Electronic Properties of Materials　　Mid-term Exam　　Oct 20 (Tue), 2014

1. (20pts) Consider an electron trapped in a one-dimensional box with infinitely high potential. The box extends from x = 0 to x = a. The electron has the mass m and the total energy E.

(a) (10ts) Find the energy eigenvalue E_n of the electron by solving Schrodinger equation,

$\frac{d^2\Psi}{dx^2} + \frac{2mE}{\hbar^2}E\Psi = 0 \quad k = \frac{\sqrt{2mE}}{\hbar}, \quad \frac{d^2\Psi}{dx^2} = -k^2\Psi$

$\Psi = A\sin kx + B\cos kx \quad (Ae^{ikx} + Be^{-ikx}$와 같은 형태)

x=0 에서 $\Psi = 0, \quad \therefore \Psi(0) = B = 0$

x=a 에서 $\Psi = 0, \quad \therefore \Psi(a) = A\sin ka = 0,$ A≠0이어야 물리적 의미를 가지므로 ka=nπ (n=1, 2, 3...)

$\therefore k = \frac{n\pi}{a}, \quad E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad (n = 1, 2, 3 \ldots)$

(b) (10pts) Find the eigenfunction ψ_n corresponding to E_n. Also, find the probability density that the electron can be found between x = 0 and a/3 for the second excited state (n = 3).

(c) $\psi_n = A\sin kx = A\sin\frac{n\pi x}{a}$. normalization : $\int_{-\infty}^{\infty} |\psi_n|^2 dx = 1$

$\therefore \int_0^a A^2 \sin^2\frac{n\pi x}{a} dx = A^2 \int_0^a \left(\frac{1}{2} - \frac{1}{2}\cos\frac{2n\pi x}{a}\right) dx$

$= A^2 \left| \frac{1}{2}x - \cancel{\frac{1}{2}\frac{a}{2n\pi}\sin\frac{2n\pi x}{a}} \right|_0^a = A^2 \cdot \frac{a}{2} = 1. \quad \therefore A = \sqrt{\frac{2}{a}}$

$\therefore \psi_n = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$

(d) · the probability density $(0 < x \le \frac{a}{3}) \Rightarrow \int_0^{\frac{a}{3}} |\psi_3|^2 dx \quad (n=3)$

$\therefore \int_0^{\frac{a}{3}} \frac{2}{a} \cdot \sin^2\frac{3\pi x}{a} dx = \frac{2}{a} \cdot \int_0^{\frac{a}{3}} \left(\frac{1}{2} - \frac{1}{2}\cos\frac{6\pi x}{a}\right) dx$

$= \frac{2}{a} \cdot \left| \frac{1}{2}x - \cancel{\frac{a}{12\pi}\sin\frac{6\pi x}{a}} \right|_0^{\frac{a}{3}} = \frac{\cancel{2}}{\cancel{a}} \cdot \frac{1}{\cancel{2}} \cdot \frac{\cancel{a}}{3} = \frac{1}{3}$

2. (25pts) Answer the following questions.

(a) (10pts) Describe the energy for a free electron, a strongly bound electron, and an electron in a periodic potential (i.e., in a crystal), respectively. Why do we get these different band schemes?

(a) · bound electrons (one-dimensional infinite potential well 고려)

$$E_n = \frac{\pi^2 \hbar^2}{2ma^2} n^2 \ (n = 1, 2, 3 \cdots) \rightarrow \text{discrete energy}$$

· free electron (no potential)

$$E = \frac{\hbar^2 k^2}{2m} \ (\text{continuous energy})$$

· electrons in crystals → 주기적인 potential 에 의해 energy band 형성
(allowed energy band, forbidden energy band 존재)

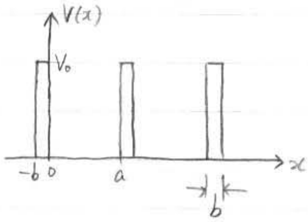
(b,c) (15pts) According to the Kronig-Penny model of one dimensional periodic potential distribution, Schrödinger equations using Bloch function as the electron wave function in the crystal have solutions if the following relation is satisfied;

$$P\frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \qquad P = \frac{maV_0 b}{\hbar^2}$$

Using this relation, explain why forbidden energy bands are formed in the crystal.

(b) Kronig - Penny model (free electrons in a periodic potential well)

① 고체는 주기적인 potential로 단순화 시킨다

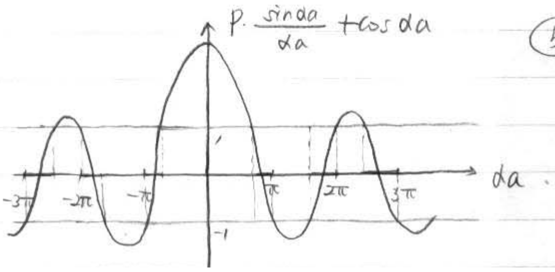


② 주기성을 가진 Bloch function,
$\psi(x) = u(x) \cdot e^{ikx}$ 를 Schrödinger equation 에 도입하여 boundary condition을 적용한다.

③ 최종적으로 얻은 해는, $P\frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$

$\left(P = \frac{maV_0 b}{\hbar^2}, \ \alpha = \frac{\sqrt{2mE}}{\hbar}, \right.$ finite $V_0 b$ 값에 대하여 b는 매우 작고 V_0는 매우 클 때)

④ 이를 αa 와 $P\frac{\sin \alpha a}{\alpha a} + \cos \alpha a$ 에 대해 plot 해 보면 다음과 같이 표현된다



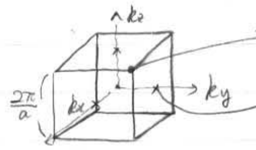
⑤ 이 때 $\cos ka$ 는 -1부터 1 사이의 값을 가지므로 해를 가지는 영역이 정해지게 된다
해가 존재하는 영역이 allowed energy band, 존재하지 않는 영역이 forbidden energy band가 된다.

3. (20pts) Answer the following questions.

(a) (5pts) Calculate how much the kinetic energy of a free electron at the corner of the first

Brillouin zone of a simple cubic lattice (three dimensions!) is larger than that of an electron at the midpoint of the face.

(a) first Brillouin zone of a simple cubic lattice ↙ 각각 ± 적용 가능.



→ at the corner, $k_c = (\pm \pi/a, \pm \pi/a, \pm \pi/a)$ $\therefore |k_c| = \sqrt{3}\,\pi/a$

→ at the midpoint of the face, $k_m = \begin{cases} (\pm \pi/a, 0, 0) \\ (0, \pm \pi/a, 0) \\ (0, 0, \pm \pi/a) \end{cases}$ $\therefore |k_m| = \frac{\pi}{a}$

(for free electron)

$\therefore E_c = \frac{\hbar^2 |k_c|^2}{2m} = \frac{3\hbar^2\pi^2}{2ma^2}$, $E_m = \frac{\hbar^2 |k_m|^2}{2m} = \frac{\hbar^2\pi^2}{2ma^2}$ $\therefore$ E_c는 E_m보다 $\frac{\hbar^2\pi^2}{ma^2}$ 만큼 더 크다. ($E_c = 3E_m$)

(b) (5pts) Calculate the main lattice vectors in the reciprocal space of an fcc crystal.

(b) FCC crystal 의 main lattice vector (in real space)

$\vec{t_1} = \frac{a}{2}(i+j)$, $\vec{t_2} = \frac{a}{2}(j+l)$, $\vec{t_3} = \frac{a}{2}(l+i)$ (a : lattice parameter, i, j, l : x, y, z 방향 unit vector)

in reciprocal space,

$\vec{b_1} = \frac{\vec{t_2}\times\vec{t_3}}{V}$, $\vec{b_2} = \frac{\vec{t_3}\times\vec{t_1}}{V}$, $\vec{b_3} = \frac{\vec{t_1}\times\vec{t_2}}{V}$ $(V = \vec{t_1}\cdot\vec{t_2}\times\vec{t_3})$

$V = \left(\frac{a}{2}\right)^3 \cdot \begin{vmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \left(\frac{a}{2}\right)^3 \cdot (1+1) = \frac{a^3}{4}$, $\therefore \vec{b_1} = \frac{4}{a^3}\cdot\left(\frac{a}{2}\right)^2 \begin{vmatrix} i & j & l \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \frac{1}{a}(i+j-l)$

$\vec{b_2} = \frac{4}{a^3}\left(\frac{a}{2}\right)^2 \cdot \begin{vmatrix} i & j & l \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \frac{1}{a}(-i+j+l)$, $\vec{b_3} = \frac{4}{a^3}\left(\frac{a}{2}\right)^2 \begin{vmatrix} i & j & l \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{vmatrix} = \frac{1}{a}(i-j+l)$

간단하게 표현, $b_1 = \frac{1}{a}(11\bar{1})$, $b_2 = \frac{1}{a}(\bar{1}11)$, $b_3 = \frac{1}{a}(1\bar{1}1)$ → bcc 의 main lattice vector (in reciprocal space)

(c) (10pts) Using the Drude postulation, derive the conductivity σ as a function of N_f (# of free electron per unit volume), electron charge *e*, electron mass *m*, and relaxation time *τ*. Decribe the temperature dependence of the electrical resistivity in pure metal on the basis of Drude conduction theory. Also, explain briefly why Drude conduction theory needs a modification and how it is modified by quantum mechanical consideration.

(a) Drude postulation → a free electron gas

전자에 electrostatic force $e\mathcal{E}$ 와 저항력 γV 가 작용한다고 생각하자 ($\gamma = \text{const.}$)

$$\therefore\ m\frac{dv}{dt} + \gamma V = e\mathcal{E} \quad \text{(운동 방정식)}$$

For steady state ($V = V_f$) → $dv/dt = 0$, $\therefore\ \gamma = \dfrac{e\mathcal{E}}{V_f}$

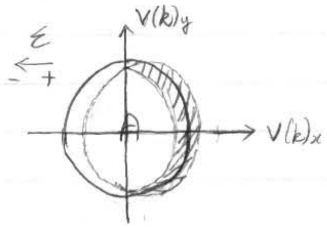
$$\therefore\ m\frac{dv}{dt} + \frac{e\mathcal{E}}{V_f}V = e\mathcal{E} \xrightarrow[\text{solution}]{} V = V_f\left[1 - \exp\left(-\left(\frac{e\mathcal{E}}{mV_f}\right)t\right)\right]$$

relaxation time, $\tau = \dfrac{mV_f}{e\mathcal{E}}$ → $V_f = \dfrac{\tau e\mathcal{E}}{m}$

대입

current density. $J = N_f V_f e = \sigma\mathcal{E}$ (Ohm's law) $\therefore\ \sigma = \dfrac{N_f e^2 \tau}{m}$

(c) Drude model 은 전기장에 의해 힘을 받은 모든 자유전자가 conduction 에 기여한다고 생각한다 하지만 실제로는 전자의 random motion 을 고려한다면 상쇄되는 움직임이 있게되어 특정 전자만 conduction 에 기여하게 된다.



Quantum mechanical consideration 은 E_F 근처의 electron 만이 conduction 에 기여한다고 생각한다.

Field 가 가해졌을 때 A 영역에서는 random motion 으로 인해 상쇄되고 빗금친 부분만이 전류형성에 기여한다.

4. (20pts) Answer the following questions

(a) (10pts) Derive the effective mass, *m** given by

$$m^* = \hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1}$$

(b) Effective mass, m^*.

$$V_g = \frac{d\omega}{dk} = \frac{d(2\pi\nu)}{dk} = \frac{d(2\pi E/h)}{dk} = \frac{1}{\hbar}\frac{dE}{dk}$$

(group velocity)

$$\therefore\ a = \frac{dV_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{dE}{dk}\right) = \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt}$$

$p = \hbar k$ 에서 $\dfrac{dp}{dt} = \hbar\dfrac{dk}{dt} \xrightarrow[\text{대입}]{}$ $= \dfrac{1}{\hbar^2}\dfrac{d^2E}{dk^2}\dfrac{dp}{dt} = \dfrac{1}{\hbar^2}\dfrac{d^2E}{dk^2}\cdot F$

$F = ma$ 에서 $m = \dfrac{F}{a}$

$$\therefore\ m^* = \hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1}$$

(b).(10pts) Consider a semiconductor with 10^{13} donors/cm^3 which has a binding energy of 10 meV. What is the concentration of extrinsic conduction electrons at 300 K ? Also, assuming a gap energy of 1 eV (and $m^* = m_0$) at 300 K, what is the concentration of intrinsic conduction electrons? Compare the concentration of extrinsic conduction electrons with that of intrinsic ones.

at 300K, band gap 1eV 가정, 300K 에서 $E_F \sim -\frac{1}{2}E_g$ 가정.

$$\therefore N_{e,ex} = N_D \times \left(1 - \frac{1}{\frac{1}{2}e^{(E_D - E_F)/kT} + 1}\right) = 10^{13} \times \left(1 - \frac{1}{0.5 \cdot e^{(-0.01+0.5)/(8.616\times10^{-5}\cdot 300)} + 1}\right) \cong 10^{13} \text{(개/cm}^3\text{)}$$

$$N_{e,in} = 4.84\times10^{15} \times (1) \times 300^{3/2} \exp\left(\frac{-1}{2\times 8.616\times10^{-5}\times 300}\right) = 9.99\times10^{10} \text{(개/cm}^3\text{)}$$

$N_{e,extrinsic} > N_{e,intrinsic}$ 이므로

extrinsic effect 에 의한 conduction 이 전체 conduction 에 더 많이 기여한다.

5. (15pts) Answer the following questions related to semiconductors.

(a) (5pts) An n-type semiconductor is brought to contact with a metal. If the work function of the metal(ϕ_M) is larger than that of the semiconductor (ϕ_S), the contact shows a rectifying (Schottky barrier) behavior. Explain the reason for it by sketching the band diagram *before* and *after* contact.

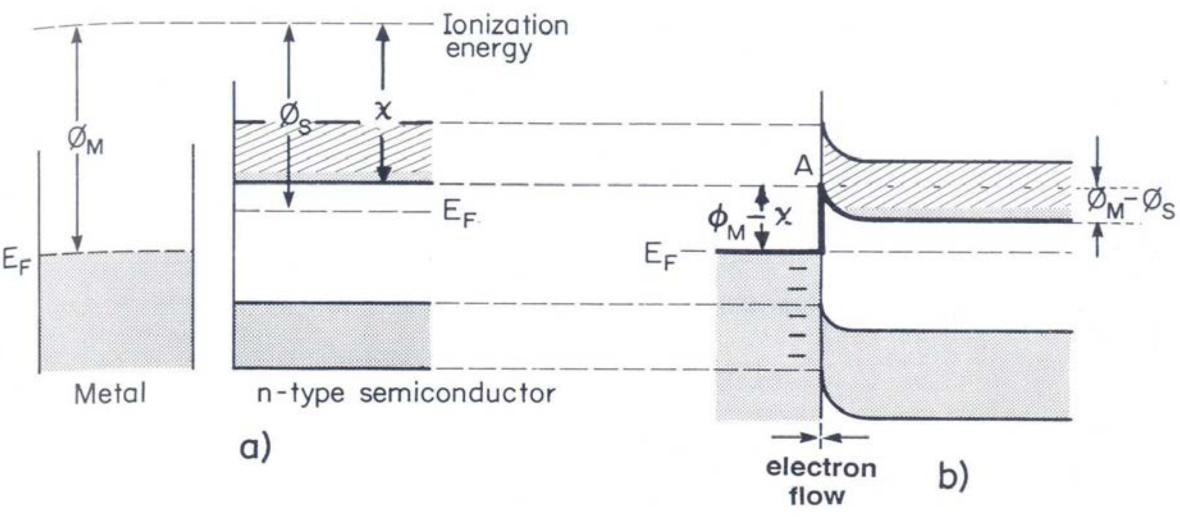


Figure 8.13. Energy bands for a metal and an n-type semiconductor (a) before and (b) after contact. $\phi_M > \phi_S$. The potential barrier is marked with heavy lines. χ is the *electron affinity*.

(b) (10pts) Draw a p-n junction in equilibrium, and explain the operation of p-n rectifier (diode) by drawing the band diagram modifications for forward and reverse bias.

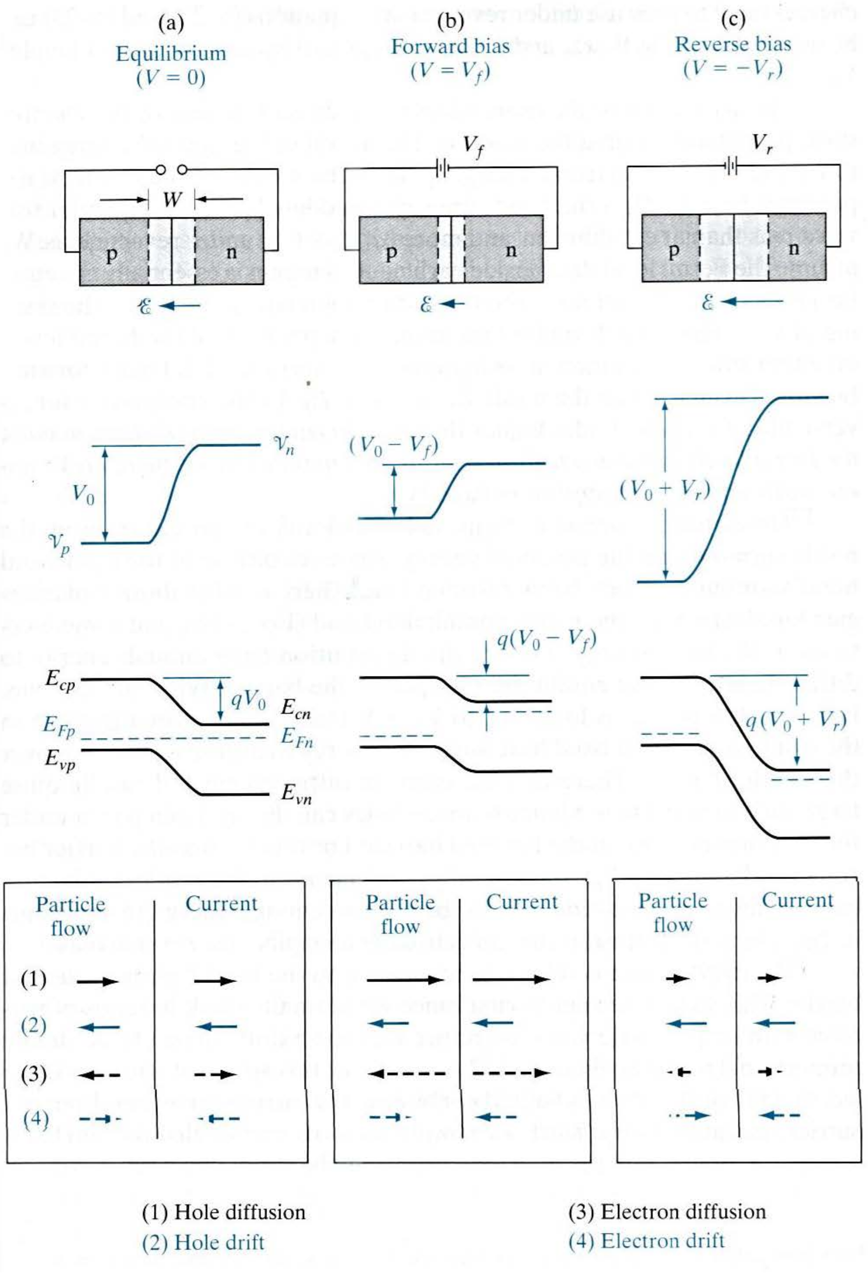


Figure 5–13 Effects of a bias at a p-n junction; transition region width and electric field, electrostatic potential, energy band diagram, and particle flow and current directions within W for (a) equilibrium, (b) forward bias, and (c) reverse bias.