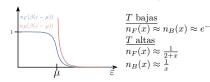
Constantes y aclaraciones

$$\begin{split} G(x) &= \frac{dN}{dx} = \text{dens. de est.}; \quad g(x) = \frac{dn}{dx} = \frac{\text{dens. de est}}{V} \\ k_B &= 1.381 \times 10^{-23} J K^{-1} = 8.62 \times 10^{-5} eV K^{-1} \\ m_e &= 9.11 \times 10^{-31} kg = 0.511 MeV c^{-2} \\ m_p &= 1.67 \times 10^{-27} kg = 938 MeV c^{-2} \\ \varepsilon_0 &= \frac{1}{4\pi K} = 8.85 \times 10^{-12} Fm^{-1} \\ \hbar &= 1.055 \times 10^{-34} Js = 6.58 \times 10^{-16} eVs \\ e &= 1.602 \times 10^{-19} C \end{split}$$

Fermions:
$$e^-, p, n \quad (n_F(x) = \frac{1}{e^x + 1})$$

Bosons: phonon, photon
$$(n_B(x) = \frac{1}{e^x - 1})$$

 $n \sim 10^{22} cm^{-3}; \tau \sim 10^{-15} s; v \sim 10^{-5} \frac{m}{}$



1 Estructura cristalina

1.1 Redes de Bravais

a	triclínica
m	monoclínica
0	ortorómbica
t	tetragonal
h	hexagonal
c	cúbica

P	Primitiva
S	Centrada en una cara
I	Centrada en el cuerpo
R	Centrada romboidal
F	Centrada en las caras

14 posibles redes de Bravais

	Tric.	Monoc.	Ortor.	Ortor. Tetra.		Cúbico	
ĺ	aP	mP, mS	oP, oS, oF, oI	tP, tI	hP, hR	cP, cF, cI	

1.2 Cosas

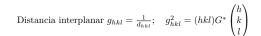
Base dual v matriz métrica

$$a^* = \frac{b \times c}{V}, \quad b^* = \frac{c \times a}{V}, \quad c^* = \frac{a \times b}{V}, \quad V = \det(\overline{a}, \overline{b}, \overline{c})$$

$$(\overline{a}^*, \overline{b}^*, \overline{c}^*) = \begin{pmatrix} \overline{a}^T \\ \overline{b}^T \\ \overline{c}^T \end{pmatrix}^{-1}, G = \begin{pmatrix} a \cdot a & a \cdot b & a \cdot c \\ b \cdot a & b \cdot b & b \cdot c \\ c \cdot a & c \cdot b & c \cdot c \end{pmatrix}, G^* = G^{-1}$$

Cambio de base

$$(\overline{a}', \overline{b}', \overline{c}') = (\overline{a}, \overline{b}, \overline{c})P, \quad \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = P^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$
$$(x, y, z) = (x^*, y^*, z^*)P, \quad \begin{pmatrix} a'^* \\ b'^* \\ c'^* \end{pmatrix} = P^{-1} \begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix}$$



Transferencia de momento $Q = \frac{4\pi \sin \theta}{\lambda}$

Condiciones de Laue $\overline{Q} = 2\pi \overline{q}_{hki}$

Ley de Bragg $q_{hkl} = \frac{2 \sin \theta_{hkl}}{\lambda}$

Módulo de Young $\nu_s = \sqrt{\frac{\gamma}{\rho}}$

Factor de estructura $F_{hkl}=\sum_p f_p e^{-i2\pi\overline{g}_{hkl}\cdot\overline{r}_p}; I\propto |F_{hkl}|^2$

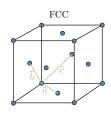
1.3 Estructuras comunes

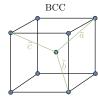
FCC (primitiva volumen 1/4)

$$\begin{cases} \overline{a} = \frac{1}{2}(1\ 1\ 0) \\ \overline{b} = \frac{1}{2}(0\ 1\ 1) \\ \overline{c} = \frac{1}{2}(1\ 0\ 1) \end{cases} \qquad \begin{cases} \overline{a}^* = (1\ 1\ -1) \\ \overline{b}^* = (-1\ 1\ 1) \\ \overline{c}^* = (1\ -1\ 1) \end{cases}$$

BCC (primitiva volumen 1/2)

$$\begin{cases} \overline{a} = \frac{1}{2}(1\ 1\ -1) \\ \overline{b} = \frac{1}{2}(-1\ 1\ 1) \\ \overline{c} = \frac{1}{2}(1\ -1\ 1) \end{cases} \qquad \begin{cases} \overline{a}^* = (1\ 1\ 0) \\ \overline{b}^* = (0\ 1\ 1) \\ \overline{c}^* = (1\ 0\ 1) \end{cases}$$





Hexagonal

_		2. 2	•			,	
G =	$\begin{pmatrix} a^2 \\ -\frac{a^2}{2} \\ 0 \end{pmatrix}$	$-\frac{a^2}{2}$ a^2 0	$\begin{pmatrix} 0 \\ 0 \\ c^2 \end{pmatrix}$,	$G^* =$	$\begin{pmatrix} \frac{4}{3a^2} \\ \frac{3a^2}{0} \end{pmatrix}$	$\begin{array}{c} \frac{2}{3q^2} \\ \frac{3}{3}a^2 \\ 0 \end{array}$	$\begin{pmatrix} 0 \\ 0 \\ \frac{1}{c^2} \end{pmatrix}$
			•	$\overline{}$	•		

 $\begin{cases} \overline{a} = (1,0) \\ \overline{b} = (-\frac{1}{2}, \frac{\sqrt{3}}{3}) \end{cases} \begin{cases} \overline{a}^* = \frac{2\sqrt{3}}{3}(\frac{\sqrt{3}}{2}, \frac{1}{2}) \\ \overline{b}^* = \frac{2\sqrt{3}}{3}(0,1) \end{cases}$







En una hcp c = 1.633a

$$(x,y,z) = (x^*,y^*,z^*)P, \quad \begin{pmatrix} a'^* \\ b'^* \\ z'^* \end{pmatrix} = P^{-1} \begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix} \qquad \qquad m_{100} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \\ n_{001} = \begin{pmatrix} \cos\left(\frac{360}{n}\right) & -\sin\left(\frac{360}{n}\right) & 0 \\ \sin\left(\frac{360}{n}\right) & \cos\left(\frac{360}{n}\right) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Cambio de base a $\mathcal{B} = \{\overline{u}, \overline{v}, \overline{w}\}$

$$M_{\mathcal{C}} = M_{\mathcal{B} \to \mathcal{C}} M_{\mathcal{B}} M_{\mathcal{B} \to \mathcal{C}}^{-1}, \quad M_{\mathcal{B} \to \mathcal{C}} = (\overline{u}, \overline{v}, \overline{w})$$

Reflexión vector director (a, b, c)

$$M = \frac{1}{a^2 + b^2 + c^2} \begin{pmatrix} -a^2 + b^2 + c^2 & -2ab & -2ac \\ -2ab & a^2 - b^2 + c^2 & -2bc \\ -2ac & -2bc & a^2 + b^2 - c^2 \end{pmatrix} \omega_{\pm}(k) = \sqrt{\frac{k_1 + k_2}{m} \pm \frac{1}{m} \sqrt{(k_1 + k_2)^2 - 4k_1 k_2 \sin^2(ka/2)}} = \sqrt{\frac{k_1 + k_2}{m} + \frac{1}{m} \sqrt{(k_1 + k_2)^2 - 4k_1 k_2 \sin^2(ka/2)}} = \sqrt{\frac{k_1 + k_2}{m} + \frac{1}{m} \sqrt{(k_1 + k_2)^2 - 4k_1 k_2 \sin^2(ka/2)}} = \sqrt{\frac{k_1 + k_2}{m} + \frac{1}{m} \sqrt{(k_1 + k_2)^2 - 4k_1 k_2 \sin^2(ka/2)}} = \sqrt{\frac{k_1 + k_2}{m} + \frac{1}{m} \sqrt{(k_1 + k_2)^2 - 4k_1 k_2 \sin^2(ka/2)}}}$$

Rotación respecto $\hat{u}=(u_x,u_y,u_z)$ $(c=\cos\theta,\quad s=\sin\theta).$

$$\begin{pmatrix} c + u_x^2(1-c) & u_x u_y(1-c) - u_z s & u_x u_z(1-c) + u_y s \\ u_y u_x(1-c) + u_z s & c + u_y^2(1-c) & u_y u_z(1-c) - u_x s \\ u_z u_x(1-c) - u_y s & u_z u_y(1-c) + u_x s & c + u_z^2(1-c) \end{pmatrix}$$

Centrosimétricos $(x, y, z) \rightarrow (-x, -y, -z)$ no tienen polarización espontánea

Dinámica de cristales

2.1 Densidad de estados

$$\overline{k} = \begin{pmatrix} \frac{2\pi}{L}n & \frac{2\pi}{L}m & \frac{2\pi}{L}l \end{pmatrix} \ \forall n, m, l \in \mathbb{Z}$$

Número de estados hasta k

$$N(k) = \int_{(\frac{2\pi}{L})^2(n^2 + m^2 + l^2) \le k^2} dV = \frac{L^3}{6\pi^2} k^3 = \frac{V}{6\pi^2} k^3$$

1, 2 y 3 dimensiones respectivamente (y se cumple $\omega = \nu_s k$)

$$\begin{cases} G(k) = \frac{L}{\pi} \\ G(\omega) = \frac{L}{\pi\nu} \end{cases} \begin{cases} G(k) = \frac{L^2}{2\pi}k \\ G(\omega) = \frac{L}{2\pi\nu^2}\omega \end{cases} \begin{cases} G(k) = \frac{V}{2\pi^2}k^2 \\ G(\omega) = \frac{V}{2\pi^2\nu_s^3}\omega^2 \end{cases}$$

2.2 Dispersión

Oscilador con masa m v constante k_s

$$F_n = m\ddot{x}_n = k_s(x_{n+1} + x_{n-1} - 2x_n)$$

$$\begin{split} &-m\omega^2Ae^{i(kna-\omega t)}=k_sAe^{i(kna-\omega t)}(e^{ika}+e^{-ika}-2)=\\ &=-4k_s\sin^2\left(\frac{ka}{2}\right)\Rightarrow \boxed{\omega=2\sqrt{\frac{k_s}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|} \end{split}$$

Oscilador con masa m v constantes alternadas k_1, k_2

$$\begin{cases}
m\ddot{x}_n = k_1(y_{n-1} - x_n) + k_2(y_n - x_n) \\
m\ddot{y}_n = k_1(x_{n+1} - y_n) + k_2(x_n - y_n)
\end{cases}$$

Ansatz

$$x_n \equiv Ae^{i(kna-\omega t)}$$
 $y_n \equiv Be^{i(kna-\omega t)}$

Ecuaciones

$$\begin{cases} -m\omega^2 A = -A(k_1 + k_2) + B(k_1 e^{ika} + k_2) \\ -m\omega^2 B = -A(k_1 e^{ika} + k_2) + B(-k_1 - k_2) \end{cases}$$

Forma matricial

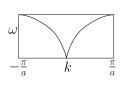
$$m\omega^2\begin{pmatrix}A\\B\end{pmatrix}=\begin{pmatrix}(k_1+k_2)&-k_1e^{ika}\\-k_2-k_1e^{ika}&(k_1+k_2)\end{pmatrix}\begin{pmatrix}A\\B\end{pmatrix}=K\begin{pmatrix}A\\B\end{pmatrix}$$

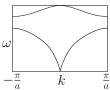
$$0 = \det(K - m\omega^2 I) = |(k_1 + k_2) - m\omega^2|^2 - |k_2 + k_1 e^{ika}|^2$$

$$\sum_{k=0}^{\infty} \omega_{\pm}(k) = \sqrt{\frac{k_1 + k_2}{m} \pm \frac{1}{m} \sqrt{(k_1 + k_2)^2 - 4k_1 k_2 \sin^2(ka/2)}}$$

 $m_1 \neq m_2$ y k_s es la misma, sea $K_i = \frac{k}{m_i}$, entonces

$$\omega_{\pm}(k) = \sqrt{(K_1 + K_2) \pm \sqrt{(K_1 + K_2)^2 - 4K_1K_2\sin^2(ka/2)}}$$





Si hay N átomos / celda: 3N ramas:

- 3 acústicas (2 trans. < 1 long.)
- 3N − 3 ópticas

2.3 Modelo de Einstein

$$E_n = \hbar\omega(n + \frac{1}{2}) \Rightarrow Z_1 = \frac{1}{2\sinh(\frac{\beta\hbar\omega}{2})}$$

 $\langle E_1 \rangle = -\frac{\partial}{\partial\beta}\ln Z_1 = \frac{\hbar\omega}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right)$

Energía v capacidad calorífica

$$\begin{split} \langle E \rangle &= \frac{3}{2} N \hbar \omega \coth \left(\frac{\beta \hbar \omega}{2} \right) \\ C_v &= \frac{\partial \langle E \rangle}{\partial T} = 3 N k_B (\beta \hbar \omega)^2 \frac{e^{\beta \hbar \omega}}{(e^{\beta \hbar \omega} - 1)^2} \end{split}$$

Definimos ahora $T_E = \frac{\hbar \omega_E}{k_B}$. En los límites

- Si $T \gg T_E$ \Rightarrow $C_v = 3Nk_b$
- Si $T \ll T_E$ \Rightarrow $C_v = 3Nk_b(\frac{T_E}{T})^2 \frac{1}{\sinh^2(\frac{T_E}{T})}$

2.4 Modelo de Debye

Aproximamos la ecuación de dispersión para k baja como $\omega = \nu k$

$$3N = \int_0^{\omega_D} 3G(\omega) d\omega = \frac{V}{2\pi^2 \nu^3} \omega_D^3 \Rightarrow \boxed{\omega_D = \sqrt[3]{\frac{6\pi^2 \nu^3 N}{V}}}$$

donde hemos contado cada partícula y cada estado 3 veces v hemos usado

$$\omega = \nu k, \qquad G(k) = \frac{V}{2\pi^2} k^2, \qquad G(\omega) = \frac{V}{2\pi^2 \nu^3} \omega^2 = 3N \frac{\omega^2}{\omega_D^3}$$

La energía y la capacidad calorífica

$$\begin{split} \langle E \rangle &= \int_0^{\omega_D} \hbar \omega 3 G(\omega) \left(\frac{1}{e^{\beta \hbar \omega} - 1} + \frac{1}{2} \right) d\omega = \\ &= E_0 + \frac{3V\hbar}{2\pi^2 \nu^3} \int_0^{\omega_D} \frac{\hbar \omega^3}{e^{\beta \hbar \omega} - 1} d\omega \qquad (x = \frac{\hbar \omega}{k_B T}) \\ T_D &:= \frac{\hbar \omega_D}{k_B} \quad \Rightarrow \boxed{\langle E \rangle = \frac{3V k_B^4 T^4}{2\pi^2 \nu^3 \hbar^3} \int_0^{\frac{T_D}{T}} \frac{x^3}{e^x - 1} dx} \end{split}$$

La capacidad calorífica $C_v = \frac{\partial \langle E \rangle}{\partial T}$ en los extremos:

- Si $T \gg T_D \quad \Rightarrow \quad \langle E \rangle \sim 3Nk_BT \quad \Rightarrow \quad C_v \sim$
- Si $T \ll T_D$ \Rightarrow $\langle E \rangle \sim \frac{3\pi^4 N k_B T^4}{5T_c^3}$ \Rightarrow $C_v \sim$ $\frac{12\pi^4}{5}Nk_B\left(\frac{T}{T_D}\right)^3$

3 Electrones en los sólidos

Modelo de Drude

$$\begin{split} n &= \frac{N}{V}; \quad \frac{dp}{dt} = -\frac{p}{\tau} + F; \quad \overline{j} = -ne\overline{v} = \sigma \overline{E} \\ \sigma_0 &= \frac{e^2 \tau n}{m}; \quad \text{si } F - e \text{Re}[E_0 e^{i\omega t}] \Rightarrow \sigma(\omega) = \frac{\sigma_0}{1 - i\omega t} \\ mv &= p = -e\tau E; \quad R_H = \frac{-1}{ne} = \frac{\rho_{yx}}{|B|} \\ \overline{E} &= \bar{\rho} \overline{j}; \quad \rho_{xx} = \rho_{yy} = \rho_{zz} \frac{m}{ne^2 \tau}; \quad \frac{1}{2} m v_0^2 = \frac{3}{2} k_B T \end{split}$$

Efecto Hall (2 portadores con la misma carga opuesta)

$$\mu_i = \frac{\tau_i}{m_i}; \quad \sigma = ne^2(\mu_1 + \mu_2); \quad R_H = \frac{\mu_2^2 - \mu_1^2}{n_0 e(\mu_1 + \mu_2)^2} e^{\beta E}$$

Hall resistivity $\rho_{xy} = -\rho_{yx} = \frac{B}{\pi c} (\overline{B} \propto \hat{z})$

Peltier coefficient $\Pi = -\frac{k_B T}{2} = \frac{-c_v T}{2}$

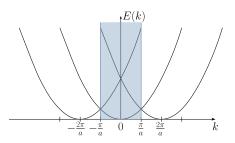
Seebeck coefficient $S = \frac{\Pi}{T}$

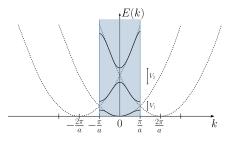
$$\langle v \rangle_{gasid.} = \sqrt{\frac{8k_BT}{\pi m}}; \quad \kappa = \frac{1}{3}nc\langle v \rangle^2 \tau = \frac{4}{\pi}\frac{n\tau k_B^2T}{m}$$

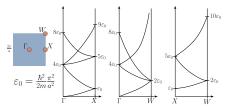
Capacidad Calorífica

$$\begin{split} g(\varepsilon) &= \frac{3n}{2(E_F)^{\frac{3}{2}}} \varepsilon^{\frac{1}{2}} = \frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3} \varepsilon^{\frac{1}{2}}, \quad k = \sqrt{\frac{2\varepsilon m}{\hbar^2}} \\ n &= \int_0^\infty \!\! d\varepsilon g(\varepsilon) n_F(\beta(\varepsilon-\mu)), \quad \frac{E_T}{V} = \int_0^\infty \!\! d\varepsilon \varepsilon g(\varepsilon) n_F(\beta(\varepsilon-\mu)) \; \varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = k_B T_F; \quad p_F = \hbar k_F; \quad U_T = \frac{3}{5} \varepsilon_F N_F \\ C &= \frac{\pi^2}{3} \left(\frac{3N k_B}{2}\right) \left(\frac{T}{T_F}\right) \\ N &= 2 \frac{V}{(2\pi)^d} \int_{|k| < k_F} dk \Rightarrow k_F = (3\pi^2 n)^{\frac{1}{3}}, \quad \varepsilon_F = \frac{\pi^2 k_F^2}{2m} = k_B T_F \end{split}$$

$$\overline{M} = g(E_F)\mu_B^2 \overline{B}; \quad \mu_B = 0.67 \left(\frac{K}{Tesla}\right) k_B$$







Teorema de Bloch $(V(\overline{r}) \text{ periódico})$

$$\psi_{\overline{k}}(\overline{r}) = u_{\overline{k}}(\overline{r})e^{i\overline{k}\cdot\overline{r}}, \quad E(\overline{k}) = E(\overline{k} + \overline{G})$$

(1D) Fourier del potencial de dos formas

$$V(x) = V_0 + \sum_{j=1}^{\infty} V_j \cos\left(\frac{2\pi j}{a}x\right) \quad \text{ 6} \quad V(x) = \sum_{j=-\infty}^{\infty} V_{\frac{2\pi j}{a}} e^{i\frac{2\pi j}{a}x}$$

Con las relaciones $V_i = 2V_{\frac{2\pi j}{2}}$, y donde los coeficientes son

$$V_{j} = \frac{2}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} dx V(x) \cos \left(\frac{2\pi j}{a}x\right); \quad V_{\frac{2\pi j}{a}} = \frac{1}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} dx V(x) e^{-i\frac{2\pi j}{a}x}$$

Gas de electrones libres

$$\begin{split} \overline{k} &= \frac{2\pi}{L}(n_x,n_y,n_z), \quad E(\overline{k}) = \frac{\hbar^2}{2m}|\overline{k}|^2, \quad n_F(x) = \frac{1}{e^x+1} \\ N &= 2\sum_{\overline{k}}n_F(\beta(E(\overline{k})-\mu)) = 2\frac{V}{(2\pi)^3}\int d\overline{k}n_F(\beta(E(\overline{k})-\mu)) \end{split}$$

Fermi energy $(E_F = \mu(T \to 0))$ (d numero de dimensiones)

$$\begin{array}{l} \varepsilon_{F} = \frac{\hbar^{2}k_{F}^{2}}{2m} = k_{B}T_{F}; \quad p_{F} = \hbar k_{F}; \quad U_{T} = \frac{3}{5}\varepsilon_{F}N \\ N = 2\frac{V}{(2\pi)^{d}}\int_{|k| < k_{F}} dk \Rightarrow k_{F} = (3\pi^{2}n)^{\frac{1}{3}}, \quad \varepsilon_{F} = \frac{\hbar^{2}(3\pi^{2}n)^{\frac{2}{3}}}{2m} \end{array}$$

Considerando los dos espines (multiplicamos por 2)

$$N_T = 2 \cdot \left(\frac{4}{3}\pi (n_x^2 + n_y^2 + n_z^2)^{3/2}\right) \Rightarrow k_{max}^2 = k_F^2 = (3n\pi^2)^{\frac{2}{3}}$$

 e^- excitados por encima de ε_F

$$n_{e^-} = 2 \cdot \frac{1}{2} \cdot (2k_BT)(\frac{1}{2}g(\varepsilon_F)) = k_BTg(\varepsilon_F); \quad \frac{n_{e^-}}{n} = \frac{3}{4}\frac{k_BT}{\varepsilon_F}$$

Electrones casi-libres

$$\begin{split} \psi_{+} &\sim \cos(\pi \frac{x}{a}), \quad \psi_{-} \sim \sin(\pi \frac{x}{a}) \\ E^{\pm} &= \frac{1}{2} (E^{0}_{\overline{k} - \overline{G}} + E^{0}_{\overline{k}}) \pm \sqrt{\frac{1}{4} (E^{0}_{\overline{k} - \overline{G}} - E^{0}_{\overline{k}})^{2} + |V_{\overline{G}}|^{2}} \end{split}$$

Enlace fuerte, celda primitiva cúbica $(B = \gamma, A = \beta)$

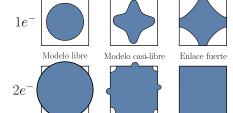
$$\begin{split} \varepsilon(\overline{k}) &= E - \left(\frac{\beta + \sum_{r_i \neq 0} \gamma(r_i) e^{i\overline{k} \cdot \overline{r}_i}}{1 + \sum_{r_i \neq 0} \alpha(r_i) e^{i\overline{k} \cdot \overline{r}_i}}\right) \\ E(\overline{k}) &\approx E_i - A - 2B(\cos k_x a + \cos k_y a + \cos k_z a) \\ A &= -\langle \varphi_{i,n} | v | \varphi_{i,n} \rangle, \quad B &= -\langle \varphi_{i,m} | v | \varphi_{i,n} \rangle \\ \overline{v} &= \nabla_{\overline{k}} \omega(\overline{k}) = \frac{1}{\hbar} \nabla_{\overline{k}} E(\overline{k}) \end{split}$$

Carga de un campo $\overline{\mathcal{E}}$

$$\dot{v}_i = \frac{1}{\hbar^2} \sum_j \frac{\partial^2 E}{\partial k_i \partial k_j} (-e \mathcal{E}_j), \quad \left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E(\overline{k})}{\partial k_i \partial k_j}$$

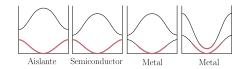
Caso totalmente degenerado

$$m^* = \frac{\hbar^2}{\left(\frac{d^2 E}{dk^2}\right)}, \quad E(\overline{k}) = E_0 + \frac{\hbar^2}{2m^*} |k|^2, \quad \sigma \simeq \frac{e^2 \tau(E_F) n}{m^*}$$



Tipos de materiales

Aislante: Banda llena ($2e^-$). $V_q > 4eV$ Semiconductor Banda llena $(2e^{-})$. $V_q < 4eV$. **Metal** Banda semillena $(1e^2 \circ 2e^- \text{ con bandas solapantes})$



4 Semiconductores

extrínseco = dopado Opacos si $h\nu > E_a$ Nivel de Fermi $E_F = \mu$ Densidad de estados (n electrones, p holes) Energía de donadores / impurezas E_D

n (negativo) N_C (conducción) N_D (donadores) p (positivo) N_V (valencia) N_A (aceptores)

$$\begin{split} g_C(\varepsilon) &= \frac{(2m_n^*)^{2/3}}{2\pi^2\hbar^3} \sqrt{\varepsilon - \varepsilon_C}; g_V(\varepsilon) = \frac{(2m_p^*)^{2/3}}{2\pi^2\hbar^3} \sqrt{\varepsilon_V - \varepsilon} \\ n &= \int_{-\varepsilon}^{\infty} d\varepsilon g_C(\varepsilon) n_F(\beta(\varepsilon - \mu)) \approx \int_{-\varepsilon}^{\infty} d\varepsilon g_C(\varepsilon) e^{\beta(\mu - \varepsilon)} \\ p &= \int_{-\infty}^{\varepsilon_V} d\varepsilon g_V(\varepsilon) (1 - n_F(\beta(\varepsilon - \mu))) \approx \int_{-\infty}^{\varepsilon_V} d\varepsilon g_V(\varepsilon) e^{\beta(\varepsilon - \mu)} \\ n &= \frac{1}{4} \left(\frac{2m_n^* k_B T}{\pi \hbar^2}\right)^{3/2} e^{\beta(\mu - \varepsilon_C)} = N_C e^{\beta(\mu - \varepsilon_C)} \\ p &= \frac{1}{4} \left(\frac{2m_p^* k_B T}{\pi \hbar^2}\right)^{3/2} e^{\beta(\varepsilon_V - \mu)} = N_V e^{\beta(\varepsilon_V - \mu)} \\ np &= N_C N_V e^{-\beta E_g} = 4 \left(\frac{k_B T}{2\pi \hbar^2}\right)^3 (m_n^* m_p^*)^{3/2} e^{-\beta E_g} \\ e^{2\beta \mu} &= \frac{N_V}{N_C} e^{\beta(\varepsilon_V + \varepsilon_C)}, \quad \mu &= \frac{\varepsilon_C + \varepsilon_V}{2} + \frac{3}{4} k_B T \ln \left(\frac{m_p^*}{m_n^*}\right) \\ \mu &= \frac{\varepsilon_T}{m^*}, \quad \sigma &= e(n\mu_n + p\mu_p), \quad E_g &= \varepsilon_C - \varepsilon_V \\ n &= p &= \sqrt{N_C N_V} e^{-\frac{\beta E_g}{2}} \quad \text{si intrinseco} \end{split}$$

Semiconductores dopados (n = 1 ionización) $\varepsilon = \varepsilon_0 \varepsilon_r$

$$\begin{split} E_n &= \frac{m^* e^4}{2(4\pi\varepsilon\hbar)^2} \frac{1}{n^2}, \quad r_n = \varepsilon \frac{4\pi\hbar^2}{m^* e^2} n^2 \\ n_n &\approx \frac{2N_D}{1 + \sqrt{1 + 4\frac{N_D}{N_C}} e^{\beta E_d}} \end{split}$$

$$\begin{split} n_n &= N_C e^{\beta(\mu-\varepsilon_C^n)}; \quad p_p = N_V e^{\beta(\varepsilon_V^p - \mu)} \\ d_n^0 &= \sqrt{\frac{2\varepsilon V_D}{e} \frac{N_A/N_D}{N_A + N_D}}; \quad d_p^0 = \sqrt{\frac{2\varepsilon V_D}{e} \frac{N_D/N_A}{N_A + N_D}} \\ d_n(V) &= d_n^0 \sqrt{\frac{V_D - V}{V_D}}; \quad d_p(V) = d_p^0 \sqrt{\frac{V_D - V}{V_D}} \\ \text{ancho de zona de carga espacial} &= d_n(V) + d_p(V) \\ eV_D &= k_B T \ln \left(\frac{n_n p_p}{n_i^2}\right); \quad I(V) = (I_n^{gen} + I_p^{gen})(e^{\beta eV} - 1) \\ \text{p-Dopado } (N_A \gg N_D); \end{split}$$

- T bajas $\Rightarrow p \approx N_V e^{-\beta E_A}$
- T intermedias $\Rightarrow p \approx N_A N_D$
- T alta $\Rightarrow p = n = \sqrt{N_C N_V} e^{-\beta \frac{E_g}{2}}$

5 Mates

$$\begin{split} \sin^2\left(\frac{x}{2}\right) &= \frac{1-\cos a}{2} \\ \int_0^\infty \frac{1}{e^x-1} dx &= +\infty, \quad \int_0^\infty \frac{1}{e^x+1} dx = \ln(2) \\ \int_0^\infty \frac{x}{e^x-1} dx &= \frac{\pi^2}{6}, \quad \int_0^\infty \frac{x}{e^x+1} dx = \frac{\pi^2}{12} \\ \int_0^\infty \frac{x^2}{e^x-1} dx &= 2\zeta(3), \quad \int_0^\infty \frac{x^2}{e^x+1} dx = \frac{3}{2}\zeta(3) \\ \int_0^\infty \frac{x^3}{e^x-1} dx &= \frac{\pi^4}{15}, \quad \int_0^\infty \frac{x^3}{e^x+1} dx &= \frac{7\pi^4}{120} \end{split}$$

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