Weeks of September 8th and 15th

Algebraic structures, ℕ and ℤ, prime numbers
Crystals and Symmetries

Exercise 1: Point Group 2/m

We consider a three dimensional Euclidean space with an orthonormal basis $\mathcal{B}_{(O,x,y,z)}$, and a set of four symmetry operators:

- The identity (1) (or 1-fold rotation):
  For a point $P(x, y, z)$ in $\mathcal{B}_{(O,x,y,z)}$, $1(P) = P$.
- A 2-fold rotation (2) (rotation of angle π) around the z axis:
  For a point $P(x, y, z)$ in $\mathcal{B}_{(O,x,y,z)}$, $2(P) = P'$ with $P'(-x, -y, z)$
- A mirror symmetry (m) across the $z = 0$ plane ((x, y) plane):
  For a point $P(x, y, z)$ in $\mathcal{B}_{(O,x,y,z)}$, $m(P) = P'$ with $P'(x, y, -z)$
- The inversion operation ($\bar{1}$) through the origin O:
  For a point $P(x, y, z)$ in $\mathcal{B}_{(O,x,y,z)}$, $\bar{1}(P) = P'$ with $P'(-x, -y, -z)$

We want to show that these for operators form a point symmetry group, noted 2/m in the Harmann-Maugin notation.

1a. Fixed point:
Can you find a point that is left unchanged by all 4 symmetry operators ?

We use the symbol "o" between two arbitrary operators f and g the same way it is used for functions: if $g(P) = P'$, $f\mathrm{o}g(P) = f\big(g(P)\big) = f(P') = P''$.
The inverse f^{-1} of a symmetry operator f is then defined as $\forall P, f\mathrm{o}f^{-1}(P) = P$, or $f\mathrm{o}f^{-1} = 1$.

1b. Show that for all symmetry operators described above, the operator is equal to its inverse.

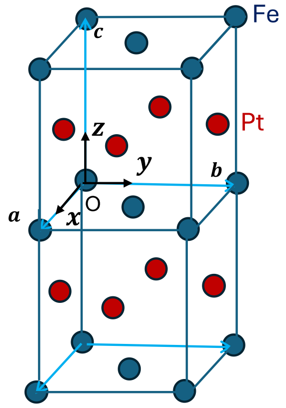
1c. Show that:

(i) $\forall P(x, y, z), 2\mathrm{o}m(P) = m\mathrm{o}2(P) = \bar{1}(P)$
(ii) $\forall P(x, y, z), \bar{1}\mathrm{o}2(P) = 2\mathrm{o}\bar{1}(P) = m(P)$
(iii) $\forall P(x, y, z), \bar{1}\mathrm{o}m(P) = m\mathrm{o}\bar{1}(P) = 2(P)$

1d. Associativity:
Deduce from 1c that $2\mathrm{o}(m\mathrm{o}\bar{1}) = (2\mathrm{o}m)\mathrm{o}\bar{1}$ and $m\mathrm{o}(\bar{1}\mathrm{o}2) = (m\mathrm{o}\bar{1})\mathrm{o}2$.

Exercise 2: Visualizing the symmetries of Iron Platinum

Iron-Platinum is a magnetic material that crystalizes in the structure shown below. In this structure, we suppose that the Iron atoms sit at the corner of a cube of edge a, as well as at the center of the top and bottom faces. Pt atoms sits at the center of the 4 other faces.



The FePt crystal can be formed by translating this cube along the **a**, **b** and **c** orthogonal vectors. On the schematic, two cubes are represented.

2a. Show schematically that the crystal structure is actually tetragonal primitive, and find its lattice parameters as a function of a.

Hint: you can check on the class slides the structure of the tetragonal primitive (you don't need to know it by heart..), and proceed like we did in class by considering neighboring cells.

2b. The FePt crystal has the space group symmetry 123, which contains 16 symmetry operations:

(i) What are the two roto-inversions ? Specify the axis and the n-fold nature.

(ii) Why there is no roto-inversion $\bar{2}$ listed ?

(iii) There are 5 2-fold rotations listed: can you identify the axis ?

(iv) There are 2 4-fold rotations listed: can you identify the axis ?

(v) There are 5 mirror symmetries listed: can you identify them ? (across the (x,y) plane for example)

(vi) What are the two remaining symmetry operations not discussed above ?

Exercise 3: Subgroups

We consider the set of real Polynomial functions of the form:

$For\ x \in \mathbb{R}, n \in \mathbb{N}, P(x) = \sum_{k=0}^{n} a_k x^k = a_0 + a_1 x + \cdots . + a_n x^n$ with $\forall k \in \mathbb{N}$, $a_k \in \mathbb{R}$.

The degree of the polynomial is defined as the highest value of the exponent $k > 0$ for which $a_k \neq 0$. If $\forall k > 0, a_k = 0$, then the degree of the polynomial is 0.

3a.

(i) Show that the set of all polynomials associated to the addition operation form a group $G_{[X]}$.

(ii) Would it still be a group if we replaced the addition operation with the multiplication ?

Given a group *G* under an operation (often called binary operation) $*$, a subset *H* of *G* is called a **subgroup** of *G* if *H* also forms a group under the operation $*$.

3b. Show that the subset of Polynomials with even coefficients form a subgroup of $G_{[X]}$.
(Hint: you can consider that 0 is an even number).

3c. Consider the subset of polynomials with an even degree. Does it form a subgroup of $G_{[X]}$?

3d. Consider the subset of polynomials with at least one real root (i.e. one real number x_0 for which $P(x_0) = 0$). Does it form a subgroup of $G_{[X]}$?

3e. (i) Show that the set of rotations around the same axis, of angles $\frac{2\pi}{6}$ (noted 6), $\frac{-2\pi}{6}$ (-6), $\frac{2\pi}{3}$ (3), $\frac{-2\pi}{3}$ (-3), π (2), and 2π (1) form a group

(ii) Show that it is a sub-group of the point group 6/mmm.

(Hint: the list of all the 24 symmetry elements in the 6/mm group can be found here: https://onlinelibrary.wiley.com/iucr/itc/Ac/ch2o3v0001/sgtable2o3o191.pdf)

Exercise 4 :

4a. 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);*

4b. Find the prime factorization of 36,112 and 132

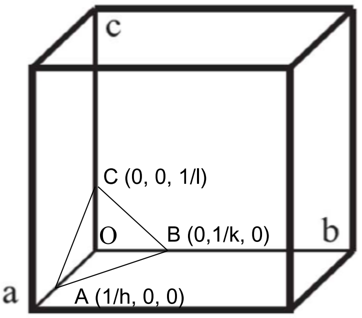
4c. Using the Bézout theorem, demonstrate:

(i) The Gauss theorem;

(ii) The Euclid Lemma.

Exercise 5 : Distance between crystal planes

We consider a crystal in the primitive cubic lattice structure of edge a. Mathematically, it means that the crystal is formed by motifs sitting on all the points in space of coordinates $P(n_1a, n_2a, n_3a)$ with $(n_1, n_2, n_3) \in \mathbb{Z}^3$, in the orthonormal basis $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$. On the schematic we show one cubic cell of this crystal, with the orthogonal basis $\mathcal{B}_{(O,\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})}$ where $\boldsymbol{a} = a\boldsymbol{x}$, $\boldsymbol{b} = a\boldsymbol{y}$, and $\mathbf{c} = a\boldsymbol{z}$.



A plane (ABC) is also represented in the cube, that intercept the edge of the cube at points A, B and C. In the $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$ basis, these points have coordinates $A(\frac{a}{h}, 0, 0), B(O, \frac{a}{k}, 0)$ and $C(0, 0, \frac{a}{l})$. For this plane to be a "crystal plane", it needs to intercept at least three points of the Bravais lattice of the crystals, i.e. the points $P(n_1a, n_2a, n_3a)$ in space describe above where motifs are located. This is a priori not obvious.

5a. We want to show that for every co-prime integers h, k and l, taken strictly positive without loss of generality, the plane (ABC) is a crystal plane.

(i) Show that the plan (ABC), that we will subsequently call $\mathcal{P}_1^{(hkl)}$, has the following equation in the $\mathcal{B}_{(O,\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}$ basis:

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

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

(ii) Using the Bézout relation for h, k and l, show that $\exists(n_1, n_2, n_3) \in \mathbb{Z}^3$ such that the point $P(n_1a, n_2a, n_3a) \in \mathcal{P}_1^{(hkl)}$.

(iii) Show that the point $Q(a(n_1 + k), a(n_2 - h), n_3a) \in \mathcal{P}_1^{(hkl)}$.

(iv) Doing a similar procedure as in (iii), find a third point that belongs to both to the Bravais lattice and to $\mathcal{P}_1^{(hkl)}$, and conclude.

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

(i) Show that the direction $\boldsymbol{u}_{[hkl]} = h\boldsymbol{x} + k\boldsymbol{y} + l\boldsymbol{z}$ (the direction $[hkl]$ in the Miller notation in crystallography) is perpendicular to $\mathcal{P}_1^{(hkl)}$.

(ii) Show that the equation of the plan $\mathcal{P}_0^{(hkl)}$ perpendicular to the direction$[hkl]$ (also noted $\boldsymbol{u}_{[hkl]}$ as above) and passing through the origin O is given by:

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

(iii) Find two other points, other than O, that belong to both the Bravais lattice (O, **a**,**b**,**c**) and the plan $\mathcal{P}_0^{(hkl)}$, and conclude that $\mathcal{P}_0^{(hkl)}$ is also a crystal plane parallel to $\mathcal{P}_1^{(hkl)}$.

5c. In the Miller notation, the crystal planes $\mathcal{P}_0^{(hkl)}$ and $\mathcal{P}_1^{(hkl)}$ belong to the family of parallel crystal planes $\{hkl\}$. We want to see if there could be a crystal plane 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. The family $\{hkl\}$ of crystal 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 crystal plane 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 5b and 5c 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. Hence, $\exists (n_1, n_2, n_3) \in \mathbb{Z}^3$, 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:

$$A''\begin{pmatrix} n_1 a + \frac{a}{h} \\ n_2 a \\ n_3 a \end{pmatrix};\ B''\begin{pmatrix} n_1 a \\ n_2 a + \frac{a}{k} \\ n_3 a \end{pmatrix};\ C''\begin{pmatrix} n_1 a \\ n_2 a \\ n_3 a + \frac{a}{l} \end{pmatrix}$$

(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 two points, one in each plane, defined by the intersection of a normal vector to the planes)

(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 $\mathbf{DM}$ and the normal $\boldsymbol{u}_{[hkl]}$ are colinear, i.e. $\exists \lambda \in \mathbb{R}, \boldsymbol{DM} = \lambda \boldsymbol{u}_{[hkl]}$.
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:

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