

1. 定态薛定谔方程:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(x, y, z) = E \psi(x, y, z)$$

束缚均为  $x$  方向,  $y, z$  方向为平面波, 得:

$$\psi(x, y, z) = \phi(x) e^{iky_y} e^{ik_z z}$$

$$\frac{\partial^2 \phi(x)}{\partial x^2} + k_x^2 \phi(x) = 0 \quad \phi(x) = A e^{ik_x x} + B e^{-ik_x x}$$

$$\phi(x)|_{x=0} = 0 \Rightarrow A + B = 0$$

$$\psi(x, y, z) = N \sin k_x x e^{iky_y} e^{ik_z z}$$

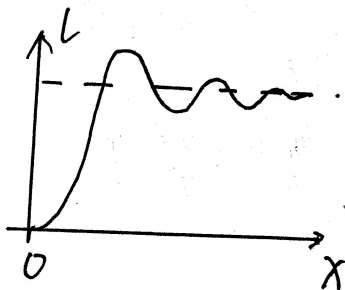
$$P(x, y, z) = \frac{e}{V} \sum_{k_x} \sum_{k_y} \sum_{k_z} |\psi|^2$$

$$= \frac{e}{V} \sum_{k_x, k_y, k_z} |\phi(x)|^2 \approx \frac{e}{V} \frac{2V}{(2\pi)^3} \int_0^{k_F} N^2 \sin^2 k_x x dk_x \int_{-k_F}^{k_F} dk_y \int_{-k_F}^{k_F} dk_z$$

$$= \frac{4N^2 e}{8\pi^3} \left( k_F - \frac{\sin 2k_F x}{2x} \right) (2k_F)^2$$

$$k_F = (8\pi^2 n)^{\frac{1}{3}} \quad \text{费米波矢}$$

$P(x, y, z)$  中含有  $\frac{N^2 e}{4\pi^3} \cdot \frac{\sin 2k_F x}{2x} (2k_F)^2$ , 为振荡项, 波长为  $2k_F$



$x \gg 0$  时趋于于零, 振荡周期为  $\frac{\pi}{k_F}$

金属  $n = 10^{23} \text{ cm}^{-3}$

半导体  $n = 10^{16} \text{ cm}^{-3}$

$$\frac{\pi}{k_F} \sim 4 \text{ \AA}$$

$$\frac{\pi}{k_F} \sim 400 \text{ \AA}$$

2. (1) 在临界点附近时  $E_c + \Delta E = E_c + \frac{\hbar^2}{2} \left( \frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z} \right)$

$\frac{2\Delta E}{\hbar^2} = \frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}$   
 k空间体积为  $\frac{4}{3}\pi \sqrt{m_x m_y m_z} \cdot \frac{2\Delta E}{\hbar^2} \sqrt{\frac{2\Delta E}{\hbar^2}}$

$\therefore D(E) \times \Delta E = \frac{V}{8\pi^2} \cdot \frac{4}{3}\pi \sqrt{m_x m_y m_z} \cdot \frac{2\Delta E}{\hbar^2} \sqrt{\frac{2\Delta E}{\hbar^2}}$   
 $D(E) \propto \sqrt{\Delta E} = \sqrt{E - E_c}$

(2) 由色散关系, 某能面内  $m$  体积为:  $E(k) = E_c$  时  $\Rightarrow 0 = \left( \frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} - \frac{k_z^2}{m_z} \right)$   
 $k_z \geq 0 \int_0^{k_B} \pi \sqrt{m_x m_y} \frac{k_z^2}{m_z} dk_z$

① 当  $E(k) > E_c$  时, 设  $E(k) = E_c + \Delta E$   $\frac{2\Delta E}{\hbar^2} + \frac{k_z^2}{m_z} = \frac{k_x^2}{m_x} + \frac{k_y^2}{m_y}$   
 体积为  $\int_0^{k_B} \pi \sqrt{m_x m_y} \left( \frac{k_z^2}{m_z} + \frac{2\Delta E}{\hbar^2} \right) dk_z$

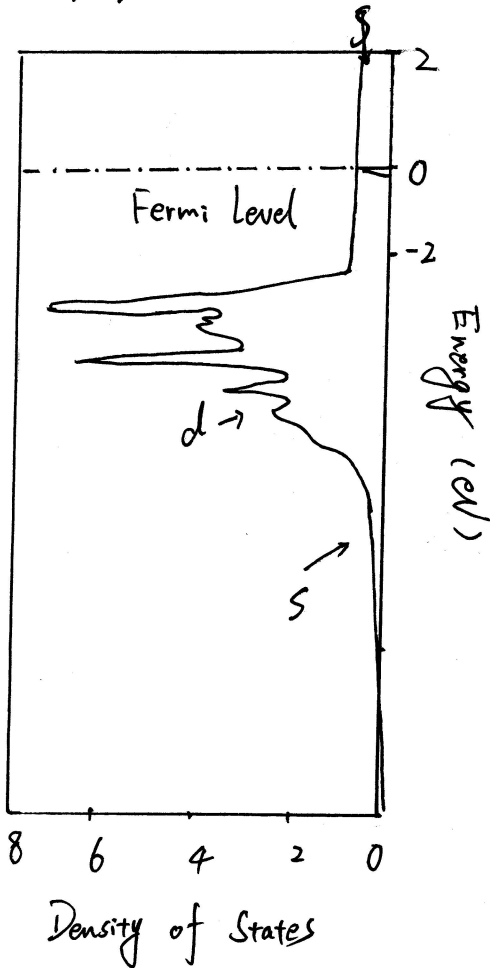
$\therefore$  改变量  $\int_0^{k_B} \frac{2\Delta E}{\hbar^2} dk_z$   
 $\Rightarrow D(E) \Delta E = \frac{V}{8\pi^2} \int_0^{k_B} \frac{2\Delta E}{\hbar^2} dk_z \Rightarrow D(E) \propto \text{const}$

② 当  $E(k) < E_c$  时, 设  $E(k) = E_c - \Delta E$   $\frac{k_z^2}{m_z} - \frac{2\Delta E}{\hbar^2} = \frac{k_x^2}{m_x} + \frac{k_y^2}{m_y}$   
 体积为  $\int_{\sqrt{\frac{2m_z \Delta E}{\hbar^2}}}^{k_B} \pi \sqrt{m_x m_y} \left( \frac{k_z^2}{m_z} - \frac{2\Delta E}{\hbar^2} \right) dk_z$

$\therefore$  改变量  $\int_0^{\sqrt{\frac{2m_z \Delta E}{\hbar^2}}} \pi \sqrt{m_x m_y} \frac{k_z^2}{m_z} dk_z + \int_{\sqrt{\frac{2m_z \Delta E}{\hbar^2}}}^{k_B} \pi \sqrt{m_x m_y} \frac{2\Delta E}{\hbar^2} dk_z$   
 $= \pi \sqrt{m_x m_y} \left[ \frac{1}{3m_z} \cdot \frac{2m_z \Delta E}{\hbar^2} \cdot \sqrt{\frac{2m_z \Delta E}{\hbar^2}} + \left( k_B - \sqrt{\frac{2m_z \Delta E}{\hbar^2}} \right) \frac{2\Delta E}{\hbar^2} \right]$

$\therefore D(E) \propto D_0 - C(E_c - E)^{1/2}$

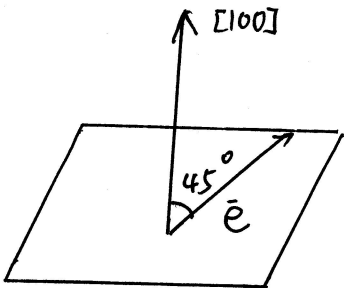
3.



right: Bandstructure  $E(k)$  for copper along directions of high crystal symmetry.

如图所示, 铜的  $d$  带位于费米面下 2 eV 以下. 可见光能量在 2.0 eV 以上, 很容易使电子从  $d$  带跃迁到  $s$  带. 容易被吸收. 2.0 eV 以下的红光则更多被反射. 使铜呈现颜色.

4.



① 电子在真空中的波矢

$$k = \sqrt{\frac{2m}{\hbar^2} (\hbar\omega - \phi - E)}$$

$$= 0.512 \sqrt{(40.8 - 4.5 - 2.2)}$$

$$= 2.99 \text{ \AA}^{-1}$$

②  $k_{\parallel} = k \sin\theta = 2.114 \text{ \AA}^{-1}$

$k_{\perp} = k \cos\theta = 2.114 \text{ \AA}^{-1}$

电子在逸透样品时,  $k_{\parallel}$  守恒,  $k_{\perp}$  不守恒.