

NANO106 Handout 1 - Linear Algebra and Lattice Computations

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1 Introduction

This document provides a summary of the basic linear algebra concepts and their application in crystallography.

2 Notation and definitions

Let us define a series of consistent notations. Note that all vectors are written in *column* format for consistency. All vectors are **bolded**.

Quantity	Notation
Lattice basis vectors	a₁ , a₂ , a₃ or a , b , c
Cartesian coordinate vectors	x or y
Crystal coordinate vectors	p or q
Metric tensor	<i>g</i>

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$\mathbf{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$$

For matrices, we will use simple **A** and **B** to denote them. **E** refers to the identity matrix. In the full form, we denote each element as a_{ij} . E.g.

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

Transposes and inverses are indicated by superscript T and -1 respectively, e.g., \mathbf{A}^T and \mathbf{A}^{-1} .

3 Required Linear Algebra Relations

We will start with the standard linear algebra relations in Cartesian coordinates. Make sure you understand the difference between Cartesian and crystal coordinates. They are not the same thing and you need to use different formulas for them.

3.1 Norm of a vector in Cartesian coordinates

$$\begin{aligned} |\mathbf{x}| &= \sqrt{\mathbf{x} \cdot \mathbf{x}} \\ &= \sqrt{\mathbf{x}^T \mathbf{x}} \\ &= \sqrt{x_1^2 + x_2^2 + x_3^2} \end{aligned}$$

3.2 Dot product in Cartesian coordinates

$$\begin{aligned} \mathbf{x} \cdot \mathbf{y} &= \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} \\ &= x_1 y_1 + x_2 y_2 + x_3 y_3 \\ &= |\mathbf{x}| |\mathbf{y}| \cos \theta \end{aligned}$$

Finding the angle between two vectors in Cartesian coordinates

$$\theta = \cos^{-1} \frac{\mathbf{x} \cdot \mathbf{y}}{|\mathbf{x}| |\mathbf{y}|}$$

3.3 Cross product in Cartesian coordinates

$$\mathbf{x} \times \mathbf{y} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \times \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} x_2 y_3 - x_3 y_2 \\ -(x_1 y_3 - x_3 y_1) \\ x_1 y_2 - x_2 y_1 \end{pmatrix}$$

3.4 Some matrix relations

$$\begin{aligned} (\mathbf{AB})^T &= \mathbf{B}^T \mathbf{A}^T \\ (\mathbf{A} + \mathbf{B})\mathbf{C} &= \mathbf{AC} + \mathbf{BC} \\ \mathbf{AA}^{-1} &= \mathbf{A}^{-1}\mathbf{A} = \mathbf{E} \end{aligned}$$

3.5 Finding the determinant and inverse of a 3×3 matrix.

$$\begin{aligned}\det(\mathbf{A}) &= \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} \\ &= a_{11}(a_{22}a_{33} - a_{32}a_{23}) - a_{12}(a_{21}a_{33} - a_{31}a_{23}) + a_{13}(a_{21}a_{32} - a_{31}a_{22}) \\ \mathbf{A}^{-1} &= \frac{1}{\det(\mathbf{A})} \begin{pmatrix} a_{22}a_{33} - a_{32}a_{23} & -(a_{21}a_{33} - a_{31}a_{23}) & a_{21}a_{32} - a_{31}a_{22} \\ -(a_{12}a_{33} - a_{32}a_{13}) & a_{11}a_{33} - a_{31}a_{13} & -(a_{11}a_{32} - a_{31}a_{12}) \\ a_{12}a_{23} - a_{22}a_{13} & -(a_{11}a_{23} - a_{21}a_{13}) & a_{11}a_{22} - a_{21}a_{12} \end{pmatrix}\end{aligned}$$

4 Crystal Coordinates

Given a lattice with basis vectors \mathbf{a} , \mathbf{b} , \mathbf{c} , any point in the lattice can be represented in *crystal coordinates* $[uvw]$. The conversion from crystal coordinates to Cartesian coordinates is given as:

$$\mathbf{x} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

5 Calculating lattice parameters

Given a set of basis vectors \mathbf{a} , \mathbf{b} , \mathbf{c} , the lattice parameters are given by:

$$\begin{aligned}a &= |\mathbf{a}| \\ b &= |\mathbf{b}| \\ c &= |\mathbf{c}| \\ \alpha &= \cos^{-1} \frac{\mathbf{b} \cdot \mathbf{c}}{|\mathbf{b}||\mathbf{c}|} \\ \beta &= \cos^{-1} \frac{\mathbf{a} \cdot \mathbf{c}}{|\mathbf{a}||\mathbf{c}|} \\ \gamma &= \cos^{-1} \frac{\mathbf{a} \cdot \mathbf{b}}{|\mathbf{a}||\mathbf{b}|}\end{aligned}$$

6 Relations in crystal coordinates

For a lattice with basis vectors \mathbf{a} , \mathbf{b} , \mathbf{c} , the metric tensor g is given by:

$$g = \begin{pmatrix} \mathbf{a} \cdot \mathbf{a} & \mathbf{a} \cdot \mathbf{b} & \mathbf{a} \cdot \mathbf{c} \\ \mathbf{b} \cdot \mathbf{a} & \mathbf{b} \cdot \mathbf{b} & \mathbf{b} \cdot \mathbf{c} \\ \mathbf{c} \cdot \mathbf{a} & \mathbf{c} \cdot \mathbf{b} & \mathbf{c} \cdot \mathbf{c} \end{pmatrix} = \begin{pmatrix} a^2 & ab \cos \gamma & ac \cos \beta \\ ab \cos \gamma & b^2 & bc \cos \alpha \\ ac \cos \beta & bc \cos \alpha & c^2 \end{pmatrix}$$

6.1 Dot product in crystal coordinates

It is important to note that dot products between crystal coordinates is not performed the same way as in Cartesian! You need to use the metric tensor to perform dot products. The dot product is given by:

$$\mathbf{p}^T g \mathbf{q}$$

6.2 Distance between points and length of vector in crystal coordinates

For two points defined by \mathbf{p} and \mathbf{q} in crystal coordinates,

$$\begin{aligned} d^2 &= (\mathbf{q} - \mathbf{p})^T g (\mathbf{q} - \mathbf{p}) \\ d &= \sqrt{(\mathbf{q} - \mathbf{p})^T g (\mathbf{q} - \mathbf{p})} \end{aligned}$$

Similarly, the length of a vector \mathbf{p} in crystal coordinates is given as:

$$d = \sqrt{\mathbf{p}^T g \mathbf{p}}$$

6.3 Angles in crystal coordinates

For three points O, P and Q defined by \mathbf{o} , \mathbf{p} , and \mathbf{q} in crystal coordinates respectively,

$$\begin{aligned} \vec{OP} &= \mathbf{p} - \mathbf{o} \\ \vec{OQ} &= \mathbf{q} - \mathbf{o} \\ \angle POQ &= \cos^{-1} \frac{\vec{OP}^T g \vec{OQ}}{|\vec{OP}| |\vec{OQ}|} \end{aligned}$$