FYS3410 - Vår 2011 (Kondenserte fasers fysikk)

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Based on Introduction to Solid State Physics by Kittel

Course content

- **Periodic structures, understanding of diffraction experiment and reciprocal lattice**
- **Crystal binding, elastic strain and waves**
- **Imperfections in crystals: point defects and diffusion**
- **Crystal vibrations: phonon heat capacity and thermal conductivity**
- **Free electron Fermi gas: density of states, Fermi level, and electrical conductivity**
- **Electrons in periodic potential: energy bands theory classification of metals, semiconductors and insulators**
- **Semiconductors: band gap, effective masses, charge carrier distributions, doping, pn-junctions**
- **Metals: Fermi surfaces, temperature dependence of electrical conductivity**

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Lecture: Impurity states in semiconductors and carrier statistics

- **Repetion: Effective mass method**
- **Intrinsic carrier concentration in semiconductors**
- **doping and conductivity in semiconductors**

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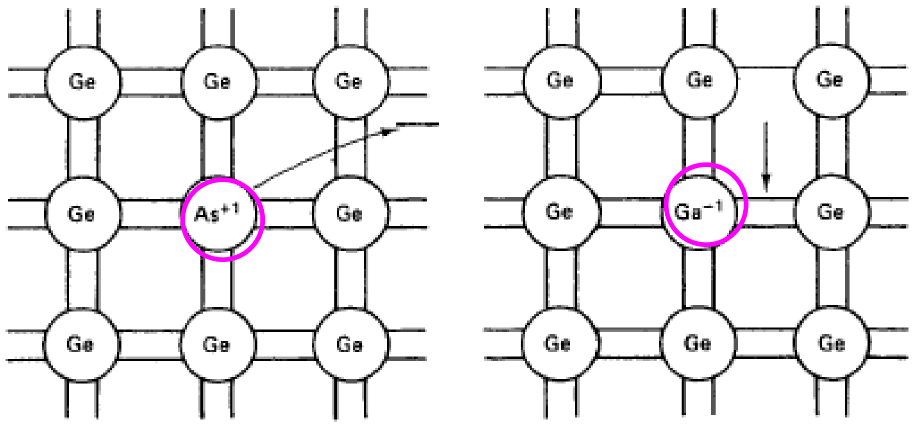
Effective mass method: solving Schrodinger equation without perodic potential for hydrogen-like behaiving impurities



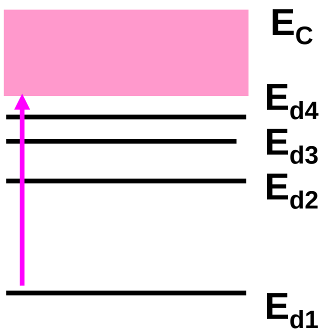
Hydrogen model:

$$E_C - E_{im} = \frac{q^4 Z^2 m^*}{2n^2(4\pi\varepsilon\hbar)^2} = 13.6\left(\frac{Z}{n\varepsilon_r}\right)^2\left(\frac{m*}{m}\right) eV$$

$$r_d = \frac{4\pi\varepsilon\hbar^2 n^2}{m^* q^2 Z} = 0.53\frac{n^2\varepsilon_r}{Z}\left(\frac{m}{m^*}\right) A$$

Ionization energy ΔE_d

$D^0 = D^+ + e^-$: ΔE_d



Lecture : Impurity states in semiconductors and carrier statistics

- Repetion: Effective mass method
- **Intrinsic carrier concentration in semiconductors**
- doping and conductivity in semiconductors

Intrinsic carrier concentration in semiconductors

- Carrier Concentration

$$n = \int \underbrace{D(\varepsilon)}_{\text{DOS}} \underbrace{f(\varepsilon)}_{\text{Fermi-Dirac distribution}} d\varepsilon$$

$$p = \int_{-\infty}^{E_v} D_h(\varepsilon) f_h(\varepsilon) d\varepsilon \qquad f_h = 1 - f_e$$

$$n = 2\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} \exp[(E_F - E_C)/k_B T]$$

$$p = 2\left(\frac{m_h k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} \exp[(E_V - E_F)/k_B T]$$

$$np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 (m_e m_h)^{\frac{3}{2}} \exp(-E_g / k_B T)$$

→ 'n-p' constant and independent of impurity concentration at a given temperature

$$n_i = p_i = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} (m_e m_h)^{\frac{3}{4}} \underline{\exp(-E_g / 2k_B T)}$$

$$E_F = \frac{1}{2}E_g + \underline{\frac{3}{4}k_B T \ln\left(\frac{m_h}{m_e}\right)}$$

⇒

{ ① $m_e = m_h$ ② $T = 0$ } ⟶ $E_F = ½\, E_g$ — The Fermi level is on the middle of E_g

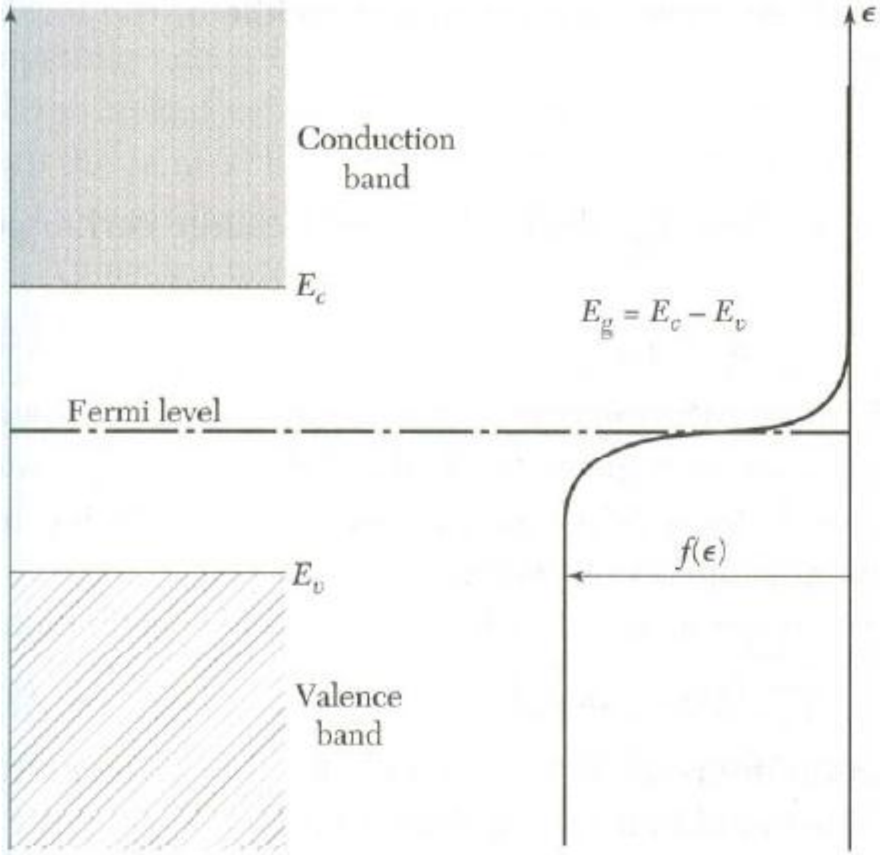
- Intrinsic conductivity & carrier concentration (n) controlled by → $\frac{E_g}{k_B T}$

$\frac{E_g}{k_B T}$ is large → the concentration of intrinsic carrier → low

Intrinsic carrier concentration in semiconductors

Fermi-Dirac distribution $$\frac{1}{\exp[(\epsilon-\mu)/k_BT]+1}$$

If $\epsilon - \mu \gg k_BT$ $$f_e \simeq \exp[(\mu-\epsilon)/k_BT]$$



$$\epsilon_k = E_c + \hbar^2k^2/2m_e$$

$$D_e(\epsilon) = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}(\epsilon - E_c)^{1/2}$$

Density of State for Electron

Figure 18. Energy scale for statistical calculations. The Fermi distribution function is shown on the same scale, for a temperature $k_BT \ll E_g$. The Fermi level μ is taken to lie well within the band gap, as for an intrinsic semiconductor. If $\epsilon = \mu$, then $f = \frac{1}{2}$.

Intrinsic carrier concentration in semiconductors

$$n = \int_{E_c}^{\infty} D_e(\epsilon) f_e(\epsilon) d\epsilon = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} \exp(\mu/k_B T) \times$$

$$\int_{E_c}^{\infty} (\epsilon - E_c)^{1/2} \exp(-\epsilon/k_B T) d\epsilon \ ,$$

Thus $$n = 2\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{3/2} \exp[(\mu - E_c)/k_B T]$$

$f_h = 1 - f_e$, If $(\mu - \epsilon) \gg k_B T$

$$f_h = 1 - \frac{1}{\exp[(\epsilon - \mu)/k_B T] + 1} = \frac{1}{\exp[(\mu - \epsilon)/k_B T] + 1}$$

$$\cong \exp[(\epsilon - \mu)/k_B T] \ ,$$

$$D_h(\epsilon) = \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2} (E_v - \epsilon)^{1/2}$$

Kittel, Solid State Physics (Chapter 8).

Intrinsic carrier concentration in semiconductors

Thus $$p = \int_{-\infty}^{E_c} D_h(\epsilon) f_h(\epsilon) d\epsilon = 2\left(\frac{m_h k_B T}{2\pi\hbar^2}\right)^{3/2} \exp[(E_c - \mu)/k_B T]$$

$$np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 (m_c m_h)^{3/2} \exp(-E_g/k_B T)$$

$$n_i = p_i = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} (m_e m_h)^{3/4} \exp(-E_g/2k_B T)$$

$$\exp(2\mu/k_B T) = (m_h/m_e)^{3/2} \exp(E_g/k_B T)$$

$$\mu = \frac{1}{2} E_g + \frac{3}{4} k_B T \ln(m_h/m_e) \quad .$$

Kittel, Solid State Physics (Chapter 8)

* **Fermi Energy of a Semiconductor**

Need to count # of electrons excited from V.B. to C.B.

The carriers excited = density of states × prob. of occupation

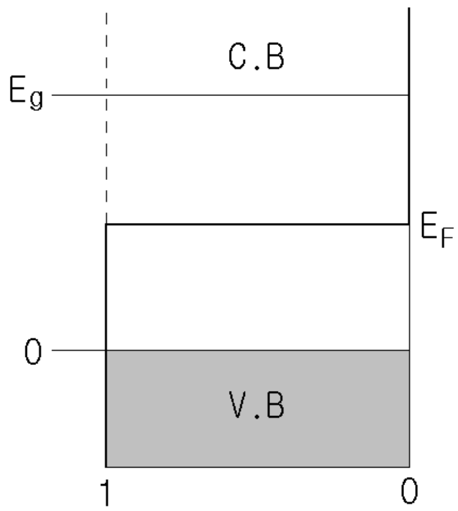
ie $$N_e = \boxed{n = \int_{E_C}^{\infty} D_C(E)\, f_{FD}(E)\, dE}$$

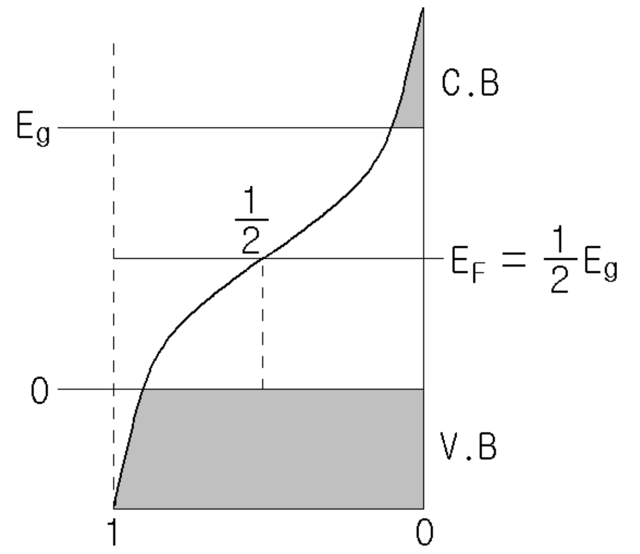
where $$f_{FD} = \frac{1}{e^{(E-E_F)/kT} + 1}$$

E_F : For metal : @ T = 0K
the energy of the hightest
occupied state

More generally,

E_F : Energy of a state for which the probability of occupation is ½.





T = 0K

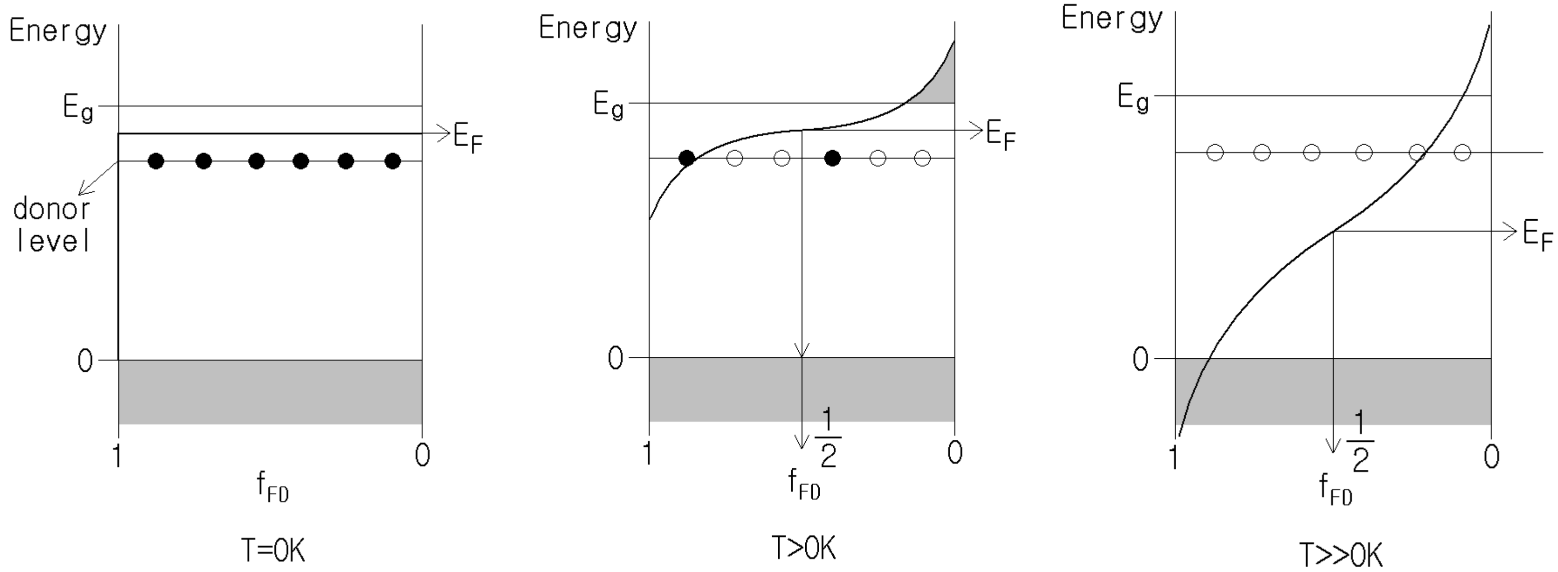
f_{FD} is a step function.
By symmetry, it is reasonable
That E_F = ½E_g

T > 0K

when DC(E) = DV(E)
It is true that EF remains at ½E_g

* The Fermi Energy for doped Semiconductors

Ex) n-type semiconductors



T = 0K **All states upto the donor levels are occupied and the conduction band is empty**

∴ E_F lies somewhere but the donor level and band edge

T > 0K E_F **falling slightly as more donors ionized basically remains in this region**

At room temperature E_F **~ at the donor level**

In a p-type material E_F **~ at the acceptor level**

The ΔE_F **for n- and p-type** $\Rightarrow$ **operation of p-n junction devices**

T >> 0K **The situation is reverted to the intrinsic case**

Charge carrier density in intrinsic semiconductor

Previously, the density of states is given by

$$D(E) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}$$

Take a unit volume ie, V=1

For conduction band

$$E_{\vec{k}} = E_o + \frac{\hbar^2 k_x^2}{2m_1^*} + \frac{\hbar^2 k_y^2}{2m_2^*} + \frac{\hbar^2 k_z^2}{2m_3^*} = E_o + \frac{\hbar^2 k^2}{2m}$$

If isotropic effective mass

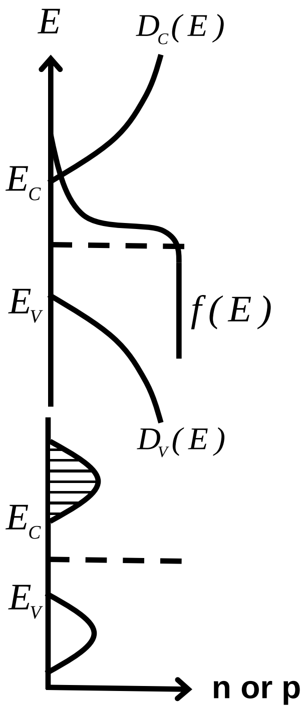
$$m_1^* = m_2^* = m_3^* = m_n^*$$

$$E_{\vec{k}} - E_c = \frac{\hbar^2 k^2}{2m_n^*}$$

Now, the density of states

$$D_c(E) = \frac{1}{2\pi^2}\left(\frac{2m_n^*}{\hbar^2}\right)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}}$$ (E > Ec) conduction band

The electron density in the conduction band



$$n = \int_{E_c}^{\infty} D_c(E)\, f(E)\, dE$$

$$f(E) = \frac{1}{e^{(E-E_F)/k_BT} + 1} \approx e^{-(E-E_F)/k_BT}$$

$$= \int_{E_C}^{\infty} \frac{1}{2\pi^2}\left(\frac{2m_n^*}{\hbar^2}\right)^{\frac{3}{2}} (E - E_C)^{\frac{1}{2}} e^{-(E-E_F)/k_BT}$$

$$e^{-\{(E-E_C)+E_F-E_C\}/k_BT}$$

put $\quad x = \dfrac{E - E_C}{k_BT}$

$$= \frac{1}{2\pi^2}\left(\frac{2m_n^*}{\hbar^2}\right)^{\frac{3}{2}} e^{(E_F-E)/k_BT} \int_o^{\infty} (k_BT)^{\frac{1}{2}} x^{\frac{1}{2}} e^{-x} dx (k_BT)$$

$$\left(\int_o^{\infty} x^{\frac{1}{2}} e^{-x} dx = \frac{\sqrt{\pi}}{2} \right)$$

$$= 2\left(\frac{m_n^* k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} e^{-(E_C - E_F)/k_B T}$$

$$= N_{eff}^C \, e^{-(E_C - E_F)/k_B T}$$

For hole, valence band $E_{\vec{k}} = E_o - \left(\frac{\hbar^2 k_x^2}{2m_1^*} + \frac{\hbar^2 k_y^2}{2m_2^*} + \frac{\hbar^2 k_z^2}{2m_3^*}\right)$

(Isotropic mass, $m_1^* = m_2^* = m_3^* = m_p^*$)

$$= E_o - \frac{\hbar^2 k^2}{2m_p^*}$$

The density of state

$$D_h(E) = \frac{1}{2\pi^2}\left(\frac{2m_p^*}{\hbar^2}\right)^{\frac{3}{2}} (E_V - E)^{\frac{1}{2}}$$

Hole density,

$$p = \int_{-\infty}^{E_V} D_h(E) f_h(E) dE$$

$$f_h(E) = 1 - f(E)$$

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

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

$$= \frac{1}{2\pi^2}\left(\frac{2m_p^*}{\hbar^2}\right)^{\frac{3}{2}} \int_{-\infty}^{E_V} (E_V - E)^{\frac{1}{2}} \underbrace{e^{-(E_F-E)/k_BT}}_{e^{[\{-(E_V-E)\}+E_V-E_F]/k_BT}} dE$$

put $x = \dfrac{E_V - E}{k_BT}$

$$= \frac{1}{2\pi^2}\left(\frac{2m_p^*}{\hbar^2}\right)^{\frac{3}{2}} \int_{\infty}^{o} (k_BT)^{\frac{1}{2}} x^{\frac{1}{2}} e^{-x} dx (-k_BT) e^{(E_V-E_F)/k_BT}$$

$$= \frac{1}{2\pi^2}\left(\frac{2m_p^*}{\hbar^2}\right)^{\frac{3}{2}}(k_BT)^{\frac{3}{2}}\left\{\int_o^\infty x^{\frac{1}{2}}e^{-x}dx\right\}e^{(E_V-E_F)/k_BT}$$

$$= 2\left(\frac{m_p^*k_BT}{2\pi\ \hbar^2}\right)^{\frac{3}{2}}e^{(E_V-E_F)/k_BT}$$

$$= N_{eff}^V e^{(E_V-E_F)/k_BT}$$

$$\therefore np = 4\left(\frac{2\pi\ k_BT}{h^2}\right)^3 (m_p^*m_n^*)^{\frac{3}{2}}e^{-(E_C-E_V)/k_BT}$$

$$= 4\left(\frac{2\pi\ k_BT}{h^2}\right)^3 (m_p^*m_n^*)^{\frac{3}{2}}e^{-E_g/k_BT}$$

or $np = N_{eff}^C N_{eff}^V e^{-E_g/k_BT}$

$n_i p_i = {n_i}^2 = {p_i}^2$: <u>Law of mass action</u>

Intrinsic type

$$n = p = (np)^{\frac{1}{2}} = 2\left(\frac{2\pi\ k_B T}{h^2}\right)^{\frac{3}{2}} (m_p^* m_n^*)^{\frac{3}{4}} e^{-E_g / 2k_B T}$$

or $m_n^{*\frac{3}{2}} e^{(E_F - E_C)/k_B T} = m_p^{*\frac{3}{2}} e^{(E_V - E_F)/k_B T}$

$$e^{2E_F / k_B T} = \left(\frac{m_p^*}{m_n^*}\right)^{\frac{3}{2}} e^{(E_C + E_V)/k_B T}$$

In fact $E_V=0$, $E_C - E_V = E_g$, also $E_C + E_V = E_g$

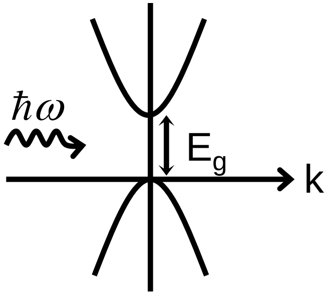
$$\frac{2E_F}{k_B T} = \frac{3}{2}\ln\frac{m_p^*}{m_n^*} + \frac{E_g}{k_B T}$$

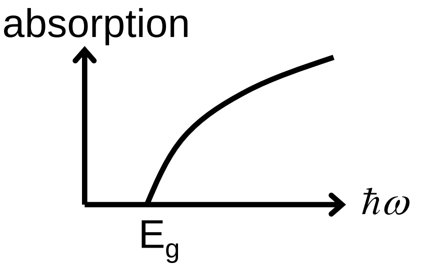
$$\therefore E_F = \frac{1}{2}E_g + \frac{3}{4}k_B T \ln\frac{m_p^*}{m_n^*}$$

If $m_n^* = m_p^*$ then $E_F = \frac{1}{2}E_g$

Measurement of E_g

1) Optical measurement : measure the penetration of photon about various frequencies





2) Electrical conductivity measurement

$$J = \sigma E = \sum nq\mu$$
$$= n(-e)v_e + pev_p = ne(-v_e) + pe\left|v_p\right|$$
$$= ne\mu_e E + pe\mu_p E = (ne\mu_e + pe\mu_p)E$$

$\therefore$ The conductivity of the semiconductor including holes and electrons

$$\sigma = ne\mu_e + pe\mu_p$$

In intrinsic type , n=p

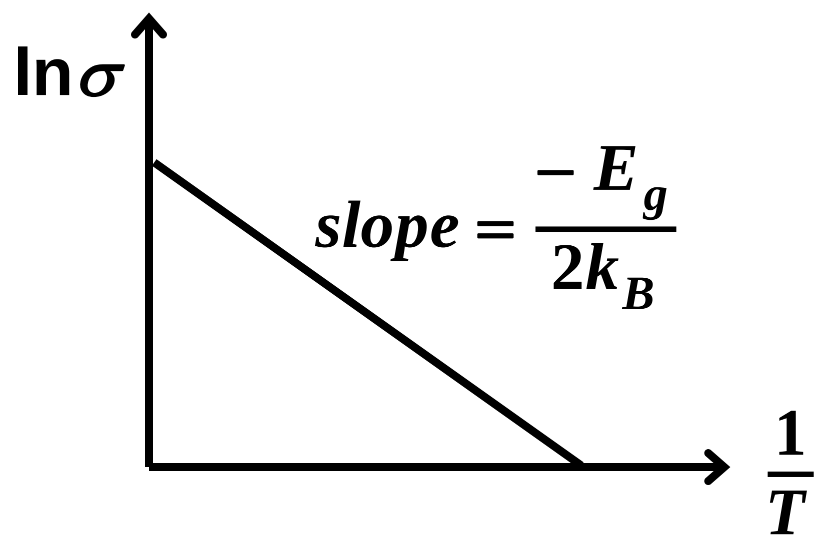
$$\sigma = n(\mu_e + \mu_p)e$$

$$= (\mu_e + \mu_p)e2\left(\frac{2\pi\ k_B T}{h^2}\right)^{\frac{3}{2}}(m_p^* m_n^*)^{\frac{3}{4}} e^{-E_g/2k_B T}$$

As T increase, σ increases

As Eg increase, σ decreases

$$\ln\sigma \sim \frac{-E_g}{2k_B T} + \frac{3}{2}\ln T$$



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- **Repetion: Effective mass method**
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- **doping and conductivity in semiconductors**

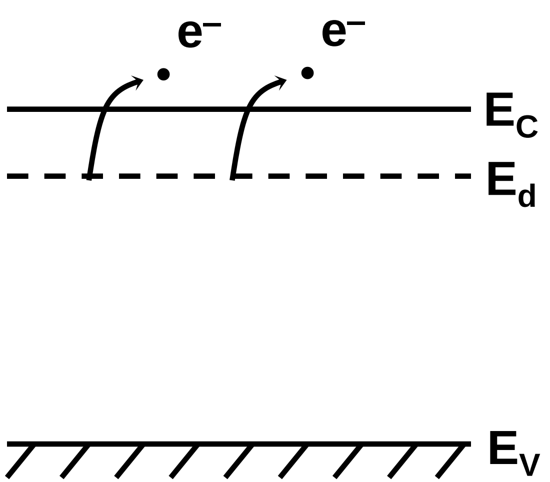
Doping of Semiconductor

For Si, Ge

- Donor $\rightarrow$ impurity atoms of valence 5(P, As, Sb)

Hydrogen energy $$H = \frac{p^2}{2m_o} - \frac{e^2}{4\pi\varepsilon_o r}$$

In solid, impurity $$m_o \rightarrow \frac{m^*}{m_o}, \; e^2 \rightarrow \frac{e^2}{\varepsilon_r}$$



donating e⁻s into the conduction band

$$E_n = -\frac{me^4}{2(4\pi\ \varepsilon_o \hbar)^2}\frac{1}{n^2}$$

$$\Rightarrow E_d = \frac{1}{\varepsilon_r^2}\left(\frac{m_n^*}{m_o}\right)\left[\frac{m_o e^4}{2(4\pi\ \varepsilon_o \hbar)^2}\right]\frac{1}{n^2}$$

$$r_n = \frac{n^2\hbar^2}{e^2 m} = a_o n^2$$

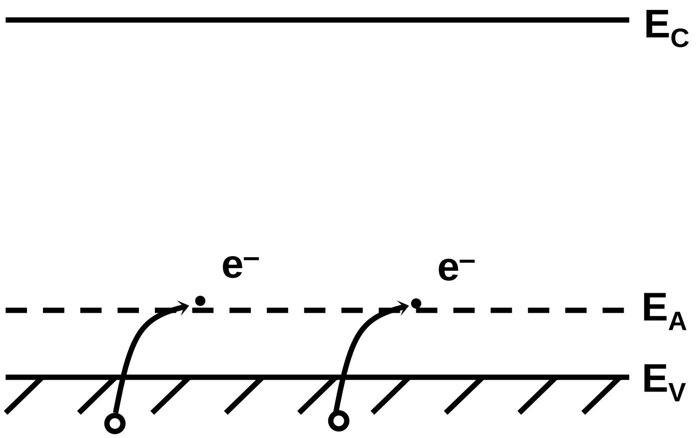
$$\Rightarrow r_d = \varepsilon_r\left(\frac{m_o}{m_n^*}\right)a_o n^2$$

Ex) Si

$$m_n^* \cong 0.2m_o, \varepsilon_r = 11.7, E_1 = 0.03eV, r_1 = 30\overset{o}{A}$$

Easy excitation to conduction band with little energy

• Acceptor : impurity atoms of valence 3(B, Al, Ga)



Carrier density in doped Semiconductor

Donors filled with electrons

$$N_d^o = N_d f(E_g - E_d)$$

$$= N_d \frac{1}{e^{(E_g - E_d - E_F)/k_B T} + 1}$$

$$n = N_d^+ = N_d - N_d^o = N_d \frac{e^{(E_g - E_d - E_F)/k_B T} + 1 - 1}{e^{(E_g - E_d - E_F)/k_B T} + 1}$$

$$= N_d \frac{1}{1 + e^{-(E_g - E_d - E_F)/k_B T}}$$

Also, previously

$$n = 2\left(\frac{2\pi m_n^* k_B T}{\hbar^2}\right)^{\frac{3}{2}} e^{(E_F - E_g)/k_B T} = n_o \underbrace{e^{(E_F - E_g)/k_B T}}_{\text{set } x}$$

Then

$$n_o x = \frac{N_d}{x e^{E_d/k_B T} + 1}$$

$$n_o e^{E_d/k_B T} x^2 + n_o x - N_d = 0$$

$$x = \frac{-n_o + \sqrt{n_o^2 + 4 n_o N_d e^{E_d/k_B T}}}{2 n_o e^{E_d/k_B T}} = \frac{-1 + \left[1 + 4\frac{N_d}{n_o} e^{E_d/k_B T}\right]^{\frac{1}{2}}}{2 e^{E_d/k_B T}}$$

i) Low T & large N_d

$$\frac{E_d}{k_B T} \rangle\rangle 1 \qquad n = n_o \sqrt{\frac{N_d}{n_0}} e^{-E_d / 2k_B T} = \sqrt{n_o N_d} e^{-E_d / 2k_B T}$$

ii) High T & small N_d

$$n = n_o \frac{-1 + \left(1 + \frac{2N_d}{n_o} e^{E_d / k_B T}\right)}{2e^{E_d / k_B T}} = n_o \frac{\frac{2N_d}{n_o} e^{E_d / k_B T}}{2e^{E_d / k_B T}} = N_d$$

Every donor will be ionized

Quatitative temperature dependence of n in the conduction band of an n-type Semiconductor