

自由电子薛定谔方程

$$\begin{cases} -\frac{\hbar^2}{2m_0} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x) \\ V(x) = 0 \end{cases}$$

$$\Rightarrow \psi(x) = A e^{ikx}$$

$$\Rightarrow \begin{cases} \psi(x) = u_k(x) e^{ikx} \\ \psi(x) = u_k(x+n\alpha) \end{cases}$$

晶体中

$$\begin{cases} -\frac{\hbar^2}{2m_0} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x) \\ V(x) = V(x+n\alpha) \end{cases}$$

$$\Rightarrow \begin{cases} \psi(x) = u_k(x) e^{ikx} \\ u_k(x) = u_k(x+n\alpha) \end{cases}$$

自由电子状态推导

$$\begin{cases} \text{波动性 } p = \hbar k \text{ (德布罗意关系)} & E = \hbar \omega \\ \text{粒子性 } p = mv & E = \frac{p^2}{2m} \end{cases} \Rightarrow E = \frac{\hbar^2 k^2}{2m_0}$$

晶体中状态推导

$$v = \frac{1}{\hbar} \frac{dE}{dk} \text{ 推导}$$

将 $E(k)$ 在 $k=0$ 处泰勒展开

$$E(k) = E(0) + \left(\frac{dE}{dk} \right)_{k=0} k + \frac{1}{2} \left(\frac{d^2 E}{dk^2} \right)_{k=0} k^2 + \dots$$

$$1^\circ k=0 \text{ 时 能量极小 } \left(\frac{dE}{dk} \right)_{k=0} = 0$$

$$\Rightarrow E(k) = E(0) + \frac{1}{2} \left(\frac{d^2 E}{dk^2} \right)_{k=0} k^2$$

$$\Rightarrow E(k) - E(0) = \frac{1}{2} \left(\frac{d^2 E}{dk^2} \right)_{k=0} k^2$$

$$\text{令 } \frac{1}{m^*} = \frac{1}{\hbar^2} \left(\frac{d^2 E}{dk^2} \right)_{k=0}$$

$$\Rightarrow E(k) - E(0) = \frac{\hbar^2 k^2}{2m^*}$$

$$E = \hbar \omega$$

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

$$= \frac{1}{\hbar} \frac{dE}{dk}$$

电子加速度 a 和 $\frac{dk}{dt}$ 推导

$$dE = f \cdot ds = + f v dt = f \cdot \frac{1}{\hbar} \frac{dE}{dk} \cdot dt \Rightarrow \frac{dk}{dt} = \frac{f}{\hbar}$$

$$a = \frac{dv}{dt} = \frac{d\left(\frac{1}{\hbar} \frac{dE}{dk}\right)}{dt} = \frac{1}{\hbar} \frac{d^2 E}{dk^2} \frac{dk}{dt} = \frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \cdot \frac{f}{1} = \frac{f}{m^*}$$

空穴推导

① 满价带中有一状态电子进入导带，留下一空态。在外电场作用下，电子和空态的运动状态是等效的。所以 $\frac{dk}{dt} = \frac{f}{\hbar}$ 是等效运动。因此可以等效

② 设价带中剩余电子的净电流为 J ，另将一电子填入空态，净电流为 $J_1 = -q v(k)$ 。

③ 由于满带不导电 $\Rightarrow J_1 + J_2 = 0 \Rightarrow J_1 = +q v(k) \Rightarrow$ 所以价带中剩余大量电子可用正电荷等效。

✓ $m_p^* = -m_n^*$ 推导

由于价带电子多带和空态都带电荷运动，所以两者加速度一致

∴ 带 $a = \frac{-qE}{m_n^*}$ ∵ $m_n^* < 0 \Rightarrow a > 0$

∴ 空带 $a = \frac{+qE}{m_p^*} > 0 \Rightarrow m_p^* = -m_n^*$

✗ 回旋频率 $\omega_c = \frac{qB}{m_n^*}$ 推导

将样本位于磁感应强度为 \vec{B} 的磁场中，由速度 \vec{v} 和 \vec{B} 夹角为 θ 。

则洛伦兹力 $\vec{F} = -q\vec{v} \times \vec{B}$

$|\vec{F}| = qvB \sin\theta = qv_{\perp}B$ 其中 $\left\{ \begin{array}{l} \text{与 } B \text{ 平行方向做匀速直线运动} \\ \text{与 } B \perp \text{ 方向做圆周运动} \end{array} \right. \Rightarrow \text{螺旋线运动}$

各向同性时

设回旋半径为 r ，角频率为 ω_c 。 $\Rightarrow v_{\perp} = \omega_c r$

则向心加速度 $a = \frac{v_{\perp}^2}{r} = \frac{F}{m_n^*} = \frac{qv_{\perp}B}{m_n^*} = \frac{qv_{\perp}B}{m_n^*}$

$\Rightarrow \frac{v_{\perp}^2}{r} = \frac{qv_{\perp}B}{m_n^*} \Rightarrow \omega_c = \frac{qB}{m_n^*}$

各向异性时

$\vec{F} = -q\vec{v} \times \vec{B} = (F_x \vec{i} + F_y \vec{j} + F_z \vec{k})$

$= -q(v_x \vec{i} + v_y \vec{j} + v_z \vec{k}) \times B(\alpha \vec{i} + \beta \vec{j} + \gamma \vec{k})$

$\left\{ \begin{array}{l} \alpha = \cos\theta_1 \\ \beta = \cos\theta_2 \\ \gamma = \cos\theta_3 \end{array} \right.$

✓ 证明大空间中k取值不连续

在一维晶体中, 由波恩卡曼边界条件得 晶体具有周期性

$$\begin{cases} \psi_k(0) = \psi_k(L) \\ L = Na \end{cases} \Rightarrow \psi_k(0) = \psi_k(L)$$

$$\because \psi_k(0) = \psi_k(L) e^{i n k L} \Rightarrow e^{i n k L} = 1 \Rightarrow n k L = 2\pi n \Rightarrow k = \frac{n}{L} (n=0, \pm 1, \pm 2, \dots)$$

\therefore 是不连续的

✓ 大空间中态密度推导

由波恩卡曼边界条件得 $\Rightarrow k = \frac{n}{L}$

$$\text{三维中, } \begin{cases} k_x = \frac{n_x}{L_1} \\ k_y = \frac{n_y}{L_2} \\ k_z = \frac{n_z}{L_3} \end{cases} \Rightarrow \text{每个允许的k值在大空间所占体积为 } \frac{1}{L_1 L_2 L_3} = \frac{1}{V}$$

\therefore k空间态密度为 $\frac{1}{V} = V$.

计入自旋后为 $2V$.

同理, 一维为 $2L$ 二维为 $2S$.

✓ 大空间中态数推导

$$E = \frac{\hbar^2 k^2}{2m_n^*} \Rightarrow k = \sqrt{\frac{2m_n^* E}{\hbar^2}}$$

一维: ① 态密度为 $2L$

② 体积为 $k \cdot 1$

$$\text{③ } Z(E) = 2L \cdot k = \frac{2L \sqrt{2m_n^* E}}{\hbar}$$

二维: ① $2S$

$$\text{② } \pi k^2 = \frac{2m_n^* \pi E}{\hbar^2}$$

$$\text{③ } Z(E) = 2S \cdot \pi k^2 = \frac{4S m_n^* \pi E}{\hbar^2}$$

三维: ① $2V$

(同) ② $\frac{4}{3} \pi k^3$ (同) ~~$\frac{4}{3} \pi k_1 k_2 k_3 \cdot \frac{1}{k}$~~

$$\text{③ } Z(E) = \frac{4}{3} \pi \cdot \frac{(2m_n^* E)^{\frac{3}{2}}}{\hbar^3} \cdot 2V = \frac{8\pi V}{3} \frac{(2m_n^*)^{\frac{3}{2}}}{\hbar^3} E^{\frac{3}{2}}$$

X 吸收峰判断推子

以 Si 为例, 从 6 个椭圆球等能面的取在轴沿 [001] 的一个为例.

再设一坐标系 k_1, k_2, k_3 . 以 [001] 上的椭圆球中心为原点, 使 k_3 与 [001] 重合. 再旋转 k_1, k_2

使 B 位于 k_1, k_3 平面内, 则 $\Rightarrow \begin{cases} \alpha = \sin\theta \\ \beta = 0 \\ \gamma = \cos\theta \end{cases}$ 且 $m_{k_1} = m_{k_2} = m_c$ $m_{k_3} = m_L$

$$\therefore E(k) = \frac{\hbar^2}{2} \left[\frac{k_1^2 + k_2^2}{m_c} + \frac{k_3^2}{m_L} \right]$$

$$\therefore \frac{1}{m^*} = \sqrt{\frac{m_x^* \alpha^2 + m_y^* \beta^2 + m_z^* \gamma^2}{m_x^* m_y^* m_z^*}} = \sqrt{\frac{m_c \sin^2\theta + m_L \cos^2\theta}{m_c^2 m_L}}$$

当 B 沿 [111] 方向时

B 与 [100] [010] [001] 夹角为 θ 与 $[\bar{1}00]$ $[0\bar{1}0]$ $[00\bar{1}]$ 夹角为 $\pi - \theta$

$$\sin^2\theta = \sin^2(\pi - \theta) = \frac{2}{3} \quad \cos\theta = \cos(\pi - \theta) = \frac{1}{3} \Rightarrow \text{只有一个 } m_n^* = \sqrt{\frac{3m_c}{2m_c + m_L}} \cdot m_L \quad 1 \uparrow \text{峰}$$

当 B 沿 [110] 方向时

$$B \text{ 与 } [100] [010] [\bar{1}00] [0\bar{1}0] \text{ 夹角为 } \frac{\pi}{4} \text{ 或 } \pi - \frac{\pi}{4} \Rightarrow \cos^2\theta = \sin^2\theta = \frac{1}{2} \\ \Rightarrow m_n^* = m_c \sqrt{\frac{2m_L}{m_c + m_L}} \quad 2 \uparrow \text{峰}$$

$$B \text{ 与 } [001] [00\bar{1}] \text{ 夹角为 } \frac{\pi}{2} \Rightarrow \cos^2\theta = 0 \quad \sin^2\theta = 1 \Rightarrow m_n^* = \sqrt{m_c m_L}$$

当 B 沿 [100] 方向时

$$B \text{ 与 } [100] [\bar{1}00] \text{ 夹角为 } 0 \text{ 或 } \pi \Rightarrow \cos^2\theta = 1 \quad \sin^2\theta = 0$$

$$B \text{ 与 } [010] [001] [0\bar{1}0] [00\bar{1}] \text{ 夹角为 } \frac{\pi}{2} \Rightarrow \cos^2\theta = 0 \quad \sin^2\theta = 1$$

$\Rightarrow 2 \uparrow \text{峰}$

当 B 沿任意方向 $\Rightarrow 3 \uparrow \text{峰}$

X 类氢模型, 用于估计 $\Delta E_0, \Delta E_A$

$$E_0 = \frac{m_0 q^4}{8\epsilon_0^2 \hbar^2} \quad E = \frac{m_n^* q^4}{8\epsilon_0 \epsilon_r \hbar^2}$$

$$\Delta E_0 = \frac{m_n^*}{m_0} \frac{E_0}{\epsilon_r^2}$$

$$\text{氢原子半径 } r_0 = \frac{\hbar^2 \epsilon_0}{\pi q^2 m_0}$$

$$\text{杂质原子半径 } r = \frac{\hbar^2 \epsilon_0 \epsilon_r}{\pi q^2 m_n^*}$$

✓ 费米分布和波尔兹曼分布.

$$\text{费米分布} f(E) = \frac{1}{1 + \exp(\frac{E - E_F}{k_B T})}$$

$$\text{波尔兹曼分布} f(E) = \frac{1}{1 + \exp(\frac{E - E_F}{k_B T})}$$

$$\text{当 } E - E_F \gg k_B T \Rightarrow \text{为波尔兹曼分布} \Rightarrow f(E) = \exp(-\frac{E - E_F}{k_B T})$$

$$1 - f(E) = \exp(-\frac{E_F - E}{k_B T})$$

导带中的电子浓度 (非简并) + (简并).

$$n_0 = \frac{1}{V} \int_{E_c}^{E_c'} g_c(E) \cdot f_B(E) dE \quad \text{非简并}$$

$$= \frac{1}{V} \int_{E_c}^{E_c'} \frac{4\pi V (2m_n^*)^{\frac{3}{2}}}{h^3} (E - E_c)^{\frac{1}{2}} \cdot \exp(-\frac{E - E_c}{k_B T}) dE$$

$$= \frac{4\pi (2m_n^*)^{\frac{3}{2}}}{h^3} \int_{E_c}^{E_c'} (E - E_c)^{\frac{1}{2}} \cdot \exp(-\frac{E - E_c}{k_B T}) \exp(-\frac{E_c - E_F}{k_B T}) dE \quad \text{令 } \frac{E - E_c}{k_B T} = x$$

$$= \frac{4\pi (2m_n^*)^{\frac{3}{2}}}{h^3} \exp(-\frac{E_c - E_F}{k_B T}) \cdot \int_0^{+\infty} (k_B T)^{\frac{1}{2}} x^{\frac{1}{2}} \exp(-x) \cdot k_B T dx$$

$$\because \int_0^{+\infty} x^{\frac{1}{2}} \exp(-x) dx = \Gamma(\frac{3}{2}) = \Gamma(\frac{1}{2}) = \frac{\sqrt{\pi}}{2}$$

$$\Rightarrow \frac{4\pi (2m_n^* k_B T)^{\frac{3}{2}}}{h^3} \cdot \frac{\sqrt{\pi}}{2} \exp(-\frac{E_c - E_F}{k_B T}) = N_c \exp(-\frac{E_c - E_F}{k_B T})$$

$$n_0 = \frac{1}{V} \int_{E_c}^{E_c'} g_c(E) f(E) dE$$

$$= \frac{4\pi (2m_n^*)^{\frac{3}{2}}}{h^3} \int_{E_c}^{E_c'} (E - E_c)^{\frac{1}{2}} \frac{1}{1 + \exp(\frac{E - E_c + E_c - E_F}{k_B T})} dE \quad \text{令 } \frac{E - E_c}{k_B T} = x \quad \frac{E_F - E_c}{k_B T} = \eta$$

$$= \frac{4\pi (2m_n^* k_B T)^{\frac{3}{2}}}{h^3} \cdot \int_0^{+\infty} x^{\frac{1}{2}} \frac{1}{1 + \exp(x - \eta)} dx \quad \text{令 } \int_0^{+\infty} \frac{x^{\frac{1}{2}}}{1 + e^{x - \eta}} dx = F_{\frac{1}{2}}(\eta)$$

$$= \frac{2(\pi m_n^* k_B T)^{\frac{3}{2}}}{h^3} \cdot \frac{2}{\sqrt{\pi}} F_{\frac{1}{2}}(\eta)$$

注意 ① 2V

(4) ② $\frac{4}{3}\pi k_1 k_2 k_3$ $k_1 = \sqrt{\frac{2m_x^* E}{\hbar^2}}$ $k_2 = \sqrt{\frac{2m_y^* E}{\hbar^2}}$ $k_3 = \sqrt{\frac{2m_z^* E}{\hbar^2}}$

③ $Z(E) = 2V \frac{4}{3}\pi k_1 k_2 k_3$

$$= \frac{8\pi V}{3} \cdot \frac{\sqrt{8m_x^* m_y^* m_z^*}}{\hbar^3} (E - E_c)^{\frac{3}{2}}$$

✓ 旋转椭球面方程

$$\frac{(k_x - k_{0x})^2}{\frac{2m_x^*(E - E_c)}{\hbar^2}} + \frac{(k_y - k_{0y})^2}{\frac{2m_y^*(E - E_c)}{\hbar^2}} + \frac{(k_z - k_{0z})^2}{\frac{2m_z^*(E - E_c)}{\hbar^2}} = 1$$

由 $E(k) - E_c = \frac{\hbar^2}{2} \left(\frac{(k_x - k_{0x})^2}{m_x^*} + \frac{(k_y - k_{0y})^2}{m_y^*} + \frac{(k_z - k_{0z})^2}{m_z^*} \right)$ 推导得

✓ Si 半导体 状态密度和 状态密度有效质量推导。

① $Z(E) = \frac{8\pi V}{3} \cdot \frac{\sqrt{8m_x^* m_y^* m_z^*}}{\hbar^3} (E - E_c)^{\frac{3}{2}} \cdot s$

$s \begin{cases} \text{Si: } 6 \\ \text{Ge: } 4 \end{cases}$

$g_c(E) = \frac{4\pi V \sqrt{8m_x^* m_y^* m_z^*}}{\hbar^3} (E - E_c)^{\frac{1}{2}} \cdot s$

② 及 $m_x^* = m_y^* = m_t$ $m_z^* = m_l$

$g_c(E) = \frac{4\pi V s \sqrt{8m_t^2 m_l}}{\hbar^3} \cdot (E - E_c)^{\frac{1}{2}}$

令 $g_c(E) = \frac{4\pi V (2m_n^*)^{\frac{3}{2}}}{\hbar^3} (E - E_c)^{\frac{1}{2}}$

$\Rightarrow (2m_n^*)^{\frac{3}{2}} = s \sqrt{8m_t^2 m_l}$

$\Rightarrow m_n^* = s^{\frac{2}{3}} (m_t^2 m_l)^{\frac{1}{3}}$

X Si 价带底同上。

① $Z(E) = \frac{8\pi V}{3} \cdot \frac{(-2m_p^*)^{\frac{3}{2}}}{\hbar^3} (E_v - E)^{\frac{3}{2}} \cdot s$

$g_v(E) = 4\pi V \cdot \frac{(-2m_p^*)^{\frac{3}{2}}}{\hbar^3} \cdot (E_v - E)^{\frac{1}{2}} \cdot s$

② 对称价带 $g_{vh}(E) = 4\pi V s \frac{(2m_{ph}^*)^{\frac{3}{2}}}{\hbar^3} (E_v - E)^{\frac{1}{2}}$

$\therefore g_v(E) = g_{vh}(E) + g_{vl}(E)$

不对称价带 $g_{vl}(E) = 4\pi V s \frac{(2m_{pl}^*)^{\frac{3}{2}}}{\hbar^3} (E_v - E)^{\frac{1}{2}}$

$\Rightarrow m_p^{\frac{3}{2}} = m_{ph}^{\frac{3}{2}} + m_{pl}^{\frac{3}{2}} \Rightarrow m_p^* = (m_{ph}^{\frac{3}{2}} + m_{pl}^{\frac{3}{2}})^{\frac{2}{3}}$

价带电子浓度推导。(中简并) + (非简并)

$$\begin{aligned}
 P_0 &= \frac{1}{V} \int_{E_V}^{E_F} g_V(E) (1 - f_V(E)) dE \\
 &= \frac{1}{V} \int_{E_V}^{E_F} \frac{4\pi V (2m_p^*)^{\frac{3}{2}}}{h^3} (E_V - E)^{\frac{1}{2}} \exp\left(-\frac{E_F - E}{kT}\right) dE \\
 &= \frac{4\pi (2m_p^*)^{\frac{3}{2}}}{h^3} \exp\left(-\frac{E_F - E_V}{kT}\right) \int_{E_V}^{E_F} (E_V - E)^{\frac{1}{2}} \exp\left(-\frac{E_V - E}{kT}\right) dE \quad \text{令 } x = \frac{E_V - E}{kT} \\
 &= \frac{4\pi (2m_p^*)^{\frac{3}{2}}}{h^3} \cdot (kT)^{\frac{3}{2}} \exp\left(-\frac{E_F - E_V}{kT}\right) \int_0^{+\infty} x^{\frac{1}{2}} \exp(-x) dx \\
 &= \frac{2(\pi m_p^* kT)^{\frac{3}{2}}}{h^3} \exp\left(-\frac{E_F - E_V}{kT}\right) = N_V \exp\left(-\frac{E_F - E_V}{kT}\right)
 \end{aligned}$$

$$\begin{aligned}
 P_0 &= \frac{1}{V} \int_{E_V}^{E_F} g_V(E) (1 - f_V(E)) dE \\
 &= \frac{4\pi (2m_p^*)^{\frac{3}{2}}}{h^3} \int_{E_V}^{E_F} (E_V - E)^{\frac{1}{2}} \frac{1}{1 + \exp\left(\frac{E_F - E_V + E_V - E}{kT}\right)} dE \quad \text{令 } x = \frac{E_V - E}{kT} \quad \xi = \frac{E_V - E_F}{kT} \\
 &= \frac{4\pi (2m_p^* kT)^{\frac{3}{2}}}{h^3} \int_0^{+\infty} x^{\frac{1}{2}} \frac{1}{1 + \exp(x - \xi)} dx \quad \text{令 } F_{\frac{1}{2}}(\xi) = \int_0^{+\infty} \frac{x^{\frac{1}{2}}}{1 + e^{x - \xi}} dx \\
 &= N_V \cdot \frac{2}{\sqrt{\pi}} F_{\frac{1}{2}}(\xi)
 \end{aligned}$$

✓ 本征半导体推导

$$\begin{aligned}
 n_i^2 &= n_0 p_0 = N_C \exp\left(-\frac{E_C - E_F}{kT}\right) \cdot N_V \exp\left(-\frac{E_F - E_V}{kT}\right) \\
 &= N_C N_V \exp\left(-\frac{E_G}{kT}\right)
 \end{aligned}$$

$$n_i = \sqrt{n_0 p_0} = \sqrt{N_C N_V} \exp\left(-\frac{E_G}{2kT}\right)$$

✓ 本征 \$E_F\$ 与禁带中位置.

$$\begin{aligned}
 n_0 = p_0 = n_i &\Rightarrow N_C \exp\left(-\frac{E_C - E_F}{kT}\right) = N_V \exp\left(-\frac{E_F - E_V}{kT}\right) \\
 &\Rightarrow \exp\left(\frac{E_F - E_C - E_V}{kT}\right) = \frac{N_V}{N_C} \\
 &\Rightarrow E_F = \frac{E_C + E_V}{2} + \frac{1}{2} kT \ln \frac{N_V}{N_C} \quad \because \frac{N_V}{N_C} = \left(\frac{m_p^*}{m_n^*}\right)^{\frac{3}{2}} \\
 &\Rightarrow E_F = \frac{E_C + E_V}{2} + \frac{3}{4} kT \ln \frac{m_p^*}{m_n^*} \quad (6i)
 \end{aligned}$$

✓ $E_g(0)$ 的求解推导 ($\ln n_i \sim \frac{1}{T}$ 关系).

设 $E_g = E_g(0) + \beta T \quad \therefore \beta = \frac{dE_g}{dT}$

$$n_i = \sqrt{N_c N_v} \exp\left(-\frac{E_g}{2k_0 T}\right) = \sqrt{N_c N_v} \exp\left(-\frac{E_g(0)}{2k_0 T} - \frac{\beta T}{2k_0 T}\right)$$

$$= \sqrt{N_c(300) N_v(300)} \cdot T^{\frac{3}{2}} \exp\left(-\frac{E_g(0)}{2k_0 T}\right) \exp\left(-\frac{\beta}{2k_0}\right)$$

$$\Rightarrow \ln(n_i \cdot T^{-\frac{3}{2}}) = \frac{1}{2} \ln[N_c(300) N_v(300)] - \frac{E_g(0)}{2k_0 T} - \frac{\beta}{2k_0}$$

$$= A - \frac{E_g(0)}{2k_0} \cdot \frac{1}{T}$$

设 $\ln\left(\frac{n_i}{T^{\frac{3}{2}}}\right) \sim \frac{1}{T}$ 图像, 则 斜率 $= -\frac{E_g(0)}{2k_0}$

$$\Rightarrow E_g(0) = -\text{斜率} \cdot 2k_0$$

✓ 半导体中电子占据能级的概率

$$f_D(E) = \frac{1}{1 + \frac{1}{2} \exp\left(\frac{E_D - E_F}{k_0 T}\right)}$$

✓ ... 空穴占据能级的概率

$$f_A(E) = \frac{1}{1 + \frac{1}{4} \exp\left(\frac{E_F - E_A}{k_0 T}\right)}$$

✓ 价带能级上电子浓度和受主能级上空穴浓度

$$n_D = N_D f_D(E) = \frac{N_D}{1 + \frac{1}{2} \exp\left(\frac{E_D - E_F}{k_0 T}\right)}$$

$$p_A = N_A f_A(E) = \frac{N_A}{1 + \frac{1}{4} \exp\left(\frac{E_F - E_A}{k_0 T}\right)}$$

✓ 电离施主和受主浓度

$$n_D^+ = N_D [1 - f_D(E)] = N_D - n_D = \frac{N_D}{1 + 2 \exp\left(-\frac{E_D - E_F}{k_0 T}\right)}$$

$$p_A^- = N_A - p_A = \frac{N_A}{1 + 4 \exp\left(-\frac{E_F - E_A}{k_0 T}\right)}$$

✓ 低温时电离平衡推导

$$n_0 = n_D^+$$

$$\Rightarrow N_c \exp\left(-\frac{E_c - E_F}{kT}\right) = \frac{N_D}{1 + 2 \exp\left(-\frac{E_D - E_F}{kT}\right)} \quad \because E_D - E_F \gg kT$$

$$\Rightarrow N_c \exp\left(-\frac{E_c - E_F}{kT}\right) = \frac{1}{2} N_D \exp\left(\frac{E_D - E_F}{kT}\right)$$

$$\Rightarrow \exp\left(\frac{E_D - E_F - E_c + E_F}{kT}\right) = \frac{1}{2} \frac{N_D}{N_c}$$

$$\Rightarrow E_F = \frac{E_c + E_D}{2} + \frac{1}{2} kT \ln \frac{N_D}{2N_c}$$

✗ 低温时 E_F 和 T 的关系推导

$$E_F = \frac{E_c + E_D}{2} + \frac{1}{2} kT \ln \frac{N_D}{2N_c (200k) \cdot T^{\frac{3}{2}}} = \frac{E_c + E_D}{2} + \frac{1}{2} kT \ln(A T^{-\frac{3}{2}})$$

$$\frac{dE_F}{dT} = \frac{k_0}{2} \ln \frac{N_D}{2N_c} + \frac{1}{2} k_0 T \left[\ln A - \ln T^{\frac{3}{2}} \right]$$

$$= \frac{k_0}{2} \ln \frac{N_D}{2N_c} - \frac{1}{2} k_0 T \cdot \frac{3}{2} \cdot \frac{1}{T}$$

$$= \frac{k_0}{2} \left[\ln \frac{N_D}{2N_c} - \frac{3}{2} \right]$$

$$\therefore \text{当 } \ln \frac{N_D}{2N_c} = \frac{3}{2} \Rightarrow E_F \text{ 达到极大值}$$

✗ 强电离能平衡推导

$$n_0 = n_D^+ = \frac{N_D}{1 + \exp\left(-\frac{E_D - E_F}{kT}\right)} \Rightarrow \frac{1}{2} N_D \exp\left(\frac{E_D - E_F}{kT}\right)$$

$$\begin{aligned} & \text{将 } E_F = \frac{E_c + E_D}{2} + \frac{1}{2} kT \ln \frac{N_D}{2N_c} \text{ 代入} \\ & n_0 = \frac{1}{2} N_D \exp\left(\frac{E_D - \frac{E_c + E_D}{2} - \frac{1}{2} kT \ln \frac{N_D}{2N_c}}{kT}\right) \Rightarrow n_0 = N_c \exp\left(-\frac{E_c - E_F}{kT}\right) \\ & \Rightarrow n_0 = N_c \exp\left(-\frac{E_c - \frac{E_c + E_D}{2} - \frac{kT}{2} \ln \frac{N_D}{2N_c}}{kT}\right) \\ & \Rightarrow n_0 = N_c \exp\left(-\frac{E_c - E_D}{2kT} + \frac{1}{2} \ln \frac{N_D}{2N_c}\right) \\ & \Rightarrow n_0 = N_c \exp\left(-\frac{\Delta E_D}{kT}\right) \left(\frac{N_D}{2N_c}\right)^{\frac{1}{2}} \\ & \Rightarrow n_0 = \left(\frac{N_c N_D}{2}\right)^{\frac{1}{2}} \exp\left(-\frac{\Delta E_D}{kT}\right) \\ & \Rightarrow \ln n_0 = \frac{1}{2} \ln \frac{N_c N_D}{2} - \frac{\Delta E_D}{kT} \\ & \Rightarrow \ln n_0 T^{-\frac{3}{2}} = -\frac{\Delta E_D}{kT} + A \end{aligned}$$

$$\therefore \frac{1}{2} kT \times k_0 = \Delta E_D$$

✓ 中间电势区

$$E_D = E_F \Rightarrow \exp\left(-\frac{E_D - E_F}{k_B T}\right) = 1$$

$$E_F = \frac{E_D + E_C}{2} + \frac{1}{2} k_B T \ln \frac{N_D}{2N_C}$$

$$n_0 = n_D^+ = \frac{N_D}{-1 + 2 \exp\left(-\frac{E_D - E_F}{k_B T}\right)} = \frac{1}{2} N_D \quad \frac{1}{2} \text{ 电离}$$

✓ 强电离区位置

$$n_0 = N_D$$

$$\Rightarrow N_C \exp\left(-\frac{E_C - E_F}{k_B T}\right) = N_D$$

$$\Rightarrow E_F = E_C + k_B T \ln \frac{N_D}{N_C}$$

$$p_0 = N_A$$

$$\Rightarrow N_V \exp\left(-\frac{E_F - E_V}{k_B T}\right) = N_A$$

$$\Rightarrow E_F = E_V + k_B T \ln \frac{N_V}{N_A}$$

✗ 弱电离百分比推导

$$n_D = \frac{N_D}{1 + \frac{1}{2} \exp\left(\frac{E_D - E_F}{k_B T}\right)} \quad \text{代入 } E_F = E_C + k_B T \ln \frac{N_D}{N_C} \quad \text{且 } E_D - E_F \gg k_B T$$

$$\Rightarrow n_D = 2 N_D \exp\left(-\frac{E_D - E_C - k_B T \ln \frac{N_D}{N_C}}{k_B T}\right)$$

$$= 2 N_D \exp\left(-\frac{E_D - E_C}{k_B T}\right) \left(\frac{N_D}{N_C}\right)$$

$$= 2 N_D \left(\frac{N_D}{N_C}\right) \exp\left(+\frac{\Delta E_D}{k_B T}\right)$$

$$\Rightarrow D_- = \frac{n_D}{N_D} = 2 \left(\frac{N_D}{N_C}\right) \exp\left(\frac{\Delta E_D}{k_B T}\right)$$

$$p_A = \frac{N_A}{1 + \frac{1}{4} \exp\left(\frac{E_F - E_A}{k_B T}\right)}$$

$$= 4 N_A \exp\left(-\frac{E_F - E_A}{k_B T}\right) \quad \text{代入 } E_F = E_V + k_B T \ln \frac{N_V}{N_A}$$

$$= 4 N_A \exp\left(-\frac{E_F - E_V}{k_B T}\right) \exp\left(-\ln \frac{N_V}{N_A}\right)$$

$$= 4 N_A \left(\frac{N_A}{N_V}\right) \exp\left(\frac{\Delta E_A}{k_B T}\right)$$

$$D_+ = \frac{p_A}{N_A} = 4 \left(\frac{N_A}{N_V}\right) \exp\left(\frac{\Delta E_A}{k_B T}\right)$$

X 杂质区方程

$$\begin{cases} n_0 = N_D + p_0 \\ n_0 p_0 = n_i^2 \end{cases} \Rightarrow n_0 = \frac{N_D}{2} + \sqrt{\left(\frac{N_D}{2}\right)^2 + n_i^2}$$

$$n_0 = N_D + p_0$$

$$\Rightarrow n_i \exp\left(-\frac{E_i - E_F}{k_B T}\right) = N_D + n_i \exp\left(-\frac{E_F - E_i}{k_B T}\right)$$

$$\Rightarrow N_D = n_i \left[\exp\left(-\frac{E_i - E_F}{k_B T}\right) - \exp\left(-\frac{E_F - E_i}{k_B T}\right) \right] = 2n_i \sinh\left(\frac{E_F - E_i}{k_B T}\right)$$

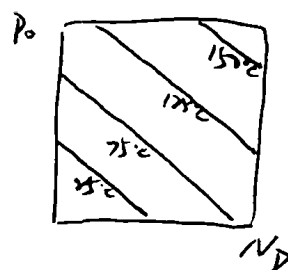
$$\Rightarrow E_F = E_i + k_B T \operatorname{arcsinh}\left(\frac{N_D}{2n_i}\right)$$

X 平衡少子浓度和 T 及取杂质浓度的关系方程 (弱电离)

则 $p_0 = \frac{n_i^2}{N_D}$

$$\therefore n_i^2 \sim T^3 \exp\left(-\frac{E_g}{k_B T}\right) \therefore p_0 \text{ 随 } T \uparrow \text{ 而 } \uparrow$$

且 p_0 随 $N_D \uparrow$ 而 \downarrow



X Si 电子有效质量的推导

因为 Si 导带底为旋矩椭球等能面,

沿 x, y, z 方向附近迁移率分别为 $\mu_1 = \frac{q\tau\hbar}{m_x} \quad \mu_2 = \frac{q\tau\hbar}{m_y} \quad \mu_3 = \frac{q\tau\hbar}{m_z}$

又因为 6 个极值, 每个能谷单位体积中有 $\frac{n}{3}$ 个电子.

设电场强度 E_x 沿 x 方向, 电流密度 J_x 为

$$\begin{aligned} J_x &= \frac{n}{3} q \mu_1 E_x + \frac{n}{3} q \mu_2 E_x + \frac{n}{3} q \mu_3 E_x \\ &= \frac{nq}{3} (\mu_1 + \mu_2 + \mu_3) E \end{aligned}$$

$$\text{令 } J_x = nq \mu_c E_x$$

$$\therefore \mu_c = \frac{1}{3} (\mu_1 + \mu_2 + \mu_3) \quad \text{且 } \mu_c = \frac{q\tau\hbar}{m_c^*}$$

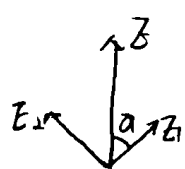
$$\therefore \frac{1}{m_c^*} = \frac{1}{3} \left(\frac{1}{m_x} + \frac{1}{m_y} + \frac{1}{m_z} \right)$$

X Ge 电子有效质量的推导

设电场 E 沿 $[001]$ 方向, 与 $[111]$ 方向夹角为 α . $\cos^2 \alpha = \frac{1}{3} \quad \sin^2 \alpha = \frac{2}{3}$

Ge 共有 8 个旋矩椭球等能面, 所以每个能谷单位体积中有 $\frac{n}{4}$ 个电子

把电场分解为 $E_1 = E \cos \alpha \quad E_2 = E \sin \alpha$



则 E_1 和 E_2 方向上的电流密度为

$$J_1 = \frac{n}{4} q \mu_1 E \cos \alpha \quad J_2 = \frac{n}{4} q \mu_2 E \sin \alpha$$

又因为总电流密度 $J = J_1 \cos \alpha + J_2 \sin \alpha$

$$= \frac{n}{4} q \mu_1 E \cos^2 \alpha + \frac{n}{4} q \mu_2 E \sin^2 \alpha$$

$$= \frac{nqE}{4} \left(\frac{\mu_1}{3} + \frac{2\mu_2}{3} \right)$$

$$\text{令 } J = \frac{nq}{4} \mu_c E$$

$$\therefore \mu_c = \frac{\mu_1}{3} + \frac{2\mu_2}{3} \quad \text{且 } \mu_c = \frac{q\tau\hbar}{m_c} \quad \mu_1 = \frac{q\tau\hbar}{m_1} \quad \mu_2 = \frac{q\tau\hbar}{m_2}$$

$$\therefore \frac{1}{m_c} = \frac{1}{3} \left(\frac{1}{m_1} + \frac{2}{m_2} \right)$$

X Si 空穴电子有效质量推导

$$\text{重掺杂带正电流密度为 } J_1 = p_1 q \mu_p E \quad \mu_p = \frac{q \tau_p}{m_{ph}^*}$$

$$\text{轻掺杂带正电流密度为 } J_2 = p_2 q \mu_p E \quad \mu_p = \frac{q \tau_p}{m_{pl}^*}$$

$$\text{又: } p_1 \propto N_{V1} \propto (m_{ph}^*)^{\frac{3}{2}} \Rightarrow J_1 = A (m_{ph}^*)^{\frac{1}{2}}$$

$$p_2 \propto N_{V2} \propto (m_{pl}^*)^{\frac{3}{2}} \Rightarrow J_2 = A (m_{pl}^*)^{\frac{1}{2}}$$

$$\therefore J_{\Sigma} = J_1 + J_2 = A [(m_{ph}^*)^{\frac{1}{2}} + (m_{pl}^*)^{\frac{1}{2}}]$$

$$\text{又: } J_{\Sigma} = p q \mu_p E \propto (m_{dp})^{\frac{3}{2}} \cdot \frac{1}{m_{cp}} \Rightarrow J_{\Sigma} = A m_{dp}^{\frac{3}{2}} \cdot \frac{1}{m_{cp}} \quad m_{cp} = (m_{ph}^{\frac{3}{2}} + m_{pl}^{\frac{3}{2}})^{\frac{2}{3}}$$

$$\Rightarrow A m_{dp}^{\frac{3}{2}} \frac{1}{m_{cp}} = A [(m_{pl}^*)^{\frac{1}{2}} + (m_{ph}^*)^{\frac{1}{2}}]$$

$$\Rightarrow \frac{1}{m_{cp}} = \frac{m_{ph}^{\frac{1}{2}} + m_{pl}^{\frac{1}{2}}}{m_{ph}^{\frac{3}{2}} + m_{pl}^{\frac{3}{2}}}$$

X 平均自由时间的推导

设有 N 个电子以 v 运动, $N(t)$ 表示在 t 时刻尚未遭受散射的电子数

则在 $t \sim t+\Delta t$ 时间内被散射的电子数为 $N(t) P \Delta t$ P 为散射几率.

$$\therefore N(t) - N(t+\Delta t) = N(t) P \Delta t$$

$$\therefore \frac{dN(t)}{dt} = \lim_{\Delta t \rightarrow 0} \frac{N(t+\Delta t) - N(t)}{\Delta t} = -N(t) P \quad \text{解为 } N(t) = N_0 e^{-Pt}$$

在 $t \sim t+dt$ 期间内被散射的电子数为

$$P \cdot N(t) = N_0 P e^{-Pt} dt$$

$$\therefore \tau = \frac{1}{N_0} \int_0^{+\infty} N_0 P e^{-Pt} dt = \frac{1}{P}$$

X 迁移率与温度的关系推导

散射概率 P

$$P_i \propto N_i T^{-\frac{3}{2}}$$

$$P_s \propto T^{\frac{3}{2}}$$

$$P_0 \propto \frac{1}{[\exp(\frac{h\nu_0}{kT}) - 1]}$$

平均自由时间

$$\tau_i \propto N_i^{-1} T^{\frac{3}{2}}$$

$$\tau_s \propto T^{-\frac{3}{2}}$$

$$\tau_0 \propto [\exp(\frac{h\nu_0}{kT}) - 1]$$

迁移率

$$\mu_i \propto N_i^{-1} T^{\frac{3}{2}}$$

$$\mu_s \propto T^{-\frac{3}{2}}$$

$$\mu_0 \propto [\exp(\frac{h\nu_0}{kT}) - 1]$$

因此总共有几种散射机制可同时存在，假设它们相互独立

$$\therefore P_{\text{总}} = P_i + P_{II} + P_{II} + \dots$$

$$\therefore \tau = \frac{1}{P} = \frac{1}{P_i + P_{II} + P_{II} + \dots}$$

$$\therefore \frac{1}{\tau} = P_i + P_{II} + P_{II} = \frac{1}{\tau_i} + \frac{1}{\tau_{II}} + \frac{1}{\tau_{II}} + \dots$$

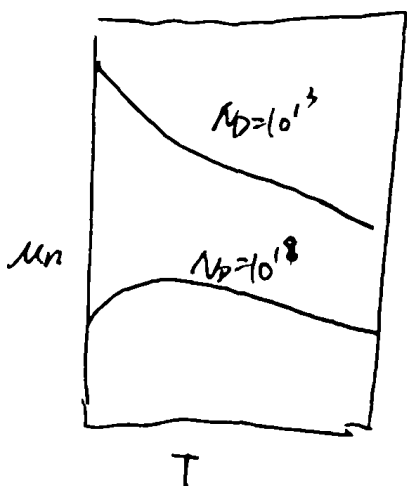
$$\therefore \frac{1}{\mu} = \frac{1}{\mu_i} + \frac{1}{\mu_{II}} + \frac{1}{\mu_{II}} + \dots$$

对 Si Ge 等半导体，散射机制是电离杂质和声学波散射

$$\mu_i \propto \frac{1}{BN_i T^{-\frac{3}{2}}} \quad \mu_s \propto \frac{1}{AT^{\frac{3}{2}}}$$

$$\text{且 } \frac{1}{\mu} = \frac{1}{\mu_i} + \frac{1}{\mu_s}$$

$$\Rightarrow \mu \propto \frac{1}{AT^{\frac{3}{2}} + BN_i T^{-\frac{3}{2}}}$$



当 $N_D = 10^{13} \text{ cm}^{-3}$ 时 即掺杂 N_i 不大，
晶格振动散射起主要作用， μ_n 随 $T \uparrow$ 而 \downarrow 。

当 $N_D \geq 10^{18} \text{ cm}^{-3}$ 时，

低温时，电离杂质散射起主要作用

高温时，晶格振动散射起主要作用

\therefore 曲线先升高再降低

✓ 电导率最小值所推导 (对n型)

$$\begin{cases} \sigma = n_0 q \mu_n + p_0 q \mu_p \\ n_0 = \frac{n_i^2}{p_0} \end{cases} \Rightarrow \sigma = \frac{n_i^2}{p_0} q \mu_n + p_0 q \mu_p$$

$$\frac{d\sigma}{dp_0} = -\frac{n_i^2}{p_0^2} q \mu_n + q \mu_p = 0 \Rightarrow p_0 = n_i \sqrt{\frac{\mu_n}{\mu_p}}$$

$$\text{同理 } p_0 = n_i \sqrt{\frac{\mu_p}{\mu_n}}$$

$$\sigma_{min} = n_i \sqrt{\frac{\mu_p}{\mu_n}} q \mu_n + n_i \sqrt{\frac{\mu_n}{\mu_p}} q \mu_p = 2 n_i q \sqrt{\mu_n \mu_p}$$

$$\therefore \rho_{max} = \frac{1}{\sigma_{min}} \quad \text{又 } \mu_p < \mu_n \therefore \text{P型半导体电阻率较大}$$

X 附加光电子的测量法

$$\Delta \sigma = \Delta p q (\mu_n + \mu_p)$$

$$\text{则 } \Delta p = \frac{1}{\sigma} - \frac{1}{\sigma_0} = \frac{1}{(\sigma_0 + \Delta \sigma)} - \frac{1}{\sigma_0} \quad \text{因 } \sigma \approx \sigma_0$$

$$= \frac{-\Delta \sigma}{\sigma_0^2} \quad \therefore \Delta p \propto \Delta \sigma$$

$$\text{又: } \Delta r = \Delta p \frac{L}{S} \quad \therefore \Delta r \propto \Delta \sigma$$

$$\text{又: } \Delta V = I \Delta r \quad \therefore \Delta V \propto \Delta \sigma$$

\therefore 示波器上的电压变化直接反映附加电子率的微小
间接的验证「非平衡」少数载流子的注入。

✓ 准费米能级公式

$$n = N_c \exp\left(-\frac{E_c - E_{Fn}}{k_B T}\right) = n_i \exp\left(-\frac{E_i - E_{Fn}}{k_B T}\right) = n_0 \exp\left(-\frac{E_i - E_{Fn}}{k_B T}\right)$$

$$p = N_v \exp\left(-\frac{E_F - E_v}{k_B T}\right) = n_i \exp\left(-\frac{E_F - E_i}{k_B T}\right) = p_0 \exp\left(-\frac{E_i - E_F}{k_B T}\right)$$

$$np = n_i^2 \exp\left(-\frac{E_{Fn} - E_{Fp}}{k_B T}\right)$$

$\therefore E_{Fn}$ 和 E_{Fp} 偏离 E_i 大小直接反映出 np 和 n_i^2 的相差程度

反映偏离热平衡态的程度

寿命 τ 的推导

IX 直接复合中的寿命推导

复合率 $R = rnp$ 产生率 $G = r n_0 p_0 = r n_i^2$ (热平衡时 $R = G$ 所得)

净复合率 $U_d = R - G = r(np - n_i^2)$

$$= r[(n_0 + \Delta n)(p_0 + \Delta p) - n_i^2] = r[n_i^2 + n_0 \Delta p + p_0 \Delta n + \Delta n \Delta p - n_i^2]$$

$$= r(n_0 + p_0) \Delta p + r \Delta p^2$$

\therefore 寿命 $\tau = \frac{\Delta p}{U_d} = \frac{1}{r(n_0 + p_0) + r \Delta p}$

小注入时 $\Delta p \ll (n_0 + p_0) \Rightarrow \tau = \frac{1}{r(n_0 + p_0)}$ 对 n 型 $\Rightarrow \tau = \frac{1}{r n_0}$ $\left. \begin{array}{l} T \text{ 和 } N_i - E \\ \tau \text{ 近似为常数} \\ \text{随 } n_0 \text{ 或 } \sigma \text{ 增加} \end{array} \right\}$

大注入时 $\Delta p \gg (n_0 + p_0) \Rightarrow \tau = \frac{1}{2 \Delta p}$ 除非平衡 Δp 变化而变化, 不是常数

IX 间接复合求 U_d 和 τ

甲: (俘获) $= r_n n (N_t - n_t)$ 乙: (发射) $= s_- n_t$

丙: (俘获) $= r_p p n_t$ 丁: (发射) $= s_+ (N_t - n_t)$

平衡时 $\text{甲} = \text{乙}$

$\Rightarrow r_n n_0 (N_t - n_t) = s_- n_t$

$\Rightarrow r_n \cdot n_0 \cdot \frac{N_t \exp(\frac{E_t - E_f}{k_B T})}{1 + \exp(\frac{E_t - E_f}{k_B T})} = s_- \cdot \frac{N_t}{1 + \exp(\frac{E_t - E_f}{k_B T})}$

$\Rightarrow s_- = r_n N_t \exp(-\frac{E_t - E_f}{k_B T}) = r_n n_i$ $n_i = N_t \exp(-\frac{E_t - E_f}{k_B T})$

同理 $s_+ = r_p \cdot p_i$ $p_i = N_t \exp(-\frac{E_t - E_v}{k_B T})$

又: 甲+丁为复合能级上的总速率 乙+丙为产生和减少

$\therefore \text{甲} + \text{丁} = \text{乙} + \text{丙} \Rightarrow r_n n (N_t - n_t) + r_p p_i (N_t - n_t) = r_n n_i n_t + r_p p_i n_t$

$\Rightarrow n_t = N_t \frac{r_n n_i + r_p p_i}{r_n (n_i + n_t) + r_p (p_i + p_t)}$

又: 净复合率 $U_d = \text{甲} - \text{乙} = \text{丙} - \text{丁}$

且 $n_i p_i = n_i^2$

$U_d = \frac{N_t r_n r_p (np - n_i^2)}{r_n (n_i + n_t) + r_p (p_i + p_t)}$

$\therefore \tau = \frac{\Delta p}{U_d} = \frac{r_n (n_0 + n_i) + r_p (p_0 + p_i)}{N_t r_n r_p (n_0 + p_0)}$