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A New Consideration of Carrier Transport Through Carbon Nanotubes Which Has Been Placed as a Channel of Field Effect Transistor

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Abstract: In this paper we have reported a mechanism which corrects Fermi level of Single Wall Carbon NanoTubes (SWCNT). We solved Boltezman equation for electron-phonon scattering to obtain electron-phonon distribution function. After that we renormalized distribution function in presence of electric field then we calculated Source Drain current. Our simulation results show that electrons scatter into all energy level of carbon NanoTube while holes don't.

Key words: CNTFET · Electron Phonon Scattering · Boltezman Equation · Monte Carlo · SWCNT

INTRODUCTION

The ability of using Carbon Nanotubes (CNT) as a channel of Field Effect Transistor (FET) have been recently considered by many scientist [1-8]. CNTs could be considered as a graphene sheet which be rolled around a cylinder circumference [1]. This rolling could be done by many ways, so CNTs could be found on various types. One of them which is semiconductor is called Zig-Zag. Our calculation shows that, Zig-zag CNT band gap is comparable to Si or Ge.

Many workers have recently computed electric current on Zig-Zag CNTs [2-6] or those metallic armchair ones [7, 8]. Liang and coworkers used some approximation to find Fermi level of CNT [9]. T. S. Li and coworkers calculated the effect of external field on energy level of a CNT by concerning Zemann effect and perturbation theory [10]. Many other workers although have simulated electric current in a CNTFET but they didn't attend to the effect of electric field on Fermi level [2-8, 11-16]. We have tried to apply the effect of external electric field on Fermi level of CNT by renormalization of electron distribution function. More accurate result's will be obtain by considering the effect of electric field on energy level of CNT but in this work we didn't do that.

Theory: When we use an armchair or metallic CNT as a channel of FET, ballistic transport is explained Source - Drain Current and electrons don't scatter from any thing. On the other hand if we use a Zig-Zag CNT as a channel of FET electron - phonon scattering must be considered.

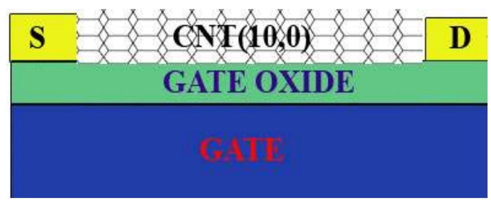

Fig. 1: Schematic view of a CNTFET.

This effect has been calculated before by many workers [11-16]. Fermi level is determined by the number of electrons in the CNT. In our experiment, this is controlled through a Gate placed next to the CNT with a dielectric layer in between (see Figure.1). Define C as the gate capacitance per unit length and assume the threshold voltage then Fermi level obtains by solving below equation.

$$n = \int f(k)dk, \quad n = \frac{Q}{e} = \frac{CV_{G-Th}}{e}$$

Where $f(k)$ is Fermi-Dirack distribution function.

We obtain electron distribution on presence of electric field by solving Boltezman equation numerically (MC) [17].

$$\frac{\partial g_n\left(\vec{r},\vec{k},t\right)}{\partial t} + \vec{v}.\vec{\nabla}_r g_n\left(\vec{r},\vec{k},t\right) + F.\vec{\nabla}_k g_n\left(\vec{r},\vec{k},t\right) = \sum_{\vec{k}'}\left(W_{k,k'} g_n(\vec{r},\vec{k},t)(1-g_n(\vec{r},\vec{k}',t)\right) - \sum_{\vec{k}'} W_{k',k} g_n(\vec{r},\vec{k}',t)(1-g_n(\vec{r},\vec{k},t)$$

Where W is electron phonon scattering rate which obtain from Fermi Golden Rule [8, 17]. Figure 2 show Total scattering rate of some CNTs.

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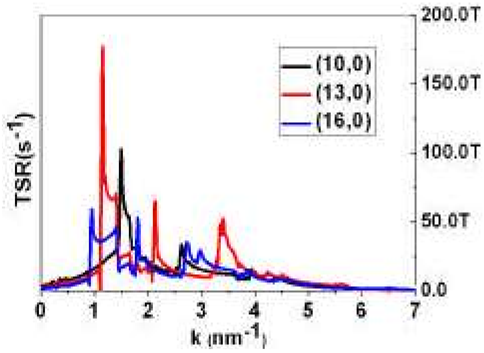

Fig. 2:

$$W_{k,k'}^{op} = \frac{D_{op}^2 \cdot DOS(k')}{\rho.d.\omega_p}\left(N_p + \frac{1}{2} \pm \frac{1}{2}\right)$$

$$W_{k,k'}^{oc} = q^2 \frac{D_{ac}^2 \cdot DOS(k')}{\rho.d.\omega_p}\left(N_p + \frac{1}{2} \pm \frac{1}{2}\right)$$

Figure. 2: Total Scattering Rate (TSR) of minimum conduction band of various CNTs. To obtain this data we break first Brillouin of electronic band and phonon band to 2000 grid point and investigated conservation rule for any transition. If the number of grid point was grown then we had more accurate data. But this need a huge time cost of computer calculations.

Conservation of electron energy and momentum determined an allowable transition. Electronic band structure of CNTs is provided from those graphen one (Zone Folding) [14]. Electronic band structure of graphen can be calculated by tight binding theory [18]. Our result's show that there are tow deferent type of semi-conducting Zig Zag CNT which is labeled with (3n+1, 0), (3n+2, 0). In this paper, we consider first type CNT properties. We have calculated phonon dispersion of graphen by FCM (Force Constant Model) [18]. In this model we have applied the effect of 4 nearest neighbors. Since there are two carbon atoms, in the unit cell of graphen, one must consider 6 coordinates. The secular equation to be solved is thus a dynamical matrix of rank 6, such that 6 phonon branches are achieved.

In order to determine phonon dispersion relation we consider the sum of the forces on the *i* th atom, F_i, for N atoms in the unit cell as follow.

$$\vec{F}_i = \sum_j K^{ij}\left(\vec{u}_j\left(\vec{R}_j\right) - \vec{u}_i\left(\vec{R}_i\right)\right)$$

$$M\ddot{\vec{u}}\left(\vec{R}_i\right) = \sum_j K^{ij}\left(\vec{u}_j\left(\vec{R}_j\right) - \vec{u}_i\left(\vec{R}_i\right)\right)$$

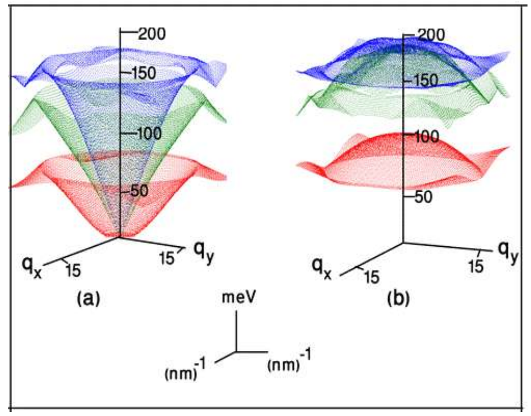

Fig. 3: a) Acoustic branch of phonon dispersion of graphene
b) Optical Branch of phonon dispersion of graphene.

$\vec{u}_i\left(\vec{R}_i\right)$ can be found by using Fourier transform as below

$$\vec{u}_i\left(\vec{R}_i\right) = C\exp(i\omega t)\sum_q \exp\left(-i\vec{q}\cdot\vec{R}_i\right)\vec{u}_i(\vec{q})$$

When we let this Fourier transform to equation of motion we find below equation.

$$\left(\sum_j K^{ij} - \omega^2 M_i \hat{I}\right)\sum_{\vec{q}} \exp\left[-i\left(\vec{q}\cdot\vec{R}_i - \omega t\right)\right]\vec{u}_i(\vec{q})$$
$$= \sum_j K^{ij}\sum_{\vec{q}} \exp\left[-i\left(\vec{q}\cdot R_j - \omega t\right)\right]\vec{u}_j(\vec{q})$$

By multiply both side of this equation to $\exp\left(i\vec{q}\cdot\vec{R}_i\right)$ and sum over all $\vec{R}_i$ we have

$$\left(\sum_j K^{ij} - \omega^2 M_i \hat{I}\right)\vec{u}_i(\vec{q}) - \sum_j K^{ij}\exp\left(i\Delta\vec{R}_{ij}\right)\vec{u}_j(\vec{q}) = 0$$

By solve this equation we can extract out phonon dispersion of graphen. More detailed of calculation can be found at [18] Fig. 3 shows phonon dispersion of graphen along high symmetry lines. The phonon dispersion relations of SWCNTs can be understood by zone folding of the phonon dispersion branches of graphen. Fig. 4 shows electron distribution function of first conduction band of CNTs (10, 0), (13,0), (16,0) while they are used as a channel of CNTFET and an electric field is applied along their axis. As you see the electron distribution is completely deflected from its original Fermi-Dirac shape.

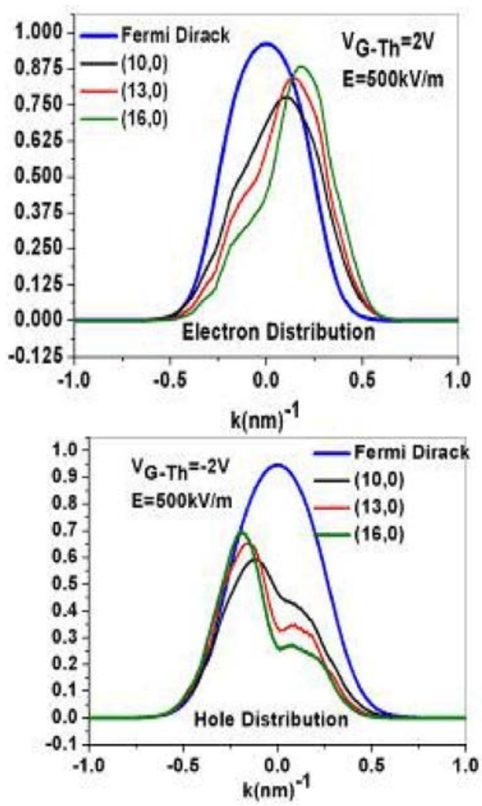

Fig. 4: This figure shows electron and hole distribution function.

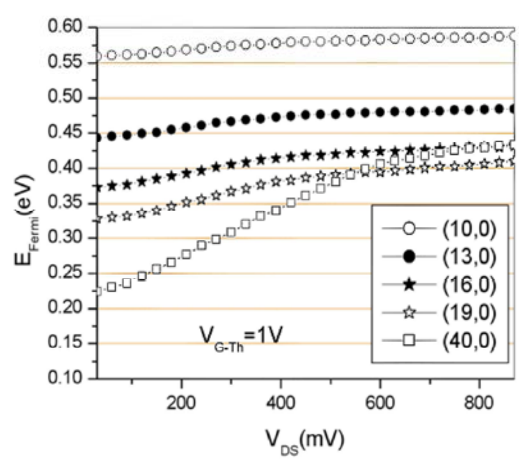

Fig. 5: This figure shows Fermi level via as Source-Drain voltage.

So the validity of Equation $n = \int f(k)dk$ is now contravened. Therefore we must find a new Fermi level which satisfies below equation.

$$n = \int g(k)dk$$

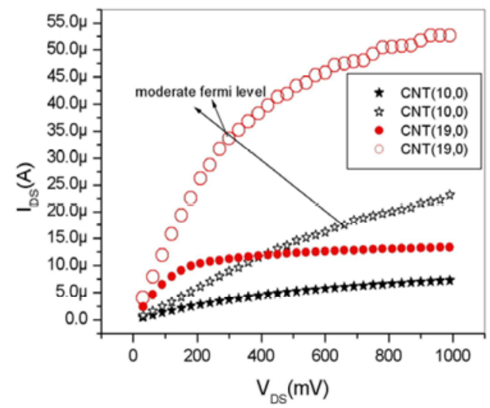

Fig. 6: This figure compares moderate Fermi level current via as those fixed Fermi level which applied for CNT (10, 0) and CNT (19, 0).

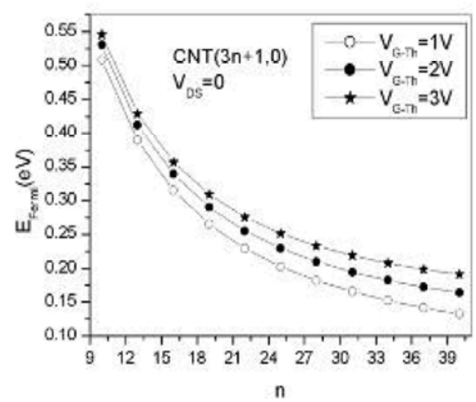

Fig. 7: This figure illustrates Fermi level of various Zig-Zag CNTs. As you see, under absence of V_{DS}, Fermi level of Zig-Zag CNT decays with increment on its geometric parameter.

Although this Equation is written on stable condition but at no equilibrium condition we can use below relation.

$$n = \int g(k,t)dk$$

We use a CNTFET with SiO_2 insulator. Insulator thickness is taken to 10nm and CNT length is taken to μm. Fig. 5 shows Fermi level of a CNTFET which use various Zig-Zag CNT as its Channel. Electric current can be obtained from below equation.

$$I = \sum_j 2 \times 2 \frac{|\vec{T}|}{\pi} \int V_j(k) g_j(k) dk$$

Where V is electron velocity which obtains from semi classical relation of motion.

$$\vec{V}_j(k) = \frac{\vec{\nabla} E_j(k)}{\hbar}$$

$\vec{T}$ is translation vector of CNT. One of 2 factors refers to electron spin and other refers to degeneracy of energy level of Zig-Zag CNT. You can see the effect of reclaimed Fermi level on electric current at Figure6. Many researchers have extracted out those branch which use fixed Fermi level [2- 8]. Figure.7 shows Fermi level on various CNTs and its dependence on gate voltage which applied perpendicular to its axis.

CONCLUSIONS

Electric field changes the Fermi level of CNT. To find a correct Fermi level which satisfied the conservation of free electron density we must renormalize electron distribution function. You can find when there is not any field along tube axis Fermi level decays by increment in CNT geometric number, on the other hand when we applied an electric field along tube axis this general rhyme was disarrangement.

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