618327-2560

Physics of Electronic Materials and Devices

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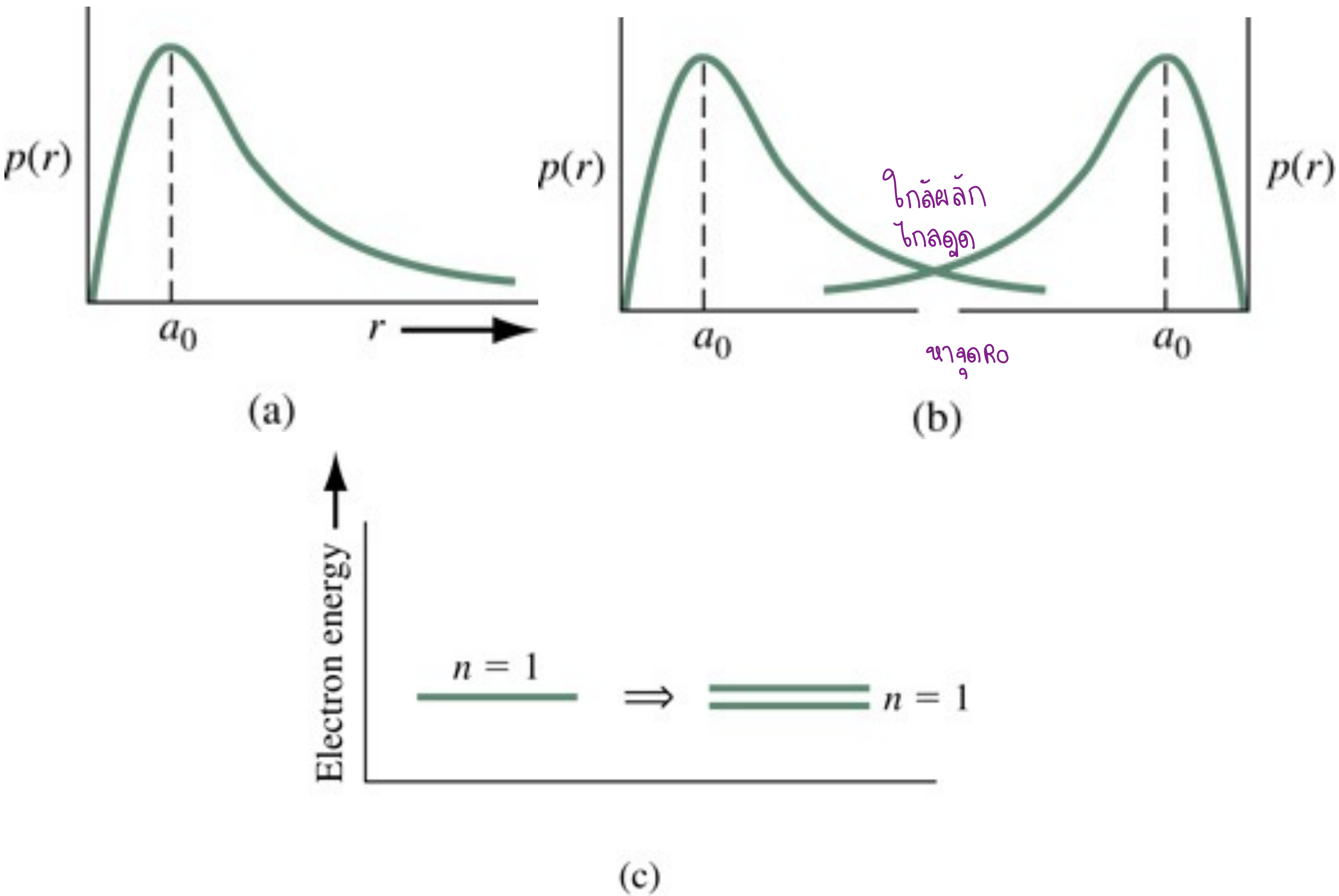
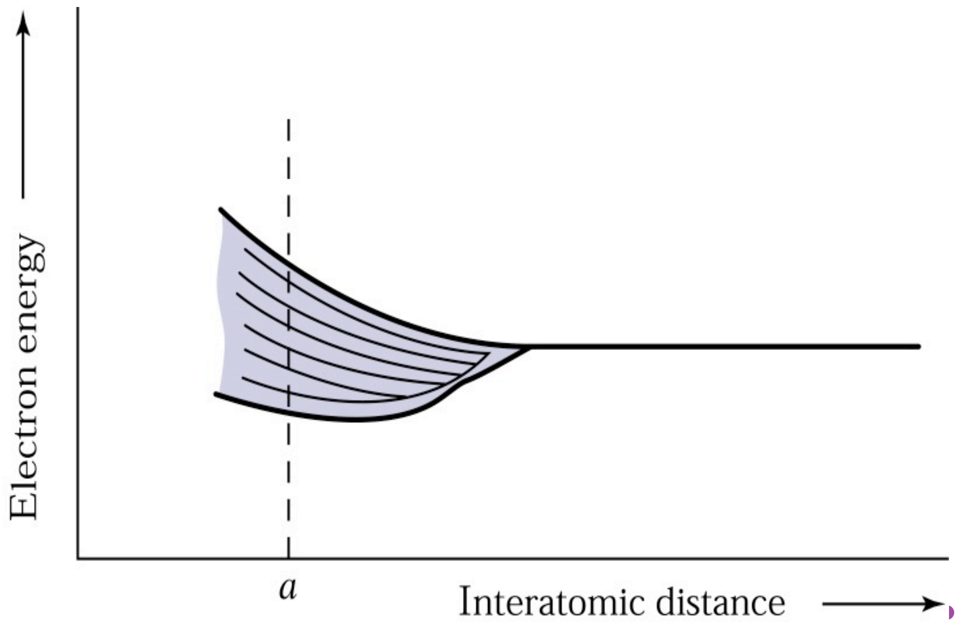
Lecture 5

Energy Bands

แถบพลังงาน



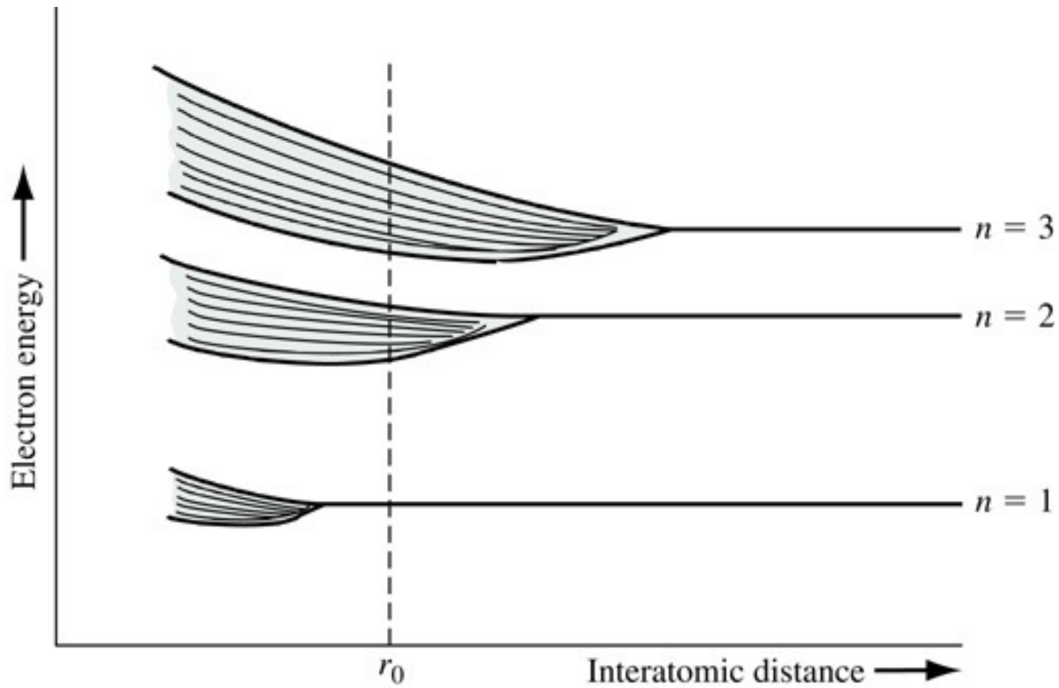
Energy Bands



- Consider two identical atoms, when they are far apart, the allowed energy levels for a given principal quantum number (**n** = 1) consist of one doubly degenerate level (both atoms have exactly the same energy).

- When they are brought closer, the doubly degenerate energy levels will spilt into two levels by the interaction between the atoms.

Energy Bands



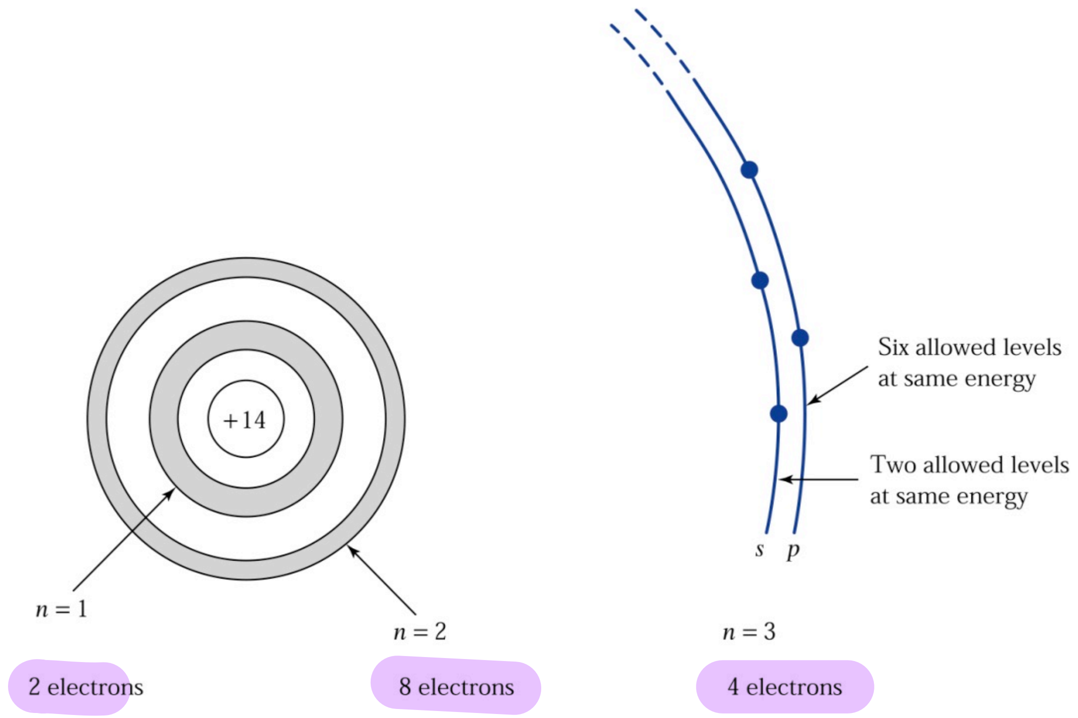
- **N** isolated atoms are brought together to form a solid, the orbits of the outer electrons of different atoms overlap and interact with each other.

- This causes a shift in the energy levels and **N** separate closely spaced levels are formed.

Energy Bands

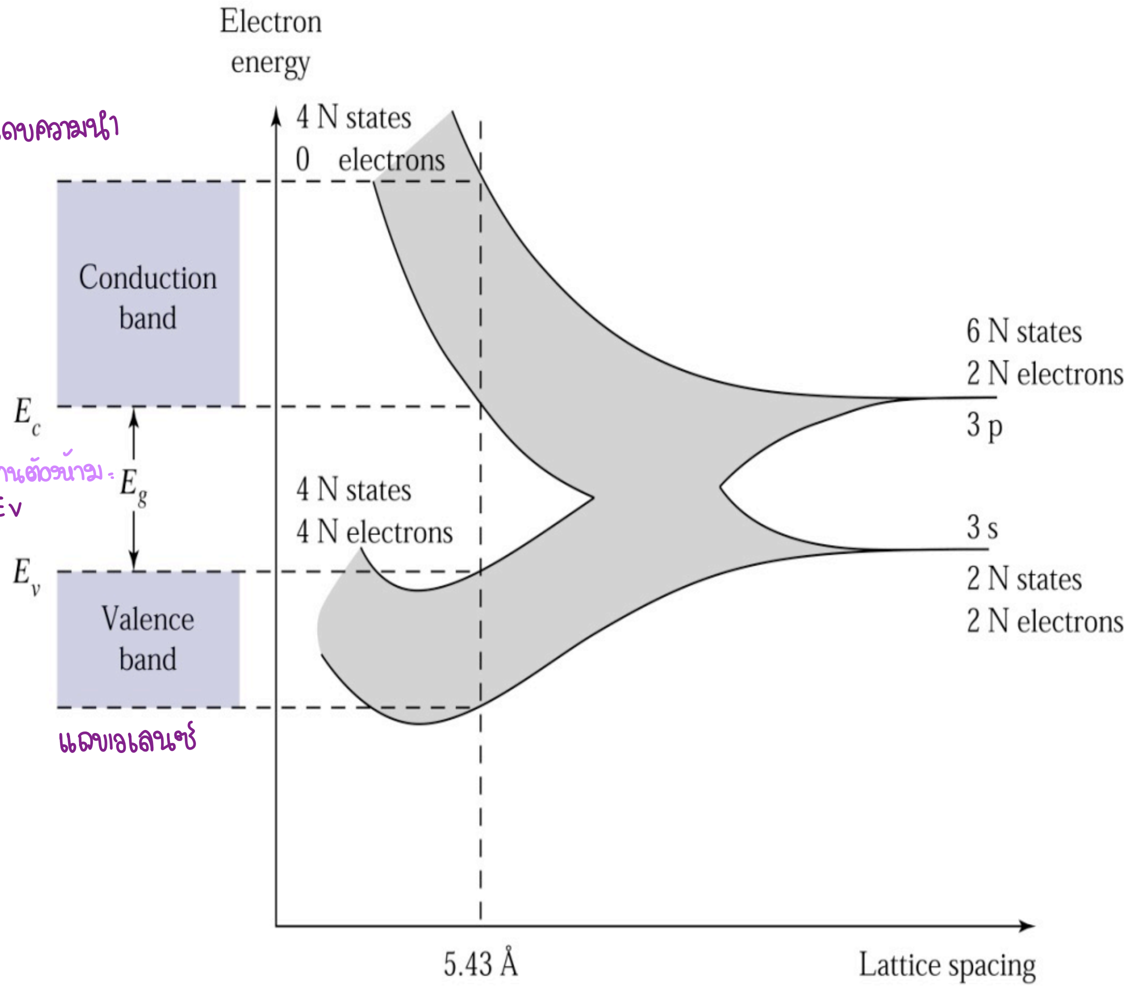
- Consider isolated silicon atom, 10 of the 14 electrons occupy energy levels whose orbital radius is much smaller than the inter-atomic separation in the crystal.
- The four remaining valence electrons are relatively weakly bound and can be involved in chemical reactions.
- Therefore, the valence electrons are the ones that will be considered.
- The two inner shells are completely full and tightly bound to the nucleus.

Energy Bands



- As the inter-atomic distance decreases, the 3s and 3p subshell of the **N** silicon atoms will interact and overlap.

Energy Bands



อยากให้นำไฟฟ้าโดยกระตุ้น ต้องมากกว่าEg e ที่อยู่ใน Valence e โดนปล่อยไปEc เลยนำไฟฟ้า

พอโดดไป Ev จะมี hole ของ e ตัวใหม่มา

- At the equilibrium interatomic distance, the bands will again split with four quantum states per atom in the lower band (***valence band***) and four quantum states per atom in the upper band (***conduction band***).

Energy Bands

- At absolute zero temperature (T = 0 K), electrons occupy the lowest energy states, so that all states in the lower band will be full and all states in the upper band will be empty.
- The bottom of the conduction band is called $\boldsymbol{E_c}$, and the top of the valence band is called $\boldsymbol{E_v}$.

Energy Bands

- The bandgap energy E_g is the width of the forbidden energy level between the bottom of the conduction band and the top of the valence band.
- The bandgap energy is the energy required to break a bond in the semiconductors to free and electron to the conduction band and leave a hole in the valence band.

Energy Bands

The energy-momentum diagram

- The energy ***E*** of a free electron is given by

$$\boxed{E = \frac{p^2}{2m_0}} \qquad (1)$$

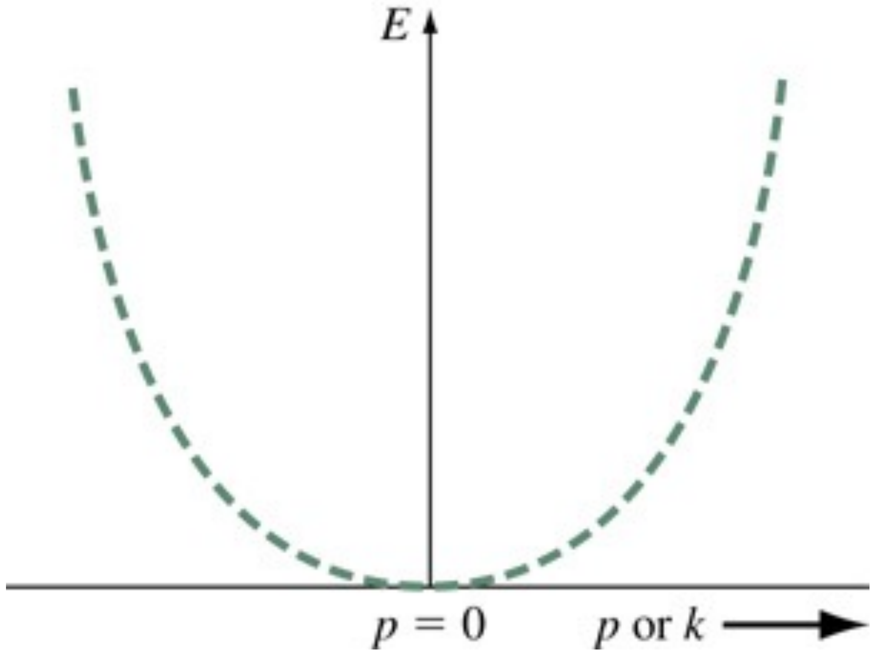
momentum

where p is the momentum

m_0 is the free-electron mass

Energy Bands

- In a semiconductor, an electron in the conduction band is similar to a free electron in that it is free to move about inside the crystal as shown in the right figure.



แกนx ตรงข้าม momentum

แกนY ค่า E (พลังงาน)

Energy Bands

- However, the above equation for ***E*** can not be used due to the periodic potential of the nucleus.

mo แทน → me*

- Anyway, if replacing mo with an effective mass, in an equation (1), it yields the energy ***E*** of an electron as

เกิดจาก mo แทนตัว me*

$$E = \frac{p^2}{2m_e^*} \quad (2)$$

Energy Bands

m_e^* ขึ้นกับคุณสมบัติสารกึ่งตัวนำนั้นๆ

- The effective mass in a solid is a result of charged particle moving under nucleus of applied electric field in presence of a periodic potential.
- This differs from the mass in free space.
- The electron effective mass depends on the properties of the semiconductor.

Energy Bands

- In quantum-mechanic, the velocity of electron is described by its group

$$v_g = \frac{d\omega}{dk}$$

$$E = h\nu = \hbar\omega$$

$$v_g = \frac{1}{\hbar}\frac{\partial E}{\partial k} \qquad \omega = \frac{E}{\hbar}$$

Energy Bands

ความเร่ง

The acceleration can be obtained by

diff จะได้

$$a = \frac{dv_g}{dt} = \frac{d}{dt}\left[\frac{1}{\hbar}\frac{\partial E}{\partial k}\right]$$

$$a = \frac{1}{\hbar}\frac{\partial^2 E}{\partial k^2}\frac{\partial k}{\partial t} \qquad (2)$$

Energy Bands

- For classical part, it expresses dE as the work done by a particle traveling a distance $v_g dt$ under the influence of a force eE.

$W = F \times S$

$$dE = F.\underline{dx}$$ ဒ:ဗြ:က၉

$S = v_g dt$

$$= F.(v_g dt)$$

$S = vt$

$$dE = F.\left(\frac{1}{\hbar}\frac{\partial E}{\partial k}\right)dt$$

Energy Bands

This leads to

$$\frac{dk}{dt} = \frac{F}{\hbar} \qquad (3)$$

Substituting (3) into (2)

F: ma

$$a = \frac{1}{\hbar}\frac{\partial^2 E}{\partial k^2}\left(\frac{F}{\hbar}\right)$$

F: ma

$$a = \underline{\frac{1}{\hbar^2}\overset{m}{\frac{\partial^2 E}{\partial k^2}}}\,F \qquad (4)$$

$$F : \frac{\left[\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial u^2}\right]^{-1} a}{m}$$

Energy Bands

$$\beta_1 : \frac{\Sigma_i (x_i y_i) - n\bar{x}\bar{y}}{[\Sigma_i (x_i^2)] - n\bar{x}^2}$$

$$r : \frac{n\,\Sigma xy - \Sigma x \Sigma y}{\sqrt{(n\Sigma_i (x_i^2) - (\Sigma_i x_i)^2)(n\Sigma_i (y_i^2) - (\Sigma_i y_i)^2)}}$$

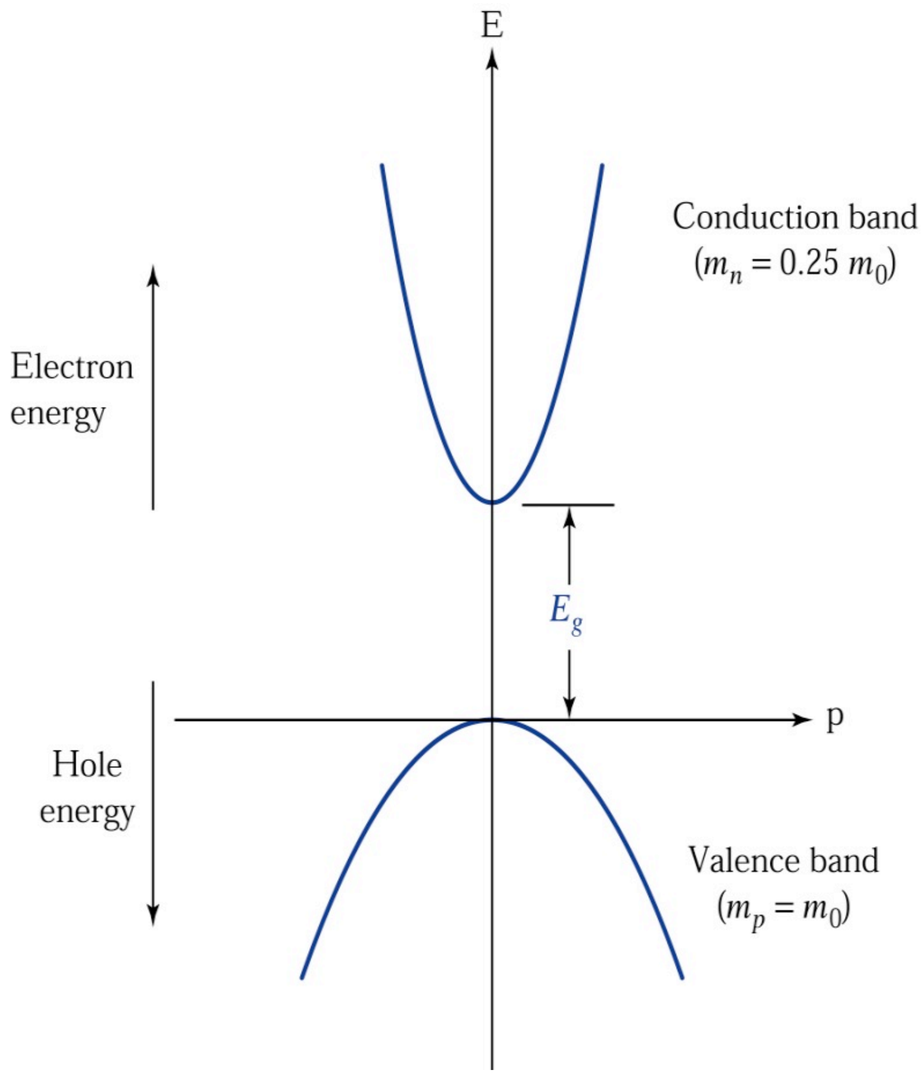
From F = ma, we have

$$m_e^* = \left(\frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} \right)^{-1} = \left(\frac{\partial^2 E}{\partial p^2} \right)^{-1} \qquad (5)$$

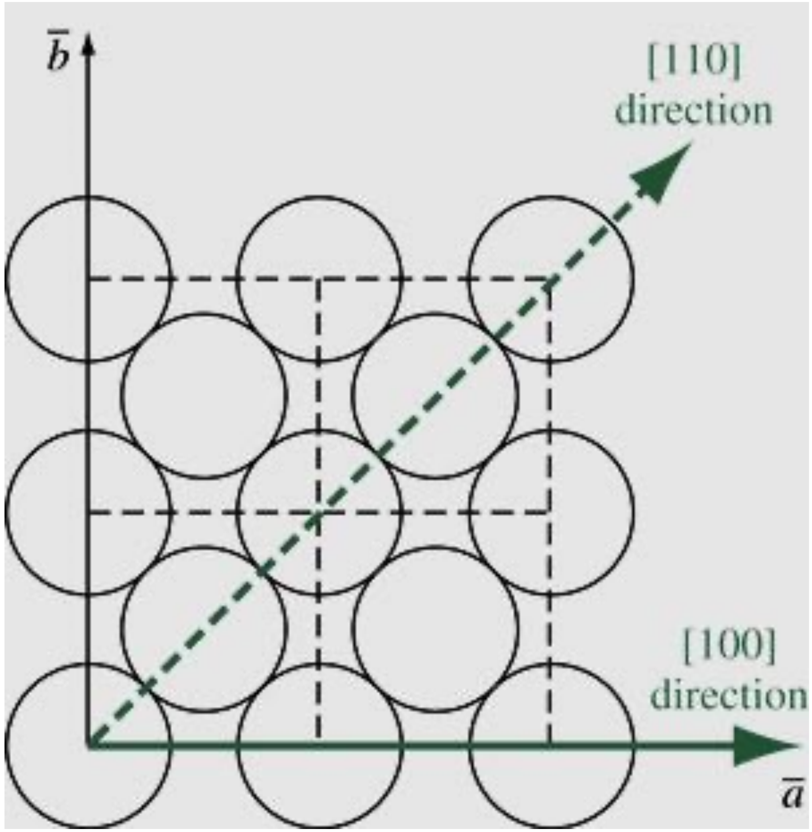
A similar expression can be written for holes with effective mass m_h^* .

Energy Bands

- A schematic energy-momentum diagram for a special semiconductor with $m_e^* = 0.25\,m_0$ and $m_h^* = m_0$.
- The electron energy is measured upward and hole energy is measured downward.
- This energy-momentum relationship is called "*energy-band diagram*".



Energy Bands



Consider 3D crystal structure,

Lattice spacing varied with

crystal direction.

Ex. FCC with [110] and [100] ,

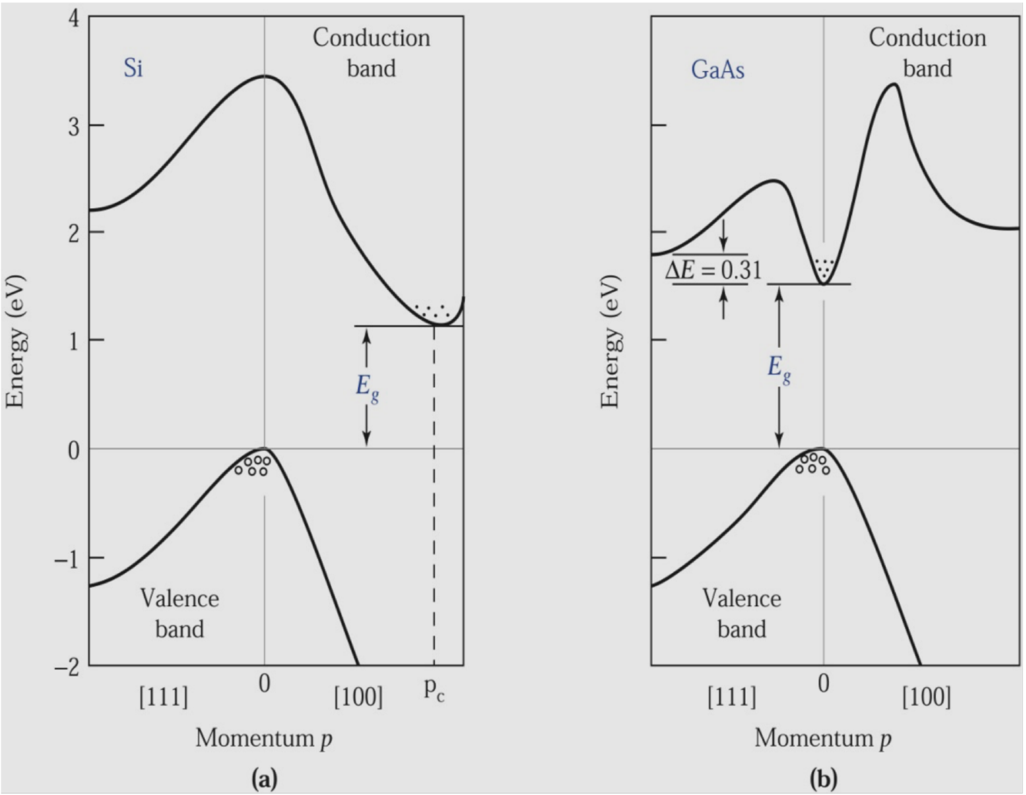
electron moving in different

direction, cause different both

periodic potential pattern and

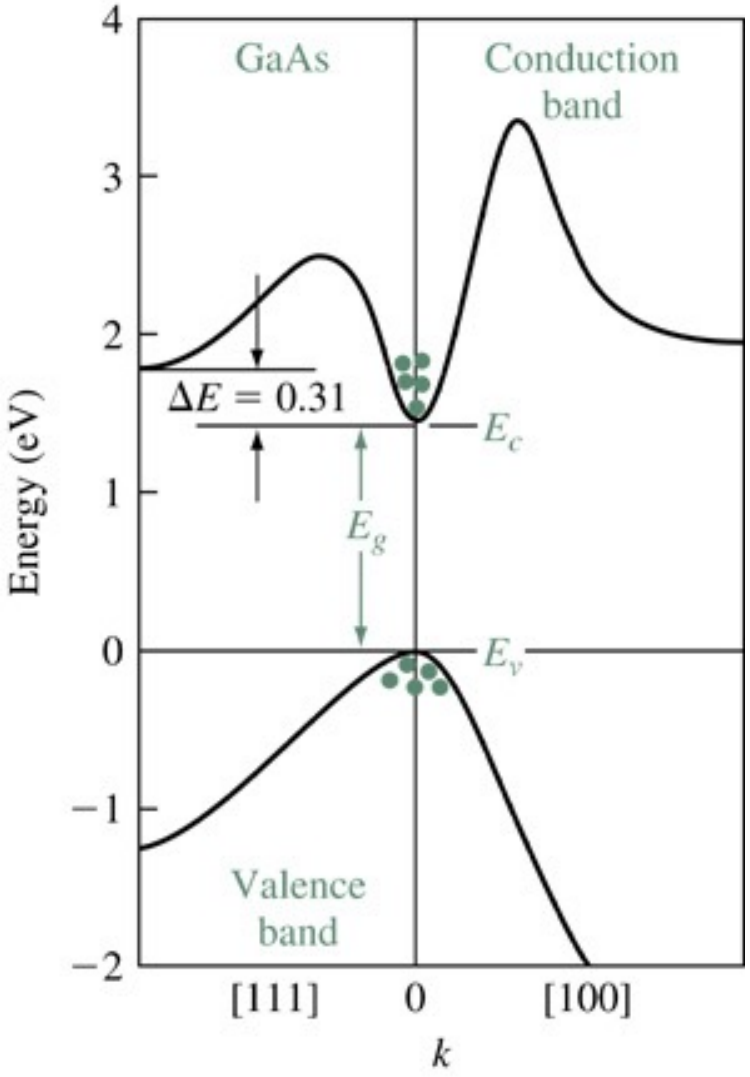
k-space boundary condition.

Energy Bands



- Energy band diagram may be classified semiconductors into 2 groups as direct semiconductors and indirect semiconductors.
- Energy band structures of Si and GaAs. Circles (o) indicate holes in the valence bands and dots (•) indicate electrons in the conduction bands.

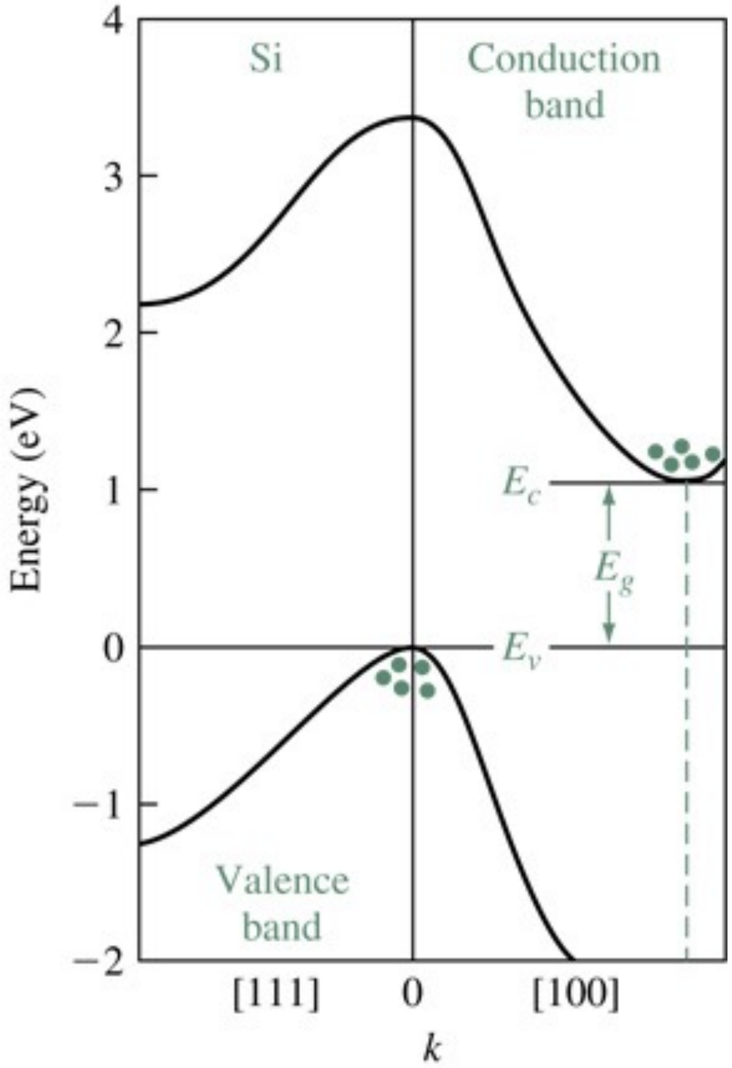
Energy Bands



(a)

- Let us consider the figure, **GaAs** is a direct semiconductors with a direct bandgap since it does not require a change in momentum for an electron transition from the valence band to the conduction band.

Energy Bands



(b)

- Unlike in the case of **Si**, an electron transition from the valence band to the conduction band requires not only an energy change but also momentum change (called indirect semiconductors).

Energy Bands

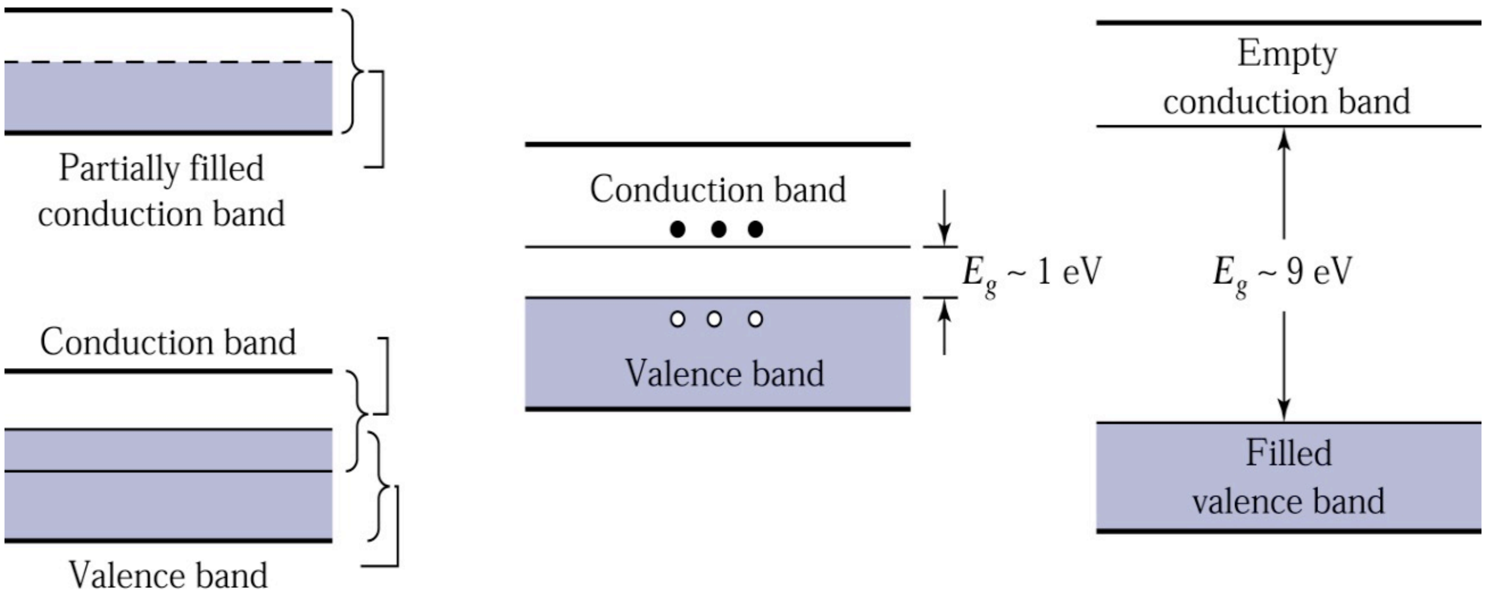
- This difference between direct and indirect bandgap is crucial for making the light sources such as LEDs or LASERs.
- These light sources require direct semiconductors for efficient generation of photons.

Energy Bands

Conduction in Metals, S/C, and Insulators

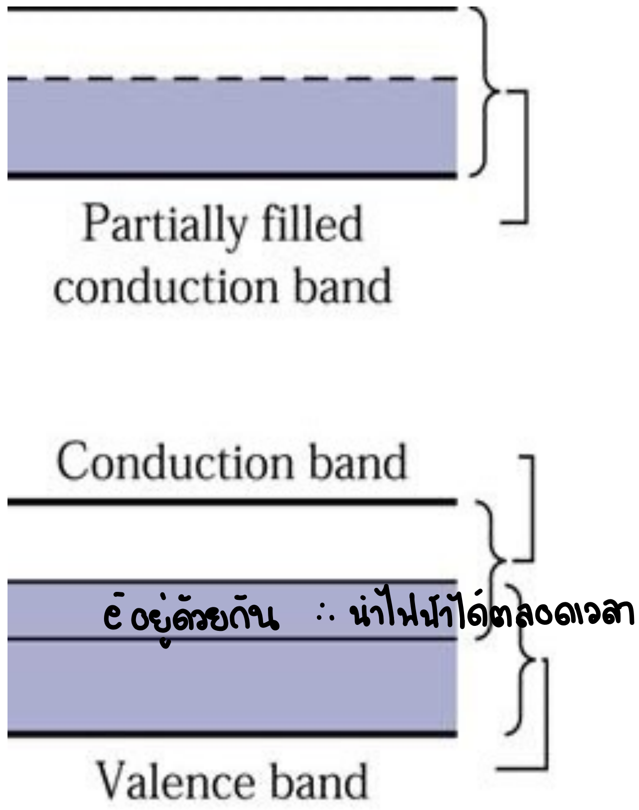
- The electrical conductivity of metals, semiconductors, and insulators could be explained by their energy bands.
- These can be done by considering the highest two bands, valence and conduction bands, of the materials.
- Electron occupation of the conduction band determines the conductivity of a solid.

Energy Bands



- (*Left*) a conductor with two possibilities (either the partially filled conduction band shown at the upper portion or the overlapping bands shown at the lower portion)
- (*Middle*) a semiconductor
- (*Right*) an insulator.

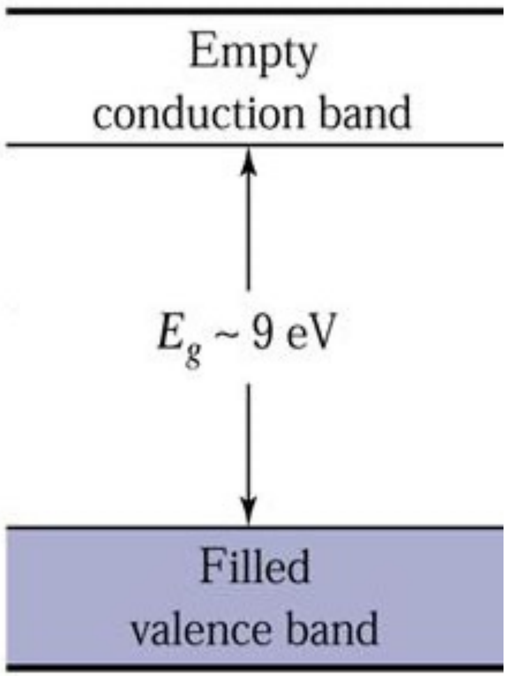
Energy Bands



โลหะ:นำไฟฟ้าอยู่แล้ว ในภาวะปกติ

- **Metals:** Highest allowed occupied band or conduction band is partially filled (such as Cu) or overlaps the valence band (such as Zn or Pb). Therefore, electrons are free to move to the next energy level with only a small applied field.

Energy Bands



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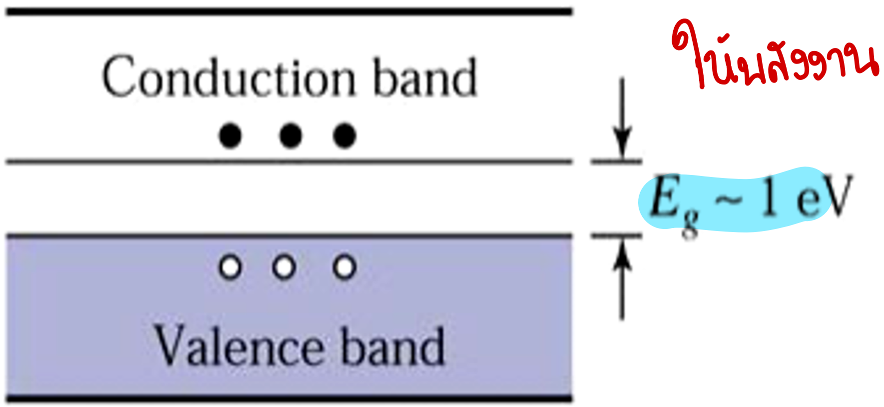
- **Insulators**: The valence electrons form strong bonds between their neighboring atoms. These bonds are difficult to break.
- Therefore, valence band is fully filled and the conduction band is totally empty.

Energy Bands

- Also, these two bands are separated by a wide bandgap.
- Thermal energy or the energy from applied electric field is not enough to raise the uppermost electron in the valence band up to the conduction band.
- Therefore, there is <u>no</u> conductivity.

Energy Bands



- **Semiconductor**: This is similar to the insulators, but the bandgap is much smaller than in the case of insulators.

- At T = 0 K, all electrons are in the valence band and no electron in the conduction band.

- Therefore, semiconductors are poor conductors at low temperatures. At room temperature, some electrons are thermally excited from the valence band to the conduction band.

- Also, it needs just small applied electric field to move these electrons and that results in conductivity.