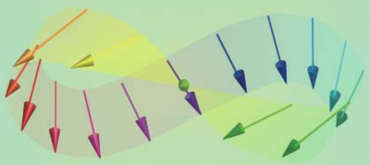
Introductory Nanotechnology

~ Basic Condensed Matter Physics ~



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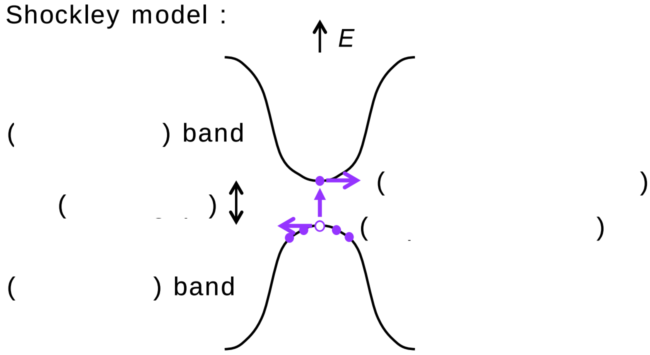
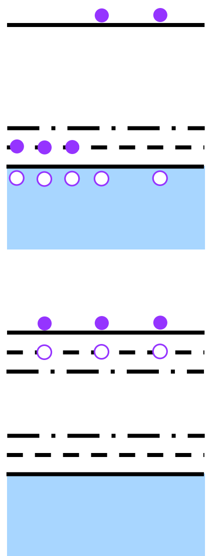
Quick Review over the Last Lecture 1

Shockley model :



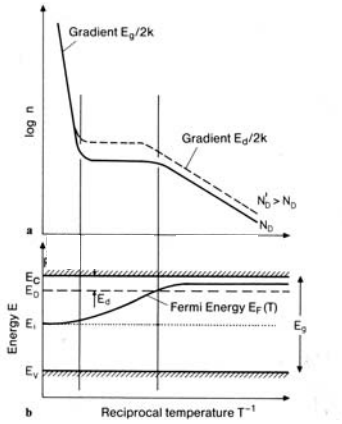


Semiconductors :

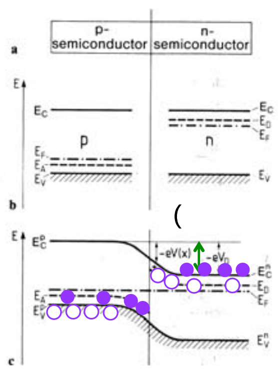
• E_F = • *np* =	• • -type : • -type : • *np* =

Quick Review over the Last Lecture 2

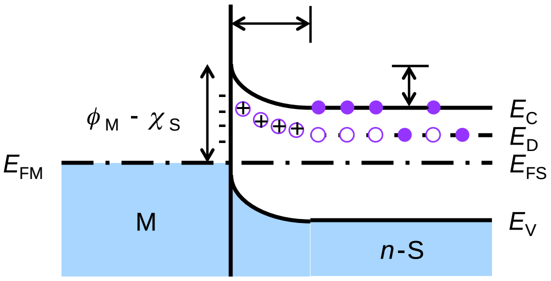
Temperature dependence of an extrinsic semiconductor :

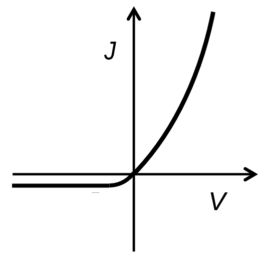


pn junction :



Metal - semiconductor junction :





Contents of Introductory Nanotechnology

First half of the course :

Basic condensed matter physics

1. Why *solids* are *solid* ?
2. What is the *most common atom* on the earth ?
3. How does an electron travel in a material ?
4. How does lattices vibrate thermally ?
5. What is a *semi*-conductor ?
6. How does an electron tunnel through a barrier ?
7. Why does a magnet attract / retract ?
8. What happens at interfaces ?

Second half of the course :

Introduction to nanotechnology (nano-fabrication / application)

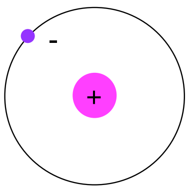
How Does an Electron Tunnel through a Barrier ?

- De Broglie wave
- Schrödinger equation
- 1D quantum well
- Quantum tunneling
- Reflectance / transmittance
- Optical absorption
- Direct / indirect band gap

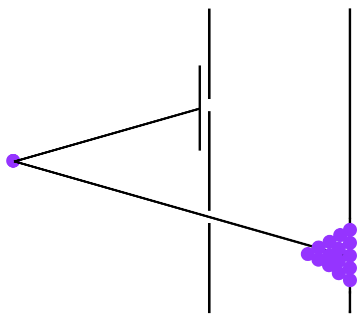
Electron Interference

Davisson-Germer experiment in 1927 :

Electrons are introduced to a screen through two slits.



Electron as a particle should not interfere.
≠ Photon (light) as a wave



→ Electron interference observed !

→ Wave-particle duality

* http://www.wikipedia.org/

Scrödinger's Cat

Thought experiment proposed by E. Schrödinger in 1935

The observer cannot know

- if a radioactive atom has decayed.
- if the vial has been broken and the hydrocyanic acid has been released.
- if the cat killed.

→ The cat is both dead and alive according to quantum law :
superposition of states

The superposition is lost :

- only when the observer opens the box and learn the condition of the cat.
- then, the cat becomes dead or alive.

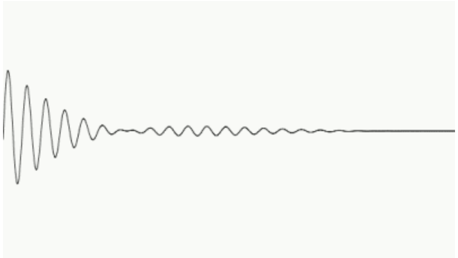
→ quantum indeterminacy

* http://www.wikipedia.org/

De Broglie Wave

Wave packet :

contains number of waves, of which amplitude describes probability of the presence of a particle.



$$\lambda = \frac{h}{m_0 v}$$

where λ : wave length, h : Planck constant and m_0 : mass of the particle.

→ de Broglie hypothesis
(1924 PhD thesis → 1929 Nobel prize)

According to the mass-energy equivalence :

$$E = m_0 c^2 = m_0 c \cdot c = p \cdot \lambda \nu$$

where p : momentum and ν : frequency.
By using $E = h\nu$,

$$\lambda = \frac{h}{p} = \frac{h}{m_0 v}$$

* http://www.wikipedia.org/

Schrödinger Equation

In order to express the de Broglie wave, Schrödinger equation is introduced in 1926 :

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

E : energy eigenvalue and ψ : wave function

Wave function represents probability of the presence of a particle $|\psi|^2 = \psi^*\psi$

ψ^* : complex conjugate (*e.g.*, $z = x + iy$ and $z^* = x - iy$)

Propagation of the probability (flow of wave packet) :

$$\boldsymbol{j} = \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$$

Operation = observation :

de Broglie wave

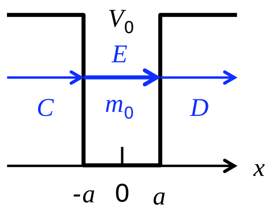
$$-\frac{\hbar^2}{2m}\nabla^2\psi = (E - V)\psi$$

operator   observed results

1D Quantum Well Potential

A de Broglie wave (particle with mass m_0) confined in a square well :

$$\begin{cases} \frac{\hbar^2}{2m_0}\frac{d^2\psi_1}{dx^2} + (E - V_0)\psi_1 = 0 & (x < -a) \\ \frac{\hbar^2}{2m_0}\frac{d^2\psi_2}{dx^2} + E\psi_2 = 0 & (-a < x < a) \\ \frac{\hbar^2}{2m_0}\frac{d^2\psi_3}{dx^2} + (E - V_0)\psi_3 = 0 & (a < x) \end{cases}$$



General answers for the corresponding regions are

$$\begin{cases} \psi_1 = Ce^{\beta x} + C_1e^{-\beta x} & (x < -a) \\ \psi_2 = A\sin\alpha x + B\cos\alpha x & (-a < x < a) \\ \psi_3 = De^{-\beta x} + D_1e^{\beta x} & (a < x) \end{cases} \qquad \begin{cases} \alpha = \frac{\sqrt{2m_0E}}{\hbar} \\ \beta = \frac{\sqrt{2m_0(V_0 - E)}}{\hbar} \end{cases}$$

Since the particle is confined in the well, $\psi_1, \psi_3 \to 0 \;\; (x \to \pm\infty)$

For $E < V_0$, $C_1 = 0, D_1 = 0$

1D Quantum Well Potential (Cont'd)

Boundary conditions :

At x = -a, to satisfy $\psi_1 = \psi_2$, $\quad -A\sin\alpha a + B\cos\alpha a = Ce^{-\beta a}$

$\psi_1' = \psi_2'$, $\quad \alpha A\cos\alpha a + \alpha B\sin\alpha a = \beta Ce^{-\beta a}$

At x = a, to satisfy $\psi_2 = \psi_3$, $\quad A\sin\alpha a + B\cos\alpha a = De^{-\beta a}$

$\psi_2' = \psi_3'$, $\quad \alpha A\cos\alpha a - \alpha B\sin\alpha a = -\beta De^{-\beta a}$

$$\therefore \begin{cases} 2A\sin\alpha a = (D-C)e^{-\beta a} \\ 2\alpha A\cos\alpha a = -\beta(D-C)e^{-\beta a} \\ 2B\cos\alpha a = (C+D)e^{-\beta a} \\ 2\alpha B\sin\alpha a = \beta(C+D)e^{-\beta a} \end{cases}$$

For $A \neq 0$, $D - C \neq 0$: $\quad \alpha\cot\alpha a = -\beta$

For $B \neq 0$, $D + C \neq 0$: $\quad \alpha\tan\alpha a = \beta$

For both $A \neq 0$ and $B \neq 0$: $\quad \tan^2\alpha a = -1 \;\rightarrow \alpha$: imaginary number

Therefore, either $A \neq 0$ or $B \neq 0$.

1D Quantum Well Potential (Cont'd)

(i) For $A = 0$ and $B \neq 0$, $C = D$ and hence,

$$\xi\tan\xi = \eta \quad (\alpha a = \xi,\ \beta a = \eta) \qquad (1)$$

(ii) For $A \neq 0$ and $B = 0$, $C = -D$ and hence,

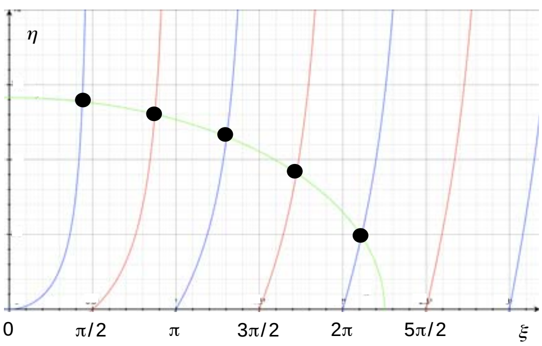
$$\xi\cot\xi = -\eta \qquad (2)$$

Here,

$$\alpha = \frac{\sqrt{2m_0E}}{\hbar},\ \beta = \frac{\sqrt{2m_0(V_0 - E)}}{\hbar}$$

$$\therefore \alpha^2 + \beta^2 = \frac{2m_0V_0}{\hbar^2}$$

$$\therefore \xi^2 + \eta^2 = \frac{2m_0V_0a^2}{\hbar^2} \qquad (3)$$

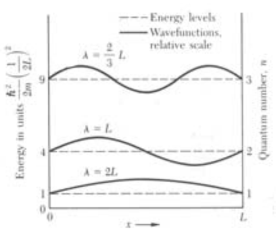


Therefore, the answers for ξ and η are crossings of the Eqs. (1) / (2) and (3).

Energy eigenvalues are also obtained as

$$E = \frac{\hbar^2}{2m_0a^2}\xi^2$$

→ Discrete states

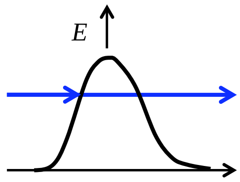


Quantum Tunneling

In classical theory,

Particle with smaller energy than the potential barrier

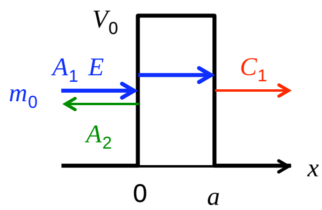
cannot pass through the barrier.



In quantum mechanics, such a particle have probability to tunnel.

For a particle with energy E ($< V_0$) and mass m_0,

Schrödinger equations are



$$\begin{cases} \dfrac{\hbar^2}{2m_0}\dfrac{d^2\psi}{dx^2} + E\psi = 0 & (x < 0,\ a < x) \\ \dfrac{\hbar^2}{2m_0}\dfrac{d^2\psi}{dx^2} + (E - V_0)\psi = 0 & (0 < a < x) \end{cases}$$

Substituting general answers $k_1 = \sqrt{2m_0 E}/\hbar$, $k_2 = \sqrt{2m_0(V_0 - E)}/\hbar$

$$\begin{cases} \psi = \boxed{A_1 \exp(ik_1 x)} + \boxed{A_2 \exp(-ik_1 x)} & (x < 0) \\ \psi = B_1 \exp(k_2 x) + B_2 \exp(-k_2 x) & (0 < a < x) \\ \psi = \boxed{C_1 \exp(ik_1 x)} + C_2 \exp(-ik_1 x) & (a < x) \end{cases}$$

Quantum Tunneling (Cont'd)

Now, boundary conditions are

$$\begin{cases} A_1 + A_2 = B_1 + B_2,\ ik_1(A_1 - A_2) = k_2(B_1 - B_2) & (x = 0) \\ B_1 \exp(k_2 a) + B_2 \exp(-k_2 a) = C_1 \exp(ik_1 a),\ k_2[B_1 \exp(k_2 a) - B_2 \exp(-k_2 a)] = ik_1 C_1 \exp(ik_1 a) & (x = a) \end{cases}$$

$$\therefore \begin{cases} \dfrac{C_1}{A_1} = \dfrac{4ik_1k_2 \exp(-ik_1 a)}{(k_2 + ik_1)^2 \exp(-k_2 a) - (k_2 - ik_1)^2 \exp(k_2 a)} \\ \dfrac{A_2}{A_1} = \dfrac{(k_1^2 + k_2^2)[\exp(k_2 a) - \exp(-k_2 a)]}{(k_2 - ik_1)^2 \exp(-k_2 a) - (k_2 + ik_1)^2 \exp(k_2 a)} \end{cases}$$

Now, transmittance T and reflectance R are

$$\begin{cases} T = \left|\dfrac{C_1}{A_1}\right|^2 = \dfrac{4k_1^2k_2^2}{(k_1^2 + k_2^2)^2 \sinh^2(k_2 a) + 4k_1^2k_2^2} = \dfrac{4E(V_0 - E)}{V_0^2 \sinh^2(a/2b) + 4E(V_0 - E)} \\ R = \left|\dfrac{A_2}{A_1}\right|^2 = \dfrac{(k_1^2 + k_2^2)^2 \sinh^2(k_2 a)}{(k_1^2 + k_2^2)^2 \sinh^2(k_2 a) + 4k_1^2k_2^2} = \dfrac{V_0 \sinh^2(a/2b)}{V_0^2 \sinh^2(a/2b) + 4E(V_0 - E)} \end{cases}$$

$$\left(b = \frac{\hbar}{2\sqrt{2m_0(V_0 - E)}} \right)$$

→ $T \neq 0$ (tunneling occurs) !

Quantum Tunneling (Cont'd)

For $V_0 - E >> \hbar^2 / 2m_0 a^2$

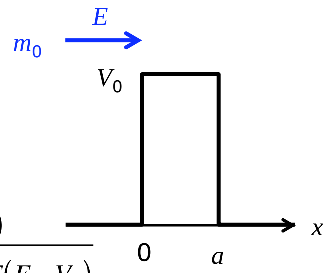
$$\therefore \hbar / a << \sqrt{2m_0(V_0 - E)}, \quad a/2b >> 1$$

$$\therefore V_0^{\,2}\sinh^2(a/2b) + 4E(V_0 - E) \approx V_0^{\,2}\sinh^2(a/2b) \approx V_0^{\,2}\exp(a/b) \approx V_0^{\,2}\exp\left(\frac{2\sqrt{2m_0(V_0 - E)}a}{\hbar}\right)$$

$$\therefore T \approx \frac{4E(V_0 - E)}{V_0^{\,2}}\exp\left(-\frac{2\sqrt{2m_0(V_0 - E)}a}{\hbar}\right)$$

→ T exponentially decrease with increasing a and (V_0 - E)

For $V_0 < E$, as k_2 becomes an imaginary number, k_2 should be substituted with



$$k_2' = \frac{\sqrt{2m_0(E - V_0)}}{\hbar} \quad (k_2 \rightarrow ik_2')$$

$$\begin{cases} T = \dfrac{4k_1^{\,2}k_2'^{\,2}}{\left(k_1^{\,2} - k_2'^{\,2}\right)^2 \sin^2(k_2' a) + 4k_1^{\,2}k_2'^{\,2}} = \dfrac{4E(E - V_0)}{V_0^{\,2}\sin^2(k_2' a) + 4E(E - V_0)} \\[2ex] R = \dfrac{\left(k_1^{\,2} + k_2'^{\,2}\right)^2 \sin^2(k_2' a)}{\left(k_1^{\,2} + k_2'^{\,2}\right)^2 \sin^2(k_2' a) + 4k_1^{\,2}k_2'^{\,2}} = \dfrac{V_0 \sin^2(k_2' a)}{V_0^{\,2}\sin^2(k_2' a) + 4E(E - V_0)} \end{cases}$$

→ $R \neq 0$!

Reflectance and Transmittance

At an energy level E, wave function is expressed as $\psi = \varphi(x)\exp(-iEt/\hbar)$

$$|\psi|^2 = |\varphi(x)|^2 \qquad \therefore \frac{\partial|\psi|^2}{\partial t} = \frac{\partial|\varphi(x)|^2}{\partial t} = 0$$

According to the equation of continuity : $\dfrac{\partial\rho}{\partial t} + \operatorname{div}\boldsymbol{j} = 0 \quad \left(\operatorname{div}\boldsymbol{j} = \dfrac{\partial j_x}{\partial x} + \dfrac{\partial j_y}{\partial y} + \dfrac{\partial j_z}{\partial z}\right)$

$$\operatorname{div}\boldsymbol{j} = 0$$

For 1D, $\dfrac{dj_x}{dx} = 0 \qquad \therefore j = j_x = \text{const.}$

At the incident side, the incident wave ψ_i and the reflection wave ψ_r satisfy

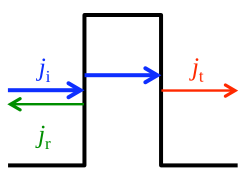
$$\psi = \psi_i + \psi_r \qquad \therefore j = j_i + |j_r|$$

Here, $j = \dfrac{\hbar}{2m_0 i}\left(\psi^*\psi' - \psi\psi^{*\prime}\right),\ j_i = \dfrac{\hbar}{2m_0 i}\left(\psi_i^{\,*}\psi_i' - \psi_i\psi_i^{\,*\prime}\right),\ j_r = \dfrac{\hbar}{2m_0 i}\left(\psi_r^{\,*}\psi_r' - \psi_r\psi_r^{\,*\prime}\right)$

At the transmission side, only the transmission wave ψ_t exists, and thus $j = j_t$

$$\therefore j_i + |j_r| = j_t \qquad \therefore j_i = j_t + |j_r|$$

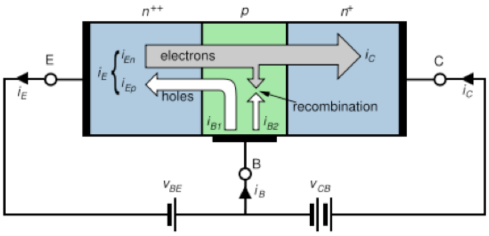
$$\therefore 1 = \frac{j_t}{j_i} + \frac{|j_r|}{j_i} \qquad \therefore 1 = T + R$$



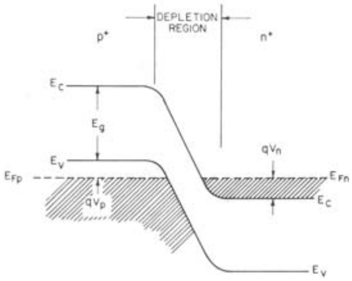
→ T : transmittance and R : reflectance
(j_t / j_i) (|j_r| / j_i)

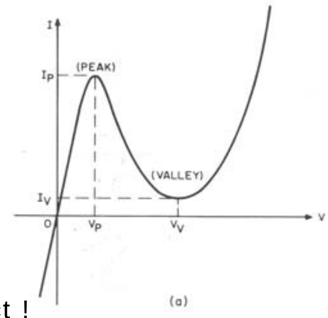
Transistor and Esaki Diode

First bipolar transistor (transfer resistor) was invented by J. Bardeen , W. Shockley and W. Brattainin 1947 :



Tunneling diode was invented by L. Esaki in 1958 :





→ First observation of tunneling effect !

* http://www.wikipedia.org/; http://photos.aip.org/;
** S. M. Sze, *Physics of Semiconductor Devices* (John Wiley, New York, 1981).

Absorption Coefficient

Absorption fraction A is defined as

$$A + R + T = 1$$

Here, $j_r = Rj_i$, and therefore $(1 - R)\ j_i$ is injected.

Assuming j at x becomes $j - dj$ at $x + dx$,

$$-dj = \alpha j dx \qquad (\alpha : \text{absorption coefficient})$$

With the boundary condition : at $x = 0$, $j = (1 - R)\ j_i$,

$$j = (1 - R)\ j_i \exp(-\alpha x)$$

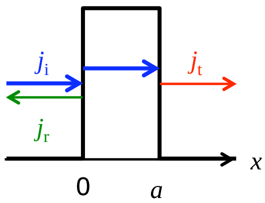
With the boundary condition : $x = a$, $j = (1 - R)\ j_i e^{-\alpha a}$,

part of which is reflected ; $R\ (1 - R)\ j_i\ e^{-\alpha a}$

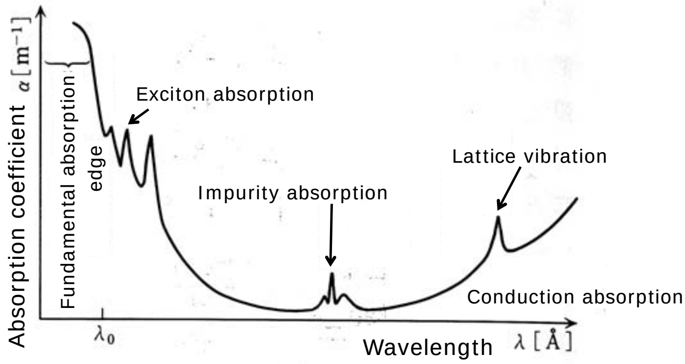
and the rest is transmitted ; $j_t = [1 - R - R\ (1 - R)]\ j_i\ e^{-\alpha a}$

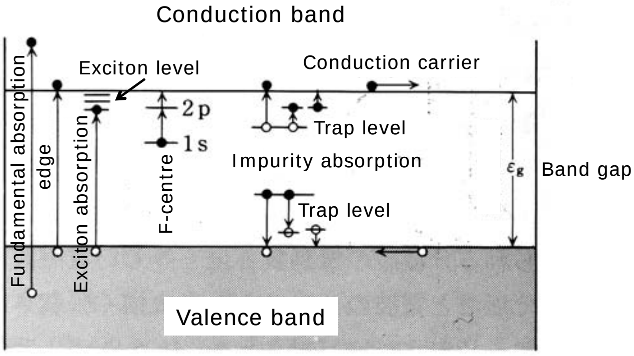
$$j_t = (1 - R)^2\ j_i \exp(-\alpha x)$$

$$\therefore T = \frac{j_t}{j_i} = (1 - R)^2 \exp(-\alpha x)$$



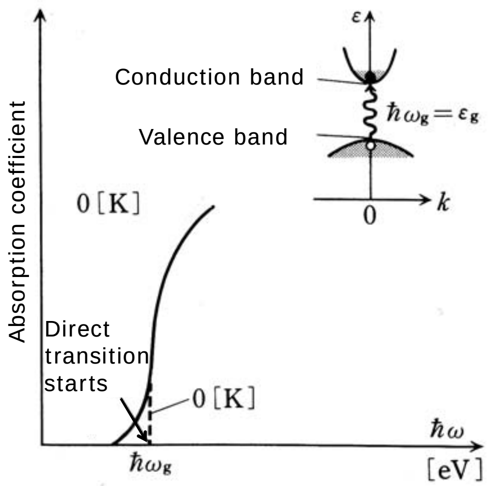
Optical Absorption

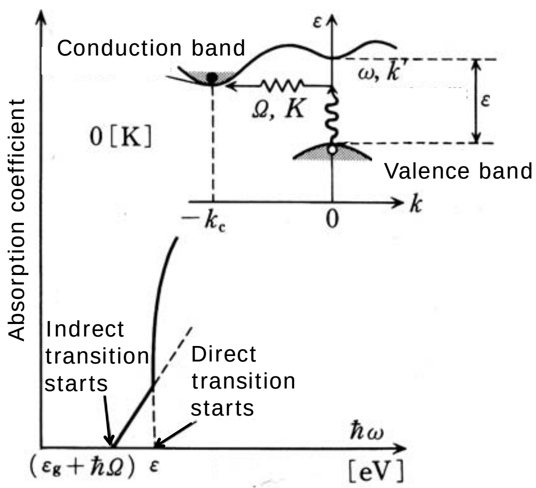




* M. Sakata, *Solid State Physics* (Baifukan, Tokyo, 1989).

Semiconductor Band Gap





Excited electrons will be recombine with holes with emitting photon.

→ Light emitting diode (LED)

* M. Sakata, *Solid State Physics* (Baifukan, Tokyo, 1989).

Semiconductor Band Gap in Si, Ge and GaAs

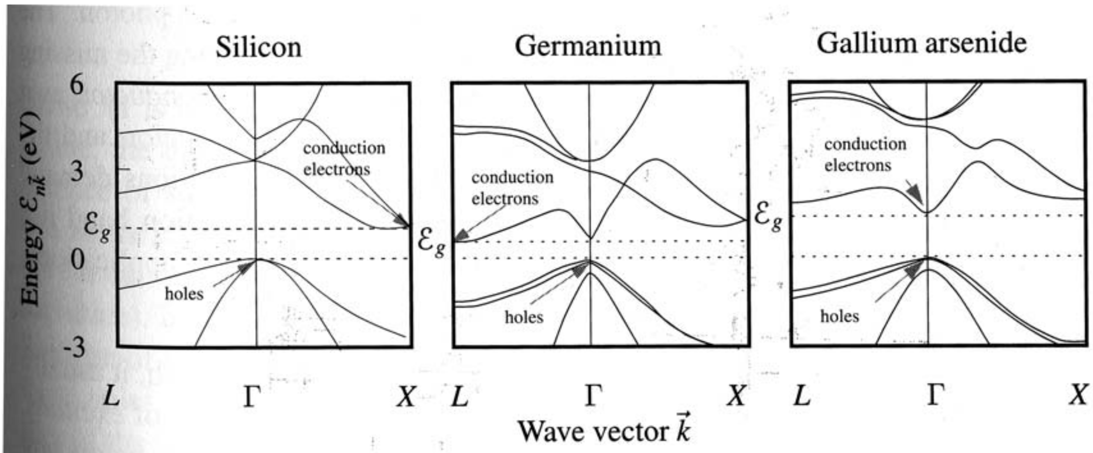
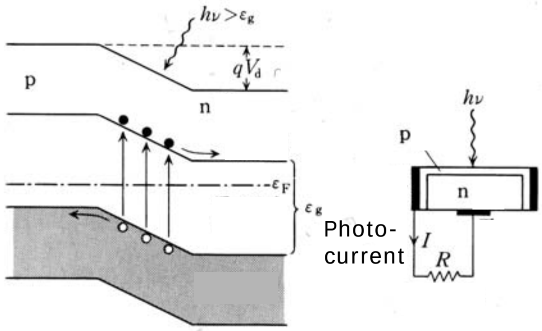


Figure 19.8. Essential features of band structures of silicon, germanium, and gallium arsenide. All have band gaps on the order of 1 eV. The bottom of the conduction band for silicon and germanium does not lie at Γ, so these materials have an indirect gap. Gallium arsenide, by contrast, has a direct gap. These diagrams are extracted from Figures 23.15 and 23.16, which contain information on how they were obtained.

* M. P. Marder, *Condensed Matter Physics* (John-Wiley, New York, 2000).

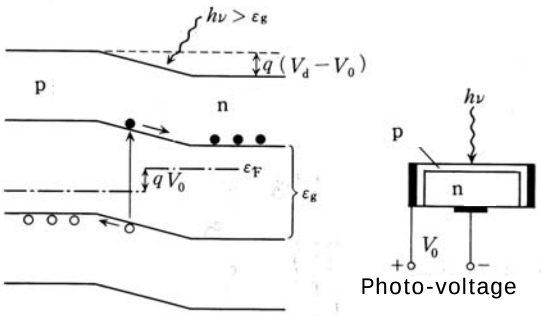
Photo Diode

Photovoltaic effect :



→ Photo diode

Direct energy conversion



→ Solar cell

* M. Sakata, *Solid State Physics* (Baifukan, Tokyo, 1989).