

Constantes

$$k_B = 1.381 \times 10^{-23} JK^{-1} = 8.26 \times 10^{-5} eVK^{-1}$$

$$m_e = 9.11 \times 10^{-31} kg = 0.511 MeVc^{-2}$$

$$\varepsilon_0 = \frac{1}{4\pi K} = 8.85 \times 10^{-12} Fm^{-1}$$

$$\hbar = 1.055 \times 10^{-34} Js = 6.58 \times 10^{-16} eVs$$

$$e = 1.602 \times 10^{-19} C$$

1 Estructura cristalina

1.1 Redes de Bravais

a	triclínica
m	monoclínica
o	ortorrómbica
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.	Tetra.	Hex.	Cúbico
aP	mP, mS	oP, oS, oF, oI	tP, tI	hP, hR	cP, cF, cI

1.2 Cosas

Base dual y matriz métrica

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

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

Cambio de base

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

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

Red recíproca y distancia interplanar $g_{hkl} = \frac{1}{d_{hkl}}$

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

Condiciones de Laue $\bar{Q} = 2\pi \bar{g}_{hkl}$

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

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

Factor de estructura

$$F_{hkl} = \sum_p f_p e^{-i2\pi \bar{g}_{hkl} \cdot \bar{r}_p}, \quad I \propto |F_{hkl}|^2$$

1.3 Estructuras comunes

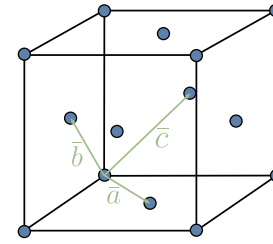
FCC

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

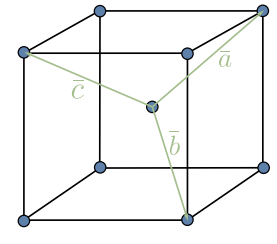
BCC

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

FCC



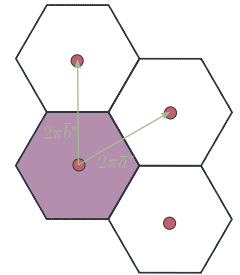
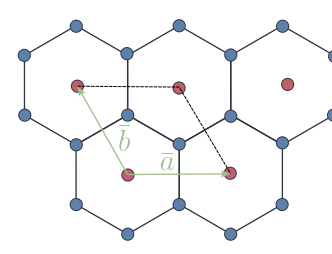
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Hexagonal

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

$$G = \begin{pmatrix} a^2 & -\frac{a^2}{2} & 0 \\ -\frac{a^2}{2} & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}, \quad G^* = \begin{pmatrix} \frac{4}{3a^2} & \frac{2}{3a^2} & 0 \\ \frac{2}{3a^2} & \frac{4}{3a^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{pmatrix}$$



En una hcp $c = 1.633a$

1.4 Grupos

$$m_{100} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} n_{001} = \begin{pmatrix} \cos\left(\frac{360}{n}\right) & -\sin\left(\frac{360}{n}\right) & 0 \\ \sin\left(\frac{360}{n}\right) & \cos\left(\frac{360}{n}\right) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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

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

Reflexión vector director (a, b, c)

$$M = \frac{1}{a^2 + b^2 + c^2} \begin{pmatrix} -a^2 + b^2 + c^2 & -2ab & -2ac \\ -2ab & a^2 - b^2 + c^2 & -2bc \\ -2ac & -2bc & a^2 + b^2 - c^2 \end{pmatrix}$$

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

$R =$

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

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

2 Dinámica de cristales

2.1 Densidad de estados

$$\bar{k} = \left(\frac{2\pi}{L}n \quad \frac{2\pi}{L}m \quad \frac{2\pi}{L}l \right) \quad \forall n, m, l \in \mathbb{Z}$$

Número de estados hasta k

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

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

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

2.2 Dispersión

Oscilador con masa m y constante k_s

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

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

Oscilador con masa m y 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

$$x_n = A e^{i(kna - \omega t)} \quad y_n = B e^{i(kna - \omega t)}$$

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

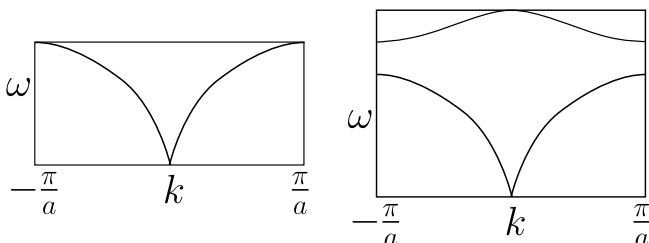
$$m\omega^2 \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} (k_1 + k_2) & -k_2 - k_1 e^{ika} \\ -k_2 - k_1 e^{ika} & (k_1 + k_2) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = K \begin{pmatrix} A \\ B \end{pmatrix}$$

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

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

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

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



2.3 Modelo de Einstein

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

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

Energía y capacidad calorífica

$$\langle E \rangle = \frac{3}{2} N \hbar\omega \coth\left(\frac{\beta\hbar\omega}{2}\right)$$

$$C_v = \frac{\partial \langle E \rangle}{\partial T} = 3Nk_B (\beta\hbar\omega)^2 \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}$$

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

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

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 y hemos usado

$$\omega = \nu k, \quad g(k) = \frac{V}{2\pi^2} k^2, \quad g(\omega) = \frac{V}{2\pi^2 \nu^3} \omega^2$$

La energía y la capacidad calorífica

$$\begin{aligned} \langle E \rangle &= \int_0^{\omega_D} \hbar\omega 3g(\omega) \left(\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2} \right) d\omega = \\ &= E_0 + \frac{3V\hbar}{2\pi^2 \nu^3} \int_0^{\omega_D} \frac{\hbar\omega^3}{e^{\beta\hbar\omega} - 1} d\omega \quad \left(x = \frac{\hbar\omega}{k_B T} \right) \end{aligned}$$

$$T_D := \frac{\hbar\omega}{k_B} \Rightarrow \boxed{\langle E \rangle = \frac{3V k_B^4 T^4}{2\pi^2 \nu^3 \hbar^3} \int_0^{\frac{T_D}{T}} \frac{x^3}{e^x - 1} dx}$$

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

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

3 Mates

$$\begin{aligned} \sin^2\left(\frac{x}{2}\right) &= \frac{1 - \cos x}{2} \\ \int_0^\infty \frac{x}{e^x - 1} dx &= \frac{\pi^2}{6} \\ \int_0^\infty \frac{x^2}{e^x - 1} dx &= 2\zeta(3) \approx 2.40411 \\ \int_0^\infty \frac{x^3}{e^x - 1} dx &= \frac{\pi^4}{15} \end{aligned}$$