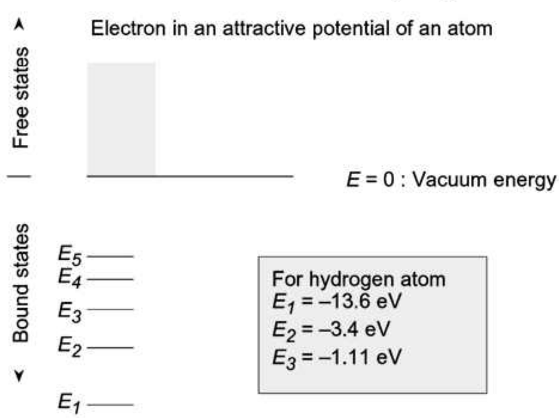
# Introduction to Solid State Physics

**Class: Integrated Photonic Devices**
**Time: Fri. 8:00am ~ 11:00am.**
**Classroom: 資電206**
**Lecturer: Prof. 李明昌(Ming-Chang Lee)**



# Electrons in An Atom

- Before examining electrons in a solid, let us examine electronic states in an atom. Let us first examine a hydrogen atom.



## Electrons in An Atom

Allowed energy levels:

$$E_n = \frac{-me^4}{2(4\pi\varepsilon_0)^2\hbar^2 n^2} = \frac{13.6}{n^2}\ \text{eV}$$

Wavefunctions:

$\psi n\ell m$: $n$: principle quantum number.

$\ell$: orbital quantum number; angular momentum of the electron $= \ell\hbar$.

$m$: magnetic quantum number; projection of the angular momentum; $m$ lies between $-\ell$ and $+\ell$.



## Electrons in Two atoms

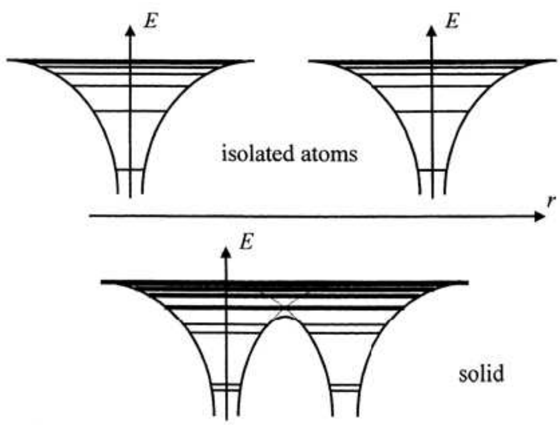
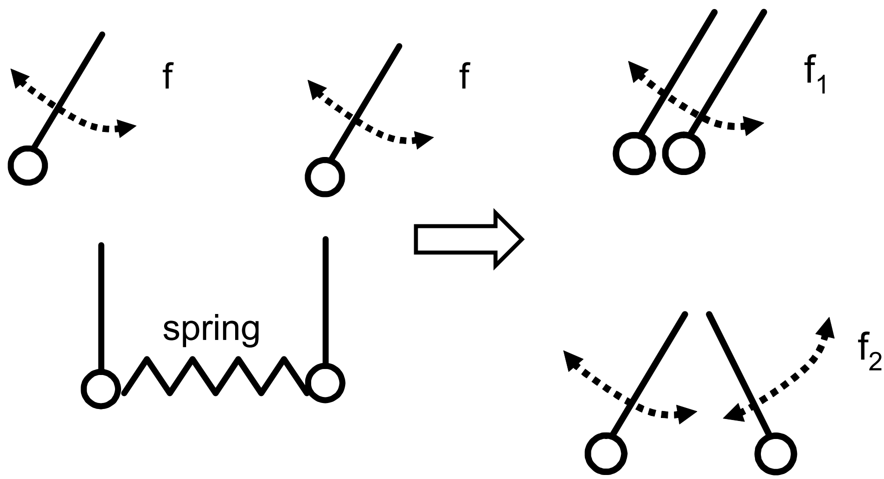


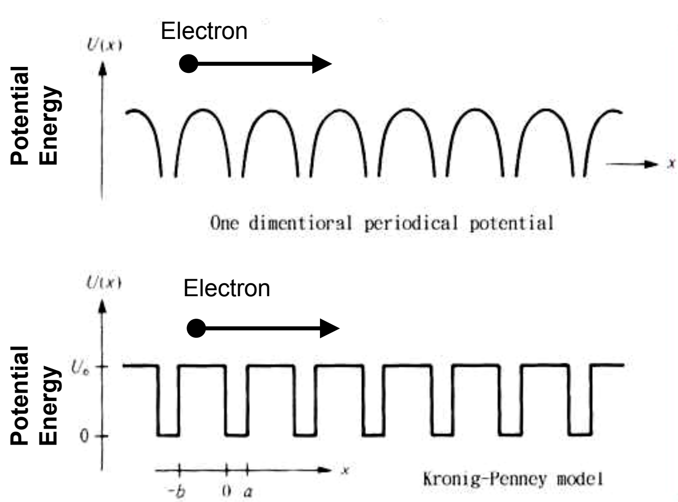

*Fig. 4.10. Change in energy spectrum from single atoms to a solid. Each of the discrete energy levels in two isolated atoms split into two separate energy levels when the atoms are bound in a solid.*

## Analogy to A Coupled Two-Pendulum System



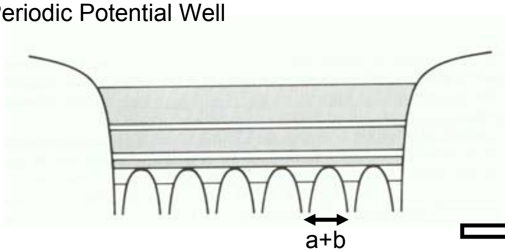



## One-dimensional Kronig-Penney Model

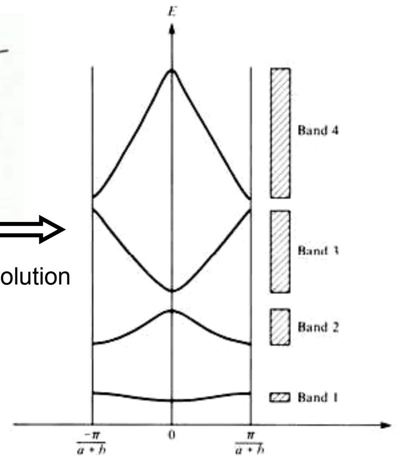


# Solutions of the S.E. in Kronig-Penny Model

Periodic Potential Well




solution




E-k diagram

Schrödinger's equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi+\left(U(x)-E\right)\Psi=0$$

Bloch Theorem

If $U[x+(a+b)]=U(x)$

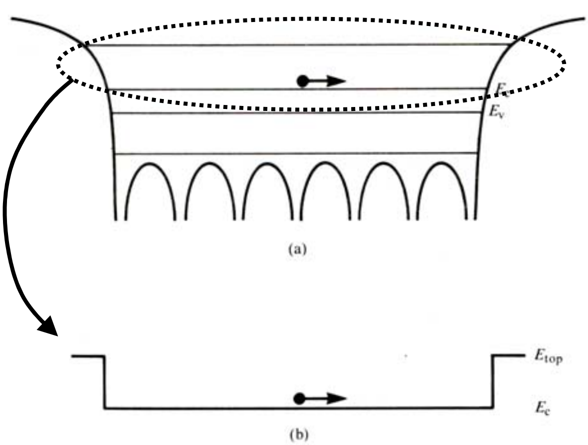
Then $\Psi(x)=\exp(jk\cdot x)u(x)$

where $u[x+(a+b)]=u(x)$



# Density of States as a function of k and E

- **For electrons near the bottom of the band, the band itself form a pseudo-potential well. The well bottom lies at $E_c$ and the termination of the band at the crystal surfaces forms the walls of the well**



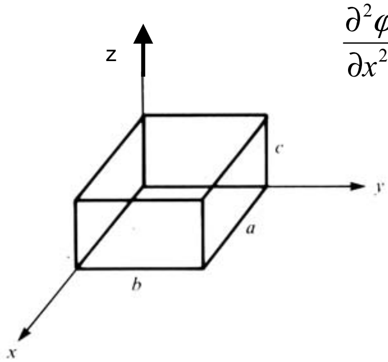
# Density of States as a function of k and E

- **The density of states near the band edges can therefore be equal to the density of states available to a particle of mass m* in a three dimension box with the dimension of the crystal**

$U(x) = 0$ except boundary

**(Time-independent S.E.)**

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} + k^2 \varphi = 0 \quad \text{(a)}$$




$$0 < x < a,\ 0 < y < b,\ 0 < z < c$$

Boundary

$$k \equiv \sqrt{2mE/\hbar^2}$$

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



# Density of States as a function of k and E

- **To solve the equation, we employ the separation of variables technique; that is**

$$\varphi(x, y, z) = \varphi_x(x)\varphi_y(y)\varphi_z(z) \quad \text{(b)}$$

- **Substitute (b) to (a)**

$$\frac{1}{\varphi_x}\frac{d^2\varphi_x}{dx^2} + \frac{1}{\varphi_y}\frac{d^2\varphi_y}{dy^2} + \frac{1}{\varphi_x}\frac{d^2\varphi_z}{dz^2} + k^2 = 0$$

$$\boxed{\frac{1}{\varphi_x}\frac{d^2\varphi_x}{dx^2} = \textbf{constant} = -k_x^{\ 2}}$$

$$\varphi(x, y, z) = A \sin k_x x \cdot \sin k_y y \cdot \sin k_z z$$

(Solution)

where $$k^2 = k_x^{\ 2} + k_y^{\ 2} + k_z^{\ 2}$$

$$k_x = \frac{n_x \pi}{a}; k_y = \frac{n_y \pi}{b}; k_z = \frac{n_z \pi}{c} \qquad n_x, n_y, n_z = \pm 1, \pm 2, \pm 3, \ldots$$

# Density of States as a function of k and E

**- Densities of states in k-space**

A unit cell of volume:

$$(\frac{\pi}{a})(\frac{\pi}{b})(\frac{\pi}{c})$$

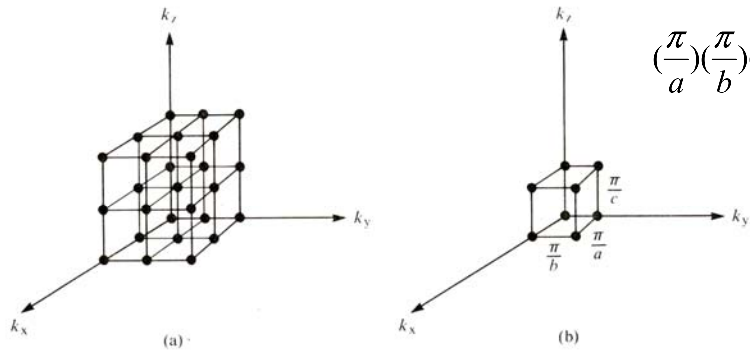



**Fig. 4.3** (a) *k*-space representation of Schrödinger equation solutions for a particle in a crystal-sized three-dimensional box. (b) *k*-space unit cell for solution points.

- **The larger the a,b and c, the smaller the unit cell volume**



# Density of States as a function of k and E

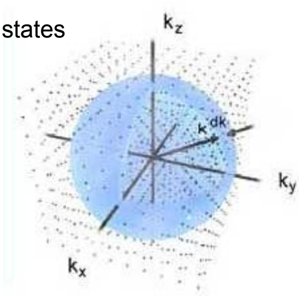
- **How many states are within k and k+dk?**

spin up and down

$$\sigma(k)dk \equiv \begin{pmatrix} Energy\ states\ with\ k \\ between\ k\ and\ k+dk \end{pmatrix} = \frac{abc}{\pi^3}\cdot(4\pi k^2)\cdot\frac{1}{8}\cdot 2\cdot dk$$

Density of states

Redundancy



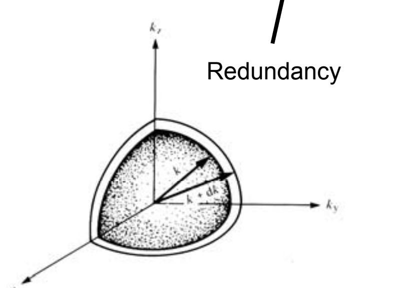



**Fig. 4.4** *k*-space spheres of radius *k* and *k* + *dk* used to determine the allowed electronic states in an incremental *dk* range.

## Density of States as a function of k and E

- **How many states are within E and E+dE?**

$$\sigma(E)dE = \sigma(k)dk \longrightarrow \sigma(E) = \sigma(k)\frac{dk}{dE}$$

**From the previous equation,**

$$E = \frac{\hbar^2 k^2}{2m} \longrightarrow \frac{dE}{dk} = \frac{\hbar^2 k}{m} \qquad \text{Therefore} \quad \sigma(E) = (abc)\frac{m\sqrt{2mE}}{\pi^2\hbar^3}$$

**Density of states per unit volume**

$$\rho(E) = \sigma(E)/V = (abc)\frac{m\sqrt{2mE}}{\pi^2\hbar^3}/V = \frac{m\sqrt{2mE}}{\pi^2\hbar^3}$$

$$V = abc$$



## Electrons and Holes in Semiconductors

Electric Field

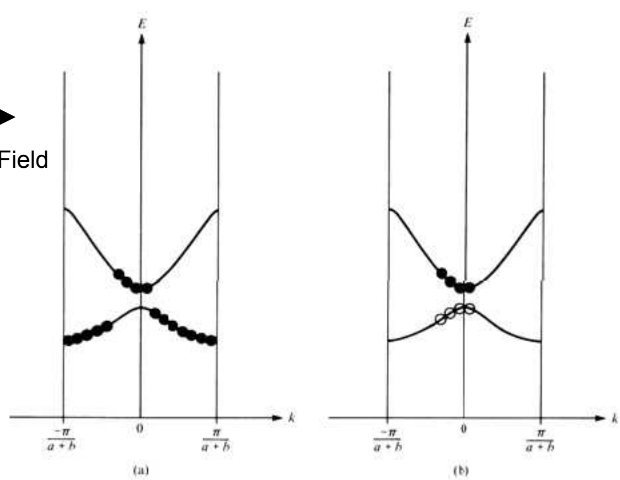


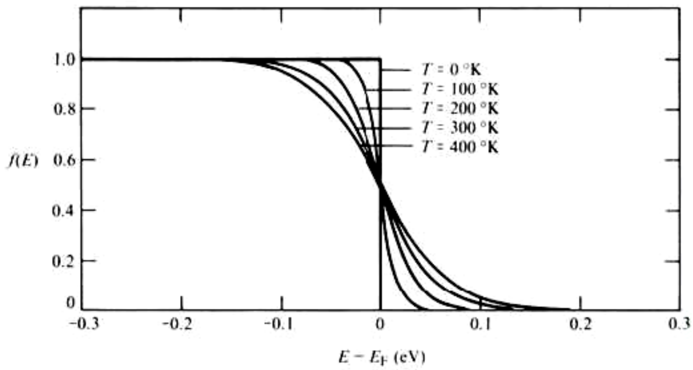

**Fig. 3.11** (a) The skewed filled-state distribution under steady-state conditions subsequent to the application of an external force. (b) Introduction of the hole. Alternative description of the electronic configuration in the lower energy band.

# Electron Distribution Functions

**The probability density function of electron residing in energy level E can be represented by Fermi-Dirac distribution**

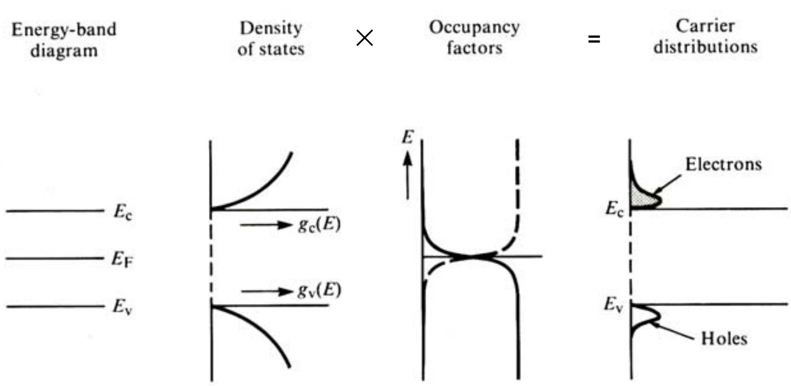
$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$

where $E_F$: Fermi Energy Level






# Carrier Density Distribution of Intrinsic Semiconductors




(b) $E_F$ near midgap

# Metal, Insulator, and Semiconductor

Metal Metal Insulator Semiconductor

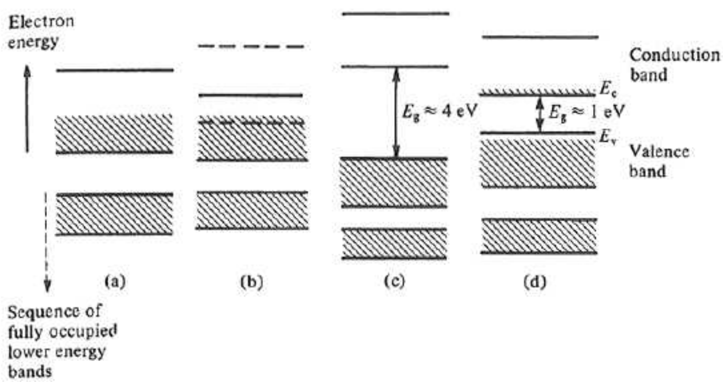



FIG. 2.7 Schematic representation of the energy bands in various materials: (a) a metal with partially filled valence band, e.g. monovalent metals; (b) a metal with two overlapping partially filled bands, e.g. divalent metals; (c) an insulator; and (d) an intrinsic semiconductor. In this, and succeeding diagrams, shading is used to signify occupied electron energy levels.



# Work Function

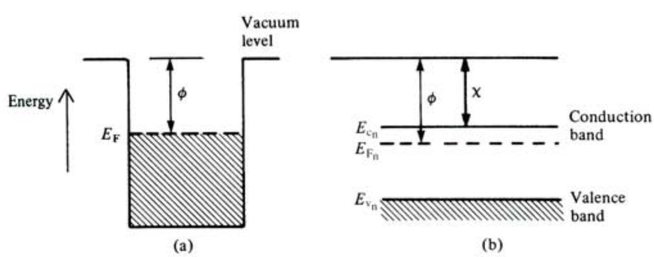
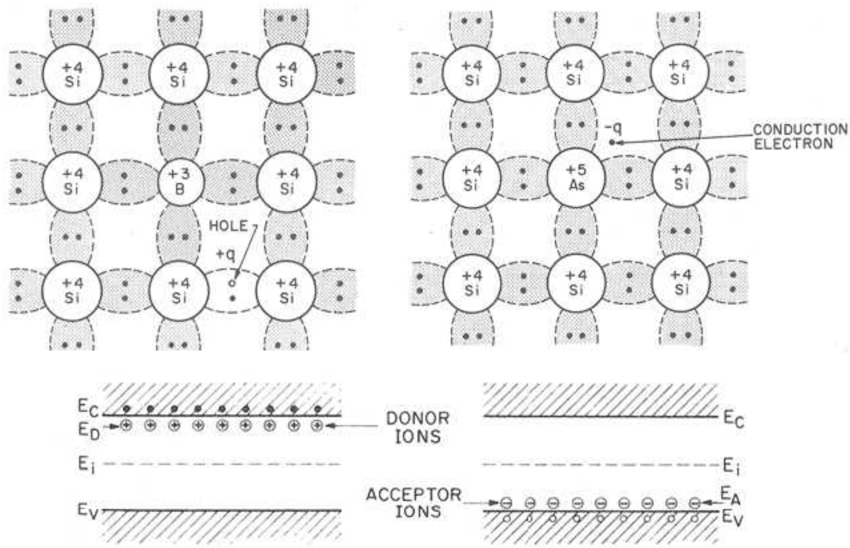



FIG. 2.17 Diagram showing the work function of (a) a metal and (b) an n-type semiconductor.

- **Work function is the minimum energy required to enable an electron to escape from the surface of solid.**
- **Work function $\varphi$ is the energy difference between Fermi level and the vacuum level.**
- **In semiconductors, it is more usual to use the electron affinity $\chi$, defined as the energy difference between the bottom of the conduction band and the vacuum level.**

# Extrinsic Semiconductors

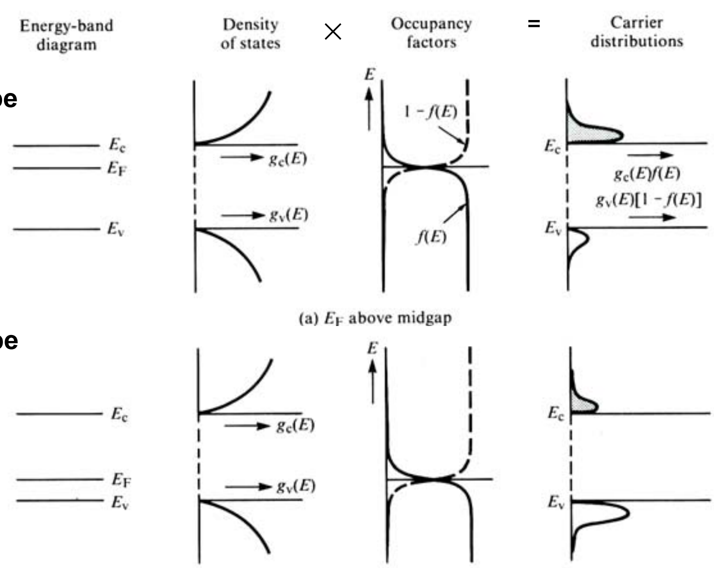





# Carrier Density Distribution of Extrinsic Semiconductors

**n-type**

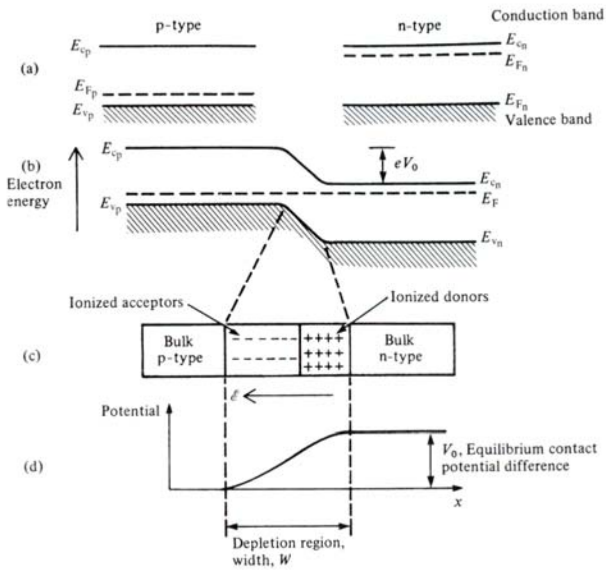
**p-type**




(a) $E_F$ above midgap

(c) $E_F$ below midgap

# p-n Junction




(a). Initially separated p-type and n-type semiconductor;

(b) the energy band distortion after the junction is formed;

(c) the space charge layers of ionized impurity atoms within the depletion region W; and

(d) the potential distribution at the junction.



# Contact Potential on p-n junction

- **Contact potential $V_0$**

**The electron concentration in the conduction band of p-type side as**

$$n_p = N_c \exp\left[-\left(\frac{E_{C_p} - E_{F_p}}{kT}\right)\right]$$

**Similarly the electron concentration in the n-type side is**

$$n_n = N_c \exp\left[-\left(\frac{E_{C_n} - E_{F_n}}{kT}\right)\right]$$

**Since the Fermi level is constant.** $E_{F_n} = E_{F_p} = E_F$

$$E_{C_p} - E_{C_n} = kT \ln\left(\frac{n_n}{n_p}\right) = eV_0 \rightarrow V_0 = \frac{kT}{e}\ln\left(\frac{n_n}{n_p}\right)$$

## Minority Carrier Distribution

• At the temperature in the range of 100K ≤ T ≤ 400K, the majority carrier concentrations are equal to the doping levels, that is $P_p = N_a$ and $n_n = N_d$ ,

$$V_0 = \frac{kT}{e} \ln\left(\frac{N_a N_d}{n_i}\right) \quad \text{(recall } np = n_i^2 \text{ )}$$

• Carrier concentration difference between p- and n-type semiconductor

$$n_p = n_n \exp\left[-\frac{eV_0}{kT}\right]$$

and

$$p_n = p_p \exp\left[-\frac{eV_0}{kT}\right]$$



## Current flow in a forward-biased p-n junction

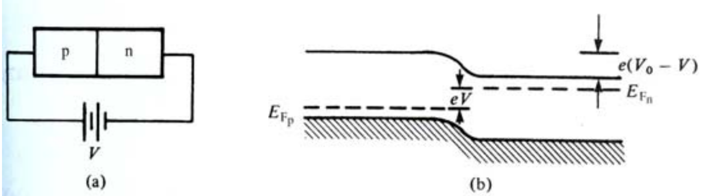



FIG. 2.21 Forward bias voltage V applied to a p–n junction (a) and the resulting energy band structure (b).

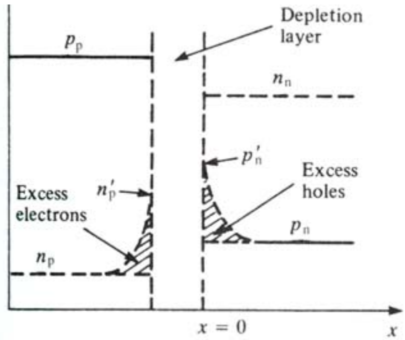
• The junction is said to be forward biased if the p region is connected to the positive terminal of the voltage source

• The external voltage is dropped across the depletion region and lower down the potential barrier by ($V_0$-V). So the diffusion current becomes larger than the drift current. There is a net current from the p to the n region.

• The Fermi levels are no longer aligned across the junction in light of the external voltage.

# Current flow in a forward-biased p-n junction

**Carrier densities**




- **Once the majority carriers flow across depletion region, they become minority carriers. The minority concentrations near the junction rise to new value $n_p$' and $p_n$'. The majority carrier concentration is almost unchanged unless a large current injection**
- **Due to the minority concentration gradient, the injected current diffuses away from the junction. The nonlinear gradient indicates minority holes (electrons) are recombined with electrons (holes) that are replenished by external voltage source.**



# Current flow in a forward-biased p-n junction

- **The injected carrier concentration at the edge of depletion region**

$$n_p' = n_n \exp\left[-\frac{e(V_0 - V)}{kT}\right]$$

$$p_n' = p_p \exp\left[-\frac{e(V_0 - V)}{kT}\right]$$

**Since**

$$p_n = p_p \exp\left[-\frac{eV_0}{kT}\right] \quad \text{and} \quad n_p = n_n \exp\left[-\frac{eV_0}{kT}\right]$$

**Then**

$$p_n' = p_n \exp\left[\frac{eV}{kT}\right] \quad \text{and} \quad n_p' = n_p \exp\left[\frac{eV}{kT}\right] \qquad \text{(a)}$$

## Current flow in a forward-biased p-n junction

**As we noted in previous slides, the excess minority carrier concentration will decrease due to recombination**

$$\Delta p(x) = \Delta p(0)\exp(-\frac{x}{L_h})$$

**where** $\Delta p(x) = p_n'(x) - p_n$

**Therefore, from (a)**

$$\Delta p(0) = p_n\left[\exp\left(\frac{eV}{kT}\right) - 1\right]$$



## Current flow in a forward-biased p-n junction

- **The diffusion current**

$$J_h = \frac{eD_h}{L_h}\Delta p(0)\exp(-\frac{x}{L_h})$$

**At x = 0**

$$J_h = \frac{eD_h}{L_h}p_n\left[\exp(\frac{eV}{kT}) - 1\right]$$

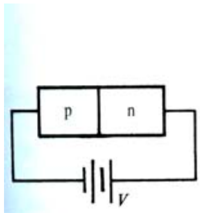
**Similarly, for electron diffusion current at the depletion edge**

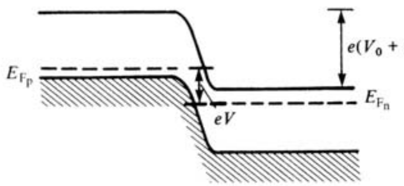
$$J_e = \frac{eD_e}{L_e}n_p\left[\exp(\frac{eV}{kT}) - 1\right]$$

**The total current**

$$J = J_0\left[\exp\left(\frac{eV}{kT}\right) - 1\right]$$ **where** $$J_0 = e\left(\frac{D_h}{L_h}p_n + \frac{D_e}{L_e}n_p\right)$$

## Current flow in a reverse-biased p-n junction




(b)

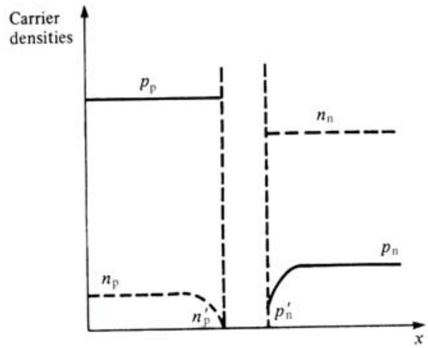



FIG. 2.24 Carrier densities in the bulk regions of a reverse-biase extraction the minority carrier densities close to the depletion lay

$$J = J_0\left[\exp\left(\frac{eV}{kT}\right) - 1\right]$$ V is negative



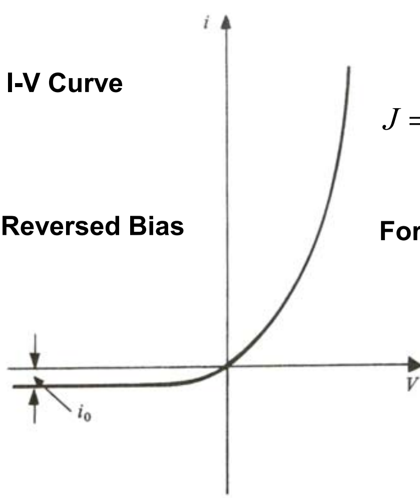
## I-V curves of p-n junction

**I-V Curve**

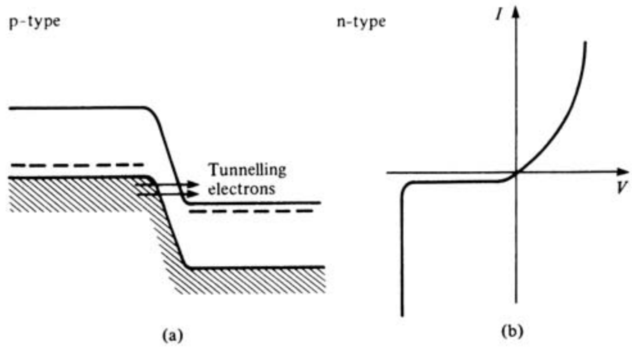
$$J = J_0\left[\exp\left(\frac{eV}{kT}\right) - 1\right]$$

**Reversed Bias**

**Forward Bias**



## Zener Breakdown

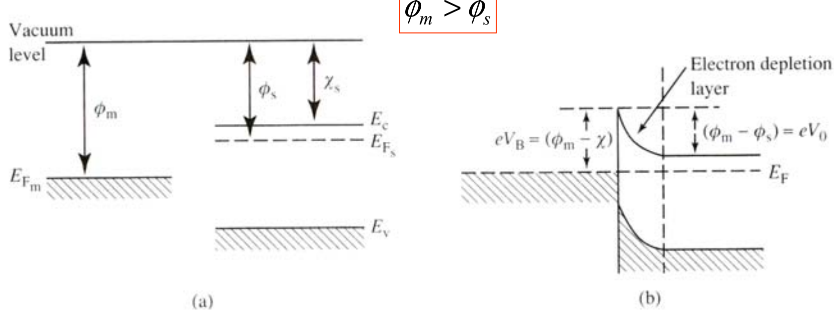



•Tunnelling of carriers across the depletion region and the process is independent of temperature
•Doping densities must be high to occur before avalanching
•Breakdown current is independent of voltage



## Metal-semiconductor Junction --- Schottky Contact

$$\boxed{\phi_m > \phi_s}$$




**A schottky barrier formed by contacting a metal to an n-type semiconductor with the metal having the larger work function: band diagrams (a) before and (b) after the junction is formed.**

# Work Function of Metal

Table 8.1 Work functions of some elements

| Element | Work Function, $\phi_m$ |
|---|---|
| Ag, silver | 4.26 |
| Al, aluminum | 4.28 |
| Au, gold | 5.1 |
| Cr, Chromium | 4.5 |
| Mo, molybdenum | 4.6 |
| Ni, nickel | 5.15 |
| Pd, palladium | 5.12 |
| Pt, platinum | 5.65 |
| Ti, titanium | 4.33 |
| W, tungsten | 4.55 |

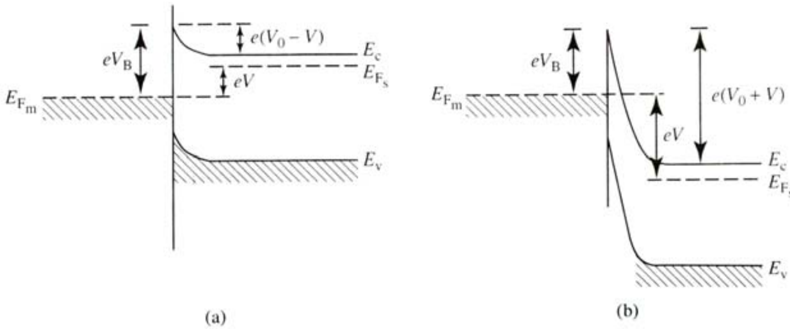


# Electron Affinity of Semiconductor

Table 8.2 Electron affinity of some semiconductors

| Element | Electron Affinity, $\chi$ |
|---|---|
| Ge, germanium | 4.13 |
| Si, silicon | 4.01 |
| GaAs, gallium arsenide | 4.07 |
| AlAs, aluminum arsenide | 3.5 |

# Metal-semiconductor Junction --- Schottky Contact




**The metal to n-type semiconductor junction shown under (a) forward bias and (b) reverse bias.**



# Metal-semiconductor Junction --- Ohmic Contact

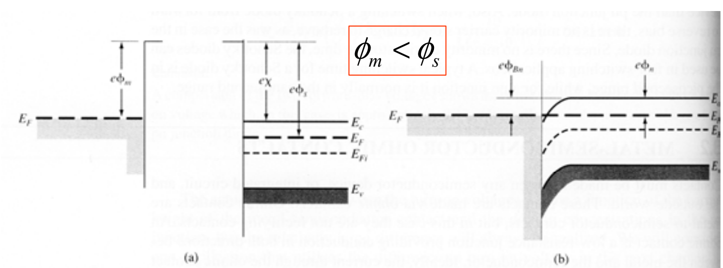



**Figure 8.11** Ideal energy-band diagram (a) before contact and (b) after contact for a metal–n-semiconductor junction for $\phi_m < \phi_s$

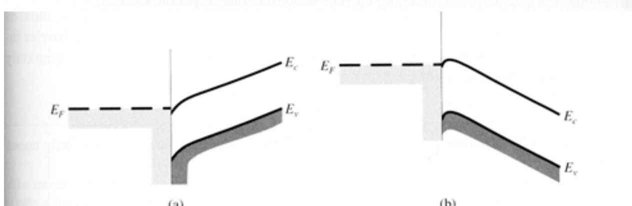
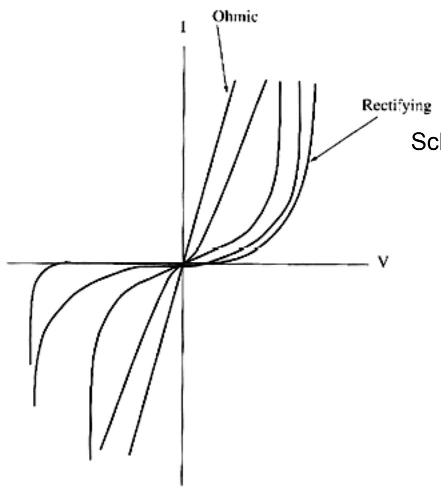



**Figure 8.12** Ideal energy-band diagram of a metal–n-semiconductor ohmic contact (a) with a positive voltage applied to the metal and (b) with a positive voltage applied to the semiconductor

# Summary of Metal-semiconductor Junction Contact




Schottly



# p-N heterojunction

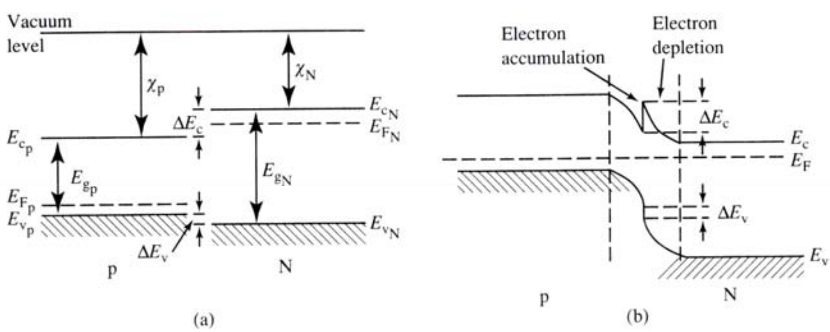



**FIG. 2.28** A p–N heterojunction: (a) shows the energy bands of the semiconductors separately; (b) show the energy bands after junction formation. (For a GaAs/$Ga_{0.3}Al_{0.7}As$ heterojunction, $E_{g_p}$ = 1.43 eV,

# n-P heterojunction

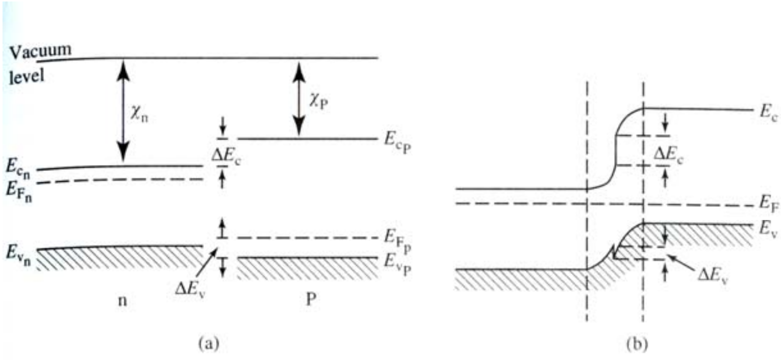
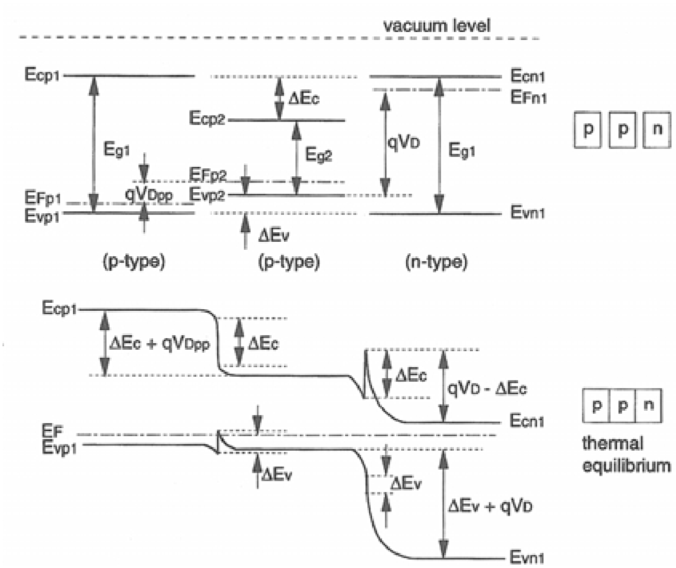



FIG. 2.29 An n–P heterojunction before (a) and after (b) junction formation.



# Double Heterojunctions



# Carriers Confined in Double Heterojuncitons

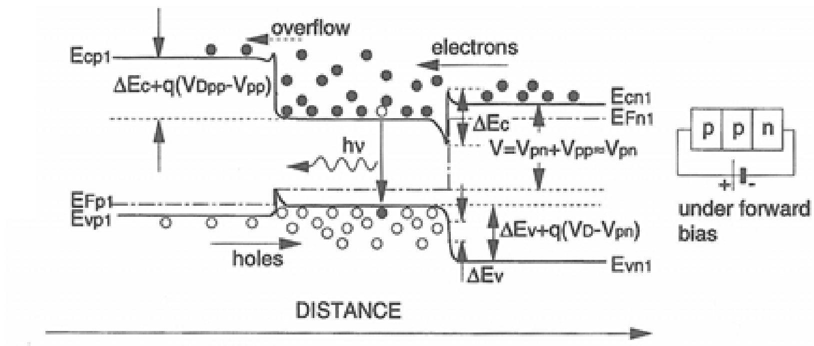



FIGURE 1.47 Energy band diagram of a double heterostructure.

**It is extremely efficient to enhance electron-hole recombination**



# Fundamentals of Electromagnetic Waves

| | | |
|---|---|---|
| Electrical field | $\vec{E}(r,t)$ | V/m |
| Electrical displacement | $\vec{D}(r,t)$ | C/m$^2$ |
| Magnetic field | $\vec{H}(r,t)$ | A/m |
| Magnetic induction | $\vec{B}(r,t)$ | webers/m$^2$ |

space time

- **E and B are fundamental fields**
- **D and H are derived from the response of the medium**
- **How many variables in Electromagnetic Wave?**