Limitation and Diameter Effects on Carrier Drift Velocity in Carbon Nanotubes

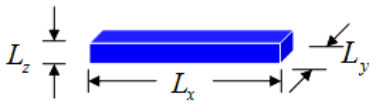
M. T. Ahmadi, R. Ismail, and V. K. Arora

***Abstract*—Due to the chemical stability and perfection of Carbon Nanotubes (CNTs) structure, carrier mobility is not affected by processing and roughness scattering as it is in the conventional semiconductor channel. Therefore, CNTs are being considered as viable candidates for high-speed applications. The mobility and saturation velocity are the two important parameters that control the charge transport in a conducting MOSFET channel. It is shown that the high mobility does not always lead to higher carrier velocity. Owing to the high electric-field streaming, the ultimate drift velocity in semiconducting CNTs are based on the asymmetrical distribution function that converts randomness in zero-field to streamlined one in a very high electric field. The limitation drift velocity is found to be appropriate thermal velocity for non- degenerate regime, increasing with the temperature, but independent of carrier concentration. In this condition, velocity rises with increasing the diameter. However, the limitation drift velocity is the Fermi velocity for degenerate regime which increasing with carrier concentration but independent of the temperature. Moreover, in degenerate regime, degeneracy occurs at lower values of the carrier concentration with increasing the CNTs diameter.**

***Index Terms*—Carbon nanotube, carrier statistic, Quantum limit, one dimensional device.**

I. Introduction

THE GROWING interest for the design of smaller devices, higher operating power and minimum power consumption of integrated circuits leads to a pressing, need to downscale semiconductor components [1]. The research for approaching to high-speed devices for future electronic is continuing. The speed is calculated by how the carrier (electron or holes) can propagate through the length of the device. The low scattering probability is responsible for high on-current in semiconducting Carbon nanotubes (CNTs) [2]. In nanoscale devices it became clear that the saturation velocity plays an important role. The higher mobility brings an electron closer to saturation as a high electric field is encountered, but saturation velocity remains the same [3]. The reduction in conducting channel length of the device brings about reducing transit-time-delay and hence enhancing the operational frequency. There isn't any agreement on the interdependence of saturation velocity on low-field mobility that is scattering-limited [4]. On the other hand, in any solid state device, it is very clear that the band structure parameters, doping profiles (degenerate or nondegenerate) and ambient temperatures play a variety of roles in limiting optoelectronic properties. It is not supported by experimental observations that higher mobility leads to higher saturation [5]. Therefore, this research focused on the controlling of the ultimate saturation velocity. In the following, the fundamental processes that limit drift velocity are delineated.



$$L_x >> \lambda_D \approx 10nm$$
$$L_{y,z} \le \lambda_D \approx 10nm$$

Fig .1. scheme of two-dimensional quantum limits.

II. Theory

In one-dimensional semiconductor, only one Cartesian direction is much larger than the De - Broglie wavelength Fig. 1.

According to Fig. 1 in quasi one-dimensional (Q1D) devices energy spectrum is continues-type in x direction and discrete-type in y and z directions with the eigen-function $\psi_k(\vec{r})$ given by

$$\psi_k(x,y,z) = \frac{1}{\sqrt{L_x}} e^{j(k\ .x)} \times \sqrt{\frac{2}{L_z}} Sin(\frac{n\pi}{L_z} z) \sqrt{\frac{2}{L_y}} Sin(\frac{m\pi}{L_y} y) \quad (1)$$

This wave function describes the propagating waves in one direction. Here k is the wave-vector component with momentum $\vec{p} = \hbar\vec{k}$, $L_{x,y,z}$ is the length in Cartesian directions. Single wall CNTs as a one- dimensional device is a one-atom thick sheet of graphite (called graphene) rolled up into a cylinder with nanometer diameter, as shown in Fig. 2.

The property of CNTs depends on the roll up direction with chiral vector $\vec{C} = n\vec{a}_1 + m\vec{a}_2 = (n,m)$. Here $\vec{a}_1$ and $\vec{a}_2$ are the basic vectors of the lattice.

If $n - m = multiple\ of\ 3$ they are metallic, otherwise they are semiconductor.

In semiconducting CNTs very near the minimum energy, band structure is parabolic [6]. Therefore

$$E(k) = \frac{E_G}{2}\sqrt{1+(\frac{3kd}{2})^2} \quad (2)$$

$$E_G = \frac{0.8(ev)}{d(nm)} \quad (3)$$

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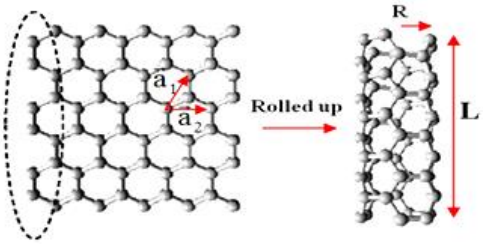

Fig. 2. A Prototype single wall CNT with diameter less than De-Broglie wavelength.

These equations show the E *(k)* and the band gap (E_G) which are function of the CNTs diameter, and we can expand equation E (k) as follow

$$E \approx \frac{E_G}{2} + \frac{\hbar^2 k_x^2}{2m^*} \tag{4}$$

Here m^* is effective mass. For semiconducting (9, 2) Carbon nanotube, $m^* = 0.189\, m_0$ [7] which we used in our equations for plotting all graphs.

$$\frac{m^*}{m_0} = \frac{4\hbar^2}{9a_{c-c}dt} = \frac{0.08}{d(nm)} \tag{5}$$

where $a_{C-C} = 1.42^{o}A$ is Carbon-Carbon (C-C) bond length, $t = 2.7$ eV is the nearest neighbor C-C tight binding overlap energy and d is diameter of the CNT [8], [9]. The distribution function of the energy E_k is given by the Fermi-Dirac distribution function

$$f(E_k) = \frac{1}{e^{\frac{E_k - E_{F1}}{k_B T}} + 1} \tag{6}$$

where E_{F1} is the one-dimensional Fermi energy at which the probability of occupation is half and T is the ambient temperature.

In non- degenerately doped semiconductors the '1' in the denominator of (6) is negligible compared to the exponential factor, the distribution is then Maxwellian

$$f(E_k) = e^{-\frac{E_k - E_{F1}}{k_B T}} \tag{7}$$

This simplified distribution function is extensively used in determining the transport parameters. This simplification is true for nondegenerately-doped semiconductors. However, nowadays most nanoelectronic devices are degenerately doped. Hence any design based on the Maxwellian distribution is not strictly correct and often leads to errors in our interpretation of the experimental results [8]. In the other extreme, for strongly degenerate carriers, the probability of occupation is 1, where $E_k < E_F$ and it is zero if $E_k > E_F$.

Arora [3] modified the equilibrium distribution function of (6) by replacing E_{F1} (the chemical potential) with the electrochemical potential $E_{F1} + q\varepsilon.l$. Here $\vec{\varepsilon}$ is the applied electric field, q is the electronic charge and l the mean free path during which carriers are collision free or ballistic. Arora's distribution function is thus given by

$$f(E_k) = \frac{1}{e^{\frac{E_k - E_{F1} + q\vec{\varepsilon}.\vec{l}}{k_B T}} + 1} \tag{8}$$

This distribution has simpler interpretation as given in the tilted band diagram of Fig. 3.

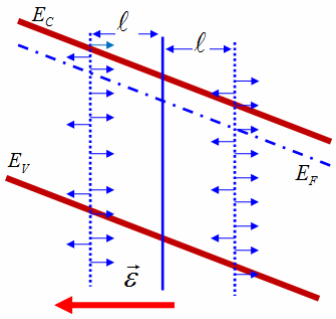

Fig. 3. Partial streamlined of electron motion on a tilted band diagram in an electric-field [10].

The carriers at a point x arrive from left or right a mean-free-path l away from either side of x. In the tilted band diagram a channel of CNT can be thought as a series of ballistic resistors, each with a length of l, where the end of each free path can be considered as virtual contacts with different quasi Fermi levels separated in energy by $q\varepsilon l$. It can be seen that the Fermi level on the left is $E_{F1} + q\varepsilon l$ and on the right is $E_{F1} - q\varepsilon l$. These are the two quasi Fermi levels with E_{F1} at the point x. The current flow is due to the gradient of Fermi energy $E_{F1}(x)$ when an electric field is applied.

Because of this asymmetry in the distribution of electrons, the electrons tend to drift opposite to the electric field $\vec{\varepsilon}$ applied in the negative x-direction (right to left). In an extremely large electric field, virtually all the electrons travel in the positive x-direction (opposite to the electric field). This explains conversion of completely random motion into a streamlined one with ultimate velocity per electron equal to v_i. Consequently, the ultimate velocity is ballistic independent of scattering interactions. The ballistic motion in a mean-free path is interrupted by the onset of a quantum emission of energy $\hbar\omega_0$. This quantum may be an optical phonon or a photon or any discrete energy difference between the quantized energy levels with or without external stimulating effect. The mean-free path with the emission of a quantum of energy is related to l_0 (zero-field mean free path) by the following expressions [11]

$$l = l_0[1 - e^{-\frac{E_Q}{q\varepsilon l_0}}] = l_0[1 - e^{-\frac{l_Q}{l_0}}] \tag{9}$$

$$q\varepsilon l_Q = E_Q = (N_0 + 1)\hbar\omega_0 \tag{10}$$

$$N_0 = \frac{1}{e^{\frac{\hbar\omega_0}{k_B T}} + 1} \tag{11}$$

Here $(N_0 + 1)$ gives the probability of a quantum emission. N_O is the Bose-Einstein distribution function determining the probability of quantum emission. The degraded mean free path (l) is now smaller than the low-field mean free path (l_o). In the Ohmic low-field regime $l \approx l_o$ and in high electric field $l \approx l_Q$. The value of inelastic scattering length when a quantum is emitted is given by [12].

$$l_Q = \frac{E_Q}{q\varepsilon} \tag{12}$$

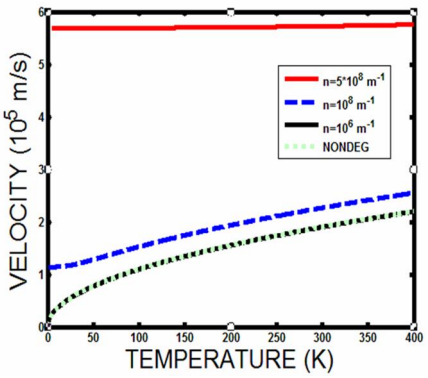

Fig. 4. Ultimate velocity and nondegenerate approximation versus temperature for (9, 2) carbon nanotube, for various concentration values.

Obviously $l_Q = \infty$ in zero –electric field and will not modify the traditional scattering described by mean free path l_0 as $l_Q >> l_0$. Therefore, the low-field mobility andassociated drift motion are scattering-limited. So, the effect of all possible scattering interactions is buried in the mean free path l_0. However, the presence of high electric field makes $l_Q << l_0$. In that extreme

$$l \approx l_Q = \frac{E_Q}{q\varepsilon} \tag{13}$$

This may be enough to explain the degradation of mobility (μ) in a high electric field. Mobility is defined as

$$\mu = \frac{q\tau_c}{m^*} = \frac{ql}{m^* v_{i1}} \approx \frac{ql_Q}{m^* v_{i1}} \tag{14}$$

Here τ_c is the mean free time in which the electron motion is ballistic. v_{i1} is the mean intrinsic velocity [13] for semiconductors. v_{i1} is the average of $|v| = \sqrt{2E_k / m^*}$ with the Fermi-Dirac distribution of (6) multiplied by the density of quantum states as given by [14]

$$v_{i1} = v_{th} \frac{\Gamma(1)}{\Gamma\left(\frac{1}{2}\right)} \frac{F_{\frac{(D-1)}{2}}(\eta_1)}{F_{\frac{(D-2)}{2}}(\eta_1)} \tag{15}$$

$$v_{th} = \sqrt{\frac{2k_B T}{m^*}} \tag{16}$$

$$F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{x^j}{e^{(x-\eta)}+1} dx \tag{17}$$

Here, $F_j(\eta)$ is the Fermi-Dirac integral of order j and $\Gamma(j+1)$ is a Gamma function. Its value for an integer j is $\Gamma(j+1) = j\Gamma(j) = j!$. For half integer values, it is $\Gamma(3/2) = (1/2)\Gamma(1/2) = (1/2)\sqrt{\pi}$. D is the dimensionality that is $D = 1$ for quasi-one-dimensional semiconductor CNTs. The Fermi integral with Maxwellian approximation is always an exponential for all values of j and is given by [15]

$$F_j(\eta) \approx e^\eta \quad \text{(Nondegenerate)} \tag{18}$$

In the strongly degenerate regime, the Fermi integral transforms to

$$F_j(\eta) \approx \frac{1}{\Gamma(j+1)} \frac{\eta^{j+1}}{j+1} = \frac{\eta^{j+1}}{\Gamma(j+2)} \quad \text{(Degenerate)} \tag{19}$$

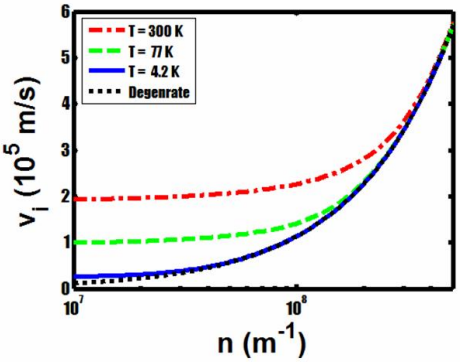

Fig. 5. Velocity versus carrier concentration for $T = 4.2$ K (liquid helium), $T = 77$ K (liquid nitrogen) and $T = 300$ K (room temperature). The 4.2 K curve is closer to the degenerate limit.

For quasi-one-dimensional CNTs, the ultimate average velocity per electron is v_{i1} which a function of temperature and doping concentration is as

$$v_i = \sqrt{\frac{2k_B T}{\pi m^*}} \times \frac{N_{C1}}{n_1} F_0(\eta_{F1}) \tag{20}$$

with

$$N_{c1} = \left(\frac{2m^* k_B T}{\pi \hbar^2}\right)^{\frac{1}{2}} \tag{21}$$

where N_{C1} is the effective density of states for the conduction band, with m^* s the density-of-states effective mass. n_1 is the carrier concentration per unit length.

Fig. 4 indicates the ultimate velocity and nondegenerate approximation as function of temperature. The velocity for low carrier concentration follows $T^{1/2}$ behavior, which is independent of carrier concentration. However, for high concentration the velocity depends strongly on concentration and becomes independent to the temperature. The ultimate saturation velocity is thus the thermal velocity appropriate for 1D carrier motion as follow

$$v_{i1ND} = v_{th1} = \frac{1}{\sqrt{\pi}} v_{th} = \sqrt{\frac{2k_B T}{\pi m^*}} \text{ (Nondegenrate)} \tag{22}$$

Fig. 5 shows the graph of ultimate intrinsic velocity as a function of carrier concentration for three temperatures (T = 4.2 K, 77 K, and 300 K). As expected, at low temperatures, carriers follow the degenerate statistics and hence their velocity is limited by appropriate average of the Fermi velocity that is a function of carrier concentration. When degenerate expression for the Fermi energy as a function of carrier concentration is utilized, the ultimate saturation velocity is given by

$$v_{i1D} = \frac{\hbar}{4m^*}(n_1 \pi) \text{ (Degenerate)} \tag{23}$$

The ultimate velocity in quasi-one-dimensional CNTs may become lower when quantum emission is considered. The inclusion of the quantum or optical phonon or any other similar emission will change the temperature dependence of the saturation velocity.

Fig. 6 shows by increasing the diameter of the CNTs in semiconductor CNTs, degeneracy occurs at lower values of carrier concentration in degenerate regime at the same temperature.

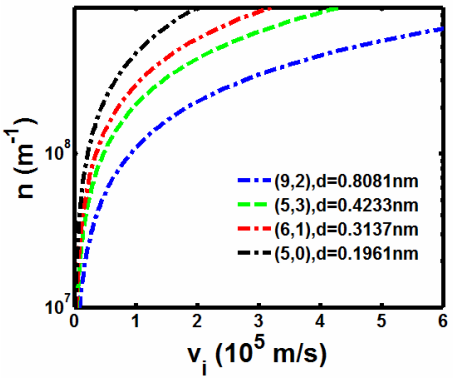

Fig. 6. Velocity versus carrier concentration in T=300 K for different diameters in degenerate regime.

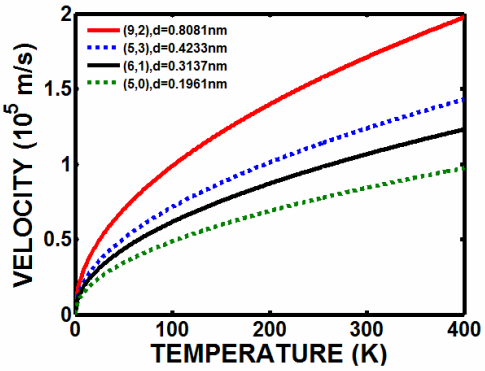

Fig. 7. Velocity versus temperature for CNTs, for various diameter values in nondegenerate regime.

According to the Fig. 7 the velocity depends on the temperature and diameter in nondegenerate regime. Furthermore, it is independent of carrier concentration. Any increase in the diameter of CNTs results a higher velocity.

III. Conclusion

Using the distribution function, the asymmetrical distribution of drifting electrons in an electric field is presented. This distribution function transforms the random motion of electrons into a streamlined one. It gives the ultimate saturation velocity that is a function of temperature in nondegenerate regime and a function of carrier concentration in the degenerate regime. The ultimate drift velocity is found to be appropriate thermal velocity for a given dimensionality for nondegenerately doped samples. However, the ultimate drift velocity is the appropriate average of the Fermi velocity for quasi-one-dimensional degenerately doped CNTs and any samples. On the other hand, by increasing the diameter of CNTs ultimate drift velocity of carrier increases in non-degenerate regime, and degeneracy occurs at lower values of carrier concentration in the degenerate regime.

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