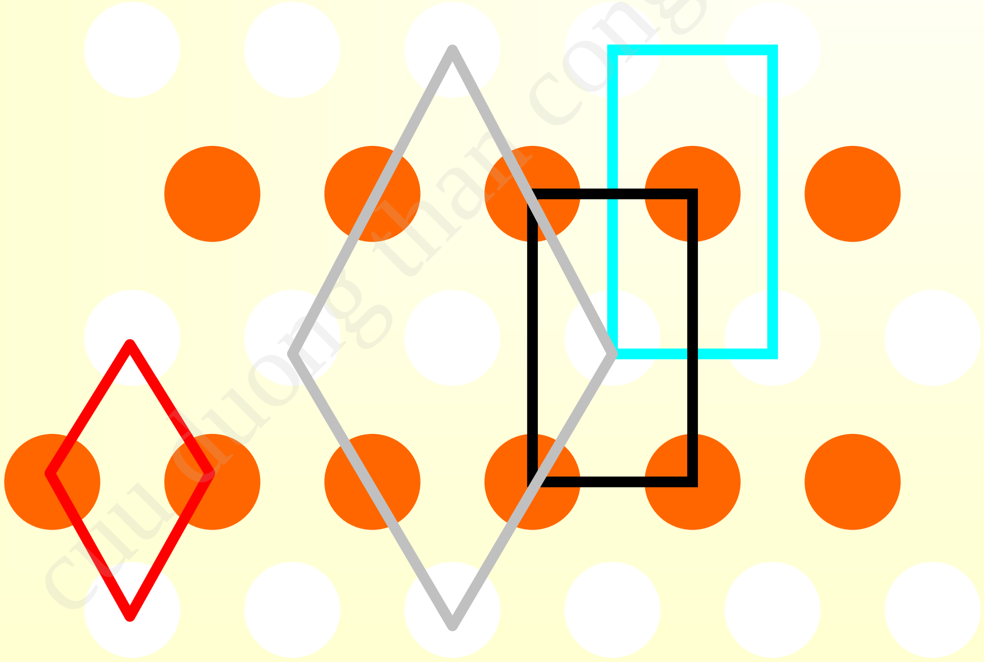
2. Technical Review – Materials

Crystal structure

❑ Basics

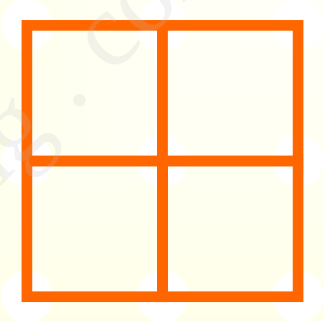
- A crystal is a repeating array
  = lattice + unit cell
- Lattice: pattern of repetition; point with identical surroundings for periodic stacking
- Unit cell: what is repeated; the simplest choice for a representative structural unit
- Lattice constant: length of unit cell edges (a, b, c) and angles between crystallographic axes (α, β, γ)

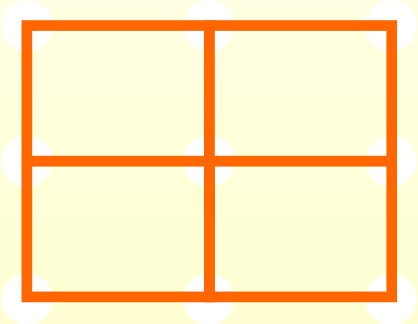
Example



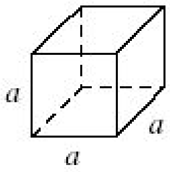
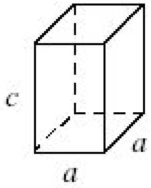
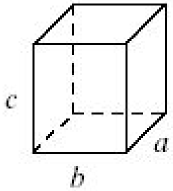
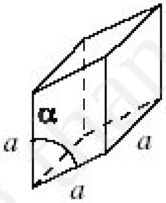
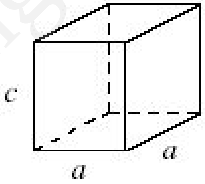
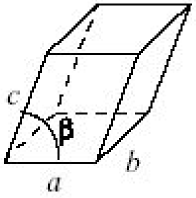
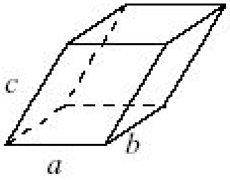
Point lattices for 2-D crystal

- Simple square
- Simple rectangle
- ____________________
- ____________________
- ____________________



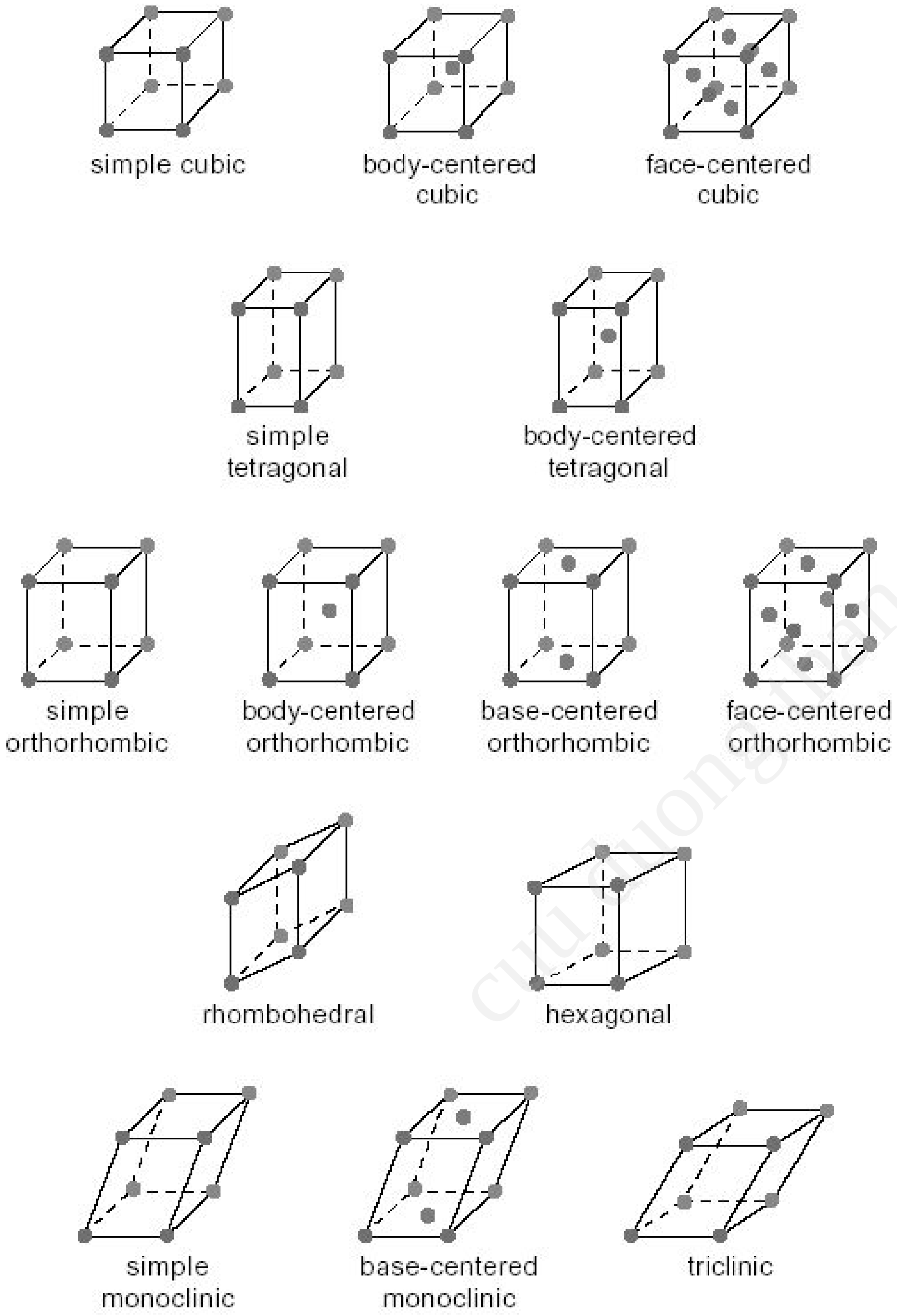


7 crystal systems

cubic	$a = b = c$, $\alpha = \beta = \gamma = 90°$	
tetragonal	$a = b \neq c$, $\alpha = \beta = \gamma = 90°$	
orthorhombic	$a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$	
rhombohedral	$a = b = c$, $\alpha = \beta = g \neq 90°$	
hexagonal	$a = b \neq c$, $\alpha = \beta = 90°$, $g = 120°$	
monoclinic	$a \neq b \neq c$, $\alpha = \gamma = 90°$, $b \neq 90°$	
triclinic	$a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$	

There are only seven unique unit cell shapes to fill 3-D space

14 Bravais lattices



There are only 14 ways to arrange lattice points in 3-D space

Indices of crystals

- Point

xyz or (x,y,z) along a,b and c axis

e.g. 100, 111, ½½½, (1,0,0)

- Direction

<hkl> family of directions

[hkl] individual direction

Use the smallest integer positions

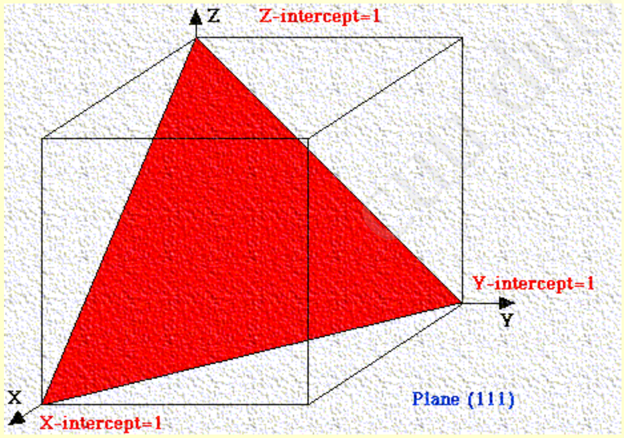
<111> = [111], [111], [ ], [ ], [ ], [ ], [ ], [ ]

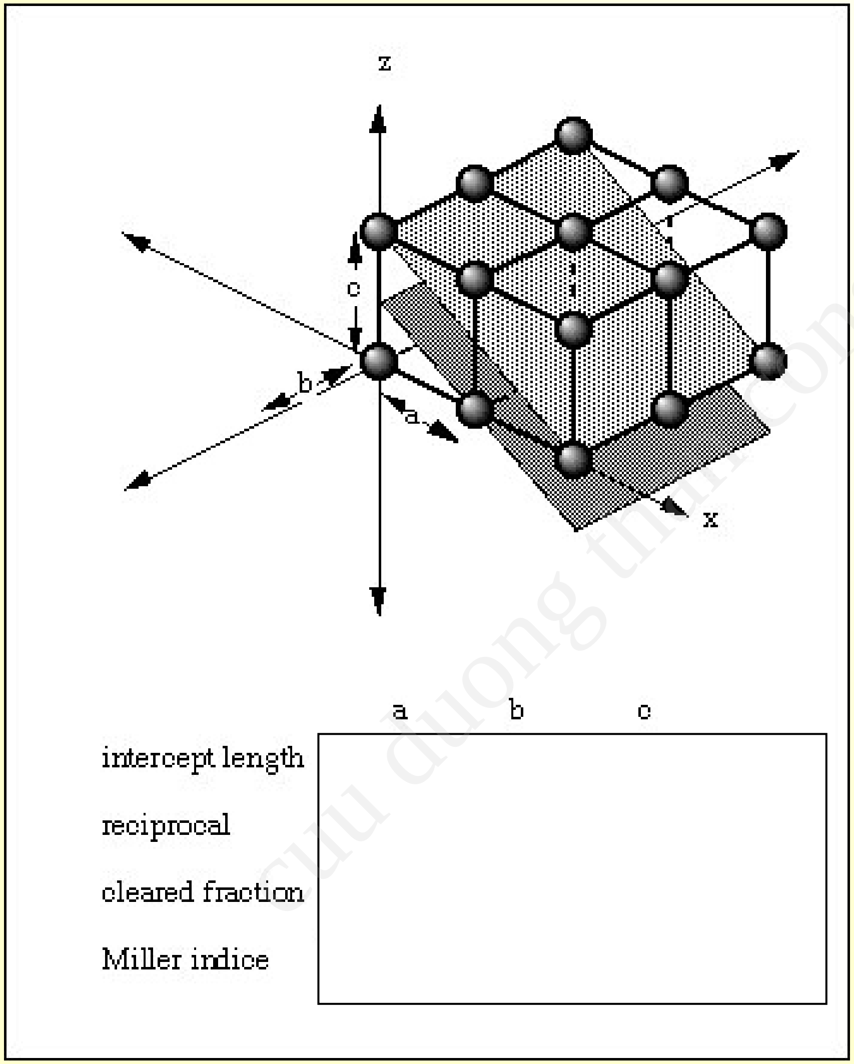
- ❑ Plane

{hkl} family of planes: integer representing inverse of axial intercept

(hkl) individual plane: Miller indices expressed by the inverse of axial intercept

(hklm) for hexagonal system: Miller-Bravais indices



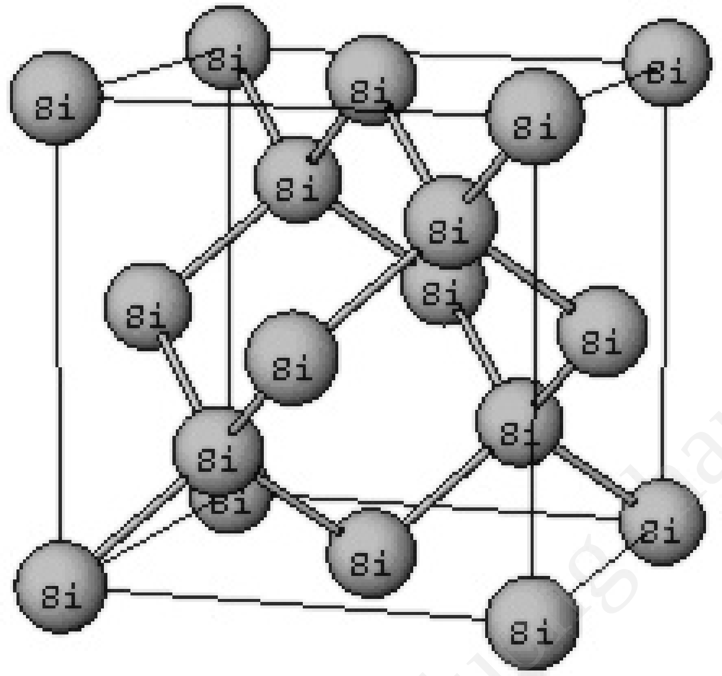

z
c
b
a
x
a
b
c
intercept length
reciprocal
cleared fraction
Miller indice

Cubic system

- Angle between [hkl] and [mnp]

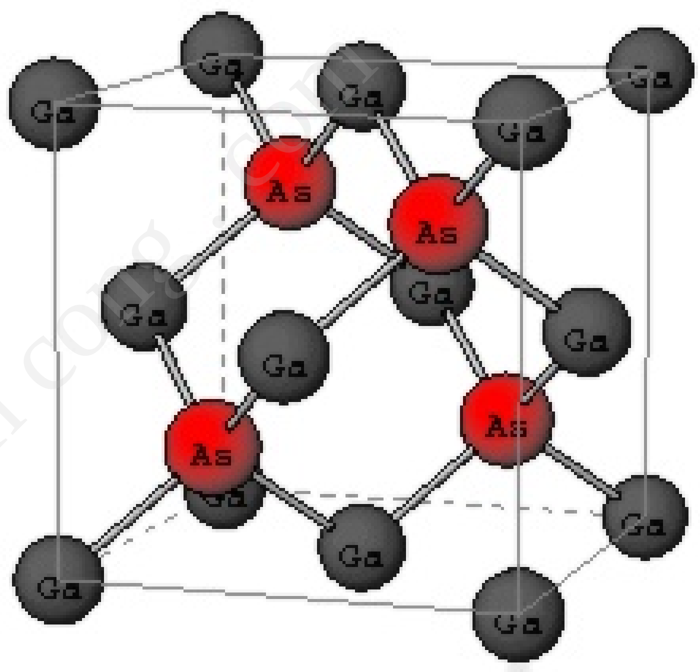
$$\cos\theta = \frac{(hm + kn + lp)}{\sqrt{(h^2+k^2+l^2)}\,\sqrt{(m^2+n^2+p^2)}}$$

- (hkl) $\perp$ [hkl]
- $d_{hkl} = a / \sqrt{(h^2+k^2+l^2)}$



Diamond (Si, Ge, C)

Interpenetrating FCC (1/4a offset)



Zincblende (GaAs, GaP)

Sublattice of Ga and As

from http://www.numis.nwu.edu/internet/Staff/el_picts.html

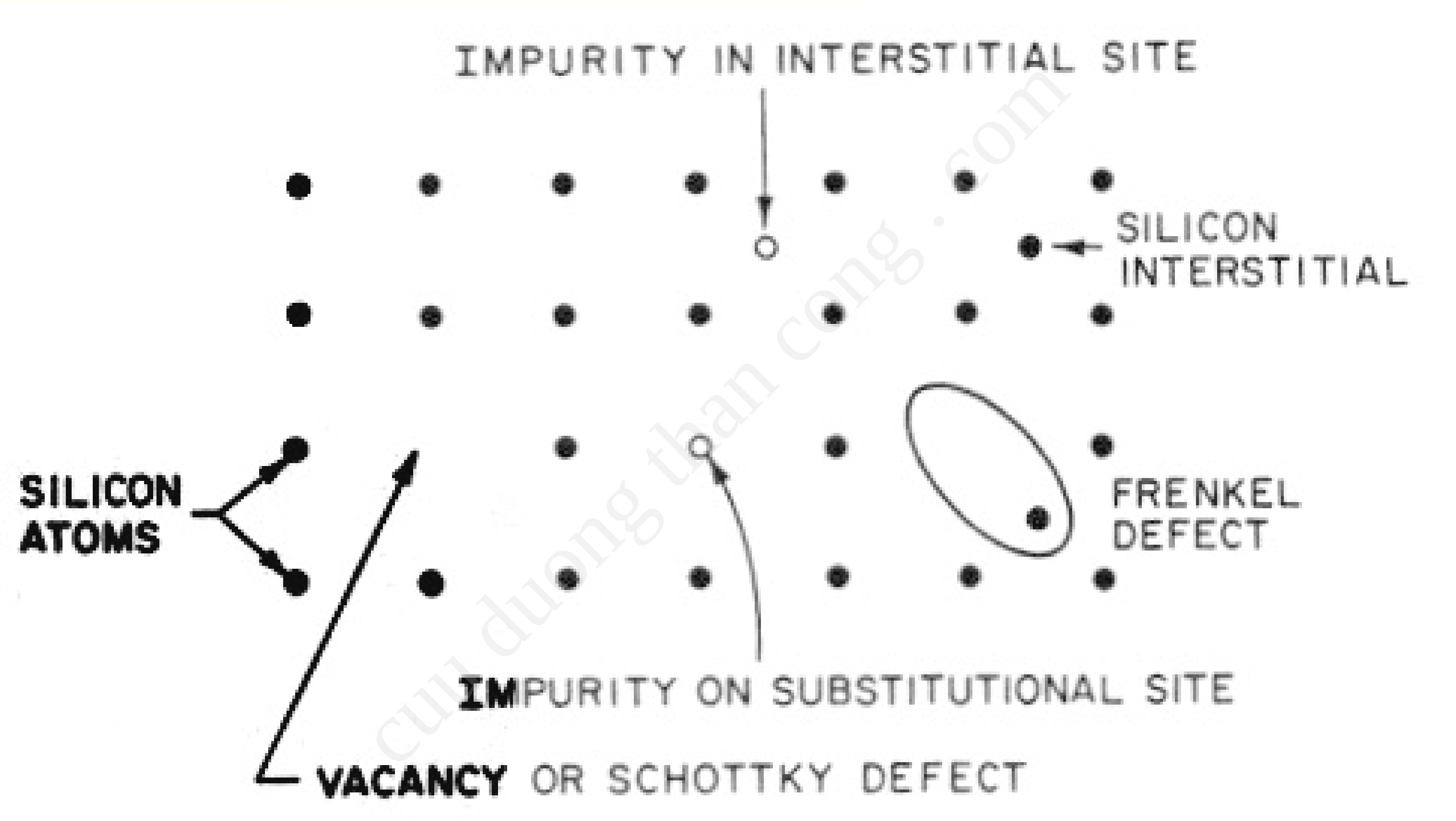
Point defects: 0-D

- Substitutional
- Interstitial
- Schottky:Vacancy by missing atom
- Frenkel : Interstitial lattice Si + Vacancy

$N_d = A \exp(-E_a/kT)$

N_d : Conc. of point defect

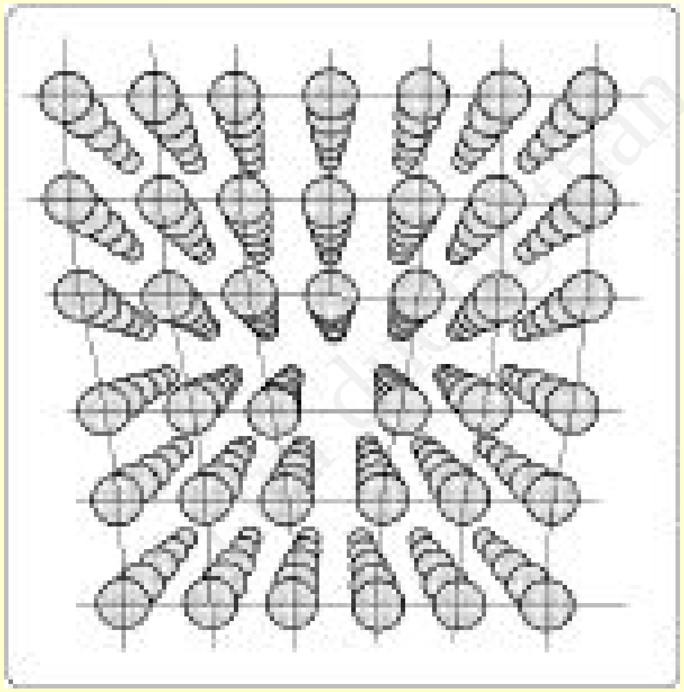
E_a : Activation energy, A : const.



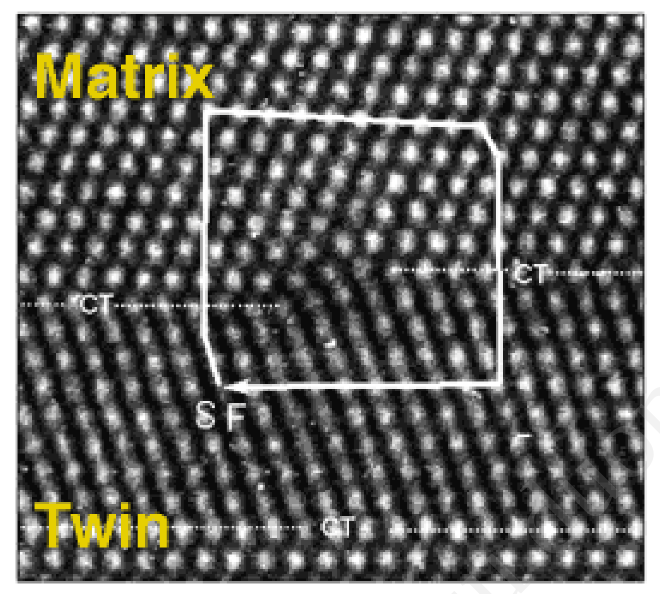
from Sze, "VLSI Technology"

Linear defects: 1-D

- Dislocation: extra half plane of atoms



Planar defects: 2-D



- Twin boundary: highly symmetrical 2-d discontinuity in the lattice
- Grain boundary: mismatched region of two adjacent grains of different orientations

From http://www.ca.sandia.gov/Materials&EngineeringSciences/FocusAreas/thinfilm.html

Volume defects: 3-D

- Precipitates of dopants or impurities

  - Precipitates are undesirable : active sites for dislocation generation from volume mismatch between precipitates and lattice

- Void

Properties and crystal structure

{111}

- Highest planar density
- Crystal grows most easily
- Oxidize faster than {100}

<111>

- Highest tensile strength

Preferred applications

<100> MOS, MEMS

<111> Bipolar circuit

Crystal growth

- CZ(Czochralski) method
  - 80-90 % of Si crystal production
  - Solidification of silicon from a liquid phase at an interface
  - Mass transport + temperature gradient
- FZ(Float Zone) method

CZ Si crystal growth

- Sand(SiO_2) to MGS(metallurgical grade silicon)

  $SiC + SiO_2 \rightarrow Si(l) + SiO_2(g) + CO(g)$

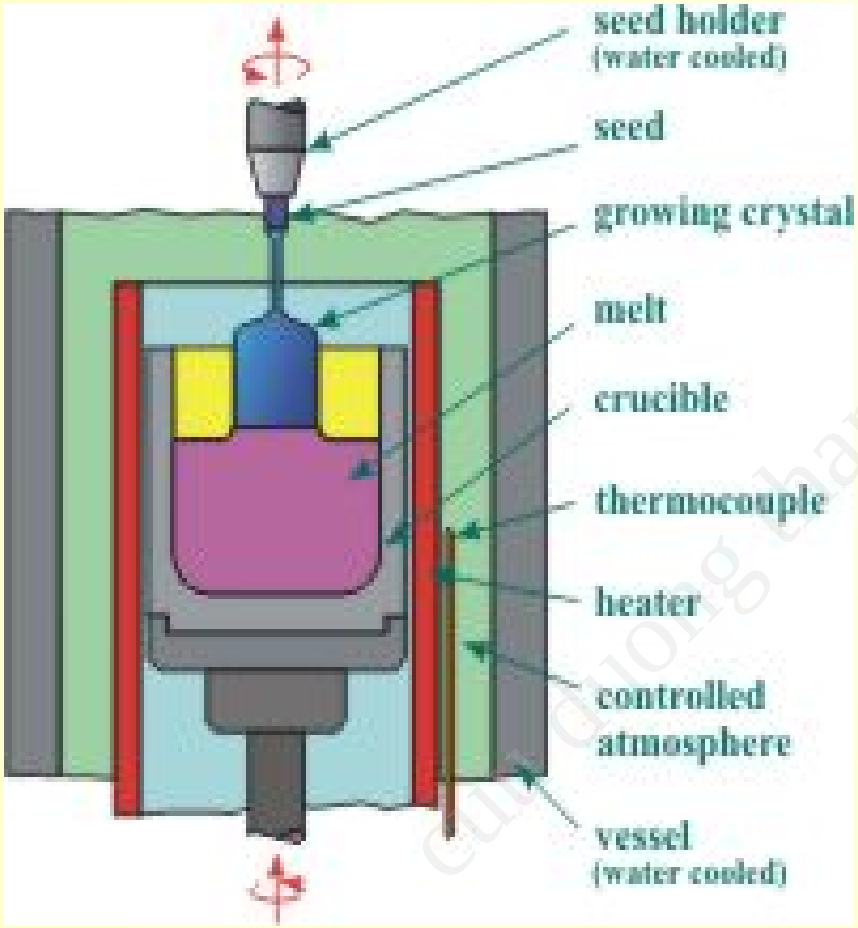
  @ 2000°C
- MGS to Trichlorosilane

  $Si + 3HCl(g) \rightarrow SiHCl_3(g) + H_2(g) + heat$ @300°C
- Trichlorosilane to polysilicon

  $2SiHCl_3(g) + 2H_2(g) \rightarrow 2Si + 6HCl(g)$
- CZ > T_m, 1415°C

CZ steps

- A cylindrical crystal rod (d = 4-8”) is pulled vertically from the melt in a heated crucible.
- The crystal rod and the crucible are usually rotated in opposite directions.
- Solid crystals are afterwards cut to form thin semiconductor wafers from which, e.g., integrated circuits, are produced.



http://www.mpi-stuttgart.mpg.de/crystal/facilities.html *http://www.mticrystal.com/furnace.html*

CZ theory

- ❑ Macroscopic model from heat transfer condition

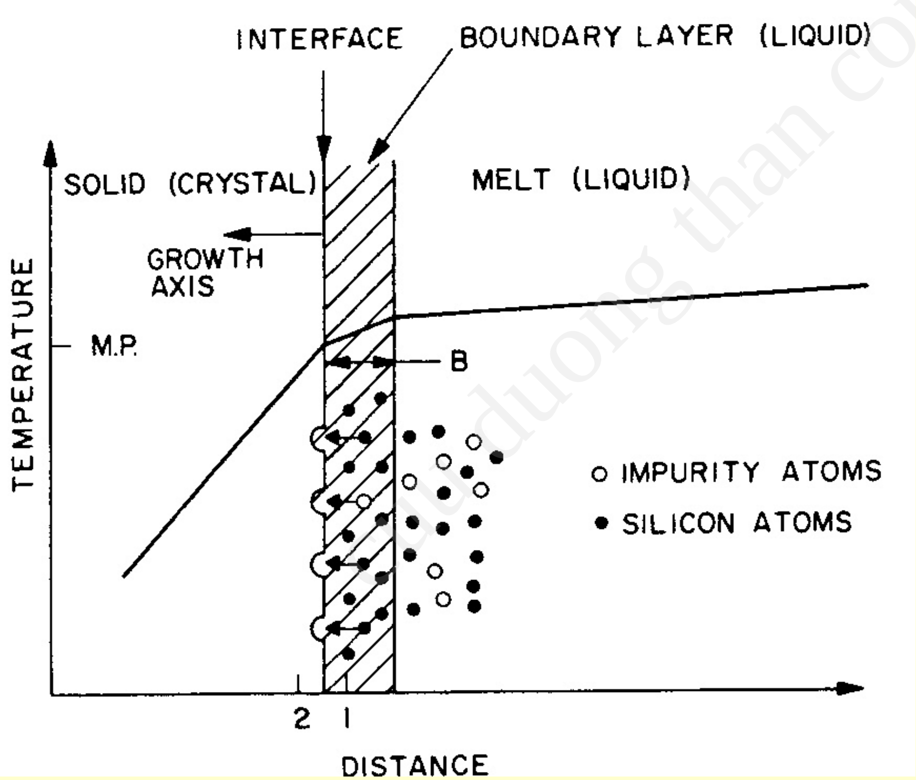
$L\ dm/dt + k_l\ (dT/dX_1)A_1 = k_s\ (dT/dX_2)A_2$

L: latent heat of fusion
dm/dt: mass solidification rate
T: temperature
k_l, k_s: thermal conductivities of solid and liquid
dT/dX_1, dT/dX_2 : thermal gradient at points 1 and 2
A_1, A_2 : Areas of the isotherm at point 1 and 2

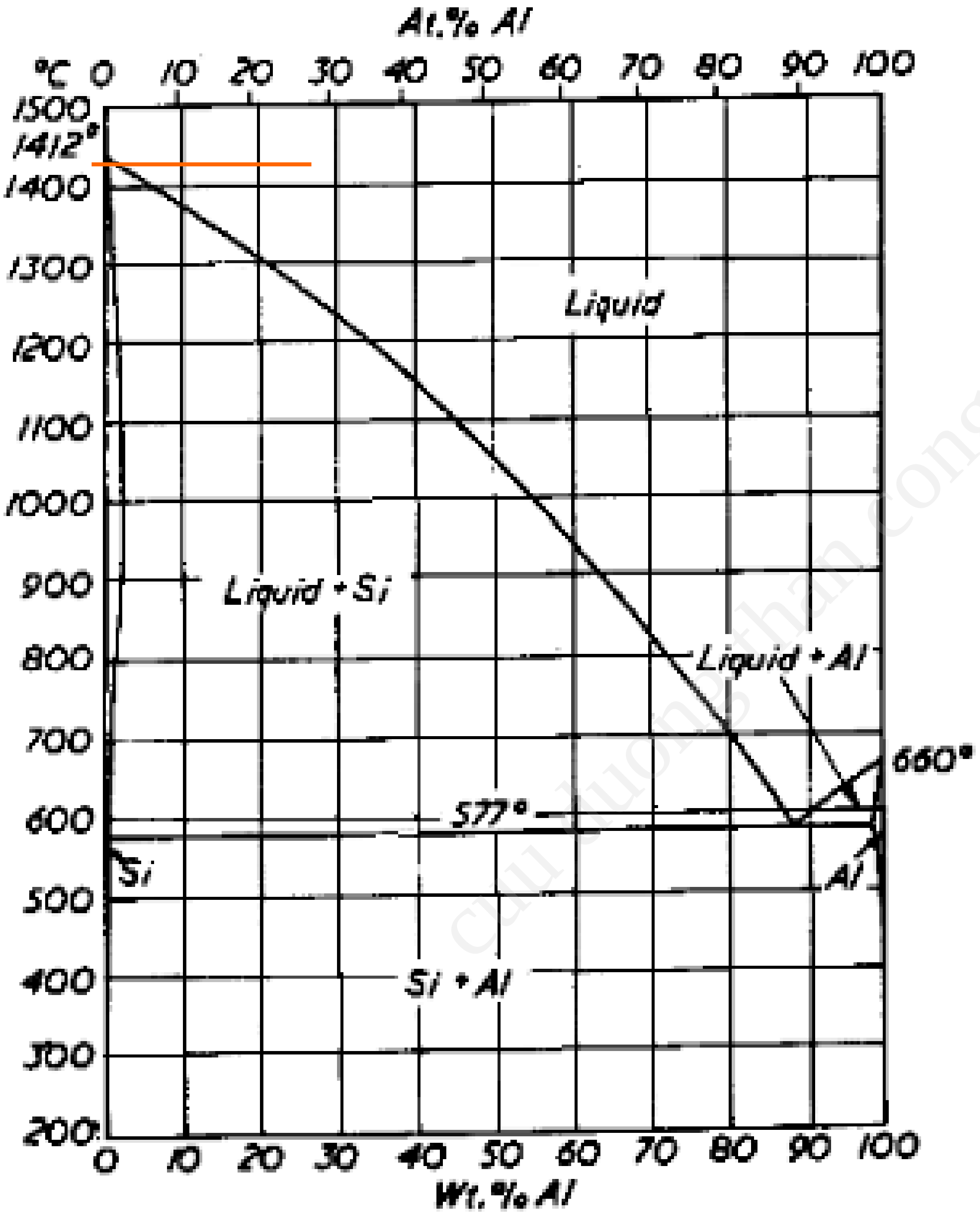
Under the zero thermal gradient in melt, $dT/dX_1 = 0$

Maximum pull rate: $V_{max} = (k_s/Ld)\,(dT/dX)$

where, d: density of solid silicon



from Sze, "VLSI Technology"



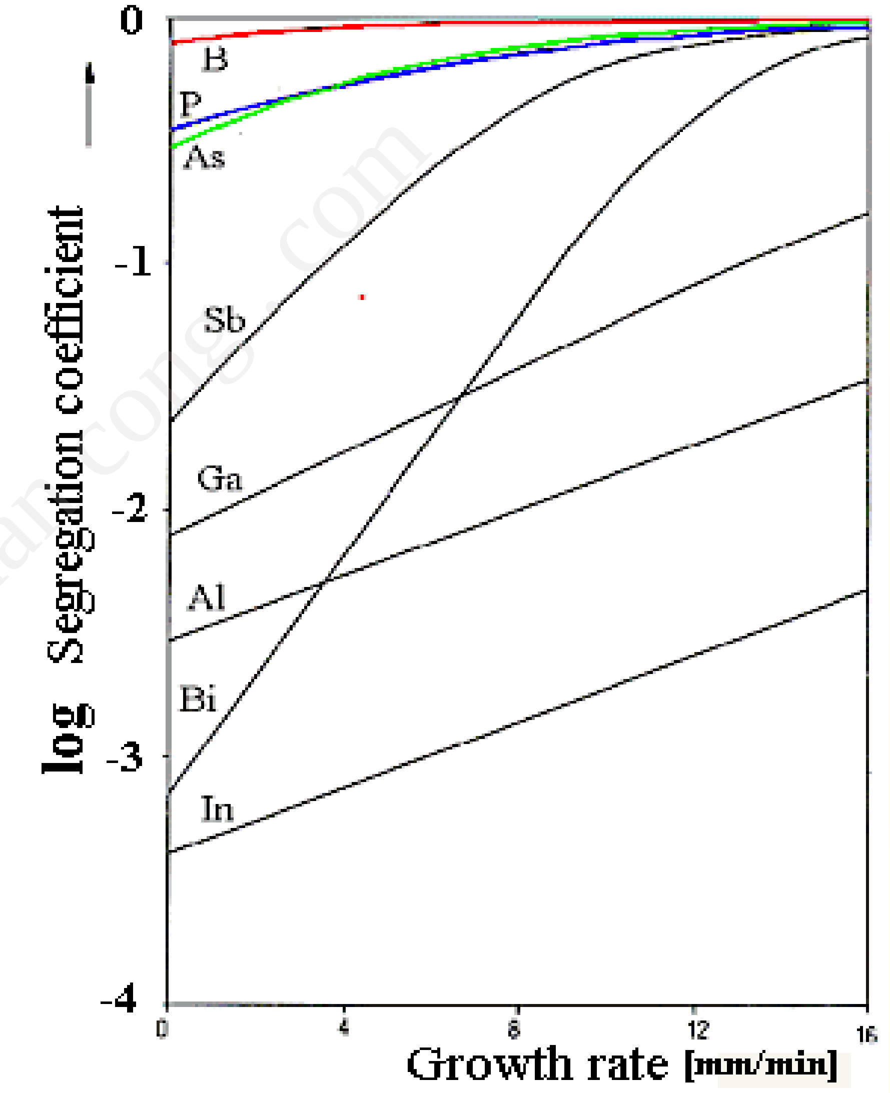
- Segregation coeff.

$$k_{seg} = C_s/C_l < 1$$

Cs , Cl :

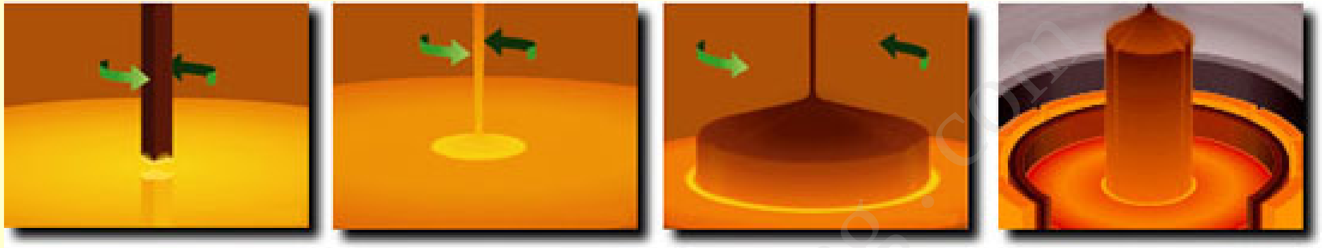
equil. conc. of impurity in the solid and liquid near the interface

- Requirement
  - impurity segregation
  - uniform distribution



http://www.tf.uni-kiel.de/matwis/amat/elmat_en/kap_5/backbone/r5_1_2.html

- CZ



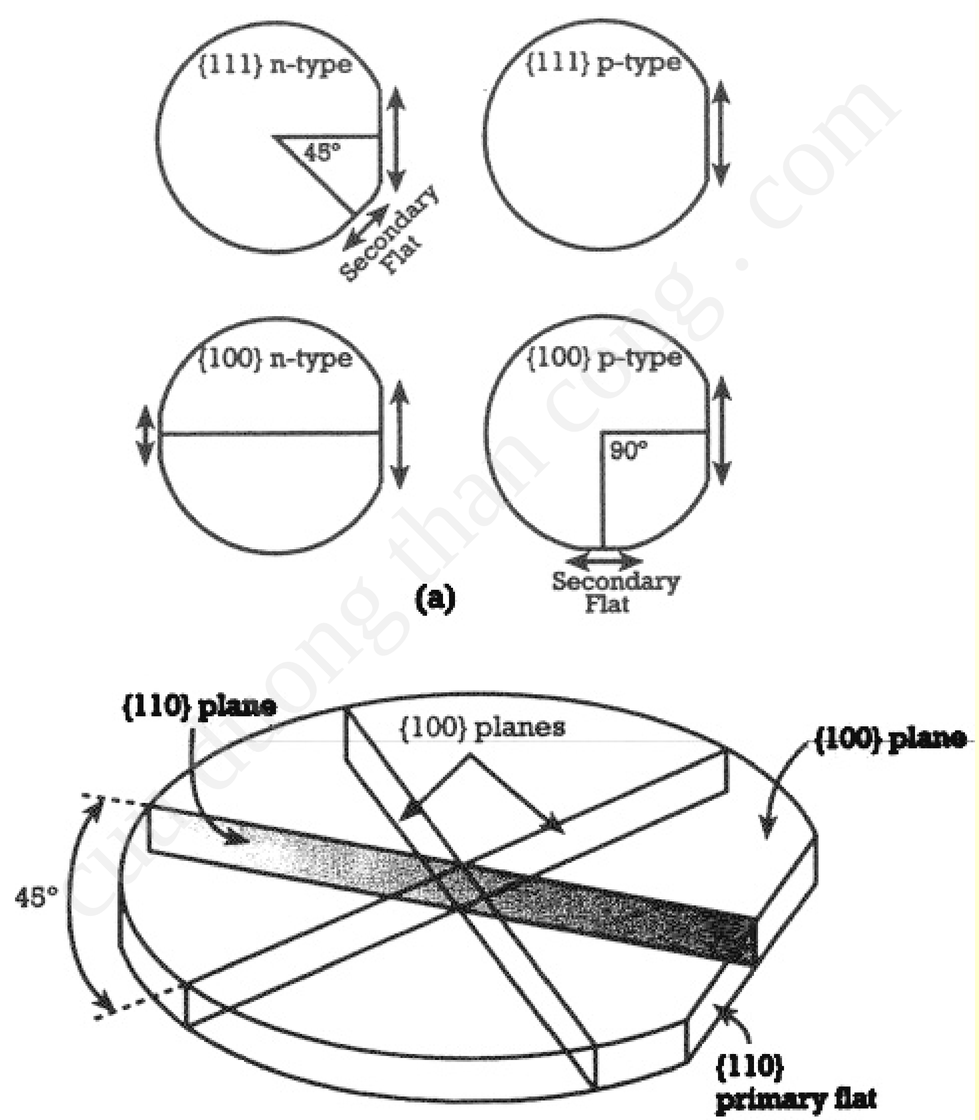
- Ingot

- Wafer

1. Slicing
2. Lapping and etching
3. Thickness sorting & flatness measurement
4. CMP (chemical mechanical polishing)
5. Quality inspection (electrical, dimensional)

http://www.ami.bolton.ac.uk/courseware/mdesign/ch2/mdesign02notes.html

Fianally…..Wafer



Si Semiconductor - Background

- Waves and matter

Newton's law : particle motion

Maxwell equation : wave propagation

Quantum physics :

1. Particle = wave
2. Energy is discrete not continuous
3. Probability and uncertainty

- de Broglie’s equation: matter wave

$\lambda = h/p$; $p = \hbar k$

where $\hbar = h/(2\pi)$, $k = 2\pi/\lambda$;wave number

p:momentum of particle

h=Planck’s constant

- Einstein equation: photon energy

$E = h\nu$; $E = \hbar\omega$: Energy of photon

ν : frequency of radiation

ω : radian frequency of radiation

- Example

Atomic spectra: absorption and emission of light by atoms corresponding discrete wavelengths rather than a continuous distribution

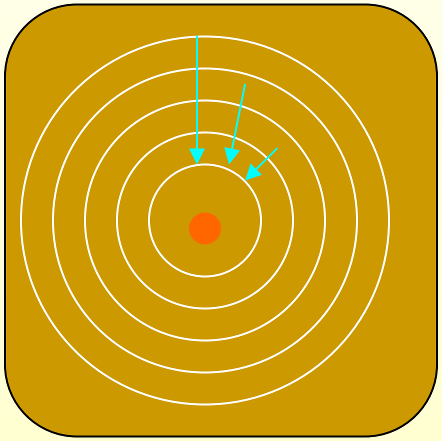
Photoelectric effect: radiation from a heated materials is emitted in discrete units of energy (quanta); a characteristic minimum energy is required to remove electrons from material

$\phi = h\nu$: work function

- Bohr model

1. Electrons exist in certain stable circular orbits about nucleus
2. Electron may shift to an orbit of higher or lower energy
3. Angular momentum p is given by

$P(\theta)=n\hbar$ n=1,2,3,..



Frequency of light given off by transition betweem orbits is,

ν = Const x $(1/n_1^2 - 1/n_2^2)$

- Hamilton’s formulation

$E = T + V$

E: tot. energy

T:kinetic energy

V:potential energy

$T = p^2/2m, \quad p = mv$

Hamiltonian, H is defined by,

$H(p,x,t) = T(p) + V(x,t)$

- Schrödinger equation

Approach from wave mechanics

$\hat{H}\psi = E\psi$

(example) $\hat{H} = \hat{p}^2/2m + V(x)$

$\hat{H} = -(\hbar^2/2m)(\angle^2/\angle x^2) + V(x)$

$$\int_{-\infty}^{\infty} \psi^*\psi dx = 1$$

$$\langle G\rangle = \frac{\int_{-\infty}^{\infty} \psi^*\hat{G}\psi dx}{\int_{-\infty}^{\infty} \psi^*\psi dx}$$

❑ Time-independent 1-D Schrödinger equation

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E-V(x)]\,\psi(x) = 0$$

- ☐ Heisenberg uncertainty principle

It is physically impossible to measure simultaneously the position and momentum of an object

Product of uncertainty of momentum and uncertainty of position is at least on the order of Planck’s constant

$\delta p \, \delta x > h$

- Maxwell-Boltzmann distribution

$f(E) = C \exp(-E/kT)$

1. Distinguishable particles
2. Any # of particles with same energy state
3. Statistically independent particles

- Bose-Einstein distribution

$$f(E) = \frac{1}{\exp[(E-E_b)/kT] - 1}$$

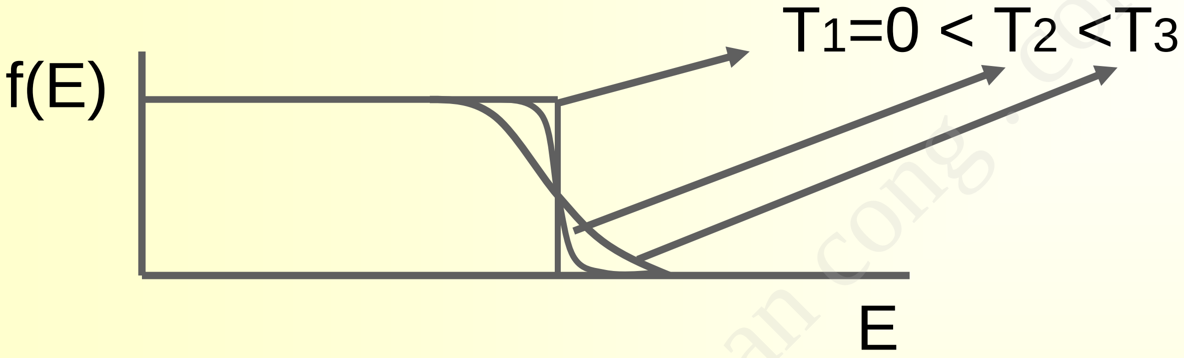
1. Indistinguishable particles
2. Any # of particles with same energy state
3. Statistically independent particles

- Fermi-Dirac distribution

$$f(E) = \frac{1}{1 + \exp[(E - E_f)/kT]}$$

1. Indistinguishable particles
2. Only one particle for any given energy state (Pauli's exclusion principle)
3. Statistically independent particles

❑ Fermi energy



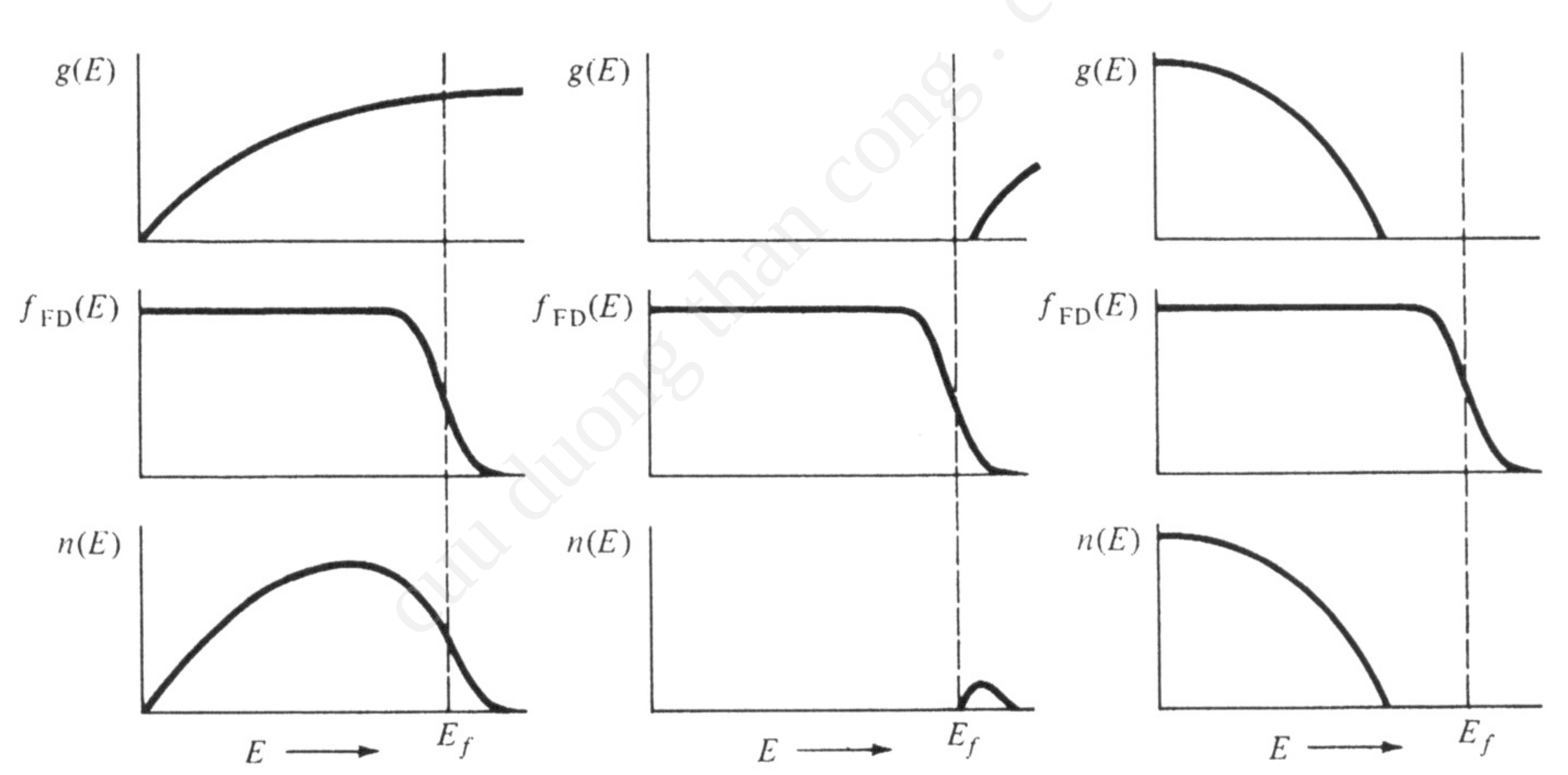
- At T=0K

States below Fermi energy is full, and above, empty

- At all temperature above 0K

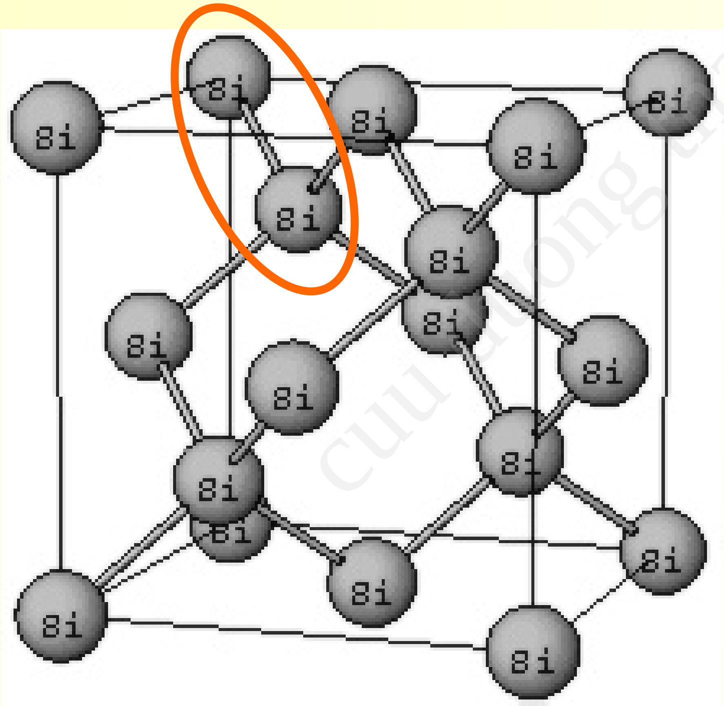
Probability that a state will be occupied at $E=E_f$ equals 1/2

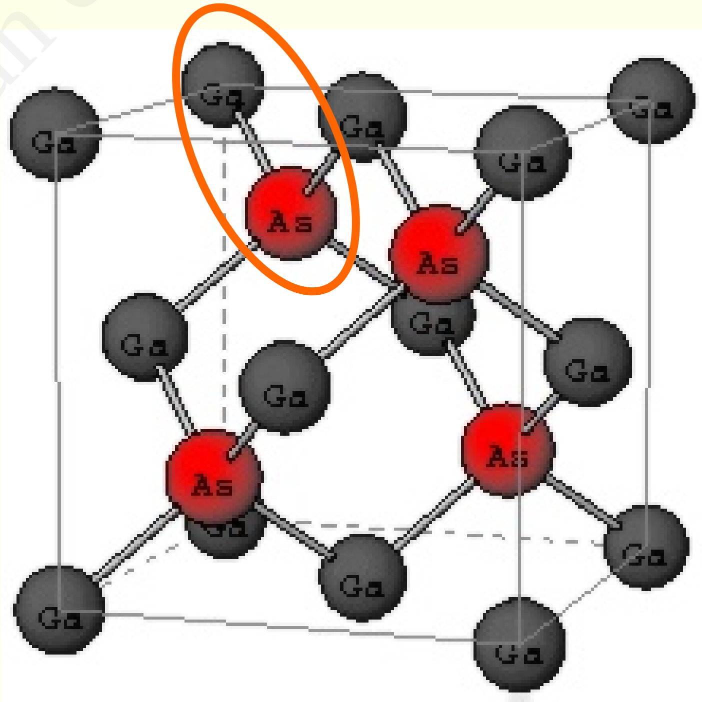
- ❑ Electron distributions; $n(E)=f(E)g(E)$ where $g(E)$=density of states

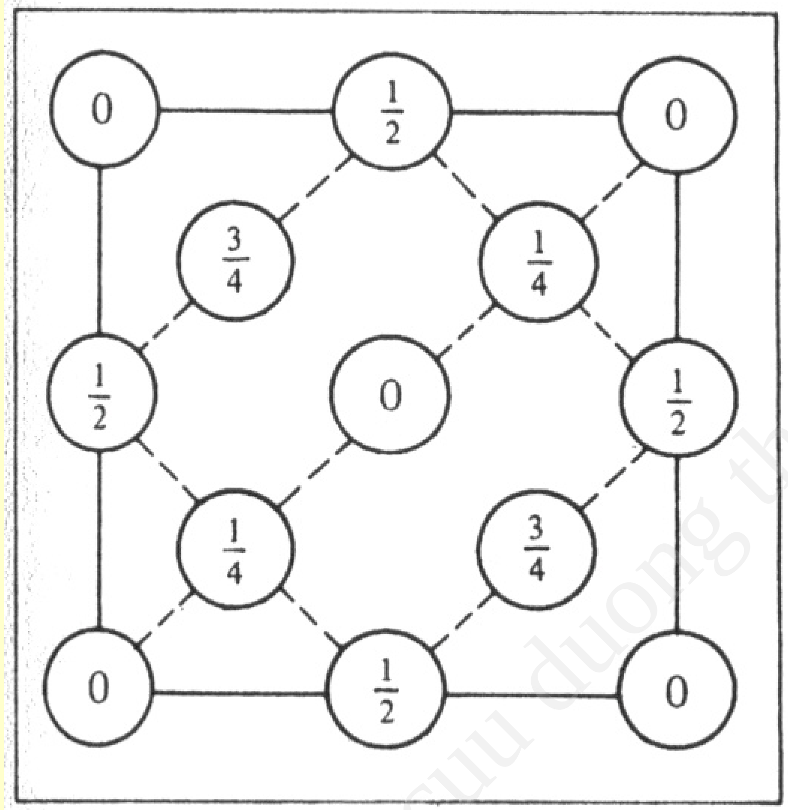


Atoms and crystals

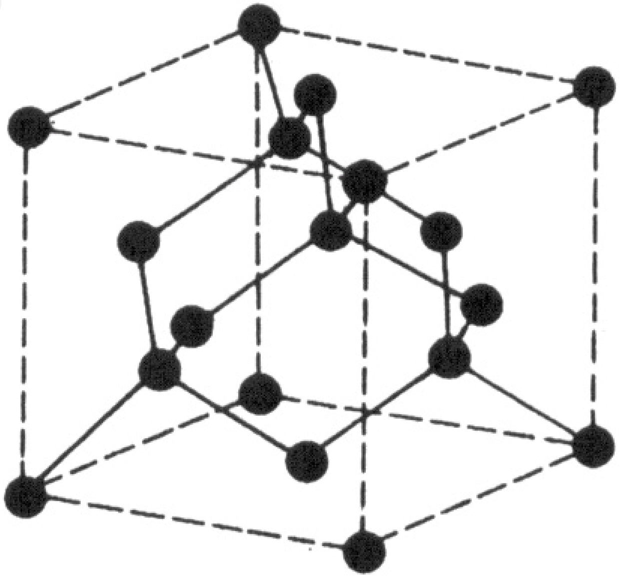
- In many crystals, groups of atoms can occupy each lattice site, which are often called “basis” of the lattice.





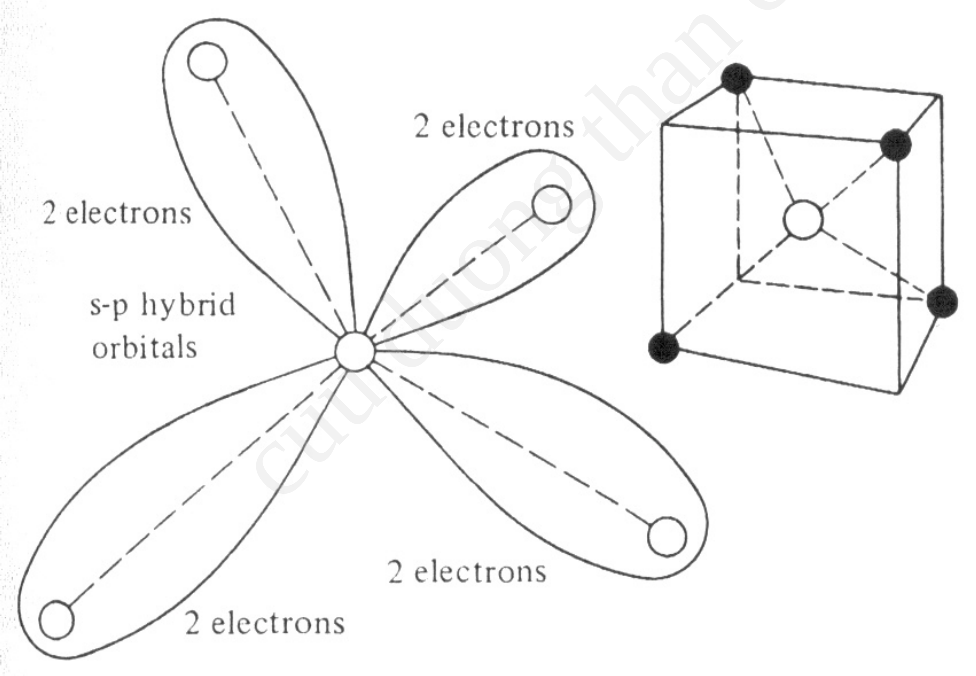


(*a*)



(*b*)

- Since lattice vectors are rather arbitrarily chosen, there is no pre-determined relation between lattice vectors and chemical bonds.



- Atomic density

FCC

BCC

❑ Reciprocal lattice

- An infinite array with points that represent values of the wave number, k=p/ħ

a.k.a momentum space

- The reciprocal lattice is generated by the set of all G's with periodicity of the direct Bravais lattice.

$$\mathrm{Exp}\,(jG\bullet R) = 1$$

- The set of vectors, G generates the reciprocal lattice of the direct lattice generated by the set of R

http://www.chembio.uoguelph.ca/educmat/chm729/recip/3vis.htm

$$\exp(j\mathbf{G}\cdot\mathbf{R}) = 1 \tag{4.2}$$

The set of vectors **G** that satisfy this relationship generates the reciprocal lattice of the direct lattice generated by the set **R**.

The reciprocal lattice has a specific time-independent orientation with respect to the space lattice. When a crystal is rotated, both the direct and reciprocal lattices rotate. The primitive vectors of the reciprocal Bravais lattice are given by

$$\mathbf{b}_i = \frac{2\pi(\mathbf{a}_j \times \mathbf{a}_k)}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)} \tag{4.3}$$

where $i, j, k = 1, 2, 3$ are cyclic values. The denominator in the above expression is the volume of the primitive cell in position space V_s. The primitive vectors of the two lattices are related by

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij} \tag{4.4}$$

where δ_{ij} is the Kronecker delta, given by

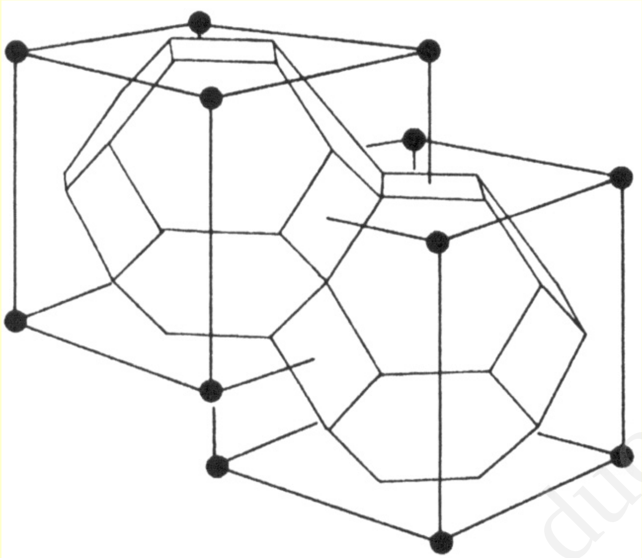
$$\delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases}$$

Thus the translation vectors that generate the reciprocal lattice can be written

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 \tag{4.5}$$

where $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$ are the primitive vectors of the reciprocal lattice and h, k, and l are integers. Note that while the dimensions of **R** are length, those of **G** are 1/length, or reciprocal length.

- ☐ Simple cubic with a > simple cubic with $2\pi/a$
- ☐ FCC with a > BCC with $4\pi/a$ in reciprocal lattice



Brillouin zone of FCC lattice

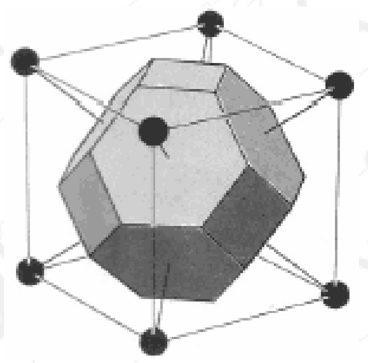
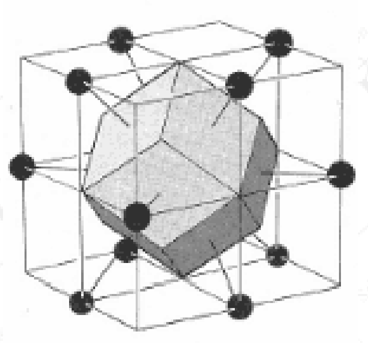
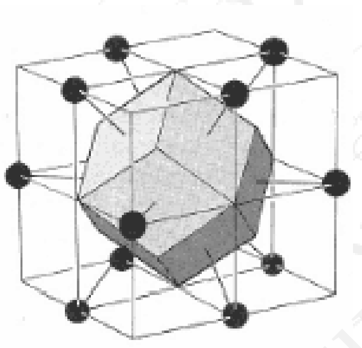
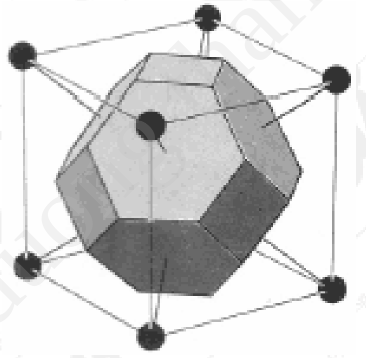
- SC W-S cell
- BCC W-S cell

- ☐ Wigner-Seitz cell

-A cell constructed by drawing perpendicular bisector planes in the lattice from the chosen center to the nearest lattice point

- ☐ Brillouin Zone

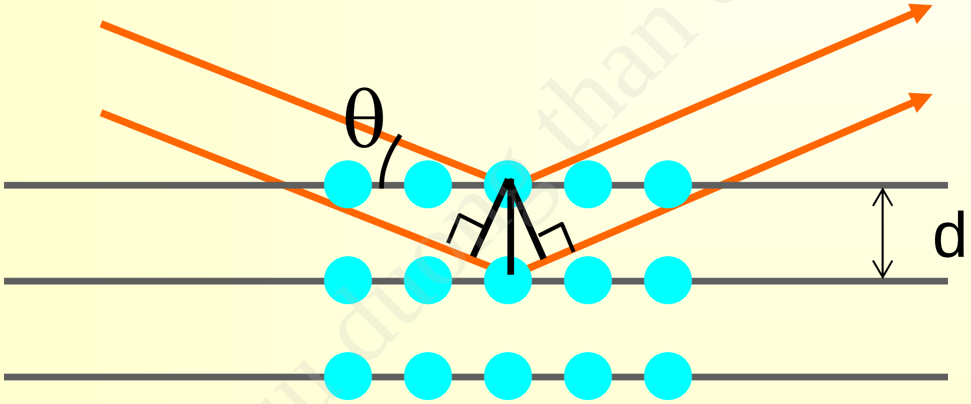
-Wigner-Seitz cell in reciprocal lattice

Lattice Real Space	Lattice k-space
 bcc WS cell	 bcc BZ (fcc lattice in k-space)
 fcc WS cell	 fcc BZ (bcc lattice in k-space)

http://britneyspears.ac/physics/crystals/wcrystals.htm

- ❑ XRD

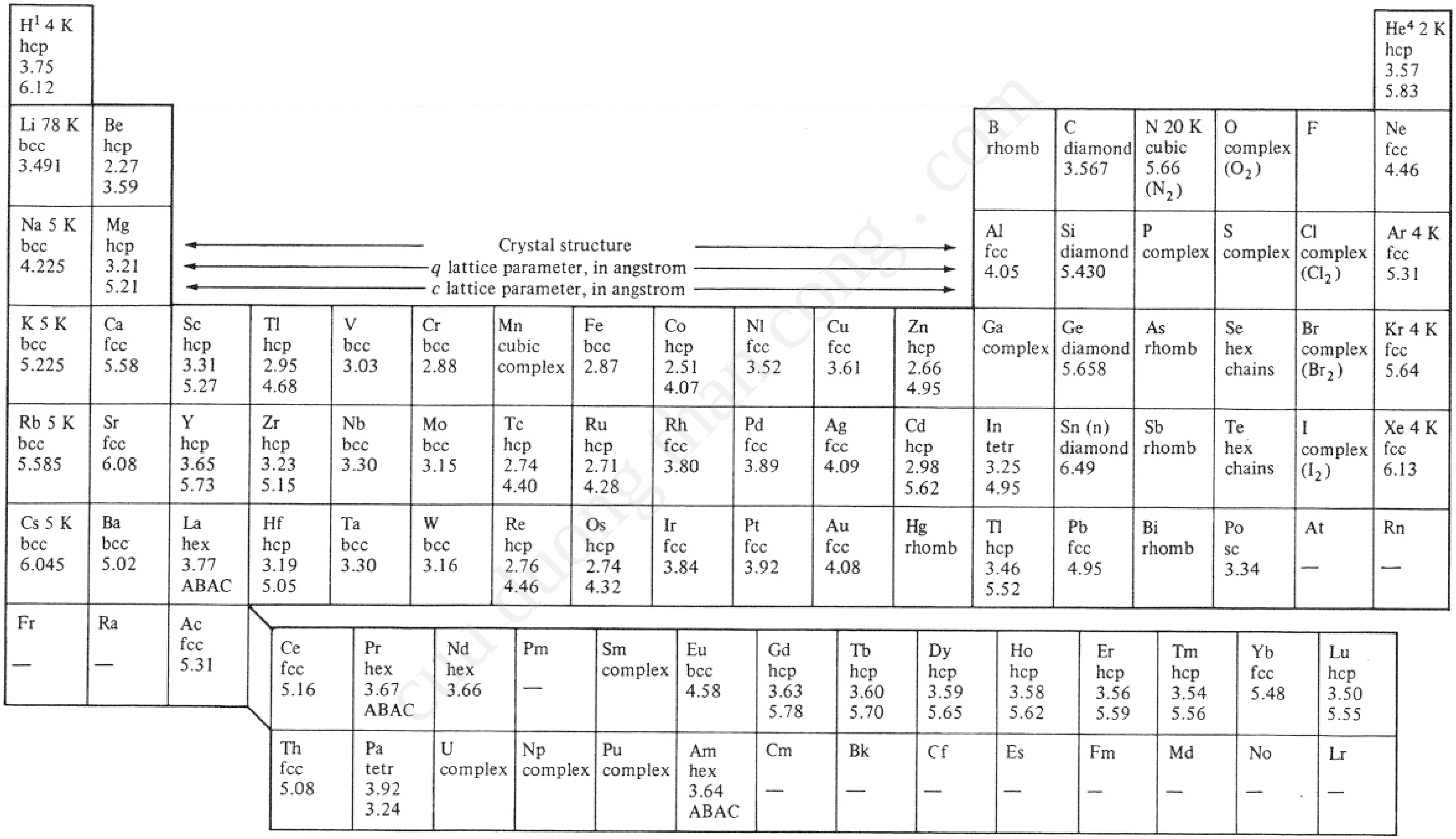
- Distances in reciprocal lattice corresponds to the distances separating planes in direct lattice
- XRD measures reflection from lattice planes: by reciprocal-lattice, reveals direct lattice.



Bragg diffraction

$2d\sin\theta = n\lambda$

Table 4.2 Crystal structures of the elements†

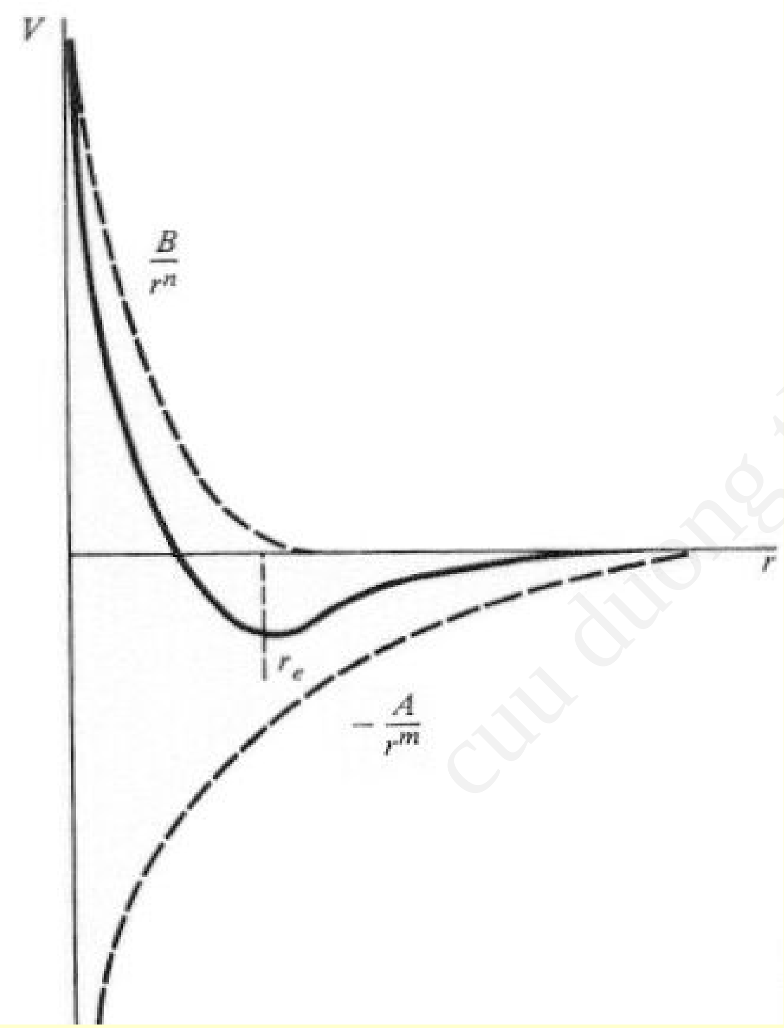


H^1 4 K hcp 3.75 6.12																	He^4 2 K hcp 3.57 5.83
Li 78 K bcc 3.491	Be hcp 2.27 3.59											B rhomb	C diamond 3.567	N 20 K cubic 5.66 (N_2)	O complex (O_2)	F	Ne fcc 4.46
Na 5 K bcc 4.225	Mg hcp 3.21 5.21	← Crystal structure → ← q lattice parameter, in angstrom → ← c lattice parameter, in angstrom →										Al fcc 4.05	Si diamond 5.430	P complex	S complex	Cl complex (Cl_2)	Ar 4 K fcc 5.31
K 5 K bcc 5.225	Ca fcc 5.58	Sc hcp 3.31 5.27	Ti hcp 2.95 4.68	V bcc 3.03	Cr bcc 2.88	Mn cubic complex	Fe bcc 2.87	Co hcp 2.51 4.07	Ni fcc 3.52	Cu fcc 3.61	Zn hcp 2.66 4.95	Ga complex	Ge diamond 5.658	As rhomb	Se hex chains	Br complex (Br_2)	Kr 4 K fcc 5.64
Rb 5 K bcc 5.585	Sr fcc 6.08	Y hcp 3.65 5.73	Zr hcp 3.23 5.15	Nb bcc 3.30	Mo bcc 3.15	Tc hcp 2.74 4.40	Ru hcp 2.71 4.28	Rh fcc 3.80	Pd fcc 3.89	Ag fcc 4.09	Cd hcp 2.98 5.62	In tetr 3.25 4.95	Sn (n) diamond 6.49	Sb rhomb	Te hex chains	I complex (I_2)	Xe 4 K fcc 6.13
Cs 5 K bcc 6.045	Ba bcc 5.02	La hex 3.77 ABAC	Hf hcp 3.19 5.05	Ta bcc 3.30	W bcc 3.16	Re hcp 2.76 4.46	Os hcp 2.74 4.32	Ir fcc 3.84	Pt fcc 3.92	Au fcc 4.08	Hg rhomb	Tl hcp 3.46 5.52	Pb fcc 4.95	Bi rhomb	Po sc 3.34	At —	Rn —
Fr —	Ra —	Ac fcc 5.31															
			Ce fcc 5.16	Pr hex 3.67 ABAC	Nd hex 3.66	Pm —	Sm complex	Eu bcc 4.58	Gd hcp 3.63 5.78	Tb hcp 3.60 5.70	Dy hcp 3.59 5.65	Ho hcp 3.58 5.62	Er hcp 3.56 5.59	Tm hcp 3.54 5.56	Yb fcc 5.48	Lu hcp 3.50 5.55	
			Th fcc 5.08	Pa tetr 3.92 3.24	U complex	Np complex	Pu complex	Am hex 3.64 ABAC	Cm —	Bk —	Cf —	Es —	Fm —	Md —	No —	Lr —	

† hcp = hexagonal close-packed, bcc = body-centered cubic, fcc = face-centered cubic, hex = hexagonal, tetr = tetragonal, rhomb = rhombic, and sc = simple cubic.

Source: From C. Kittel, *Introduction to Solid State Physics*, 5th ed., Wiley, New York, 1976; used by permission.

Energy of crystals



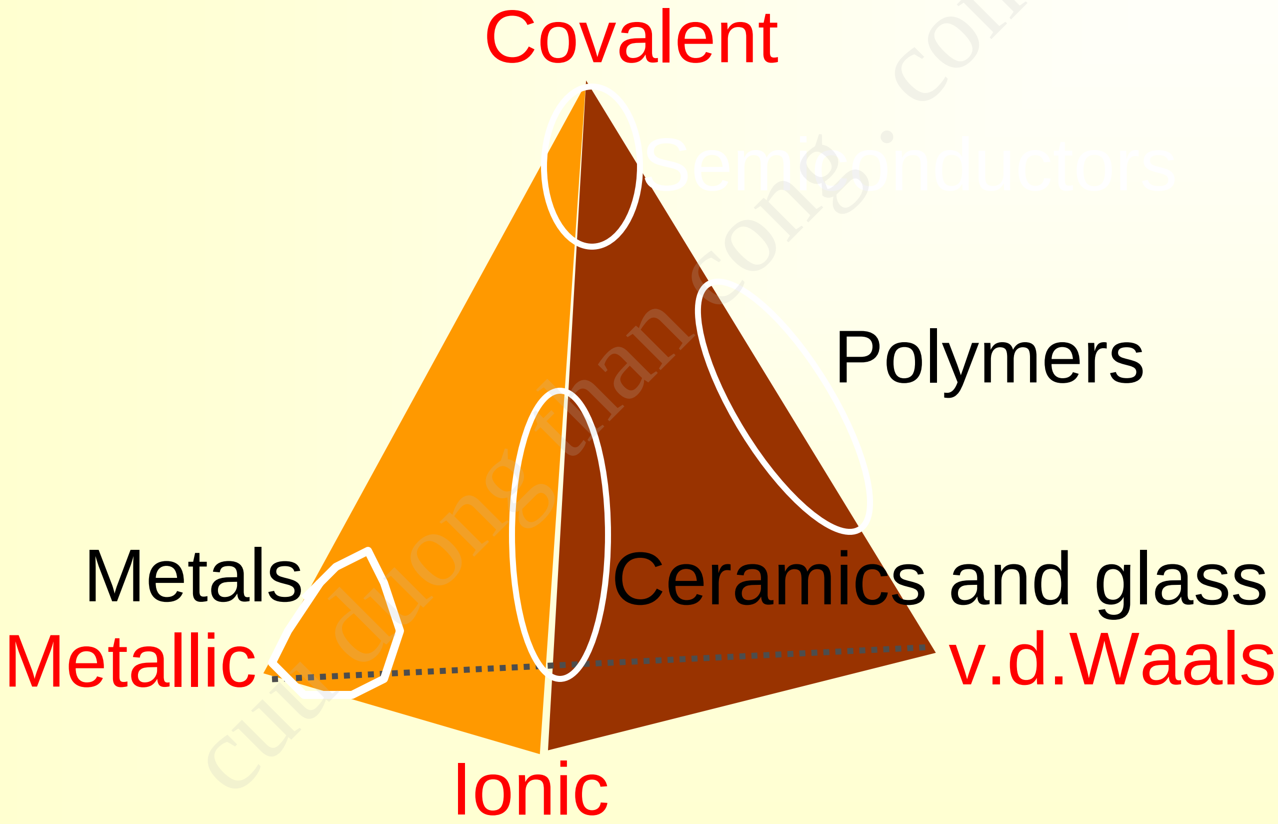
- Atom in crystal

$V = -A/r^m + B/r^n$ (n>m)

r: atomic spacing

r_e: equil. spacing

- Repulsive interaction
  - Electron orbitals overlap > overlapping electrons with parallel spins enter higher energy state > system energy lowered by increased r.
- Attractive interaction
  - Covalent bonding: cooperative sharing of valence electrons between two adjacent lattice atoms, highly-directional e.g. bond angle of Si = 109.5°
  - Metallic bonding: sharing of valence electrons by many ionic cores in lattice, de-localized
  - Ionic bonding: inert-gas electron configuration formed by transferred electrons resulting in two oppositely charged ions, nondirectional
  - van der Waals: interaction from induced dipole moments between neighboring atoms



Covalent

Semiconductors

Polymers

Metals

Metallic

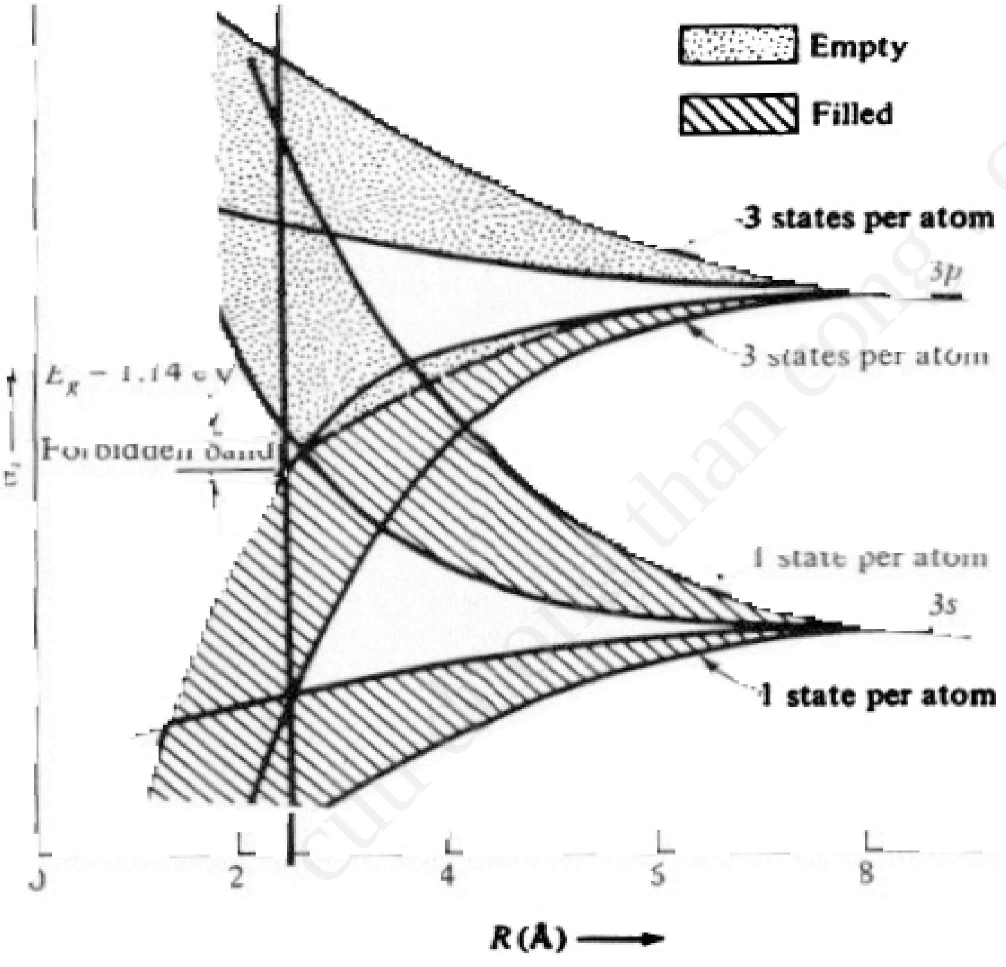
Ceramics and glass

v.d.Waals

Ionic

- Atom → crystal
- Discrete atomic energy level → energy band
- Total # of energy levels constant but closely packed
- A band can be viewed as a continuum of states, because the thermal energy of electrons within a band allow them to move freely between the closely spaced levels

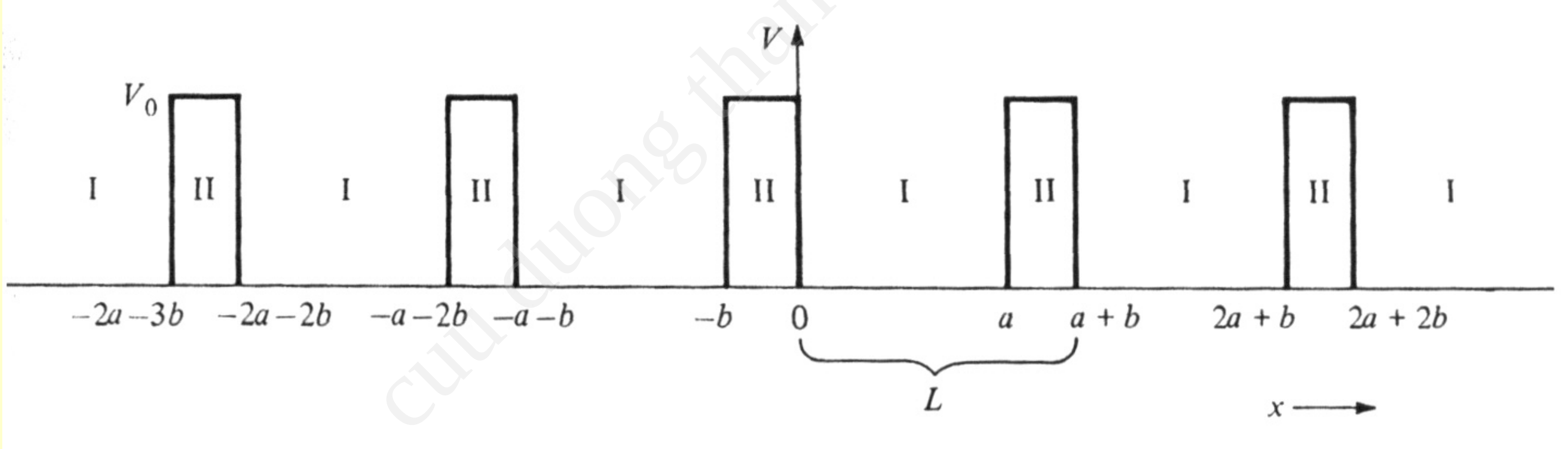
Formation of energy bands



(b)

Kronig-Penney model

- Math treatment for energy levels allowed for a single electron experiencing 1-D periodic potential



$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0$$

$$\psi(x) = U(x) \exp jkx \tag{5.2}$$

where $U(x) = U(x + L) = U(x + NL)$. Therefore, $U(a) = U(-b)$.

In regions labeled I

$$\psi_{\mathrm{I}} = U_{\mathrm{I}} \exp jkx$$

$$\frac{d\psi_{\mathrm{I}}}{dx} = jkU_{\mathrm{I}} \exp jkx + \frac{dU_{\mathrm{I}}}{dx} \exp jkx$$

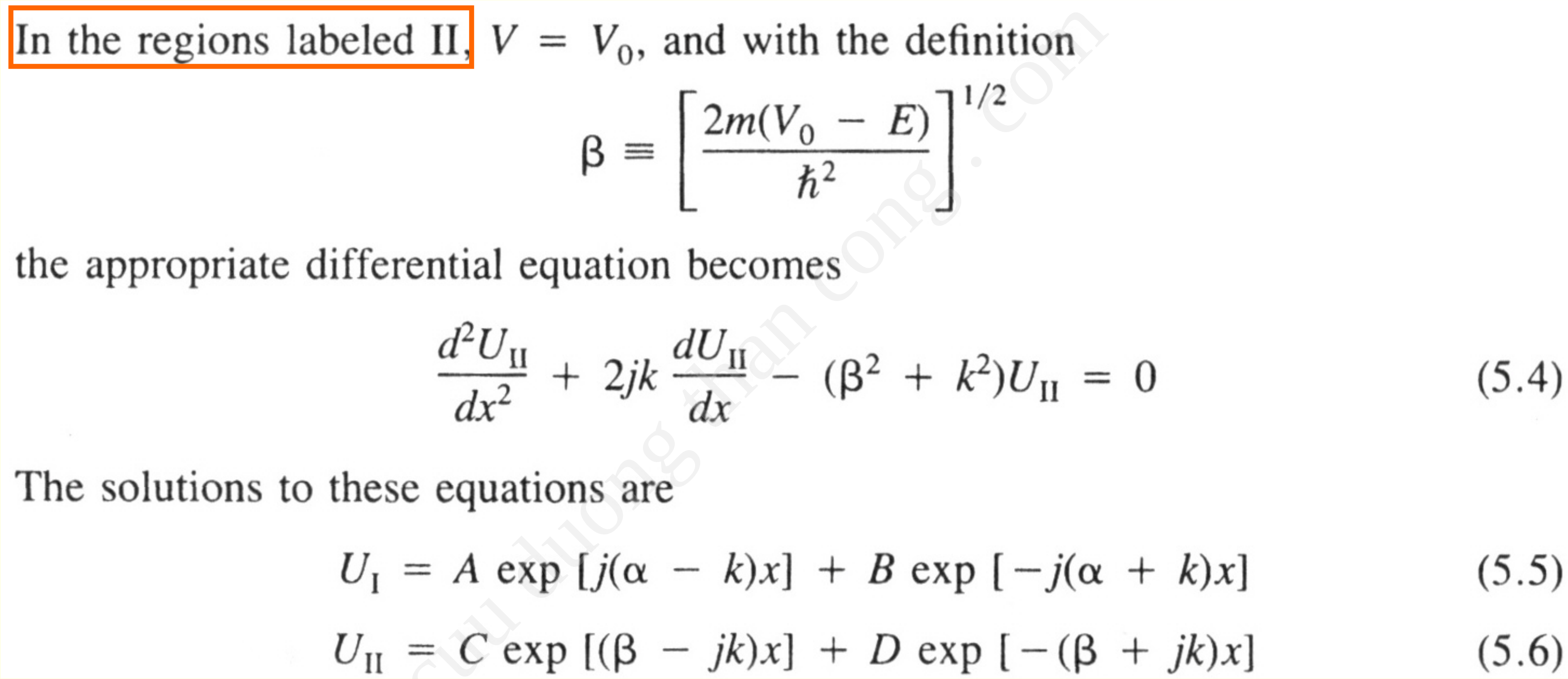
$$\frac{d^2\psi_{\mathrm{I}}}{dx^2} = -k^2U_{\mathrm{I}} \exp jkx + jk\frac{dU_{\mathrm{I}}}{dx} \exp jkx + jk\frac{dU_{\mathrm{I}}}{dx} \exp jkx + \frac{d^2U_{\mathrm{I}}}{dx^2} \exp jkx$$

When we make the substitution

$$\alpha \equiv \left(\frac{2mE}{\hbar^2}\right)^{1/2}$$

the appropriate differential equation for region I becomes

$$\frac{d^2U_{\mathrm{I}}}{dx^2} + 2jk\frac{dU_{\mathrm{I}}}{dx} + (\alpha^2 - k^2)U_{\mathrm{I}} = 0 \tag{5.3}$$



In the regions labeled II, $V = V_0$, and with the definition

$$\beta \equiv \left[\frac{2m(V_0 - E)}{\hbar^2}\right]^{1/2}$$

the appropriate differential equation becomes

$$\frac{d^2U_{\mathrm{II}}}{dx^2} + 2jk\,\frac{dU_{\mathrm{II}}}{dx} - (\beta^2 + k^2)U_{\mathrm{II}} = 0 \qquad (5.4)$$

The solutions to these equations are

$$U_{\mathrm{I}} = A \exp\,[j(\alpha - k)x] + B \exp\,[-j(\alpha + k)x] \qquad (5.5)$$

$$U_{\mathrm{II}} = C \exp\,[(\beta - jk)x] + D \exp\,[-(\beta + jk)x] \qquad (5.6)$$

Both U and dU/dx must be continuous at the boundaries, and since U is a periodic function, $U(a) = U(-b)$. The boundary conditions are satisfied if

$$\text{Continuity condition}\left\{\begin{aligned} U_{\mathrm{I}}(0) &= U_{\mathrm{II}}(0) \\ \left.\frac{dU_{\mathrm{I}}}{dx}\right|_0 &= \left.\frac{dU_{\mathrm{II}}}{dx}\right|_0 \\ U_{\mathrm{I}}(a) &= U_{\mathrm{II}}(-b) \\ \left.\frac{dU_{\mathrm{I}}}{dx}\right|_a &= \left.\frac{dU_{\mathrm{II}}}{dx}\right|_{-b} \end{aligned}\right.$$

or

$$A + B = C + D$$

$$j(\alpha - k)A - j(\alpha + k)B = (\beta - jk)C - (\beta + jk)D$$

$$A \exp\,[j(\alpha - k)a] + B \exp\,[-j(\alpha + k)a] =$$

$$C \exp\,[-(\beta - jk)b] + D \exp\,[(\beta + jk)b]$$

$$j(\alpha - k)A \exp\,[j(\alpha - k)a] - j(\alpha + k)B \exp\,[-j(\alpha + k)a] =$$

$$(\beta - jk)C \exp\,[-(\beta - jk)b] - (\beta + jk)D \exp\,[(\beta + jk)b]$$

$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} \sinh \beta b \sin \alpha a + \cosh \beta b \cos \alpha a = \cos [k(a + b)]$$

b → 0, $V_o \to \infty$, a→L, sinhβb→βb, coshβb→1

$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} \beta b \sin \alpha L + \cos \alpha L = \cos kL$$

but $\beta^2 >> \alpha^2$. Therefore

$$\frac{\beta^2 b}{2\alpha} \sin \alpha L + \cos \alpha L = \cos kL$$

or

$$\frac{P}{\alpha L} \sin \alpha L + \cos \alpha L = \cos kL$$

Keep in mind that $\alpha = (2mE/\hbar^2)^{1/2}$.

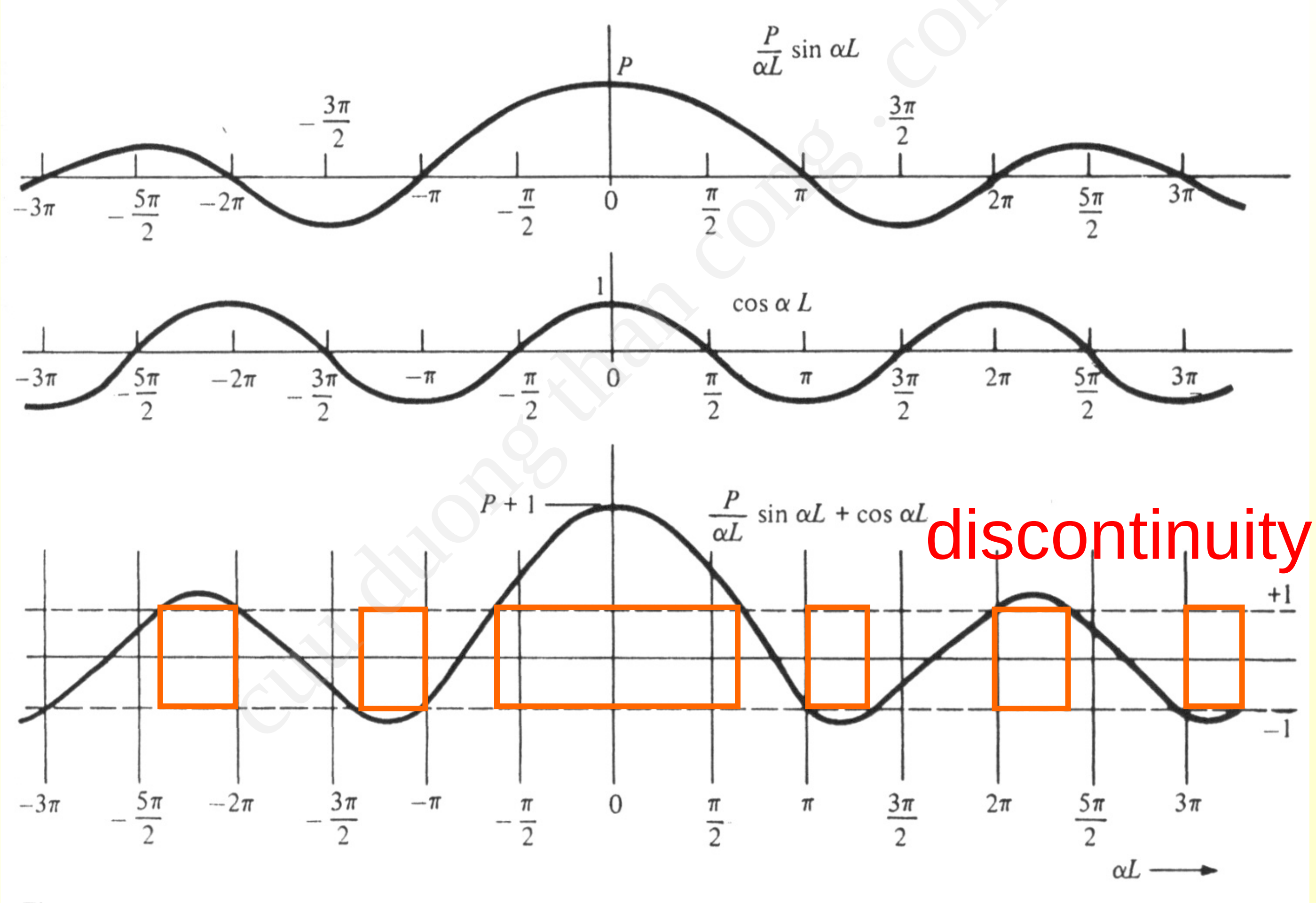
where

$$\lim_{\substack{\beta\to\infty \\ b\to 0}} \frac{\beta^2 ab}{2} = P$$

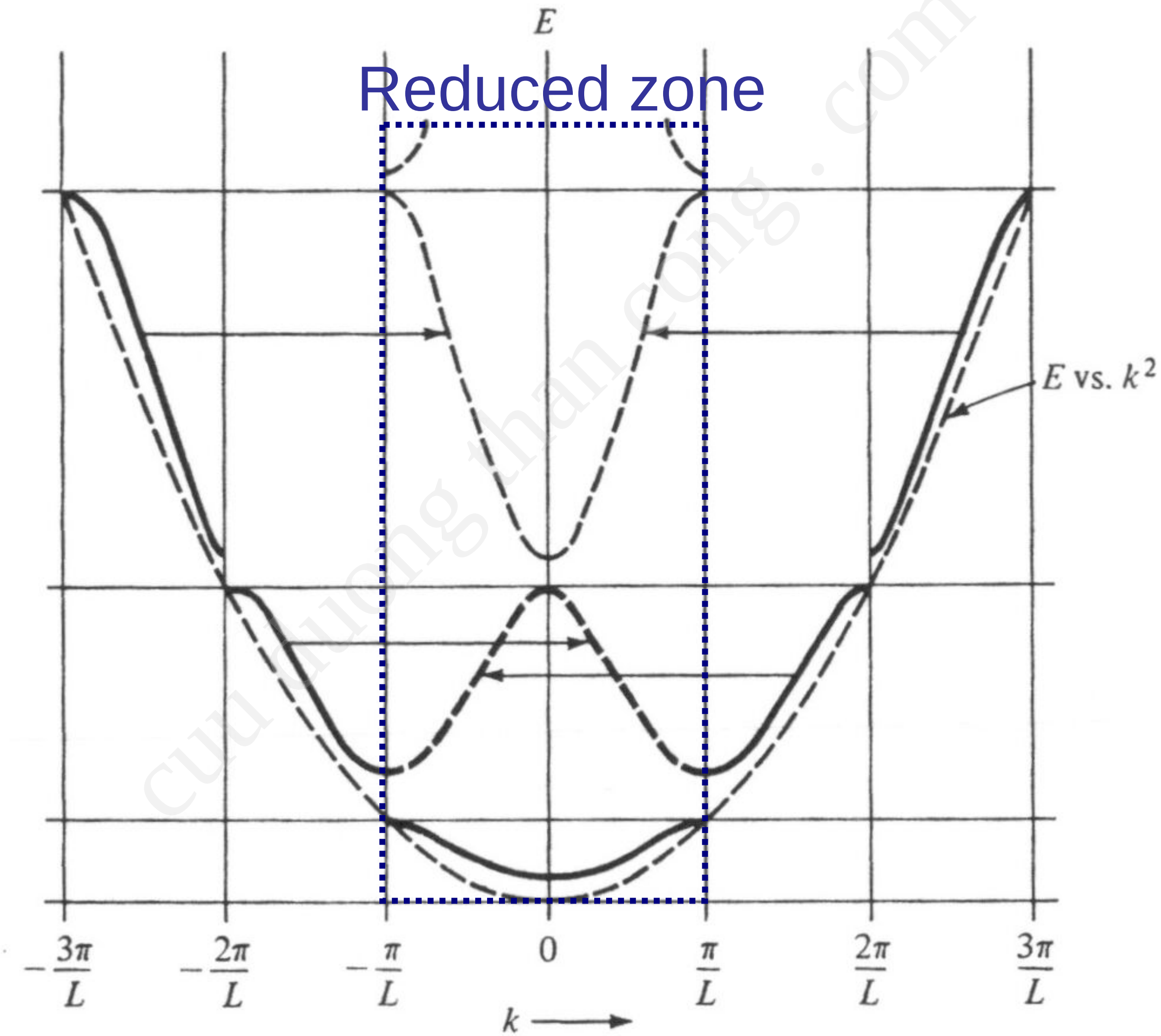
Then

$$\beta = \left[\frac{2m(V_0 - E)}{\hbar^2}\right]^{1/2} \approx \left[\frac{2mV_0}{\hbar^2}\right]^{1/2} \qquad \text{as } V_0 \to \infty$$

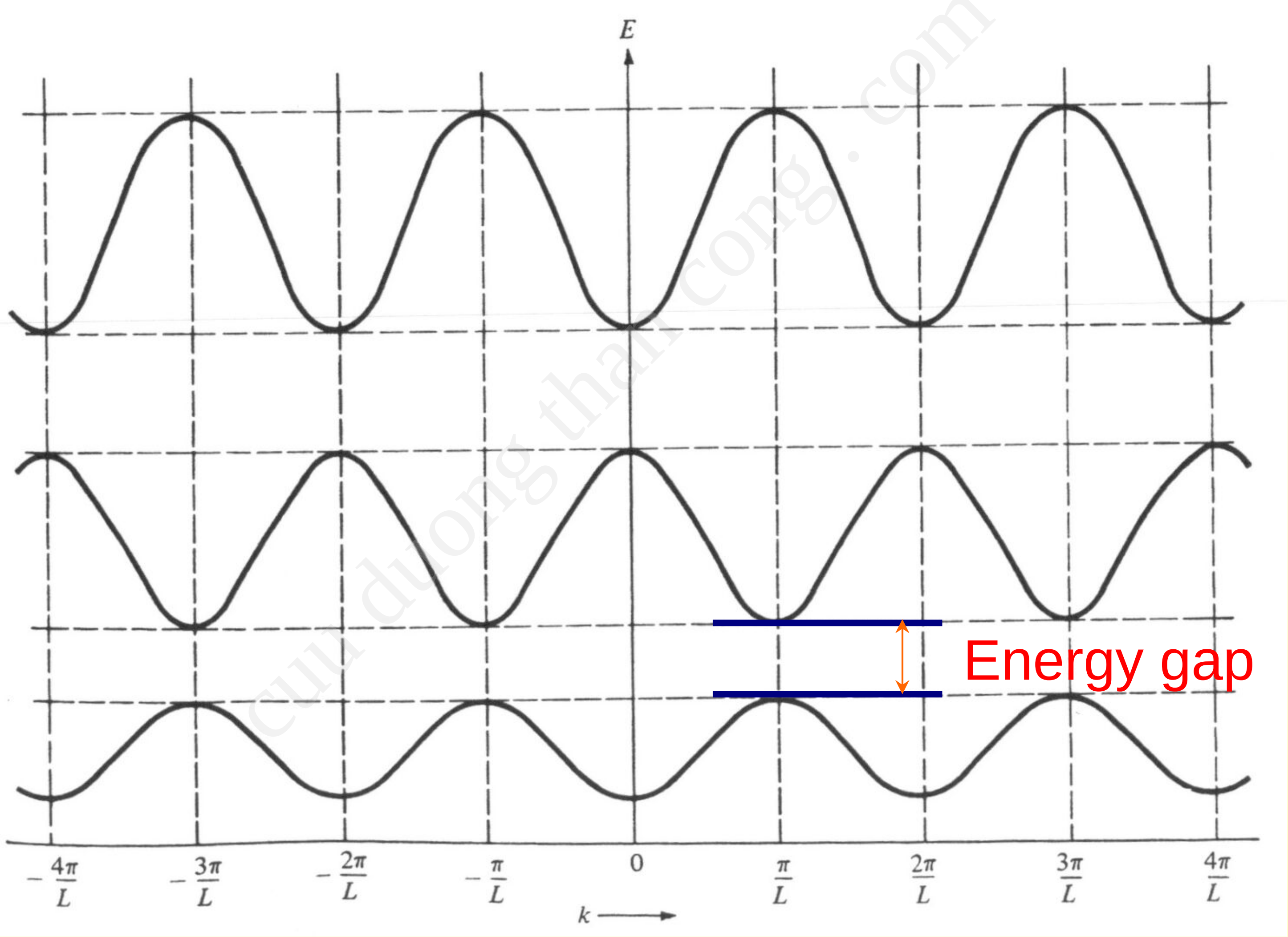
- Graphical solution



- Extended and reduced zone scheme



- Periodic zone scheme



- Electrons in crystals are arranged in energy bands separated by regions in energy for which no wavelike electron orbital exist. Such forbidden regions are called energy gaps or band gaps.
- Extended zone scheme: different bands are drawn in different zones in wavevector (k) space
- Reduced zone scheme: all bands are drawn in the first B-zone
- Periodic zone scheme: every band is drawn in every zone

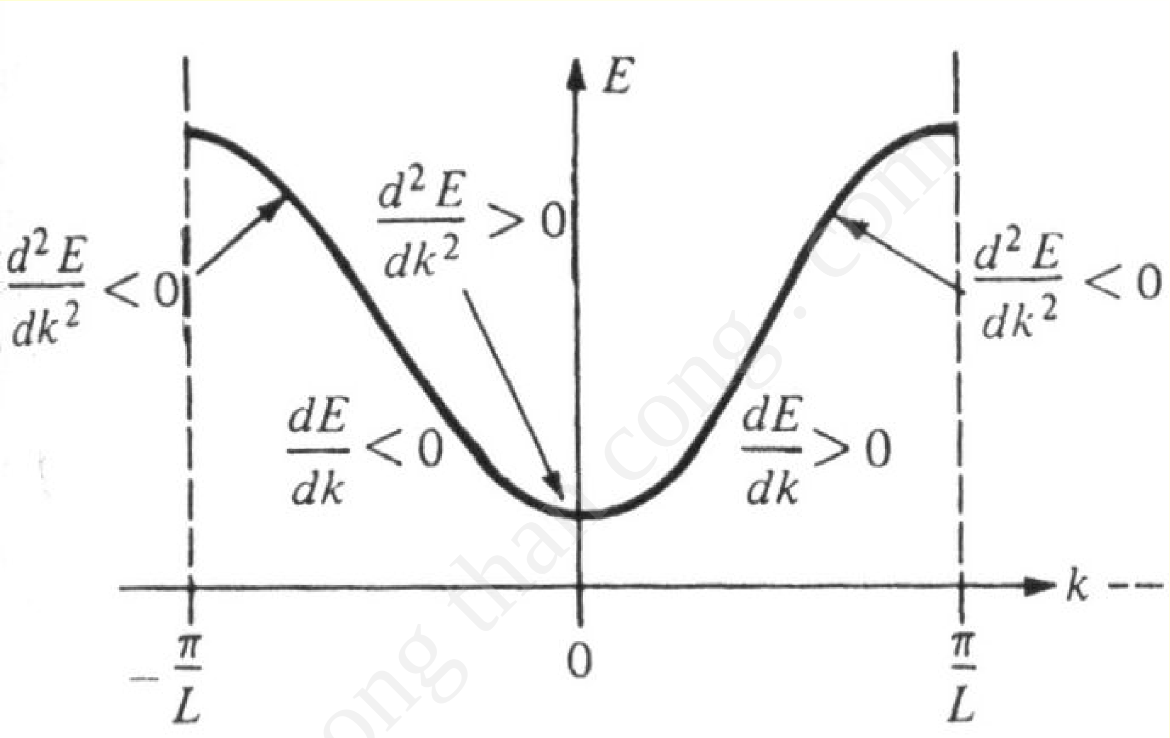
Effective mass

- Concept of packing periodic lattice into particle > "effective mass"

$E=p^2/2m= (\hbar k)^2/2m$

$dE/dk = \hbar^2 k/m \ (= \hbar v)$

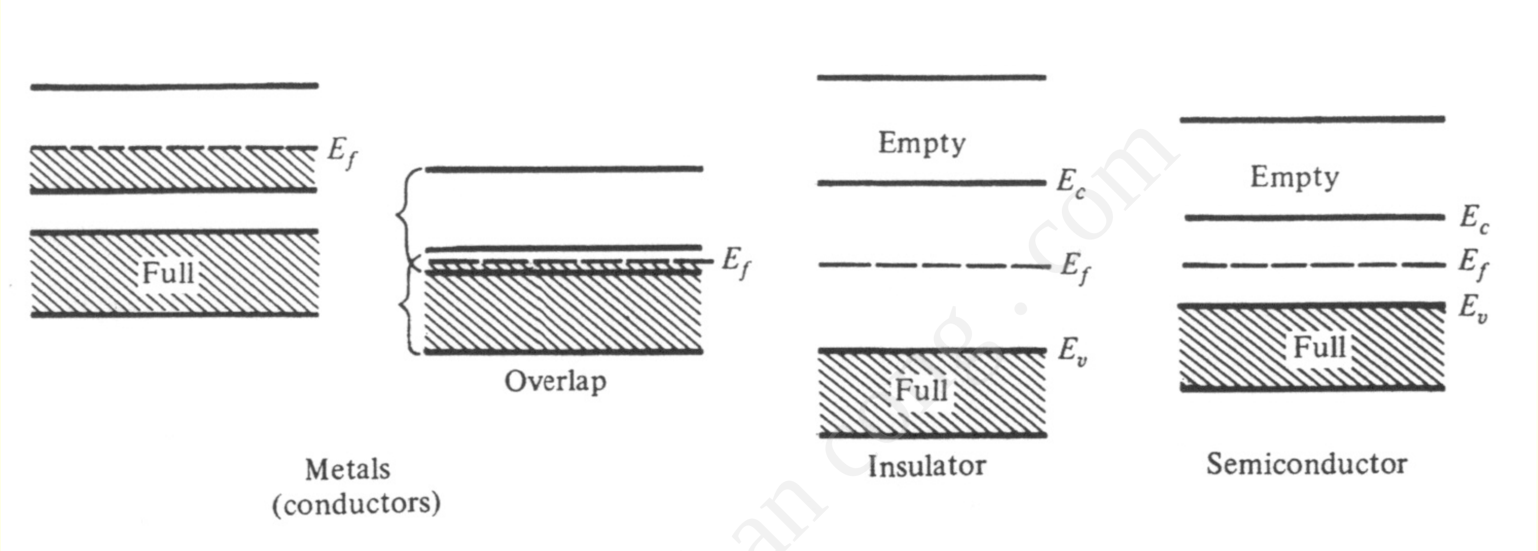
$m^* = \hbar^2 / (d^2E/dk^2)$



- ❑ Interpretation

+m* > acceleration

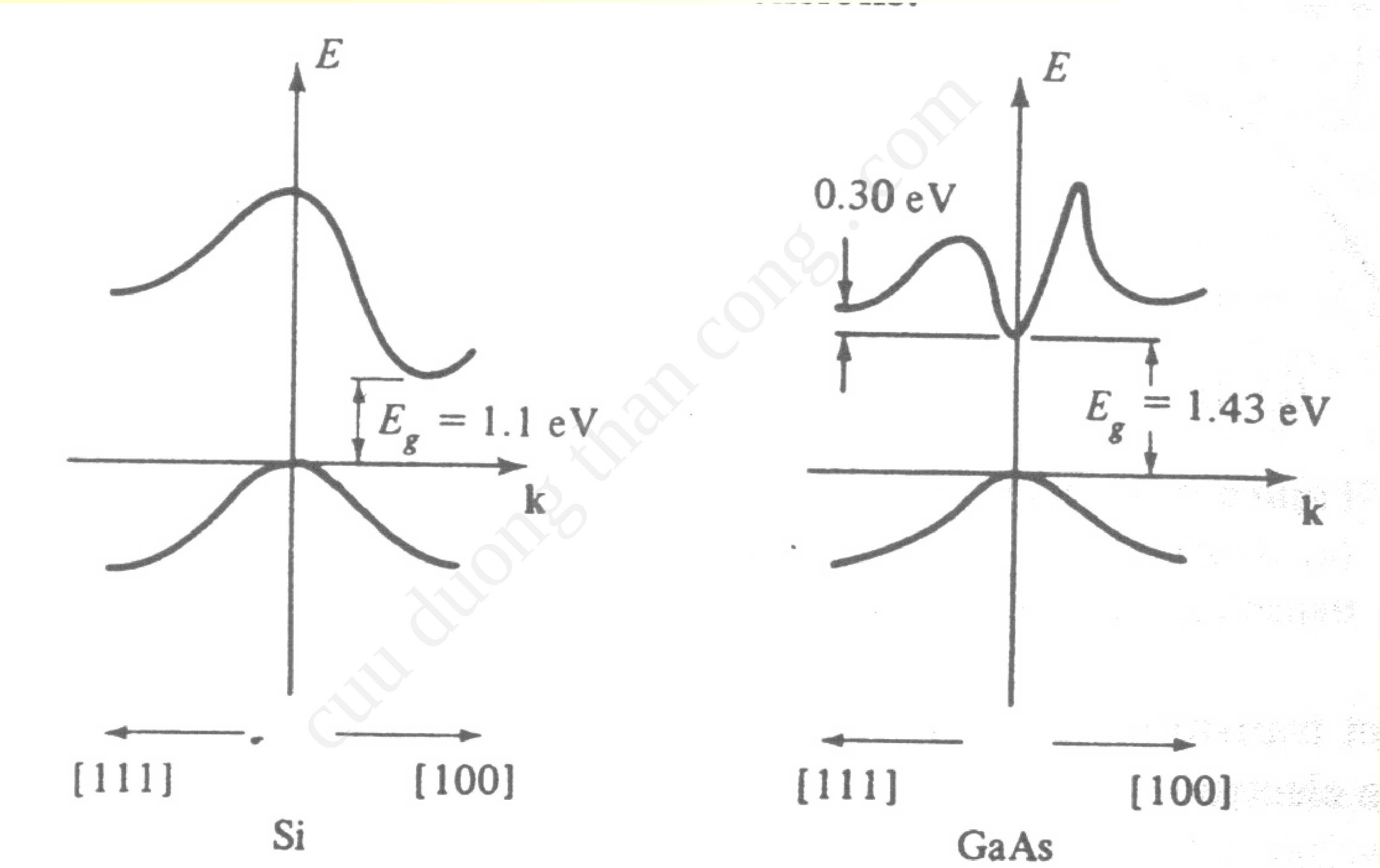
-m* > deceleration



- Valence band: highest energy levels that is fully occupied by (valence) electrons (at 0K)
- Conduction band: vacant or partially occupied energy levels in which electrons can move freely
- Band gap: Eg=Ec-Ev

Holes

- Imaginary particle of +e
- Vacant orbitals on an otherwise filled band
- $k_h = -k_e$
- $E(k_h) = -E(k_e)$
- $v_h = v_e$
- $m_h = -m_e$


E
E_g = 1.1 eV
k
[111]
[100]
Si
E
0.30 eV
E_g = 1.43 eV
k
[111]
[100]
GaAs

Density of States

$L = n_x\lambda$: standing wave condition

$p_x = h/\lambda$

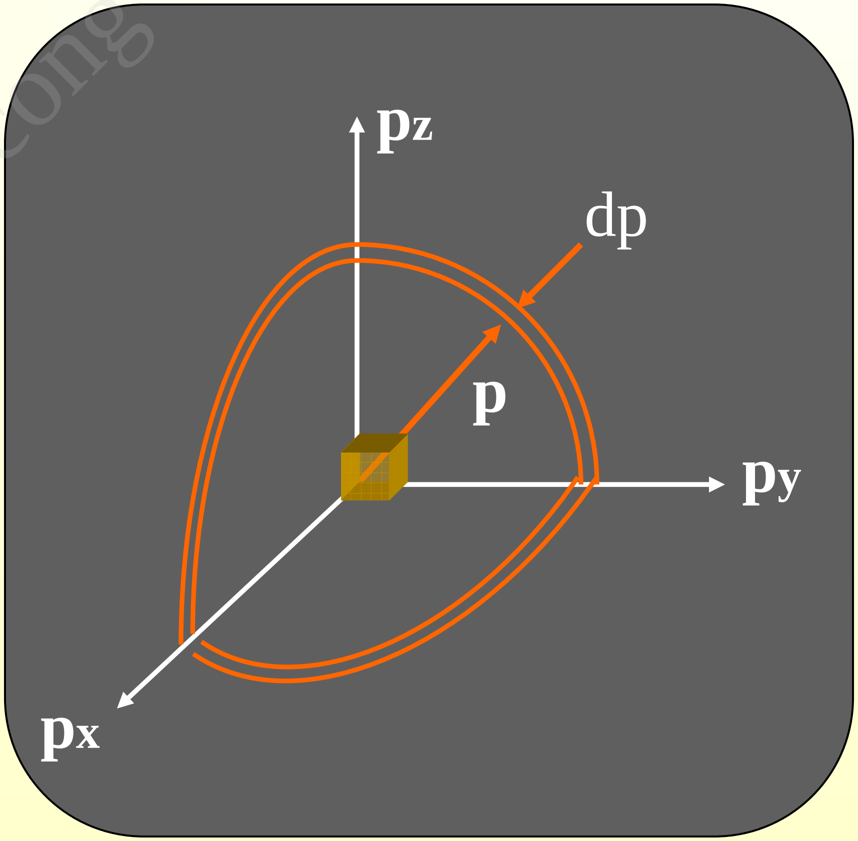
$Lp_x = hn_x$

$Ldp_x = h\ (dn_x = 1)$

For 3-D cube of side L,

$L^3dp_xdp_ydp_z = h^3$

Unit cube (L=1) = h^3



Volume between two concentric spheres,

$dV = 4\pi p^2 dp$

# of energy states contained,

$2(4\pi p^2 dp)/h^3$

$N(E)dE = 8\pi p^2 dp/h^3 = 4\pi(2m_n/h^2)^{3/2} E^{½}\, dE$

Therefore,

$N(E) = 4\pi(2m_n/h^2)^{3/2} E^{½}$: density of states

Intrinsic carrier concentration

n = (density of states) x (probability of occupying)

$n = \int N(E)f(E)dE$, from 0 to E_{top}

$$f(E) = \frac{1}{1 + \exp[(E-E_f)/kT]}$$

Approximation

$f(E) = \exp[-(E-E_f)/kT]$ for $E-E_f > 3kT$

$f(E) = 1- \exp[-(E_f-E)/kT]$ for $E-E_f < -3kT$ (hole)

$n = 4\pi(2m_n/h^2)^{3/2} \int E^{½} \exp[-(E-E_f)/kT]\, dE$

from 0 to ∞

Set $x=E/kT$ then, solve $\int x^{½} e^{-x} dx$

$n = 2(2\pi m_n kT/ h^2)^{3/2} \exp(E_f/kT)$

General expression: for electron, use E_f-E_c

$n = N_c \exp[- (E_c-E_f)/kT]$

Where Nc = effective density of states in conduction band = $2(2\pi m_n kT/ h^2)^{3/2}$

Similarly,

$p = N_v \exp [- (E_f-E_v)/kT]$

where $N_v = 2(2\pi m_p kT/ h^2)^{3/2}$

For intrinsic semicoductor, $n=p=n_i$

where n_i = Intrinsic carrier density.

$$E_f = E_i = (E_c + E_v)/2 + kT/2 \ln(N_v/N_c)$$
$$= (E_c + E_v)/2 + 3kT/4 \ln(m_p/m_n)$$

$n_i^2 = np$

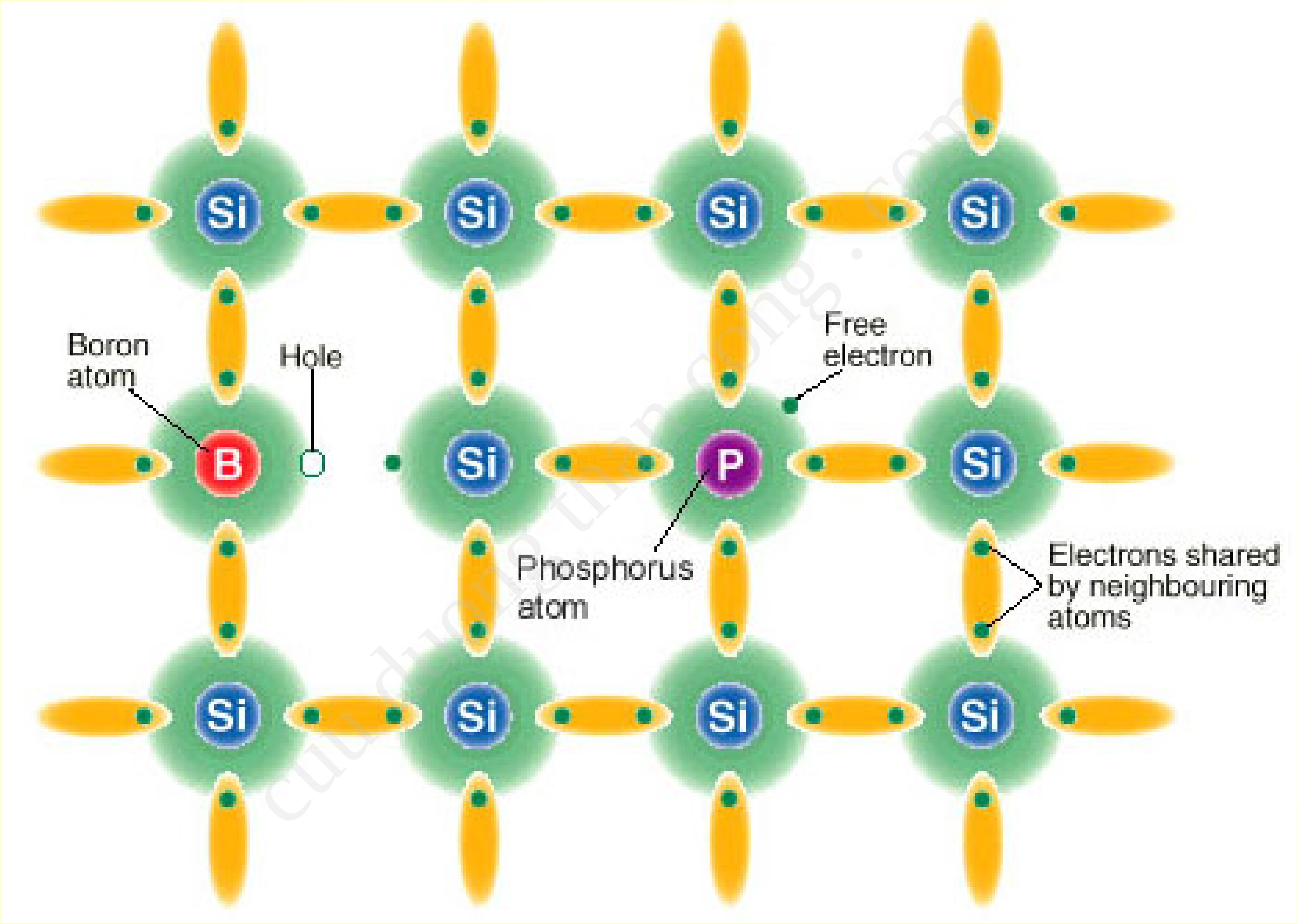
$n_i = \sqrt{N_c N_v} \exp(-E_g/2kT)$: mass action law

where $E_g = E_c - E_v$

Valid for intrinsic and extrinsic (with dopants) semiconductor under thermal equilibrium condition

Extrinsic semiconductor

- Dopants : purposely introduced impurities to change conductivity of semiconductors
- Doping electron donor (coulmn V :P, As, Sb) > introducing extra electrons > n-type
- Acceptor (column III: B, Al, Ga) > holes > p-type
- When a crystal is doped such that equilibrium carrier concentration n_0 and p_0 are different from the intrinsic carrier concentration n_i, it is said to be extrinsic.



from http://acre.murdoch.edu.au/refiles/ pv/text.html

- Under complete ionization condition,

$n = N_D$

N_D: donor concentration

$E_c – E_f = kT/ \ln(N_C/N_D)$

$p = N_A$

N_A: acceptor concentration

$E_f - E_v = kT/ \ln(N_V/N_A)$

- Relation between intrinsic and extrinsic

$n = N_c \exp[-(E_c-E_f)/kT]$

$= N_c \exp[-(E_c-E_i)/kT] \exp[(E_f-E_i)/kT]$

$= n_i \exp[(E_f-E_i)/kT]$

$p = n_i \exp[(E_i-E_f)/kT]$

- If donor and acceptor are present together,

From charge neutrality,

$n + N_A = p + N_D$

$n_n = f\ (N_D, N_A, n_i) =$

$p_n = n_i^2/n_n$

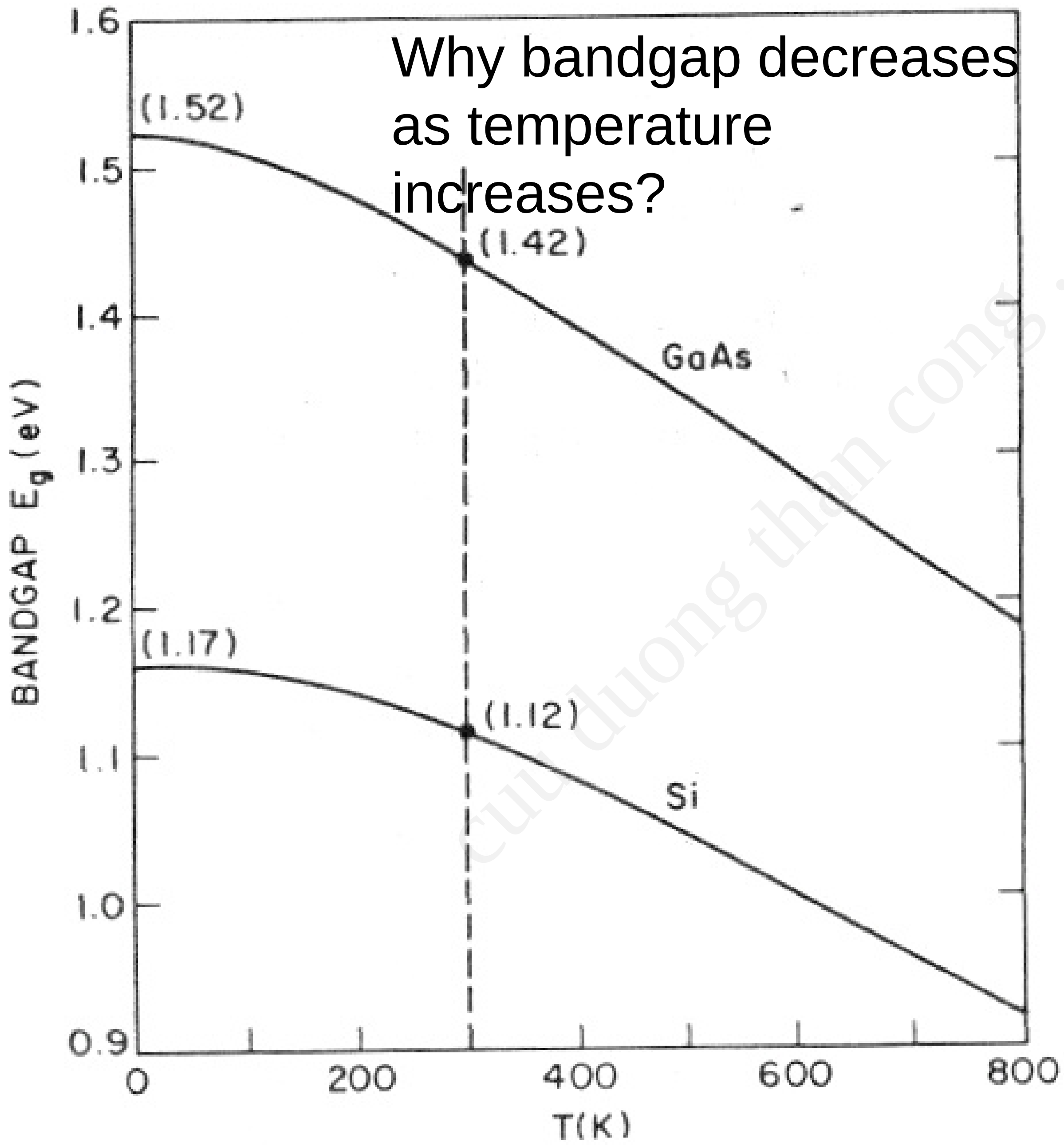
Subscript n refers n-type semiconductor

Similarly,

$p_p =$

$n_p = n_i^2/p_p$

Why bandgap decreases as temperature increases?



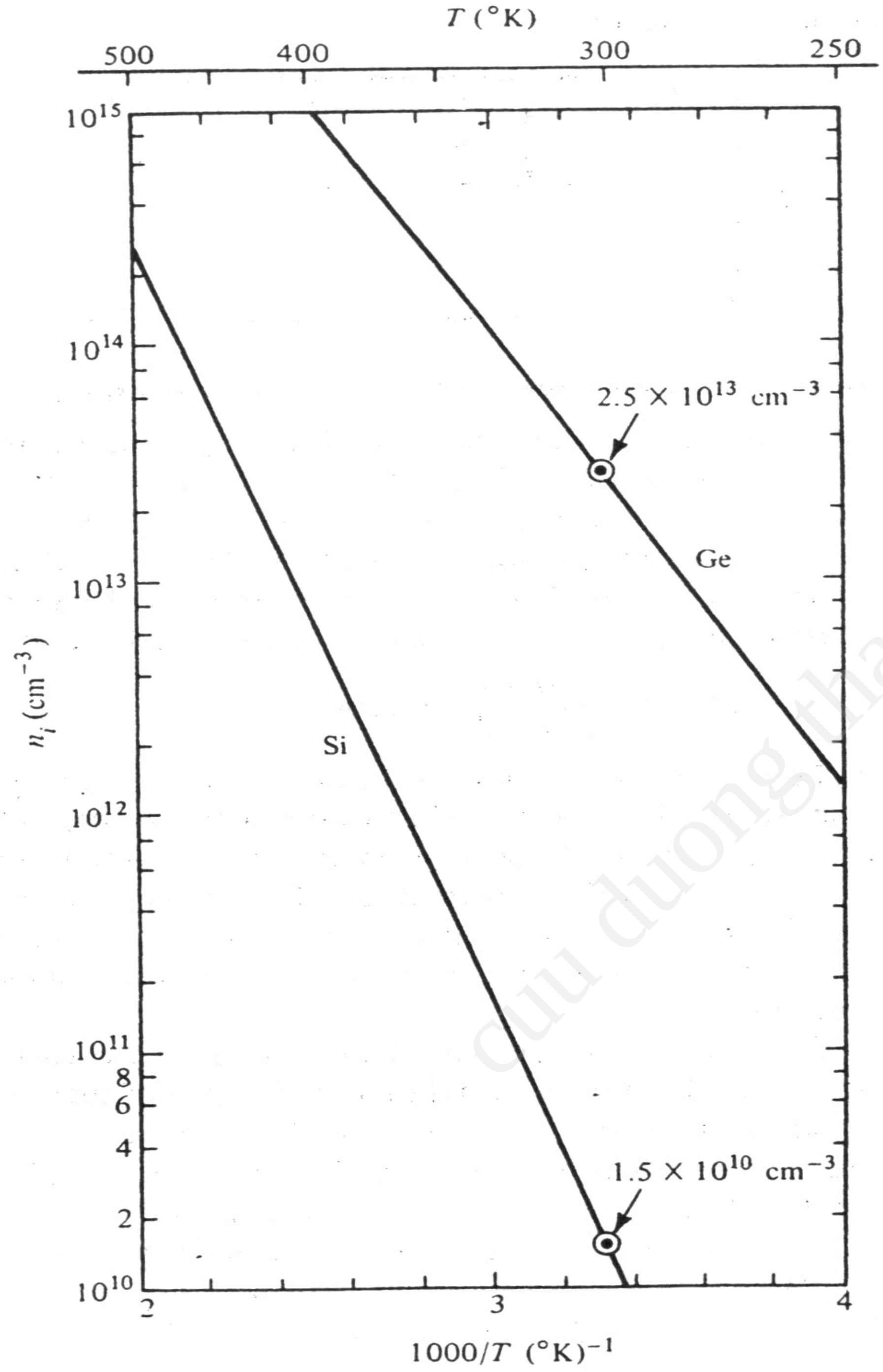
T ↑

Vibration amplitude ↑

Interatomic distance ↑

Potential on electron ↓

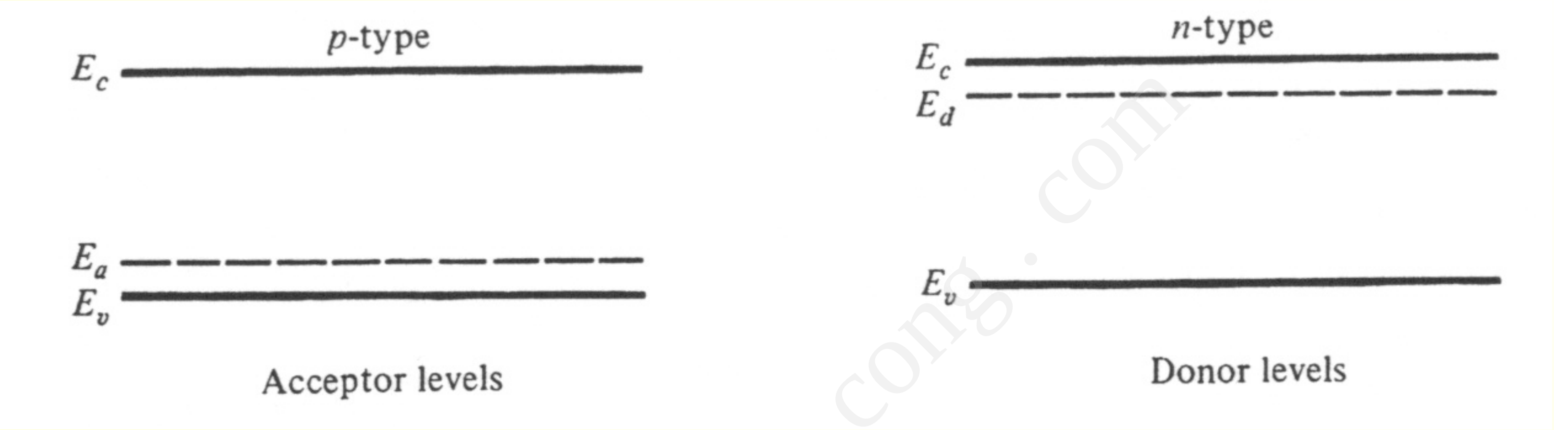
Bandgap ↓



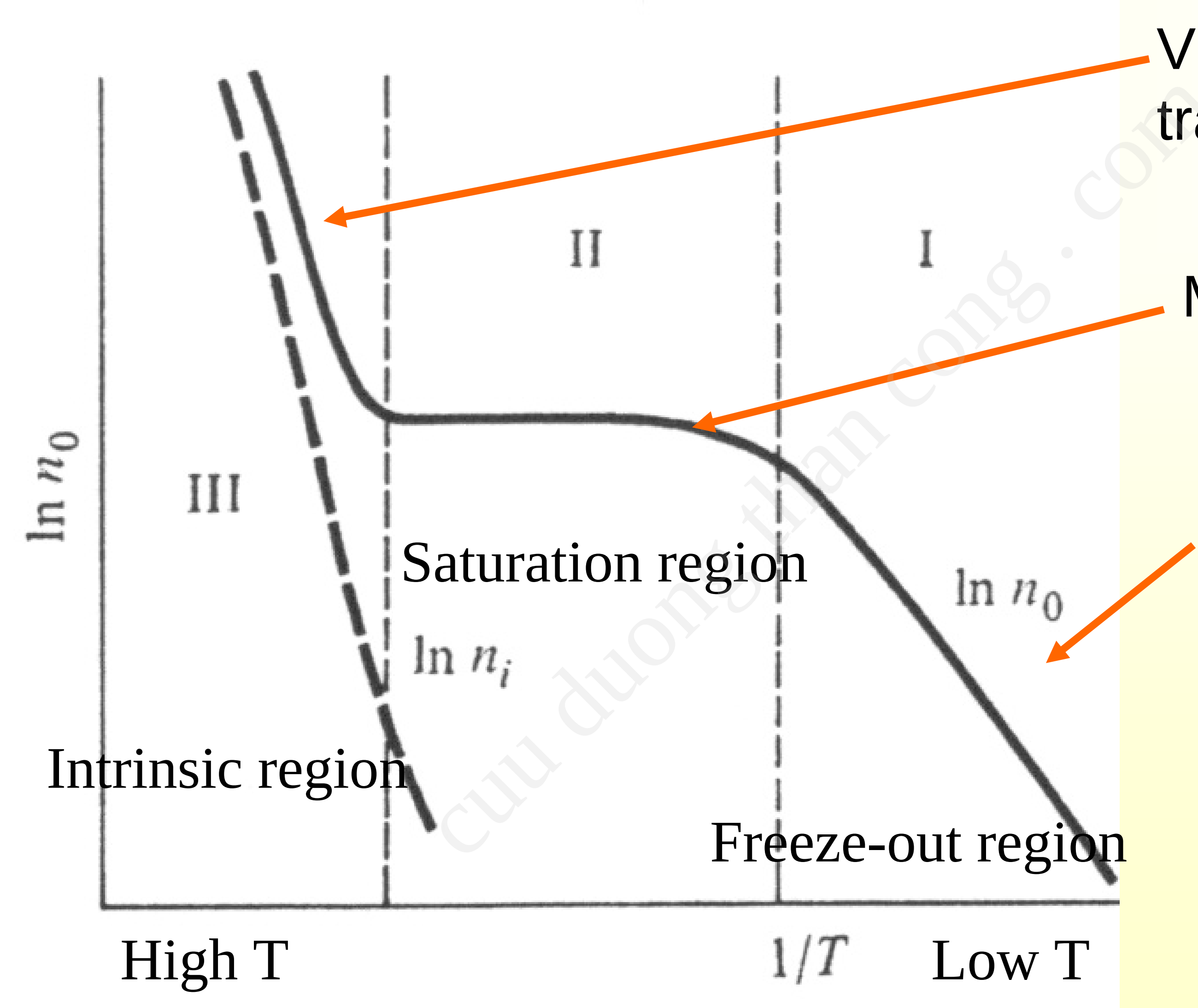
Why carrier concentration increases as temperature increases?

n_i vs. 1000/T

$n_i = \sqrt{N_c N_v} \exp(-E_g/2kT)$



Extra energy levels are formed from impurities.
Excess electrons or holes are localized in a single energy level (at low temperature); donor energy level or acceptor energy level.
Donors or acceptors produce conduction electrons or valence-band holes.



Valence-conduction transition dominant

Most impurities ionized

No ionization

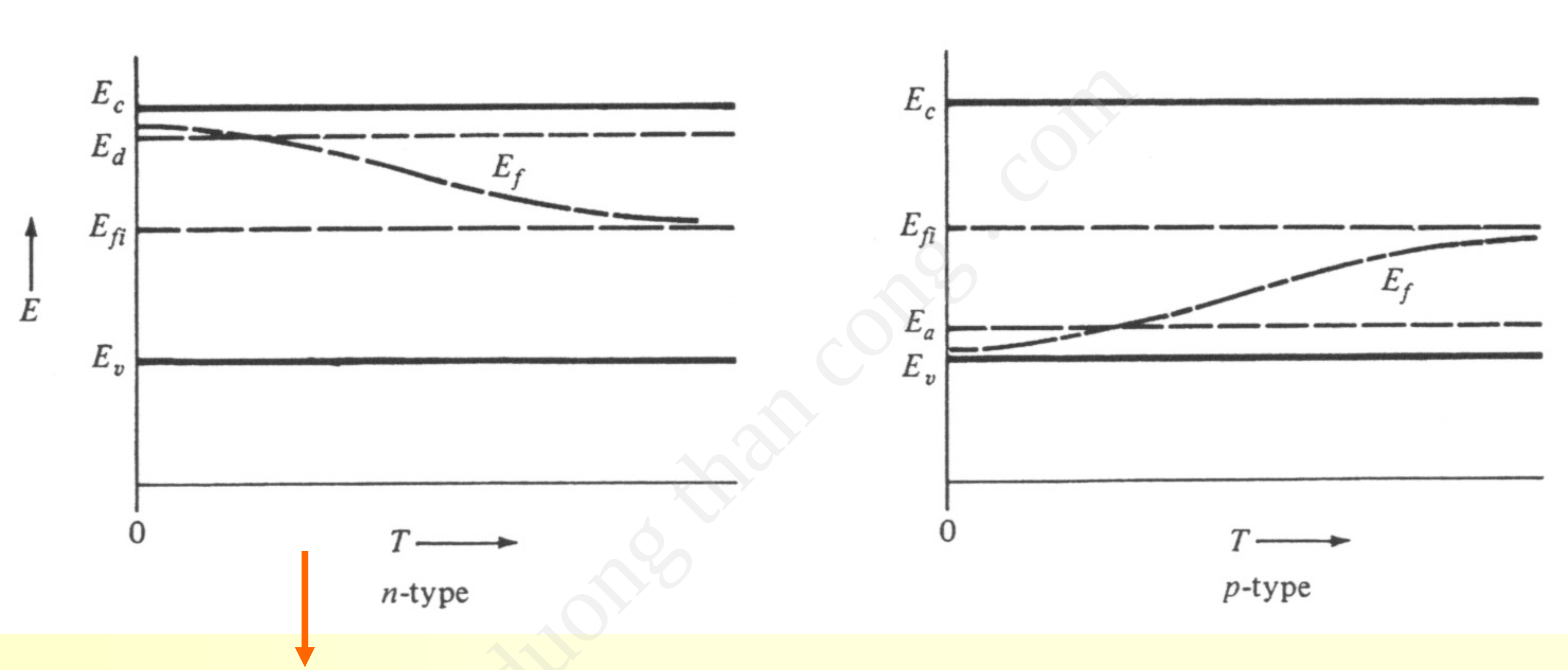
Saturation region

Intrinsic region

Freeze-out region

High T

Low T



At low T, donor level is completely filled; $E_c > E_f > E_d$
As T increases, E_f approaches E_i

References

S. M. Sze, “Semiconductor Devices - Physics and Technology”

S. M. Sze, “Physic of semiconductor devices”

R. A. Colclaser and S. Diehl-Nagle, “Materials and devices”

C. Kittel, “Introduction to Solid State Physics”

B. G. Streetman, “Solid state electronic devices”

J. F. Shackelford, “Introduction to materials science for engineers”

Mobility

- Ideal gas law: pV=NkT

  Assumption:

  Particles

  - Obey Newton's law of motion.
  - Move in all direction with equal probability.
  - Have no interactions between them.
  - Collide with the walls elastically.

- Kinetic Energy

Change of momentum

$$m\Delta v = F\Delta t = 2mv_x$$

Average time between collision

$$\Delta t = 2L/v_x$$

Average force

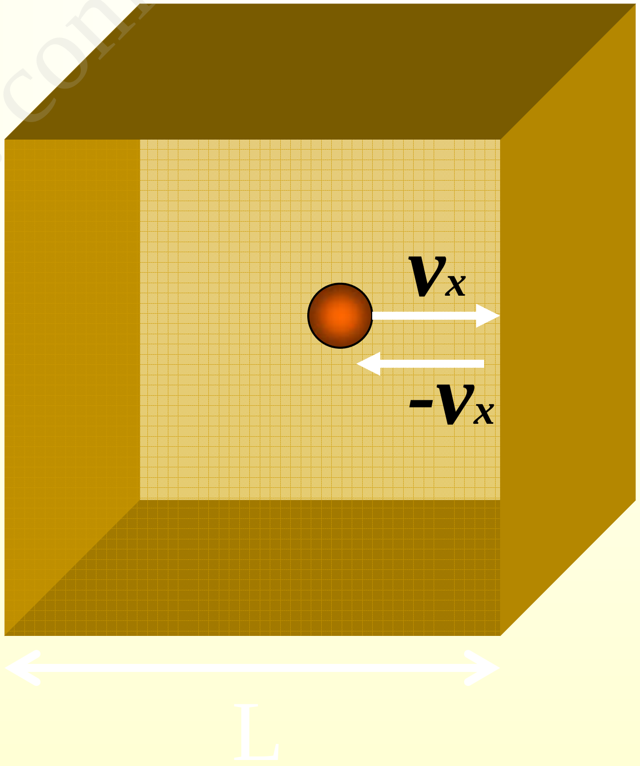
$$F = mv_x^2/L$$

Considering 3-D and N particles,

$$F = (1/3)\ N\ mv^2/L$$

Pressure on each wall

$$p = (1/3)\ N\ mv^2/L^3 = (1/3)N\ mv^2/V = (2/3)N/V\ \tfrac{1}{2}mv^2$$



Therefore,

$$p = 2/3\ N/V\ (KE)$$

Where, KE: Kinetic Energy,

$p = kT\ N/V$ from ideal gas law

$$\therefore KE = 3/2\ kT$$

For any x, y or z component,

KE per degree of freedom ,

$$KE_i = ½\ kT$$

At 300K,

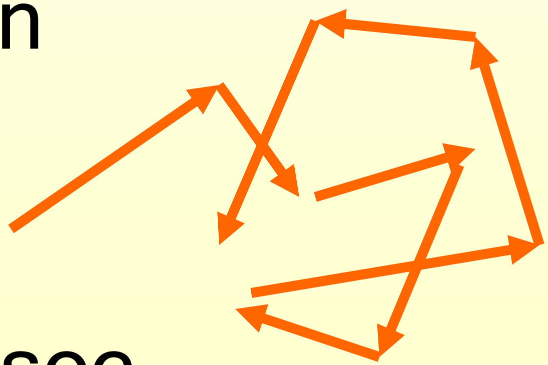
$3/2\ kT = 38.8$ meV

$kT = 25.8$ meV

$½\ kT = 12.9$ meV

- Thermal motion of an electron: random scattering from collisions with lattice atoms, impurities and other atoms.
- No net motion of n electrons/cm^3 over any period of time > no net current
- However, an individual electron moves at certain velocity
- At room temperature,

  thermal velocity of Si ~ 10^7 cm/sec



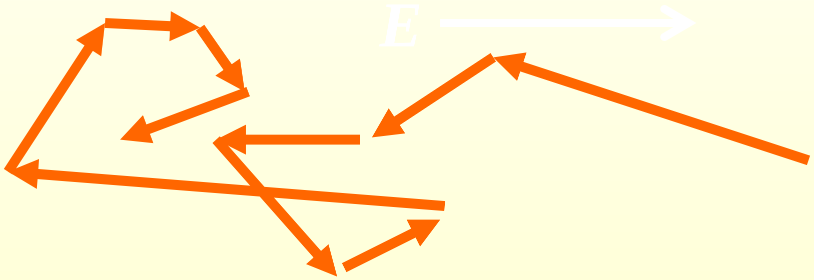
Applying $\boldsymbol{E}$ to x-direction,

force experienced by an electron is, $-q\boldsymbol{E}$

Net motion occurs in –x direction.

Force acting on the n electrons/cm^3 by electric field is

$F_{appl} = -q\boldsymbol{E}$



Then, electrons are accelerated continuously?

- Net acceleration is balanced in steady state by the collision process.
- Momentum applied = momentum gained

$$-q\boldsymbol{E}\tau = m_n v_n$$

Where,

v_n = drift velocity : additional velocity component superimposed on random thermal motion

τ = mean free time: mean time between collisions

- $v_n = -(q\tau / m_n)E = -\mu_n E$
- $\mu_n = -v_n / E$
- Mobility is the proportionality factor describing how well the electron motion respond to an applied electrical field.
- Electron mobility, $\mu_n = q\tau / m_n$
- Hole mobility, $\mu_p = q\tau / m_p$

- Scattering

Lattice scattering from thermal vibration of lattice atoms, dominant at high T

resulting in $\mu_L \propto T^{-3/2}$

Impurity scattering from Coulombic interaction between charge carriers and ionized dopant impurities

resulting in $\mu_i \propto T^{3/2}/N_i$

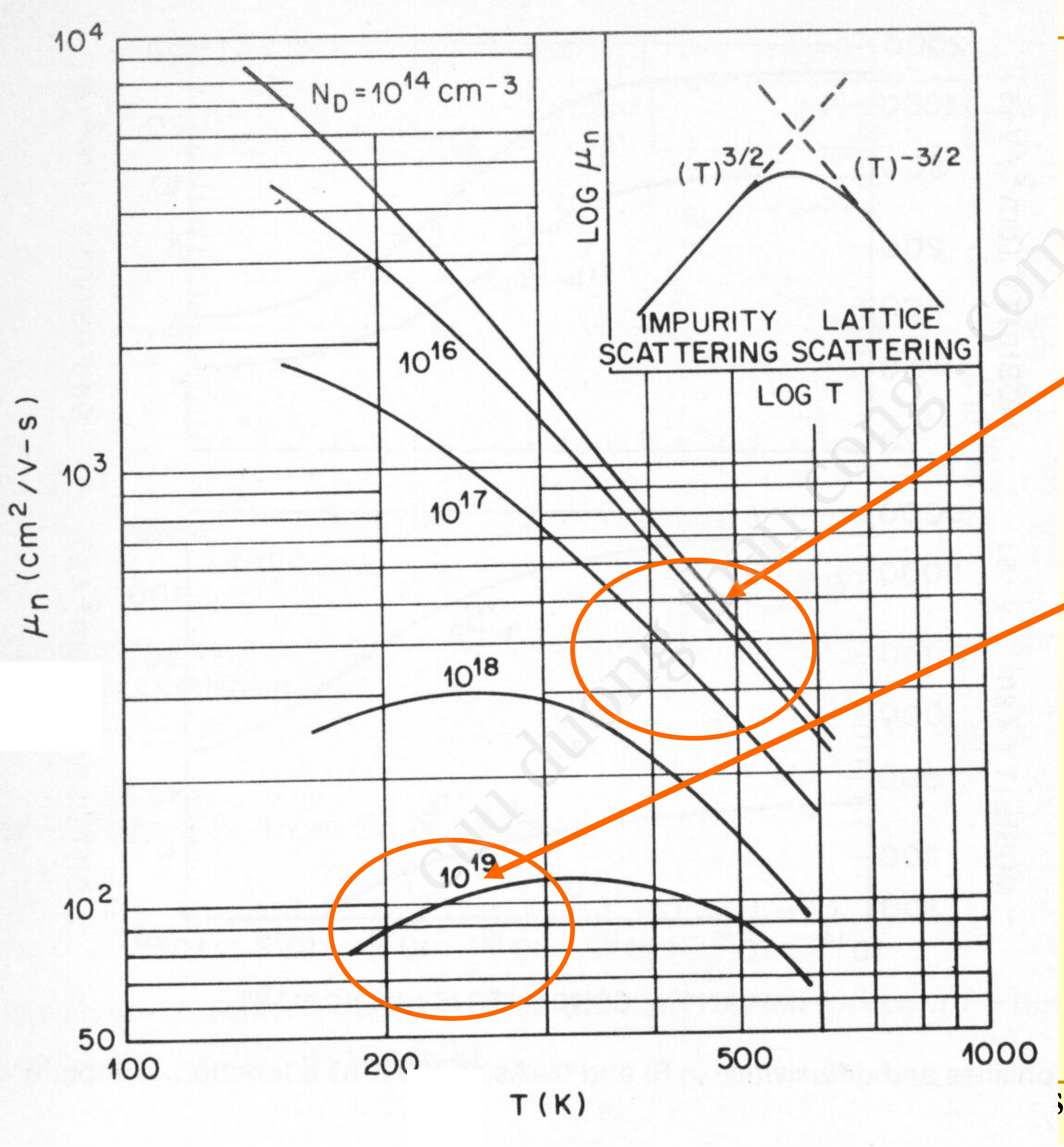
N_i : Total impurity conc.

- Probability of a collision taking a place in unit time is,

$$1/\tau = 1/\tau_{\text{lattice}} + 1/\tau_{\text{impurity}}$$

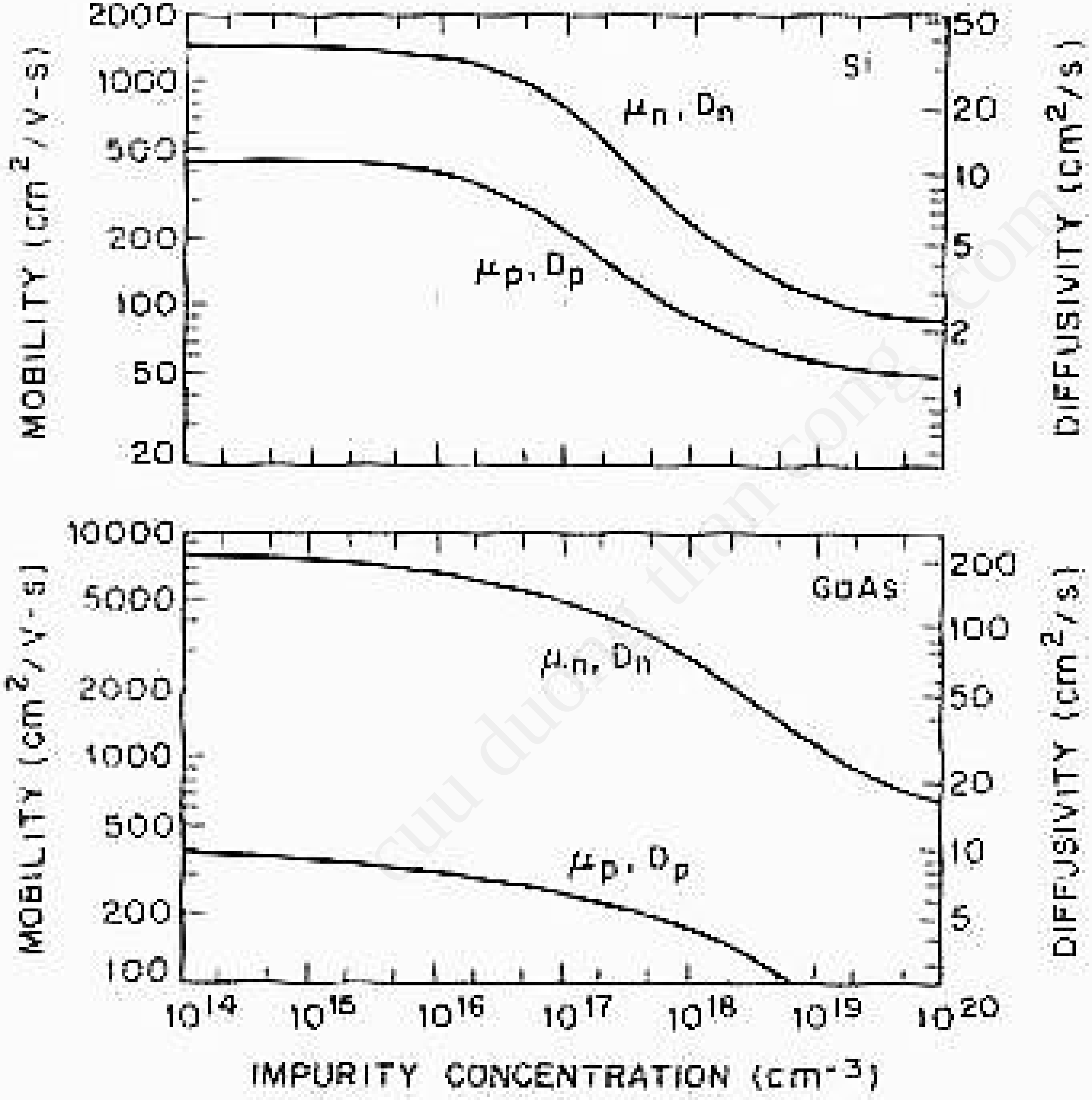
Therefore,

$$1/\mu = 1/\mu_L + 1/\mu_i$$

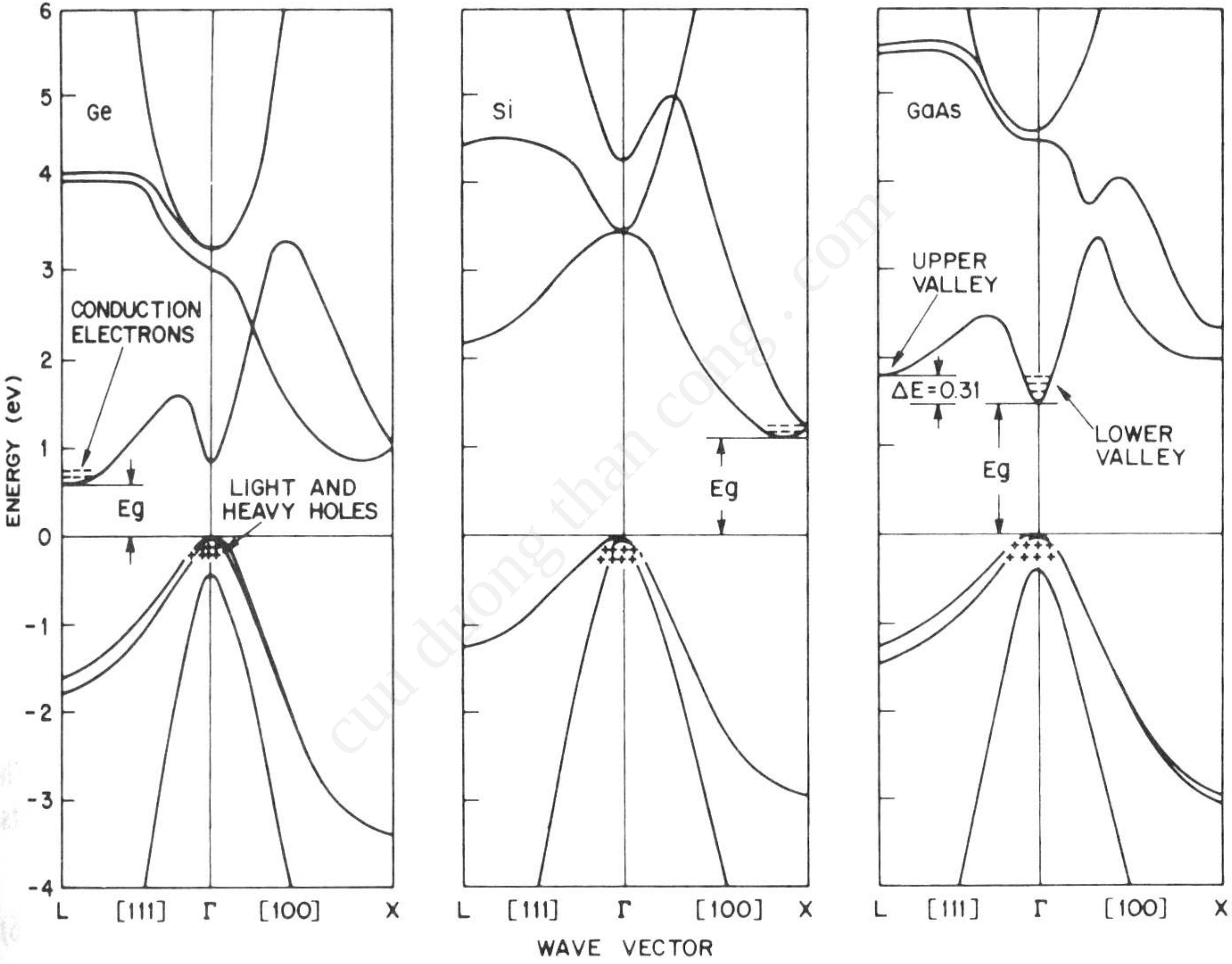


Lattice scattering dominates

Impurity scattering dominates



Electron mobility > hole mobility, why?


Ge
Si
GaAs
ENERGY (eV)
6
5
4
3
2
1
0
-1
-2
-3
-4
CONDUCTION ELECTRONS
LIGHT AND HEAVY HOLES
Eg
UPPER VALLEY
LOWER VALLEY
ΔE=0.31
L
[111]
Γ
[100]
X
WAVE VECTOR

Resistivity

- Drift current: transport of carriers under the influence of electric field
- Electron current density:

  $J_n = I_n/A = -qv_nN/V = -qnv_n = qn\mu_n \boldsymbol{E}$

  where I_n = electron current

  A = cross sectional area
- Hole current density:

  $J_p = I_p/A = qpv_n = qp\mu_p \boldsymbol{E}$
- Total current density:

  $J = J_n + J_p = (qn\mu_n + qp\mu_p)\boldsymbol{E} = \sigma \boldsymbol{E}$

- Conductivity

  $\sigma = qn\mu_n + qp\mu_p$

- Resistivity

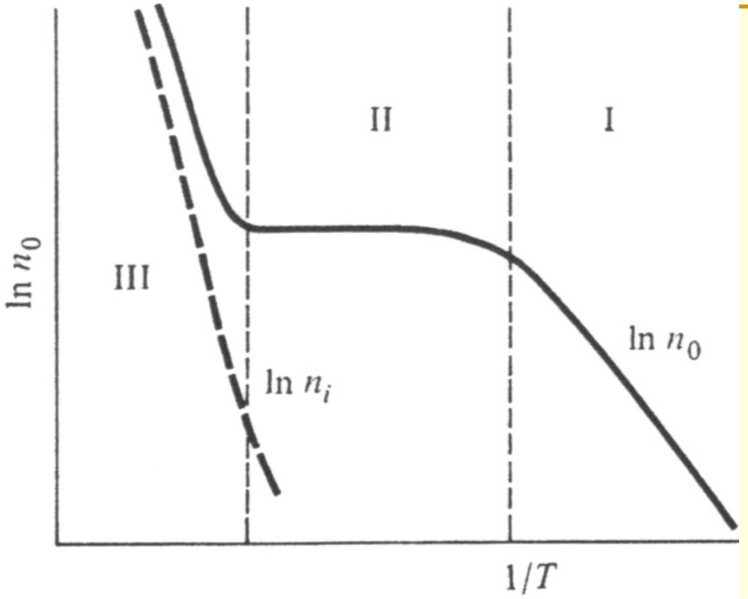
  $\rho = 1/(qn\mu_n + qp\mu_p)$

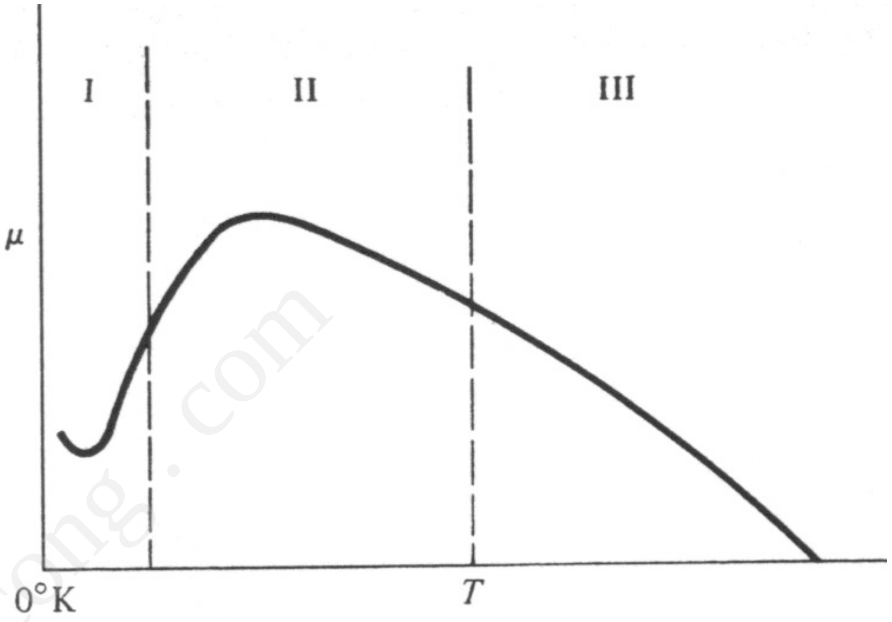
- For n-type

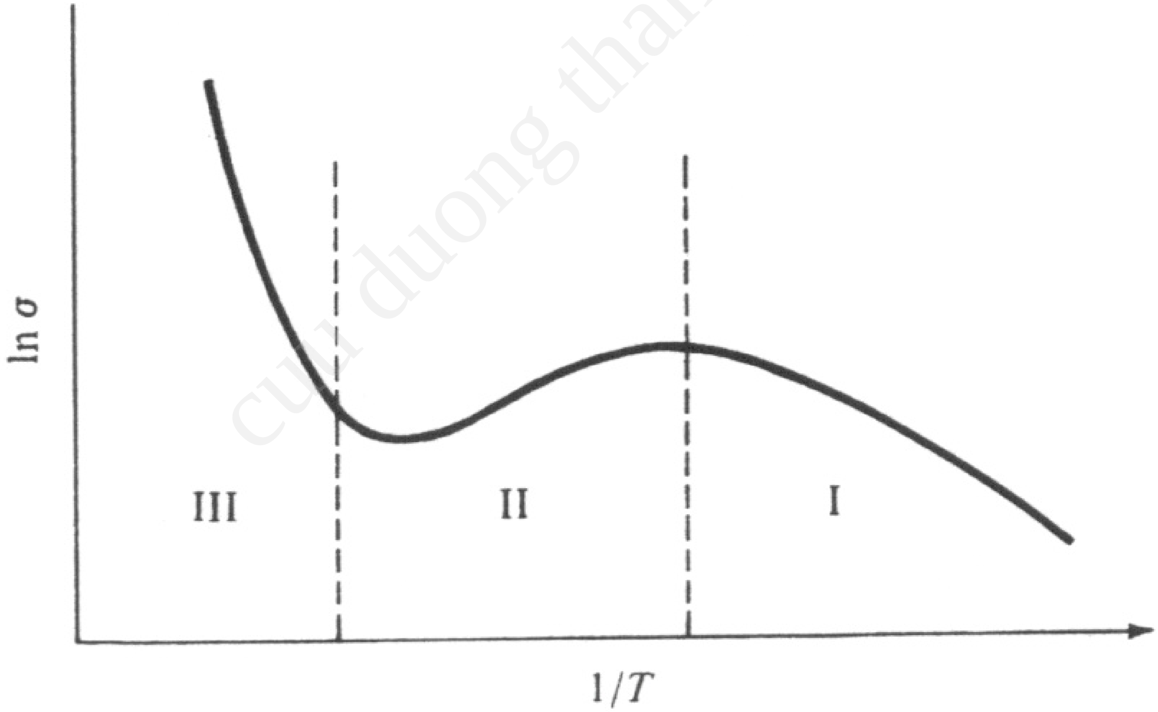
  $\rho = 1/qn\mu_n$

- For p-type

  $\rho = 1/qp\mu_p$

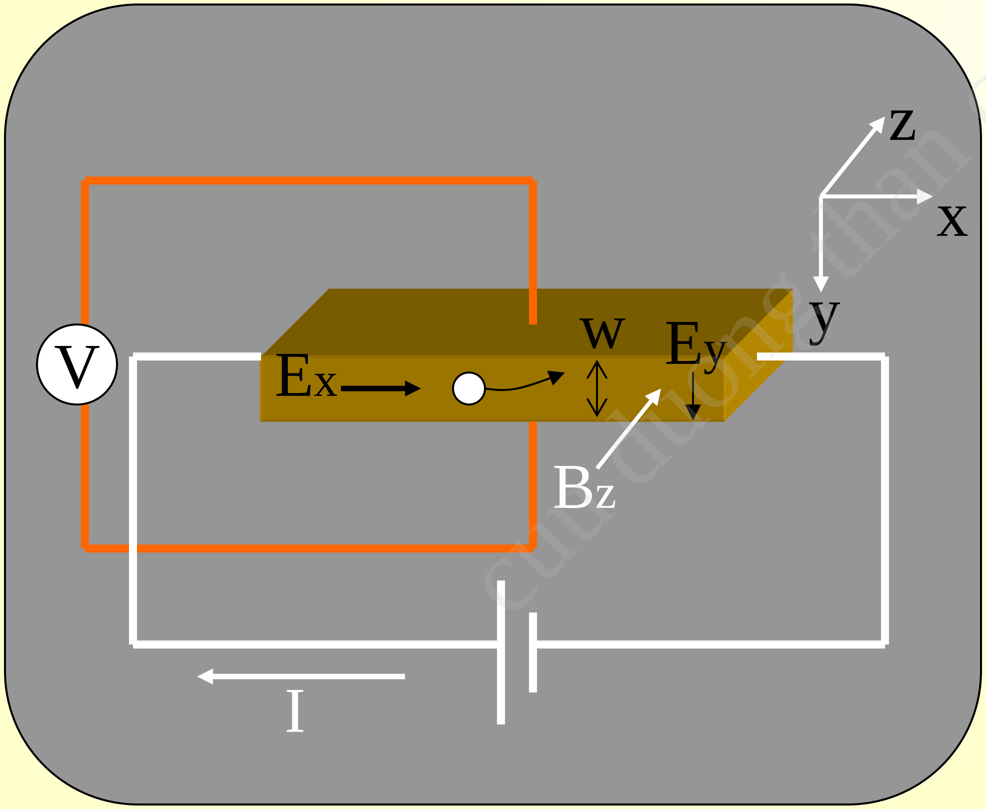

ln n_0
III
II
I
ln n_i
ln n_0
1/T


I
II
III
μ
0°K
T


ln σ
III
II
I
1/T

Hall effect

- Hall effect: establishment of electric field from Lorentz force



$qE_y = qv_xB_z$

$qE_y = qv_xB_z$: Hall field

Hall voltage, $V_H = E_yw$

$E_y = (J_p/qp)B_z = R_HJ_pB_z$

Hall coefficient

$R_H = 1/qp$ (for hole)

$R_H = -1/qn$ (for electron)

$p = 1/(qR_H) = J_pB_z/qE_y$

$= (I/A)B_z/[q(V_H/w)] = IB_zw/qV_HA$

By Hall measurement, carrier concentration can be obtained.

Drift and diffusion

- Diffusion current: transport of carriers from a spatial variation of carrier concentration
- Total current density:

$$J_n = qn\mu_n \boldsymbol{E} + qD_n\, dn/dx$$

$$J_p = qp\mu_p \boldsymbol{E} - qD_p\, dp/dx$$

- Total conduction current density:

$$J = J_n + J_p$$

- Einstein relation:

$$D_n = (kT/q)\mu_n$$

p-n Junction

- Electrostatic potential

When electric field is applied,

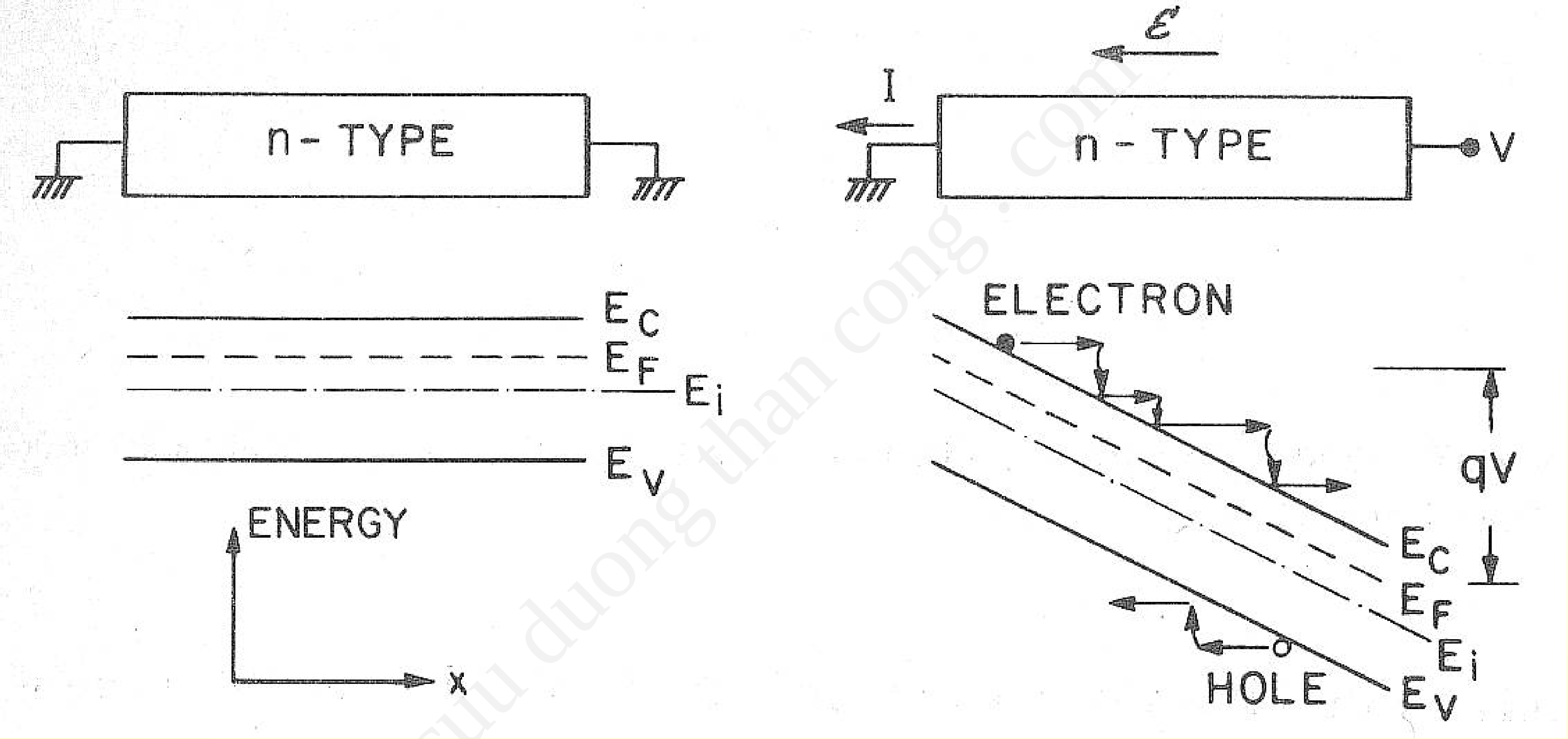
Force on electron= -q$\mathcal{E}$ = -grad(E),

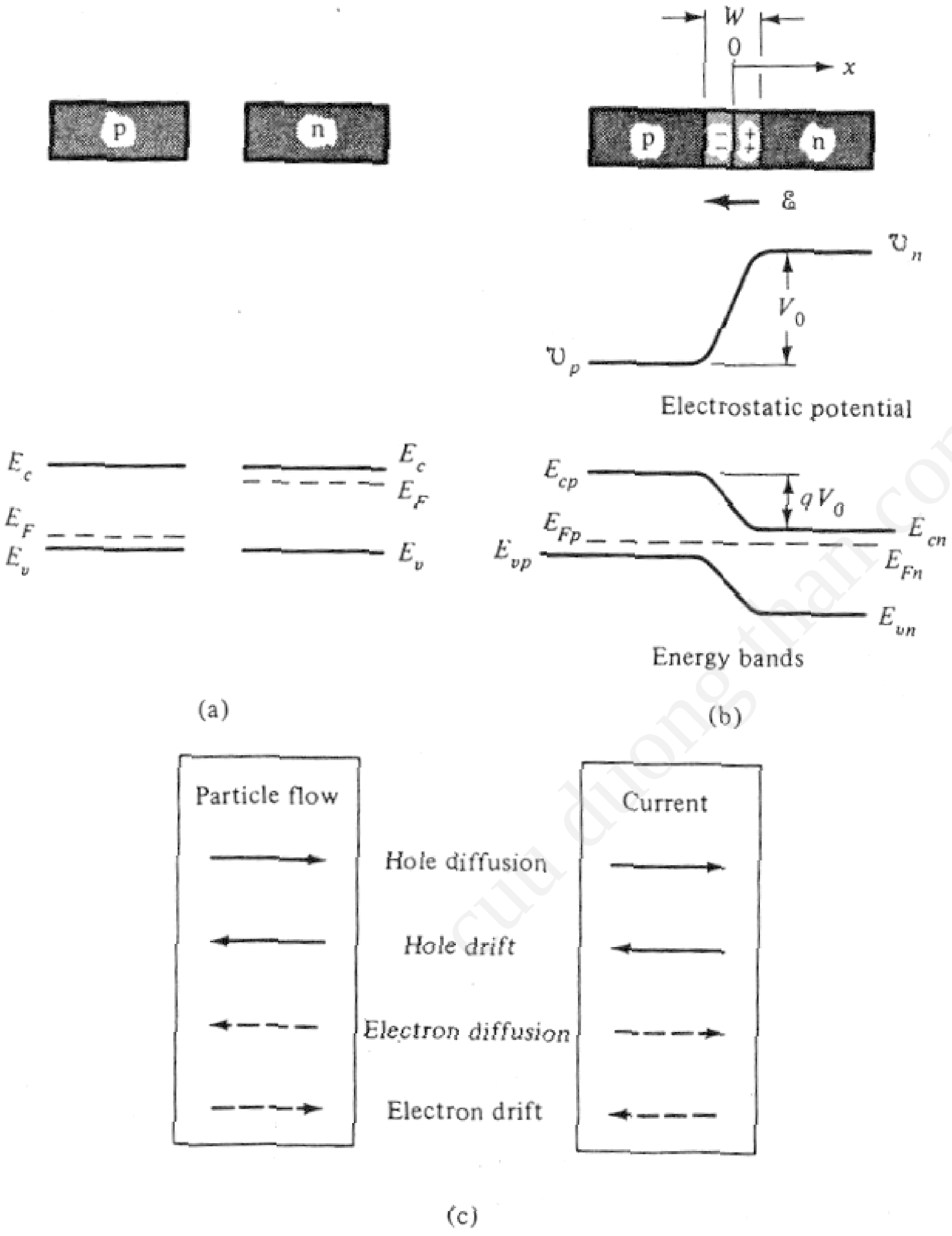
where E = electron potential energy

$$\mathcal{E} = (1/q)dE_i/dx \quad (1)$$

$$\mathcal{E} = -\,dV/dx \quad (2)$$

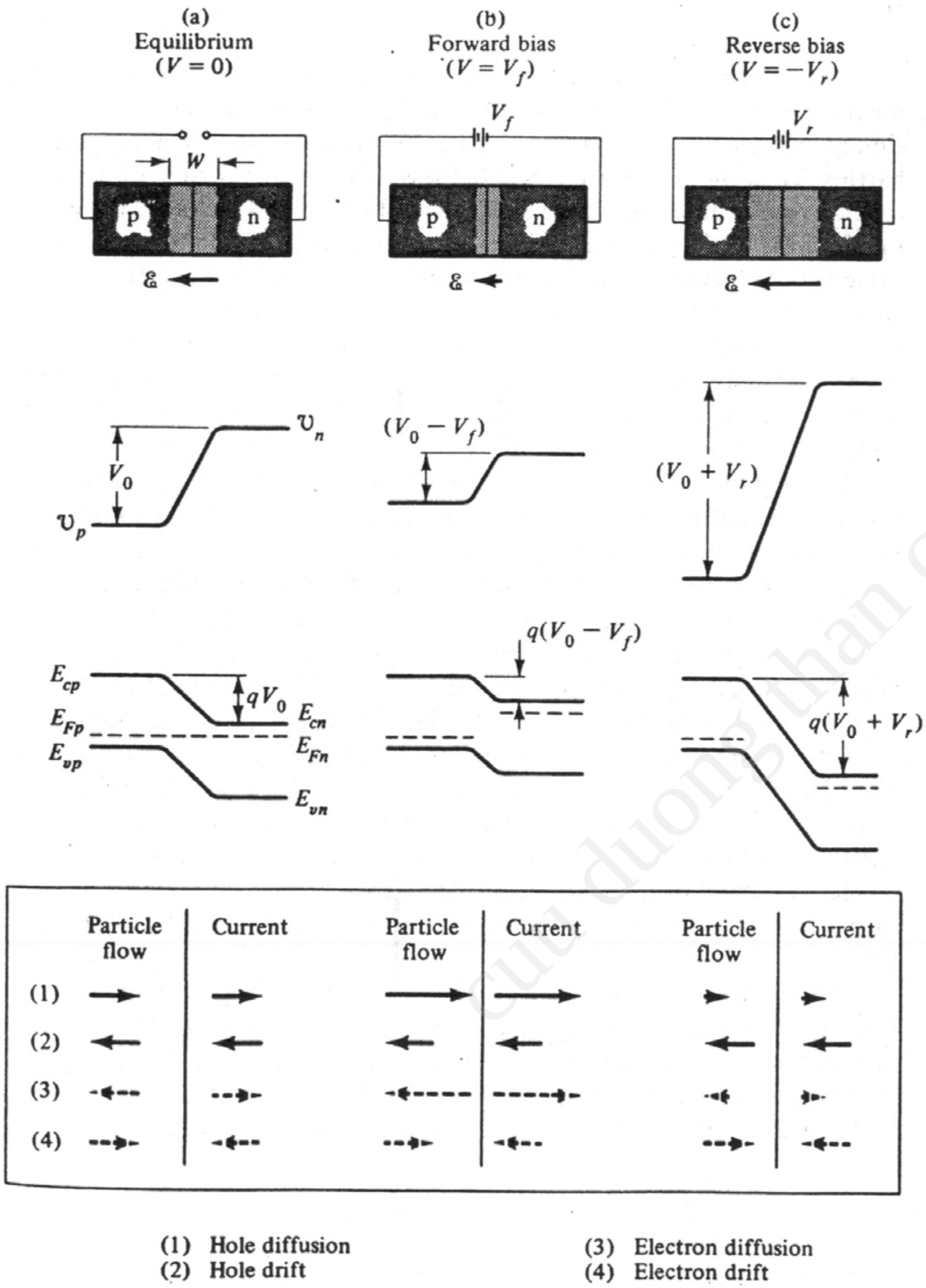
Electrostatic potential: $V = -E_i/q$ from (1) and (2)


n-TYPE
E_C
E_F
E_i
E_V
ENERGY
x
ℰ
I
n-TYPE
V
ELECTRON
qV
E_C
E_F
E_i
E_V
HOLE

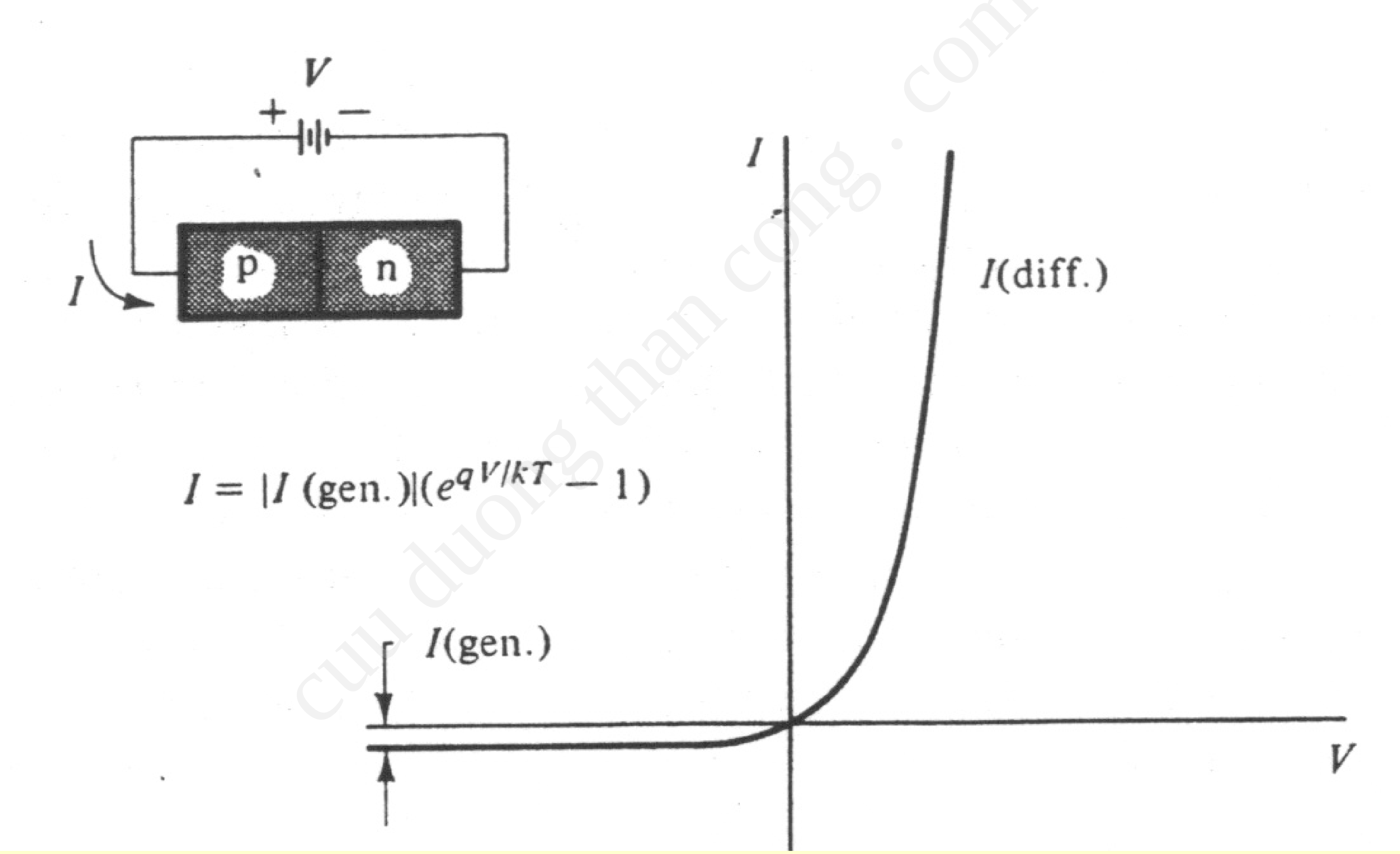


p
n
W
0
x
p
n
ℰ
𝒱_n
V_0
𝒱_p
Electrostatic potential
E_c
E_F
E_v
E_c
E_F
E_v
E_cp
E_Fp
E_vp
qV_0
E_cn
E_Fn
E_vn
Energy bands
(a)
(b)
Particle flow
Current
Hole diffusion
Hole drift
Electron diffusion
Electron drift
(c)

- Effects of bias
  - Built-in potential
  - Transition region



❑ I-V characteristics



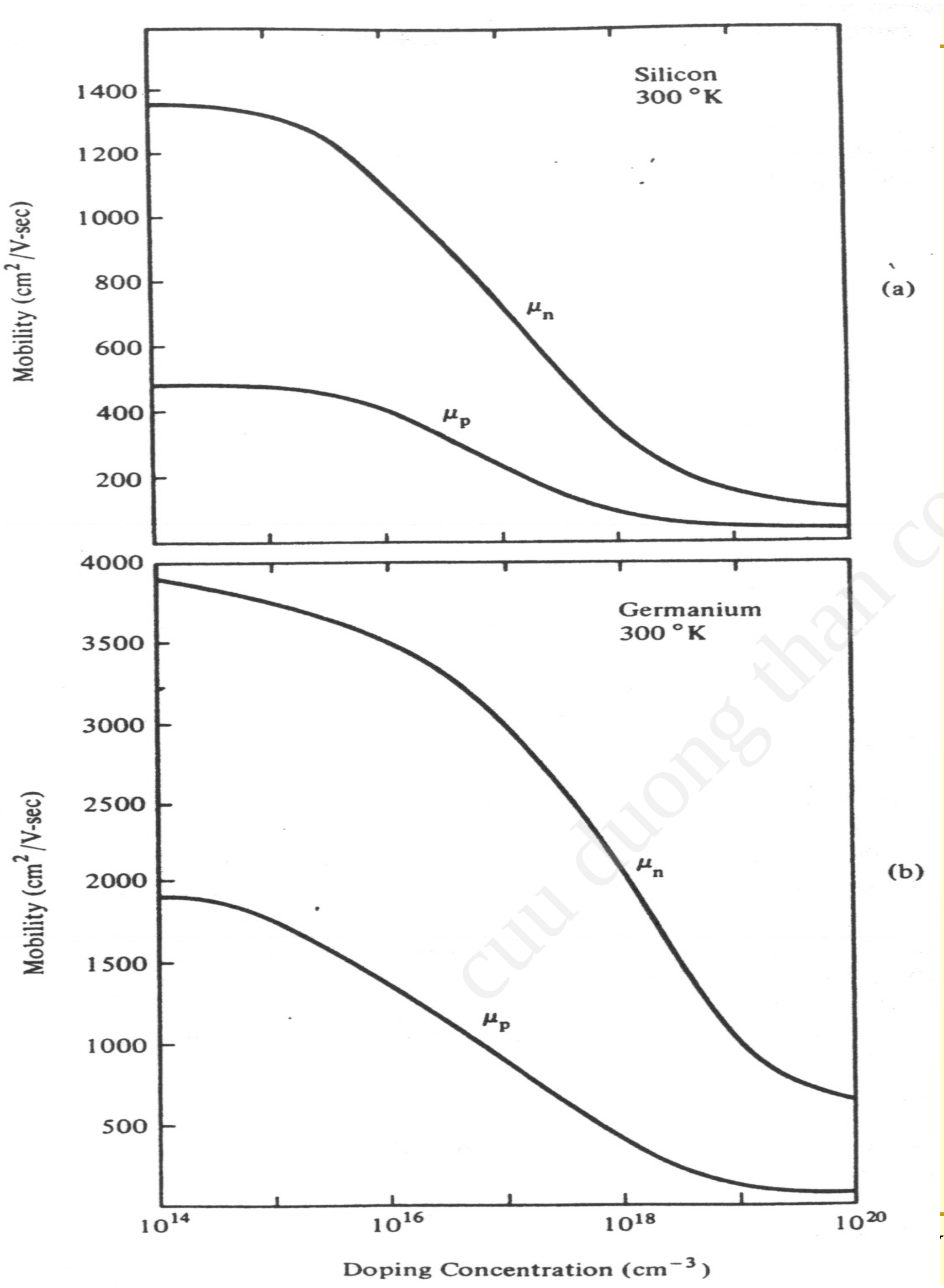
$$I = |I\,(\text{gen.})|(e^{qV/kT} - 1)$$

Important physical constants

Quantity	Symbol	Value
Angstrom unit	Å	1 Å = 10^{-4} μm = 10^{-8} cm
Boltzmann's constant	k	1.38×10^{-23} J/K = 8.6×10^{-5} eV/K
Electron charge	$-q$	-1.6×10^{-19} C
Electron rest mass	m_0	9.11×10^{-31} kg
Electron volt	eV	1.6×10^{-19} J
Permeability in vacuum	μ_0	$4\pi \times 10^{-9}$ H/cm
Permittivity in vacuum	ϵ_0	8.85×10^{-14} F/cm
Planck's constant	h	6.63×10^{-34} J·s

Properties of silicon at 300 K

Atomic density	5.0×10^{22} Atoms/cm^3
Bandgap energy	1.12 eV
Effective density of states	
Conduction band, N_c	2.8×10^{19} cm^{-3}
Valence band, N_v	1.04×10^{19} cm^{-3}
Intrinsic carrier concentration, n_{i0}	1.5×10^{10} cm^{-3}
Lattice constant	5.43 Å
Relative permittivity, ϵ_s	11.7
Mobility (intrinsic), μ_n	1350 cm^2/V·s
μ_e	480 cm^2/V·s


Silicon
300 °K
1400
1200
1000
800
600
400
200
Mobility (cm^2/V-sec)
μ_n
μ_p
(a)
Germanium
300 °K
4000
3500
3000
2500
2000
1500
1000
500
Mobility (cm^2/V-sec)
μ_n
μ_p
(b)
10^{14}
10^{16}
10^{18}
10^{20}
Doping Concentration (cm^{-3})

References

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