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# EFFECT OF DOPING ON THE MOBILITY OF SEMICONDUTING SINGLE-WALLED CARBON NANOTUBES

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## ABSTRACT

The single walled carbon nanotube as a 1-D device is studied by evaluating the various electrical parameters such as mobility, velocity, critical electric field etc. Comparison of these parameters eventually reveals that nano-devices are ideal replacement for current 2-D solid state silicon devices. Monte Carlo simulation technique was used to evaluate above parameters for both intrinsic as well as extrinsic carbon nanotubes. Thermal analysis showed that carbon nanotubes exhibit similar trend as that of silicon. It is also found that carbon nanotubes devices exhibits exceptionally high mobility in order of 10^5 (cm^2/V-s).the main factor governing the mobility in case of carbon nanotubes devices is the electron phonon interaction.

**Keywords**: 1-D, single walled ,Monte Carlo, electron-phonon interaction, doping.

## INTRODUCTION

SOLID-STATE devices in which electrons are confined to two dimensional planes have provided some of the most exciting scientific and technological breakthroughs of the last 50 years. From metal-oxide-silicon field effect transistors to high mobility gallium-arsenide heterostructures, these devices have played a key role in the microelectronics revolution. But with the growth of technology and according to Moore's Law the number of components on the chip doubles every 18 months. And hence the length of the channel of MOSFET has to decrease. However, there is a practical limit on this due to characteristics of silicon. It is observed that the velocity of the carrier saturates after certain critical field and the mobility starts decreasing thereafter. These problems force us to go for new devices which give better characteristic for small dimensions. Recent studies and research have showed that carbon nano-devices offer better characteristics as compared to silicon at lower dimensions.

Carbon nanotubes are wires of pure carbon with diameter of few nanometers and length of few hundred microns. A single walled carbon nanotubes may be considered as a single layer sheet of graphite (called grapheme) rolled into cylinder. They are quasi 1-D materials made of sp2 hybridized carbon network as called graphene. Carbon nanotubes have very high mobility and exceptional conductivity as dominant scattering is only electron-phonon scattering as stated earlier and also because it has more or less a hollow structure. Another parameter that describes the structure and properties of carbon nanotube is its chiral angle. This angle is specified by how the graphene sheet is rolled into cylinder (fig 1). Carbon nanotube becomes either metallic or semiconducting depending on this chiral angle. A nanotube with its axis collinear with the horizontal line (θ=0) is called zigzag nanotube. Zigzag nanotubes can be either metallic or semiconducting depending on the index of wrapping. In general an (n,m) carbon nanotube is metallic if n-m=3q, where q is an integer. All armchair nanotubes (n=m) are metallic as are one third of zigzag nanotubes. Nanotubes can form with axes collinear to several lines forming chiral angles from 0 to 30 degrees. Other than zigzag or armchair there also exist chiral nanotube which can be either metallic or semiconducting depending on its band structure.

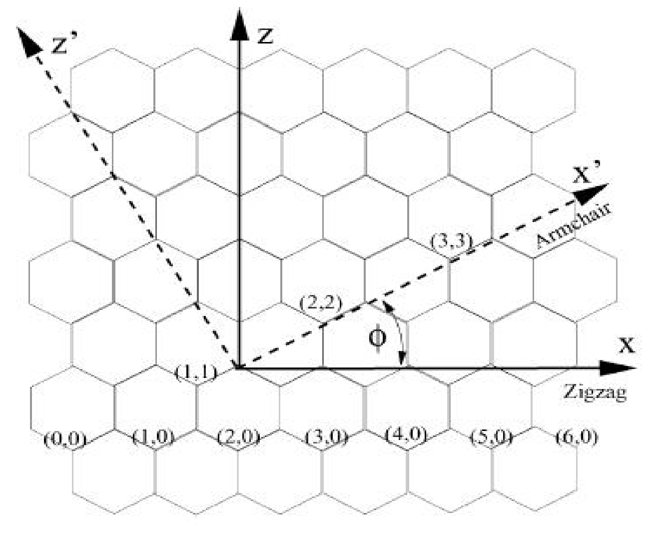

Fig. 1. Schematic of SWCTs in the 2-D graphite sheet.

The properties of carbon nanotubes are determined by their diameter and their chiral angle both of which depend on n and m i.e. indexes of carbon nanotubes. The diameter, $d_t$, is simply the length of the chiral vector divided by ¼, and we find that $d_t = (\ 3/\ )a_{c\text{-}c}(m^2 + mn + n^2)^{1/2}$, where $a_{c\text{-}c}$ is the distance between neighboring carbon atoms in the flat sheet. In turn, the chiral angle is given by $\tan^{-1}(\ 3n/(2m + n))$.

Although the choice of n and m determines whether the nanotube is metallic or semiconducting, the chemical bonding between the carbon atoms is exactly the same in both cases. This surprising result is due to the very special electronic structure of a two-dimensional graphene sheet, which is a semiconductor with a zero band gap. In this case, the top of the valence band has the same energy as the bottom of the conduction band, and this energy equals the Fermi energy for one special wavevector, the so-called K-point of the two-dimensional Brillouin zone (i.e. the corner point of the hexagonal unit cell in reciprocal space). Theory shows that a nanotube becomes metallic when one of the few allowed wavevectors in the circumferential direction passes through this K-point. As the nanotube diameter increases, more wavevectors are allowed in the circumferential direction. Since the band gap in semiconducting nanotubes is inversely proportional to the tube diameter, the band gap approaches zero at large diameters, just as for a graphene sheet. At a nanotube diameter of about 3 nm, the band gap becomes comparable to thermal energies at room temperature.

A few comparisons between silicon and carbon properties will reveal that carbon can be a better substitute to silicon in future years.

| Property | Silicon | Carbon |
|---|---|---|
| 1.Bandgap(eV) | 1.21 | Can be modelled anything between 0 to 2eV |
| 2.Mobility<br>electrons<br>(cm^2/V-s)<br>holes | 1300<br>500 | 10000(for n=10)<br>10000(for n=10) |
| 3.Max. Temperature | 850° | 1800° |
| 4. Ion/Ioff | low | high |

## Model description

## METHODOLOGY

In this paper the electron transport phenomenon in single walled carbon nanotubes (SWNT), is studied by Monte Carlo simulation method. The effect of mobility is investigated here. The role of electronic bandstructure, electron-phonon interaction, electron-impurity scattering and quantum transport are taken into account during simulation. We have considered the case of perfect carbon nanotube and without defects and injected electrons are scattered only by phonons for intrinsic type of tubes. Phonons and impurity electrons are both accounted for scattering in doped case. The Phonon energy spectrum is derived from the phonon wavevector. The phonons considered in this paper are longitudinally polarized acoustic modes (LA) of graphene.

### *Scattering Rates*

Free carriers (electron of holes) interact with the phonons and with each other through a variety of scattering processes, which relax the energy and momentum of the particle. Scattering rates calculated by Fermi’s Golden rule are typically used in MC device simulation as well as simulation of ultra fast processes. Phonon scattering involves different modes of vibration, either acoustic or optical, as well as both transverse and longitudinal modes. Carriers may either emit or absorb quanta of energy from the lattice in the form of phonons, in individual scattering events. The designation of inter-valley and intra-valley scattering comes from the multi-valley band structure model and refers to whether the initial states and final states are in the same valley or different valley. Since theory predicts that the change in the p-electronic energy under longitudinal strain is larger than under torsional or transverse34 strain, electron scattering by longitudinal polarizations is treated as the most dominant of the acoustic modes. The importance of these longitudinal modes has been observed in thermal relaxation studies of nanotubes. We therefore consider just the longitudinal acoustic modes. The phonon energy as a function of phonon wavevector is shown in fig 2.

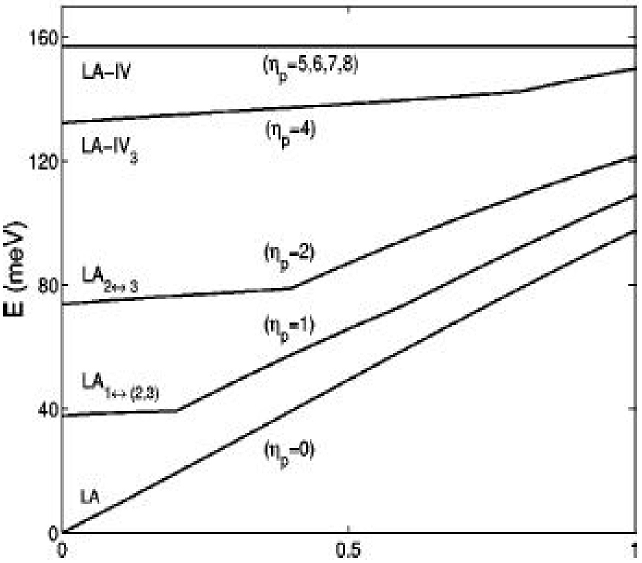

Fig2.Phonon energy as a function of phonon wavevector. [1]

| Phonon | Energy |
|---|---|
| $\hbar\mu 1$ | 0.038 eV |
| $\hbar\mu 2$ | 0.074 eV |
| $\hbar\mu 3$ | 0.160 eV |
| $\hbar\mu 4$ | 0.132 eV |
| $\hbar\mu 5$ | 0.160 eV |

Fig 3. Phonon energy table. [1]

The nonpolar scattering rate $1/\tau_{ep}(k)$ between an electron of wavevector $k$ and a phonon has been calculated from the Fermi golden-rule expression [4]:

$$1/^{2}{}_{ep}(k) = \sum_{V',q} (\Pi/{}^{\circ}\mu_{n,q})\Delta_{n,V'}(q^{2})\,|\,\Phi(k,k')\,|^{2}$$
$$\cdot\text{¢}\,(E_{V} - E_{V'} \pm \hbar\mu_{n,q})(\text{¦}_{n,q} + (1/2) \pm (1/2)). \qquad (1)$$

where, $E_v$ and $E_v$’ are the initial and final energies respectively and $\Phi$ is overlap integral.$\Delta_{n,V'(q)}$is a coupling constant, $\omega_{n,q}$is the frequency of phonon of type $n,q$, wavevector $q,k'$ is the final wavevector.

The scattering rate of electrons due to impurity is given by,

$$1/^{2}{}_{imp}(k) = [N_{imp} Z^{2} e^{4} / 4\text{®}^{2} \hbar\,\text{£}^{2}]$$
$$\cdot \sum_{V'k'G} (|\,\Phi(k,k')\,|^{2} / ({}_{s}{}^{2} + |\,k - k' + G\,|^{2})^{2})$$
$$\cdot\ (\text{¢}\,(E_{V}(k) - E_{V}(k'))) . \qquad (2)$$

ε is dielectric constant, Nimp is concentration of dopant, Z is electron number, β can be calculated by using Debye approximation.

$$\text{¦}_{LA} = 1/(\exp(\hbar\text{´}\ /k_{B}T) - 1). \qquad (3)$$

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Monte Carlo simulation

The charge transport in zigzag carbon nanotubes are studied using standard Monte Carlo. The simulation is homogeneous and is carried for sufficient long time duration using single electron method. The simulation carried out by injecting electrons and the free fight estimation of the electrons scattered by various instantaneous random events. Free flights for electrons are generated by Monte Carlo algorithms, changing their final states after scattering events and then repeating the same procedure for next flight. The particle motion is sampled at various time steps throughout the simulation, which helps for statistical estimation of the physical quantities like average drift velocity and mobility in presence of the applied electric field.

For the scattering process,we need to know the type of scattering (absorption or emission), which terminates the free flight of the electrons. The final energy and momentum needs to be calculated. To compute the direction of the scattered electron the azimuth and polar angles are needed. We have considered cylindrical coordinate system. The velocity of electron at nth time instant is given as,

$$v_n = \sqrt{(2E_n / m^*)} \qquad (4)$$

For every time step the energy of electron and subsequently the velocity is calculated. This process is applied on all electrons and properly iterated for specified steps. The coordinates at each time instant is calculated. It is also necessary to correct the path angle inclined to the electric field in z direction at every time step. Thus the displacements in the three directions are calculated.

where $R$ is a random number and $B_n$ is calculated as,

The average drift velocity is calculated by taking ratio of averages of the total displacement and drift times. The ratio of drift velocity to the applied electric field gives the mobility. The intrinsic mobility for our model is studied at different temperature levels (100˚K-600˚K). Further, we consider tube is doped with phosphorous impurities in order to study the effect of doping on electron transport. For various doping concentrations of phosphorous, mobility of SWCNTs is calculated.

## RESULTS AND CONCLUSION

### *Temperature dependence of mobility*

Simulations at different temperatures have been carried out for intrinsic SWCNTs. Results are taken for different temperature values ranging from 100˚K to 600˚K, for the electric field of 100V/cm. Fig. 4 shows intrinsic mobility of SWCNT for different temperature values

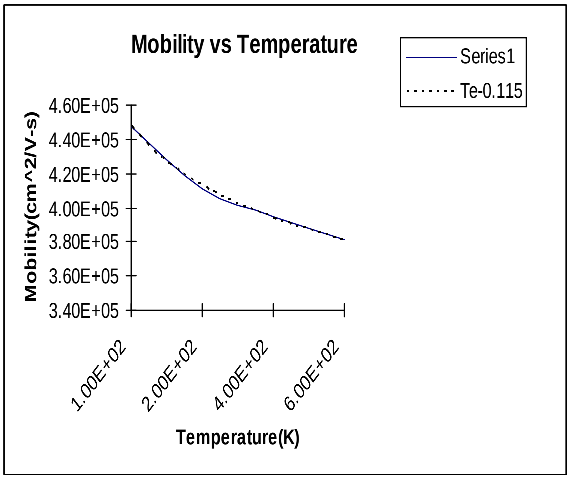

Fig 4.Temperature dependence of mobility at electric field of 100 V/cm

### *Doping dependence of mobility*

Introduction of impurities such as phosphorus, nitrogen or boron to enhance physical properties of semiconductor is a common practice in microelectronics. To induce N-type of behavior, donor impurities such as phosphorus are added. The mobility of phosphorus doped SWCNTs is calculated for different doping concentrations. We plot electron mobility for various doping concentration. Experimental results show that for low impurity concentration mobility falls quickly and remains constant for larger extent of doping. This condition of constant mobility suggests that effect of impurity phonons are less pronounced for this profile. Also, mobility falls sharply for doping concentration larger than 1e18 cm$^{-3}$.

In conclusion, transport mechanism in semiconducting SWCNT at various temperature and doping levels is studied with Monte Carlo simulation approach. Results show that mobility dependence on temperature obeys power law, which is also observed experimentally. This suggests validity of the proposed approach. It has been shown that mobility of SWCNTs can be tuned by selective doping of impurities. This model can be efficiently employed for the simulation of CNT based FETs.

## REFERENCES

[1] N. Koratkar et al., “Mobility of carbon nanotubes in high electricfields,” Journal of Nanoscience and. Nanotechnology, vol. 4, pp.69-71, 2004.

[2] R. Saito, M. Fujita, G. Dresselhaus, and M. Dresselhaus,“Electronic structure of chiral graphene tubules,” Applied PhysicsLetters, vol. 60, issue 18, pp. 2204-2206, May 1992 .

[3] J. Hone, B. Batlogg, Z. Benes, A. T. Johnson, and J. E. Fischer“Quantized Phonon Spectrum of Single-Wall Carbon Nanotubes”,Science, vol. 289, issue 5485, pp.1730-1733, Sep. 2000 .

[4] J. H. Davies, The Physics of Low-dimensional Semiconductors:An Introduction, Cambridge University Press, 1998, pp. 249-328.

[5] T. Dürkop, T. Brintlinger, and M. S. Fuhrer, ”Nanotubes are highmobility semiconductors”, in AIP Conf. Proc. Structural andElectronic Properties of Molecular Nanostructures, New York,2002, pp. 242-246.