VE320 RC2

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Overview

1. Chapter 3
   - Allowed and Forbidden Energy Bands
   - Electrical Conduction in Solids
   - Extension to Three Dimensions
   - Effective Mass
   - Density of States Function
2. Review

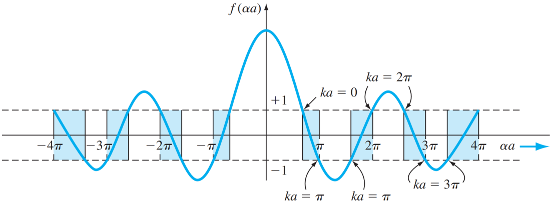
Energy Bands

- 1-D Kronig-Penney Model (not required):

$$f(\alpha a) = P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$$

- This relation gives the conditions for which Schrodinger's wave equation will have a solution.
- since $f(\alpha a) = \cos ka$, k and a are real, the value of $f(\alpha a)$ must be between -1 and 1. Then we get a list of discontinuous possible regions of α, which gives the possible regions of E. This is known as the energy band.

Energy Bands



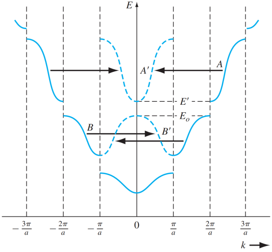


Figure 3.10 | The E versus k diagram showing 2π displacements of several sections of allowed energy bands.

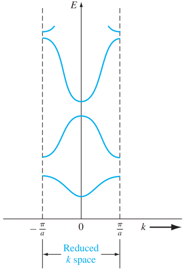


Figure 3.11 | The E versus k diagram in the reduced-zone representation.

Energy Bands and Conductivity

- Qualitatively, conductivity is related the number of carriers (electrons or holes)
- When a possible state is occupied, there is an electron. Otherwise, there is a hole.
- Usually, only electrons in the conduction band and holes in the valence band can be carriers.

Electrical Conduction in Solids

- metal

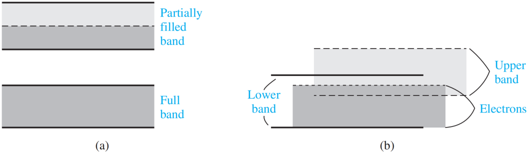
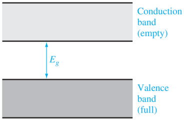
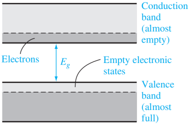


Figure 3.21 | Two possible energy bands of a metal showing (a) a partially filled band and (b) overlapping allowed energy bands.

- insulator



- semiconductor



Extension to Three Dimensions

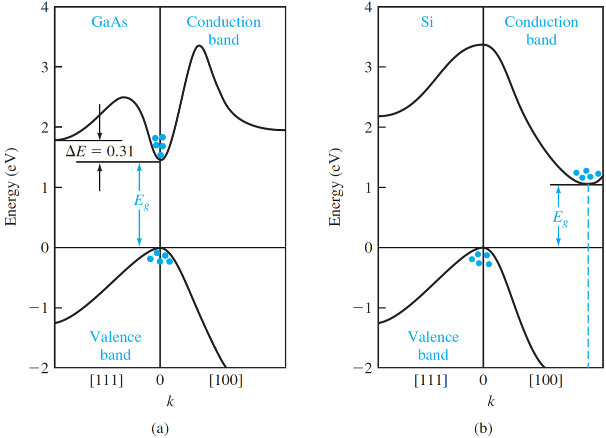


Figure: (a) Direct Bandgap Semiconductor (b) Indirect Bandgap Semiconductor

Effective Mass

- $F_{ext} = m^* a$
- for electrons in free space:
  $E = \dfrac{\hbar^2 k^2}{2m}$, $\dfrac{1}{\hbar}\dfrac{\mathrm{d}E}{\mathrm{d}k} = v$, $\dfrac{1}{\hbar^2}\dfrac{\mathrm{d}^2 E}{\mathrm{d}k^2} = \dfrac{1}{m}$
- for electrons in crystalline semiconductors:
  use parabola approximation for electrons near the bottom of the conduction band and the top of the valence band
  $\dfrac{1}{\hbar^2}\dfrac{\mathrm{d}^2 E}{\mathrm{d}k^2} = \dfrac{1}{m^*}$
- $E(k) = E_c + \dfrac{\hbar^2}{2m_n^*}(k - k_1)^2$
- $E(k) = E_v - \dfrac{\hbar^2}{2m_p^*}(k - k_2)^2$
- k_1, k_2: k axis coordinate of bottom point and top point
  m_n^*, $m_p^* > 0$

Exercise

textbook exercise 3.17:
Figure P3.17 shows the parabolic E versus k relationship in the valence band for a hole in two particular semiconductor materials. Determine the effective mass (in units of the free electron mass) of the two holes.

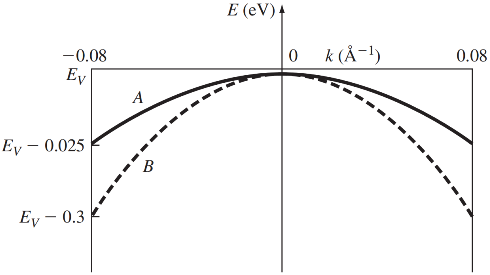


Figure P3.17 | Figure for Problem 3.17.

Answer

valence band: $E(k) = E_v - \frac{\hbar^2}{2m_p^*}k^2$

A:

$$m_p^* = \frac{\hbar^2 k^2}{2(E_v - E)}$$
$$= \frac{(1.054 \times 10^{-34})^2 (0.08 \times 10^{10})^2}{2 \times 0.025 \times (1.6 \times 10^{-19})} = 8.8873 \times 10^{-31}\text{kg}$$

B:

$$m_p^* = \frac{\hbar^2 k^2}{2(E_v - E)}$$
$$= \frac{(1.054 \times 10^{-34})^2 (0.08 \times 10^{10})^2}{2 \times 0.3 \times (1.6 \times 10^{-19})} = 7.406 \times 10^{-32}\text{kg}$$

Density of States Function

- for electrons in the lattice:

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

- for electrons at the bottom of conduction band:

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

- for electrons at the top of valence band:

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

Exercise

textbook exercise 3.27:
Determine the total number ($\#/cm^3$) of energy states in silicon between E_v and $E_v - 3kT$ at $T = 300K$

Answer

silicon: $m_p^* = 0.56 m_0$

$$
\begin{aligned}
N &= \int_{E_v-3kT}^{E_v} g_v(E)\mathrm{d}E \\
&= \frac{4\pi(2m_p^*)^{3/2}}{h^3}\int_{E_v-3kT}^{E_v}\sqrt{E_v - E}\mathrm{d}E \\
&= \frac{4\pi(2m_p^*)^{3/2}}{h^3}(-\frac{2}{3})(E_v - E)^{3/2}\Big|_{E_v-3kT}^{E_v} \\
&= \frac{4\pi[2\times 0.56\times(9.11\times 10^{-31})]^{3/2}}{(6.625\times 10^{-34})^3}(-\frac{2}{3})[-(3\times 1.38\times 10^{-23}\times 300)^{3/2}] \\
&= 4.116\times 10^{25}\mathrm{m}^{-3}
\end{aligned}
$$

Charge Density Calculation

$$\text{surface atom density} = \frac{\#\ \text{atom per lattice plane}}{\text{area of the lattice plane}}$$

$$\text{volume atom density} = \frac{\#\ \text{atom per lattice}}{\text{volume of the unit lattice}}$$

Quantum Mechanics Basic Equations

- photons: $E = h\nu$, $\lambda\nu = c$, $p = \dfrac{h\nu}{c}$
- matters: $p = mv$, $E = \dfrac{1}{2}mv^2$
- general: $k = \dfrac{2\pi}{\lambda}$, $\hbar = \dfrac{h}{2\pi}$
- de Brogile wavelength$= \dfrac{h}{p}$
- uncertainty principle: $\Delta p \Delta x \geq \hbar$, $\Delta E \Delta t \geq \hbar$

Solution of Second Order Differential Equations

$$
\begin{aligned}
\frac{\partial^2 y}{\partial x^2} &= k^2 y \\
y &= A_1 e^{kx} + A_2 e^{-kx} \\
\frac{\partial^2 y}{\partial x^2} &= -k^2 y \\
y &= A_1 e^{ikx} + A_2 e^{-ikx} \\
y &= A_1^{'} \cos kx + A_2^{'} \sin kx
\end{aligned}
$$

One-Dimensional Schrodinger's Equation

- One-dimensional Schrodinger's equation (seperate variables):

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

- PDF: $f_X(x) = |\psi(x)|^2$
- Boundary condition:
  1. $\int_{-\infty}^{\infty} |\psi(x)|^2 = 1$
  2. $\psi(x)$ is finite, single-valued and continuous
  3. $\frac{\partial \psi(x)}{\partial x}$ is finite, single-valued and continuous when $V(x)$ in the region is finite. However, when $V(x)$ is infinite, $\frac{\partial \psi(x)}{\partial x}$ may be not continuous.
- The essence of solving $\psi(x)$ is just solving a BVP. Following slides provide three typical $V(x)$ and corresponding solutions.

Free Space

- $V(x) = 0$
- $\dfrac{\partial^2 \psi(x)}{\partial x^2} + \dfrac{2m}{\hbar^2} E\psi(x) = 0$
- Solution: $\psi(x) = Ae^{ikx} + Be^{-ikx}$
  $k = \sqrt{\dfrac{2mE}{\hbar^2}}$
- Other features of the wave can be calculated with the relationships mentioned previously.

Infinite Quantum Well

- $\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$
- $V(x) = \begin{cases} \infty & x \leq 0 \text{ or } x \geq a \\ 0 & \text{otherwise} \end{cases}$

Infinite Quantum Well

- general solution in the region $(0, a)$:
  $\psi(x) = Ae^{ikx} + Be^{-ikx}$
  $k = \sqrt{\dfrac{2mE}{\hbar^2}}$
- general solution in the region $(-\infty, 0)$ and $(0, \infty)$:
  $\psi(x) = 0$
- apply boundary condition:
  $A + B = 0$
  $Ae^{ika} + Be^{-ika} = 0$
  $\int_{-\infty}^{\infty} |\psi(x)|^2 = 1$
- conclusion:
  $\psi(x) = \sqrt{\dfrac{2}{a}} \sin k_n x$
  $k_n = \dfrac{n\pi}{a},\ E_n = \dfrac{k^2\hbar}{2m} = \dfrac{\hbar^2 n^2 \pi^2}{2ma^2}$

Finite Quantum Well

- $\dfrac{\partial^2\psi(x)}{\partial x^2} + \dfrac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$
- $V(x) = \begin{cases} V_0 & x \leq 0 \text{ or } x \geq a \\ 0 & \text{otherwise} \end{cases}$

Finite Quantum Well

- general solution in the region $(-\infty, 0)$ and (a, ∞):
  $\psi(x) = Ae^{ik_1x} + Be^{-ik_1x}$
  $k_1 = \sqrt{\frac{2m(E - V_0}{\hbar^2}}$
- general solution in the region $(0, a)$:
  $\psi(x) = Ce^{ik_2x} + De^{-ik_2x}$
  $k_2 = \sqrt{\frac{2mE}{\hbar^2}}$
- apply boundary condition:
  $\psi(x)$ continuous at 0 and a
  $\frac{\partial\psi(x)}{\partial x}$ continuous at 0 and a
  $\int_{-\infty}^{\infty} |\psi(x)|^2 = 1$

Reference

1. Semiconductor Physics and Devices: Basic Principles 4th ed. Donald A. Neamen.
2. 2023Summer Ve320_RC_2, Shuo Deng
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4. 2023Summer RC1, Qian Zhao
5. 2023Summer VE320 RC3, Jiajun Sun