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Archives of Physics Research, 2010, 1 (2): 31-36
(http://scholarsresearchlibrary.com/archive.html)

Archives of Physics Research
Scholars Research Library
ISSN 0976-0970

Nano scale contact junctions between SWCNT Channel and gate dielectric of CNTFET

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Abstract

Shrinking transistors causes some problems such as leakage current, tunneling and boron diffusion through the ultra thin gate SiO_2. Some researchers believe that CNT (carbon nano tube) can play silicon role in the future of nano transistors. However, the key factors of the next CNTFET (carbon nano tube field –effect-transistor) are SWCNT/Si contacts. The schottky barrier exits at this contact and the energy barrier height is mainly determined by the difference between the SWCNT (metal) work function and Si affinity. Henceforth, much more complexity could arise at a nano scale contact junctions, where just a few carbon atoms could form the contact and the actual schottky barrier height can no longer infer from the traditional contact properties. We have studied analytically and numerically the effects of these contacts on the carrier transport through the SWCNT.

Key words: Nano transistors, Carbon nano tube, Gate dielectric and Schottky barrier.

INTRODUCTION

In the last decade, FETs (field-effect-transistors) based on semiconducting CNTs have been generated considerable and remarkable interest due to their quasi-ideal electronic and mechanical properties and have a high level of performance [1-3]. Among numerous remarkable properties of CNTs, some issues related to transport mechanisms and device physics are still the main problem of the CNTFET generations.

Significant efforts have been made recently to solve these problems, nevertheless there are still key points to be addressed and understood. In particular there has been no modeling and fabrication process – compatible doping method for CNTs. However, the quasi one-dimensional

(1D) CNTFETs can be doped via charge transfer processes [4] which there 1D nature yields a very good charge confinement and electrostatic control [5].
Moreover, in contrast to silicon in these materials carrier transport properties are excellent and nearly similar for holes and electrons in zigzag type CNT (10, 0) semiconducting nano tubes. Mean free path of 300-500 nm at low field and 10-100 nm at high field have been measured [6]. In this work, we study the contacts analytically and numerically, between SWCNT/Sio_2 to find a better and easier condition of a full-nanotube circuit design with using Monte Carlo (MC) method.

Calculations and discussion

As mentioned previously, grapheme is a two dimensional sheet consisting of connected carbon atoms in hexagons like the benzene molecule. The basis of a grapheme sheet consists of two atoms named 'a' and 'b', see Fig.1. The nearest neighbor atoms interactions , e.g. , the interaction between atom 'a' with three 'b' atoms, causes the angle between 'b' atom becomes 120°. When folding the grapheme sheet into a SWCNT (Single Walled Carbon Nano Tube) it is possible to use the concepts and calculations from grapheme sheets.

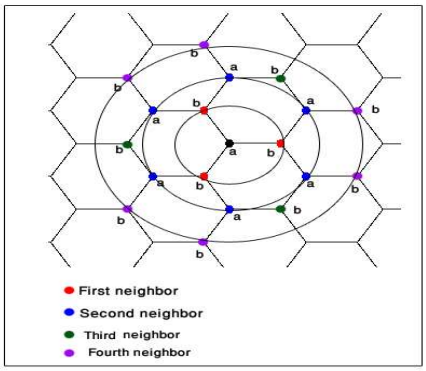

Fig.1. Neighbor atoms of a graphitic plane up to 4th nearest neighbors for an atom 'a'.
are just for understanding the process

To study these interactions, we pick out one particular atom to study and consider all of the other nearest neighbor's atoms effect on selected atom. This arbitrary carbon atom of grapheme can vibrate (move) freely while its nearest neighbor atoms are fixed at their positions leads to both bonding and anti bonding potentials in the grapheme sheet [6]. Here, we just consider bonding potential and neglect anti bonding potential (Latter will be discussed in the next paper). Bonding potential includes harmonic and Moore's potentials [7, 8] in that:

(1) $$U = U\_bond + U\_Lj$$

(2) $$U_{bond} = D\left(\left(1-e^{-\beta(r-r_0)}\right)^2 -1\right) + \frac{1}{2}K(\theta-\theta_0)^2\left(1+K'(\theta-\theta_0)^4\right)$$

$$r_0 = 1/42\text{A}^{\circ}, D = 6/03\times10^{-19}\text{Nm}, \quad \beta = 2/65\times10^{10}\text{m}^{-1}, \quad \theta_0 = 2/094\text{rad},$$
$$k = 9\times10^{-19}\text{Nm/rad}^2, \quad K' = 0/754\text{rad}^{-4}$$

Where the force corresponded to above potentials can be determined by

(3) $$\vec{F} = \vec{\nabla} U$$

We use the velocity Varlet algorithm (for more details see Ref. [5].). It represents harmonic vibrations with the same amplitude, direction and phase, where only arbitrary atom is allowed to moves or vibrates.

Assuming the motion of the first nearest neighbor atoms and doing some calculations based on velocity Varlet algorithm, the sum over the forces on the atom i, labeled to F_i , we will have:

(4) $$\vec{F}_i = \sum_j K^{ij}(\vec{u}_j(\vec{R}_j) - \vec{u}_i(\vec{R}_i)) \qquad ,i = 1,....N$$

Where $\vec{u_i}(\vec{R_i})$ and $R_i = (x_i, y_i, z_i)$ are the displacement and position of the i th atom, respectively. We can write a $3N \times 3N$ dynamical matrix $D(q)$ as follow:

(5) $$D(\vec{q})\vec{u}_q = 0$$

The dynamical matrix D for two-dimensional graphite is written in terms of the 3×3 matricesD_{aa}, D_{ab}, D_{ba} and D_{bb} for the 'a' and 'b' atoms within the unit cell as shown in Fig.1

(6) $$D(\vec{q}) = \begin{bmatrix} D_{aa} & D_{ab} \\ D_{ba} & D_{bb} \end{bmatrix}$$

The sum over j is taken up to the nearest neighbor of the i th atom and K^{ij} is a 3×3 force constant matrix between the i th and the j th atom. The force constant tensor is thus given by

(7) $$K^{ab_1} = \begin{bmatrix} \phi_r^1 & 0 & 0 \\ 0 & \phi_{ti}^1 & 0 \\ 0 & 0 & \phi_{to}^1 \end{bmatrix}$$

Where ϕ_r^n, ϕ_{ti}^n and ϕ_{to}^n represent the force constant parameters in the radial (bond-stretching), in-plane and out-of-plane tangential (bond-bending) direction of the nth nearest neighbors, respectively.

The force constant matrices for the two other atoms are obtained by rotating the matrix in Eq. (15) according to the rules for a second-rank tensor:

(8) $$K^{ij} = U^{-1}(\theta) K^{ab_1} U(\theta)$$

Where U is the rotation matrix for rotation around the z – axis, and θ is angle between x – axis and the line from one atom to another atom.

Furthermore, force constant parameters up to 3th nearest neighbor in unit of 104 dyne/cm. are determined experimentally by using inelastic neutron scattering or EELS (Electron Energy Loss Spectroscopy) techniques [9] are given in Table 1 (see Fig.5).

Table 1. Force constant parameters up to 3th nearest neighbor in unit of 104 dyne/cm

Radial	Tangential in-plane	Tangential out-of- plane
$\phi_r^1 = 36.5$	$\phi_{ti}^1 = 24.5$	$\phi_{to}^1 = 9.82$
$\phi_r^2 = 8.8$	$\phi_{ti}^2 = -3.23$	$\phi_{to}^2 = -0.4$
$\phi_r^3 = 3.00$	$\phi_{ti}^3 = -5.25$	$\phi_{to}^2 = 0.15$

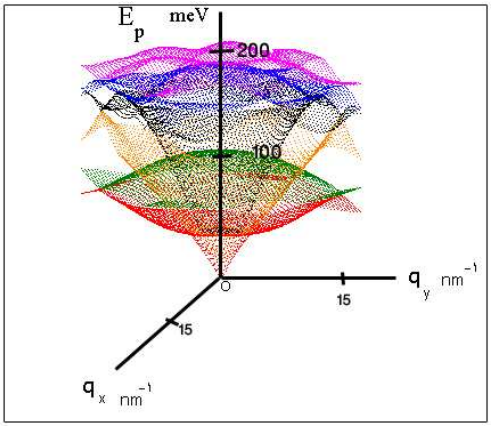

Fig.2.3d plot of the stable phonon dispersion in first Brillion zone

By assuming the time dependence of all $U_i(R_i)$ as the form of $e^{i\omega t}$. We could see in [5], how the determinant of Dynamical Matrix of a two dimension grapheme sheet as the form of Eq. (4) varies by passing vibrations time. The time dependence of displacement vector causes a time oscillating behavior on phonon frequency.

From [2] and quantum confinement along the SWCNT circumference the wave function of carrier which propagated along the CNT axis, are bound around CNT. These confinements cause the sub bands of SiO2 and SWCNT can be decoupled, in that, the first sub-band contributes mostly to the total current. According to retarded Green's function, G, we can write the below relation with considering the self-energy (E_{self}) due to the coupling of the device to the source and drain contacts, which is zero except at the boundaries, the effective mass Hamiltonians, H, and E_I [5-11].

(9) $$G = \frac{1}{E_I - H - E_{source}^{self} - E_{drain}^{self}}$$

H is discredited with using finite differences as stated in Ref. [4] for nearly four discrete sub-bands, as follow:

(10)
$$H = \begin{pmatrix} u_1 + \frac{\hbar^2}{m^* a^2} & -\frac{\hbar^2}{2m^* a^2} & 0 \\ -\frac{\hbar^2}{2m^* a^2} & u_2 + \frac{\hbar^2}{m^* a^2} - \frac{\hbar^2}{2m^* a^2} & 0 \\ 0 & -\frac{\hbar^2}{2m^* a^2} & u_3 + \frac{\hbar^2}{m^* a^2} - \frac{\hbar^2}{2m^* a^2} \end{pmatrix}$$

Where $u_{1,2,3}$ are the potential energy at the point 1, 2, 3 and a is the grid spacing. The energy depends effective mass (m^*) inside the band gap should change from $\frac{\hbar^2}{m^* a^2}$ to $\frac{\hbar^2}{2m^*(1+\frac{\varepsilon}{E_g})a^2}$ in which E_g is the band gap energy. We can now find the carrier concentration, velocity and current as follow:

(11)
$$N = \int G\ \Gamma_{source}\ G^+\ f_{source}\ dE + \int G\ \Gamma_{drain}\ G^+\ f_{drain}\ dE$$

Here Γ is the broadening due to contacts and is given by [2], i.e;

(12)
$$\Gamma = i(E_{self} - E^+_{self})$$

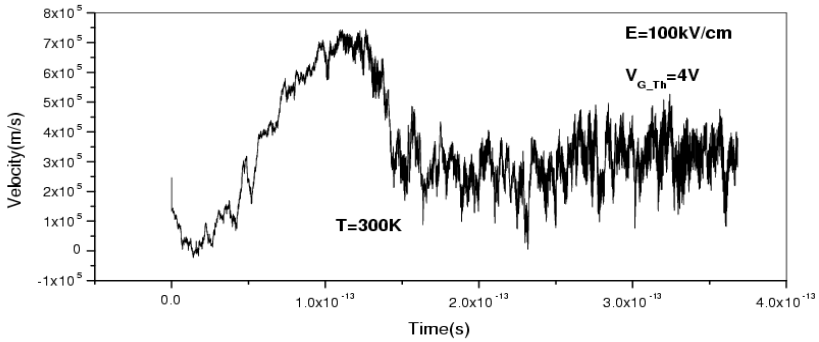

Fig.3. Applied electrical field accelerates carrier in which the velocity takes a maximum value and then tends to a constant value after about 10s

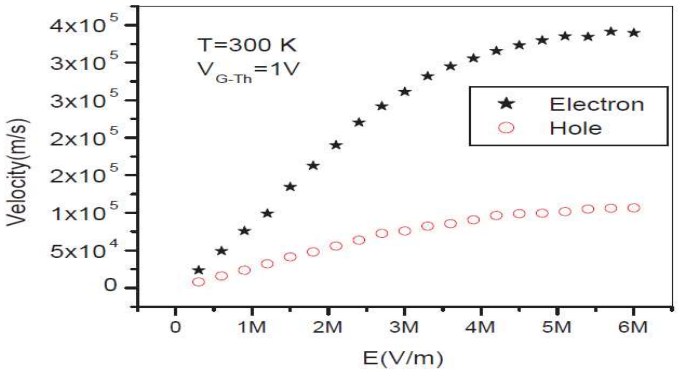

Fig.4. the electron and hole velocity versus applied electrical field

Henceforth, carriers are treated as a sheet charge distributed over the surface of the CNT. Now we take the example of what we found in the above calculations and show only the results of them in the Figs. 3 and 4.

Different transport velocities of electron and hole are obtained and revealed in Fig. 3. Holes move slower than electrons in the SWCNT channel due to their mobility, but after 10^{13} s they get the same velocities. This means that the CNTFET which is made cannot work at high electric field, in particularly, in switching devices such as CPU memory or computer memory. Usually, for such off - on devices, the slope of velocity - field is a key factor for designing a CNTFET. By looking at Fig. 4 the acceptable range for this device is estimated from 0.5 to 3 MV/m. By looking at Figs.3 and 4, we see that the electrons are scattered into the whole levels above Fermi Level, whereas holes scattered just at the maximum level of valence band.

DISCUSSIONS AND CONCLUSION

As stated above, in the CNTFETs source and drain contacts are either schottky or Ohmic –like. Ohmic boundary conditions are characterized by thermal equilibrium and to local charge neutrality, which is only condition of carrier injection in the device. But, the treatment of a schottky contact requires changing the injection SWCNT to SiO2 and the particle motions algorithm in the space charge region near schottky interface. Simulation results suggest that different electron and hole velocity (Fig. 4) under the same conditions and applied electric field at the low electric field. They behavior Boltzmann function or self-limiting tendency at high electric field , meaning, a novel model for gate dielectric/CNT contacts is needed for describing the electrostatic charge balance across the contacts and the dipole polarization along the SWCNT.

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