

Constantes

$$\begin{aligned}
 k_B &= 1.381 \times 10^{-23} JK^{-1} = 8.26 \times 10^{-5} eVK^{-1} \\
 m_e &= 9.11 \times 10^{-31} kg = 0.511 MeVc^{-2} \\
 \varepsilon_0 &= \frac{1}{4\pi K} = 8.85 \times 10^{-12} Fm^{-1} \\
 \hbar &= 1.055 \times 10^{-34} Js = 6.58 \times 10^{-16} eVs \\
 e &= 1.602 \times 10^{-19} C
 \end{aligned}$$

1 Estructura cristalina

1.1 Cosas

Base dual y matriz métrica

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

Cambio de base

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

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

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

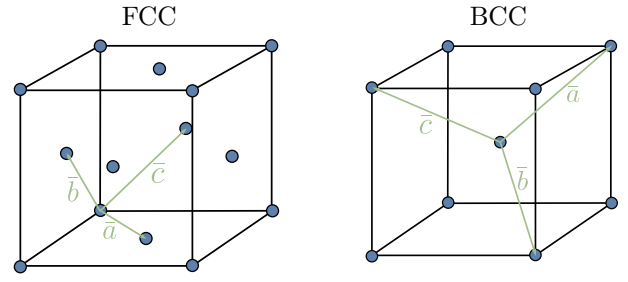
1.2 Estructuras comunes

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

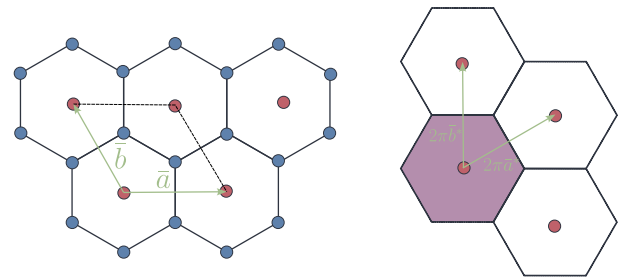
$$\begin{cases} \bar{a} = \frac{1}{2}(1 \ 1 \ -1) \\ \bar{b} = \frac{1}{2}(-1 \ 1 \ 1) \\ \bar{c} = \frac{1}{2}(1 \ -1 \ 1) \end{cases} \quad \begin{cases} \bar{a}^* = (1 \ 1 \ 0) \\ \bar{b}^* = (0 \ 1 \ 1) \\ \bar{c}^* = (1 \ 0 \ 1) \end{cases}$$



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 $c = 1.633a$

1.3 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 $\mathcal{B} = \{\bar{u}, \bar{v}, \bar{w}\}$

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

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

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

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

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

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

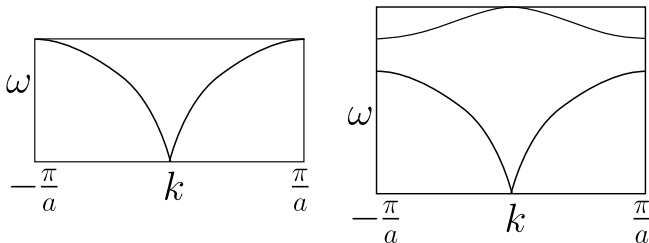
$$m\omega^2 \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} (k_1 + k_2) & -k_2 - k_1 e^{ika} \\ -k_2 - k_1 e^{ika} & (k_1 + k_2) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = K \begin{pmatrix} A \\ B \end{pmatrix}$$

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

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

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

$$\sin^2\left(\frac{x}{2}\right) = \frac{1 - \cos x}{2}$$

$$\int_0^\infty \frac{x}{e^x - 1} dx = \frac{\pi^2}{6}$$

$$\int_0^\infty \frac{x^2}{e^x - 1} dx = 2\zeta(3) \approx 2.40411$$

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}$$