Constantes

$$k_B = 1.381\times10^{-23} JK^{-1} = 8.26\times10^{-5} eVK^{-1}$$
$$m_e = 9.11\times10^{-31} kg = 0.511 MeVc^{-2}$$
$$\varepsilon_0 = \frac{1}{4\pi K} = 8.85\times10^{-12} Fm^{-1}$$
$$\hbar = 1.055\times10^{-34} Js = 6.58\times10^{-16} eVs$$
$$e = 1.602\times10^{-19} C$$

1 Estructura cristalina

1.1 Cosas

Base dual y matriz métrica

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

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

Cambio de base

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

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

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

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

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

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

Factor de estructura

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

1.2 Estructuras comunes

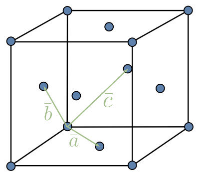
FCC

$$\begin{cases}\bar a = \frac12(1\ 1\ 0)\\ \bar b = \frac12(0\ 1\ 1)\\ \bar c = \frac12(1\ 0\ 1)\end{cases}\qquad \begin{cases}\bar a^* = (1\ 1\ -1)\\ \bar b^* = (-1\ 1\ 1)\\ \bar c^* = (1\ -1\ 1)\end{cases}$$

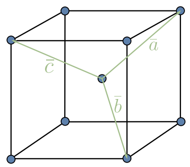
BCC

$$\begin{cases}\bar a = \frac12(1\ 1\ -1)\\ \bar b = \frac12(-1\ 1\ 1)\\ \bar c = \frac12(1\ -1\ 1)\end{cases}\qquad \begin{cases}\bar a^* = (1\ 1\ 0)\\ \bar b^* = (0\ 1\ 1)\\ \bar c^* = (1\ 0\ 1)\end{cases}$$

FCC



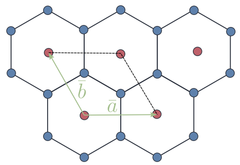
BCC

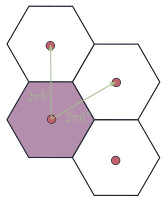


Hexagonal

$$\begin{cases}\bar a = (1, 0)\\ \bar b = (-\frac12, \frac{\sqrt3}{2})\end{cases}\qquad \begin{cases}\bar a^* = \frac{2\sqrt3}{3}(\frac{\sqrt3}{2}, \frac12)\\ \bar b^* = \frac{2\sqrt3}{3}(0, 1)\end{cases}$$

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





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 $\mathcal{B} = \{\overline{u}, \overline{v}, \overline{w}\}$

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

Reflexión vector director (a, b, c)

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

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

$$\begin{pmatrix} c + u_x^2(1-c) & u_xu_y(1-c) - u_zs & u_xu_z(1-c) + u_ys\\ u_yu_x(1-c) + u_zs & c + u_y^2(1-c) & u_yu_z(1-c) - u_xs\\ u_zu_x(1-c) - u_ys & u_zu_y(1-c) + u_xs & c + u_z^2(1-c)\end{pmatrix}$$

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

2 Dinámica de cristales

2.1 Densidad de estados

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

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 $\omega = \nu_s k$)

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

2.2 Dispersión

Oscilador con masa m y constante k_s

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

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

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

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

Ecuaciones

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

Forma matricial

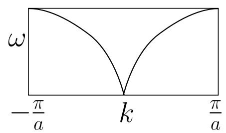
$$m\omega^2\begin{pmatrix}A\\B\end{pmatrix} = \begin{pmatrix}(k_1+k_2) & -k_2 - k_1e^{ika}\\ -k_2 - k_1e^{ika} & (k_1+k_2)\end{pmatrix}\begin{pmatrix}A\\B\end{pmatrix} = K\begin{pmatrix}A\\B\end{pmatrix}$$

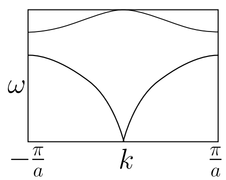
$$0 = \det(K - m\omega^2 I) = |(k_1+k_2) - m\omega^2|^2 - |k_2 + k_1e^{ika}|^2$$

$$\boxed{\omega_\pm(k) = \sqrt{\frac{k_1+k_2}{m}\pm\frac{1}{m}\sqrt{(k_1+k_2)^2 - 4k_1k_2\sin^2(ka/2)}}}$$

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

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





2.3 Modelo de Einstein

$$E_n = \hbar\omega(n + \frac12)\quad\Rightarrow\quad Z_1 = \frac{1}{2\sinh(\frac{\beta\hbar\omega}{2})}$$
$$\langle E_1\rangle = -\frac{\partial}{\partial\beta}\ln Z_1 = \frac{\hbar\omega}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right)$$

Energía y capacidad calorífica

$$\langle E\rangle = \frac32 N\hbar\omega\coth\left(\frac{\beta\hbar\omega}{2}\right)$$
$$C_v = \frac{\partial\langle E\rangle}{\partial T} = 3Nk_B(\beta\hbar\omega)^2\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}$$

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

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

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

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

La energía y la capacidad calorífica

$$\langle E\rangle = \int_0^{\omega_D}\hbar\omega 3g(\omega)\left(\frac{1}{e^{\beta\hbar\omega} - 1} + \frac12\right)d\omega =$$
$$= E_0 + \frac{3V\hbar}{2\pi^2\nu^3}\int_0^{\omega_D}\frac{\hbar\omega^3}{e^{\beta\hbar\omega} - 1}d\omega\qquad (x = \frac{\hbar\omega}{k_BT})$$
$$T_D := \frac{\hbar\omega}{k_B}\quad\Rightarrow \boxed{\langle E\rangle = \frac{3Vk_B^4T^4}{2\pi^2\nu^3\hbar^3}\int_0^{\frac{T_D}{T}}\frac{x^3}{e^x - 1}dx}$$

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

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

3 Mates

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