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Renormalization of Fermi Level of Carbon Nano Nube Field Effect Transistors

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Abstract

In this paper we have simulated electron phonon scattering in a SWCNT by solving Boltzmann equation. We have extracted electric current of a CNTFET by using a new consideration of Fermi level moderation. Finally we have reported a mechanism which moderate Fermi level in a CNT under an applied electric field. Results show Fermi level increase linearly respects to electric field and the slope of this line is proportionate to CNT diameter.

Keywords: CNTFET, Electron Phonon Scattering, Carbon Nano Tubes

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INTRODUCTION

Many researchers have simulated electron transport of CNTFETs (Carbon Nano Tube Field Effect Transistor) [1-7]. Some of them used MC (Monte Carlo) and solved Boltzmann equation to obtain distribution function of electron [8-10].The basic idea that used was that electron distribution function is changed in presence of electric or magnetic field. We know electrons are fermions and they are explained with Fermi – Dirac distribution. 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. Define C as the gate capacitance per unit length and assume the threshold voltage then Fermi level obtains by solving below equation.

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

$$n = \frac{Q}{e} = \frac{CV_{G-Th}}{e}$$

Where f is Fermi-Dirac distribution function.

RESULTS AND DISCUSSION

We obtain electron distribution by solving Boltzmann equation numerically [11].

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

Where W is the electron phonon scattering rate which obtain from Fermi Golden Rule[9].

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

To obtain electron phonon scattering we must consider momentum and energy conservation. Electronic band structure of CNTs (Carbon Nano Tube) is provided from those graphene one (Zone Folding)[5]. Electronic band structure of graphene can be calculated by tight binding theory [12, 13].

Phonon dispersion relations of CNTs can be calculated using tight-binding methods [14-16], density functional theory [17, 18], and symmetry-adapted models [19, 20]. The phonon dispersion relations of SWCNTs (Single Wall Carbon Nano Tube) can be understood by zone folding of the phonon dispersion branches of graphene. In this work we have calculated phonon dispersion of a graphene sheet by force constant model [21, 22]. In this model we have applied the effect of 4 nearest neighbors. Since there are two carbon atoms, in the unit cell of graphene, 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. Figure 1 shows phonon dispersion of graphene.

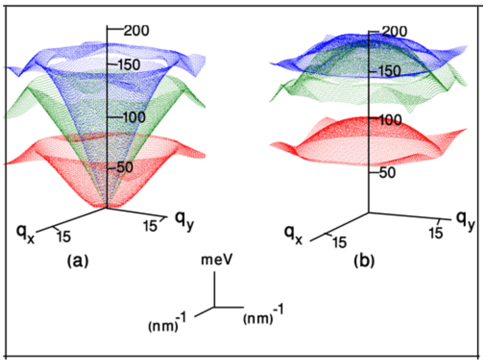

Figure1. (a) Acoustic branch of phonon dispersion of graphene (b) Optical Branch of phonon dispersion of graphene

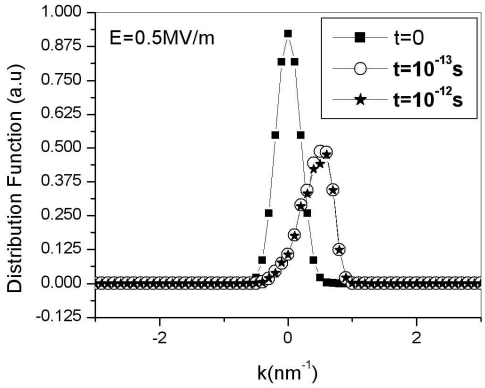

Figure 2 show electron distribution function of first conduction band of CNT (10, 0)

Figure2: This figure shows electron distribution function. Note that system take a stable condition after $10^{-13} s$.

As you see the electron distribution is completely deflected from its original Fermi – Dirac distribution. So the validity of Equation $n = \int f(k)dk$ is now contravened. Therefore we must find a new Fermi level which satisfied below equation.

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

Although this Equation is written on stable condition but on nonequilibrium condition we can use below equation.

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

This moderation of Fermi level is neglected on other works [1-10].

Figure 3 shows Fermi level of a CNTFET which use various Zig – Zag CNT as its Channel.

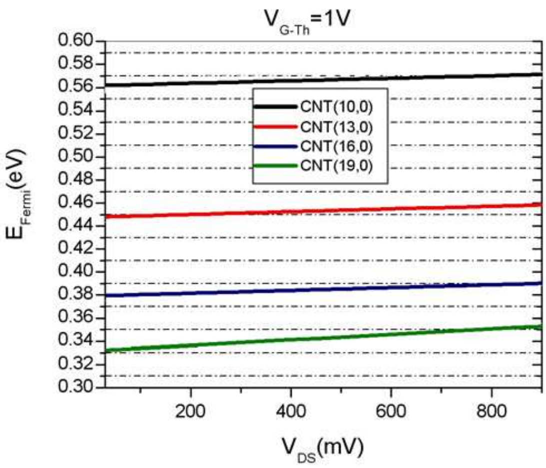

Figure3: This figure shows modification of Fermi level via as Source – Drain voltage

When the correction on Fermi level is applied we can calculate electric current by below equation on stable condition.

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

One of 2 factors refers to electron spin and other refers to degeneracy of energy level of Zig – Zag CNT. If Gate voltage is small Fermi level only cut first conduction band. V is electron velocity which obtains from semiclassical relation of motion.

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

Figure 4 compare electric current when Fermi level be a fixed number via as moderate Fermi level current.

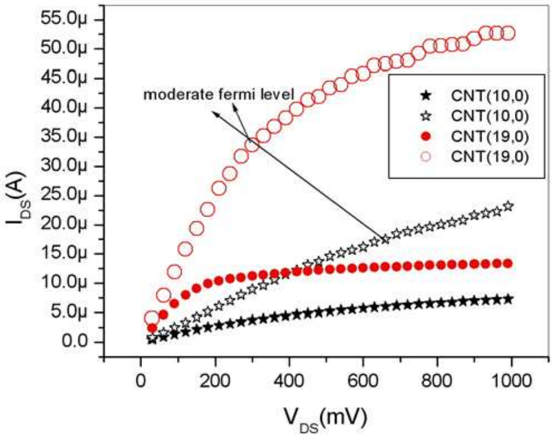

Figure 4: This figure compare moderate Fermi level current via as those fixed Fermi level

CONCLUSION

Although Electric filed can disturb energy levels of a CNT and this itself cause Fermi level deflection we have not considered this effect. But we focused to find a correct Fermi level which satisfied the conservation of free electron density.

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