundary (ZBO) mode, and 21meV radial-breathing mode (RBM) have been considered. Acoustic phonon (AP) scattering is by the longitudinal acoustic (LA) mode. The relevant e-ph coupling parameters for the (16,0) CNT can be found in Table 4-1 [35]. Figure 5.4 (a) compares the output characteristics, $I_{DS}$-$V_{DS}$, of the CNT p-i-n TFET under ballistic and dissipative transport. Here, it is seen that the influence of OP scattering (green dash-dot) becomes important only at large gate biases, even though the high-energy modes (LO and ZBO) have the strongest e-ph coupling [35]. Up to moderate gate biases, the current reduction is mainly due to carrier backscattering by AP and low-energy (RBM) phonon modes. Similar behavior on the influence of phonon scattering on the above-threshold operation of CNT-MOSFETs has already been reported [34, 35], and can be easily understood as follows.
In order to have current reduction due to scattering by high-energy phonons, a majority of forward going carriers (source → drain) should be backscattered into empty backward going states by OP emission. Thus, the energy requirements for effective backscattering depends on the condition, \( (E_{FS} - E_{C-channel}) = \eta_{FS} \geq \hbar \omega \), where \( E_{FS} \) and \( E_{C-channel} \) are the source Fermi level, and the channel conduction band position, \( \eta_{FS} \) are the scattering parameter, and \( \hbar \omega \) is the phonon energy.

Figure 5.4. (a) Above-threshold \( I_{DS} - V_{DS} \) characteristics for the CNT \( p-i-n \) TFET. All the optical phonon modes (LO, ZBO, and RBM) are considered simultaneously for OP scattering. LA mode is considered for AP scattering. (b) Energy-position resolved current density spectrum (i.e., integrand of Eq. (2.18)) at \( V_{DS} = V_{GS} = 0.5V \) confirms the reduced influence of high-energy OP scattering on DC current transport up to moderate gate biases.
respectively (see Figure 5.4 (b)) [34]. This is further exemplified in the energy-position resolved current density spectrum shown in Figure 5.4 (b). After reaching the drain region, however, carriers can be efficiently scattered by OP emission down to empty low-lying states, and thus will not possess enough energy to surmount the channel barrier and reach the source region again. On the other hand, elastic scattering due to acoustic and low-energy phonons can effectively backscatter at all gate biases, and is the dominant mechanism until high-energy OP scattering becomes effective at larger gate biases. Therefore, in Figure 5.4 (a) above-threshold performance is only moderately affected by phonon scattering. We observe, however, a lower value of the on-current (by about 4~10x) in the CNT p-i-n TFET compared to that of conventional CNT-MOSFETs [34, 35] due to the presence of the tunneling barrier. This observation confirms that the on-state performance of p-i-n TFETs is mainly dominated by the tunneling barrier properties, and moderately affected by the channel itself [98, 100, 103].

5.4 Influence of Phonon Scattering on Subthreshold Operation

The subthreshold (off-state) operation is discussed next. Figure 5.5 (a) shows the transfer characteristics, $I_{DS}-V_{GS}$, for the CNT p-i-n TFET. Note that only the 180meV ZBO phonon mode, with strongest e-ph coupling, is included here since the subthreshold properties are observed to be mainly determined by this mode. In Figure 5.5 (a) it is seen that the p-i-n TFET has ambipolar behavior, which can be easily understood by observing Figure 5.4 (b). For small gate biases (or negative biases), the bands in the channel are pulled up, and a tunneling path appears at the channel-drain junction leading to ambipolar transport. As expected, the ambipolar branch appears earlier for larger drain biases. For identical source/drain doping concentrations the $I_{DS}-V_{GS}$ curves are symmetric around the minimum point. Asymmetric doping schemes can, however, suppress the ambipolar branch up to larger gate biases and lead to more desirable device characteristics [37]. It should be noted that, unlike in a conventional MOSFET, the subthreshold swing ($S$) of a p-i-n TFET is not a constant, but is bias dependent as seen in Figure 5.5 (a) [98, 99, 103]. Interestingly, we observe less than 60mV/dec $S$ at room temperature for both ballistic and
dissipative transport (blue solid and red dashed curves); in our model device, $S < 60\text{mV/dec}$ is obtained for $V_{GS} < 0.32\text{V}$ (left of dashed vertical line).

In Figure 5.5 (a) it is evident that the presence of OPs has a significant detrimental effect on the subthreshold properties; a minimum $S$ of $20\text{mV/dec}$ for ballistic transport (at $V_{DS} = 0.1\text{V}$) degrades to $35\text{mV/dec}$ in the presence of OPs at room temperature ($T = 300\text{K}$). The degradation is even greater at higher device temperatures; minimum $S \geq 40\text{mV/dec}$ at $T = 400\text{K}$ ($V_{DS} = 0.1\text{V}$). The main reason for such deterioration of $S$ is due
to phonon absorption assisted transport as exemplified in Figure 5.5 (b). Under the ballistic approximation, the minimum off-state current is mainly due to direct source to drain tunneling through the channel barrier region, and can be made very small; longer channel lengths, $L_{ch}$, further suppresses the off-current, and $S < 10\text{mV/dec}$ can be achieved for ballistic transport. Under such biasing conditions, however, higher-order processes such as phonon absorption assisted transport become significant, and tend to dominate the off-state characteristics. From Eqs. (3.7) and (3.8) it is seen that the phonon absorption assisted process is proportional to the phonon occupation number, $n_\omega$, and increases at higher device temperatures (Eq. (3.3)). Thus, even though the direct tunneling processes are expected to be fairly temperature independent [98, 99, 103], higher-order processes such as phonon assisted transport that are temperature dependent can become important in the off-state of a BTBT device as seen here. They could also limit the desirable off-state characteristics that could have been achieved otherwise. At the same time, the on-state performance of the CNT $p-i-n$ TFET is observed to be relatively temperature insensitive, and can be attributed to the fact that the above-threshold transport is mainly due to direct tunneling. In indirect bandgap semiconductors, such as technologically important silicon and germanium, BTBT would be mainly due to phonon assisted transport [107, 108], and could have strong temperature dependence both in the off-state as well as the on-state.

In summary, we observe less than $60\text{mV/dec}$ subthreshold swings in $p-i-n$ TFETs, in contrast to that in conventional (e.g. $n-i-n$) MOSFETs operating in the over-the-barrier conduction regime. The on-current of $p-i-n$ TFETs is, however, mainly dependent on the tunneling barrier properties, and phonon scattering has only a moderate effect. On the other hand, the subthreshold operation is dominated by phonon assisted transport, and exhibits significant temperature dependence. Nevertheless, the low subthreshold swing is robust and persists even with the inclusion of phonon scattering and under higher source-to-drain biases.
6. PERFORMANCE COMPARISON BETWEEN CNT BASED P-I-N TUNNEL FET AND CONVENTIONAL MOSFET GEOMETRIES

A detailed description of the operation of CNT based p-i-n Tunnel FETs (TFETs) was presented in the previous chapter. The influence of phonon scattering on the subthreshold operation as well as the on-state performance was discussed. It was seen that phonon assisted tunneling tends to degrade the desirable subthreshold characteristics of TFETs. It also resulted in increasing the off-state leakage current at higher temperatures. Under on-state operation, phonon scattering had a relatively small effect on device current. The presence of the tunneling barrier itself was more detrimental towards the current drive capability. Therefore, it is important comprehensively compare the p-i-n device performance to the conventional MOSFET operation under realistic transport conditions. This will allow us to understand the true potentials of the p-i-n geometry over the conventional MOSFET, and any shortcomings that need to be addressed before it can become a useful device technology.

In this chapter we address this important task of a comprehensive comparison between the two geometries. We use CNTs as the model channel material due to many benefits of that system as described in section 5.1. Previous work has also compared CNT transistor performance to that of silicon transistors [109-111] and to that based on silicon nanowires [112]. Here we use similar device metrics to compare the performance between TFETs and MOSFETs using a uniform simulation environment for both the devices. Note that this chapter is adapted from [40].

The model device structure used in this study, shown in Figure 6.1, has a cylindrical wrap-around gate and doped source/drain regions. In this study we have
modified the device structure from that in Figure 5.1 (a) by removing the high-k oxide from the source/drain regions. It has been observed that having high-k gate oxide over the doped source region increases the source-channel fringing fields that result in smaller tunneling currents in the case of TFETs. Therefore, in this study we remove the high-k oxide from the source/drain regions as shown in Figure 6.1 (in realistic device fabrication these regions could be filled with a low-k spacer dielectric). We use the following device parameters and $T = 300\text{K}$ unless specified otherwise. A (13,0) zigzag CNT with intrinsic channel length, $L_{ch} = 15\text{nm}$, doped source/drain regions with $L_{S,D} = 20\text{nm}$, high-k HfO$_2$ oxide ($k = 16$) with $t_{OX} = 2\text{nm}$ have been used. Source/drain linear doping concentration is $0.8/\text{nm}$ which can be compared with the carbon atom density for a (13,0) CNT of $122/\text{nm}$. When comparing the two device geometries the source region is doped either $p$- or $n$- type accordingly, keeping all other parameters identical.

### 6.1 Comparison of the Off-State Operation

The subthreshold characteristics for the two device geometries are compared first. Here we look into the off-state current that determines the standby leakage and standby power dissipation ($P_{\text{standby}}$), as well as the influence of phonon scattering on subthreshold
operation for the two devices. Drain induced degradation of subthreshold characteristics, which is important for highly scaled devices, is also discussed.

6.1.1 Subthreshold slope, off-current ($I_{OFF}$), and standby power dissipation ($P_{standby}$)

One of the main attractions for BTBT transistors has been their potential to reduce

![Figure 6.2](image)

**Figure 6.2.** $I_{DS}-V_{GS}$ dependence on temperature for, (a) $n-i-n$ MOSFET and, (b) $p-i-n$ TFET under ballistic and dissipative transport. The latter has reduced temperature dependence under ballistic conditions. Phonon assisted tunneling can, however, degrade the subthreshold characteristics.
off-state leakage, and in turn, standby power dissipation ($P_{\text{standby}}$) in circuits. This is achieved through subthreshold operation with $S$ below the conventional limit in these devices. Figure 6.2 compares the temperature dependence of the transfer characteristics ($I_{DS}$-$V_{GS}$) for the two geometries. The ballistic results (solid curves) are discussed first. In Figure 6.2 (a) it is observed that we obtain ideal subthreshold operation with $S = 60\text{mV/dec}$ (at $T = 300\text{K}$) due to the superior electrostatic control by the wrap-around gate. At higher temperatures, however, $S$ degrades proportionately. This can be easily understood by observing Figure 6.3 (a) showing the thermionic emission mechanism in the off-state of a conventional MOSFET. The high energy tail of the Fermi distribution grows with temperature as $\sim \exp\left(-E/k_BT\right)$ leading to the aforementioned degradation of $S$. Furthermore, in integrated circuits this results in higher off-state leakage currents and $P_{\text{standby}}$. This could lead to a positive feedback mechanism between the two, known as thermal runaway, that could ultimately destroy the circuit [113].

On the other hand, the ballistic results for the TFET (Figure 6.2 (b)) clearly shows $S < 60\text{mV/dec}$ operation at room temperature. This is easily understood by examining Figure 6.3 (b) where the high energy tail of the Fermi distribution for electrons lies inside the $p$-type source bandgap region. Therefore, when the conduction band in the channel is pulled above the valence band of the source, an abrupt reduction in device current is
expected, which leads to $S$ values much smaller than the conventional limit [103]. In Figure 6.2 (b) an interesting observation is that the off-state current under ballistic transport does not significantly degrade at elevated temperatures. This is due to the elimination of high energy thermal injection within the source bandgap region. There is a slight increase in subthreshold current at higher temperatures related to the broadening of

![Figure 6.4. $I_{OFF}$ vs. $I_{ON}$ dependence on temperature at $V_{DD} = 0.3V$ under, (a) ballistic and, (b) dissipative transport. Shaded region is where the $p-i-n$ TFET has an advantage over the $n-i-n$ MOSFET due to larger $I_{ON}$ with a smaller $I_{OFF}$. Temperature dependence of $I_{OFF}$ for the $p-i-n$ TFET is also smaller than that for the latter.](image-url)
the Fermi distribution near $E_{FS}$ (see Figure 6.3 (b)). The possibility of achieving off-stage leakage currents that do not degrade at higher temperatures is an attractive feature of TFETs that could potentially alleviate the thermal runaway problem mentioned earlier.

The relative benefits of the TFET over the MOSFET geometry in the off-state can be better compared through the $I_{OFF}$ vs. $I_{ON}$ (at a constant $V_{DD}$) results shown in Figure 6.4 (a) for ballistic operation. Here, the $I_{OFF}$-$I_{ON}$ curves are generated by scanning the $I_{DS}$-$V_{GS}$ results in Figure 6.2 with a constant $V_{DD}$ bias window as explained in Ref. [109]. In Figure 6.4 (a) the increase in $I_{OFF}$ at smaller $I_{ON}$ values ($I_{ON} \leq 0.6 \mu A$/tube) observed for the TFET is due to ambipolar conduction seen in Figure 6.2 (b). Figure 6.4 (a) clearly shows the suppression of $I_{OFF}$ degradation at higher temperatures under ballistic transport in the case of TFETs compared to MOSFETs. Furthermore, the shaded region of Figure 6.4 (a) corresponds to the range of device biasing conditions where the TFET has the benefit over the MOSFET. Within this region it is observed that the former has a smaller $I_{OFF}$ (thus smaller $P_{standby}$) at a given $I_{ON}$ (looking vertically). Conversely, the TFET can deliver a larger $I_{ON}$ at a given $I_{OFF}$ (looking horizontally). It is noted that in this region the TFET can only deliver a few $\mu A$ of drive current per CNT. Therefore, these devices might be better suited for low power applications with moderate drive current requirements.

### 6.1.2 Comparative influence of phonon scattering

The influence of phonon scattering on the transfer characteristics is shown by the dashed curves of Figure 6.2 (see Refs. [34, 36, 38, 39] for detailed information on each geometry). In Figure 6.2 (a) it is observed that phonon scattering has only a small effect on the subthreshold properties of the MOSFET which are dominated by the thermionic emission component of current conduction. Nevertheless, at small gate biases the onset of ambipolar conduction is seen due to phonon assisted inelastic tunneling that turns on BTBT in CNT-MOSFETs at an earlier voltage [36, 38]. In the case of the TFET in Figure
6.2 (b) it is observed that $S$ degrades in the presence of phonon scattering even though $S < 60\text{mV/dec}$ is still attained. This deterioration is due to phonon absorption assisted transport playing an important role under off-state biasing conditions (see Figure 6.3 (b) and Figure 5.5 (b)) [39]. More importantly, the subthreshold current becomes temperature dependent due to larger phonon occupation (eq. (3.3)) at higher temperatures that increases phonon absorption assisted transport (second term of eqs. (3.7) and (3.8)).

Nevertheless, examining Figure 6.4 (b) we observe that there still exists a possible biasing region (shaded) where the TFET outperforms the MOSFET geometry. The significant increase in $I_{OFF}$ at higher temperatures is clearly observed for the TFET. Off-state leakage that is about an order of magnitude smaller compared to the MOSFET can still be attained at both room and elevated temperatures. In comparing Figure 6.4 (a) and (b), however, it is clear that the ballistic operation of TFETs could have reduced the off-state leakage significantly, especially at higher temperatures. Therefore, it can be summarized that the TFET can indeed deliver superior subthreshold characteristics under realistic transport conditions, but phonon scattering deteriorates the beneficial features that could have been attained otherwise.

### 6.1.3 Drain induced off-state degradation

In this section we examine the effect of the drain bias on subthreshold properties. In a conventional MOSFET this could lead to the well known drain induced barrier lowering (DIBL) effect [77]. In the case of a TFET in the off-state, as shown in Figure 6.3 (b), it is not clear whether DIBL could necessarily have a similar effect since the high energy tail of the Fermi distribution is already within the source bandgap region. Therefore, in order to study the effect of the drain bias on subthreshold current we use a slightly modified device geometry compared to Figure 6.1 that allows drain field penetration into the channel region in our wrap-around gate structure. In this section we use a (10,0) CNT with $t_{OX} = 5\text{nm}$ and SiO$_2$ ($k = 3.9$) for the gate oxide that covers the full length of the tube
including the source/drain regions. All other device parameters are similar to the previous case, and ballistic transport simulations are performed.

The transfer characteristics, and its drain bias dependence, for the two geometries are compared in Figure 6.5. We observe that the CNT-MOSFET still retains the well tempered operation with very small DIBL. On the other hand, the TFET shows a significant bias dependence similar to the DIBL effect of a MOSFET. A closer examination of the energy bands (Figure 6.6), however, provides insight into the origin of this bias dependence. First of all, in the case of the MOSFET in Figure 6.6 (a) it is observed that the top of the channel barrier does not get pulled down significantly at larger $V_{DS}$; thus, the smaller DIBL seen for this case. On the other hand, in Figure 6.6 (b) there is a significant shortening of the channel barrier width at large $V_{DS}$ for the case of the TFET. The transmission coefficient for direct electron tunneling through the channel region increases exponentially with decreasing barrier width. Therefore, as expected from

![Graph showing transfer characteristics and drain bias dependence for n-i-n MOSFET and p-i-n TFET](image)

Figure 6.5. Dependence of subthreshold properties on the drain bias for, (a) n-i-n MOSFET and, (b) p-i-n TFET under ballistic transport (the device geometry is slightly modified from that for the rest of the paper. See text for details). The n-i-n MOSFET shows small DIBL compared to the p-i-n TFET. For the latter the off-current is increased at high $V_{DS}$ due to drain induced barrier shortening (DIBS) (see Figure 6.6).
eq. (2.19) the off-state current increases significantly. This effect for TFETs observed here can be identified as drain induced barrier shortening (DIBS). It should be noted that DIBS would be important for a highly scaled device where short channel effects are considerable. If the original channel barrier width ($\sim L_{ch}$) were long enough, the actual magnitude of direct tunneling current would be very small even in the presence of barrier shortening effects.

6.2 Comparison of the On-State Performance

The on-state device performance of the two geometries is compared next. In this regard we use a few popular device metrics such as the on-current ($I_{on}$), intrinsic device
delay metric ($\tau$), and power-delay product (PDP) which is essentially the switching energy of the transistor [77]; The latter two metrics, $\tau$ and PDP, relate to the intrinsic operation of the transistor where it switches from the on-state to the off-state, or vice versa.

### 6.2.1 On-current ($I_{ON}$)

One of the main concerns for BTBT based transistors has been their ability to deliver considerable drive currents. The use of TFETs with only one tunneling barrier for carriers as opposed to BTBT in MOSFETs [36, 41, 42, 97] where there are two, the on-current for the former has improved. And, even though there have been many optimization strategies proposed for TFETs in order to improve $I_{ON}$ further [37, 98, 101-103] it still remains a challenge. Figure 6.7 compares $I_{DS}$-$V_{GS}$ in linear scale for the two devices shown in Figure 6.1. It is observed that the drive current for the TFET is about 3x smaller than that for the MOSFET. If the high-k oxide covers the CNT throughout, including the source region, $I_{ON}$ further degrades by about 18x compared to the MOSFET.

![Figure 6.7. Linear $I_{DS}$-$V_{GS}$ comparison for the n-i-n MOSFET and p-i-n TFET under ballistic and dissipative transport. The on-current for the latter is reduced due to the presence of the tunneling barrier.](image-url)
(not shown). In Figure 6.7, however, it is observed that phonon scattering has only a minor effect on TFET on-state current (reduces by $\sim 10\%$) compared to the MOSFET (reduces by $\sim 16\%$). This is because in the case of the former the back-scattered carriers in the channel region have a larger probability of being reflected back by the source-channel tunneling barrier, ultimately escaping into the drain. Thus, DC current transport is not significantly affected by phonon scattering. Therefore, from Figure 6.7 it can be noted that the tunneling barrier properties of a TFET have a much dominant effect on the drive current, and the channel mobility itself has only a comparatively minor influence [39, 98, 100, 103].

### 6.2.2 Intrinsic device delay metric ($\tau$)

Intrinsic device delay ($\tau$) is an important performance metric that corresponds to intrinsic limitations on switching speed and AC operation of a transistor [77]. In this

![Figure 6.8. Intrinsic device delay metric ($\tau$) vs. $I_{ON}/I_{OFF}$ comparison. Surprisingly, $p-i-n$ TFET shows similar delay compared to the $n-i-n$ MOSFET even though the former has a smaller drive current (Figure 6.7). Also, $p-i-n$ TFET even becomes faster at larger $I_{ON}/I_{OFF}$ operating regime. In the presence of a load capacitance, however, the actual drive current will become important and the $p-i-n$ TFET could be relatively slower.](image-url)
work the switching speed is calculated by, \( \tau = \left( Q_{on} - Q_{off} \right) / I_{on} \), instead of the traditional equation of \( \tau = C_s V_{dd} / I_{on} \) \[77\] due to the strong bias dependence of gate capacitance, \( C_s \) (see Section 6.3). Here, \( Q_{on,off} \) is the total charge induced in the transistor in the on- and off-states, respectively (calculated similar to \( I_{on,off} \) with a constant \( V_{dd} \) bias window \[109\]). Thus, \( \tau \) accounts for any additional charging induced by fringe capacitance effects. Figure 6.8 shows the \( \tau \) vs. \( I_{on}/I_{off} \) comparison for the TFET and the MOSFET. Surprisingly, we observe that \( \tau \) for the former is comparable to that of the latter even though the MOSFET has a much larger drive current (Figure 6.7). At larger \( I_{on}/I_{off} \) ratios (> 10^4) the TFET is even faster. The main reason for this behavior is the amount of charge involved in the on-off transition of a TFET is considerably smaller compared to that for the MOSFET (see Section 6.3). Device delay, however, increases significantly (not shown) when high-k oxide covers the full length of the CNT including the source region due to the reduction in \( I_{on} \).

In Figure 6.8 it is also observed that phonon scattering increases \( \tau \) for both the devices. Even though the drive current for the TFET does not considerably deteriorate in the presence of phonon scattering (Figure 6.7) the degradation of \( \tau \) is comparatively larger. This is due to the occupation of negative going states (-\( k \)) in the channel in the presence of back-scattering, and the occupation of low energy states with smaller band velocities, which increase the average transit time for carriers. A similar effect has also been reported in Schottky barrier CNTFETs \[114\]. Finally, it should be noted that even though the intrinsic delay in Figure 6.8 is comparable for the two geometries, the TFET could become significantly slower in the presence of a load capacitance (such as a long interconnect). In such cases the actual drive current of the device becomes important and the MOSFET would have a considerable advantage (Figure 6.7).
6.2.3 Power-delay product (PDP) and Dynamic power dissipation (P_{dynamic})

Power-delay product (PDP) is the switching energy required for on-off transition of a transistor. It is a measure of the dynamic power dissipation, \( P_{dynamic} = \alpha (PDP) f \), where \( f \) is the operating frequency and \( \alpha \) the activity factor [77]. In this work we calculate PDP by, \( PDP = (Q_{ON} - Q_{OFF}) V_{DD} \), that corresponds to charging of the MOS capacitor under the voltage bias \( V_{DD} \). Figure 6.9 compares the PDP vs. \( I_{ON}/I_{OFF} \) for the two geometries. Here, it is observed that the TFET has a smaller switching energy compared to the MOSFET. Furthermore, the relative shapes of the two curves appear to be fundamentally different; the MOSFET curve is concave down while that for the TFET is concave up, thus resulting in a smaller PDP under practical biasing conditions (similar distinctions for the two geometries have been consistently observed under various device parameters [37]).

![Figure 6.9. Comparison of the power-delay product (PDP = switching energy). p-i-n TFET has a significant benefit here, and shows a fundamentally different behavior compared to the n-i-n MOSFET.](image-url)
These apparent fundamental differences for the two can be attributed to their total gate capacitances, $C_g$ (see dashed lines of Figure 6.10). Here, $C_g = \frac{dQ_{tot}}{dV_{GS}}$ where $Q_{tot}$ is the total charge induced throughout the transistor. In Figure 6.10 we observe that the $C_g$-$V_{GS}$ curves for the two geometries at finite $V_{DS}$ have very different shapes (see Section 6.3 for details). Now, note that the switching energy of a transistor can be written in an alternative form, $PDP = C_{ave} V_{DD}^2$ [77] where the capacitance $C_{ave}$ is an average value determined from the $C_g$-$V_{GS}$ curve for the appropriate biasing window, $V_{DD}$ ($= 0.3V$ in this case). In Figure 6.9, going from smaller to larger $I_{ON}/I_{OFF}$ ratios (i.e. left to right) we are moving from the on-state to the off-state in the $C_g$-$V_{GS}$ curves of Figure 6.10 (i.e. right to left). Therefore, $C_{ave}$ will also change accordingly. Thus, it is apparent that the observed differences in the shapes of the PDP curves (Figure 6.9) for the two geometries are related to their non-equilibrium device capacitances (Figure 6.10). Furthermore, because of the use of ultra thin high-k gate oxides, the devices operate in the quantum capacitance limit. Therefore, it is evident that the important differences observed for the switching energy of the two devices are in fact related to their quantum capacitances. At this point, we take a closer look at the origin of these distinctions for the two geometries.

![Figure 6.10. Total device capacitance ($C_g$) vs. $V_{GS}$ calculated from $dQ_{tot}/dV_{GS}$ for, (a) n-i-n MOSFET and, (b) p-i-n TFET under dissipative transport. At small $V_{DS}$ both devices show similar characteristics. However, at larger $V_{DS}$ a fundamentally different behavior is observed; for the p-i-n TFET device capacitance remains small until larger gate biases are applied.](image-url)
since that provides useful insights into the fundamental differences in the relevant device physics.

6.3 Device Operation at the Quantum Capacitance Limit

The continual rise in gate oxide capacitances, along with the importance of carrier transport in confined structures, have made the quantum capacitance limit of device operation increasingly relevant; i.e. $C_{ox} \gg C_Q$ condition where $C_{ox}$ and $C_Q$ are the gate oxide and quantum capacitance, respectively [115, 116]. And, $C_Q$ is related to the average density of states (DOS) near the Fermi level, $C_Q \sim DOS(E_F)$ [21]. As discussed below, in TFET structures the DOS can become very small, thus the aforementioned condition can be easily achieved. In this case the gate capacitance is dominated by $C_Q$ itself; $C_g = \left(\frac{C_{ox} C_Q}{C_{ox} + C_Q}\right) = C_Q$.

Figure 6.10 compares the bias dependence of $C_g$ for the two devices under dissipative transport (similar behavior is obtained under ballistic transport as well). It is

![Figure 6.10](image)

Figure 6.11. Energy-position resolved electron distribution for, (a) n-i-n MOSFET and, (b) p-i-n TFET under ballistic transport at $V_{GS} = 0.5\text{V}$, $V_{DS} = 0.3\text{V}$. A significantly higher occupation of channel states is observed for the former.
observed that the equilibrium $C_gV_{GS}$ curves (solid) for the two are very similar, and carry the characteristic signature of the CNT-DOS [8]. This relationship has also been experimentally verified in the case of CNT-MOSFETs [117]. At larger $V_{DS}$, however, interesting differences arise. First of all, in the case of the MOSFET the initial peak splits into two. This is because the negative going ($-k$) half of channel DOS is filled only at a larger $V_{GS}$ compared to the positive going ($+k$) ones [116]. On the other hand, $C_gV_{GS}$ curve for the TFET remains notably small up to larger gate biases. This means that the charge induced in the channel for the TFET is considerably lower compared to that for the MOSFET. This difference can be clearly observed in the energy-position resolved electron distribution function (eq. (2.11)) shown in Figure 6.11. There, the $+k$ states in the channel of the MOSFET that are below the source Fermi energy ($E_{FS}$) are well occupied. On the other hand, in the case of the TFET even though the conduction band in the channel is well below the source $E_{FS}$ the channel states are relatively empty. This is due to the presence of the tunneling barrier that hinders carrier injection into the channel from the source reservoir [103, 116].

Since $Q_c$ in fact originates from the filling of the channel DOS by the source and

![Figure 6.12. Reservoir resolved LDOS for the n-i-n MOSFET at $V_{GS} = 0.5V$, $V_{DS} = 0.3V$: (a) source-evolving states (LODS$_S$), (b) drain-evolving states (LDOS$_D$). There is a significant amount of source-evolving states inside the channel that are filled by the source Fermi distribution. Drain-evolving states in the channel are not filled at larger $V_{DS}$.](image)
drain reservoirs, it is instructive to distinguish the origin of these states by the two contacts of the transistor. This is achieved by looking at the contact resolved LDOS (from eq. (2.14)) shown in Figure 6.12 and Figure 6.13 for the MOSFET and the TFET, respectively. This separation is strictly possible under ballistic transport, but it elucidates the underlying physical reasons for the differences seen for the two device geometries. In Figure 6.12 it is observed that there is a significant amount of source-evolving (+k) states inside the channel that is filled by that reservoir. This leads to the considerable device capacitance observed for the MOSFET in Figure 6.10 (a) (dashed curve) when quantum capacitance has a significant contribution to $C_g$. At larger gate biases the drain-evolving (-k) states also get filled by the drain reservoir, further increasing $C_g$. This behavior leads to the splitting of the single peak in $C_g$-$V_{GS}$ curve under equilibrium conditions, into two peaks under larger drain biases.

In Figure 6.13 (a), for the case of the TFET, it is observed that there is only a small amount of source-evolving states inside the channel which are filled by that reservoir. Therefore, they have only a small contribution to $C_g$. On the other hand, there
is a large number of drain-evolving states inside the channel; both \(-k\) states, as well as \(+k\) states that originate from the reflection of the former against the tunneling barrier (Figure 6.13 (b)). These states are, however, not occupied by the drain Fermi reservoir at large \(V_{DS}\). They get filled only at larger gate biases, and will subsequently increase \(C_Q\) as observed by the dashed curve of Figure 6.10 (b). On the other hand, at small drain biases these states are easily filled, and dominate \(C_Q\) (solid curve of Figure 6.10 (b)). At this point, it can be noted that the TFET would have very small \(C_Q\) under non-equilibrium conditions, and would easily get into the quantum capacitance limit of operation [103]. Furthermore, the characteristic differences in drain bias dependence of \(C_Q\) for the MOSFET and the TFET should be readily distinguishable from an experiment similar to [117].

In summary, this chapter presented a comprehensive comparison of device performance between the conventional MOSFET and the \(p-i-n\) TFET geometries. It was confirmed that the TFET can indeed operate with a subthreshold swing below the 60mV/decade conventional limit, thereby reducing off-state leakage and standby power dissipation. Phonon assisted tunneling tends to deteriorate the desirable subthreshold characteristics of a TFET that could have been achieved under ballistic conditions. Under on-state operation, the drive current and the switching speed of a TFET are dominated by the tunneling barrier properties, and phonon scattering comparatively has only a minor effect. On the other hand, at the quantum capacitance limit of device operation, the switching energy of a TFET is observed to be fundamentally smaller compared to that of a MOSFET. Therefore, the \(p-i-n\) TFET geometry is expected to be a strong candidate for future low power applications.
7. TREATMENT OF INELASTIC TRANSPORT IN CNT OPTOELECTRONIC DEVICES

Electroluminescence and the investigation of potential optoelectronic applications for CNTs have been a relatively recent research endeavor. This chapter describes the modeling and simulation of a recently demonstrated optoelectronic device based on a partially suspended CNTFET [10]. The optical emission in this device has been attributed to an excitonic process, and the experimentally observed high emission efficiencies have generated much interest in this class of devices. In section 7.1 we review optical emission in CNT based devices highlighting the importance of excitonic effects. Section 7.2 describes the simulation method we use in this study. Since the experimentally investigated devices tend to be at the long channel limit (hundreds of nanometers) we use a numerical solution of the Botzmann transport equation (BTE) instead of the NEGF formalism used up to now for quantum transport calculations. Chapter 8 presents a detailed simulation study, using the methods presented here, for experimentally demonstrated device geometries. Note that certain parts of this chapter are adapted from our publications [43, 44].

7.1 Background on Excitonic Emission in CNTs

In recent years, rapid progress in research on carbon nanotube (CNT) electronic and optoelectronic devices has occurred [5, 118]. High performance CNT transistors operating close to the ballistic limit have been experimentally realized [13, 15, 16]. The demonstration of electroluminescence in CNTs has opened up new possibilities for optoelectronic applications as well [9, 10, 46, 119]. The importance of nanoscale physical phenomena in governing the operation of CNT devices has been underscored in a
multitude of experiments [5, 118]. The first optical emission in a CNTFET was demonstrated in 2003 by the Avouris’ group at IBM [9]. Since then, a number of experiments have been reported investigating the optical emission phenomena in these devices [10, 46, 119].

All these devices had tube lengths of a few micrometers or more, and operated in the diffusive limit. Optical emission in earlier CNT devices [9, 46] was attributed to free carrier recombination under ambipolar transport, which is similar to the operation of conventional light emitting diodes (LEDs). In this case, a Schottky-barrier CNT field-effect transistor (CNTFET) is operated at high source-drain bias ($V_{DS}$) such that both electrons and holes are injected into the channel simultaneously from the two contacts, respectively [9, 46]. These free carriers radiatively recombine inside the channel region resulting in optical emission. Device operation was well modeled by drift-diffusion treatment of carrier transport and free carrier recombination [120-123]. A recent experiment [10], however, using a partially suspended CNTFET as shown in Figure 7.1 (a) demonstrated an enhancement of optical emission intensities of 100-1000x than that in the earlier work. The emission process was attributed to exciton generation under unipolar transport conditions [10].

Figure 7.1 (a) shows a schematic of this novel device. It uses a semiconducting CNT suspended over a trench that has been created on the oxidized silicon wafer by reactive ion etching. Pd metal is used for source/drain contacts, and the heavily doped substrate is used as the back-gate. Interestingly, the optical emission is spatially localized near the trench-substrate junction near the drain (Figure 7.1 (b)), and it is attributed to radiative recombination of impact excited excitons in this region [10]. It has already been well established that the optical processes in CNTs are dominated by excitonic effects [124, 125]. In the case of the partially suspended CNTFET reported in Ref. [10], as shown in Figure 7.1 (c), there exists a high electric-field region at the trench-substrate junction near the drain contact (shown for positive gate bias, $V_{GS} > 0$). This arises due to
the difference in electrostatic coupling to the back-gate in the trench and the substrate regions, respectively. Electrons injected from the source can gain enough kinetic energy in this high-field region to generate excitons by impact excitation. The subsequent radiative recombination of these excitons is expected to lead to localized optical emission at the trench-substrate junction seen in Ref. [10]. At this point it is important to differentiate the above mechanism from thermal light emission reported in suspended metallic CNTs [11, 126, 127]. In the latter case the optical emission is seen in the middle of the trench region where the local temperature is the highest [11, 128].

Note that excitonic effects in CNTs are expected to be much stronger compared to conventional semiconductors due to the enhancement of Coulomb interaction in 1D. In fact, there has been a multitude of both experimental and theoretical work clearly demonstrating that the photoluminescence (where the initial excitation is due to the

Figure 7.1. (a) A schematic of the CNTFET suspended over a trench with the back-gated geometry, (b) Experimental observation of optical emission localized at the trench-drain junction (from [10]). (c) Band diagram near the trench-substrate junction at the drain end (shown for $V_{GS} > 0$). Electrons that are injected from the source can gain enough kinetic energy at this junction for the impact excitation of excitons.
absorption of photons) in CNTs is excitonic based [119, 124, 129-149]. The reported excitonic binding energies \( (E_b) \) for CNTs are in the range of \( 100 \text{meV} \sim 1 \text{eV} \) [139, 143]. Such large binding energies for CNTs should be contrasted with that for conventional semiconductors, such as GaAs, that is only a several meV’s [150]. Therefore, observation of excitonic effects in conventional semiconductors requires ultracold experimental setups. Another important factor that influences the observation of excitonic effects, especially in devices, is the exciton ionization field \( (E_i) \). This is the field at which the bound excitons dissociate due to the opposite forces imposed on the electron and the hole, and the excitonic effects get quenched. Therefore, having a larger \( E_i \) corresponds to more stable excitons in a device, and more pronounced excitonic effects on the device characteristics. Table 7-1 compares the binding energies and the ionization field strengths for conventional semiconductors vs. CNTs; few representative cases are presented. It is clearly seen that both the binding energy and the ionization field for CNTs is about two orders of magnitude larger than that for conventional semiconductors. Therefore, efficient impact excitation of stable excitons is expected in CNT devices under suitable operating conditions [142].

<table>
<thead>
<tr>
<th>Material</th>
<th>Bandgap ( (E_G, \text{eV}) )</th>
<th>Exciton binding energy ( (E_b, \text{meV}) )</th>
<th>Ionization field ( (E_I, \times 10^6 \text{V/m}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs (^{(a)})</td>
<td>1.41</td>
<td>5.1</td>
<td>0.6</td>
</tr>
<tr>
<td>Ge (^{(a)})</td>
<td>0.80</td>
<td>1.4</td>
<td>0.06</td>
</tr>
<tr>
<td>(13,0) CNT (^{(b)})</td>
<td>0.82</td>
<td>281</td>
<td>84.5</td>
</tr>
<tr>
<td>(25,0) CNT (^{(b)})</td>
<td>0.43</td>
<td>160</td>
<td>27</td>
</tr>
</tbody>
</table>

(a) From [150]. (b) From [151].
7.2 Simulation Method

This section describes the numerical simulation scheme used in treating dissipative transport in CNTFETs including the exciton process. Solution of the 1D Boltzmann transport equation is described first followed by the finite difference scheme used in solving the Poisson’s equation.

7.2.1 Numerical solution of the Botzmann transport equation (BTE)

In this section we describe the numerical solution of the transport equation. Our model treats inelastic effects on carrier transport due to both optical phonon (OP) scattering and the excitonic process. It should be noted that the prior work [120-123] on device modeling of optical emission in CNTFETs operating in the diffusive limit did not consider the latter process. Both doped source/drain contacts (CNT-MOSFETs) as well as metal Schottky contacts (SB-CNTFETs) were treated in our simulations. The 1D Boltzmann transport equation (BTE) was numerically solved for electron transport in the lowest conduction band [24, 45],

\[
\frac{\partial}{\partial t} + v_k \cdot \frac{\partial}{\partial z} + \left( -\frac{q \xi_z}{\hbar} \right) \cdot \frac{\partial}{\partial k} f(z,k) = S^{\text{in}} - S^{\text{out}} \tag{7.1}
\]

where, \(v_k\) is the band velocity, \(\xi_z\) is the position dependent electric field, \(f(z,k)\) is the phase-space distribution function, and \(S^{\text{in/out}}\) are the in/out-scattering rates described below. In calculating \(v_k\), CNT energy dispersion of,

\[
E(k) = \left(3\alpha_{cc}\gamma/2\right)\sqrt{k^2 + \Delta k^2} - \left(E_g/2\right) \tag{7.2}
\]
has been used where $a_{CC} = 0.142\text{nm}$ is the carbon-carbon bond length, $\gamma = 3\text{eV}$ is the hopping parameter, $\Delta k$ is the angular (confinement) momentum of the sub-band, and $E_G = 3a_{CC}\gamma \Delta k$ is the CNT bandgap [152]. A similar solution of the BTE has been used in Ref. [153] to investigate hot-carrier effects in conventional CNT-MOSFETs (with doped source/drain contacts and without the trench geometry).

Transport calculations were performed self-consistently with electrostatics by solving the 2D Poisson equation using the finite difference method. Knowing the potential distribution in the device, the spatial dependent electric field $\xi_z$ can be calculated. With this eq. (7.1) is solved for the phase-space distribution function $f(z,k)$. With $f(z,k)$ known, the charge distribution in the device is calculated, which in turn is used for the determination of the potential distribution from the Poisson’s equation. This solution procedure leads to the self-consistent iterations between BTE and Poisson as shown in Figure 7.2. The convergence criteria used for the Poisson solution are similar to that explained in section 2.2.

The direct numerical solution of eq. (7.1) requires an appropriate discretization of the non-linear partial differential equation. This is performed using first order upwinding schemes for both the real and momentum space discretization [154, 155]. A full account

![Figure 7.2. Self-consistent BTE-Poisson iteration scheme used in this study.](image)
of the discretization method is given in section III(A) of [45] for the case of CNT-MOSFETs with doped source/drain contacts. The final discretized equation has the following form,

\[
\frac{\{f\}_t - \{f\}_{t-1}}{dt} + [\text{del}_t]\{f\}_{t-1} + \{f\}_{bc} + [\text{del}_k]\{f\}_{t-1} = \{S\}_{t-1}
\]

(7.3)

where \(\{f\}\) is the phase-space distribution function represented as a column vector. In eq. (7.3) \(\{f\}_t\) and \(\{f\}_{t-1}\) are the distribution functions at “t” and “t-1” time steps, and, \(\{f\}_{bc}\) originates from the fixed boundary conditions (Fermi functions) at the source/drain ends. Matrices \([\text{del}_t]\) and \([\text{del}_k]\) represent the matrix form of the corresponding operators, and \(\{S\}_{t-1}\) is the net in-scattering rate evaluated at the previous time step. Finally the time evolution is performed as,

\[
\{f\}_t = \{f\}_{t-1} + dt \times (\{S\}_{t-1} + [U]\{f\}_{t-1} - \{f\}_{bc})
\]

(7.4)

where, \([U] = -([\text{del}_t] + [\text{del}_k])\). The above time evolution procedure requires an initial distribution, for which we use the steady-state ballistic distribution,

\[
([\text{del}_t] + [\text{del}_k])\{f\}_{\text{ballistic}} = -\{f\}_{bc}
\]

(7.5)

and, is determined using Gaussian elimination. In eq. (7.4) we are using an explicit scheme for solving the PDE given in eq. (7.1). Implicit schemes, however, are expected to be more stable and achieve convergence more rapidly compared to the explicit method presently being used [155]. Therefore, the implementation of an implicit method for improving numerical properties should be investigated in the future.
When solving (7.4) appropriate boundary conditions needs to be applied near the contacts in order to account for tunneling through the Schottky barriers in the case of SB-CNTFETs. In order to account for SB-tunneling at the contacts, matrix \([U]\) of eq. (7.4) needs to be modified. This is performed in the following manner. At position \(z_i\) near the source-end for an electron with momentum \(k_j > 0\) (i.e., source-injected electron) we impose the following boundary condition on the phase-space distribution function (see Figure 7.3),

\[
f(z_i, k_j) = \bar{T} \cdot f_{F-D} \left( E_C(z_i) + E(k_j) - E_{FS} \right) \\
+ \left[ 1 - \bar{T} \right] \cdot f \left( z_i, -k_j \right)
\]  

\[(7.6)\]

where \(E_C(z_i)\) is the conduction band edge, \(E(k_j)\) is the kinetic energy of the electron from the band edge, \(E_{FS}\) is the source Fermi energy, and \(f_{F-D}\) is the Fermi-Dirac function.

Figure 7.3. Treatment of SB-tunneling near the source end. Phase-space distribution function, \(f(z, k)\), at the position \(z_i\) is considered.
In eq. (7.6) \( T \) is the transmission probability at energy \( \left( E_c(z_i) + E(k_j) \right) \) calculated using the Wentzel-Kramers-Brillouin (WKB) approximation [152]. Equation (7.6) can be intuitively understood by observing that the distribution function for positive going carriers near the source-end, \( f(z_i, k_j) \), is determined by the direct-injection from the source reservoir (first term on RHS) and the reflected component of the negative going carriers (second term on RHS).

As shown in Figure 7.3, the boundary condition, eq. (7.6), is applied to all phase-space nodes, \( f(z_i, k_j) \), at position \( z_i (i = 1, 2, \ldots) \) with momentum \( k_j \) such that \( k_j > 0 \) and \( E(k_j) < \left| E_c(z_{i-1}) - E_c(z_i) \right| \). Equation (7.6) thus modifies both the matrix \([U]\) and the vector \( \{f_{bc}\} \) of eq. (7.4) at the corresponding phase-space nodes. Source injection is considered up to a distance of \( z_{\text{cut-off}} \) taken to be 15nm in our simulations. At the beginning of the source (\( z_0 \)) a fixed boundary condition is applied according to eq. 30 of [45]. A similar approach is used to treat tunneling at the drain-end for the drain-injected electrons (with \( k_j < 0 \)).

The in/out-scattering rates in eq. (7.1), \( S_{\text{in/out}} \), are determined microscopically, accounting for the Pauli blocking of scattering events [24],

\[
S_{\text{in}}(z,k) = \sum_{k'} f(z,k') \left[ 1 - f(z,k) \right] S(k',k) \quad (7.7)
\]

\[
S_{\text{out}}(z,k) = \sum_{k'} f(z,k) \left[ 1 - f(z,k') \right] S(k,k') \quad (7.8)
\]

where \( S(k,k') \) is the transition rate from state-\( k \) to state-\( k' \), determined from Fermi’s golden rule;

\[
S_{\text{OP,exc}}(k,k') = \frac{2\pi}{\hbar} |M_{\text{OP,exc}}|^2 \delta \left( E(k') - E(k) + \hbar \omega_{\text{OP,exc}} \right) \quad (7.9)
\]
Here, both OP emission [45] and exciton emission [142] processes by the high energy carriers are treated separately where $|M_{OP,exc}|$ is the matrix element for the respective scattering mechanism. For OP scattering, the zone boundary optical mode (180meV) and longitudinal optical mode (190meV) that have the largest electron-phonon coupling in CNTs were treated [45]. In this work, excitons are assumed to have a constant energy dispersion ($\hbar\omega_{exc} = \text{constant}$) with an impact excitation energy threshold of 430meV for the (25,0) CNT considered here [140, 149]. Detailed calculations on the impact excitation of excitons vs. the impact ionization mechanisms in a (25,0) CNT show that the threshold energy for the latter process is about 150meV $\approx 6 \times k_B T$ higher compared to the former [142]. And, the impact ionization rate is less than half of that for impact excitation of excitons [142]. Furthermore, [153] has shown that quantum efficiency for impact induced processes decreases exponentially with increasing threshold energy. Therefore, since the distribution function at large energies decreases exponentially, and the impact ionization has a considerably larger energy threshold, combined with lower scattering rate, we are not considering this process presently.

In solving eq. (7.4), it becomes nonlinear due to the treatment of the in/out-scattering processes in the degenerate limit in eqs. (7.7) and (7.8). Therefore, it is solved iteratively for the steady-state distribution function using an explicit upwinding scheme for the discretization of the BTE operators [45]. A full account of the solution procedure is given in Ref. [45]. Finally, the exciton generation profile along the CNT, $R_{exc}(z)$, is determined from,

$$R_{exc}(z) = \sum_k S_{exc}^{out}(z,k)$$

(7.10)

where, $S_{exc}^{out}(z,k)$, given by eq. (7.8), is the steady-state out-scattering rate due to exciton emission by the high energy carriers.
7.2.2 Finite difference solution of the Poisson’s equation

This section describes the finite difference scheme for solving the 2D Poisson equation for a device with cylindrical symmetry. In order to discretize the Poisson equation given in eq. (2.28) it is conceptually simpler to write it in the integral form;

\[ \int \vec{D} \, d\vec{s} = \int \rho dV \]  

(7.11)

where \( \vec{D} \) is the 2D displacement field with \((\hat{r},\hat{z})\) components, and the charge distribution \( \rho \) given by eqs. (2.30) and (2.31). Now, for a volume-element \((m,n)\) completely inside a dielectric medium the 2D finite difference mesh for a device with cylindrical symmetry is given in Figure 7.4 (a). In a homogeneous region (with relative dielectric constant \( \varepsilon \)), such as inside the oxide region, eq. (7.11) can be discretized as follows,

Figure 7.4. (a) 2D finite difference mesh for solving Poisson’s equation in a cylindrically symmetric geometry. (b) Grid points around element \((m,n)\).
\[
\begin{align*}
\varepsilon & \frac{V_{m,n} - V_{m+1,n}}{dr} \left( r_{m,n} + \frac{dr}{2} \right) \uparrow \\
+ & \varepsilon \frac{V_{m,n} - V_{m-1,n}}{dr} \left( r_{m,n} - \frac{dr}{2} \right) \downarrow \\
+ & \varepsilon \frac{V_{m,n} - V_{m,n+1}}{dz} \left( r_{m,n} \frac{dr}{dz} \right) \rightarrow \\
+ & \varepsilon \frac{V_{m,n} - V_{m,n-1}}{dz} \left( r_{m,n} \frac{dr}{dz} \right) \leftarrow \\
= & 2\pi r_{m,n} dr \rho_{m,n} \frac{1}{2\pi \varepsilon_0} = \frac{\rho_{uid}}{2\pi \varepsilon_0}
\end{align*}
\]

where \( V_{m,n} \) is the electrostatic potential at the middle of the volume element \((m,n)\), and \( \rho_{m,n} \) is the net charge density in there (in units of \(1/\text{cm}^3\)). Then, due to the angular symmetry of the device, \( \rho_{uid} \) is the net linear charge density along the axial direction in units of \(1/\text{cm}\). In eq. (7.12) the arrows indicate the surface integral of the displacement field, i.e. \( \vec{D} d\vec{s} \), in that direction with respect to the grid point \((m,n)\) shown in Figure 7.4 (b). According to eqs. (2.30) and (2.31), for volume elements completely inside a given dielectric medium \( \rho_{m,n} \) would be zero unless there are some other charge impurities such as oxide charges etc.

Figure 7.5. Discretization scheme at the boundary between two dielectric regions \( \varepsilon_{\text{in}} \) and \( \varepsilon_{\text{out}} \). In this case mesh elements are created such that the boundary completely lies within them.
The discretization scheme for a volume element at the CNT/dielectric boundary is shown in Figure 7.5. In this case we need the potential values not only on the ‘x’ points but also on the ‘dots’. The potential on the ‘dots’ can be approximated through finite difference method. For example, the potential on the red dot in Figure 7.5 can be approximated by,

\[ V_{\text{red-dot}} = \frac{3}{4} V_{m,n} + \frac{1}{4} V_{m+1,n}. \]  \hspace{1cm} (7.13)

And, the final discretized form of eq. (7.11) for a mesh point \((m,n)\) at the boundary (Figure 7.5) can be written as,

\[
\begin{align*}
\varepsilon_{\text{out}} & \frac{V_{m,n} - V_{m+1,n}}{dr} \left( r_{m,n} + \frac{dr}{2} \right) \quad \uparrow \\
+ \varepsilon_{\text{in}} & \frac{V_{m,n} - V_{m-1,n}}{dr} \left( r_{m,n} - \frac{dr}{2} \right) \quad \downarrow \\
+ \varepsilon_{\text{out}} & \left( \frac{3}{4} V_{m,n} + \frac{1}{4} V_{m+1,n} - \frac{3}{4} V_{m,n+1} - \frac{1}{4} V_{m+1,n+1} \right) \left( r_{m,n} + \frac{dr}{4} \right) \frac{dr}{2 dz^2} \quad \rightarrow \text{(up)} \\
+ \varepsilon_{\text{out}} & \left( \frac{3}{4} V_{m,n} + \frac{1}{4} V_{m+1,n} - \frac{3}{4} V_{m,n-1} - \frac{1}{4} V_{m+1,n-1} \right) \left( r_{m,n} + \frac{dr}{4} \right) \frac{dr}{2 dz^2} \quad \leftarrow \text{(up)} \hspace{1cm} (7.14) \\
+ \varepsilon_{\text{in}} & \left( \frac{3}{4} V_{m,n} + \frac{1}{4} V_{m-1,n} - \frac{3}{4} V_{m,n-1} - \frac{1}{4} V_{m-1,n-1} \right) \left( r_{m,n} - \frac{dr}{4} \right) \frac{dr}{2 dz^2} \quad \rightarrow \text{(down)} \\
+ \varepsilon_{\text{in}} & \left( \frac{3}{4} V_{m,n} + \frac{1}{4} V_{m-1,n} - \frac{3}{4} V_{m,n-1} - \frac{1}{4} V_{m-1,n-1} \right) \left( r_{m,n} - \frac{dr}{4} \right) \frac{dr}{2 dz^2} \quad \leftarrow \text{(down)}
\end{align*}
\]

where \( \rho_{ld} \) (in 1/cm) corresponds to the net linear charge density along the CNT surface, and arrows have been used in a similar notation as in eq. (7.12) and Figure 7.4 (b).
The non-linear procedure in solving Poisson and transport equations to achieve self-consistency is described next. The system of equations arising from the discretization of Poisson’s equation given by eqs. (7.12) and (7.14), along with appropriate boundary conditions, can be put in the matrix form as,

\[
\begin{bmatrix}
A \\
\end{bmatrix}
\begin{bmatrix}
V_{1,1} \\
V_{1,2} \\
\vdots \\
V_{m,n-1} \\
V_{m,n} \\
V_{m,n+1} \\
\vdots \\
\end{bmatrix}
= 
\begin{bmatrix}
B.C \\
\end{bmatrix}
\tag{7.15}
\]

where, the R.H.S has the information on fixed boundary conditions and local net charge densities. Here, \(N\) is the total number of 2D grid points. Note that in the non-linear scheme for solving Poisson equation, the local charge density, rigorously calculated from transport equations, is represented as a differentiable function of the local potential, i.e: \(\rho_{m,n} = \rho(V_{m,n})\). Here, the phenomenological function \(\rho\) is related to \(V_{m,n}\) through a quasi-Fermi energy (see Appendix C of [22]). Thus, eq. (7.15) can be written in general as,

\[
F\left(\{V\}_{Nx1}\right) = \left[ A \right]_{N \times N} \{V\}_{N \times 1} - \rho\left(\{V\}_{N \times 1}\right) = 0
\tag{7.16}
\]

where, \(\{V\}_{N \times 1}\) is the column vector comprising electrostatic potential throughout the discretized mesh points; i.e. \(V_{1,1}, V_{1,2}, \ldots\), etc. Then, using the Newton-Rapson method, new potential distribution is related to the old one by,

\[
\{V\}_{\text{new}} = \{V\}_{\text{old}} + \{\Delta V\}
\tag{7.17}
\]

where,
\[
\{ \Delta V \} = -F' \left( \{ V^{old} \} \right)_{N \times N} \setminus F \left( \{ V^{old} \} \right)_{N \times N}.
\] (7.18)

Here, \( \setminus \) operator corresponds to the Gaussian elimination method for solving a linear system of equations. In eq. (7.18) the Jacobian matrix is given by,

\[
F' \left( \{ V^{old} \} \right)_{N \times N} = [A]_{N \times N} - \text{diag} \left[ \rho' \left( \{ V^{old} \} \right) \right]_{N \times N}
\] (7.19)

It should be noted that the last term of eq. (7.19) is a diagonal matrix of the form,

\[
\text{diag} \left[ \rho' \left( \{ V^{old} \} \right) \right]_{N \times N} = \begin{bmatrix}
\rho'(V_1^{old}) & 0 & 0 \\
0 & \rho'(V_2^{old}) & 0 \\
0 & 0 & \ddots & 0 \\
0 & 0 & \cdots & \rho'(V_N^{old})
\end{bmatrix}_{N \times N}
\] (7.20)

where, \( \rho' \) denotes the derivative of function \( \rho \).
8. EXCITON GENERATION IN CNTS FOR OPTOELECTRONIC APPLICATIONS

This chapter describes the numerical investigation of the CNT optical emitter reported in [10]. The modeling and simulation formalism used in this study was discussed in the previous chapter. Here, we look into exciton generation in partially suspended CNT transistors by the impact excitation process under high-field transport conditions. Carbon nanotube MOSFETs with doped source/drain contacts as well as SB-CNTFETs with metal Schottky contacts have been explored. Note that the latter type of contacts with Pd metal were in fact used in the actual experiment [10]. This chapter is adapted from our publications [43, 44].

The model device structures (which represent the more complex 3-dimensional geometry of the experiment) are shown Figure 8.1. They have cylindrical symmetry with
gate oxide and trench regions wrapping around the CNT channel. A (25,0) zigzag CNT is used unless specified otherwise. In the case of the CNT-MOSFET following device parameters have been used [43]: $T_{OX} = 10\text{nm}$ (SiO$_2$, $\varepsilon_{OX} = 3.9$), $T_{trench} = 100\text{nm}$, $L_{SD} = 60\text{nm}$, $L_{sub1} = 80\text{nm}$, $L_{trench} = 80\text{nm}$, and $L_{sub2} = 150\text{nm}$. Source/drain doping is, $N_{SD} = 1.2/\text{nm}$, which can be compared with the carbon atom density in a (25,0) CNT of 231/\text{nm}.

Figure 8.2. (a) Band diagram for the (25,0) zigzag CNT-MOSFET at $V_{GS} = 0.7\text{V}$ and $V_{DS} = 0.8\text{V}$ calculated from self-consistent simulation. (b) Energy-position resolved electron distribution function. Note that positive (negative) energy represents positive (negative) going carries with $+k$ ($-k$) momentum. Degenerately doped source/drain regions are clearly visible at the ends.
We use the following device parameters in the case of the SB-CNTFET [44]: $T_{OX} = 10$nm ($\text{SiO}_2$, $\varepsilon_{OX} = 3.9$), $T_{trench} = 100$nm, $L_{sub1} = 100$nm, $L_{trench} = 100$nm, $L_{sub2} = 180$nm, and $d_{SB-Metal} = 10$nm (Schottky barrier height, $\varphi_{SB} = 50$meV).

Device operation for the partially suspended CNT-MOSFET is discussed first (Figure 8.1 (a)). Self-consistent band diagram for this device under typical on-state operation is shown in Figure 8.2 (a). It is clearly seen that, as suggested in [10], a significant potential drop occurs at the trench-substrate junction near the drain-end (dashed circle). Electrons can gain enough kinetic energy under this field, leading to a significant hot electron population in that region. Heavily doped (n-type) source and drain regions are also observed. This can be clearly seen in the energy-position resolved electron distribution function shown in Figure 8.2 (b) where source/drain carrier reservoirs are located at the two ends. In constructing Figure 8.2 (b) the energy-momentum conversion of the phase-space distribution function, $f(z,k)$, is accomplished using the dispersion relation, $E(k)$, in eq. (7.2). The direction of electron momentum is given by the sign of the energy; i.e. $+k$ ($-k$) momentum depicted by positive (negative) energy. The detailed carrier evolution inside (and near) the trench region of the CNT-MOSFET (Figure 8.2 (b)) will be elaborated below, along with the discussion for the SB-CNTFET, since both devices behave similarly in this region (compare Figure 8.2 to Figure 8.3).
In the case of the partially suspended SB-CNTFET, the self-consistent energy band diagram under typical operation conditions is shown in Figure 8.3 (a). Device parameters used here were given above. A characteristic Schottky barrier band profile is clearly seen near the contacts. Furthermore, as suggested in Ref. [10], and similar to the operation of the CNT-MOSFET (Figure 8.2 (a)), a significant potential drop occurs at the trench-substrate junction near the drain contact (dashed circle). The band diagram

![Figure 8.3](image-url)
observed here has also been inferred by recent experimental evidence [156, 157]. In the high-field region near the drain-end of the trench, source injected electrons can gain enough kinetic energy leading to a significant hot electron population. This can be clearly observed in the energy-position resolved distribution function for conduction band electrons shown in Figure 8.3 (b) (constructed similar to Figure 8.2 (b)). Inside the trench region, as seen in Figure 8.3 (a), the carriers are gradually accelerated under the moderate electric field. When they gain energy above the 180meV OP energy, they emit optical phonons and start to populate the states near the bottom of the band with $E \approx 0$. This is manifested by the appearance of low energy electron occupation near Line-(A) of Figure 8.3 (b).

The distribution function at Line-(B) situated just beyond the drain-end of the trench shows a significant population of hot carriers, and is elaborated on in Figure 8.4.
Here, it clearly shows the main mechanisms for carrier scattering near this region; OP and exciton emission. The exciton emission rate by hot carriers satisfying the energy threshold requirement is expected to be stronger (in the range of $\sim 10^3 \text{ps}^{-1}$) [142] compared to energy loss through phonon scattering ($< 10^2 \text{ps}^{-1}$) [45]. Therefore, efficient exciton emission, accompanied by OP emission, is observed in the evolution of the distribution function in this region (Figure 8.4). By the time carriers reach Line-(C) of Figure 8.3 (b) all the hot electrons have been thermalized by emission of phonons/excitons and give rise to a stream of forward going carriers with energies delineated by the OP energy. Note that OP emission near the trench-substrate junction is not expected to lead to significant self-heating effects. This is due to effective coupling of lattice vibrations to the substrate in this region as confirmed by previous device simulation studies for on-substrate CNT-MOSFETs [45]. Furthermore, experimentally observed thermal light emission in metallic CNTs is in the suspended section of tubes, while it is absent for on-substrate tubes at comparable device currents [11, 127]. In the case of the device studied here, under very large drive currents, thermal light emission due to carrier heating near the trench-substrate junction could have some contribution towards optical emission, but exciton generation process is expected to be the dominant mechanism.

The exciton generation profile along the CNT, i.e. $R_{\text{exc}}(z)$ from eq. (7.10), is shown in Figure 8.5 (a). It clearly shows the localized nature of generation near the trench-substrate junction. Subsequent radiative recombination of these excitons leads to localized optical emission seen in the experiment [10]. Figure 8.5 (a) also shows exciton generation near the drain contact. This is expected from the large electric field at that location as seen from Figure 8.3 (a). Optical emission near the drain, however, is expected to be largely quenched because the nanotube emission yield is lower on the oxide than from the suspended tube (possibly due to increased non-radiative decay channels), and near the metal contacts the excitons are quenched by energy transfer to plasmons and screening effects. Figure 8.5 (b) shows that the highest generation rate near the trench-substrate junction is located to the right of the high-field region. This is easily
understood by the energy threshold requirement for exciton emission by carriers accelerated under this field. Furthermore, it is expected to suppress the possibility of field-induced dissociation of excitons, and improve their radiative recombination. It is also observed that the exciton generation cannot be described by a local field-dependent generation rate as would be necessary for a drift-diffusion solution of this problem.

Figure 8.5. (a) Steady-state exciton generation profile along the CNT for the device shown in Figure 8.3. Localized exciton generation near the trench-substrate junction is clearly observed (dashed circle). The radiative recombination of these excitons leads to localized optical emission seen in the experiment. Additional exciton generation near the drain contact is also observed. (b) The generation profile (solid) along with the electric field (dashed) near the trench-substrate junction. The highest generation region is located to the right of the high-field region.
Figure 8.6 shows the bias dependence of device characteristics; $I_{DS}$ vs. $V_{GS}$ and the exciton generation efficiency, $\eta_{exc} = \left( qN_{ex-tot}/I_{DS} \right)$ vs. $V_{GS}$. In calculating the generation efficiency, $q$ is the electron charge, and $N_{ex-tot}$ is the total number of excitons generated per second near the trench-substrate junction. $N_{ex-tot}$ is calculated by integrating the spatially resolved generation rate, $R_{exc}(z)$, within the interval $-50 \text{nm} \leq z \leq 120 \text{nm}$ of Figure 8.5 (a). We first concentrate on the results for the SiO$_2$ substrate oxide with $T_{trench} = 10 \text{nm}$ (solid circles). A linear increase in $I_{DS}$-$V_{GS}$ for above-threshold operation accompanied by an exponential increase in $\eta_{exc}$ vs. $V_{GS}$ is seen in this case. The latter relationship also leads to an exponential increase in the localized exciton generation rate, $N_{ex-tot}$. A key experimental result [10] was the observation of an exponential increase in light emission intensity vs. $V_{GS}$ with a linear increase of $I_{DS}$-$V_{GS}$; a relationship attributed to the impact excitation mechanism of the optical emission in these devices. Here, we confirm a similar relationship for the localized exciton generation rate that would lead to the experimentally observed device characteristics.

The effect of CNT diameter (bandgap) on exciton generation efficiency is explored in Figure 8.6 (b) by comparing the results for the (25,0) CNT to that of a (19,0) CNT device. For the latter, all device parameters are similar to that of the (25,0) CNT with SiO$_2$ substrate and $T_{trench} = 10 \text{nm}$ (solid circles). We also assume a Schottky barrier height of $\varphi_{SB} = 50 \text{meV}$ for carrier injection and the gate metal work function is chosen such that both devices have the same threshold voltage. Therefore, we obtain similar device currents ($I_{DS}$) for both the devices. The exciton generation efficiency for the (19,0) CNT, however, is observed to be significantly smaller (Figure 8.6 (b)). This is because of the larger electronic bandgap for the (19,0) CNT that increases the impact excitation energy threshold for exciton emission to 560meV. Similar behavior is also reported for the reduction of impact ionization rate with increasing energy threshold in conventional CNT-MOSFET devices (without the trench) [153]. For smaller diameter tubes the device current itself could be reduced due to larger Schottky barriers for carrier injection [158]. This would further reduce the total exciton generation rate for smaller diameter CNTs.
Figure 8.6. (a) $I_{DS}$-$V_{GS}$ comparison at $V_{DS} = 0.7V$ for a (25,0) SB-CNTFET. Device parameters used here are similar to that in Figure 8.3 (a) except for $T_{trench}$ and the substrate oxide. $d_{ox} = 10nm$, $\varepsilon_{ox} = 3.9$ (SiO$_2$) and $\varepsilon_{ox} = 16$ (HfO$_2$) have been used. A linear increase in $I_{DS}$ is observed above the threshold voltage. On-current is reduced for the deeper trench due to reduced gate coupling in that region. (b) Exciton generation efficiency at the trench-substrate junction vs. $V_{GS}$ shows an exponential increase. Exciton generation for a (19,0) CNT device with SiO$_2$ substrate oxide and $T_{trench} = 10nm$ (dash-dot curve) is compared to that of the (25,0) CNT devices (see legend of (a)).
Device optimization schemes are discussed next. Figure 8.6 compares two different trench depths, $T_{\text{trench}} = 10\text{nm}$ and $100\text{nm}$ (solid circles and dashed squares), both with SiO$_2$ substrate oxide. Figure 8.6 (a) shows that the deeper trench delivers a smaller device current. This is due to the weaker gate control of the electronic bands inside the trench region for deeper trench depths. More importantly, however, Figure 8.6 (b) shows that the exciton generation efficiency is higher for the device with a deeper trench which would result in higher optical emission intensities. This is due to the larger potential drop at the trench-substrate junction for those devices leading to a hotter carrier distribution and higher exciton generation rates. It is, however, observed that the improvement of emission efficiency with increasing trench depth has a saturation type behavior due to increased electrostatic screening effects inside the trench region [43]. Therefore, performance improvements attainable with deeper trench geometries could be limited [43].

Figure 8.6 also compares the effect of high-k substrate oxides on device characteristics, i.e. SiO$_2$ (solid circles) vs. HfO$_2$ (dotted stars). It is seen that the current drive for the two structures is nearly equal since the device current is mainly determined by the modulation of the channel barrier inside the trench region; in this case, both devices have $T_{\text{trench}} = 10\text{nm}$. On the other hand, the exciton generation efficiency for the latter device is significantly larger than that for SiO$_2$. This is due to the stronger gate coupling in the substrate region for the high-k oxide that leads to a larger potential drop at the trench-substrate junction (see Figure 8.3 (a)). This results in a hotter carrier distribution in that region and enhancement of exciton emission efficiency. Therefore, high-k substrate oxides could lead to significant improvement of optical emission intensity. It is noted that the emission efficiency could be further enhanced by using a deeper trench along with high-k oxides.

In summary, we have presented detailed numerical simulations of the partially suspended CNT optoelectronic device reported in Ref. [10]. As observed in the
experiment, our simulations show localized exciton generation by hot carriers, and an exponential increase in emission rate vs. linear increase in $I_{DS}-V_{GS}$. The emission efficiency is predicted to improve by deeper trench geometries. High-k substrate oxides could lead to even greater performance enhancements.
9. CONCLUSION AND FUTURE WORK

9.1 CNT Electronics and Band-to-Band Tunneling Devices

NEGF simulation of dissipative quantum transport in CNT transistors was a major focus of this thesis. A detailed simulation environment that models CNTs with an atomistic $p_z$ tight-binding Hamiltonian, along with self-consistent electrostatics, was developed. Electron-phonon scattering was treated within the deformation potential theory, and realistic phonon modes and their e-ph coupling in CNTs were used from force-constant calculations. Because of the use of the $p_z$ tight-binding formalism that describes both conduction and valence bands in CNTs, transport mechanisms based on band-to-band tunneling and phonon-assisted tunneling were captured naturally. To our knowledge this work is the most comprehensive treatment of dissipative quantum transport in CNT transistors to date. It allowed us to study detailed carrier transport effects in CNT based devices in particular, and explore interesting device physics that are important for nanoscale transistors in general. Conventional thermionic MOSFET operation, as well as BTBT transport, was treated in a uniform simulation environment that allowed us to identify important performance merits of each device category in particular. A personal outlook on the future potentials for CNT based electronics is given in section 9.3.

At this point some possible future directions for the work presented in this thesis on BTBT based devices are envisaged. As seen from our work (Chapter 6 in particular), the $p$-i-$n$ Tunnel FET geometry offers some unique performance advantages over the conventional CNT-MOSFETs. Nevertheless, one main drawback for tunneling transistors is the lower drive currents that limit circuit performance, especially in the presence of
large load capacitances such as interconnects. Therefore, further work is required to identify optimization strategies for increasing the device current while maintaining steep subthreshold slopes. It should comprehensively understand the dependence of various device characteristics on device parameters such as doping density and profile, bandgap, channel length, gate oxide, etc. Different material systems such as heterostructures that could improve tunneling current near the source-channel junction while allowing large $V_{DD}$ operation and better scaling properties should also be explored. Furthermore, circuit level comparisons, beyond the intrinsic device metrics we have used so far, are required for a better assessment of the $p-i-n$ Tunnel FET technology over the conventional CNT-MOSFETs. And, device optimization strategies for the best circuit level performance should be investigated.

Finally, since there is a resurgence of interest on BTBT based devices for potential low-power technologies it is important to extend the modeling and simulation infrastructure beyond the 1D case considered here. As a first step, an extension of the nanoMOS program for ultra-thin body dual gate MOSFETs can be developed for BTBT transistors by introducing a two-band effective-mass Hamiltonian similar to that used in [80]. This model, however, would only be valid for direct bandgap semiconductors; for technologically important silicon and SiGe, the indirect nature of the band-structure as well as phonon assisted tunneling needs to be treated. Barring a few exceptions [107], most of simulation studies performed on BTBT devices in conventional semiconductors, such as silicon, rely on physical models of questionable validity (the ones available in commercial device simulation packages such as MEDICI). This is simply due to the sheer computational complexity involved in the rigorous treatment of phonon assisted transport in conventional (3D) semiconductors. Because of the renewed interest in possible technological applications for BTBT devices, it is imperative to develop simulation tools that accurately treat phonon mediated processes in conventional material systems.
9.2 CNT Optoelectronic Devices

Our work on modeling and simulation of optical emission in CNT devices has been very promising. It clearly showed that the localized optical emission seen in the experimental devices [10] is well described by our transport simulations based on the exciton emission model. We further explored device optimization strategies such as the use of high-k substrate oxides and deeper trench geometries in order to improve optical emission intensities. There are, however, a number of future directions for the work presented in this thesis. The numerical solution procedure described in section 7.2.1 used an explicit scheme for the discretization of the BTE operators. On the other hand, implicit schemes are expected to have better and more stable numerical convergence properties [155]. Therefore, introducing an implicit solution scheme in the future will be beneficial for improving the simulation time and the ability to handle larger device sizes. In section 7.2.1, we also assumed optical phonons to be in equilibrium with the external thermal bath (kept at room temperature). Optical phonon emission in the high-field region near the trench-substrate junction, however, could lead to hot-phonon effects as reported in [45]. A significant hot-phonon population can in turn increase exciton generation rate through phonon absorption mediated processes [142]. This effect could especially become important under large drive currents. Therefore, it will be useful to extend the simulation procedure presented in section 7.2.1 to include hot-phonon effects as described in [45].

Finally, we have so far only treated electron transport in the conduction band. The experimental devices instead show ambipolar behavior, therefore requiring hole transport in the valence band as well. Previous observations of optical emission in CNTFETs were in fact attributed to free carrier recombination instead of the novel excitonic mechanism. Introduction of hole transport into the BTE simulator (thus two band transport) will allow the treatment of free carrier recombination, along with exciton emission, in one unified simulation environment. Treating both these processes on the same footing in the future will allow the exploration of relative importance of the two emission mechanisms under
different regimes of device operation. This will undoubtedly be a very useful contribution to the scientific community, and provide a comprehensive understanding of the operation of CNT optoelectronic devices.

9.3 Future Outlook

Since the discovery of CNTs in early 1990’s the research on their physical properties and possible technological applications has been extensive [5]. Carrier transport in CNTs has been well studied by many groups, and high performance transistors that surpass silicon transistors have been experimentally demonstrated [109]. CNTs have also been an excellent “learning tool” for investigating many interesting device physics. The ability to rigorously model and simulate CNT based devices, as accomplished here, is due to its simplified material structure. Nevertheless, the advent of CNTs into semiconductor technology has been hampered by a few major challenges that are yet to be solved. These are mainly related to their synthesis and deterministic placement in order to build large scale circuits that is imperative for technological manufacturability.

First of all, present techniques used for the synthesis of CNTs have large variations in tube chiralities; i.e. semiconductor vs. metallic CNTs, as well as tube diameters, is not well controlled. Therefore, even though individual high performance CNT based devices can be fabricated in laboratories, the controllability required for mass-scale manufacturing is yet to be achieved. There have been some demonstrations of post-synthesis separation techniques, but mass-scale production of CNTs with a well defined chirality is yet to be accomplished. Another challenge is the deterministic placement of CNTs (both in position and direction) for wafer-scale fabrication. Even though there has been some initial success in this regard, such as directed CVD (chemical vapor deposition) growth techniques, it still remains a major hurdle. Aforementioned challenges, mainly related to material science aspect of IC fabrication, need to be solved
before ubiquitous use of CNTs in conventional electronics. Nevertheless, there might be attractive niche markets with less stringent requirements where CNT based electronics can have initial market penetration. One example is thin film transistors, or flexible electronics, that could be based on CNT networks (or mats) instead of well defined individual tubes. In the long run, other challenges pertinent to high performance IC manufacturing can be overcome, and CNTs could one day become the technological workhorse that silicon has had been for many decades.
List of References


