SOLUTIONS - Tutorials N°1

Ex 3 :

Cubic lattice - The angle Φ between the two planes (h_1, k_1, l_1) and (h_2, k_2, l_2) is equal to the angle between the 2 vectors

$$\vec{G_1}\begin{pmatrix} h_1 \\ k_1 \\ l_1 \end{pmatrix} \text{ and } \vec{G_2}\begin{pmatrix} h_2 \\ k_2 \\ l_2 \end{pmatrix}$$

$$\vec{G_1} \cdot \vec{G_2} = h_1 h_2 + k_1 k_2 + l_1 l_2 = G_1 G_2 \cos \Phi$$

Then $$\cos \Phi = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\left[(h_1^2 + k_1^2 + l_1^2)(h_2^2 + k_2^2 + l_2^2)\right]^{1/2}}$$

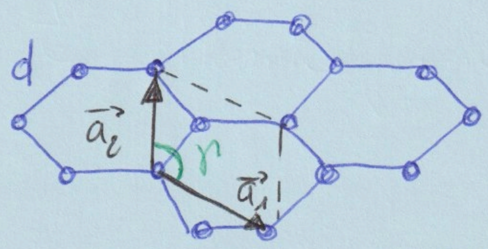
Specific case of (100) and (110) planes :

$$\cos \Phi = \frac{1}{\sqrt{2}} = \frac{\sqrt{2}}{2}$$

So $$\boxed{\Phi = \frac{\pi}{4}}$$

Ex 4 : 2D Bravais lattice .

1- Direct space

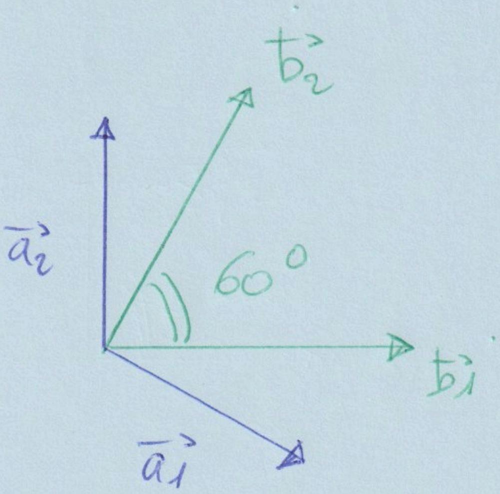


The unit cell is defined by the 2 vectors $\vec{a_1}, \vec{a_2}$.

$$\|\vec{a_1}\| = \|\vec{a_2}\| = d\sqrt{3}$$

$$\gamma = 120°$$

2- Reciprocal space

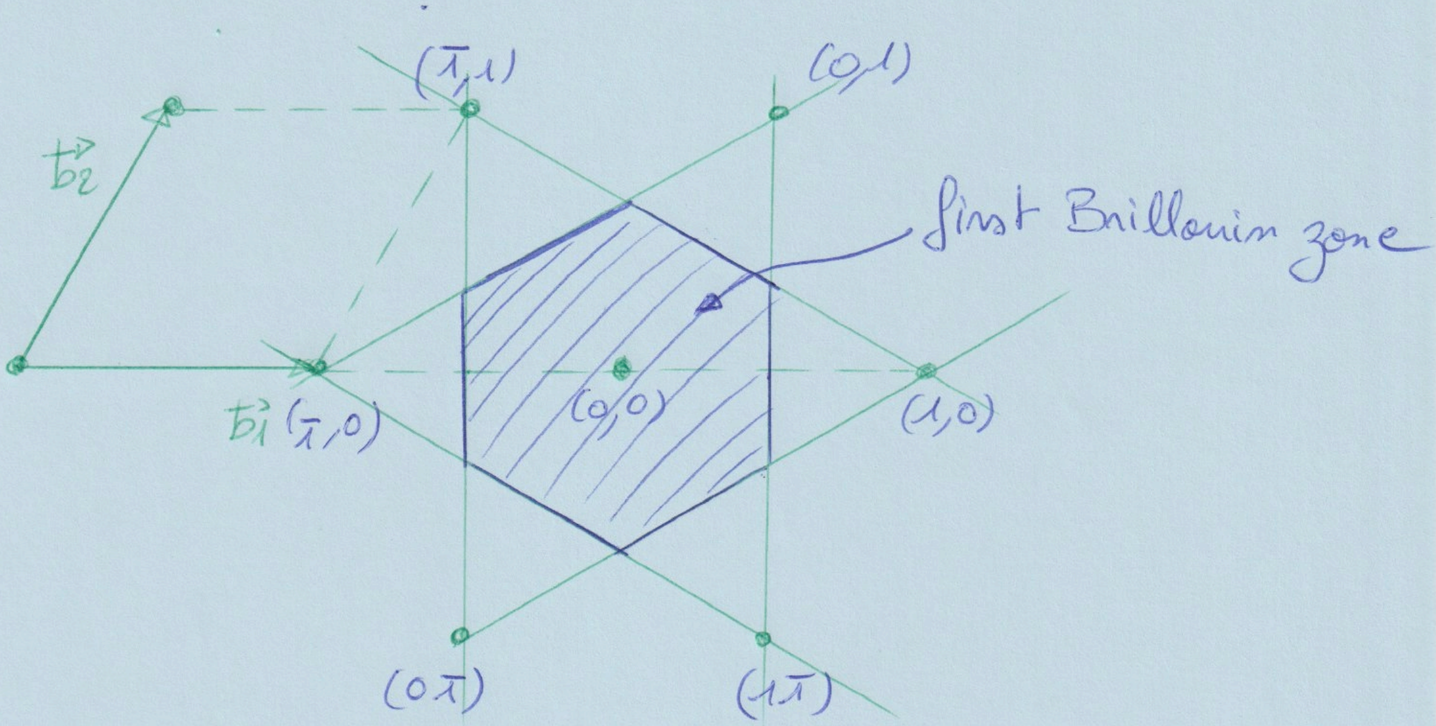


by definition :

$\vec{a_1} \cdot \vec{b_1} = 2\pi = \vec{a_2} \cdot \vec{b_2}$

$\vec{a_1} \perp \vec{b_2}$ since $\vec{a_1} \cdot \vec{b_2} = 0$

$\vec{a_2} \perp \vec{b_1}$ since $\vec{a_2} \cdot \vec{b_1} = 0$



3- Structure factor

$$F(h,k) = Nf\left(1 + e^{-i2\pi\left(\frac{h}{3} + \frac{2k}{3}\right)}\right)$$

← Atomic form factor.

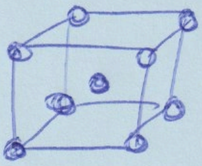
Ex5: General formula of structure factor.

$$F(h,k,l) = N \sum_j f_j \, e^{-i2\pi(x_j h + y_j k + z_j l)}$$

- **Simple Cubic:** 1 atom per unit cell in (0,0,0)

$F_{sc} = Nf \neq 0$ All planes of (h,k,l) indices give rise to a diffraction peak.

- **Centered Cubic:** 2 atoms per unit cell in (0,0,0) and (½, ½, ½)



(Z = 2) $F_{cc} = Nf\left(1 + e^{-i\pi(h+k+l)}\right)$

If $h+k+l = (2n+1) \Rightarrow$ an odd integer number

$F_{cc} = 0$ (no peaks)

If $h+k+l = 2n \Rightarrow$ an even integer number

$F_{cc} = 2Nf$ (peaks are present)

- **Centered faces cubic:** 4 atoms / unit cell.

$$F_{cfc} = Nf\left[1 + e^{-i\pi(h+k)} + e^{-i\pi(h+l)} + e^{-i\pi(k+l)}\right]$$

(0, 0, 0)
(½, ½, 0)
(0, ½, ½)
(½, 0, ½)

If all indices are odd numbers } $F_{cfc} = 4Nf$
——— even numbers }

If one index is odd and the 2 others even $\Rightarrow F_{cfc} = 0$
——— even ——— odd $\Rightarrow F_{cfc} = 0$