NANO106 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	$\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$
Cartesian coordinate vectors	$\mathbf{x}$ or $\mathbf{y}$
Crystal coordinate vectors	$\mathbf{p}$ or $\mathbf{q}$
Metric tensor	g

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

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

Let us denote a basis transformation from basis vectors $\mathbf{a_i}$ to $\mathbf{a_i'}$ 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:

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

In the new coordinate ssytem, 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 transformas. 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 C!

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