Recitation Class 1

Zexi Li

lzx12138@sjtu.edu.cn

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Outline

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Semiconductor Materials

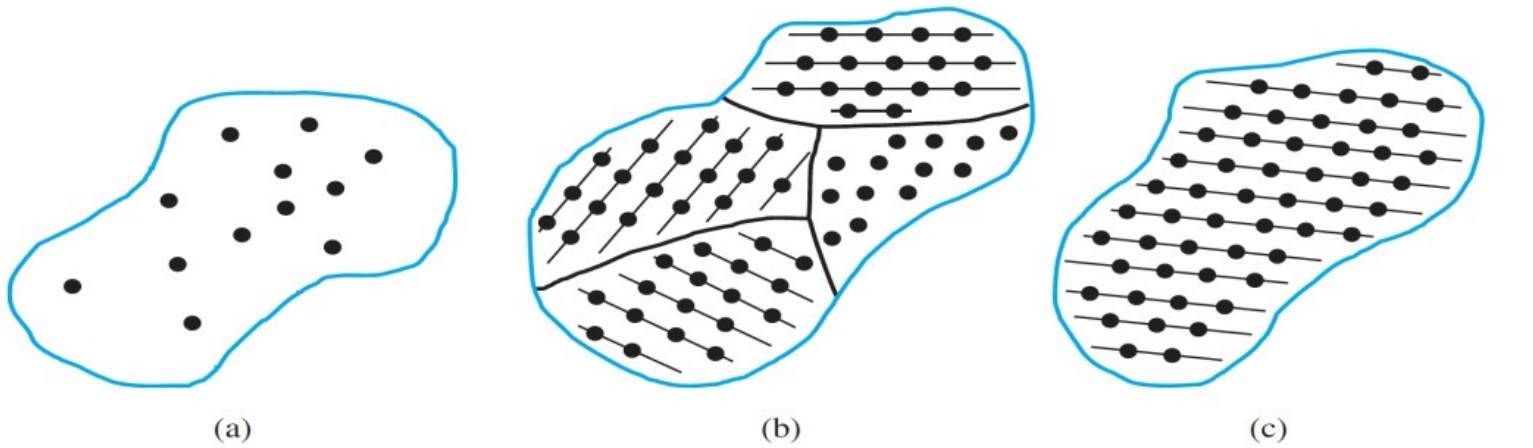
Conductors	Semiconductors	Insulators
$< 10^{-3}\Omega \cdot \text{cm}$	$10^{-3} - 10^{9}\Omega \cdot \text{cm}$	$> 10^{9}\Omega \cdot \text{cm}$
Metals (Au, Al, Cu, Hg, ...)	Si, Ge, GaAs, InP, ...	SiO_2, HfO_2, ...
Solids, liquids (Hg)	Solids	Solids, liquids gases

Table: Semiconductor

Semiconductors are the materials that have resistivities between $10^{-3} - 10^{9}\Omega \cdot \text{cm}$ depending on light illumination, temperature, electric field, magnetic field and impurities.

Type of Solids

- Amorphous
- Polycrystals
- Single crystals



(a) (b) (c)

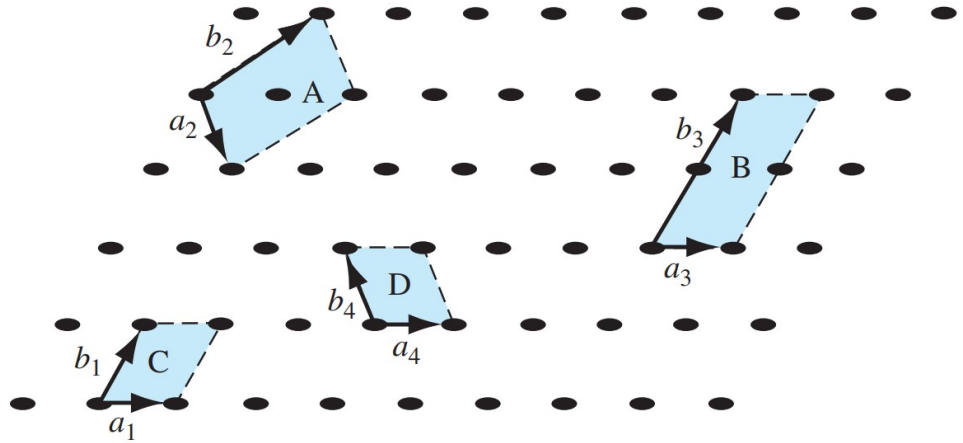
All atoms or ions are periodically ranged in a short range (a few atoms)

Multiple crystalline grains randomly packed

All atoms or ions are periodically ranged in a long range (μm scale)

All semiconductors covered in this course are assumed to be single crystalline.

Primitive and unit cell



Unit Cell: small volume of the crystal that can be used to reproduce the entire crystal.
A unit cell is not a unique entity
Primitive Cell: the smallest unit cell that can be repeated to form the lattice.

Lattice types

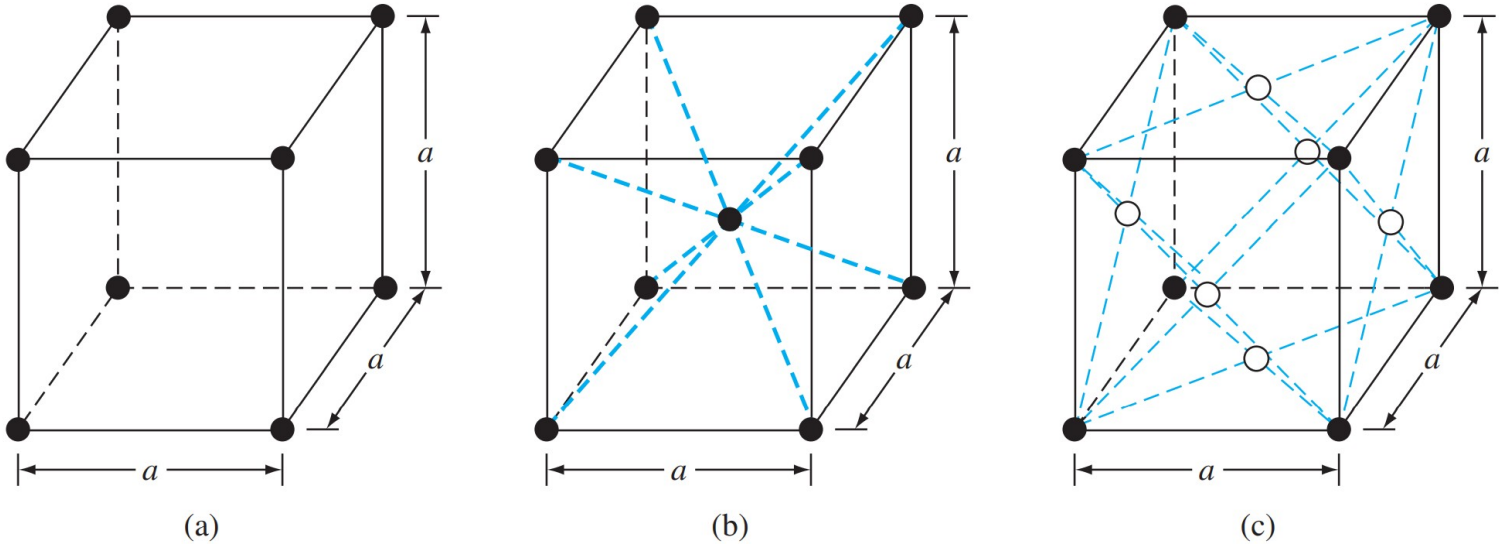


Figure: (a) simple cubic(sc), (b) body-centered cubic(bcc), (c) face-centered cubic(fcc)

$$\#\text{number of atoms per unit cell}$$

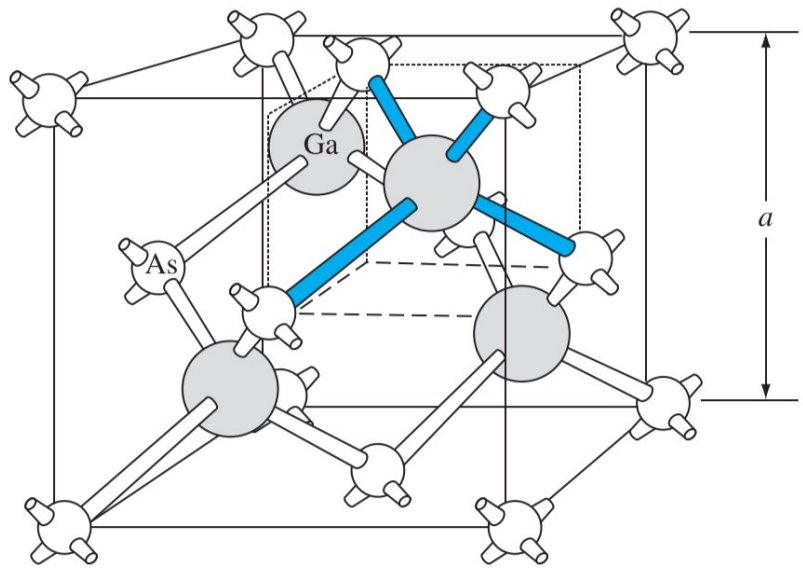
$$\text{Volume Density} = \frac{\#\text{ atoms per unit cell}}{\text{volume of unit cell}}$$

$$\text{Surface Density} = \frac{\#\text{ atoms per lattice plane}}{\text{area of lattice plane}}$$

(Example after reviewing Miller index)

The diamond structure

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



The diamond structure: To help remember

Method 1:

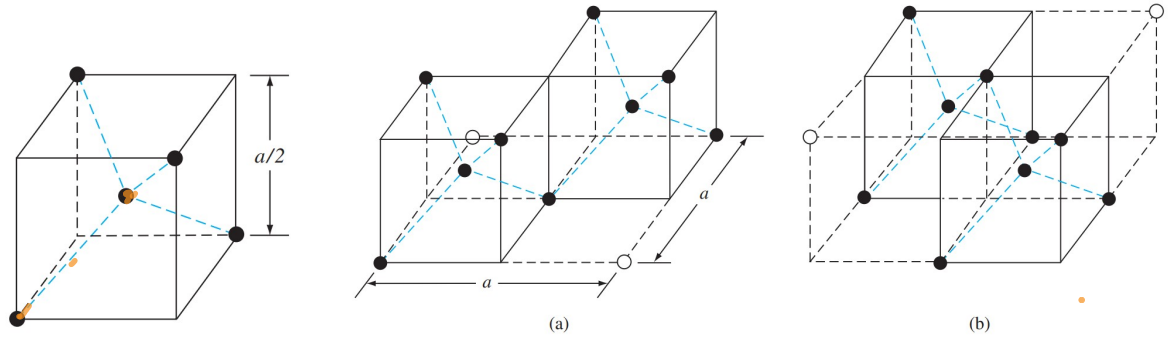
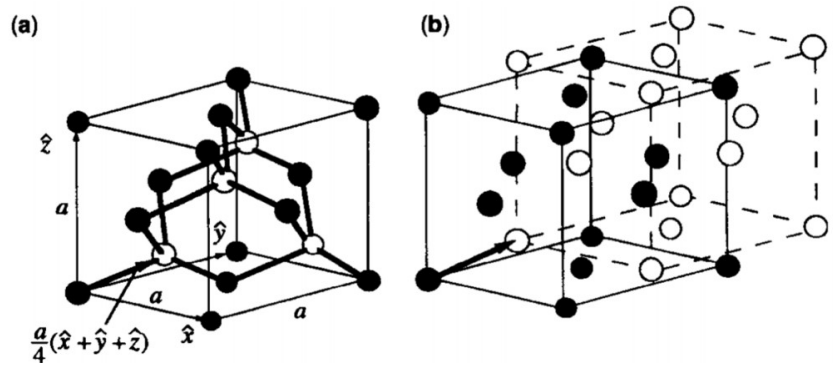


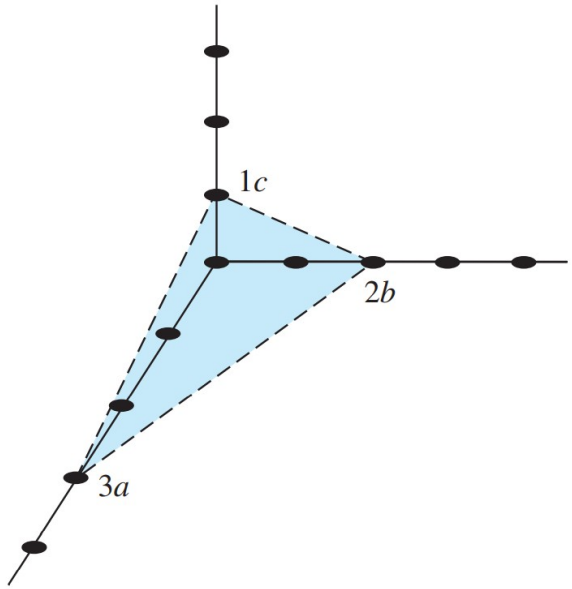
Figure: Tetrahedral structure & (a) bottom half, (b) top half

Method 2:



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

Crystalline Plane and Miller Index

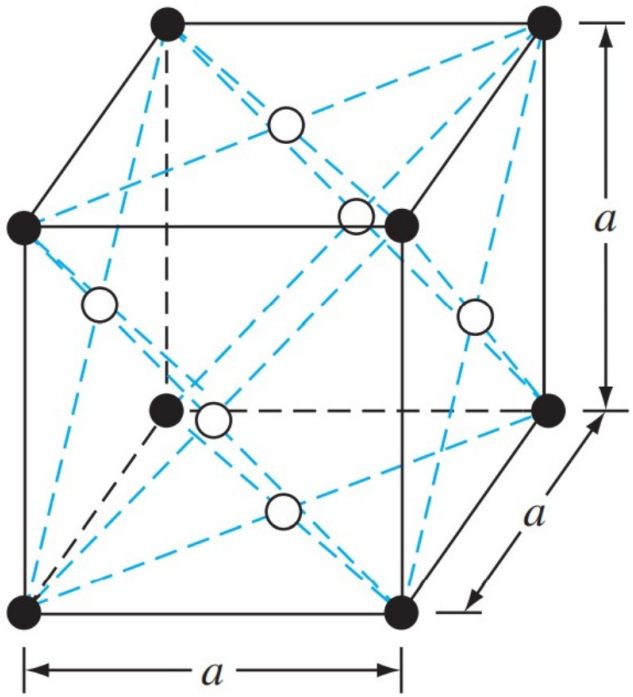


$$(3,2,1) \xrightarrow{\text{Reciprocal}} (\frac{1}{3},\frac{1}{2},1) \xrightarrow{\text{multiply lcd}} (2,3,6)$$

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

Example: Surface density

The lattice constant of a single crystal is 4.50 $\AA$. Calculate the surface density of atoms (# per cm^2) on the plane (111) for face-centered cubic lattice.



Doping

n-type semiconductors: Charge carriers are negative, i.e. electrons doped by donor-type of dopants.
p-type semiconductors: Charge carriers are positive, i.e. holes doped by acceptor-type of dopants.

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Basic concepts

Wave function:

$$\Psi(x)$$

Probability density function:

$$|\Psi(x)|^2 = \Psi(x) \cdot \Psi^*(x)$$

Schrodinger Equation:

$$-\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = j\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

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

E: total energy of the particle.

Infinite quantum well

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V(x)\Psi=E\Psi,\quad \begin{cases} V(x)=+\infty, & x\le 0 \text{ or } x\ge a \\ V(x)=0, & 0<x<a \end{cases}$$

General solution:

$$\Psi(x)=A\mathrm{e}^{-ikx}+B\mathrm{e}^{ikx}$$

Boundary condition:

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

$$\int_0^a \Psi(x)\Psi^*(x)\,\mathrm{d}x=1$$

conclusion:

$$k=\frac{n\pi}{a}, n=0,\pm1,\pm2,\ldots$$

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

Finite quantum well

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

General solution:

$$\Psi(x)=\begin{cases} Ae^{-ik_1x}+Be^{ik_1x}, & k_1=\sqrt{\frac{2m(E-V_0)}{\hbar^2}}, \quad x\le 0 \text{ or } x\ge a \\ Ce^{-ik_2x}+De^{ik_2x}, & k_2=\sqrt{\frac{2mE}{\hbar^2}}, \quad 0<x<a \end{cases}$$

Boundary condition:

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

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

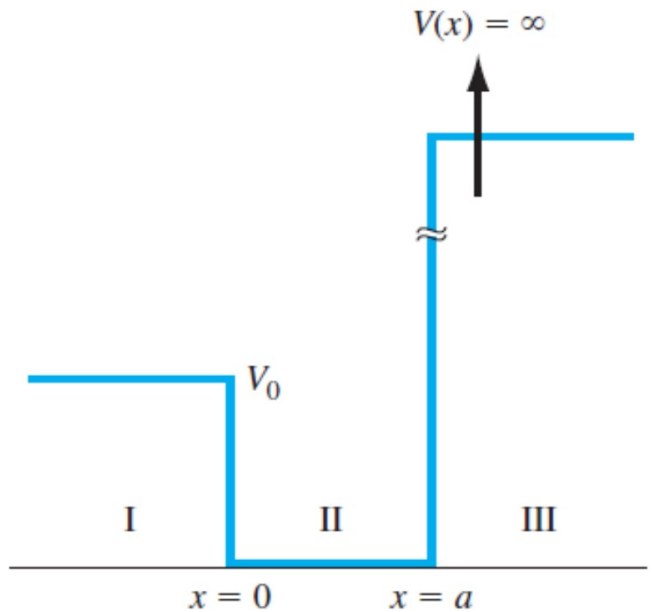
Example

Consider the one-dimensional potential function shown in the figure below. Assume the total energy of an electron is $E < V_0$.

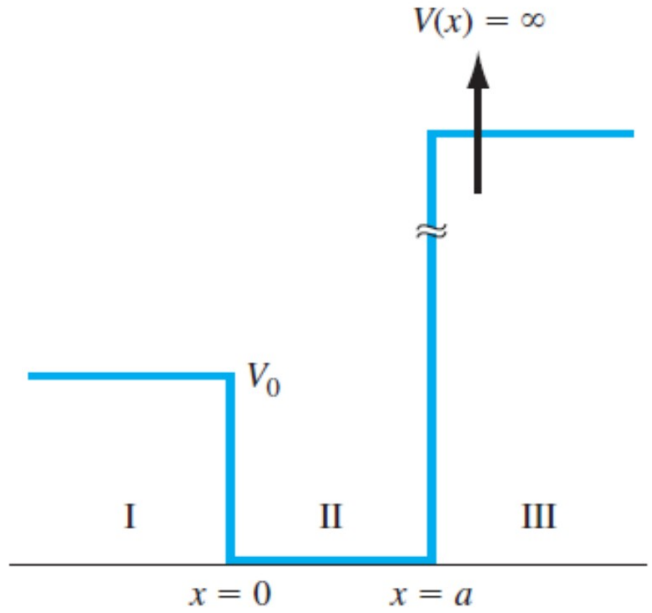
a) Write the wave solutions that apply in each region.

b) Write the set of equations that result from applying the boundary conditions.

c) Show explicitly why, or why not, the energy levels of the electron are quantized.



Example



$$\Psi(x) = \begin{cases} A\mathrm{e}^{-ik_1 x} + B\mathrm{e}^{ik_1 x}, & x \leq 0 \\ C\mathrm{e}^{-ik_2 x} + D\mathrm{e}^{ik_2 x}, & 0 < x < a \\ 0, & x \geq a \end{cases}$$

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

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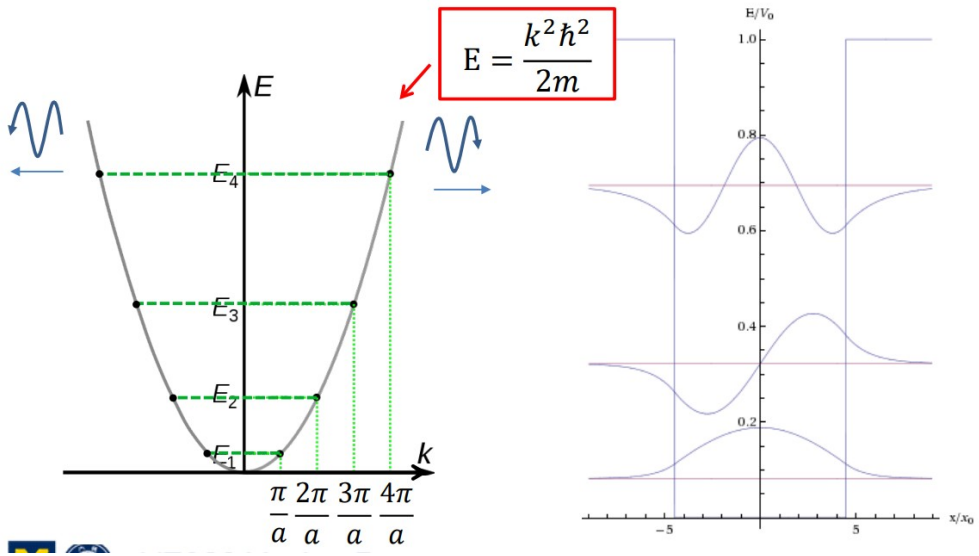
Energy bands



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

Effective mass

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

Taking derivative:

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

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

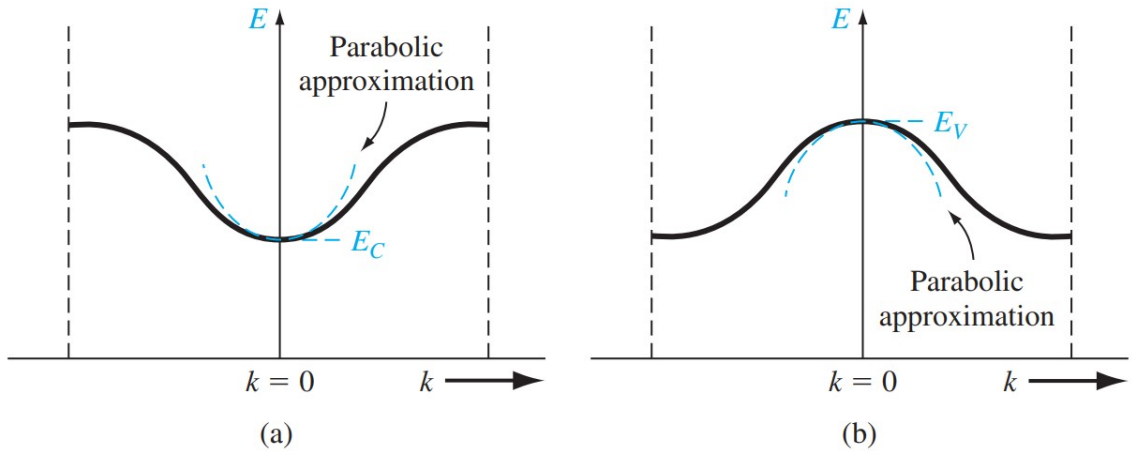


Figure: (a) The conduction band in reduced k space, and the parabolic approximation. (b) The valence band in reduced k space, and the parabolic approximation

$$E - E_c = C_1 k^2$$

Effective mass

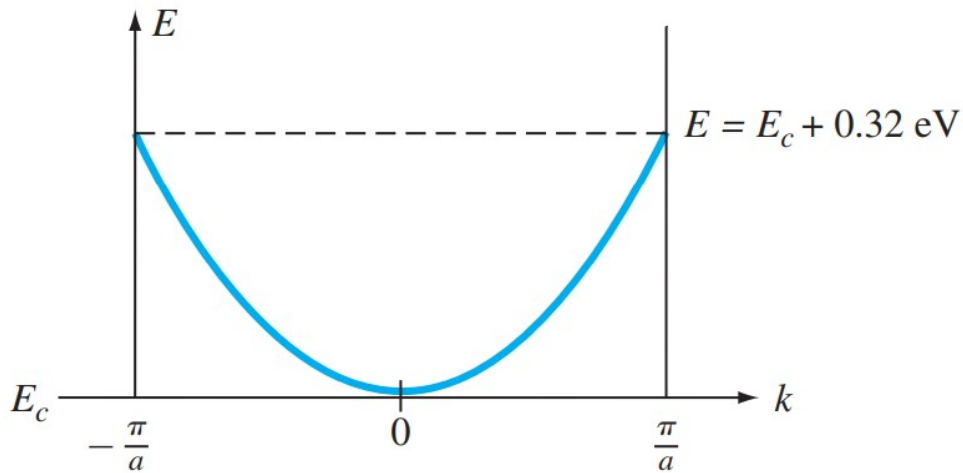
$$\boxed{\frac{1}{\hbar^2}\frac{\mathrm{d}^2E}{\mathrm{d}k^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*}}$$

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

$$E = E(k) = E_v - \frac{\hbar^2}{2m_p^*}(k - k_2)^2$$

Example

A simplified E versus k curve for an electron in the conduction band is given. The value of a is 10 $\mathring{A}$. Determine the relative effective mass m^*/m_0.



Answer:

End