Recitation Class for Mid I Chapter 1-4

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Outline

Overview

Chapter 1 The Crystal Structure of Solids

Chapter 2 Introduction to Quantum Mechanics

Chapter 3 Introduction to the Quantum Theory of Solids

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Chapter 1 The Crystal Structure of Solids

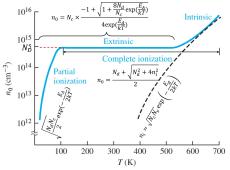
Chapter 2 Introduction to Quantum Mechanics

Chapter 3 Introduction to the Quantum Theory of Solids

Overview

Chapter 5 Carrier Transport Phenomena

$$J = qn\mu_n E_x + qp\mu_p E_x + qD_n \nabla n + qD_p \nabla$$



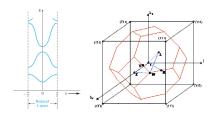
$$n_0 = \int_{E_c}^{\infty} g_c(E) f_F(E) dE = N_c \exp\left(\frac{E_F - E_c}{kT}\right)$$

Overview

▶ Chapter 3 Introduction to the Quantum Theory of Solids

$$g(E) = \frac{4\pi (2m)^{\frac{3}{2}}}{h^3} \sqrt{E}$$

$$f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$



Overview

► Chapter 2 Quantum Mechanics

$$E=\frac{k^2\hbar^2}{2m}$$

► Chapter 1 Introduction

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Lattice types

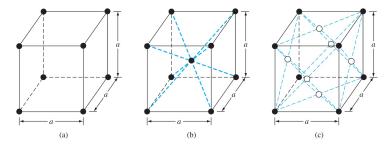


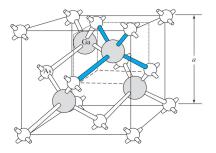
Figure: (a) simple cubic(sc), (b) body-centered cubic(bcc), (c) face-centered cubic(fcc)

$$\label{eq:Volume Density} \begin{split} &\#\text{number of atoms per unit cell} \\ &\text{Volume Density} = \frac{\#\text{ atoms per unit cell}}{\text{volume of unit cell}} \\ &\text{Surface Density} = \frac{\#\text{ atoms per lattice plane}}{\text{area of lattice plane}} \end{split}$$

The diamond structure

The diamond structure all atoms are of the same species **The zincblende structure** two different types of atoms. e.g,

GaAs.

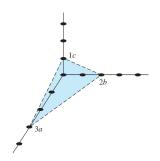


Equivalent to two face-centered cubics sliding 1/4 diagonal length along a diagonal.

atoms per unit cell = 8.



Crystalline Plane and Miller Index



$$(3,2,1) \stackrel{\mathsf{Reciprocal}}{\longrightarrow} (\frac{1}{3},\frac{1}{2},1) \stackrel{\mathsf{multiply}}{\longrightarrow} \mathsf{lcd} (2,3,6)$$

Any parallel plane is entirely equivalent to any other. The [hkl] direction is perpendicular to the (hkl) plane.

Example: Determine the Miller index of x-y plane.



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Infinite quantum well

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi = E\Psi, \quad \left\{ \begin{array}{ll} V(x) = +\infty, & x \leq 0 \text{ or } x \geq a \\ V(x) = 0, & 0 < x < a \end{array} \right.$$

General solution:

$$\Psi(x) = Ae^{-ikx} + Be^{ikx}$$

Boundary condition:

$$\Psi(x)|_{x=a,0} = 0$$

$$\int_0^a \Psi(x)\Psi^*(x) dx = 1$$

conclusion:

$$k = \frac{n\pi}{a}, n = 0, \pm 1, \pm 2, \dots$$

$$E = \frac{k^2 \hbar^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

Finite quantum well

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi = E\Psi, \quad \left\{ \begin{array}{l} V(x) = V_0, & x \le 0 \text{ or } x \ge a \\ V(x) = 0, & 0 < x < a \end{array} \right.$$

General solution:

$$\Psi(x) = \begin{cases} A e^{-ik_1 x} + B e^{ik_1 x}, & k_1 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}, & x \le 0 \text{ or } x \ge a \\ C e^{-ik_2 x} + D e^{ik_2 x}, & k_2 = \sqrt{\frac{2mE}{\hbar^2}}, & 0 < x < a \end{cases}$$

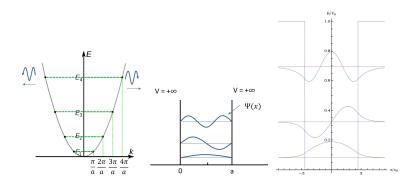
Boundary condition:

$$\begin{aligned} &\Psi(x)|_{x=0} \text{ continuous} \\ &\Psi(x)|_{x=a} \text{ continuous} \\ &\int_{-\infty}^{\infty} \Psi(x) \Psi^*(x) \, \mathrm{d}x = 1 \end{aligned}$$

Note: depending on the relationship between E and V_0 , $\Psi(x)$ is different.



Energy bands



For same energy level, the k can have two values, Because the wave can move to positive and negative directions.

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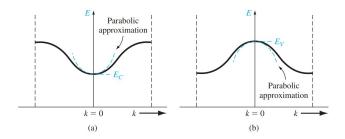
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Effective mass



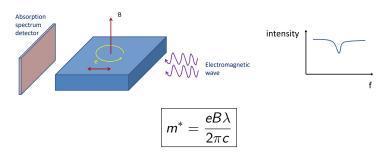
$$\boxed{\frac{1}{\hbar^2} \frac{\mathrm{d}^2 E}{\mathrm{d}k^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*}}$$

$$E = E(k) = E_c + \frac{\hbar^2}{2m_n^*}(k - k_1)^2$$

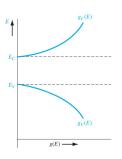
$$E = E(k) = E_{v} - \frac{\hbar^{2}}{2m_{r}^{*}}(k - k_{2})^{2}$$

Effective Mass: experimentally

Cyclotron resonance



Density of States Function



$$g(E) = \frac{4\pi (2m)^{\frac{3}{2}}}{h^3} \sqrt{E}$$

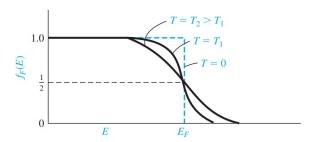
$$g_c(E) = \frac{4\pi (2m_n^*)^{\frac{3}{2}}}{h^3} \sqrt{E - E_c}$$

$$g_v(E) = \frac{4\pi (2m_p^*)^{\frac{3}{2}}}{h^3} \sqrt{E_v - E}$$

Distribution Function

► Fermi-Dirac probability function:

$$f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$



Distribution Function

▶ Boltzmann distribution When $\exp\left(\frac{E-E_F}{kT}\right) >> 1 \Rightarrow E-E_F > 3kT$

$$f_F(E) \approx exp\left(-\frac{E-E_F}{kT}\right)$$

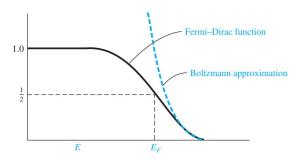


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n_0 and p_0 Equations

$$n_0 = \int_{E_c}^{\infty} g_c(E) f_F(E) dE$$

$$\Rightarrow n_0 = N_c \exp\left[\frac{-(E_c - E_F)}{kT}\right], \quad N_c = 2\left(\frac{2\pi m_n^* kT}{h^2}\right)^{3/2}$$

$$p_0 = \int_{-\infty}^{E_v} g_v(E) (1 - f_F(E)) dE$$

$$\Rightarrow p_0 = N_v \exp\left[\frac{-(E_F - E_v)}{kT}\right], \quad N_v = 2\left(\frac{2\pi m_p^* kT}{h^2}\right)^{3/2}$$

$$kT = 0.0259 \text{ only for } T = 300K$$

Always be careful about the temperature!

Intrinsic Semiconductor

$$n_0 p_0 = n_i^2 = N_c N_v \exp\left[\frac{-(E_c - E_v)}{kT}\right] = N_c N_v \exp\left[\frac{-E_g}{kT}\right]$$

$$\boxed{E_{Fi} - E_{midgap} = \frac{1}{2}kT \ln\left(\frac{N_v}{N_c}\right) = \frac{3}{4}kT \ln\left(\frac{m_p^*}{m_n^*}\right)}$$

Self-consistency

$$n_i^2 = N_c N_v \exp\left[\frac{-(E_c - E_v)}{kT}\right] = N_c N_v \exp\left[\frac{-E_g}{kT}\right]$$

For
$$Si$$
 at $300K$:
$$n_i = 1.5 \times 10^{10} cm^{-3},$$

$$E_g = 1.12 eV,$$

$$N_c = 2.8 \times 10^{19} cm^{-3},$$

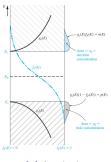
$$N_v = 1.04 \times 10^{19} cm^{-3},$$

$$kT = 0.0259 eV$$

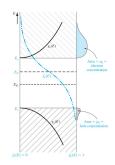
$$LHS = 2.25 \times 10^{20} \neq 4.82936 \times 10^{19} = RHS$$

Write down the steps with all equations and constants used!

The Extrinsic Semiconductor



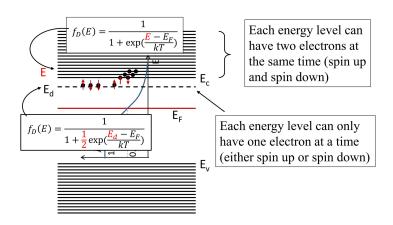
(a) Intrinsic



(b) n-type semiconductor

$$n_0 p_0 = N_c N_v \exp\left(-\frac{E_g}{kT}\right) = n_i^2$$

Statistics of Donors and Acceptors



Statistics of Donors and Acceptors

$$f_d(E) = \frac{1}{1 + \frac{1}{2} \exp\left(\frac{E_d - E_F}{kT}\right)}$$
$$n_d = f_d(E)N_d = N_d - N_d^+$$

where N_d^+ is the concentration of ionized donors.

$$f_a(E) = \frac{1}{1 + \frac{1}{g} \exp\left(\frac{E_F - E_a}{kT}\right)}$$

1/g is the degeneracy factor, normally taken as 4 for acceptor level in silicon and gallium arsenide (because of detailed band structure).

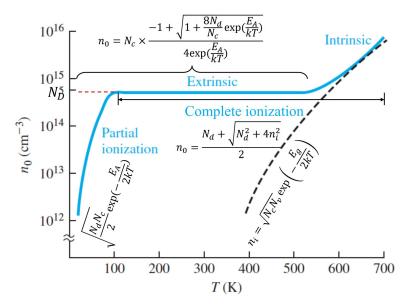
$$p_a = f_a(E)N_a = N_a - N_a^+$$

Statistics of Donors and Acceptors

We calculate the relative number of electrons in the donor state compared with the total number of electrons: (assuming $(E_d - E_F) \gg kT$)

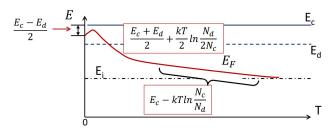
$$\frac{n_d}{n_d + n_0} = \frac{1}{1 + \frac{N_c}{2N_d} \exp\left[\frac{-(E_c - E_d)}{kT}\right]}$$

Example: Determine the fraction of total electrons still in the donor states at T=300K. Consider phosphorus doping in silicon, for T=300K, at a concentration of $N_d=10^{16}cm^{-3}$. **Answer:** 0.41%. Very few electrons remains in the donor states (completely ionized).



Fermi Level Position

$$\begin{split} E_F &= E_c + kT \ln \left(\frac{\sqrt{1 + \frac{8N_d}{N_c} \exp\left(\frac{E_A}{kT}\right)} - 1}{4 \exp\left(\frac{E_A}{kT}\right)} \right) \\ &= \begin{cases} \frac{E_c + E_D}{2} + \frac{kT}{2} \ln \frac{N_d}{2N_c}, & T \text{ small} \\ E_c - kT \ln \frac{N_c}{N_d}, & T \text{ big} \end{cases} \end{split}$$



Good luck to your midterm exam!