

# Handout 2 - Summary of Coordinate Transformations

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## 1 Introduction

This document provides a summary of the various coordinate transformations relations and formulas.

## 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	<b>a<sub>1</sub></b> , <b>a<sub>2</sub></b> , <b>a<sub>3</sub></b>
Cartesian coordinate vectors	<b>x</b> or <b>y</b>
Crystal coordinate vectors	<b>p</b> or <b>q</b>
Metric tensor	<i>g</i>

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

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

Let us denote a basis transformation from basis vectors **a<sub>i</sub>** to **a'<sub>i</sub>** as:

$$\begin{pmatrix} \mathbf{a}'_1 \\ \mathbf{a}'_2 \\ \mathbf{a}'_3 \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{pmatrix} \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix}$$

or more compactly as:

$$\mathbf{A}' = \mathbf{C}\mathbf{A}$$

In the new coordinate system, we add a ', e.g.,  $\mathbf{p}'$  denotes the crystal coordinates in the new basis.

### 3 Transformation relations

The following table summarizes all the coordinate transformations. Be very careful to note whether we are using the transpose of the vector (i.e., writing it in terms of a row instead of a column), the order of the multiplication, and whether we are using the inverse or the direct transformation matrix  $\mathbf{C}$ !

Transformation	Old basis-> New basis	New basis-> Old basis
Position/Vector -> Position/Vector	$\mathbf{p}'^T = \mathbf{p}^T \mathbf{C}^{-1}$	$\mathbf{p} = \mathbf{p}'^T \mathbf{C}$
Position/Vector -> Reciprocal Position/Vector	$\mathbf{p}^{*T} = \mathbf{p}^T g$	$\mathbf{p}^T = \mathbf{p}^{*T} g^{-1}$
Reciprocal Position/Vector -> Reciprocal Position/Vector	$\mathbf{p}^{*'} = \mathbf{C} \mathbf{p}^*$	$\mathbf{p}^* = \mathbf{C}^{-1} \mathbf{p}^{*'}$
Metric Tensor -> Metric Tensor	$g' = \mathbf{C} g \mathbf{C}^T$	$g = \mathbf{C}^{-1} g' (\mathbf{C}^{-1})^T$