# Theory and Design of Field-Effect Carbon Nanotube Transistors

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*Abstract*- **In this work we study the effects of the application of an electric field perpendicular to the axis of a Carbon nanotube. We find that such a field acts to lower the bandgap and alter the wavefunctions around the circumference of the tube. We simulate the quantum transport properties of a resonant-tunneling FET as an application of these effects using the Wigner-function formalism. The results of our theoretical model indicate that the current in this device can be effectively manipulated by the gate potential.**

## I. Introduction

Carbon Nanotubes (CNTs) are at the forefront of current research in nanoelectronics. It has been shown experimentally that the current in semiconducting CNTs can be manipulated by external fields, and CNT-FETs have been demonstrated[1]. In this work we determine the effect of an external electric field($F_\perp$) applied perpendicular to the axis of a CNT. We find a number of changes in the CNT electronic structure as $F_\perp$ increases. The energy bandgap decreases while the energy gap between the lowest two subbands increases. Also the wavefunctions around the CNT circumference becomes a mixture of the $F_\perp = 0$ wavefunctions.

Presently the most active area of research in CNT devices involves the study of the transistor action of metal-CNT contacts when a gate potential is applied nearby. In this work, we propose a few unique types of CNT-based tunneling-FETs that take advantage of both the bandstructure tunning by a perpendicular field and the special structural properties of carbon nanotubes. These structural properties include a nanoscale diameter and the ability to seamlessly connect two CNTs of different diameter.

The proposed device we theoretically model is a double barrier resonant-tunneling CNT-FET. We consider a gated carbon nanotube connected on either side to larger diameter tubes. The defects in the periodic lattice at the connections are modeled as barriers to electron flow along the device. Quantum transport within the nanotube is modeled using the Wigner-function formalism[2]. It is found that the current in the CNT-FET can be manipulated effectively by the gate voltage which changes the electronic structure of the gated nanotube.

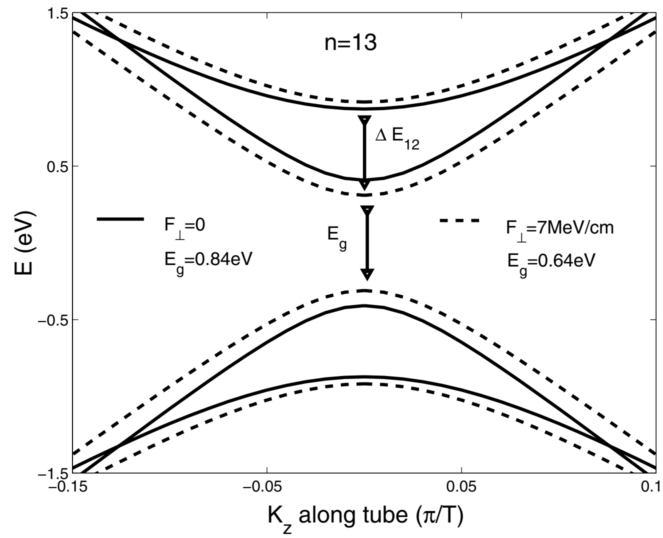


Figure 1. CNT Bandstructure

## II. Effect of Perpendicular Field

Since the CNT diameter is small, electrons are quantized into discrete energy levels around the circumference of the tube[3]. Here we determine how these energy levels are altered when a uniform electric field is applied perpendicular to the nanotube axis. Using second-order perturbation theory, the change in the bandgap energy is

$$\Delta E_g = -2\left(\frac{eF_\perp d}{4}\right)^2 \left(\frac{1}{|\Delta E^o_{12}|} + \frac{1}{|\Delta E^o_{13}|}\right), \qquad (1)$$

where $e$ is the electron charge, $F_\perp$ is the perpendicular field, $d$ is the CNT diameter, and $\Delta E^o_{1j}$ is the energy difference between band 1 and band j when $F_\perp$=0. So we find that $F_\perp$ reduces the bandgap. Also, the electronic wavefunction along the circumference ($\theta$) is altered according to

$$\Psi_1(\theta) = \sqrt{\frac{1}{1+|\beta|^2}}\left(\Psi^o_1(\theta) + \beta\Psi^o_2(\theta)\right), \qquad (2)$$

where $\beta$=($ieF_\perp d/4\Delta E^o_{12}$).

In Fig. 1 we show the bandstructure of a semiconducting zig-zag CNT when a perpendicular field of $7MeV/cm$ is applied. This tube has a tube index of $n$=13 and a diameter of $d$=$1nm$. We see that the bandgap decreases,

 

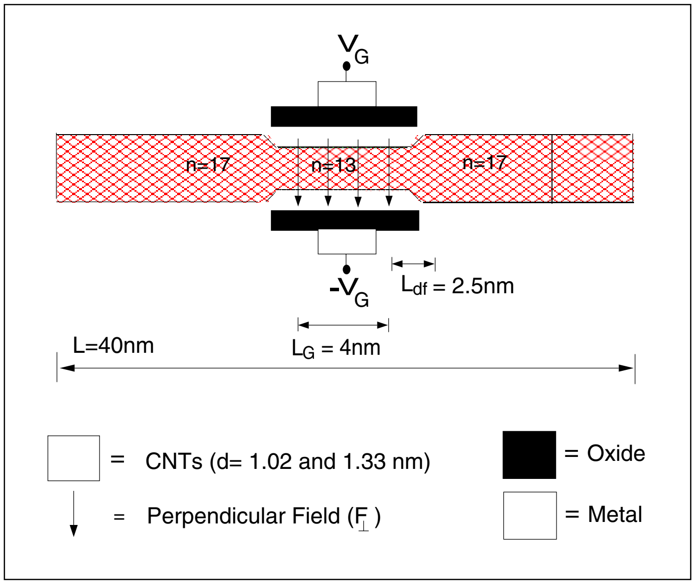


Figure 2. CNT-Junction FET

while the energy gap $\Delta E_{12}$ increases in both the conduction and valence bands. As $F_\perp$ increases, the effective mass of the first band increases while that of the second band decreases. This tunning of the electronic structure leads to effects that maybe useful in electronic applications. The increasing effective mass of the first band would lead to the increase of tube resistance while the changes in the bandgaps could find applications in resonant-tunneling devices. We propose devices which will utilize the latter application.

## III. CNT Tunneling FET

The ability of the perpendicular field to perturb the bandstructure of the CNT provides a basis for some interesting applications. One that we will consider here is a CNT-based tunneling FET. In Fig. 2 we show a proposed device composed of 3 nanotube segments. The middle segment is a $4nm$ long $1nm$ diameter tube located under the gate. On either side of this gate tube($1nm$) are nanotube segments with a larger diameter($1.33nm$). The seamless connections between the segments produce defects in the periodic structure of the nanotube which will localize and trap some charge. These defects will therefore be modeled as tunneling barriers for electrons transversing the gate region and a double barrier device will result.

The device is similar to a prototype AlGaAs double-barrier resonant-tunneling(RT) diode, except here the depth of the potential well can be manipulated by the gate field. The effective masses of the nanotubes in the device are also very close to that of GaAs, $m = 0.07m_e$, so a comparison with the AlGaAs RT diode is interesting. The potential diagram for the CNT-FET is shown in Fig. 3, where an applied voltage $Va$ is dropped over the device. All the potential is dropped over the gate region since we consider the case of heavy doping, $8.33X10^5 cm^{-1}$, outside of the gated region of the device. Here we set the unknown defect barrier height equal to $2.8nm$, the typical value for the bandoffset in AlGaAs. Since increasing the gate potential to $0.3eV$ lowers the depth of the nanotube quantum well, the gate can potentially manipulate the current through the device.

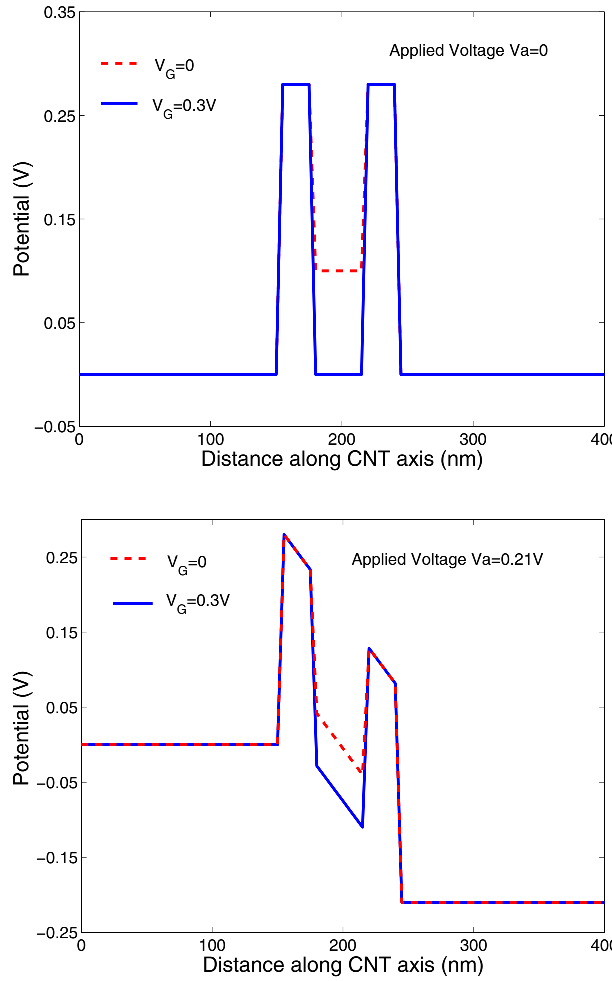


Fig. 3 Potential diagrams for CNT-FET

## IV. Wigner Function Simulation

In order simulate the transport properties of the CNT-FET, we discretize the Liouville equation and calculate the Wigner distribution function [2]. We used 80 mesh points along the 40nm tube and 60 mesh points for the wavevector $k$. Using a CNT Monte Carlo simulator[4-5], the mean free path for phonon scattering is about $50nm$ for the nanotube considered here. We therefore have ballistic transport along the 40nm device, and ignore phonon scattering. We also only consider the lowest subband, but this is a good approximation because the subband spacing is about $0.5eV$. Considering steady-state transport in the CNT-FET, the Wigner distribution function $f$ satisfies the discretized equations

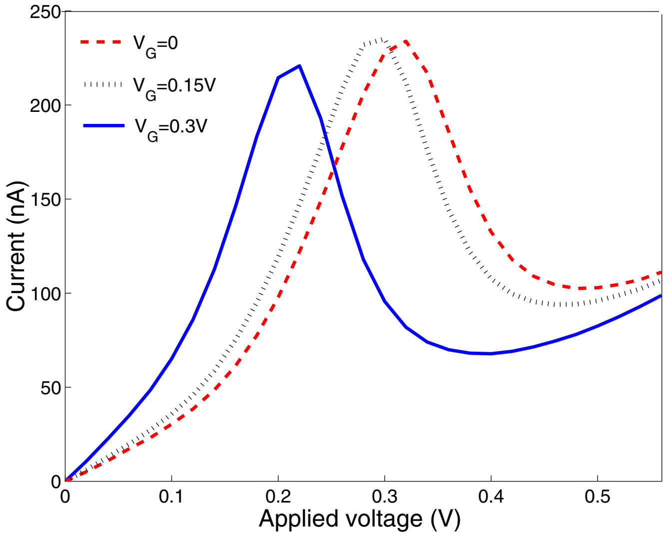


Figure 4. IV for CNT-Junction FET 1

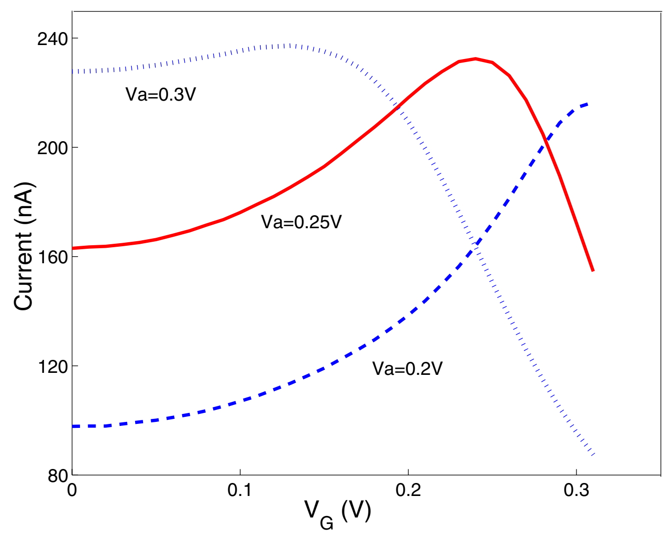


Figure 5. I vs $V_G$ for CNT-Junction FET 1

$$\frac{\hbar^2 k}{m\Delta x}\left[f(x-\Delta x,k)-f(x,k)\right] = \sum_{k'}\Phi(x,k-k')f(x,k'), \quad k>0 \tag{3}$$

and

$$\frac{\hbar^2 k}{m\Delta x}\left[f(x,k)-f(x+\Delta x,k)\right] = \sum_{k'}\Phi(x,k-k')f(x,k'), \quad k<0. \tag{4}$$

Here $m$ is the effective mass of the CNT and the distance along the CNT axis is $x$ with a mesh spacing of $\Delta x$. The term $\Phi$ is kernel of the potential operator in the Liouville equation which can be expressed as

$$\Phi(x,k-k') = \frac{2}{N_k}\sum_{x'}\sin\left((k-k')x'\right)\left(V(x+\frac{x'}{2}) - V(x-\frac{x'}{2})\delta_{gcd(x'/\Delta x,2),2}\right). \tag{5}$$

In this expression, $V$ is the potential due to the applied bias, the defects, and the bandoffset between the two different carbon nanotubes and $N_k = 60$ is the number of wavevector mesh points. Only the $x'$ mesh points that are even multiples of the position mesh spacing, when the greatest common divisor(gcd) of $x'/\Delta x$ and 2 is 2, contribute to $\Phi$.

Considering an open system, the boundary conditions on the left and the right of the device are

$$f(0,k>0) = \ln\left(1+exp\left(\frac{\hbar^2k^2}{2m} - E_F(0) - V(0)\right)\right)$$
$$f(L,k<0) = \ln\left(1+exp\left(\frac{\hbar^2k^2}{2m} - E_F(L) - V(L)\right)\right). \tag{6}$$

The Fermi energy, $E_F$, is found by requiring

$$\sum_k f(0,k) = \sum_k f(L,k) = 2Nd\Delta xNk, \tag{7}$$

where $Nd$ is the doping density per unit length ($8.33X10^5 cm^{-1}$ outside the gate region).

In the case of the CNT, the Wigner function $f(x,k)$ corresponds to the probability of a particle being at the position $x$ in the state $k$ because there is charge confinement perpendicular to the tube axis. The current $I$ through the device is found from the Wigner function according to

$$I(x+\Delta x/2) = \left(\frac{1}{1+|\beta|^2}\right)\frac{\Delta k}{2\pi}\left(\sum_{k>0}\frac{\hbar k}{m}f(x,k) + \sum_{k<0}\frac{\hbar k}{m}f(x+\Delta x,k)\right), \tag{8}$$

where $\Delta k$ is the spacing of the wavevector mesh points. The tunneling between states perpendicular to the tube axis is also considered with the term $\beta$.

Simulations for the CNT-FET are shown in Fig.s 4-5. In Fig. 4, we see that as the gate voltage is increased from 0 to $0.3eV$, the peak current in the resonant-tunneling device decreases from $0.31eV$ to $0.21eV$. The peak occurs at lower applied voltages when the gate voltage increases because the lowest bound state in the quantum well, formed by the defects, is pushed down to lower energies relative to the electrons outside of the well. This allows resonant tunneling to occur at lower biases. We find that the peak current shift is approximately $\propto V_G^2$.

In Fig. 5 the current vs. the gate voltage curves for applied voltages $Va$ of ($0.2V$,$0.25V$,$0.3V$) are shown. The curve when $Va = 0.3V$ is interesting in that it remains roughly constant at $230nA$ for $0.15V$ and then drops sharply to $80nA$ after another $0.15V$. It is expected that this curve will flatten out beyond $V_G = 0.3V$ somewhat, displaying an inverter type of characteristic, but we need to go beyond the perturbation analysis in section II to study higher gate voltages. Furthermore it would be interesting to determine the effects of altering the length of the gated CNT which would adjust the energy of bound state within.

The effect of the perpendicular wavefunction mismatch with increasing $V_G$ can also be seen in Fig.s 4-5. As the gate voltage increases the lowest subband around the gate nanotube circumference becomes a mixture of the two lowest $V_G = 0$ subbands. For an electron in the lowest subband to tunnel from the left side into the gated region, and then back into the lowest subband on the right side of the gate, the electron must enter into the perturbed lowest subband inside the gated CNT. The probability of this is the square of the overlap in (2). The appropriate factor was included in (8) above. The effect of the subband mixing in the gated CNT is to decrease the current in the device.

## IV. Conclusion

In this work we determine that the bandstructure of a CNT is altered by the application of an external electric field perpendicular to the tube axis. Our perturbation analysis shows that the bandgap decreases as this field is increased. The mixing of the energy eigenstate wavefunctions for the subbands along the CNT circumference was also determined. These results not only give insight into how the electric properties of CNTs change when placed in electric fields, but also may serve as the basis of unique device applications, such as the tunneling CNT-based FETs we describe here.

We propose an example CNT tunneling FET based on the connection of carbon nanotubes with different diameters. The regions where these tubes connect are treated as tunneling barriers for electrons flowing through the device. These barriers can potentially confine electrons in a quantum well along the tube axis, creating essentially a quantum dot in a CNT. Here the nanotube region between two barriers is gated and quantum transport simulations are used to determine how the properties of the the device are controlled by the gate potential. For this the Wigner distribution function is used to simulate the transport properties in the steady state. We find that within our model, the resonant peak and thus the current through the device can be manipulated effectively with the gate potential.

Another possible resonant-tunneling device that could take advantage of the effect of the perpendicular field is shown in Fig. 6. Here a voltage is applied across the nanotube circumference and electrons tunnel from the source to the drain. A fixed applied voltage of $0.64V$ across the nanotube is considered. The gate can be used to manipulate the tunneling probability by lowering the conduction band of the nanotube relative to the Fermi level in the source. In this device the gated region of the nanotube is

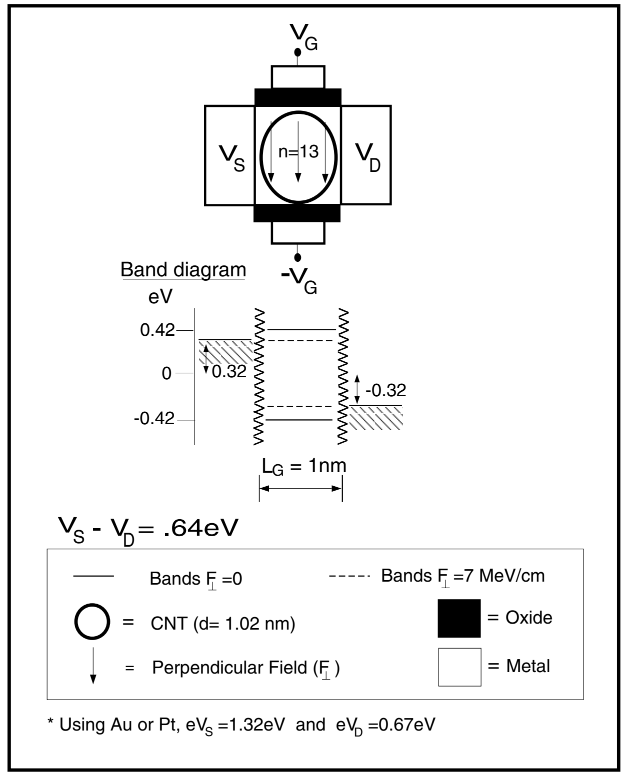


Figure 6. IV for CNT-Junction FET 2

very close to the source and drain contacts and the effects of these contacts on the electronic structure and tunneling barriers would likely be significant. Such devices might be feasible though if the dimensions are scaled to comply with production abilities.

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