Chapter IV

Electron field emission of carbon nanotube

In this chapter, our study has been extended to individual single-wall carbon nanotubes on field emission characteristics by employing the vacuum potential energy barrier and the electric field at nanotip. Then the characteristic of field emission current versus energy band of armchair carbon nanotube including the carbon nanotubes which chiral vectors at (5,5), (10,10), (15,15), and (20,20) are determined.

4.1 Circumferential boundary condition of armchair carbon nanotube

The radial dimension of carbon nanotube is comparable with de Brogelie wavelength, so that carbon nanotube can be considered as a quasi-one-dimensional material. For all armchair nanotubes, the energy bands show a large degeneracy at the zone boundary, where $k = \pi/a$. From the discrete allowed values for $E_q^a(k)$ given by following periodic boundary condition Eq.(4.1) yields the energy dispersion relations (a stand for the armchair nanotube), $\overrightarrow{C_h} = (n, n)$, here we calculate the dispersion relation for armchair nanotubes (5,5), (10,10), (15,15) and (20,20). By applying Eq.(2.18) as our boundary condition for armchair nanotubes, we have

following possible transverse wave vectors as following:

$$k_{x,q} = \frac{2\pi q}{na\sqrt{3}} \quad ; q = 1, 2, ..., 2n \tag{4.1}$$

For example CNT(5,5)

$CNT(5,5) : q = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10$

$k_x = \frac{2\pi q}{5\sqrt{3}a} = \frac{2\pi}{5\sqrt{3}a}\{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$

The circumferential boundary condition forces the possible values of transverse wave vectors to be discrete which we can see from Eq.(4.1). By assuming very large longitudinal length of carbon nanotube, we have continuous values of possible wave vectors along the nanotube axis. We have the energy dispersion relation as that in Eq.(2.19). From Figure 4.1, we can consider only the conduction

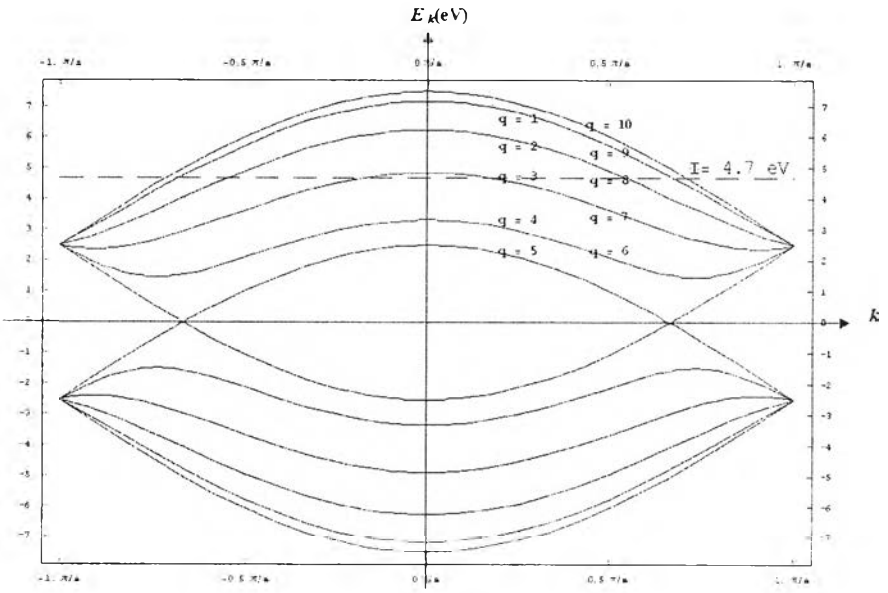

Figure 4.1: Energy dispersion relation of armchair carbon nanotube (5,5) along the longitudinal wave vector k

electrons as the carriers that contribute to the emission. Thus, only the electrons in the conduction band(anti-π bond electrons) are considered.

4.2 The characteristic of field emission current versus energy band of nanotube

By neglecting electronic collision, we can apply the function N(E), which is the density of electronic states reached at unit nanotip in unit time

$$dN(E_q(k)) = \frac{1}{\pi h} f(E_q(k)) \frac{\partial E_q(k)}{\partial k} dk, \tag{4.2}$$

where $f(E)$ is the Fermi-Dirac distribution function at the energy level E, and $(1/\hbar)\partial E_q(k)/\partial k$ represents the electronic group velocity along the nanotube axis. In this research, we apply only positive group velocity to be our incident electrons reach to our carbon nanotubes. The electron emission can be described by the WKB theory[24], and the tunneling probability $D(F, E_q(k))$ through vacuum potential energy barier $W(x, F)$ is calculated as follows:

$$D(F, E_q(k)) = \exp\left\{ -\frac{2}{\hbar}\sqrt{2m^*} \times \int_{x_1}^{x_2} \sqrt{W(x,F) - E_q(k)}dx \right\} \quad ; E_q(k) < \chi \tag{4.3}$$

$$D(F, E_q(k)) = 1 \quad ; E_q(k) > \chi \tag{4.4}$$

where x_1 and x_2 are the classical turning points of the vacuum potential barrier, respectively. F is the magnitude of an external applied electric field. $\hbar = h/2\pi$, h is the Planck constant, m^* is the electronic effective mass of carbon nanotube. We use m^* of $0.06m_e$ Ref.[25] where m_e is the free electron mass. Tunneling probability strongly depends on the local electric field at the tip of CNT. According to Eqs. (4.2)-(4.4), the characteristic of emission current versus applied field can be obtained as

$$I = \frac{e}{\pi\hbar} \sum_q \int_{FBZ} f(E_q(k)) \times \frac{\partial E_q(k)}{\partial k} D(E_q(k), F) dk \tag{4.5}$$

where FBZ represents the first Brillouin zone, the range of q depends on the crystal lattice structure of carbon nanotube. We can see from Eq.(4.6) that emission current depends on the energy band, thus on the chirality of carbon nanotube.

4.3 Nanotip local electric field concentration

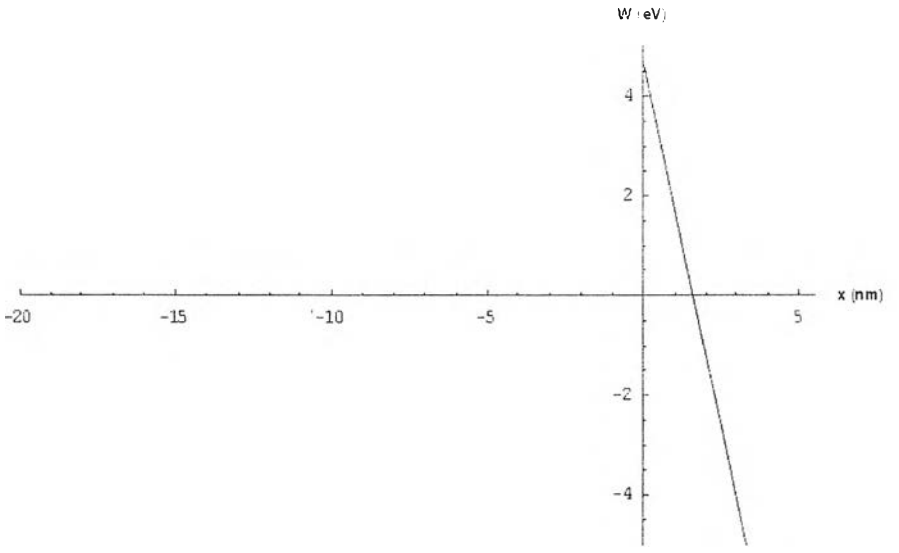

Figure 4.2: Potential barrier using the parameter $F = 5V/\mu m$ and plotted along the longitudinal axis of nanotube from location -20 nm to 5 nm

In our calculation here, we need to assume that there is local concentration of electric field at the end of nanotip which is exactly the location of our triangular potential barrier. This local electric field intensity also have large effect to electron emission of carbon nanotube. We assume the local electric field concentration as

$$\varepsilon = F/\alpha R \tag{4.6}$$

where R is the radius of carbon nanotube and α is an adjusting parameter. We use $\alpha = 5$ in our calculation. This value was previously used by Liu, et al.[[1]]. For simplicity, we will concern only with the armchair carbon nanotube.

4.4 Numerical calculation for electron field emission characteristic of armchair carbon nanotube

For simplicity of calculation, we start from the possible range of integration separated by the junction of transmission coefficient value at k which gives the transmission coefficient equal to one. This means the range of k that makes the energy dispersion higher than or equal to the work function of electrons in our material. In our case the work function is 4.7 eV above fermi energy. The second condition that we have to consider is our range of integration for our simulation program. k range gives positive incident group velocity of electron given by

$$v_g = \frac{1}{\hbar}\frac{\partial E}{\partial k} \tag{4.7}$$

where k is the longitudinal wave vector along the nanotube axis. By both conditions, we explain above, we can get following integration range for the Eq.(4.6) as

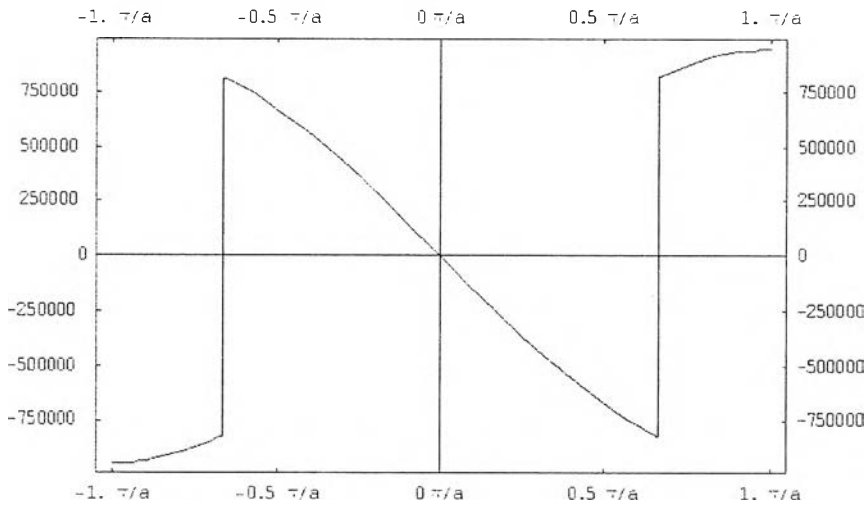

Figure 4.3: Electrons group velocity of armchair carbon nanotube (5,5) at q=5 in the unit of m/s.

q_i	1st k range	2nd k range($D=1$)	3rd k integration range
1	$-\pi/a, -0.675185\pi/a$	$-0.675185\pi/a, 0$	
2	$-\pi/a, -0.544209\pi/a$	$-0.544209\pi/a, 0$	
3	$-0.901241\pi/a, -0.168064\pi/a$	$-0.168064\pi/a, 0$	$0.901241, \pi/a$
4	$-0.734885\pi/a, 0$		$0.734885\pi/a, \pi/a$
5	$-2\pi/3a, 0$		$2\pi/3a, \pi/a$
6	$-0.734885\pi/a, 0$		$0.734885\pi/a, \pi/a$
7	$-0.901241\pi/a, -0.168064\pi/a$	$-0.168064\pi/a, 0$	$0.901241\pi/a, \pi/a$
8	$-\pi/a, -0.544209\pi/a$	$-0.544209\pi/a, 0$	
9	$-\pi/a, -0.675185\pi/a$	$-0.675185\pi/a, 0$	
10	$-\pi/a, -0.709957\pi/a$	$-0.709957\pi/a, 0$	

Table 4.1: The range of k value for positive incident electrons group velocity of armchair carbon nanotube (5,5).

4.5 Fermi-Dirac distribution function along the k value of carbon nanotube

The relation between probability of degenerate states at the room temperature at 300 K.

$$f(E) = \frac{1}{1 + \exp[\frac{E-\mu}{k_B T}]} \tag{4.8}$$

This Fermi-Dirac distribution shows the distribution of possible electron states of our conduction carriers which can compose to our emitted electrons giving the current characteristic of our electrons emission of carbon nanotube.

4.6 Calculation result of I-V chacteristic of armchair carbon nanotube.

The emission of electrons follow the Eq.(4.6) is depicted in Fig. 4.4 for armchair carbon nanotubes (5,5), (10,10), (15,15), and (20,20).

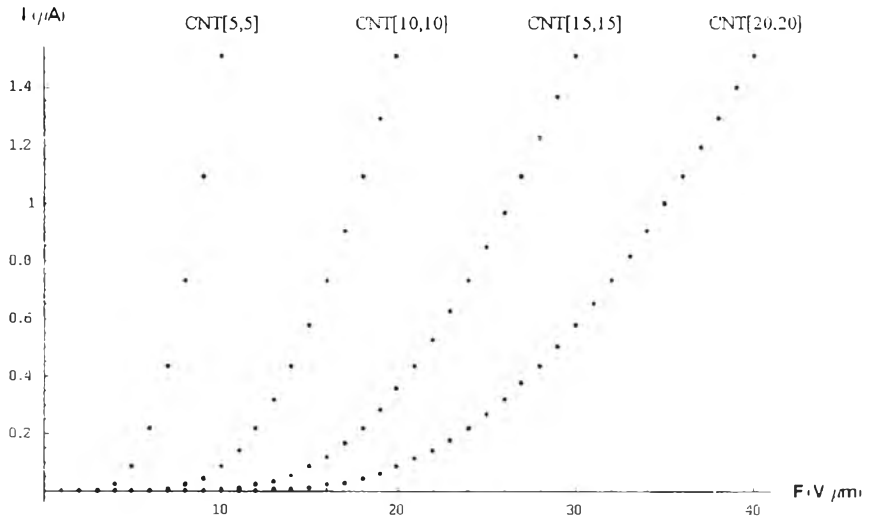

Figure 4.4: I-V characteristic of armchair Carbon nanotube (5,5), (10,10), (15,15), and (20,20) by using effective mass=0.06 m_e.

4.7 Conclusion and further suggestion

By using the tight binding approximation we come to the good agreement with the experimental result that local electric field at nanotip affects the electron emission current significantly. The local electric field is the major priority to affect the emission current result.

The source code which we develop in Mathematica software is provided in an appendix of this thesis. This enables us to see easily that if we supply the same diameter of carbon nanotube even in different chiral parameters, we still

get the same set of current characteristic. The review about effective mass and group velocity, which are important parameters for our calculation, is also provided in appendices. Saturation at high external electric field should be developed to explain the other range of emission characteristic. Better more theories have to be developed to get better explanation about saturation point of current. This review research just aim to review the basic theory that relates to molecular physics, discrete mathematics, WKB approximation, etc. which we hope to motivate more researchers in Thailand who wish to develop nanoelectronics which would take the major roles in semiconductor industry in the near future.