Mathematical Methods for Materials Science

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Additional Exercises

Complex Numbers Reciprocal spaces, X-ray diffraction

Exercise A1: irrationality of $\sqrt{2}$ and \sqrt{n}

A1a. We want to show that $\sqrt{2}$ is irrational, or in other words, there is no $(n, m) \in \mathbb{N}^2$, with gcd(n, m) = 1, such that $2 = \left(\frac{m}{n}\right)^2$.

- (i) Show that 2 divides m.
- (ii) Show then that 2 divides n.
- (iii) Express a contradiction with gcd(n, m) = 1.

A1b. We want to show that $\forall n \in \mathbb{N}, (\sqrt{n} \in \mathbb{R} \setminus \mathbb{Q} \text{ or } \sqrt{n} \in \mathbb{N})$. We consider $n \in \mathbb{N}$ and suppose that $\sqrt{n} \in \mathbb{Q}$. Hence, $\exists (a,b) \in \mathbb{N}^2, \sqrt{n} = \frac{a}{b}$ and gcd(a,b) = 1. Consider a prime number p in the factorization of b:

- (i) Show that $p|a^2$, and hence necessarily we must have p|a.
- (ii) Show that b = 1 and conclude.

Exercise A2: Inequalities of Cauchy-Schwartz and Minkowski

2a. For $n \in \mathbb{N}^*$ and $x_1, \dots, x_n, y_1, \dots, y_n \in \mathbb{R}$, we define the function T of $\lambda \in \mathbb{R}$ such as

$$T(\lambda) = \sum_{i=1}^{n} (\lambda x_i + y_i)^2$$

- (i) Show that $\forall \lambda \in \mathbb{R}, T(\lambda) \geq 0$.
- (ii) Show that $T(\lambda) = \left(\sum_{i=1}^n x_i^2\right) \lambda^2 + 2\left(\sum_{i=1}^n x_i y_i\right) \lambda + \sum_{i=1}^n y_i^2$
- (iii) Consider the equation $T(\lambda)=0$ (assuming $\sum_{i=1}^n x_i^2 \neq 0$). What is the sign of the determinant ?
- (iv) Deduce the inequality of Cauchy-Schwartz: $(\sum_{i=1}^n x_i y_i)^2 \le (\sum_{i=1}^n x_i^2)(\sum_{i=1}^n y_i^2)$

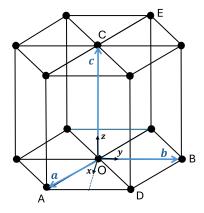
2b.

- (i) Using 2a, show: $\sum_{i=1}^{n} (x_i + y_i)^2 \le (\sum_{i=1}^{n} x_i^2) + 2\sqrt{\sum_{i=1}^{n} x_i^2} \sqrt{\sum_{i=1}^{n} y_i^2} + \sum_{i=1}^{n} y_i^2$
- (ii) Deduct the inequality of Minkowski: $\sqrt{\sum_{i=1}^{n}(x_i+y_i)^2} \le \sqrt{\sum_{i=1}^{n}x_i^2} + \sqrt{\sum_{i=1}^{n}y_i^2}$

Exercise A3: Distance between crystal planes in the hexagonal structure

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

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



АЗа.

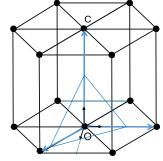
- (i) What are the coordinates of the vectors a, b, c in the basis $\mathcal{B}_{(O,x,y,z)}$?
- (ii) What are the coordinates in the basis $\mathcal{B}_{(O,x,y,z)}$ and $\mathcal{B}_{(O,a,b,c)}$ of the points A,B, C, D and E shown on the schematic?

A3b.

- (i) What is the volume of the cell defined by the vectors a, b, c?
- (ii) Show that the reciprocal lattice vectors are given by, in the $\mathcal{B}_{(O,x,y,z)}$ basis:

$$a^* = \frac{4\pi}{a\sqrt{3}}x$$
; $b^* = \frac{4\pi}{a\sqrt{3}}(\frac{1}{2}x + \frac{\sqrt{3}}{2}y)$; $c^* = \frac{2\pi}{c}z$

A3c. We consider the crystal plane (hkl) (h,k,l three relative integers) shown on the schematic, that intercepts the a,b,c axis at positions $\frac{a}{h},\frac{b}{k},\frac{c}{l}$ respectively.



- (i) What is the normal to the plane in the orthonormal $\mathcal{B}_{(\mathcal{O},x,y,z)}$ basis ?
- (ii) Show that the equation of the plane in $\mathcal{B}_{(0,x,y,z)}$ 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 (hkl) plane parallel to \mathcal{P} is the one passing through the origin, show that the distance between the (hkl) plane is given by:

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