MA1-3 F. Sorin

Fall 2024 **Mathematical Methods for Materials Science** SMX

Serie n°2 – September 17th

Algebraic structures

Prime numbers, Fields and vectorial spaces, basics on vectors and 3D geometry, Crystallography

Exercise 1 :

1a. Find the following gcd and lcm:

(i) *gcd(3,15,45,90); gcd(4,6,12,30); gcd(3,5,7);*

(ii) *lcm(3,15,45,90); lcm(4,6,12,30); lcm(3,5,7);*

1b. Find the prime factorization of 36,112 and 132

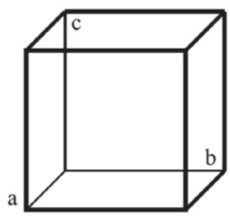
1c. Using the Bézout theorem, demonstrate:

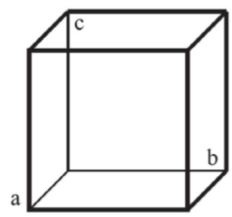
(i) The Gauss theorem;

(ii) The Euclid Lemma.

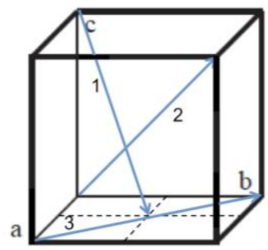
Exercise 2: Miller indices

2a. Draw the crystal directions [101], [$1\bar{1}2$] in the cubes to the right representing the cubic structure:

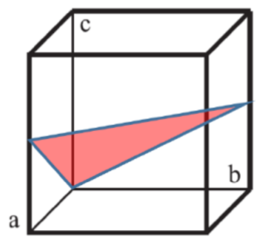


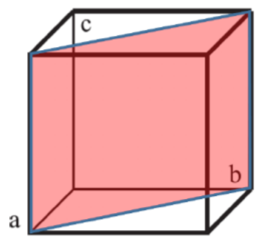


2b. Find the Miller indices of the directions (1, 2 and 3) shown in the cube on the right. What is the angle between directions 1 and 3 ?
To which plan do directions 1 and 3 both belong ?



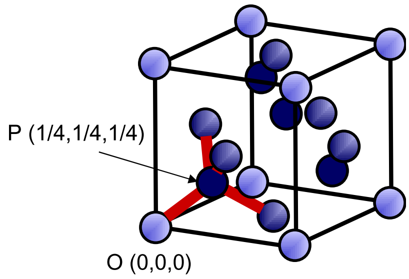
2c. What are the Miller indices of the crystal planes below:





Exercise 3: Diamond structure

The diamond structure shown below consists of tetrahedra of carbon atoms arranged in space to form the crystal. This arrangement turns out to be represented by a motif of two carbon atoms translated in the face-centered cubic Bravais lattice. The atoms can be represented by a sphere of radius R. 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).



3a. Is the point of coordinate (¼, ¼, ¼) a lattice point ?

3b.

(i) How many atoms are in the conventional FCC cell for Diamond ?

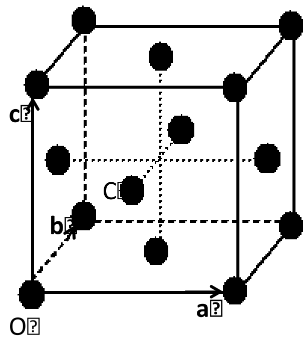
(ii) What is the coordination number ?

3c. Deduce the packing fraction of the Diamond structure.

3d. Find a condition on mutually prime relative integers (h,k,l) so that the plan (hkl) goes through the point P(¼, ¼, ¼).

Exercise 4 : Primitive cell of the FCC structure

Consider the Face-centered cubic conventional cell shown to the right with the origin marked as O and the three orthogonal axis of length the cube edge a.



4a. In the basis (O, **a**, **b**, **c**), what are the coordinate of the point C at the center of a face of the cube ? Is this basis a Bravais lattice for the FCC cubic structure ?

4b. We consider the same origin O and three new vectors **a'**, **b'** and **c'** such that :

$$\vec{a}' = \frac{1}{2}\left(\vec{b} + \vec{c}\right) ; \vec{b}' = \frac{1}{2}(\vec{a} + \vec{c}) ; \vec{c}' = \frac{1}{2}\left(\vec{a} + \vec{b}\right)$$

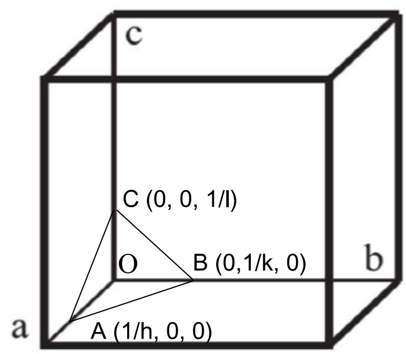
(i) Show that for all point M of the FCC lattice, one can find relative integers n, p and q, such that: $\overrightarrow{OM} = \frac{n}{2}\vec{a} + \frac{p}{2}\vec{b} + \frac{q}{2}\vec{c}$, with *(n,p,q)* either all even numbers, or 1 is odd and 2 are even numbers.

(ii) Express the **OM** vector in the (O, **a'**, **b'**, **c'**) basis and conclude whether this basis is indeed a primitive basis for the FCC structure.

4c. Calculate the volume occupy by the FCC primitive cell in two ways:
(i) Using the vectorial formula seen in class;
(ii) Making an argument regarding the number of motifs should be present in the primitive and conventional cells of the FCC.

Exercise 5 : Distance between crystal planes

We consider a family of plans $\{hkl\}$ in a primitive cubic lattice structure of edge a, with the basis (O, **a**, **b**, **c**) as shown in the schematic. One of these plans is the one intercepting the points A, B and C on the schematic.



We want to establish a general form for their equations, and deduce the distance between the plans $d_{(hkl)}$, a very important parameter in crystallography. To simplify the visualization, we consider without loss of generality that h, k and l are positive integers (as in the schematic).

5a. We want to show that for every co-prime integers h, k and l, we can find a family of crystal planes $\{hkl\}$ in the cubic structure lattice.

(i) Show that the plan that intercepts the axis **a**, **b** and **c** at the points A ,B and C shown on the schematic has the equation:

$$\mathcal{P}_1^{(hkl)} = \{(x, y, z) \in \mathbb{R}^3 / hx + ky + lz = a\}$$

We need to find three points of the Bravais lattice that also belong to $\mathcal{P}_1^{(hkl)}$, to conclude that $\mathcal{P}_1^{(hkl)}$ is a crystal plan.

(ii) We call $d = gcd(h, k)$. Show that $gcd(d, l) = 1$.

(iii) Using Bézout twice, show that $\exists (n_1, n_2, n_3) \in \mathbb{Z}^3, hn_1 + kn_2 + ln_3 = 1$.
Deduct that the point $P(n_1 a, n_2 a, n_3 a) \in \mathcal{P}_1^{(hkl)}$.

(iv) Doing the same for $gcd(h, l)$ and $gcd(k, l)$, find 2 more points that belong both to the Bravais lattice and to $\mathcal{P}_1^{(hkl)}$, and conclude.

5b. The $\{hkl\}$ passing through the origin O

(i) Show that the equation of the plan $\mathcal{P}_0^{(hkl)}$ perpendicular to the direction $[hkl]$ and passing through the origin O is given by:

$$\mathcal{P}_0^{(hkl)} = \{(x,y,z) \in \mathbb{R}^3 / hx + ky + lz = 0\}$$

(ii) Find two other points, other than O, that belong to both the Bravais lattice (O, **a**,**b**,**c**) and the plan $\mathcal{P}_0^{(hkl)}$.

(iii) Conclude that $\mathcal{P}_0^{(hkl)}$ belongs to the family of crystal plans $\{hkl\}$.

5c. We want to see if there could be a crystal plan of the $\{hkl\}$ family that could intercept the axis **a**, **b** and **c** closer to the origin O, that is at points A' $(a/H,0,0)$, B' $(0,a/K,0)$ and C' $(0,0,a/L)$ with (H,K,L) integers and $H \geq h, K \geq k, L \geq l$. In other words, we translate $\mathcal{P}_0^{(hkl)}$ along its normal $[hkl]$, and see if we intercept a crystal plan of the $\{hkl\}$ family before $\mathcal{P}_1^{(hkl)}$:

(i) Show that one equation of this plan containing A', B' and C', is given by:

$$\mathcal{P}^{(HKL)} = \left\{(x,y,z) \in \mathbb{R}^3 / hx + ky + lz = \frac{ah}{H}\right\}$$

(ii) Since we supposed that $\mathcal{P}^{(HKL)}$ is a crystal plane, show that

$$\exists (n_1,n_2,n_3) \in \mathbb{N}^3, H \times (hn_1 + kn_2 + ln_3) = h$$

(iii) Conclude that necessarily, $H = h$ and so that $\mathcal{P}^{(HKL)} = \mathcal{P}_1^{(hkl)}$

5d. Sequence of planes $\mathcal{P}_n^{(hkl)}$

We want to show by induction that as we translate the plan $\mathcal{P}_0^{(hkl)}$ along its normal $[hkl]$, the nth plan intercepted by $\mathcal{P}_0^{(hkl)}$ that belongs to the $\{hkl\}$ family has the equation:

$$\mathcal{P}_n^{(hkl)} = \{(x,y,z) \in \mathbb{R}^3 / hx + ky + lz = na\}$$

(i) Deduct from 6b and 6c that it is true for $n = 0$ and $n = 1$.

(ii) Suppose it is true for an integer $n > 1$, i.e. that the nth $\{hkl\}$ plan has the equation:

$$\mathcal{P}_n^{(hkl)} = \{(x,y,z) \in \mathbb{R}^3 / hx + ky + lz = na\}$$

Since it is a crystal plane, it intercepts crystal lattice points. $\exists (n_1,n_2,n_3) \in \mathbb{Z}^3$, such that the point O'$(n_1 a, n_2 a, n_3 a)$ belongs to $\mathcal{P}_n^{(hkl)}$, with $hn_1 a + kn_2 a + ln_3 a) = na$.

Considering the point O' as a new origin of the Bravais lattice, explain why the (n+1)th $\{hkl\}$ crystal plane is the plane that passes through the three points:

$$A''\begin{pmatrix} n_1a+\frac{a}{h} \\ n_2a \\ n_3a \end{pmatrix};\quad B''\begin{pmatrix} n_1a \\ n_2a+\frac{a}{k} \\ n_3a \end{pmatrix};\quad C''\begin{pmatrix} n_1a \\ n_2a \\ n_3a+\frac{a}{l} \end{pmatrix}$$

(iii) Expressing the equation of the plane containing A'', B'' and C'', conclude that the proposition is true for the (n+1)th $\{hkl\}$ plan.

5e. We consider now an arbitrary n and want to calculate the distance between $\mathcal{P}_n^{(hkl)}$ and $\mathcal{P}_{n+1}^{(hkl)}$.

(Reminder: the distance between two parallel planes is the distance between the two points defined by the intersection of a normal vector with each plane)

(i) Show that the point $D\begin{pmatrix} \frac{na}{h} \\ 0 \\ 0 \end{pmatrix} \in \mathcal{P}_n^{(hkl)}$

(ii) We look for a point $M\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ such that $M \in \mathcal{P}_{n+1}^{(hkl)}$ and the vectors **DM** and the normal $\boldsymbol{n_{(hkl)}}$ are colinear, i.e. $\exists\lambda \in \mathbb{R}, \boldsymbol{DM} = \lambda \boldsymbol{n_{(hkl)}}$.
Show that we must have: $\lambda = \frac{a}{h^2+k^2+l^2}$

(iii) Conclude that the distance between two (hkl) planes in the cubic system is given by:

$$d_{(hkl)} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$