References

[1] Liu Xinghui, Zhu Changchun, Li Yukui, *Physica B* **334**, (2004): 243-248.

[2] Knapp, W. et al., *Vacuum* **69**, (2003): 339-344.

[3] Saito, Y. et al., *Carbon* **38**, (2000): 169-182.

[4] Saito, Y. et al., *Applied Surface Science* **146**, (1999): 305-311.

[5] Collins, P. G., Zettl, A., *Physics Review B* **55**, (1997): 9391-9399.

[6] Gomer, R., *Surface Science* **299-300**, (1994): 129.

[7] Collins, P. G., Zettl, A., *Applied Physics Letters* **69**, (1996): 1969-1971.

[8] Xu, X., Brandes, G.R., *Applied Physics Letters* **74**, (1996): 2549-2551.

[9] Peter Y. Yu and Manuel Cardona, *Fundamentals of Semiconductors Physics and Materials Properties*, Springer, Heidelberg (1996).

[10] W. A. Harrison, *Electronic Structure and the Properties of Solids: The Physics of the Chemical Bond*, Dover, New York (1989).

[11] D.J. Chadi, M.L.Cohen, *Phys. Stat. Solidi B* **68**, (1975): 405-419.

[12] F. Herman, *Proc. Int'l Conf. on Physics of Semiconductors*, Dunod, Paris (1964): 3-22.

[13] G. S. Painter and D. E. Ellis, *Phys. Rep.* **1**, (1970): 4747.

[14] R. Saito, M. S. Dresselhaus, G. Dresselhaus., *Physical Properties of Carbon Nanotubes*, Imperial College Press, London (1998).

[15] S. J. Tans, M. H. et al., *Nature, London*386, (1997): 474.

[16] R. Saito, M. Fujita, G. Dresselhaus, and M. S. Dresselhaus. *Appl. Phys. Lett.* **60**, (1992): 2204-2206.

[17] R. A. Jishi, D. Inomata, K. Nakao, M. S. Dresselhaus, and G. Dresselhaus, *J. Phys. Soc. Jpn.* **63**, (1994): 2252-2260.

[18] A. M. Rao, E. et al., *Science* **275**, (1997): 187-191.

[19] J. W. Mintmire and C. T. White, *Carbon* **33**, (1995): 893.

[20] C. H. Olk and J. P. Heremans, J., *Mater. Res.* **9**, (1994): 259-262.

[21] J. W. G. Wildoer, et al., *Nature (London)* **391**, (1998): 59-62.

[22] A. G. Rinzler, J. H. Hafner, P. Nikolaev, *Science* **269**. (1995): 1550.

[23] S. Han, J. Ihm, *Phys. Rev. B* **66**, (2002): 241402.

[24] R. Stratton, *Phys. Rev.* **125**(1), (1962): 67.

[25] Hideaki Sakai, Hidekatsu Suzuura, and Tsuneya Ando, *J. Phys. Soc. Jpn.* **72**, (2003): 1698-1705.

Appendices

Appendix A

Electron velocity

Since the E v.s. k curves correspond to the dispersion relationship for electron waves, the group velocity for electronic transport can be calculated if the E v.s. k relations are known as a function of k,

$$v_g = \frac{\partial \omega}{\partial k} = \frac{1}{\hbar}\left(\frac{\partial E}{\partial k}\right) \tag{A.1}$$

whenever E is of the form $\hbar^2 k^2/2m^*$, $v_g = \hbar k/m^*$; for a free electron $v_g = \hbar k/m$.

The conditions required for $m^* v_g = \hbar k$ can be seen by expressing these various quantities in terms of the E v.s. k dependence. In order for the relation to hold $[\hbar^2/(\partial^2 E/\partial k^2)][(\partial E/\partial k)/\hbar]$ must be equal to $\hbar k$. This leads to the differential equation

$$\frac{\partial E}{\partial k} = k\frac{\partial^2 E}{\partial k^2} \tag{A.2}$$

which has solutions of the form

$$E = Ak^2 + B \tag{A.3}$$

where A and B are not functions of k. Thus the relationship $m^* v_g = \hbar k$ holds for an energy band with extremum at $k = 0$, but does not hold as written for an energy band with extremum at some non-zero value of k, such as $k = k'$. In this case, we need to write $m^* v_g = \hbar(k' - k)$.

In general, in three dimensions

$$\mathbf{v}_g = \frac{1}{\hbar}\nabla_{\mathbf{k}} E(\mathbf{k}) \tag{A.4}$$

where

$$\partial_{\mathbf{k}} E(\mathbf{k}) = \mathbf{e}_1 \frac{\partial E}{\partial k_1} + \mathbf{e}_2 \frac{\partial E}{\partial k_2} + \mathbf{e}_3 \frac{\partial E}{\partial k_3} \tag{A.5}$$

$$\mathbf{k} = \mathbf{e}_1 k_1 + \mathbf{e}_2 k_2 + \mathbf{e}_3 k_3 \tag{A.6}$$

The physical meaning of $\nabla_{\mathbf{k}} E(\mathbf{k})$ is that it is the derivative of E(k) in the direction normal to the energy surface at the point $\mathbf{k}$. The velocity is zero at band extrema

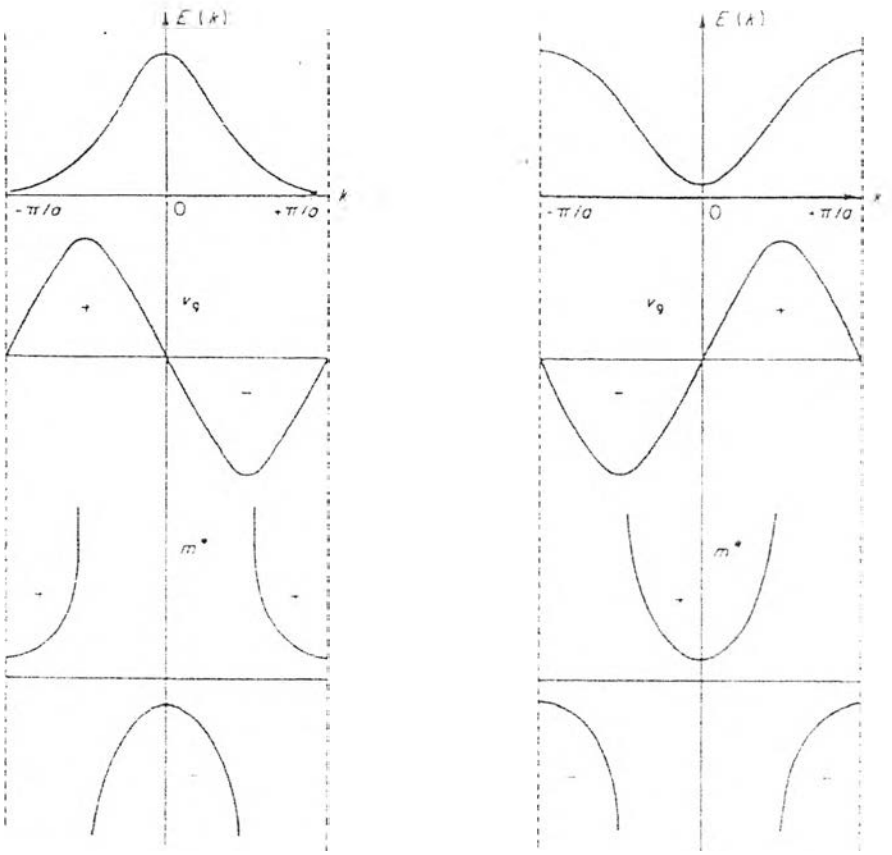

Figure A.1: Typical variation of group velocity v_g and effective mass m^* as a function of k.

and at zone faces. Representative $E(\mathbf{k})$ variations are shown in Fig. A.1 in one dimension, together with the dependence of v_g on k. In thermal equilibrium there are an equal number of electron-occupied states with positive velocity and with negative velocity; hence there is no net charge transport. There is also no way to cause an imbalance in the velocities by the application of an electric field

since, in spite of the effects of the field, an equal number of positive and negative velocities remain. Therefore there is no net charge transport, e.g., why there is no conductivity due to the valence electrons in the filled band of an insulator, and why a partially filled band is the requirement for electrical conduction.

Appendix B

Effective mass

In Appendix A we introduced the concept of an effective mass as a way of describing a situation where the energy depended on k in the same way as for free electrons, but the proportionality constant was not the same as for the free electrons. The proportionality constant is not the same as for free electrons because we are dealing with electrons in a periodic potential; many of their properties are like those of free electrons but some "fudge factor" needs to be introduced to account for the actual environment. The relationship between this effective mass m^* that enters the energy relation: $E = \hbar^2 k^2 / 2m^*$, and the E vs $\mathbf{k}$ dependence. can be obtained in the following way.

The significance of mass is as a proportionality factor between force and acceleration, so that we can calculate the acceleration experienced by an electron, e.g., if we apply an electric field. Now the effect of an external force can be described in terms of the change in momentum caused by the force acting for a time, i.e.,

$$\mathbf{F}dt = d\mathbf{p} = \hbar d\mathbf{k} \tag{B.1}$$

$$\mathbf{F} = \hbar \frac{d\mathbf{k}}{dt} \tag{B.2}$$

This is a general relationship correlating the effect of an external force $\mathbf{F}$ with the time rate of change of $\mathbf{k}$. Under the action of an external force $\mathbf{F}$, the $\mathbf{k}$ of all occupied states changes with a rate equal to $\mathbf{F}/h$. If F is positive, the k of all occupied states is shifted toward positive k values, and vice versa if F is negative. If a band is only partially filled, net transport is possible, since now there

is an unbalance between occupied positive-velocity states and occupied negative-velocity states in the presence of an external force such as an electric field.

But we would like to be able to write $\mathbf{F} = m^*\mathbf{a}$ for this case, or

$$\mathbf{F} = m^* \frac{d\mathbf{v}_g}{dt} \tag{B.3}$$

where m^* is a proportionality constant between force and acceleration, and hence called an effective mass. Let's see what form m^* must have in order for Eqs. (B.2) and (B.3) to be consistent. Since in one dimension

$$\frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{dE}{dk}\right) = \frac{1}{\hbar}\frac{d}{dk}\left(\frac{dk}{dt}\frac{dE}{dk}\right) \tag{B.4}$$

we can substitute from Eq. (B.2) to obtain

$$F = \left(\frac{\hbar^2}{d^2E/dk^2}\right)\frac{dv_g}{dt} \tag{B.5}$$

we conclude that the effective mass m^* must be defined as

$$m^* = \frac{\hbar^2}{d^2E/dk^2} \tag{B.6}$$

for the one-dimensional case. For a free electron $m^* = m$, for an electron displaying free behavior $m^* = constant$, and for a general case, m^* is a function of E and ceases to be an especially helpful construct.

The effective mass of two illustrative band shapes is also given in Fig. A.1. The effective mass m^* is positive for electrons at the bottom of a band and negative for electrons at the top of a band. A negative mass simply implies that the induced acceleration is in the opposite direction to the force that caused it. This provides an example of the effective mass including effects of the crystal potential; the existence of a negative effective mass is the result of Bragg reflection effects in which an electron acted on by a force in one direction is actually accelerated in the opposite direction because it undergoes reflection at the zone face. As shown in Fig. A.1. in one dimension the effective mass becomes infinite at some point within the zone, but three-dimensional effects allow the electron to gain energy

beyond the point by shifting to a different k direction since m^* does not become infinite for the same $E(k)$ for all k directions.

Geometrically the velocity of an electron as given by Eq. (A.1) is the *slope* of the E vs k curve, whereas the effective mass of an electron as given by Eq. (B.6) is the reciprocal of the *curvature* of the E vs $\mathbf{k}$ plot.

To calculate the effective mass in a three-dimensional case, we replace Eq.(B.4) by

$$\frac{d\mathbf{v}_g}{dt} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\left(\mathbf{F}\cdot\nabla_{\mathbf{k}}E(\mathbf{k})\right). \tag{B.7}$$

If the components of the acceleration are a_i and of the force are F_j, then the tensor element $(1/m^*_{ij})$ is the proportionality constant between the ith component of the acceleration and the jth component of the force, and is given by

$$\frac{1}{m^*_{ij}} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}. \tag{B.8}$$

Appendix C

Mathematica program for electron field emission of armchair carbon nanotube

In this Appendix, we show first a simple program for generating parameters of integration boundary, which is discussed in Chapter 4. The next program is used to calculate the result of I-V characteristic of electron field emission of armchair carbon nanotube which is also already discuss in Chapter 4. Any reader can use these codes by citing the content of this thesis.

C.1 Parameters for carbon nanotube field emission

This program need just a few parameters to input. Following here is a example to input parameter and call the program for I-V characteristic curve result. The parameters used here are armchair carbon nanotube (5,5) and integration range which can be receive from first program fkr and the range of external applied electric field in this case in from 0 to 10 $V/\mu m$ and the last parameter is the working temperature which we use 300 K as a room temperature for our calculation.

Example: Input and output of the program fkr , CNTFieldEmission and Graphic result for I-V characteristic of carbon nanotube.

```
MatrixForm[kr5=fkr[5]]
```

{-1, -0.675185}	{-0.675185, 0}	
{-1, -0.544209}	{-0.544209, 0}	
{-0.901241, -0.168064}	{-0.168064, 0}	{0.901241, 1}
{-0.734885, 0}	{}	{0.734885, 1}
$\{-\frac{2}{3}, 0\}$	{}	$\{\frac{2}{3}, 1\}$
{-0.734885, 0}	{}	{0.734885, 1}
{-0.901241, -0.168064}	{-0.168064, 0}	{0.901241, 1}
{-1, -0.544209}	{-0.544209, 0}	{}
{-1, -0.675185}	{-0.675185, 0}	{}
{-1, -0.709957}	{-0.709957, 0}	{}

```
cnt5=CNTFieldEmission[5,kr5,10,300]//Chop
```

{0,0.0000138183,0.00173236,0.0194133,0.0827728,0.217667,
0.434258,0.728996,1.09072,1.50561}

```
Pcnt5=ListPlot[cnt5,AxesLabel→{FontForm["F (V/μ
m)",{"Arial-Bold",12}],FontForm["I (μA)",{"Arial-
Bold",12}]},PlotRange→{{0,10.5},{0,1.75}}];
```

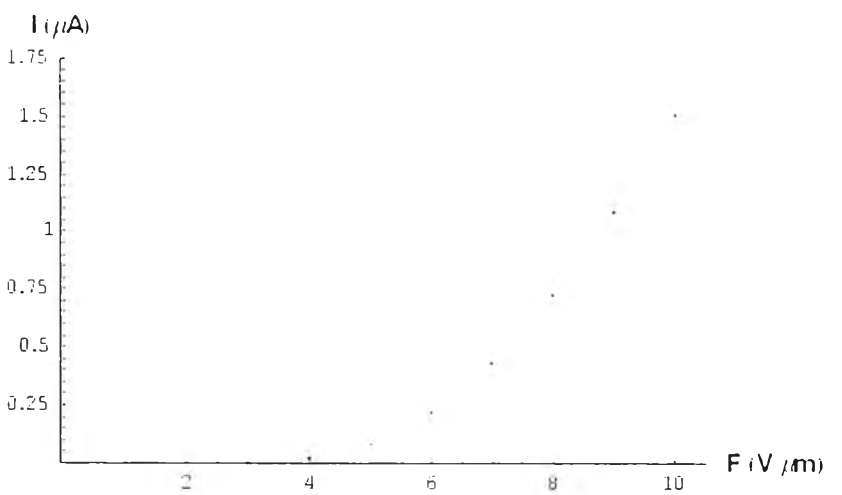

Figure C.1: Input and output of the program fkr, CNT field.

C.2 Carbon nanotube field emission program

Following here is source code for integration limit fkr and current I-V characteristic of carbon nanotube program.

```
Clear[Eaqp]
t = 2.5; (* eV *)
acc = .144 ; (* nm *)
a = acc√3 ; (* nm *)
Eaqp[k_, q_, n_] := t√(1 + 4 Cos[q π / n] Cos[k (10^-9 a) / 2] + 4 Cos[k (10^-9 a) / 2]^2)
Clear[DEaqp]
DEaqp[k_, n_, qi_: 5] := ∂k Eaqp[k, qi, n]
Clear[fkr]
fkr[n_] := Module[{qi, kpeak, krange, krangeo},
  qi = Table[i, {i, 2 n}];
  kpeak = (Solve[Eaqp[k, #, n] == ε + μ, {k}] & /@ qi);
  krange = Table[Take[Table[kpeak[[j, i, 1, 2]] (10^-9 a) / π, {i, Length[kpeak]}], {2, 3}],
    {j, Length[qi]}];
  krange = Table[If[Abs[Im[krange[[i, 1]]]] > 0, {}, krange[[i]]], {i, Length[krange]}];
  krangeo =
   Table[If[i == n, {{-2/3, 0}, {2/3, 1}},
     {{Max[-1, FindRoot[qe DEaqp[k, n, i] / hbar == 0, {k, -If[4 Abs[i - n] < n, 2/3, 1] π / (a 10^-9)}][[1, 2]]
         a / (π 10^9)], 0}, If[{FindRoot[qe DEaqp[k, n, i] / hbar == 0, {k, 1 π / (a 10^-9)}][[1, 2]] a / (π 10^9)} >= 1,
       {}, {FindRoot[qe DEaqp[k, n, i] / hbar == 0, {k, If[4 Abs[i - n] < n, 2/3, 1] π / (a 10^-9)}][[1, 2]]
         a / (π 10^9), 1}]}], {i, 2 n}];
  kr =
   Table[
    {{Flatten[krangeo[[qi]]][[1]], If[Length[krange[[qi]]] < 1, krangeo[[qi]][[1, 2]],
       krange[[qi, 1]]]}, If[Length[krange[[qi]]] < 1, {},
      {krange[[qi, 1]], Min[krangeo[[qi]][[1, 2]], Last[Flatten[krangeo[[qi]]]]]}],
     If[Length[krangeo[[qi, 2]]] < 2, {}, {krangeo[[qi]][[2, 1]], krangeo[[qi]][[2, 2]]}]},
    {qi, 2 n}];
  Return[kr]]
```

Figure C.2: Limit of integration program fkr source code.

```
Clear[CNTFieldEmission]
CNTFieldEmission[n_, kr_, F_:20, T_:300] :=
 Module[{qi, kpeak, krange, krangeo, kb, α, acc, a, L, R, hbar, me, meff, qe, μ, fI},
  (* Material Parameters *)
  kb = 1.3806503 10^-23; (* m^2 kg s^-2 K^-1 *)
  α = 5;
  acc = .144 ; (* nm *)
  a = acc √3 ; (* nm *)
  L = a n √3 ; (* nm *)
  R = L / (2 π) ; (* nm *)
  hbar = 1.05457148 10^-34; (* m^2 kg/s *)
  me = 9.10938188 10^-31; (* kg *)
  meff = 0.06 me; (* kg *)
  qe = 1.60219 10^-19; (* C *)
  μ = 0; (* eV *)
  Ξ = 4.7; (* eV *)
  (* Electron Field Emission *)
  fI =
   Table[
    10^6
     Sum[
      NIntegrate[
       qe π / hbar { f[Eaqp[k, qi, n], T, kb] qe DEaqp[k, n, qi]
          Exp[-2/hbar NIntegrate[√(2 meff qe (μ + Ξ - (V/(α R)) x - Eaqp[k, qi, n])) 10^-9,
            {x, 0, (μ + Ξ - Eaqp[k, qi, n])/(V/(α R))}]] },
       {k, kr[[qi, 1, 1]] Pi / (10^-9 a), kr[[qi, 1, 2]] Pi / (10^-9 a)}] +
      If[Length[kr[[qi, 2]]] < 1, 0,
       NIntegrate[qe π / hbar (f[Eaqp[k, qi, n], T, kb] qe DEaqp[k, n, qi]),
        {k, kr[[qi, 2, 1]] Pi / (10^-9 a), kr[[qi, 2, 2]] Pi / (10^-9 a)}]] +
      If[Length[kr[[qi, 3]]] < 1, 0,
       NIntegrate[qe π / hbar { f[Eaqp[k, qi, n], T, kb] qe DEaqp[k, n, qi]
          Exp[-2/hbar NIntegrate[√(2 meff qe (μ + Ξ - (V/(α R)) x - Eaqp[k, qi, n]))
            10^-9, {x, 0, (μ + Ξ - Eaqp[k, qi, n])/(V/(α R))}]] },
        {k, kr[[qi, 3, 1]] Pi / (10^-9 a), kr[[qi, 3, 2]] Pi / (10^-9 a)}]], {qi, 2 n}], {V, F}];
  Return[fI]]
```

Figure C.3: Program CNTFieldEmission source code.

Vitae

Mr. Kamol Tantanasiriwong was born on October 29, 1972 in Bangkok province, Thailand. He obtained a Bachelor Degree in Civil Engineering (2nd class honor) from Chulalongkorn University in 1994. During 1994 to 1996, he obtained a Monbusho scholarship to study in Japan and has spent his time in the Bridge and Structure Laboratory in Tokyo University. In 1995, he worked as an engineer trainee at Kyoto Takaraike Subway Project with Obayashi Japanese Company in Kyoto for 3 weeks. From 1999 to 2001, he worked as a structural engineer for Taksin Petchkasem (2nd Extension) Elevated Highway Project. In 2002, he started a renewable energy project and set up his own biodiesel plant. In 2003, he came back to study for a master degree in Physics and aimed at research on Nanoelectronics. In 2004, he also worked as a structural engineer in Warnes Associates Co.,Ltd. for 9 months. In 2005, he started his own IT company, MagicShine Network Corp.,Ltd., which mainly focused on wireless internet services and made to order application software. In 2006, he has eventually finished his graduate physics research project on Field Emission of Single Walled Carbon Nanotubes.