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PHYSICS OF ELECTRONIC MATERIALS AND DEVICES

Dr. Orrathai Watcharakitchakorn

Lecture 6

The band theory of solids

ทฤษฎีของแถบพลังงาน (สามารถอธิบายคุณสมบัติของวัสดุ)

- Band theories help explain the properties of materials.
- There are three popular models for band theory:

  - Kronig-Penney model

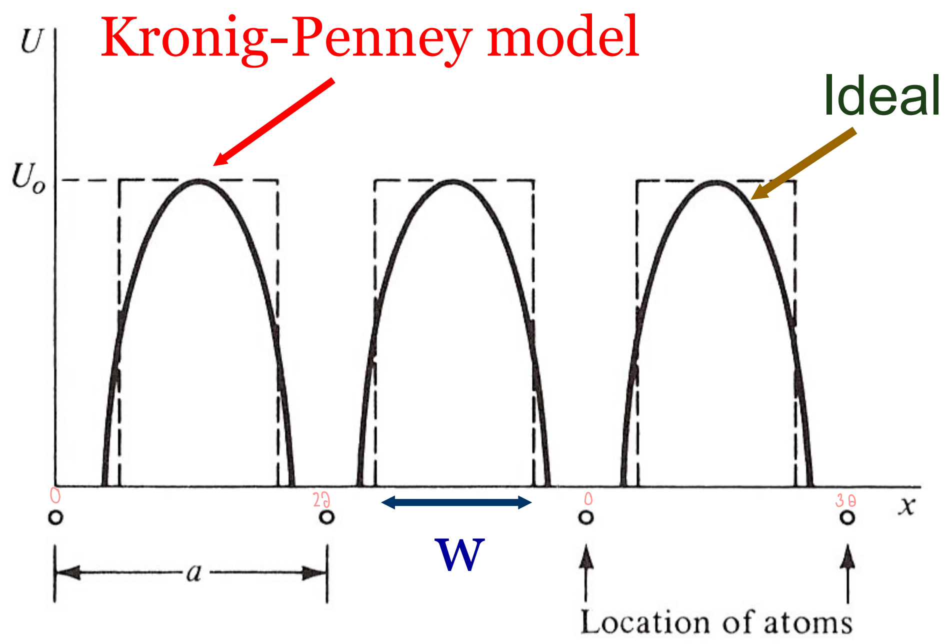
  - Ziman model

  - Feynman model

Kronig-Penney Model

ลักษณะของศักย์พลังงานไม่ต่อเนื่องเป็นคาบ

- Band theory uses $V \neq 0$. The potential is periodic in space due to the presence of immobile lattice ions.



Kronig-Penney Model

- Ions are located at $x = 0, a, 2a$, and so on. The potential wells are separated from each other by barriers of height U_0 and width w.
- From time-independent Schrödinger equation in 1-dimension (x-only), we have

สมการคลื่นเริ่มต้น

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}\{E-V(x)\}\psi(x)=0 \qquad (1)$$

Kronig-Penney Model

- For this equation to have solution, the following must be satisfied

เขียนสมการให้อยู่ในรูปนี้

Plot Graph

$$\cos(ka) = \frac{P\sin(\alpha a)}{\alpha a} + \cos(\alpha a) \qquad (2)$$

สูงสุดได้ 1

ต่ำสุดได้ -1

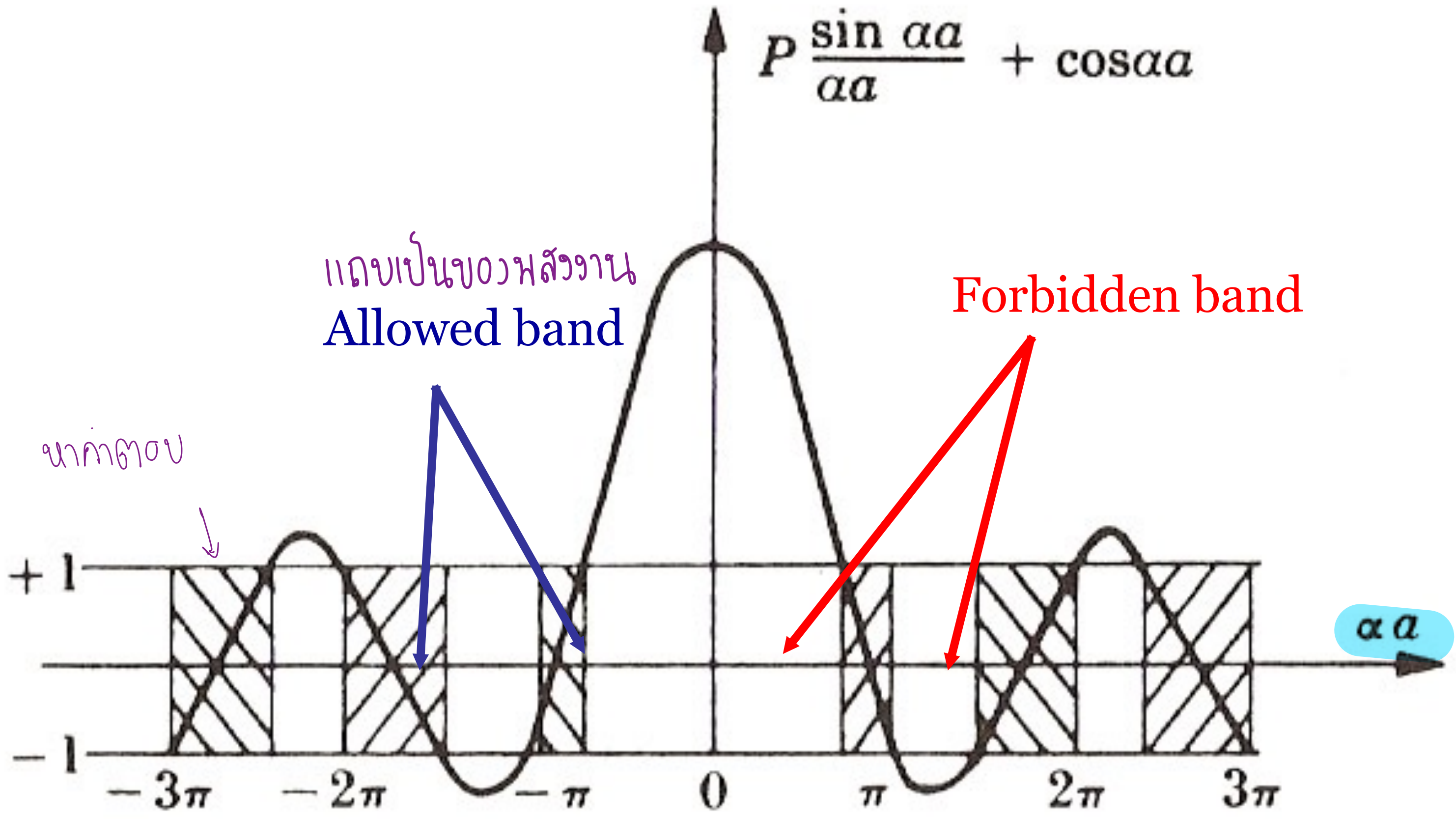
ถ้า P = 0

$\cos(ka) = \cos(\alpha a)$

$$P = \frac{maV_0 w}{\hbar^2} \qquad (3)$$

$$\alpha = \frac{1}{\hbar}\sqrt{2mE} \qquad (4)$$

Kronig-Penney Model



Kronig-Penney Model

- We plot the right-hand side of (2) as a function of αa and since the left-hand side of the same equation is always between -1 and +1, a solution exists only for the shaded region and no solution outside the shaded region.
- These regions are called "*allowed and forbidden bands of energy*" due to the relation between α and E.

Kronig-Penney Model

From equation (2), we have

P↑ แถบพลังงานแคบลง

- If P increases, allowed bands get narrower and the forbidden bands get wider. ลดลง
- If P decreases, allowed bands get wider and forbidden bands get narrower.
- If P = 0, then *cos(αa) = cos(ka)*

$$\alpha^2 = k^2 = \frac{2mE}{\hbar^2} \quad \text{or}$$

$\hbar^2 \cdot k^2 = 2mE$

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

$$E = \frac{\hbar^2 k^2}{2m} \quad \text{(like a case of free electron of V = 0)}$$

Kronig-Penney Model

- If $P \rightarrow \infty$, then $\sin(\alpha a) = 0$

$$\alpha a = n\pi$$

$$\alpha^2 = \left(\frac{n\pi}{a}\right)^2 = \frac{2mE}{\hbar^2}$$

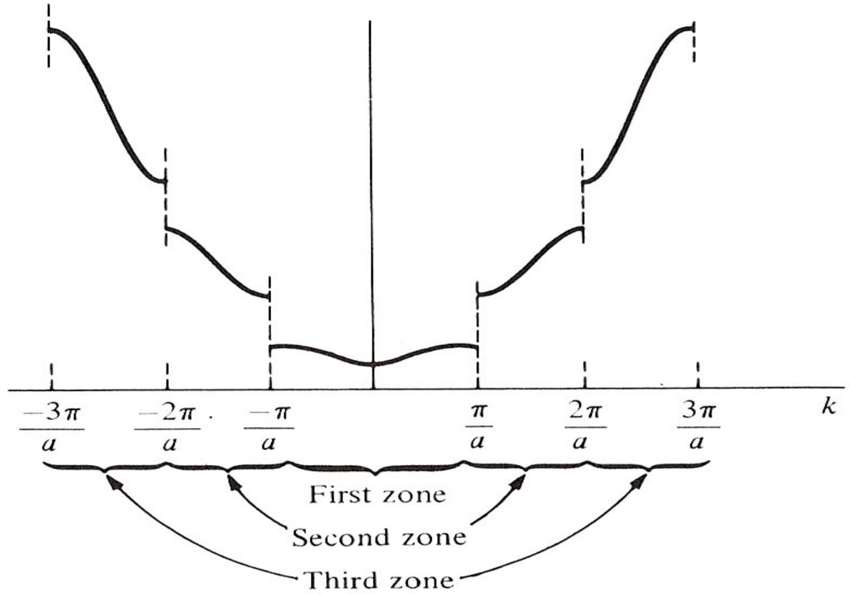
ระดับชั้นพลังงาน

$$E = \frac{n^2 h^2}{8ma^2}$$ (a case of infinite potential well V = ∞ with width *a*)

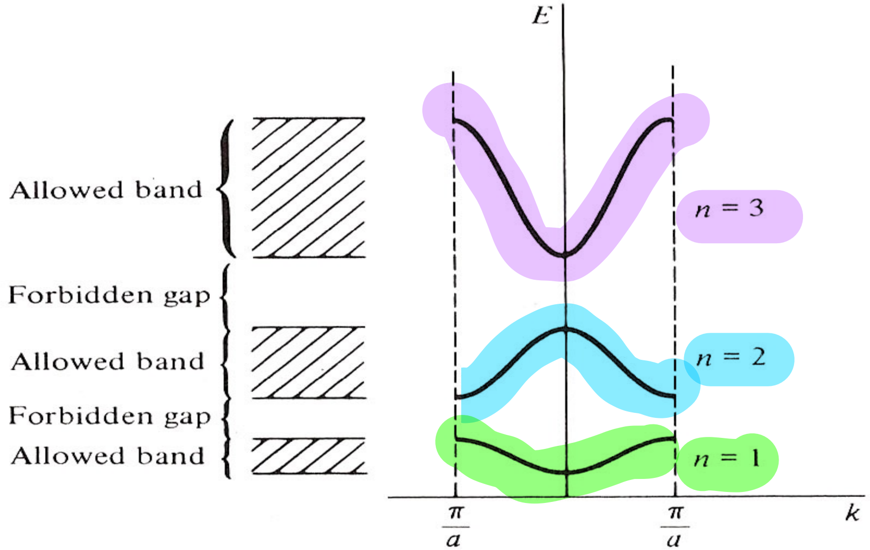
- At the boundary of an allowed band cos(ka) = ±1 , this implies k = nπ/a for n = 1, 2, 3, …

E-k diagram

Brillouin Zone



(a)



Reduced Brillouin Zone

Number of electrons per unit volume

- The total number of electrons per unit volume in the range dE (between E and E + dE) is given

ถ้าอยากหาจำนวน e^- ต่อหน่วยปริมาตรในพื้นที่แคบ

$$n = \int_{0}^{\infty} n(E)d(E) = \int_{0}^{\infty} N(E)F(E)dE \qquad (5)$$

จำนวน e^- หรือ hole : e^- . จำนวน e^- ต่อหน่วยปริมาตร

where N(E) = density of states (number of energy levels per energy range per unit volume)

F(E) = a distribution function that specifies expectancy of occupation of state or called *"probability of occupation"*.

ความน่าจะเป็นของเฟอร์มิ - ดิแรก

f^n โอกาสที่พบ e^- ที่ครอบครองอยู่ ณ พลังงานนั้นๆ

Number of electrons per unit volume

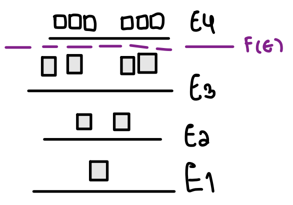
- The density of states per unit volume in three dimensions can be expressed as

$$N(E) = 4\pi \left(\frac{2m}{h^2} \right)^{3/2} E^{1/2}$$

ถ้ามี probability 0.5

ถ้าE ต่ำจะมี e^-

ถ้าE สูงจะไม่มี e^-



ถ้าไม่มี e^- เลย probability : 0

Number of electrons per unit volume

- The probability of occupancy is given by the *Fermi-Dirac- distribution* as

$$F(E) = \frac{1}{1 + e^{(E - E_F)/kT}}$$

where E_F = Fermi energy level (the energy at F(E) = 0.5)

k = Boltzmann's constant

T = absolute temperature (K)

Number of electrons per unit volume

ถ้า E-Ef ถ้าE>Ef : ⊕

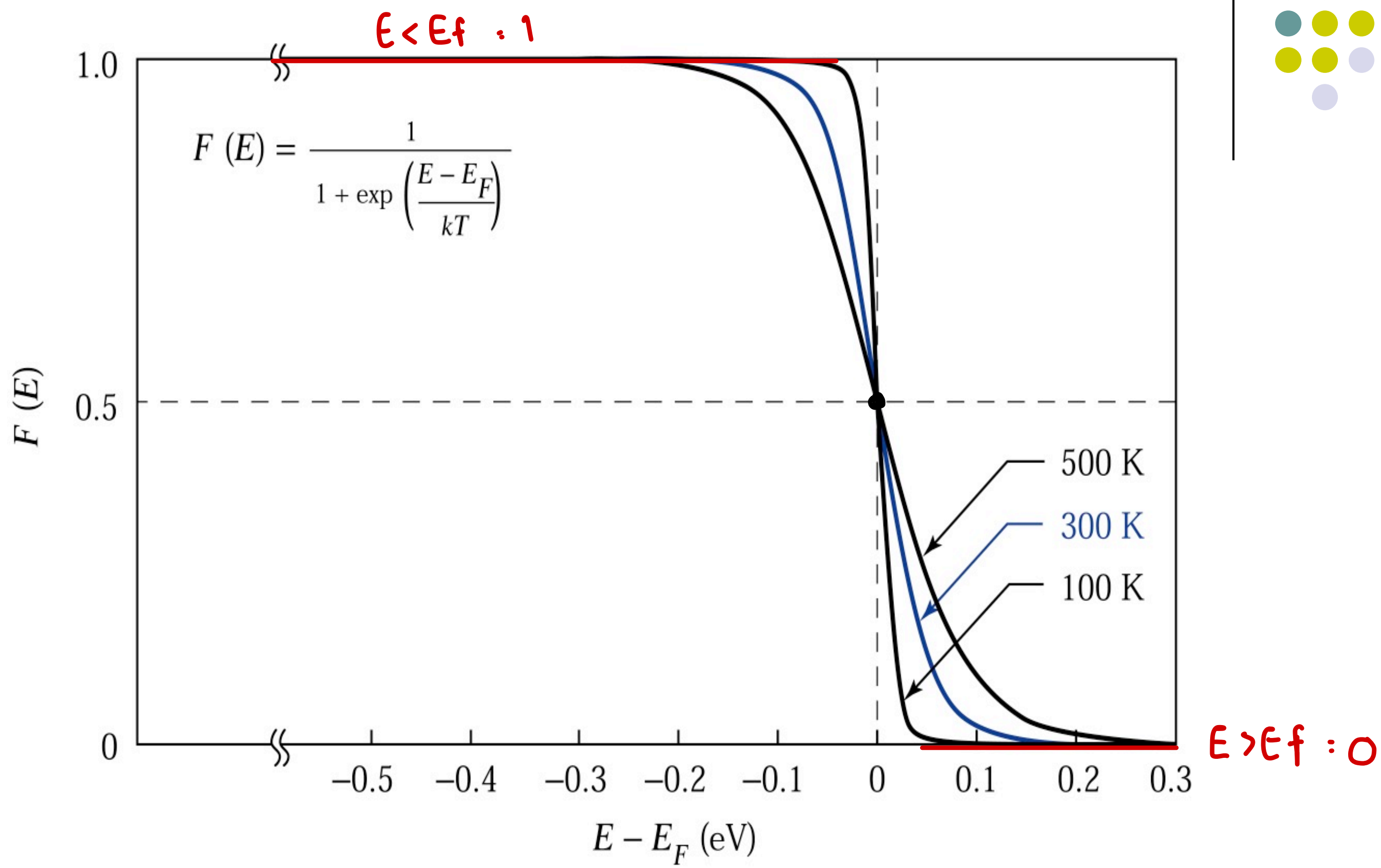
ถ้า E-Ef ถ้าE<Ef : ⊖

$F(E) = \frac{1}{1+e^{(E-E_f)/kT}}$

E=Ef

$F(E) = \frac{1}{1+e^{0}}$

$F(E) = \frac{1}{1+1} = \frac{1}{2}$



- For T = 0 K:
  - If $E > E_F$, $F(E) = 0 \rightarrow F(E) = 1/(e^{\infty}+1) = 0$
  - If $E < E_F$, $F(E) = 1 \rightarrow F(E) = 1/(e^{-\infty}+1) = 1$
- For T > 0 K, $F(E_F) = 0.5$

Number of electrons per unit volume

- From equation (5),

$$n = \int_0^{\infty} N(E)F(E)dE = \int_0^{E_F} N(E)F(E)dE$$

- For T = 0 and E < E_F

$$n = \int_0^{E_F} N(E)(1)dE$$

$$= \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left(\frac{2}{3}E_F^{3/2}\right)$$

Number of electrons per unit volume

- For T = 0 and E < E_F

$$E_F(T=0) = \left(3\pi^2 n\right)^{2/3} \left(\frac{\hbar^2}{2m}\right)$$

- For T > 0

$$E_F(T) = E_F(0)\left[1 - \frac{\pi^2}{12}\left(\frac{kT}{E_F(0)}\right)^2 + \ldots\right]$$

Fermi levels of various materials

1 eV = 1.6 × 10^{-19} C

Li	4.72 eV
Na	3.12 eV
K	2.14 eV
Cu	7.04 eV
Ag	5.51 eV
Al	11.70 eV

Characteristics of F(E)

กรณี E=Ef

1. F(E), at E = E_F, equals to 0.5.

ระดับพลังงานเฟอร์มิ

2. For (E – E_F) > 3kT

ลดรูป

$$F(E) = \frac{1}{1+e^{(E-E_f)/kT}}$$

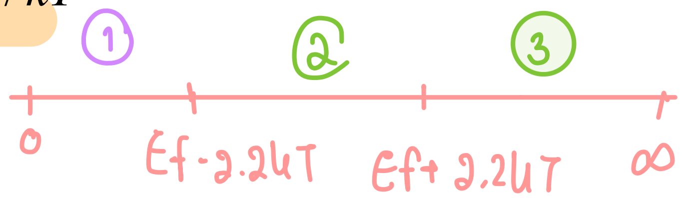
$$F(E) \approx e^{-(E-E_F)/kT}$$

This is called "**Maxwell–Boltzmann distribution**".

Characteristics of F(E)

3. For $(E - E_F) < 3kT$

$$F(E) \approx 1 - \mathrm{e}^{-(E-E_F)/kT}$$



4. F(E) may be distinguished into 3 regions for T > 0 as

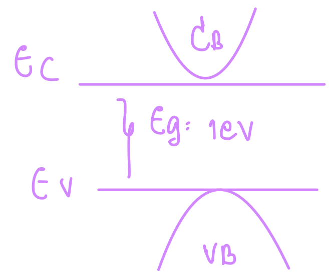
- $E = 0$ to $(E = E_F - 2.2kT)$: F(E) is close to unity. เข้าใกล้ 1
- $(E = E_F - 2.2kT)$ to $(E = E_F + 2.2kT)$: F(E) changes from nearly 1 to nearly 0. เข้าใกล้ 0
- $(E = E_F + 2.2kT)$ to $E = \infty$: F(E) is close to zero. เข้าใกล้ 0

ธาตุจากหมู่ 4 ที่ไม่โดนเจือปน

Intrinsic carrier concentration

- Free charge carrier density or the number of electrons per unit volume

$$e^- \quad n = \int_0^{\infty} N(E)F(E)dE$$



hole p

$$N(E) = 4\pi\left(\frac{2m_e}{h^2}\right)^{3/2} E^{1/2}$$

$E_g = E_C - E_V$

- For electrons: $E^{1/2} = (E - E_C)^{1/2}$ and
- For holes: $E^{1/2} = (E_V - E)^{1/2}$ and

① สารกึ่งตัวนำบริสุทธิ์

Intrinsic carrier concentration

$1\,J = \frac{1}{1.6\times10^{-19}}\,eV$

$1.38\times10^{-23}\times300\,K = \frac{4.14\times10^{-21}\,J}{1.6\times10^{-19}\,eV} = 0.0259\,eV$

ที่อุณหภูมิห้อง 25° = 300K

- At room temperature, kT = 0.0259 eV and (E – E_F) >> kT, so Fermi function can be reduced to Maxwell-Boltzmann distribution.

$$F(E) \approx e^{-(E-E_F)/kT}$$

Intrinsic carrier concentration

ฟ function ไอทส

F(E)

$$n = \int_0^\infty 4\pi \left(\frac{2m_e^*}{h^2} \right)^{3/2} . e^{-(E-E_F)/kT} . (E - E_C)^{1/2} \, dE$$

Let $\dfrac{E - E_C}{kT} = x_C$,

then $\dfrac{dx_C}{dE} = \dfrac{1}{kT}$ or $dE = kT\,dx_C$

so $e^{-(E-E_F)/kT} = e^{-(kTx_C + E_C - E_F)/kT} = e^{-x_C} . e^{-(E_C - E_F)/kT}$

Intrinsic carrier concentration

Then

$$n = \int_0^\infty 4\pi \left(\frac{2m_e^*}{h^2}\right)^{3/2} .e^{-x_C} .e^{-(E_C - E_F)/kT} .(kTx_C)^{1/2} kT dx_C$$

$$= 4\pi \left(\frac{2m_e^*}{h^2}\right)^{3/2} (kT)^{3/2} e^{-(E_C - E_F)/kT} \int_0^\infty x_C^{1/2} e^{-x_C} dx_C$$

Intrinsic carrier concentration

- Therefore, the electron density in the conduction band at room temperature can be expressed by

e^- ←
$$n = N_C \exp\left[-(E_C - E_F)/kT\right] \qquad (6)$$

hole : p

where $N_C = 2\left(2\pi m_e^* kT/h^2\right)^{3/2}$ is effective density of states in the conduction band.

N_C : fⁿ ความหนาแน่นสถานะที่ทั้งหมดในแถบความจริง

Intrinsic carrier concentration

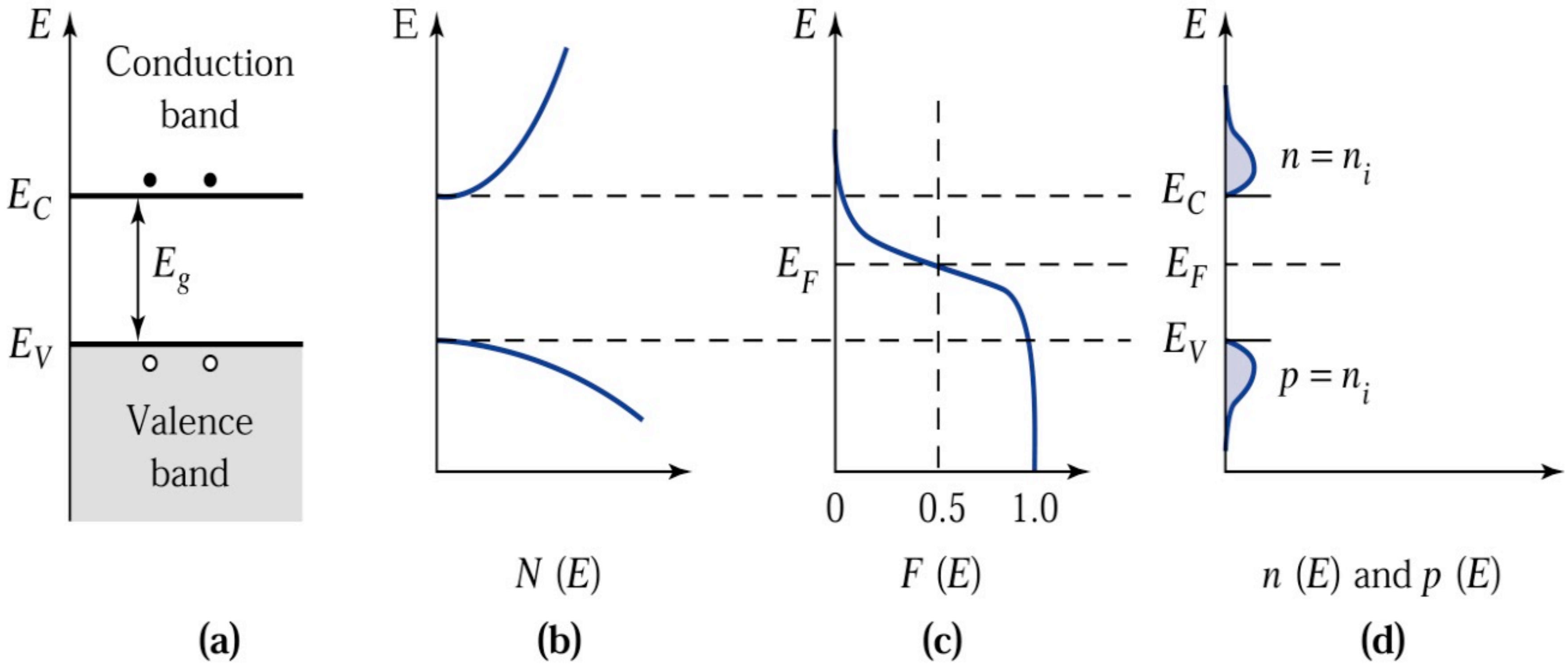
- Similarly, we can obtain the hole density *p* in the valence band as

hole $\leftarrow$ $$p = N_V \exp\left[-(E_F - E_V)/kT\right] \quad (7)$$

where $N_V = 2\left(2\pi m_h^* kT/h^2\right)^{3/2}$ is effective

density of states in the valence band.

Intrinsic carrier concentration



(a) Schematic band diagram.

(b) Density of states.

(c) Fermi distribution function.

(d) Carrier concentration

Intrinsic carrier concentration

- For intrinsic semiconductors, the number of electrons per unit volume in the conduction band equals to the number of holes per unite volume in the valence band.

$$n = p = n_i \qquad n_i \times n_i = n_i^2 \qquad (8)$$

$$n.p = n_i^2$$

where n_i = intrinsic carrier density

Intrinsic carrier concentration

- From (8);

สมการ 6 สมการ 7

$$N_C \exp\left[-(E_C - E_F)/kT\right].N_V \exp\left[-(E_F - E_V)/kT\right] = n_i^2$$

$$N_C.N_V.\exp\left[-(E_C - E_V)/kT\right] = n_i^2$$

$$E_C - E_V = E_g$$

$$n_i^2 = N_C.N_V.\exp\left(-E_g/kT\right)$$

สมการคำนวณหา

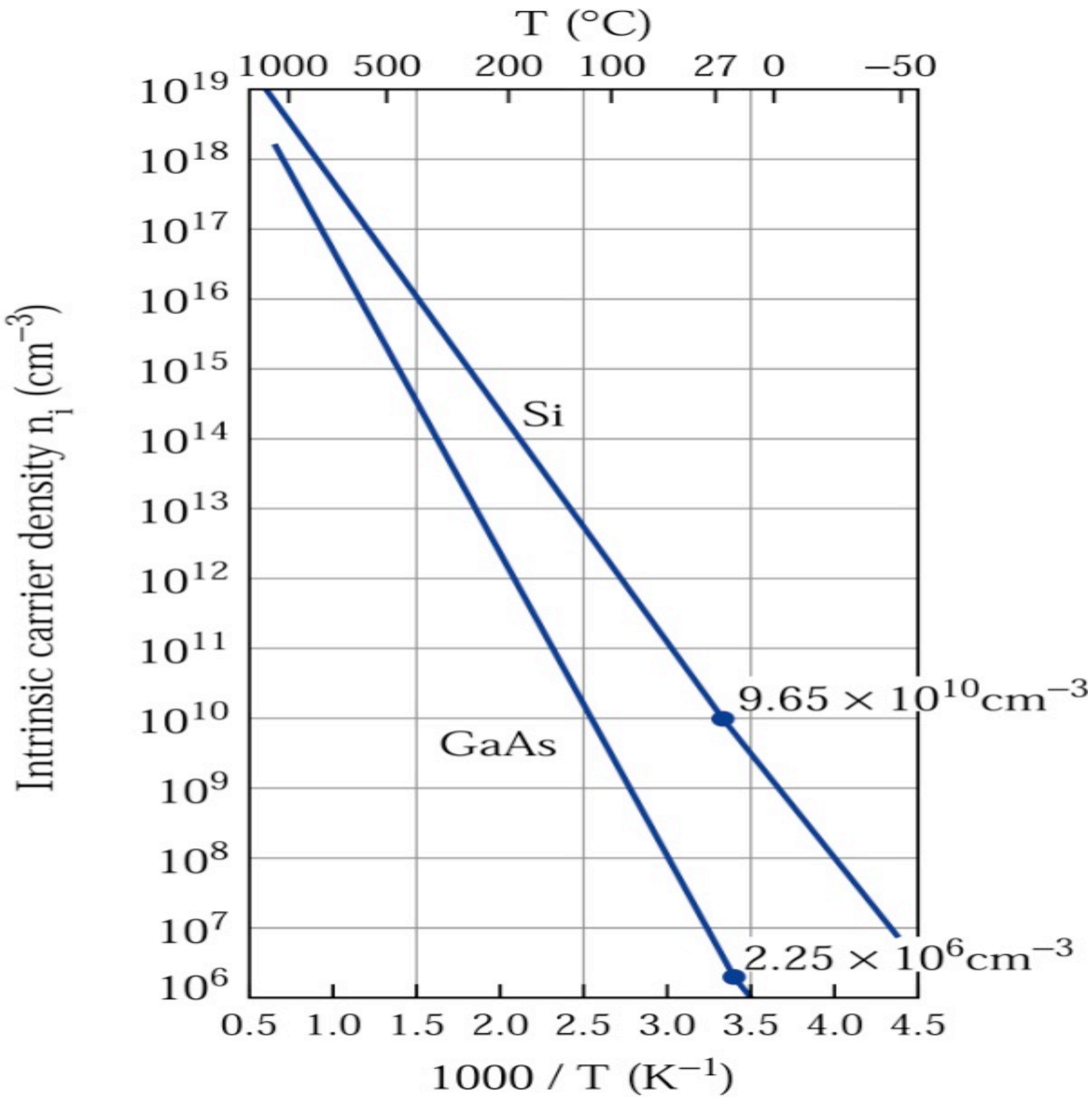
$$n_i = \sqrt{N_C N_V}\exp\left(-E_g/2kT\right)$$

Intrinsic carrier concentration

- The Fermi level of an intrinsic semiconductor can be found by equating (6) = (7) as

$$E_F = E_i = \left(E_C + E_V\right)/2 + \left(kT/2\right)\ln\left(N_V / N_C\right)$$

Intrinsic carrier concentration



Example 1 ทดรบ้าน

$h: 6.63 \times 10^{-34}$

$m_0: 9.1 \times 10^{-31}$ kg

- Calculate effective density of states N_C and N_V for GaAs at room temperature (300 K) if GaAs has

$$m_e^* = 0.067 m_0 \quad \text{and} \quad m_h^* = 0.65 m_0$$

$$N_C = 2\left[\frac{2\pi m_e^* \times k}{h^2}\right]^{\frac{3}{2}} = 2\left[\frac{2\times\pi\times 0.067\times 9.1\times 10^{-31}\times 1.38\times 10^{-23}}{(6.63\times 10^{-34})^2}\right]^{\frac{3}{2}}$$

เฉลย $N_C = 4.34 \times 10^{17}\ cm^{-3}$

$N_V : 1.31 \times 10^{19}\ cm^{-3}$

Example 2

- From previous example, calculate intrinsic carrier density n_i for GaAs at room temperature where energy gap of GaAs is 1.43 eV. $E_g (eV)$

$$n_i = \sqrt{N_C N_V} \exp(-E_g/2kT)$$