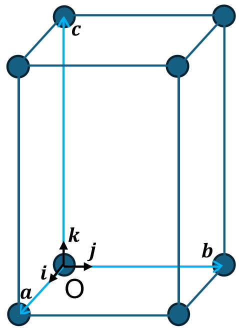
Week 05

Crystallography
Crystal planes, Reciprocal space, Diffraction

Exercise 1 : Answer these questions by true or false

	True	False
1. The reciprocal lattice is always an orthogonal basis	☐	☐
2. If $\mathcal{R}$ is the reciprocal lattice of a direct lattice $\mathcal{D}$, then the reciprocal lattice of $\mathcal{R}$ is $\mathcal{D}$.	☐	☐
3. A plane (hkl) in a direct Bravais lattice is orthogonal to the vector of coordinates h, k, l in the reciprocal basis	☐	☐
4. The probing wavelength of a X-ray beam must be comparable to the size of the atoms.	☐	☐
5. In the Laue Condition, the difference between the incoming and diffracted wave vectors must belong to the direct lattice	☐	☐

Exercise 2:

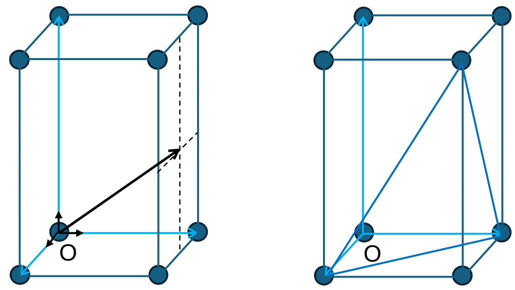


We consider the tetragonal primitive structure as shown to the right. We represent the origin, the orthonormal basis $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$, and the orthogonal basis $\mathcal{B}_{(O,\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})}$, with:

$\boldsymbol{a} = a\boldsymbol{x},\ \boldsymbol{b} = a\boldsymbol{y}, \boldsymbol{c} = c\boldsymbol{z}$, and $a \neq c$.

2a. Is the $\mathcal{B}_{(O,\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})}$ a Bravais lattice for the primitive tetragonal structure ?

2b. What are the Miller indices of the direction and plane below:

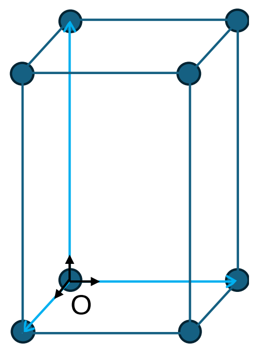


2c.

(i) Draw the plane (111) in the schematic to the right.

(ii) This plan goes through the points of coordinates $A\begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix}$; $B\begin{pmatrix} 0 \\ a \\ 0 \end{pmatrix}$ and $C\begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix}$ in the orthonormal $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$ basis. Show that: $\boldsymbol{AB} \times \boldsymbol{AC} = c\begin{pmatrix} a \\ a \\ \frac{a^2}{c} \end{pmatrix}$.

(iii) Is the plane (111) perpendicular to the direction [111] ?



2d. Can you find a new basis $\mathcal{B}_{(O,\boldsymbol{a'},\boldsymbol{b'},\boldsymbol{c'})}$ for which the vector $\boldsymbol{a'} + \boldsymbol{b'} + \boldsymbol{c'}$ is perpendicular to the plan (111) ?

2e.

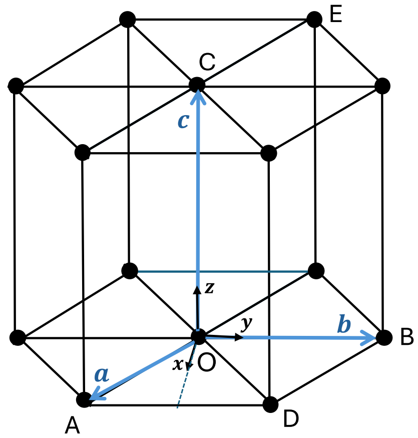
(i) What is the Reciprocal lattice of $\mathcal{B}_{(O,\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})}$?

(ii) How does it compare to the basis $\mathcal{B}_{(O,\boldsymbol{a'},\boldsymbol{b'},\boldsymbol{c'})}$ found above ?

Exercise 3: Distance between crystal plane in the HC structure

We consider the hexagonal comapct structure shown to the right. We represented the origin, the orthonormal basis $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$, and the Bravais lattice $\mathcal{B}_{(O,\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})}$, with:

- $\|\boldsymbol{a}\| = \|\boldsymbol{b}\| = a$, $\|\boldsymbol{c}\| = c$, and $a \neq c$ (where $\|\boldsymbol{a}\|$ is the norm of the vector $\boldsymbol{a}$);
- $\widehat{(\boldsymbol{a},\boldsymbol{b})} = \frac{2\pi}{3}$, $\widehat{(\boldsymbol{a},\boldsymbol{c})} = \widehat{(\boldsymbol{b},\boldsymbol{c})} = \frac{\pi}{2}$ (where $\widehat{(\boldsymbol{a},\boldsymbol{b})}$ is the angle between vectors $\boldsymbol{a}$ and $\boldsymbol{b}$).



3a.

(i) What are the corrdinates of the vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ in the basis $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$?

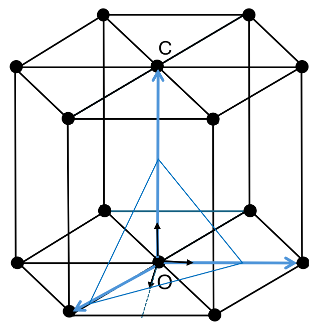
(ii) What are the corrdinates in the basis $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$ and $\mathcal{B}_{(O,\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})}$ of the points A,B, C, D and E shown on the schematic ?

3b.

(i) What is the volume of the cell defined by the vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$?

(ii) Show that the reciprocal lattice is given by, in the $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$ basis:

3c. We consider the crystal plane (hkl) (h,k,l three relative integers) shown on the schematic, that intercepts the $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ axis at positions $\frac{\boldsymbol{a}}{h}, \frac{\boldsymbol{b}}{k}, \frac{\boldsymbol{c}}{l}$ respectively.



(i) What is the normal to the plane in the orthonormal $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$ basis ?

(ii) Show that the equation of the plane in $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$ is given by:

$$\mathcal{P} = \left\{ M \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \frac{(2h+k)}{a\sqrt{3}} x + \frac{k}{a} y + \frac{l}{c} z = 1 \right\}$$

4d. Assuming that the closest plane in the $\{hkl\}$ family is the one passing through the origin, show that the distance between the $\{hkl\}$ plane is given by:

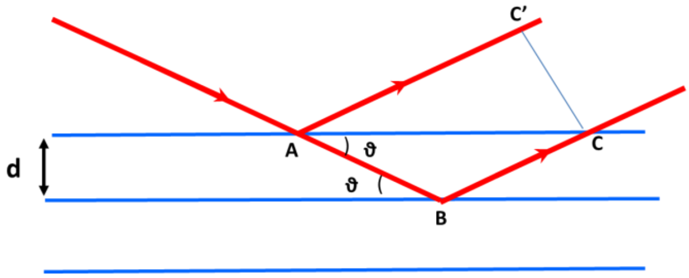
$$d_{(hkl)} = \frac{1}{\sqrt{\frac{4}{3a^2}(h^2 + k^2 + hk) + \frac{l^2}{c^2}}}$$

Exercise 4. Bragg law

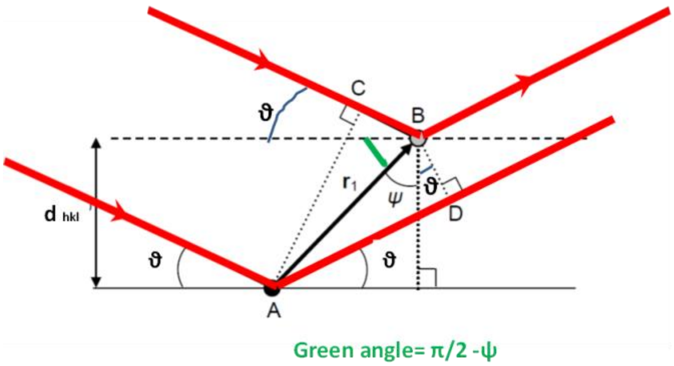
Two general descriptions of the Bragg law are depicted here. The path difference between the two red reflected rays should be an entire number of λ for constructive interference.

Show that Bragg law is fulfilled for

a)



b)



c) does it matter where on the plane the atoms are located?

d) Calculate the angles at which there will be reflections for the following sets of planes in KCl which is cubic with α = 6.27 Å and CuKα radiation, λ = 1.54 Å.

i) (001)

ii) (110)

iii) (111)

e) What is the difference when using a smaller wavelength i.e. X.rays with higher energy?

f) What does the order *n* represent in the Bragg law?