

Mathematics for Materials

Problem Set B for 'Vectors, Matrices...' Course

(overall 4th set in the Michaelmas Term maths provision)

1. (a) Consider a crystal defined by three non-coplanar vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$. Make a diagram showing the three vectors, the unit cell of the crystal, and the position of lattice vector $2\mathbf{a} + \mathbf{b} - \mathbf{c}$.
(b) If the crystal is orthorhombic, calculate the length and direction cosines of the given lattice vector, giving your answers in terms of the vectors' magnitudes a , b and c .
2. (a) Explain what is meant by the Miller indices $(1\bar{1}2)$.
(b) For an orthorhombic crystal defined by lattice vectors $[a, 0, 0]$, $[0, b, 0]$, and $[0, 0, c]$, make diagrams showing the position of the planes described by the Miller indices $(23\bar{2})$ and (011) .
(c) Construct the equation of the plane $(23\bar{2})$.
(d) Find the shortest distance between the above plane and the point $3\mathbf{a} - \mathbf{c}$.
3. Using a sketch, explain the geometrical meaning of the scalar triple product.
4. Find the angle between each of the following pairs of planes:
(a) $\mathbf{r} \cdot \begin{pmatrix} 2 \\ 3 \\ 1 \end{pmatrix} = -2$ and $\mathbf{r} \cdot \begin{pmatrix} -1 \\ 4 \\ 7 \end{pmatrix} = 3$.
(b) $\mathbf{r} = \begin{pmatrix} 2 \\ 0 \\ 5 \end{pmatrix} + \lambda \begin{pmatrix} 1 \\ 1 \\ -3 \end{pmatrix} + \mu \begin{pmatrix} 0 \\ -2 \\ -2 \end{pmatrix}$ and the plane containing points $(1, 2, 1)$, $(0, 5, -1)$, $(1, 3, -3)$.
5. (a) Define the term *linear independence*.
(b) Thus explain why the scalar triple product can test if three vectors are linearly independent.
(c) Are $\begin{pmatrix} 2 \\ -1 \\ 1 \end{pmatrix}$, $\begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix}$, and $\begin{pmatrix} -1 \\ -1 \\ -3 \end{pmatrix}$ dependent or independent?
(d) Prove that $\alpha \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} + \beta \begin{pmatrix} 1 \\ -1 \\ 3 \end{pmatrix} + \gamma \begin{pmatrix} 1 \\ 3 \\ 3 \end{pmatrix} \neq \begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix}$ for any α , β , and γ .
(e) Consider again the three vectors from left hand side of the equation in (d). Without computing the scalar triple product, explain whether they are linearly independent.
6. (a) Write down the definitions of $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$
(b) For a general crystal, explain how the reciprocal lattice vectors are oriented relative to the faces of the crystal and to $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$.
(c) Use your answer to (a) to show that $\mathbf{a} \cdot \mathbf{a}^* = 1$ and $\mathbf{b} \cdot \mathbf{a}^* = \mathbf{c} \cdot \mathbf{a}^* = 0$ and explain how this relates to your answer to (b).
(d) How are the reciprocal lattice vectors are oriented relative to the faces of the crystal and to $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ in the special case of an orthorhombic crystal?
7. For a triclinic crystal with a unit cell defined by vectors $\mathbf{a} = \begin{pmatrix} 3 \\ 2 \\ 2 \end{pmatrix}$, $\mathbf{b} = \begin{pmatrix} 1 \\ 5 \\ 0 \end{pmatrix}$, $\mathbf{c} = \begin{pmatrix} 1 \\ 1 \\ 4 \end{pmatrix}$, find:
(a) The volume of the unit cell
(b) The reciprocal lattice vectors

8. Consider a crystal with basis vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$.

- (a) Write down three points in the plane (hkl) .
- (b) Construct a normal to the plane (hkl) .
- (c) Show that the angle θ between planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ is defined by

$$\cos \theta = \frac{(h_1\mathbf{a}^* + k_1\mathbf{b}^* + l_1\mathbf{c}^*) \cdot (h_2\mathbf{a}^* + k_2\mathbf{b}^* + l_2\mathbf{c}^*)}{|h_1\mathbf{a}^* + k_1\mathbf{b}^* + l_1\mathbf{c}^*||h_2\mathbf{a}^* + k_2\mathbf{b}^* + l_2\mathbf{c}^*|}$$

- (d)* Simplify the expression in (c) for the orthorhombic case where $\mathbf{a} = a\mathbf{i}$, $\mathbf{b} = b\mathbf{j}$ and $\mathbf{c} = c\mathbf{k}$.

9. For a triclinic crystal with a unit cell defined by vectors $\mathbf{a} = \begin{pmatrix} 3 \\ 2 \\ 4 \end{pmatrix}$, $\mathbf{b} = \begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix}$, and $\mathbf{c} = \begin{pmatrix} -2 \\ -3 \\ 2 \end{pmatrix}$,

- (a) Find the angle between planes (100) and (001)
 - (b) Find the angle between planes $(1\bar{2}2)$ and (310) [Ans: $\theta = 148.3^\circ = 31.7^\circ$]
10. (a) Why must basis vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ for a crystal always be linearly independent?
- (b) Thus explain why for any position vector $\mathbf{p}$, $\mathbf{p} = \alpha\mathbf{a} + \beta\mathbf{b} + \gamma\mathbf{c}$ for some α , β , and γ .
 - (c) If $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ are orthogonal to one another, how can you use the dot product operation to write expressions for α , β , and γ ? Why does this not work in the general case when $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ are not orthogonal?
 - (d) Use the properties of reciprocal lattice vectors to find expressions for α , β , and γ in the general case.
- (e) Resolve $\begin{pmatrix} 14 \\ -4 \\ 1 \end{pmatrix}$ along the directions $\begin{pmatrix} 1 \\ 3 \\ 1 \end{pmatrix}$, $\begin{pmatrix} 0 \\ 2 \\ 2 \end{pmatrix}$, and $\begin{pmatrix} -3 \\ 4 \\ -1 \end{pmatrix}$.
11. (a) We can also write $\mathbf{p} = \alpha\mathbf{a}^* + \beta\mathbf{b}^* + \gamma\mathbf{c}^*$. Explain why, and how we can use this to solve a system of simultaneous equations.
- (b) Hence solve the following set of simultaneous equations. Verify your solution.

$$\begin{aligned} 3x + 2y + 2z &= 7 \\ x + 5y &= -37 \\ x + y + 4z &= 23 \end{aligned}$$

(N.B. The reciprocal lattice vectors you need should be those that you already found in Q7).