

I. CRISTAL·LOGRAFIA

Xarxa de Bravais:

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \quad n_i \in \mathbb{Z}$$

Cel·la primitiva: unitària de volum mínim.

$$V_p = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$$

Xarxa recíproca: $\{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3\}$

$$\mathbf{G} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3 \quad k_i \in \mathbb{Z}$$

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_p} \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V_p} \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V_p}$$

$$\mathbf{b}_i \cdot \mathbf{a}_j = \delta_{ij} \quad \exp(i\mathbf{G} \cdot \mathbf{R}) = 1$$

$$V_p^* = \frac{(2\pi)^3}{V_p}$$

Funció $n(\mathbf{r})$ amb la peridocitat de la X.D.

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}} \quad n_{\mathbf{G}} = \frac{1}{V_c} \int_C dV n(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r})$$

Plans Cristal·lins

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 \quad |\mathbf{G}| = \frac{2\pi}{d}$$

Xarxes Cúbiques:

Cúbica simple (sc): 1 nus/cel·la conv. $V = a^3$, 6 lrs. v.

$$\mathbf{a}_i = a\mathbf{e}_i, \quad \mathbf{b}_j = \frac{2\pi}{a}\mathbf{e}_j$$

Cúbica centrada a l'interior (bcc): 2 nusos/cel·la conv.

$V_p = a^3/2$, $|a_i| = a\sqrt{3}/2$, $\theta_{ij} = 110^\circ$, 8 lrs. v.

$$\mathbf{a}_1 = \frac{a}{2}(-\mathbf{x} + \mathbf{y} + \mathbf{z}), \quad \mathbf{a}_2 = \frac{a}{2}(\mathbf{x} - \mathbf{y} + \mathbf{z}), \quad \mathbf{a}_3 = \frac{a}{2}(\mathbf{x} + \mathbf{y} - \mathbf{z})$$

$$\mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y} + \mathbf{z}), \quad \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x} + \mathbf{z}), \quad \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x} + \mathbf{y})$$

Cúbica centrada a les cares (fcc): 4 nusos/cel·la conv.

$V_p = a^3/4$, $|a_i| = a\sqrt{2}/2$, $\theta_{ij} = 60^\circ$, 12 lrs. v.

$$\mathbf{a}_1 = \frac{a}{2}(\mathbf{y} + \mathbf{z}), \quad \mathbf{a}_2 = \frac{a}{2}(\mathbf{x} + \mathbf{z}), \quad \mathbf{a}_3 = \frac{a}{2}(\mathbf{x} + \mathbf{y})$$

$$\mathbf{b}_1 = \frac{2\pi}{a}(-\mathbf{x} + \mathbf{y} + \mathbf{z}), \quad \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x} - \mathbf{y} + \mathbf{z}), \quad \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x} + \mathbf{y} - \mathbf{z})$$

Altres xarxes:

Hexagonal: $V_p = a^2 c \sqrt{3}/2$

$$\mathbf{a}_1 = a\mathbf{x}, \quad \mathbf{a}_2 = \frac{a}{2}(\mathbf{x} + \sqrt{3}\mathbf{y}), \quad \mathbf{a}_3 = c\mathbf{z}$$

$$\mathbf{b}_1 = \frac{2\pi}{a\sqrt{3}}(-\mathbf{y} + \sqrt{3}\mathbf{x}), \quad \mathbf{b}_2 = \frac{4\pi}{a\sqrt{3}}\mathbf{y}, \quad \mathbf{b}_3 = \frac{2\pi}{c}\mathbf{z}$$

$$d = \frac{a}{\sqrt{\frac{3}{3}(h^2 + k^2 - 4k) + \frac{a^2}{c^2}l^2}}$$

Base 2 àtoms:

$$\mathbf{r}_1 = \mathbf{0} \quad \mathbf{r}_2 = \frac{\mathbf{a}_1 + \mathbf{a}_2}{3} + \frac{\mathbf{a}_3}{2}$$

II. DIFRACCIÓ ELÀSTICA

Llei de Bragg

$$2d \sin \theta = n\lambda$$

Amplitud de dispersió:

$$F = \int_V dV n(\mathbf{r}) e^{i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}} = \sum_{\mathbf{G}} \int_V dV n_{\mathbf{G}} e^{i(\mathbf{G} - \Delta\mathbf{k}) \cdot \mathbf{r}}$$

Condicció de difracció:

$$\Delta\mathbf{k} = \mathbf{G}$$

Llei de Laue:

$$2\mathbf{k} \cdot \mathbf{G} = G^2$$

Factor d'estructura i de forma atòmica

$$S_{\mathbf{G}} = \int_C dV n(\mathbf{r}) \exp(i\mathbf{G} \cdot \mathbf{r}) = \sum_j e^{-i\mathbf{G} \cdot \mathbf{r}_j} \int_C dV n_j(\boldsymbol{\rho}) e^{-i\mathbf{G} \cdot \boldsymbol{\rho}}$$

$$f_j = \int_C dV n_j(\boldsymbol{\rho}) e^{-i\mathbf{G} \cdot \boldsymbol{\rho}} \quad S_{\mathbf{G}} = \sum_j f_j e^{-i\mathbf{G} \cdot \mathbf{r}_j}$$

Exemples:

S.C.

1 sola espècie: $S = f$

2 espècies diferents: $S = f_1 + f_2 \exp(-i\pi l)$

2 espècies iguals: $S = f[1 + \exp(-i\pi l)]$, ext. si l senar

B.C.C.

1 espècie: $S = f\{1 + \exp[-i\pi(h+k+l)]\}$ cal que $h+k+l$ parell.

F.C.C.

1 espècie: cal que índex mateixa paritat

$$S = f\{1 + \exp[-i\pi(h+k)] + \exp[-i\pi(h+l)] + \exp[-i\pi(k+l)]\}$$

III. GAS DE FERMI. TEOREMA DE BLOCH

Gas d'electrons lliures:

$$\psi_{\mathbf{k},s}(\mathbf{r}) = \frac{1}{\sqrt{V}} \exp(i\mathbf{k} \cdot \mathbf{r}) \chi_{\frac{1}{2},m_s} \quad E_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}$$

Dens. espais ocupats en espai \mathbf{k} :

$$\frac{1 \text{ estat}}{(2\pi/L)^3} = \frac{V}{8\pi^3}$$

Estat fonamental:

$$N = 2 \left(\frac{4\pi}{3} k_F^3 \right) \left(\frac{V}{8\pi^3} \right) \quad \rho = \frac{N}{V} = \frac{k_F^3}{3\pi^2}$$

$$k_F = \left(3\pi^2 \frac{N}{V} \right)^{1/3} = (3\pi^2 \rho)^{1/3} \quad E_F = \frac{\hbar^2}{2m} (3\pi^2 \rho)^{2/3}$$

$$E_{tot} = 2 \int_0^{k_F} E_{\mathbf{k}} N_{\mathbf{k}} dV_{\mathbf{k}} = 2 \int_0^{k_F} \frac{\hbar^2 k^2}{2m} \frac{V}{8\pi^3} 4\pi k^2 dk = \frac{3}{5} N E_F$$

Estats excitats:

$$f(E, T) = \frac{1}{\exp\left[\frac{E-\mu}{k_B T}\right] + 1} \quad \mu \approx E_F \left[1 - \frac{1}{3} \left(\frac{\pi k_B T}{2E_F}\right)^2\right]$$

Densitat d'estats $D(E)$:

$$\begin{aligned} dN &= \left(\frac{V}{2\pi^2}\right) \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} dE \\ D(E) &= \left(\frac{V}{2\pi^2}\right) \left(\frac{2m}{\hbar^2}\right) E^{1/2} = \frac{3}{2} \frac{N}{E} \\ D(E)dE &= D(k)dk = \frac{V}{4\pi^3} dV_k = \frac{V}{\pi^2} k^2 dk \end{aligned}$$

Número de partícules:

$$N = \int_0^\infty dE D(E) f(E)$$

Energia interna i capacitat calorífica:

$$\begin{aligned} U &= \int_0^\infty dE E D(E) f(E) \\ \Delta U &= \int_0^\infty dE E D(E) f(E) - \frac{3}{5} N E_F \approx \frac{\pi^2}{6} (k_B T)^2 D(E_F) \\ C &= \frac{d(\Delta U)}{dT} = \frac{\pi^2}{3} k_B T^2 D(E_F) = \frac{\pi^2}{2} \left(\frac{k_B T}{E_F}\right) N k_B \end{aligned}$$

Teorema de Bloch

$$\begin{aligned} V(\mathbf{r}) &= \sum_{\mathbf{G}} V_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r}) \quad V_{\mathbf{G}} = \frac{1}{V_c} \int d\mathbf{r} V(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r}) \\ \phi_{\mathbf{k}}(\mathbf{r}) &= e^{i\mathbf{k} \cdot \mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}} e^{i(\mathbf{k}-\mathbf{G}) \cdot \mathbf{r}} \\ \left[\frac{\hbar^2 |\mathbf{k}-\mathbf{G}|^2}{2m} - E_{\mathbf{k}} \right] C_{\mathbf{k}-\mathbf{G}} + \sum_{\mathbf{G}''} V_{\mathbf{G}''-\mathbf{G}} C_{\mathbf{k}-\mathbf{G}} &= 0 \end{aligned}$$

IV. CONSEQÜÈNCIES DEL TEOREMA DE BLOCH

Model de Xarxa Buida:

$$V_{\mathbf{G}} = 0 \quad \phi_{\mathbf{k}}(\mathbf{r}) = C_{\mathbf{k}-\mathbf{G}} e^{i(\mathbf{k}-\mathbf{G}) \cdot \mathbf{r}} \quad E_{\mathbf{k}-\mathbf{G}} = \frac{\hbar^2}{2m} |\mathbf{k}-\mathbf{G}|^2$$

Electrons quasilliers:

$$\phi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}} e^{i(\mathbf{k}-\mathbf{G}) \cdot \mathbf{r}} \quad k^2 \approx |\mathbf{k}-\mathbf{G}|^2$$

No degenerat:

$$\phi_{\mathbf{k}}(\mathbf{r}) = C_{\mathbf{k}-\mathbf{G}} e^{i(\mathbf{k}-\mathbf{G}) \cdot \mathbf{r}}$$

$$E(\mathbf{k}-\mathbf{G}) = \frac{\hbar^2}{2m} |\mathbf{k}-\mathbf{G}|^2 + V_0 + \sum_{\mathbf{G}'' \neq 0} \frac{|V_{\mathbf{G}''}|^2}{\frac{\hbar^2}{2m} |\mathbf{k}-\mathbf{G}|^2 - \frac{\hbar^2}{2m} |\mathbf{k}-\mathbf{G}-\mathbf{G}''|^2}$$

Degenerat (x2):

$$E_{\pm} = \frac{\hbar^2}{2m} |\mathbf{k}-\mathbf{G}|^2 \pm |V_{\mathbf{G}'}|$$

Electrons fortament lligats:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_j e^{i\mathbf{k} \cdot \mathbf{r}_j} \Omega(\mathbf{r}-\mathbf{r}_j)$$

Bandes:

$$E(\mathbf{k}) = E_0 - \alpha - \gamma \sum_m e^{i\mathbf{k} \cdot \boldsymbol{\rho}_m}$$

Superfície de Fermi:

$$E_n(\mathbf{k}) = E_F$$

2n orbitals per banda.

VI. DINÀMICA DELS ELECTRONS DE BLOCH

Model semiclàssic

Velocitat de grup

$$\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} E_n(\mathbf{k}) \Big|_{\mathbf{k}=\mathbf{k}_0}$$

Eq. moviment espai de vectors d'ona:

$$\mathbf{F} = \hbar \frac{d\mathbf{k}}{dt}$$

Evolució temporal en presència de camps:

$$\hbar \frac{d\mathbf{k}}{dt} = -e[\boldsymbol{\mathcal{E}} + \mathbf{v}_n(\mathbf{k}) \times \boldsymbol{\mathcal{B}}]$$

Corrent elèctric

$$\mathbf{j}_e = -e v_e(\mathbf{k}_e)$$

Massa efectiva

$$a_i = \frac{1}{\hbar^2} \sum_{j=1}^3 \frac{\partial^2 E}{\partial k_i \partial k_j} F_j \quad \left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}$$

$$\frac{d^2 \mathbf{r}}{dt^2} = \left(\frac{\mathbf{1}}{m^*}\right) \mathbf{F}$$

VII. MOVIMENT DELS IONS. FONONS

1D; base monoatòmica

$$V = \sum_s \frac{C}{2} (u_{s+1} - u_s)^2 \quad F_s = -\frac{\partial V}{\partial u_s} = C[u_{s+1} + u_{s-1} - 2u_s]$$

$$u_s(x, t) = u e^{i(kx - \omega t)} = u e^{i(ksa - \omega t)} \quad \omega = \sqrt{\frac{4C}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

Solució general i velocitat de grup:

$$u_s(x, t) = \sum_k A_k e^{i(ksa - \omega_k t)} \quad v_g = \frac{d\omega}{dk} \Big|_{k=k_0} = a \sqrt{\frac{C}{m}} \cos\left(\frac{ka}{2}\right)$$

Velocitat de fase, velocitat del sol i ω_{\max} :

$$v_f = \frac{\omega}{k} \Big|_{k \rightarrow 0} = a \sqrt{\frac{C}{m}}, \quad v_{so} = \frac{d\omega}{dk} \Big|_{k \rightarrow 0} = a \sqrt{\frac{C}{m}}, \quad \omega_{\max} = \sqrt{\frac{4C}{m}} = \frac{2v_{so}}{a}$$

D branques acústiques, Dp - D branques òptiques.

1D; base diatòmica

$$F_{us} = C[v_s + v_{s-1} - 2u_s] \quad F_{vs} = C[u_s + u_{s-1} - 2v_s]$$

$$\omega^2 = C \left(\frac{m+M}{mM} \pm \left[\left(\frac{m+M}{mM} \right)^2 - \frac{2(2-\cos ka)}{mM} \right]^{1/2} \right)$$

ω_+ : branca òptica, ω_- : branca acústica
 $k \rightarrow 0$

$$\omega_+(k) \approx \sqrt{2C} \left(\frac{m+M}{mM} \right)^{1/2} \quad \omega_-(k) \approx \left(\frac{C/2}{m+M} \right)^{1/2} ka$$

$k \rightarrow \pm\pi/a$

$$\omega_+ = \sqrt{\frac{2C}{m}} \quad \omega_- = \sqrt{\frac{2C}{M}}$$

3D, base monoatòmica

$$F_{s,\alpha} = - \sum_r \sum_\beta \phi_{\alpha\beta}(s,r) u_{r,\beta} \quad \alpha, \beta \in \{x, y, z\}$$

$$\phi_{\alpha,\beta} = \frac{\partial^2 V}{\partial u_{s,\alpha} \partial u_{r,\beta}} \quad m_s \frac{d^2 u_{s,\alpha}}{dt^2} = - \sum_r \sum_\beta \phi_{\alpha\beta}(s,r) u_{r,\beta}$$

$$\det[\phi_{\alpha\beta}(s,r) - m_r \omega^2 \delta_{sr} \delta_{\alpha\beta}] = 0 \quad \mathbf{u}_s(t) = \mathbf{A} e^{i(\mathbf{k} \cdot \mathbf{R}_s - \omega t)}$$

A. RELACIONS ÚTILS

$$\sin(x) \approx x - \frac{x^3}{3!} \quad \cos(x) \approx 1 - \frac{x^2}{2}$$

$$\sin\left(\frac{\pi}{2} + x\right) = \cos(x) \quad \cos\left(\frac{\pi}{2} + x\right) = -\sin(x)$$

$$\sin(\alpha + \beta) = \sin \alpha \cos \beta + \cos \alpha \sin \beta$$

$$\cos(\alpha + \beta) = \cos \alpha \cos \beta - \sin \alpha \sin \beta$$

$$\sin(\alpha - \beta) = \sin \alpha \cos \beta - \cos \alpha \sin \beta$$

$$\cos(\alpha - \beta) = \cos \alpha \cos \beta + \sin \alpha \sin \beta$$

$$\sin(2\alpha) = 2 \sin \alpha \cos \alpha \quad \cos(2\alpha) = \cos^2 \alpha - \sin^2 \alpha$$

$$\sin^2(\alpha) = \frac{1}{2}[1 - \cos(2\alpha)] \quad \cos^2(\alpha) = \frac{1}{2}[1 + \cos(2\alpha)]$$

$$\sin \alpha + \sin \beta = 2 \sin \frac{\alpha + \beta}{2} \cos \frac{\alpha - \beta}{2}$$

$$\sin \alpha - \sin \beta = 2 \cos \frac{\alpha + \beta}{2} \sin \frac{\alpha - \beta}{2}$$

$$\cos \alpha + \cos \beta = 2 \cos \frac{\alpha + \beta}{2} \cos \frac{\alpha - \beta}{2}$$

$$\cos \alpha - \cos \beta = 2 \sin \frac{\alpha + \beta}{2} \sin \frac{\alpha - \beta}{2}$$

$$\sin \alpha \sin \beta = \frac{1}{2}[\cos(\alpha - \beta) - \cos(\alpha + \beta)]$$

$$\cos \alpha \cos \beta = \frac{1}{2}[\cos(\alpha - \beta) + \cos(\alpha + \beta)]$$

$$\sin \alpha \cos \beta = \frac{1}{2}[\sin(\alpha - \beta) + \sin(\alpha + \beta)]$$

$$\frac{\hbar^2}{2m_e} 4\pi^2 \approx 150 \text{ eV} \text{Å}^2$$

$$x^2 - 2jx + c^2 = 0 \quad \rightarrow \quad x_{\pm} \approx j \left[1 \pm \sqrt{1 - \frac{c}{j^2}} \right]$$