Crystallographic Algebra. Exercises

La Plata, Argentina. April-May 2014

April 26, 2014

Abstract

Vector. Basis. Scalar product. Metric Tensor. Matrices. Determinant. Cross product.

1 Vectors

1.1. Find the sum $\vec{r} + \vec{q}$ and draw the resulting vector:

- 1.1.1. $\vec{q} = 2.3\vec{a} - 1.5\vec{b} + 6.7\vec{c}$; $\vec{r} = 1.2\vec{a} + 4.5\vec{b} - 8.3\vec{c}$
- 1.1.2. $\vec{q} = 2.3\vec{a} - 1.5\vec{b} + 6.7\vec{c}$; $\vec{r} = -1.2\vec{a} - 4.5\vec{b} - 6.7\vec{c}$
- 1.1.3. $\vec{q} = -3\vec{a} - 4\vec{b} - 5\vec{c}$; $\vec{r} = 3\vec{a} + 4\vec{b} + 9\vec{c}$

1.2. The vectors $\hat{i}$, $\hat{j}$ and $\hat{k}$ are used to designate orthogonal basis with unit length (Cartesian or orthonormal basis). Consider a vector which makes equal angles with $\hat{i}$, $\hat{j}$ and $\hat{k}$. Calculate its components.

1.3. The components of a vector $\vec{r}$ in a given basis $\vec{a}$, $\vec{b}$ and $\vec{c}$ can be writen as:

$$r_1 = r\ \cos\phi_1; r_2 = r\ \cos\phi_2; r_3 = r\ \cos\phi_3$$

where $r = |\vec{r}|$ and ϕ_1, ϕ_2 and ϕ_3 are known as the direction cosine. In a Cartesian basis it can be shown that $\cos^2\phi_1 + \cos^2\phi_2 + \cos^2\phi_3 = 1$. Calculate the components of a unit vector that can be spawned by $\hat{i}$ and $\hat{j}$ vectors and make equal angles with each of them.

1.4. A triangle is defined by the vertices of three vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ that extends from the origin. In terms of this three vectors show that the vector sum of the successive sides of the triangle is zero.

1.5. Find the diagonal vectors of a unit cube with one corner at the origin and its three sides lying along Cartesian basis. Show that there are four diagonals with length $\sqrt{3}$. Representing these as vectors, what are their components. Show that the diagonals of the cube's faces have length $\sqrt{2}$ and determine their components.

1.6. Consider basis vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$, which forms angles $\alpha = \pi/2$, $\beta = \pi/2$ and $\gamma = 2\pi/3$ and have length $a = b \neq c$. Such base is known as an hexagonal base in crystallography. Define a cartesian basis and express each vector $\vec{a}$, $\vec{b}$ and $\vec{c}$ in terms of $\hat{\imath}$, $\hat{\jmath}$ and $\hat{k}$.

1.7. Calculate the metric tensor of the basis vectors:

1.7.1. $a = b = c$, $\alpha = \beta = \gamma = \pi/2$. This is called a cubic basis in crystallography.

1.7.2. $a = b \neq c$, $\alpha = \beta = \gamma = \pi/2$. This is called a tetragonal basis in crystallography.

1.7.3. $a \neq b \neq c$, $\alpha = \beta = \gamma = \pi/2$. This is called an orthorhombic basis in crystallography.

1.7.4. $a = b \neq c$, $\alpha = \beta = \pi/2$, $\gamma = 2\pi/3$. This is called a hexagonal basis in crystallography.

1.7.5. $a = b = c$, $\alpha = \beta = \gamma$. This is called a rhombohedral basis in crystallography.

1.7.6. $a \neq b \neq c$, $\alpha = \gamma = \pi/2 \neq \beta$. This is called a monoclinic basis in crystallography.

1.7.7. $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$. This is called a triclinic basis in crystallography.

1.8. Calculate the scalar product $\vec{r} \cdot \vec{q}$. which pair of vectors are orthogonal ?:

1.8.1. $\vec{q} = 2.3\vec{a} - 1.5\vec{b} + 6.7\vec{c}$; $\vec{r} = 1.2\vec{a} + 4.5\vec{b} - 8.3\vec{c}$ and $a = b = 1$, $c = 2$, $\alpha = \beta = \gamma = \pi/2$

1.8.2. $\vec{q} = 1.5\vec{a} - 4.2\vec{b}$; $\vec{r} = -6.7\vec{c}$ and $a = b = 0.456$, $c = 1.345$, $\alpha = \beta = \pi/2$, $\gamma = 2\pi/3$

1.8.3. $\vec{q} = 2.3\vec{a} - 1.5\vec{b} + 6.7\vec{c}$; $\vec{r} = -1.2\vec{a} - 4.5\vec{b} - 6.7\vec{c}$ and $a = b = c = 1$, $\alpha = \beta = \gamma = \pi/3$

1.8.4. $\vec{q} = 2.3\vec{a} + 2.3\vec{b} + 2.3\vec{c}$; $\vec{r} = 1.3\vec{a} + 1.3\vec{b} - 2.6\vec{c}$ and $a = b = c = 1.23$, $\alpha = \beta = \gamma = \pi/5$

1.8.5. $\vec{q} = -3\vec{a} - 4\vec{b} - 5\vec{c}$; $\vec{r} = 3\vec{a} + 4\vec{b} + 9\vec{c}$ and $a = b = c = 1.234$, $\alpha = \beta = \gamma = \pi/2$

1.9. Calculate the scalar product between the diagonals of the unit cube. Which angle forms the daigonals with each other and with the edges of the cube ? Calculate the angle between the diagonals of the cube and the diagonals of the faces.

1.10. Calcule $\vec{r} \cdot \vec{q}$ in an orthorhombic basis.

1.11. Calcule $\vec{r} \cdot \vec{q}$ in a hexagonal basis.

1.12. Calcule $\vec{r} \cdot \vec{q}$ in a tetragonal basis.

1.13. Calcule $\vec{r} \cdot \vec{q}$ in a cubic basis.

1.14. Calculate the scalar product between the basis vector in a Cartesian system. Write down the metric tensor.

2 Matrices

2.1. Calculate :

2.1.1. $$\begin{pmatrix} 2 & 1 & 5 \\ 1 & 5 & 2 \\ 5 & 1 & 2 \end{pmatrix} \cdot \begin{pmatrix} 1 & -1 & 3 \\ -1 & 1 & 3 \\ 1 & -1 & -3 \end{pmatrix}.$$

2.1.2. $$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1/2 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

2.1.3. $$\begin{pmatrix} -1 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

2.1.4. $$\begin{pmatrix} 1 & 0 & 1 \\ -1 & 1 & 1 \\ 0 & -1 & 1 \end{pmatrix} \cdot \begin{pmatrix} 2/3 & -1/3 & -1/3 \\ 1/3 & 1/3 & -2/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}.$$

2.2. The matrix $P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ could represent a symmetry operation for certain crystals. Calculate $P^3 = P \cdot P \cdot P$. Calculate $P \cdot (x\,y\,z)^T$

2.3. The matrices $P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$ and $Q = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$ represent symmetry operations for certain crystals. Calculate $P \cdot Q$. Calculate $P \cdot (x\,y\,z)^T$ and $Q \cdot (z\,y\,-x)^T$

2.4. Given the matrix $Q = \begin{pmatrix} 0 & 1 & 0 & 1/2 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$. Calculate $Q \cdot (x\,y\,z\,1)^T$

2.5. Calculate $Q = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \cdot (x\,y\,z)^T + (\frac{1}{2}\;0\;0)^T$. Compare to the previous exercise.

2.6. Given $Q = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$. Calculate $Q \cdot Q^T$. What can be said of the matrix Q.

2.7. Determine which of the following matrices are orthogonal:

2.7.1. $Q = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

2.7.2. $P = \begin{pmatrix} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

2.7.3. $R = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

2.8. Calculate the determinant of:

2.8.1. $Q = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

2.8.2. $P = \begin{pmatrix} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

2.8.3. $R = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

2.9. Calculate the determinant of the metric tensor for the tetragonal basis

2.10. Calculate the determinant for the hexagonal basis

2.11. Calculate the cross product $\vec{r} \cdot \vec{q}$:

2.11.1. $\vec{q} = 2.3\vec{a} - 1.5\vec{b} + 6.7\vec{c}$; $\vec{r} = 1.2\vec{a} + 4.5\vec{b} - 8.3\vec{c}$ and $a = b = 1$, $c = 2$, $\alpha = \beta = \gamma = \pi/2$

2.11.2. $\vec{q} = 1.5\vec{a} - 4.2\vec{b}$; $\vec{r} = -6.7\vec{c}$ and $a = b = 0.456$, $c = 1.345$, $\alpha = \beta = \pi/2$, $\gamma = 2\pi/3$

2.11.3. $\vec{q} = 2.3\vec{a} - 1.5\vec{b} + 6.7\vec{c}$; $\vec{r} = -1.2\vec{a} - 4.5\vec{b} - 6.7\vec{c}$ and $a = b = c = 1$, $\alpha = \beta = \gamma = \pi/3$

2.11.4. $\vec{q} = 2.3\vec{a} + 2.3\vec{b} + 2.3\vec{c}$; $\vec{r} = 1.3\vec{a} + 1.3\vec{b} - 2.6\vec{c}$ and $a = b = c = 1.23$, $\alpha = \beta = \gamma = \pi/5$

2.11.5. $\vec{q} = -3\vec{a} - 4\vec{b} - 5\vec{c}$; $\vec{r} = 3\vec{a} + 4\vec{b} + 9\vec{c}$ and $a = b = c = 1.234$, $\alpha = \beta = \gamma = \pi/2$