Week 04

Crystallography
Mathematical description of crystals
Miller indices

Exercise 1 : Answer these questions by true or false

	True	False
1. A plane (hkl) for a given Bravais lattice is orthogonal to the vector of coordinates h, k and l in the primitive cell basis.	☐	☐
2. The reciprocal lattice is always an orthogonal basis.	☐	☐
3. Two planes that have the same normal are parallel to each other .	☐	☐
4. A family of parallel crystal planes (hkl) contains all the lattice points.	☐	☐

Exercise 2 :

We consider points and vectors in an orthonormal basis $(O, \vec{\imath}, \vec{\jmath}, \vec{k})$.

2a.

(i) What are the coordinates of the vector $\overrightarrow{AB}$ formed by the points $A(1,0,0)$ and $B(0,1,0)$?

(ii) For $C(0,0,1)$, calculate $\overrightarrow{AB}.\overrightarrow{AC}$ and $\overrightarrow{AB} \times \overrightarrow{AC}$.

2b.

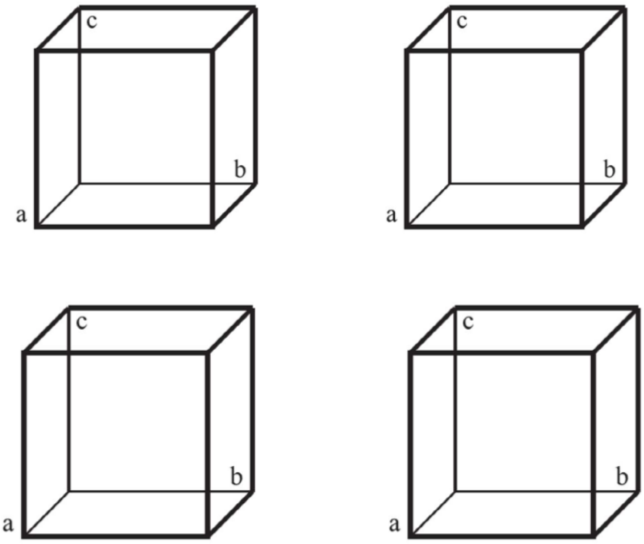
(i) What is the angle between the vectors $\overrightarrow{AB}$ and $\overrightarrow{AC}$?

(ii) What is the equation of the line passing through the points A and B ?

(iii) What is the equation of the plane passing through the points A, B and C ?

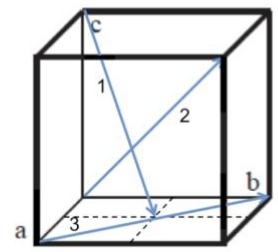
Exercise 3: Miller indices

3a. Draw the crystal directions [101], $[1\bar{1}2]$, and planes $(10\bar{1})$ et $(11\bar{1})$ in the cubes representing the cubic structure below

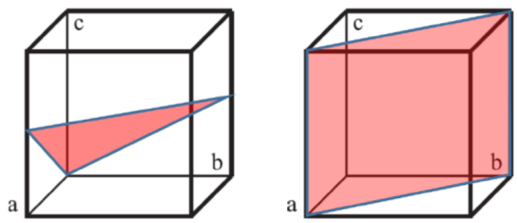


3b. Find the Miller indices of the directions 1, 2 and 3 shown in the cube on the right. What is the angle between directions 1 and 3 ?

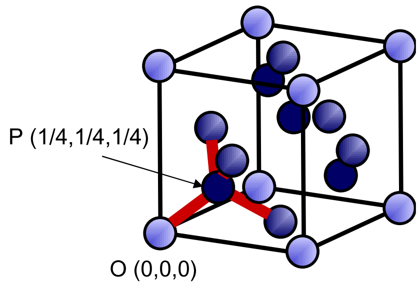
To which plan do directions 1 and 3 both belong ?



3c. What are the Miller indices of the crystal planes below :



3d. The diamond structure shown below was described in the exercises of week 01. In the motif, one atom has its center at one corner of the cube that could be an origin O (0,0,0), and the other one is shifted along the diagonal at position (¼, ¼, ¼). The two spheres representing the two atoms are in contact with each other (to the contrary of what is shown on the schematic below for clarity).

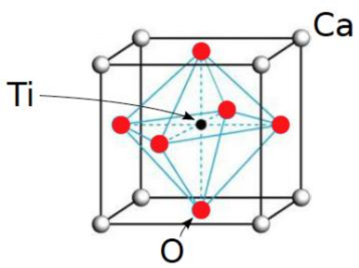


(i) Is the point P of coordinate (¼, ¼, ¼) a lattice point ?

(ii) What is the equation of the plane passing through the point P and parallel to the plan (100) ? Is it a crystal plane for the diamond structure ?

(iii) Find the family of crystal plans {*hkl*} that goes through the point P(¼, ¼, ¼).

Exercise 4



Consider the material we already saw in exercise week 2 for finding the motif and the crystal system.

Represent on a schematic the structure of the atoms in the plans (100), (200), (110) et (111).

Exercise 5 :

We consider a cubic structure and a plan shown to the right, that intercepts the axis **a**, **b** and **c** at points A, B and C respectively. The cube edge is a, we define an origin O and an orthonormal basis $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$, and an orthogonal basis $\mathcal{B}_{(O,\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})}$ as represented, with $\boldsymbol{a} = a\boldsymbol{x}, \boldsymbol{b} = a\boldsymbol{y}$ and $\boldsymbol{c} = a\boldsymbol{z}$:

5a. What are the coordinates of the points A, B and C in the basis $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$ and $\mathcal{B}_{(O,\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})}$?

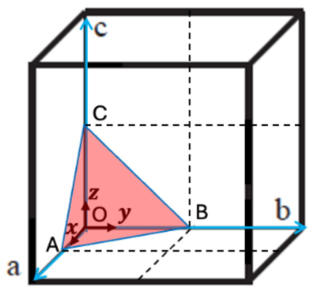
5b. What are the Miller indices of the plan ?

5c. We want to find the equation of this plane in the $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$ basis. The plan can be expressed as a set of points that are a linear combination of the vectors $\boldsymbol{AB}$ and $\boldsymbol{AC}$:

$$\mathcal{P} = \left\{ M = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \boldsymbol{AM} = \lambda \boldsymbol{AB} + \mu \boldsymbol{AC}, (\lambda, \mu) \in \mathbb{R}^2 \right\}$$

(i) For an arbitrary point $M = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ with $M \in \mathcal{P}$, express a set of linear equations that link x, y, z, a and two real parameters λ and μ.

(ii) By eliminating λ and μ, show that the equation of the plan in the $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$ basis is given by: $\mathcal{P} = \left\{ M = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, x + y + z = \frac{a}{2} \right\}$



5d.

(i) Can you find a point $D = \begin{pmatrix} na \\ pa \\ qa \end{pmatrix}$ (in the $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$basis), with $(n, p, q) \in \mathbb{Z}^3$ that belong to the plane $\mathcal{P}$?

(ii) Conclude whether this plane is a lattice plane for the primitive cubic structure ?

5e. Is $\mathcal{P}$ a lattice plane for the BCC and the FCC structures ?