Electronic Transport Parameter of Carbon Nanotube Metal-Semiconductor On-Tube Heterojunction

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Abstract. Carbon Nanotubes research is one of the top five hot research topics in physics since 2006 because of its unique properties and functionalities, which leads to wide-range applications. One of the most interesting potential applications is in term of nanoelectronic device. Carbon nanotubes heterojunction has been modeled, which was built from two different carbon nanotubes, that one is metallic and the other one is semiconducting. There are two different carbon nanotubes metal-semiconductor heterojunction. The first one is built from CNT(10,10) as metallic carbon nanotube and CNT (17,0) as semiconductor carbon nanotube. The other one is built from CNT (5,5) as metallic carbon nanotube and CNT (8,0). All of the semiconducting carbon nanotubes are assumed to be a pyridine-like N-doped. Those two heterojunctions are different in term of their structural shape and diameter. It has been calculated their charge distribution and potential profile, which would be useful for the simulation of their electronic transport properties. The calculations are performed by using self-consistent method to solve Non-Homogeneous Poisson's Equation with aid of Universal Density of States calculation method for Carbon Nanotubes. The calculations are done by varying the doping fraction of the semiconductor carbon nanotubes The electron tunneling transmission coefficient, for low energy region, also has been calculated by using Wentzel-Kramer-Brillouin (WKB) approximation. From the calculation results, it is obtained that the charge distribution as well as the potential profile of this device is doping fraction dependent.

Keywords: *carbon nanotube heterojunction; potential profile; molecular devices; doped carbon nanotubes.*

1 Introduction

Since the first time it was discovered in 1991 by Sumio Iijima [1], carbon nanotube (CNT) has become an object for intense scientific research and recently, engineering research; moreover, it also become the most influencing materials in nanotechnology development. CNT is a seamless tubule shaped all-carbon molecules which is a new kind of carbon molecules allotrope. It can be considered as wrapped-graphene, honeycomb carbon atom lattice which

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transformed into quasi-one-dimensional lattice with its bond arrangements conservation [2]. If both ends of CNT are closely capped, it could be considered as a long form of fullerene, classification for "buckyball" carbon molecules or buckmisterfullerene. The diameter of CNT varies in nanometer size, from 0.6 nm[1] [3] up to tens of nanometer; however, it can be grown up to more than 1 μm long.

The properties and symmetries of CNT are depends on its chiral vector [4][5], the way how the graphene rolled up which show its helicity, especially its electronic properties. It is possible to connect carbon nanotubes to become on-tube structures by introducing the presence of topological defects, in form of pentagonal or heptagonal ring, in addition of hexagonal ring in honeycomb graphene structure [6]. On-tube structures which could be formed are independent of the CNTs electronic properties; therefore, there could be CNT metal-semiconductor junction, CNT metal-metal [6][7] or CNT semiconductor-semiconductor junction [3] and metal-semiconductor-metal CNT junction [8] as well as T-shaped metal-semiconductor-metal CNT junction [9], which is different kind of junction that is not on-tube junction. On-tube connected structures of CNT may show behavior as new nanoscale devices.

It has been known that the metal-semiconductor junction exhibit Schottky-barrier effect, so that the metal-semiconductor junction itself named as Schottky-barrier diode [10][11]. CNT has prospect to be developed as Schottky-barrier diode. In recent years, most studies investigated the presence of Schottky-barrier effect in structures which connects semiconducting CNT with various kinds of metal [12]-[16] or metal CNT with Silicon as the semiconductor [17]. However, there are only few study about Schottky barrier in metal-semiconductor heterojunction which fully-built from CNT. Odintsov [18] has investigated it theoretically by presume the presence of applied gate voltage from encircled cylindrical electrode; and also the CNTs are undoped. The presence of Schottky barrier effect in CNT devices will give expectation of future CNT-based solar cell, especially after recent discovery of CNT-sheet which can be mass-produced [19].

The electronic properties of CNT, especially SWNT, are also determined by its growth environment. The carbon atom bonding type in CNT makes possibility that CNT is sensitive to gas exposures; consequently, there might be weak binding between carbon atoms of CNT with gas molecules or substitution of several carbon atoms with exposé gas atoms [20]. In recent years, there are many experimental result prove the existence of doped-CNTs together with several theoretical studies of their properties such as B-doped CNT [21]-[23],

[1] The smallest diameter has been observed

N-doped CNT [21][24][25], Oxidized CNT [20], etc., which can be considered as *n-type* CNT or *p-type* CNT. Therefore, it is possible to create such nanodevices which are built from CNT heterojunction which exhibit *p-n* junction [26] or *n-i-p* junction.

The investigation comprise the calculation of individual CNT's electronic properties, and the charge distribution as well as potential profile calculation formed by the heterojunction, which will become the basis of the calculation of electron transmission coefficients and also the calculation of direct-tunneling current flew in the heterojunction since the transport in CNT exhibit ballistic transport, instead of classical diffusive transport [3][27][28][29]; therefore, the direct tunneling current could be calculated by using Landauer Formula in the future. The calculation of individual CNT's electronic properties are done by using tight binding approximation of graphene and constructed to be CNT's using zone-folding of energy dispersion relation [27][28]. Afterward, the charge distribution and potential profile are calculated by using self-consistent method of Poisson's Equation with aid from universal density of states for carbon nanotubes [30] and method to calculate charge distribution of *n-type* CNT in *p-n* CNT junction [26].

In this paper, the comparison of electronic transport parameter of carbon nanotube metal-semiconductor on-tube heterojunction will be explained. The first one is built from CNT(10,10) as metallic carbon nanotube and CNT (17,0) as semiconductor carbon nanotube. The second one is CNT (5,5) as metallic carbon nanotube and CNT (8,0) as asemiconductor carbon nanotube. All of the semiconducting carbon nanotubes are assumed to be a pyridine-like N-doped.

2 Geometrical Modeling and Simulation of Electron Transport of Heterojunctions

Carbon nanotube can be perceived as a wrapped graphene, where graphene is a 2-dimensional carbon atom lattice. In an analogy with paper, there are so many ways to wrap the graphene into cylindrical-shaped form. The way how to wrap the graphene to be carbon nanotube become the most important concept to comprehend structure and properties of carbon nanotube since graphene consists carbon atoms.

Graphene sheet is a single-layer 2-dimensional carbon atom lattice which is actually a part of 3-dimensional graphite, one of the well-known carbon allotrope. In graphene, carbon atom is arranged in hexagonal honey-comb structure. In this planar lattice, carbon atom possesses sp^2 bonding state so there is still one dangling bond in each atom carbon. The nearest-neighbor distance

between carbon atoms is $a_{c-c} = 1.44\,\mathring{A}$, which is a very small value. The physical reason why carbon nanotube formed from similar structure of graphene is because the presence of many edge atoms with dangling bonds which correspond to high energy states.

On the 2-dimensions graphene-sheet reference, the chiral vector is defined as

$$\vec{C}_h = n\vec{a}_1 + m\vec{a}_2 \tag{2.1}$$

Where n and m are integer, which satisfies $0 \le |m| \le n$. $\vec{a}_1$ and $\vec{a}_2$ are the primitive translation vector of 2-dimensions graphene hexagonal lattice which consists of carbon atoms.

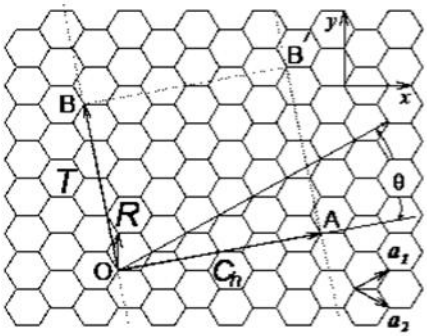


Figure 1 Illustration of Chiral Vector and Translational Vector in 2-dimensional Graphene [27].

From those two basic parameters of carbon nanotube, many others nanotube geometrical parameter can be derived. Since the chiral vector gives the circumference of nanotube, the diameter of nanotube can be obtained as

$$d_{NT} = \frac{|\vec{C}_h|}{\pi} = \frac{\sqrt{\vec{C}_h \cdot \vec{C}_h}}{\pi} = \frac{a\sqrt{n^2 + m^2 + nm}}{\pi} \tag{2.2}$$

From the geometrical structure parameters of carbon nanotube, which define the unit cell of carbon nanotube with chiral vector and translational vector as the real space unit vector, it can be obtain the reciprocal lattice vector of carbon nanotube by using the Laue Condition [31]

$$\vec{X}_i \cdot \vec{K}_j = 2\pi\delta_{ij} \tag{2.3}$$

where $\vec{X}_i$ is the real space vector and $\vec{K}_j$ is the reciprocal space vector.

The electronic structure of single-walled carbon nanotube can be derived from the electronic structure of two-dimension graphene [27] with an addition factor from the effect of wrapping. For the graphene, the electronic structure can be calculated by Tight-Binding Approximation Method (TBA) where it can also be limited by only considering the nearest-neighbor interaction. In a crystalline structure or quasi-crystalline structure, substance comes with symmetries in its unit cell of lattice with respect to its basis because of the periodicity. As a consequence, for 3-dimensions crystal, every state function must satisfy

$$\mathrm{T}_{\alpha_i}\,\Psi = \exp\left[i\vec{k}\cdot\vec{a}_i\right]\Psi, \quad i = 1,2,3 \tag{2.4}$$

which is the representation of periodicity, the Bloch-Floquet function. In order to satisfy eq. (2.4), there are two possible functions which are by using linear combination of plane wave or by using the linear combination of atomic orbital function. The eigenfunction of solids is defined as the linear combination of the Bloch function which are

$$\Psi_j\left(\vec{k},\vec{r}\right) = \sum_{j'\neq 1}^{n} C_{jj'}\left(\vec{k}\right)\Phi_{j'}\left(\vec{k},\vec{r}\right) \tag{2.5}$$

where n denotes the number of Bloch function. $C_{jj'}$ are coefficients that must be found which weigh the Bloch function to the eigenfunction. The corresponding energy eigenvalue of eigenfunction states in eq. (2.5) could be defined as

$$E_j\left(\vec{k}\right) = \frac{\left\langle \Psi_j \middle| \mathrm{H} \middle| \Psi_j \right\rangle}{\left\langle \Psi_j \middle| \Psi_j \right\rangle} \tag{2.6}$$

$$E_j\left(\vec{k}\right) = \frac{\left\langle \sum_{j'\neq 1}^{n} C_{jj'}\left(\vec{k}\right)\Phi_{j'}\left(\vec{k},\vec{r}\right) \middle| \mathrm{H} \middle| \sum_{j'\neq 1}^{n} C_{jj'}\left(\vec{k}\right)\Phi_{j'}\left(\vec{k},\vec{r}\right) \right\rangle}{\left\langle \sum_{j'\neq 1}^{n} C_{jj'}\left(\vec{k}\right)\Phi_{j'}\left(\vec{k},\vec{r}\right) \middle| \sum_{j'\neq 1}^{n} C_{jj'}\left(\vec{k}\right)\Phi_{j'}\left(\vec{k},\vec{r}\right) \right\rangle} \tag{2.7}.$$

By applying index changes in dual space as j becomes i and $j'=j$ as well as in real Hilbert space as j becomes i only, eq. (2.7) describe as

$$E_i = \frac{\sum_{j=1}^{n}\sum_{j'=1}^{n} C_{ij}^{*} C_{ij'} \left\langle \Phi_j\left(\vec{k},\vec{r}\right)\middle|\mathrm{H}\middle|\Phi_{j'}\left(\vec{k},\vec{r}\right)\right\rangle}{\sum_{j=1}^{n}\sum_{j'=1}^{n} C_{ij}^{*} C_{ij'} \left\langle \Phi_j\left(\vec{k},\vec{r}\right)\middle|\Phi_{j'}\left(\vec{k},\vec{r}\right)\right\rangle} \tag{2.8}$$

which its expression can be reduced as

$$\frac{\sum_{j,j'=1}^{n} \mathrm{H}_{jj'}\left(\vec{k}\right) C_{ij}^{*} C_{ij'}}{\sum_{j,j'=1}^{n} S_{jj'}\left(\vec{k}\right) C_{ij}^{*} C_{ij'}} \tag{2.9}$$ where $\mathrm{H}_{jj'} = \left\langle \Phi_j \middle| \mathrm{H} \middle| \Phi_{j'} \right\rangle, \quad j, j' = 1,...,n$ (2.10)

is called as transfer integral matrices and $\mathrm{S}_{jj'} = \left\langle \Phi_j \middle| \Phi_{j'} \right\rangle, \quad j = 1,...,n$ (2.11)

is called as overlap integral matrices. Finally, those equations become

$$\left[\mathrm{H} - E_i\left(\vec{k}\right)\mathrm{S}\right] C_i = 0 \tag{2.12}.$$

From the equation above, it can be derived the energy eigenvalue by treat the equation to have non-trivial solution. It should be realized that the energy eigenvalue obtained is as function of wave-number $\vec{k}$, thus the energy dispersion relation could be acquire.

To obtain the carbon nanotube density of states is by using universal density of states [30]. This method is effective to construct the density of states in the vicinity of Fermi energy level, ε_F. In this method, the density of states is expressed by

$$n(E) = \frac{2\sqrt{3}}{\pi^2} \frac{1}{\left|V_{pp\pi}\right|} \frac{a_{C-C}}{r} \sum_{\eta=-\infty}^{\infty} g\left(E, \varepsilon_\eta\right) \tag{2.13}$$

Where

$$g\left(E,\varepsilon_\eta\right) = \begin{cases} \left|E\right| \Big/ \sqrt{E^2 - \varepsilon_\eta^2}, & \left|E\right| > \left|\varepsilon_\eta\right| \\ 0, & \left|E\right| < \left|\varepsilon_\eta\right| \end{cases}, \tag{2.14}.$$

r is the nanotube radius and $V_{pp\pi}$ is equal to the transfer integral. The ε_η is the energy from the quantized perpendicular wave vector component which states by

$$\left|\varepsilon_\eta\right| = \frac{\left|3\eta - n + m\right|}{2}\left|V_{pp\pi}\right|\frac{a_{C-C}}{r} \tag{2.15}$$

with *n* and *m* are integer which denotes the chiral vector of nanotube.

Physical and chemical properties of a SWNT can also be modified by the adsorption of foreign atoms or molecules [2]. This process is named functionalization and become the way on how to tailor new nanostructures for engineering them for desired application. A certain functionalization can modify the bandgap of SWNT to become a wide bandgap material, while others can give rise to a substantially changes in the density of states. These functionalization not only can form bonds with ligands for chemical and biology application, but also modify the electronic and magnetic properties of SWNT.

There are two types on how the nitrogen could become dopant in the carbon nanotube. Firstly, the nitrogen atom coordinated to three carbon atoms in sp^2 like. Therefore the sharp localized states will be formed above the Fermi level since the nitrogen gives additional electrons which are injected into the nanotube structure. Secondly is the pyridine-type nitrogen dopant. The nitrogen atom is incorporated into the nanotube since a carbon atom is removed from the nanotube to leave a vacancy. This pyridine-like structure of N-doping nanotube gives effect to create a prominent-donor-like feature close-above the Fermi energy level [25].

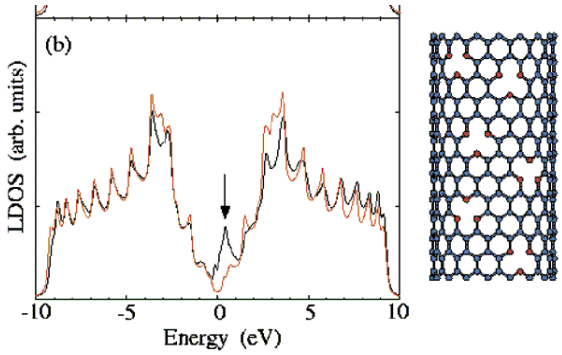


Figure 2 Pyridine-like N-doped CNT (17,0) Structure and Its Theoretical Local Density of States (LDOS). The arrow shows the electron donor states.

Czerw, et al. [25] have been identified the electron donor states for N-doped CNT. For pyridine-like N-Doped CNT, where one of 18 C atom is replaced by a N atom, it has been observed that there is donor state occurs at ~0.18 eV above the Fermi energy level. Different from the B-doped CNT which possess work function 1.7 eV much than pristine (undoped)-CNT [7], N-doped CNT still has work function 5 eV, 0.08 eV lower that pristine-CNT. The calculated electron mean free path of B/N-doped CNT is in vicinity of 175-275 nm [21], which is decreased due to the dopant concentration.

In the program, the metal carbon nanotube is used as the first nanotube which has the exact coordinates. And then, the atomic coordinates of the semiconductor carbon nanotubes was translated as long as the length of the metallic carbon nanotube with an addition of 1 Å. Afterward, the semi conductor carbon nanotube atomic coordinates is moved approaching the metallic carbon nanotube with a step of 0.01 Å. The aim is to find out the right distance between both nanotubes, so the length of atomic bonds among the edge atoms are match with the carbon-carbon atomic bond, which is 1.40 Å until 1.44 Å.

From the method above, the carbon nanotube heterojunction atomic coordinate could be obtain as in Figure 3. In the junction tapering area, pentagonal, heptagonal, and trigonal-like hexagonal rings were formed instead of normal hexagonal ring whereas in the part of individual nanotube. These rings shapes are possible to be formed in the nanotube. In this study, realizing that it is no more than 1 Å in length, the joint structure length is neglected for the calculation of the heterojunction electronic properties.

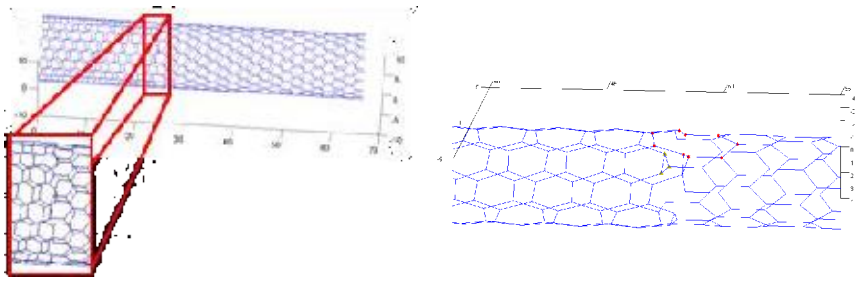


Figure 3 The geometry construction of the carbon nanotube on-tube metal-semiconductor heterojunction, which constructed from CNT(10,10) and CNT (17,0) (left) and from CNT(5,5) and CNT(8,0) (right)

The charge distribution in the semiconductor carbon nanotube is calculated by using one-sided of the way how to calculate the charge distribution in a *p-n* junction carbon nanotube [26]. It is stated that in the *n-type* part of carbon nanotube, the charge distribution per carbon atom as a function of position could be stated as

$$\sigma(z) = \frac{e}{\varepsilon} f - \frac{e}{\varepsilon} \int_{E_c(z)}^{\infty} n(E,z)\, F(E)\, dE \tag{2.16}$$

To calculate the charge distribution, the density of states used is the Universal Density of States [30], instead of the method used to find the individual carbon nanotube density of states. The reason why Universal Density is used is because of the density of states needed is a density of states which could be dependent on position in the nanotube, the bias voltage applied as well as the potential profile of the heterojunction itself.

By using the Universal Density of States, the Van Hove Singularity values are presumably could be shifted by the appearance of potential. Consequently, the Van Hove Singularity factor becomes

$$g(E,\varepsilon_\eta) \rightarrow g(E,\varepsilon_\eta - e\psi(z)) \tag{2.17}$$

where the $\psi(z)$ is the appeared electric potential, which might be varied as function of position, and *e* is the charge of an electron. Therefore,

$$g(E,\varepsilon_\eta - \psi(z)) = \begin{cases} |E| \Big/ \sqrt{E^2 - (\varepsilon_\eta - e\psi(z))^2}, & |E| > |\varepsilon_\eta - e\psi(z)| \\ 0, & |E| < |\varepsilon_\eta - e\psi(z)| \end{cases} \tag{2.18}$$

Meanwhile, potential profile in semiconductor CNT is calculated from charge distribution which is obtained by using Green Function for electrical potential by using approximation that CNT is a charged cylinder.

$$\psi(z) = \frac{1}{4\pi} \int_{-\infty}^{\infty} 2\pi R \frac{\rho(z')}{\varepsilon \sqrt{R^2 + (z - z')^2}}\, dz' \tag{2.19}$$

The self-consistent method is used to calculate eq. (2.18) and eq. (2.19) simultaneously. The result of the calculation itself is the charge distribution per square area as well as the potential profile, while the input is the guessed potential profile.

The calculation is performed using standard parameters which are in the room temperature (300 K), 3.9 in electrical permittivity of CNT, 1.44 Å of a_{C-C}, 2.50 eV of $V_{pp\pi}$ as well as no voltage bias. The other parameters are obtained from identifying properties of each CNT, such as the length of semiconductorCNT, its diameter as well as the number of atoms in the nanotube rings. The calculation is executed by using MATLAB and using several kinds guess potential. The calculation is also performed with various doping fraction.

The usual method to figure out how an electric potential profile in a system is by solving out the Poisson's Equation and putting in all of the boundary conditions. The Poisson's equation itself is expressed as

$$\nabla^2\psi = \frac{\rho}{\varepsilon} \tag{2.20}$$

where ρ is the charge distribution and ε is the permittivity of the material. A homogeneous Poisson's equation is described by Laplace's Equation,

$$\nabla^2\psi = 0 \tag{2.21}$$

which has physical meaning that there is no external charges which affect the potential profile. Therefore, the Poisson's equation itself is a non-homogeneous equation if the charge distribution term is present.

In microscopic point of view, charges are usually represented as point charge. Since the Coulomb's Equation gives

$$\psi = \frac{1}{4\pi\varepsilon}\frac{q}{r} \tag{2.22}.$$

3 Calculation Result and Discussion

The geometrical structure of specific individual carbon nanotube could be derived from the definition of chiral vector, eq. (2.1). As consequences, the other parameter of the carbon nanotubes could also be derived, such as the diameter as well as the length of one unit cell of the nanotube. Therefore the number of atom in one unit cell of nanotube could be calculated. The calculation result of some parameters could be tabulated in Table 1, which the chiral vector were varied.

In order to minimize the tapering structure, a specific chiral vector has been chosen from the second condition which is used in building the heterojunction. Based on raw classification of the effect of chiral vector to nanotube electronic properties, where if $n-m=0$ or $n-m=3d$ the carbon nanotube becomes metallic one and the other are semiconductor, the selection has been made. It is has been chosen that CNT (10,10) as the metallic carbon nanotube (mCNT) and CNT (17,0) as the semiconductor carbon nanotubes (CNT).

The atomic coordinate of one unit cell of carbon nanotube has been calculated by using carbon nanotube coordinate generator program from R. Saito's book [27] where the calculation perform using FORTRAN. It has been made a program to plot the atomic coordinate of one unit cell of carbon nanotube by using MATLAB. For CNT (10,10) and CNT (17,0), it is obtained the coordinate plot as in figure 8. It could be seen that the CNT (10,10) is an armchair nanotube and CNT (17,0) is a zigzag nanotube. The diameter of both carbon nanotube are 1.356 nm for CNT (10,10) and 1.331 for CNT (17,0). The length of the 50 cells individual nanotubes was obtained of 12.47 nm for CNT (10,10) and 21.60 nm for CNT (17,0).

Table 1 Parameters of Some Carbon Nanotube.

chirality vector	diameter (´)	translation vector length (´)	number of atoms
(5,5)	6.78477	2.49000	20
(6,4)	6.82986	18.79908	152
(7,4)	7.55521	13.86372	124
(9,0)	7.05094	4.31281	36
(9,2)	7.95103	43.77021	412
(10,10)	13.56955	2.49000	40
(12,5)	11.85557	65.26459	916
(17,0)	13.31845	4.31281	68
(17.9)	17.91660	98.63039	2092
(17,10)	18.52297	101.96846	2236

In the modified program, the metal carbon nanotube, which is the CNT (10,10), is used as the first nanotube which has the exact coordinates, generated by the coordinate generator procedure. And then, the atomic coordinates of the semiconductor carbon nanotube was translated as long as the length of the metallic carbon nanotube with an addition of 1 Å. Afterward, the semiconductor carbon nanotube atomic coordinates is moved approaching the metallic carbon

nanotube with a step of 0.01 Å. The aim is to find out the right distance between both nanotubes, so the length of atomic bonds among the edge atoms are match with the carbon-carbon atomic bond, which is 1.40 Å until 1.44 Å.

From the method above, the carbon nanotube heterojunction atomic coordinate could be obtained as in Figure 4. The length of the heterojunction generated is 34.014 nm. In the junction tapering area, it was formed pentagonal, heptagonal and trigonal-like hexagonal rings instead of normal hexagonal ring whereas in the part of individual nanotube. These ring shapes are possible to be formed in the nanotube [34].

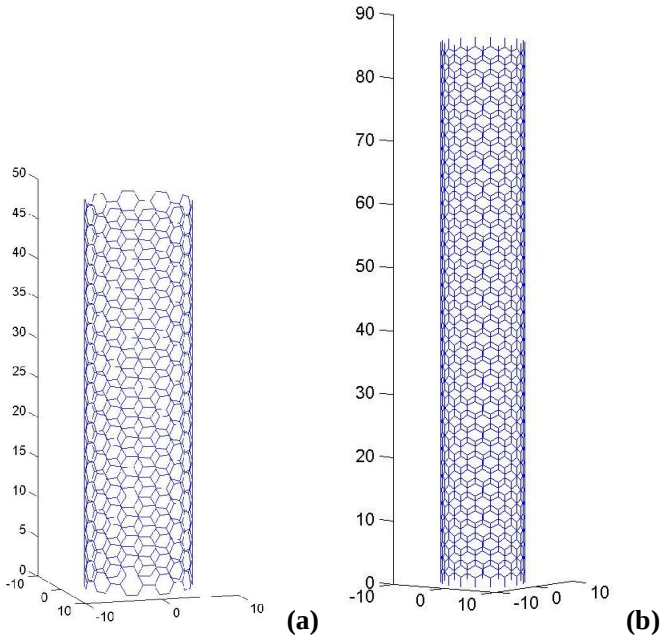


Figure 4 Plot of 20 unit cells of carbon nanotube **(a).** CNT (10,10) **(b)**. CNT (17,0), units are in Å

The energy dispersion relations of the building blocks carbon nanotubes, CNT (10,10) and CNT (17,0), were calculated and derived from the Tight Binding Approximation. To calculate the energy dispersion relation, the running number of μ is limited up to a number where the energy dispersion plot is not exceeded the work function of the nanotube, instead from zero until the number of hexagon. It is obtained the plot of CNT (10,10) energy dispersion as in the Figure 6.

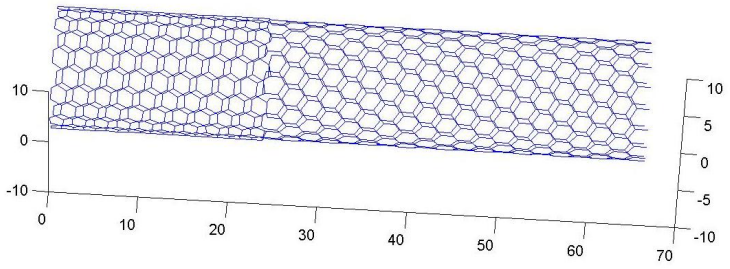


Figure 5 The junction of CNT (10,10) – left – and CNT (17,0) – right – , 20 cells each, all scale are in Å.

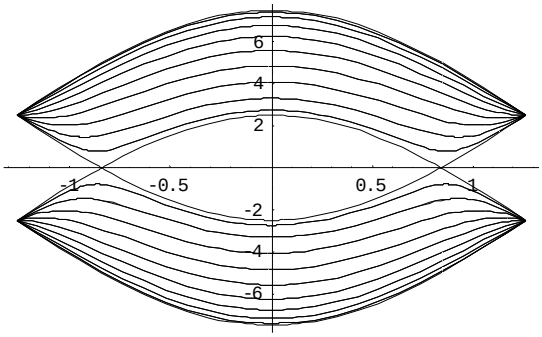


Figure 6 The plot of energy dispersion relation of CNT (10,10). The vertical axis denotes the energy value in eV with the Fermi energy level is set arbitrarily zero and the horizontal axis denotes the wavenumber for one Brillouin Zone.

From the plot of energy dispersion relation, it could inferred that the there are overlaps at the Fermi level. It means that electrons may have energy at the Fermi level as well as at its vicinity. Therefore, there is no forbidden band observed in the CNT (10,10). This point is a nature of metallic material where electrons could move freely between the conductance and the valence band. It could be really concluded, from the energy dispersion relation obtained, that CNT (10,10) is a carbon nanotube which possesses properties as a metallic material.

The calculation result of energy dispersion relation of CNT (17,0) obviously gives insight that there is a forbidden gap. It is not observed any present of overlaps among the dispersion relation. It could be inferred that CNT (17,0) possess a semiconducting properties since there is a bandgap. From the position of the HOMO (Highest Occupied Molecular Orbital), also known as the top of

valence band, and the position of LUMO (Lowest Unoccupied Molecular Orbital), the bottom of conduction band; It could be deduced that this nanotube has a direct-bandgap instead of indirect bandgap. The direct bandgap itself lies at the zero value of wavenumber. The value of the bandgap itself is 0.5431 eV.

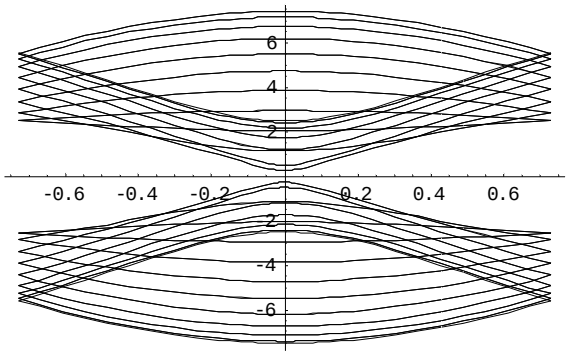


Figure 7 The plot of energy dispersion relation of CNT (17,0). The vertical axis denotes the energy value in eV with the Fermi energy level is set arbitrarily zero and the horizontal axis denotes the wavenumber for one Brillouin Zone.

From the electronic properties identification of both CNT (10,10) and CNT (17,0), it could be noticed that these two nanotubes is possible to be used as the building blocks of a metal-semiconductor heterojunction. The CNT (10,10) acts as the metallic material and CNT (17,0) acts as the semiconductor material with a certain bandgap.

The Density of States calculation is performed by using eq. (2.44) since the carbon is a one-dimensional material. The calculation is done by using that equation instead of Universal Density of States method since the energy dispersion relation of individual carbon nanotube has been known in previous sub-chapter and the density of states which will be calculated is in equilibrium condition and without any modification in the structure. From the equation, it could be inferred that the density of states could be obtained from the energy dispersion relation where it is a function of wavenumber.

To calculate this matter, the root find by using Two-way Newton-Rhapson method [35] which is believed to be accurate enough. The nature of each energy dispersion relation of carbon nanotube has no more than two roots for each level in a Brillouin Zone; therefore, the Two-way Newton-Rhapson method is sufficient. The Dirac Delta itself will determine which differentiation of wave number, in respect with its energy, is taking account into the calculation since

$$\int \delta(x-a)\, f(x)\, dx = f(a) \tag{3.1}$$

The differentiation of the wave number in respect with the energy could be obtained as one over the differentiation of the energy in respect with the wave number, namely

$$\frac{\partial E}{\partial k} = -t \frac{\left(-4\cos\left[\frac{ak}{2}\right]\sin\left[\frac{ak}{2}\right] + 2a\cos\left[\frac{\pi\mu}{10}\right]\sin\left[\frac{ak}{2}\right]\right)}{2\sqrt{1+4\cos^2\left[\frac{ak}{2}\right]-4\cos\left[\frac{ak}{2}\right]\cos\left[\frac{\pi\mu}{10}\right]}} \tag{3.2}$$

for CNT (10,10), where μ is the quantization number of wave vector parallel to nanotube chiral vector and

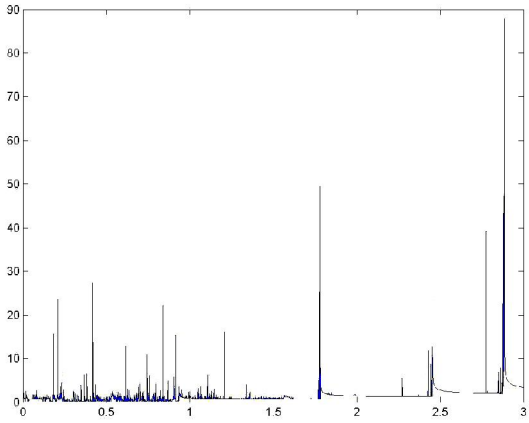
$$\frac{\partial E}{\partial k} = -t \frac{\sqrt{3}a\cos\left[\frac{\pi\mu}{17}\right]\sin\left[\frac{\sqrt{3}ak}{2}\right]}{\sqrt{1-4\cos\left[\frac{\sqrt{3}ak}{2}\right]\cos\left[\frac{\pi\mu}{17}\right]+4\cos^2\left[\frac{\pi\mu}{17}\right]}} \tag{3.3}$$

for CNT (17,0).

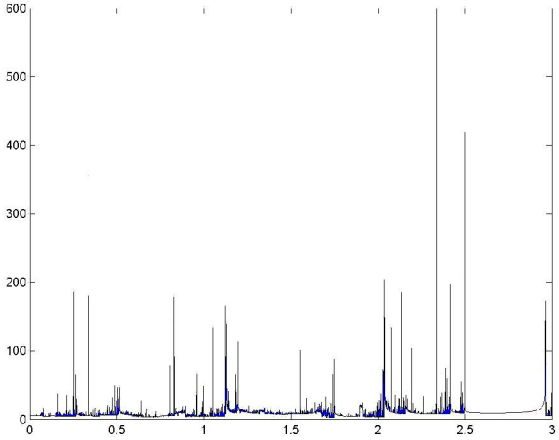
The calculation itself was done by using MATLAB with code in Appendix B. The parameter used are standard parameters, such as 2.50 eV for the $V_{pp\pi}$, 1.44Å for the a_{C-C}. The calculation performed is not taking account all of the energy dispersion relation level, but limited up to the value of carbon nanotube work function. The result of the calculation could be obtained in Figure 8 (a) for CNT (10,10) and Figure 8 (b) for CNT (17,0). From both figures of individual carbon nanotube energy dispersion relation, it could be observed that there are van Hove Singularities in the Density of States. The van Hove singularities value might be different from one nanotube to the others, so it would become a kind of fingerprints of the nanotube. For the semiconductor Carbon Nanotube, CNT (17,0) for this case, the first van Hove singularity become lies the edge of the conduction and valence band, 0.5431 eV if the valence band is set arbitrarily to zero.

The heterojunction is built up from metalCNT, the CNT (10,10) and pyridine-like N-doped semiconductorCNT (*n*-type), the CNT (17,0). The parameters of individual nanotubes have been known from previous sub-chapters. In addition, since the pyridine-like N-doped CNT is used as semiconductor nanotube instead of pristine undoped CNT, the Fermi level is shifted 0.18 eV above its original Fermi level as stated in Chapter 2. For the isolated metalCNT and

semiconductorCNT, the energy band diagram is shown in Figure 16. It can be seen that the electron affinity value of the semiconductorCNT could be obtained from the difference between the bottom of the conduction band and the vacuum level.



(a)



(b)

Figure 8 Plot of the Density of States **(a)** CNT (10,10) and **(b)** CNT (17,0) – the horizontal scale denotes the energy value in eV and the vertical axis shows the number of states (arbitrarily). The plot only includes the positive value of energy, above the Fermi level, the conduction band region only since it is symmetric in equilibrium condition

In a metal-semiconductor junction, a potential barrier usually is formed. By presumably this thing happens to this semiconductor heterojunction, the height of barrier could be calculated by using $q\phi_{Bn} = q\left(\phi_m - \chi\right)$ and the result given is 0.2415 eV. If the semiconductorCNT in the heterojunction has enough length, the potential height will be suppressed at the relatively infinite position from the junction, which gives result 0.08 eV. If this thing really happens, the energy band diagram would give result as in Figure 9.

The charge distribution is calculated by using the one sided abrupt junction approach, which is usually done to illustrate the properties of metal-semiconductor junction. The charge distribution in the semiconductor carbon nanotube is calculated by using one-sided of the way how to calculate the charge distribution in a *p-n* junction carbon nanotube [26]. It is stated that in the *n-type* part of carbon nanotube, the charge distribution per carbon atom as a function of position could be stated as

$$\sigma\left(z\right) = \frac{e}{\varepsilon} f - \frac{e}{\varepsilon} \int_{E_c(z)}^{\infty} n\left(E,z\right) F\left(E\right) dE \tag{3.4}$$

where ε is the electrical permittivity of carbon nanotube and f is the doping fraction. From the equation, it could be inferred that the charge distribution depends on the carbon nanotube density of states, $n\left(E,z\right)$, as well as the Fermi-Dirac distribution function, $F\left(E\right)$, which is integrated from the bottom of the conduction band.

By using the Universal Density of States, the van Hove singularity values are presumably could be shifted by the appearance of potential [26]. Consequently, by limiting the van Hove singularities to be less than the work function, the value of each van Hove singularities is tabulated in Table 2.

The potential profile in the semiconductor carbon nanotube is calculated from the charge distribution with the $\rho\left(\vec{r}_2\right)$ is the charge distribution, not per atom, but per area. The kernel used for the equation is a kernel which compatible with cylindrical system. The calculation is performed using standard parameters which are in the room temperature (300 K), 3.9 in electrical permittivity of carbon nanotube, 1.44Å of a_{C-C}, 2.50 eV of $V_{pp\pi}$ as well as no voltage bias. The other parameters are obtained from previous sub-chapters, such as the length of semiconductorCNT, its diameter as well as the number of atoms in the nanotube rings. The calculation is executed by using MATLAB and using

several kinds guess potential. The calculation is also performed with various doping fraction.

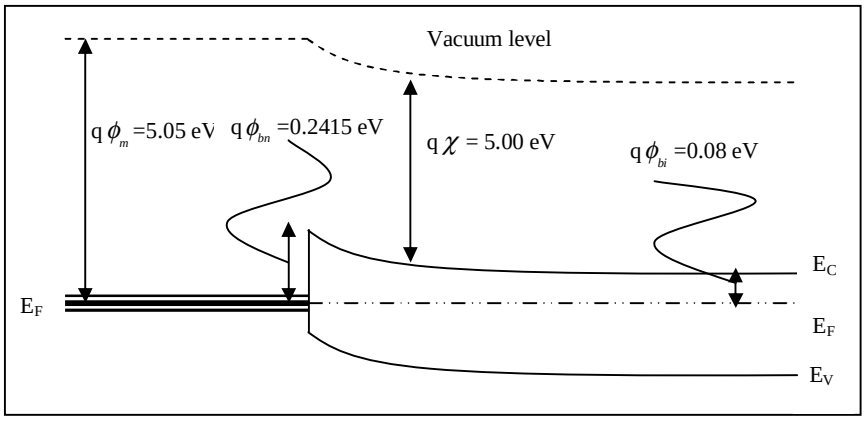


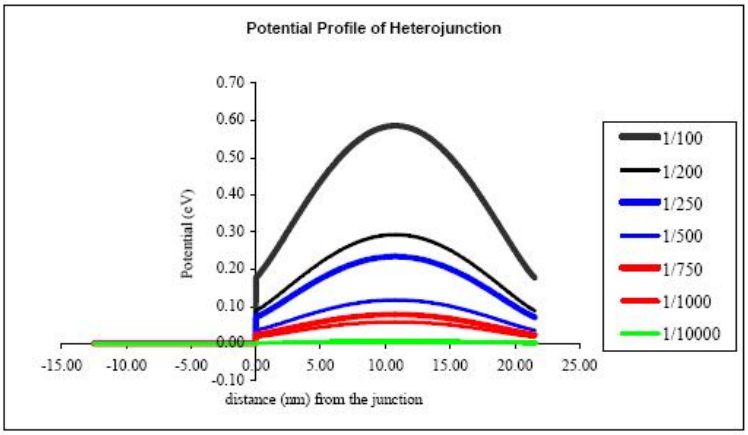
Figure 9 Expected energy band diagram of CNT(10,10) and N-doped CNT(17,0) heterojunction.

Table 2 Value of van Hove Singularities below the semiconductorCNT work function – Fermi energy level is set arbitrarily to zero.

η	ε_η (eV)
0	4.5953
1	3.7844
2	2.9734
3	2.1625
4	1.3516
5	0.5406
6	0.2703
7	1.0812
8	1.8922
9	2.7031
10	3.5140
11	4.3250

However, the result of the charge distribution calculation has a good agreement with the gold-semiconductor CNT-gold junction [13] Kim, et.al. obtained that in the gold-semiconductor CNT-gold heterojunction, the charge distribution has valleys nearby the joint between the metal and the CNT where the charge distribution is almost similar along the nanotube. As the second output, it has been obtained the potential profile of the carbon nanotube heterojunction.

From the potential profile result, it can be inferred that the potential formed has it peak in the vicinity of semiconductor-CNT center point, with non-zero potential at both ends. This may make a barrier structure for the electron which flow from metallic CNT through the semiconductor CNT. Even though the potential profile looks to be symmetric, the exact values of the potential at both ends are different. At the surface of the junction, the potential value is smaller than the other.



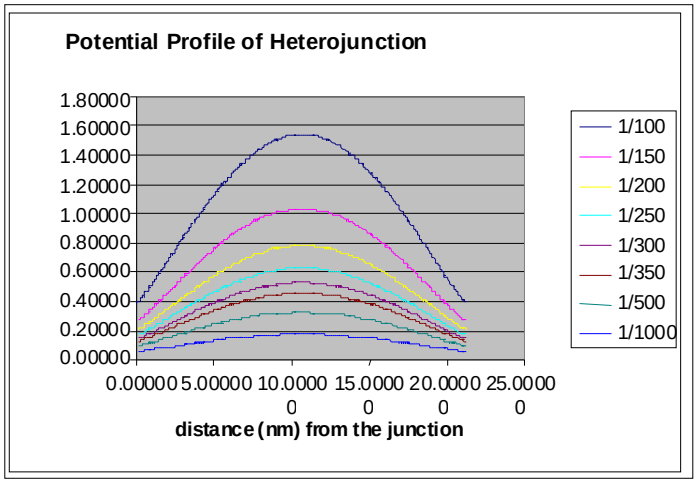


Figure 10 The plot of profile potential of the CNT(10,10)/CNT(17,0) heterojunction **(a)** and CNT(5,5)/CNT(8,0) heterojunction **(b)**

In the future calculation, it must be also anticipated some new things regarding the electronic transport in carbon nanotubes. One of the new things is that there is an expectation that the electron transported in a carbon nanotube is not move straightly inside the nanotube or parallel to the nanotube axis, but in such helical way [35].

4 Conclusion

From the explanations and calculation results of this work, it could be concluded that there is a possibility to make an on-tube heterojunction which built by two different types of carbon nanotubes, the metallic ones and the semiconductor ones. Since the electronic properties of individual carbon nanotubes depend on their chiral vector, it has been chosen two nanotubes to build this heterojunction. 50 cells carbon nanotube CNT (10,10) is chosen to become metallic carbon nanotube and 50 cells carbon nanotube CNT (17,0) is chosen to be the semiconductor carbon nanotube. From the Tight Binding Approximation, it has been obtained that the CNT (17,0) is a semiconductor carbon nanotube with a band-gap of 0.5431 eV. In this case, the semiconductor CNT is an N-doped carbon nanotube which has donor states at 0.18 eV above the Fermi level. The heterojunction structure becomes 34.014 nm long.

The calculation of charge distribution and potential profile has been done by using self-consistent method to solve non-homogeneous Poisson's Equation, with support of the Universal Density of States and neglecting the effect which could come out from the joint area as well as the interaction between the tubes. At relatively high doping fraction, there are valleys of electron distribution at the vicinity near the carbon nanotube edges with some other peaks at the edge of semiconductor nanotube. The rest of the low doping fraction nanotubes have slightly higher charge distribution at the middle of the nanotubes. It could be concluded that the electrons tend to be confined in the center area of the nanotubes. The change in doping fraction gives difference in term of number of electrons distributed in the nanotube.

The potential profile makes the highest peak in the vicinity of semiconductor-CNT center, instead of near the semiconductor-CNT surface. This potential makes barriers for electron which flow from the metallic-CNT through the semiconductor-CNT. The higher the doping fraction in the nanotube, the higher the potential barrier will be. The potential value is slightly suppressed at the metal-semiconductor junction if compared with the value at the other end. It is happened because of the effect from the induced image charge at the metal surface.

From the comparison of charge distribution and potential profile of both carbon nanotube metal-semiconductor heterojunctions, which are CNT(10,10)/CNT(17,0) and CNT(5,5)/CNT(8,0), some similar anomalies as well as some differences were obtained.

Further calculation can be done to calculate the transmission coefficient and direct tunneling current. Those parameters are needed to be calculated in order to identify the characteristic of the heterojunction if it is used as electronic device. The calculation result could be compared with the result of the experiment in the near future.

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