Constantes

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

1 Estructura cristalina

1.1 Redes de Bravais

a	triclínica
m	monoclínica
o	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.	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

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

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

Cambio de base

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

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

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

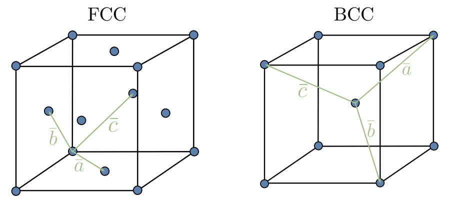
1.3 Estructuras comunes

FCC

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

BCC

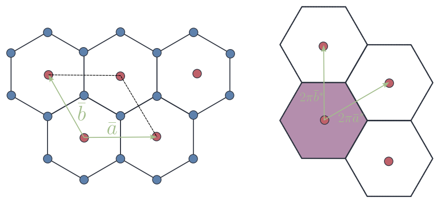
$$\begin{cases}\overline{a} = \frac{1}{2}(1\ 1\ -1)\\ \overline{b} = \frac{1}{2}(-1\ 1\ 1)\\ \overline{c} = \frac{1}{2}(1\ -1\ 1)\end{cases}\qquad \begin{cases}\overline{a}^* = (1\ 1\ 0)\\ \overline{b}^* = (0\ 1\ 1)\\ \overline{c}^* = (1\ 0\ 1)\end{cases}$$



Hexagonal

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

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



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

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

Reflexión vector director (a,b,c)

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

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

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

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

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

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

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

2.2 Dispersión

Oscilador con masa m y constante k_s

$$F_n = m\ddot{x}_n = k_s(x_{n+1}+x_{n-1}-2x_n)$$
$$-m\omega^2Ae^{i(kna-\omega t)} = k_sAe^{i(kna-\omega t)}(e^{ika}+e^{-ika}-2) =$$
$$= -4k_s\sin^2\left(\frac{ka}{2}\right)\Rightarrow \boxed{\omega = 2\sqrt{\frac{k_s}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|}$$

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

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

Forma matricial

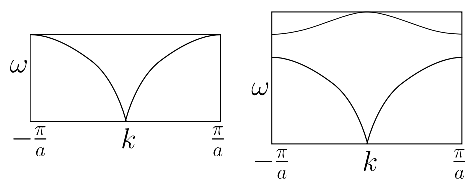
$$m\omega^2\begin{pmatrix}A\\B\end{pmatrix} = \begin{pmatrix}(k_1+k_2) & -k_2-k_1e^{ika}\\ -k_2-k_1e^{ika} & (k_1+k_2)\end{pmatrix}\begin{pmatrix}A\\B\end{pmatrix} = K\begin{pmatrix}A\\B\end{pmatrix}$$

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

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

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

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

Energía y capacidad calorífica

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

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

- Si $T\gg T_E\quad\Rightarrow\quad C_v = 3Nk_b$
- 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 $\omega = \nu k$

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

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

$$\langle E\rangle = \int_0^{\omega_D}\hbar\omega3g(\omega)\left(\frac{1}{e^{\beta\hbar\omega}-1}+\frac{1}{2}\right)d\omega =$$
$$= E_0+\frac{3V\hbar}{2\pi^2\nu^3}\int_0^{\omega_D}\frac{\hbar\omega^3}{e^{\beta\hbar\omega}-1}d\omega\qquad(x = \frac{\hbar\omega}{k_BT})$$
$$T_D := \frac{\hbar\omega}{k_B}\quad\Rightarrow\boxed{\langle E\rangle = \frac{3Vk_B^4T^4}{2\pi^2\nu^3\hbar^3}\int_0^{\frac{T_D}{T}}\frac{x^3}{e^x-1}dx}$$

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

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