Chapter III

Electron field emission

This chapter is a review of necessary basic quantum mechanics which related to electron field emission theory that necessary for carbon nanotube.

3.1 Cold emission: Fowler-Nordheim equation

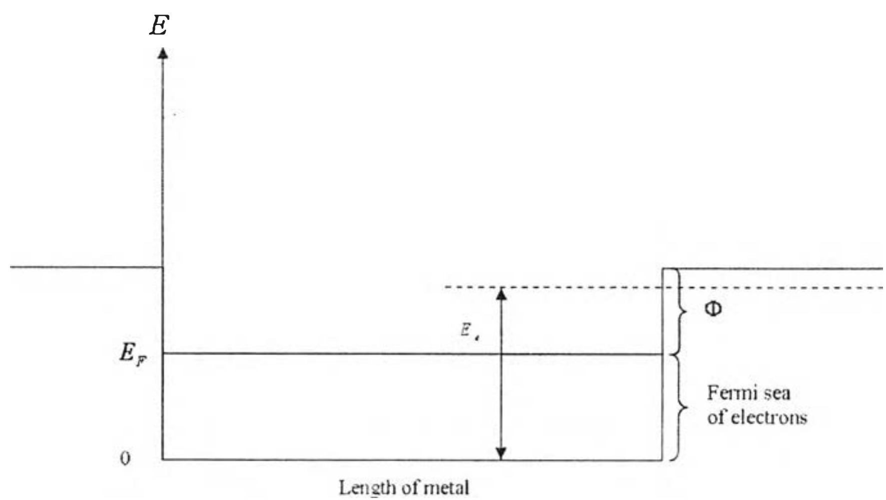

Figure 3.1: Sommerfeld model for energy distribution of electrons in a metal.

In the phenomenon of cold emission, electrons are drawn from a metal at room temperature by an external electric field. The potential well of the metal, before the electric field is turned on. is depicted in Figure 3.1. After applying a constant electric field ε, the potential at the nanotube surface slopes down as shown in Fig. 3.2, there by allowing electrons in the Fermi sea to tunnel through

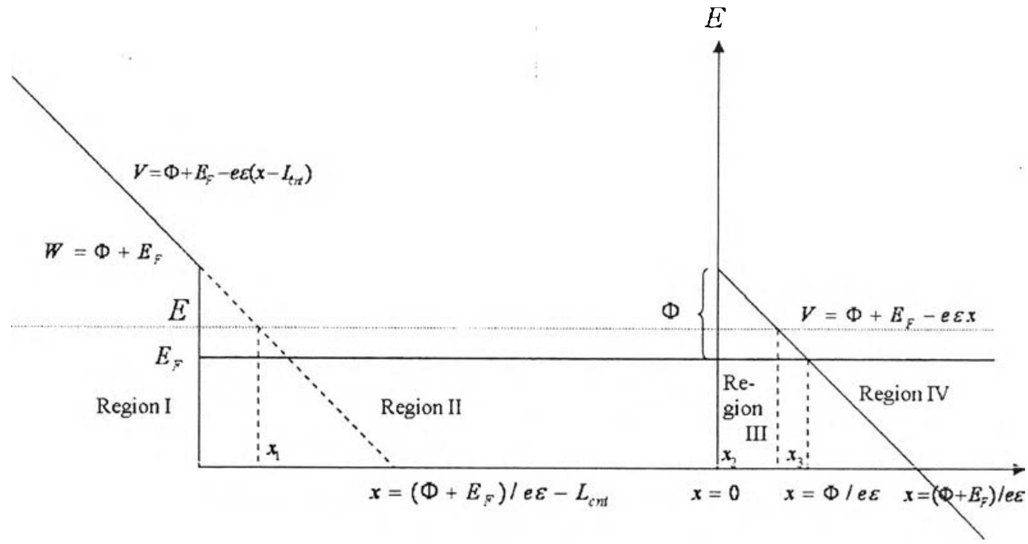

Figure 3.2: Potential configuration for the phenomenon of cold emission due to external applied electric field inducing the potential barrier slope change which gives the possibility of electron tunneling at the right end of metal as shown for any electron energy E in the conduction band.

the potential barrier. If the surface of the metal is taken as the x=0 plane, the new potential outside the surface is

$$V(x) = \Phi + E_F - e\varepsilon x \tag{3.1}$$

where E_F is the Fermi level and Φ is the work function of the metal. For any particle at energy level E, we consider at the end of emission tip. The difference between potential energy and particle energy is

$$V - E = \Phi + E_F - E - e\varepsilon x. \tag{3.2}$$

The unbound wavefunction in region IV by WKB approximation method is

$$\begin{aligned} \varphi_{IV} &= \frac{A}{\sqrt{k}} \exp\left[i\left(\int_{x_3}^{x} k dx - \frac{\pi}{4}\right)\right] \\ &= \frac{A}{\sqrt{k}}\left[\cos\left(\int_{x_3}^{x} k dx - \frac{\pi}{4}\right) + i \sin\left(\int_{x_3}^{x} k dx - \frac{\pi}{4}\right)\right] \end{aligned} \tag{3.3}$$

In region III, we apply the connection formulas of WKB approximation method to obtain the wave function in region IV as

$$\varphi_{III} = \frac{A}{2\sqrt{\kappa}} \exp\left[-\int_{x}^{x_3} \kappa dx\right] - \frac{iA}{\sqrt{\kappa}} \exp\left[\int_{x}^{x_3} \kappa dx\right] \tag{3.4}$$

where κ is defined by

$$\frac{\hbar^2\kappa^2}{2m} = V - E > 0 \tag{3.5}$$

Define r as the integral

$$r \equiv \exp\left[\int_{x_2}^{x_3} \kappa dx\right] \tag{3.6}$$

Substituting this r into Eq.(3.5) gives

$$\varphi_{III} = \frac{A}{2r\sqrt{\kappa}} \exp\left[\int_{x_2}^{x} \kappa dx\right] - \frac{iAr}{\sqrt{\kappa}} \exp\left[-\int_{x_2}^{x} \kappa dx\right] \tag{3.7}$$

So the allowed wave function in region II is

$$\varphi_{II} = -\frac{A}{2r\sqrt{k}} \sin\left[\int_{x}^{x_2} kdx - \frac{\pi}{4}\right] - \frac{i2Ar}{\sqrt{k}} \cos\left[\int_{x}^{x_2} kdx - \frac{\pi}{4}\right] \tag{3.8}$$

where z is defined by

$$z \equiv \int_{x}^{x_2} kdx - \frac{\pi}{4} \tag{3.9}$$

Eq. (3.8) can be rewritten as

$$\begin{aligned} \varphi_{II} &= -\frac{A}{2r\sqrt{k}}\frac{e^{iz} - e^{-iz}}{2i} - \frac{i2Ar}{\sqrt{k}}\frac{e^{iz} + e^{-iz}}{2} \\ &= \frac{iA}{\sqrt{k}}\left(\frac{1}{4r} - r\right) e^{iz} - \frac{iA}{\sqrt{k}}\left(\frac{1}{4r} + r\right) e^{-iz} \end{aligned} \tag{3.10}$$

The second term of above equation represents the incident component of the wave function. Thus, we can get the transmission coefficient T from this term and amplitude of wave function in outbound region IV in Eq.(3.5) as following

$$T = \frac{1}{\left(\frac{1}{4r} + r\right)^2} = \frac{1}{r^2 + \frac{1}{2} + \frac{1}{16r^2}} \tag{3.11}$$

Eq.(3.11) may be approximated as

$$T \simeq \frac{1}{r^2} = \exp\left[-2\int_{x_2}^{x_3} \kappa dx\right] = \exp\left[-2\int_{x_2}^{x_3} \sqrt{\frac{2m}{\hbar}(V-E)}dx\right] \tag{3.12}$$

By following the WKB criteria,

$$\kappa a = \sqrt{2ma^2(V-E)/\hbar} >> 1. \tag{3.13}$$

For transmission at the Fermi level $V - E_F = \Phi - e\varepsilon x$,

$$\begin{aligned} T &= \exp\left[-\frac{2}{\hbar}\int_0^{\Phi/e\varepsilon} \sqrt{2m(\Phi - e\varepsilon x)}dx\right] \\ &= \exp\left[-\frac{4}{3}\frac{\sqrt{2m}}{\hbar}\frac{\Phi^{3/2}}{e\varepsilon}\right] \end{aligned} \tag{3.14}$$

The above equation is the Fowler-Nordheim equation. At any energy level E, $V - E = E_F - E + \Phi - e\varepsilon x$ we have the transmission coefficient

$$T = \begin{cases} \exp\left[-\frac{2}{\hbar}\int_0^{(\Phi+E_F-E)/e\varepsilon} \sqrt{2m(\Phi + E_F - e\varepsilon x - E)}dx\right] & ; E < \Phi + E_F \\ 1 & ; E \geq \Phi + E_F \end{cases} \tag{3.15}$$

3.2 Electron field emission of carbon nanotube

To calculate the characteristic of field emission, we need to know how much current can tunnel through potential barrier at nanotip. The current can be calculated by the number of electrons that come to the nanotube by group velocity at each level of energy describing by the Fermi-Dirac distribution at room temperature. The number of electrons for both spins in each infinitesimal degenerate energy band distribution dE is described by

$$dN = \frac{2f(E)dE}{h} = \frac{f(E)}{\pi\hbar}\frac{\partial E}{\partial k}dk \tag{3.16}$$

where $f(E)$ is the Fermi-Dirac distribution function which describes the possibility of electron state distribution at each energy level given by

$$f(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]} \tag{3.17}$$

From the previous section, we can conclude the total current which depends on the number of electrons tunneling through that the triangular barrier at the end of nanotube is given by

$$\begin{aligned} I &= e \int\limits_{FBZ} T dN = \frac{e}{\pi\hbar} \int\limits_{FBZ} f(E[k]) \frac{\partial E[k]}{\partial k} T[E[k], \varepsilon] dk \\ &= \frac{e}{\pi\hbar} \sum_q \int\limits_{FBZ} f(E_q[k]) \frac{\partial E_q[k]}{\partial k} \exp\left(-\frac{2}{\hbar}\sqrt{2m} \int\limits_{x_2}^{x_3} \sqrt{V - E_q[k] dx} \right) dk \quad ; E_q[k] < V \\ &= \frac{e}{\pi\hbar} \sum_q \int\limits_{FBZ} f(E_q[k]) \frac{\partial E_q[k]}{\partial k} dk \quad ; E_q[k] > \Phi + \mu \end{aligned} \tag{3.18}$$

where e is the electronic charge and $E_q[k]$ is the energy dispersion relation of π and anti π electrons of carbon nanotube at each specific possible discrete values of wave vectors from the circumferential boundary condition of carbon nanotube.

In the next chapter, we will formulate the comprehensive calculation for the field emission. We compare the results with the experiments to see how the behaviour of carbon nanotube field emission is.