Coordiate McCoordinates

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1 Introduction

This bit of maths goes through the transformations required to generally calculate the directional derivative of the displacement field component parallel to the g vector in a hexagonal crystal structure.

The component of strain used by the Howie-Whelan equations [**?**] will change the local lattice curvature and therefore the local deviation from the Bragg reflection condition: $s'_g = s_g + \delta s_g$. Tunstall et al [**?**] showed that there is a second component given by the change in lattice parameter which contributes with a lower effect to the new s'_g.

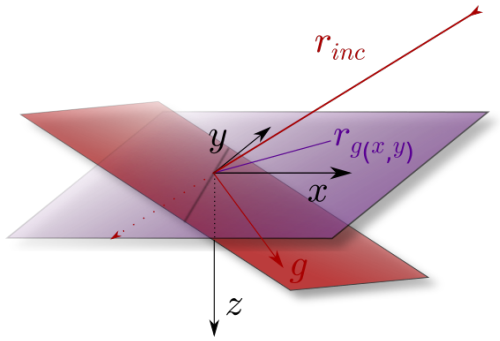

Figure 1: Coordinate system used throughout. We make the assumption that g is perpendicular to r_{inc}

In Cartesian coordinates (x, y, z) with the origin on the surface of the sample and z going inside the sample and the incident beam parallel to z (the z axes is defined in the same direction as that of the vector **k**):

$$s'_g = s_g + \beta'$$

$$s'_g = s_g + |\boldsymbol{g}| \left(\frac{\partial u_g}{\partial z}\right)_{x,y} + \theta_B |\boldsymbol{g}| \left(\frac{\partial u_g}{\partial r_g}\right)_z \tag{1}$$

where $u_g(x, y, z)$ is the component of the displacement field parallel to $\mathbf{g}$, r_g is the coordinate in the x, y plane parallel to $\mathbf{g}$ and θ_B is the Bragg angle.

For a non-normal incidence electron beam (r_{inc}) Elena thinks equation (1) can be generalised to:

$$s'_g = s_g + |\boldsymbol{g}| \frac{\partial u_g(x,y,z)}{\partial r_{inc}(x,y,z)} + \theta_B |\boldsymbol{g}| \left(\frac{\partial u_g(x,y,z)}{\partial r_g(x,y,z)} \right)_{r_{inc}} \tag{2}$$

r_g is this time the coordinate parallel to $\mathbf{g}$ living in the plane with the normal parallel to r_{inc} .

u_g is the displacement field in the g direction or it's projection on the $\mathbf{g}$ vector:

$$\begin{aligned} u_g(x,y,z) &= \boldsymbol{u}(u_x, u_y, u_z) \cdot \hat{\boldsymbol{g}}(x,y,z) \\ &= \frac{u_x(x,y,z)g_x + u_y(x,y,z)g_y + u_z(x,y,z)g_z}{|\boldsymbol{g}|} \end{aligned}$$

where $\hat{\boldsymbol{g}}$ is the unit vector parallel to g. Also equal to $\boldsymbol{r_g}$.

We are interested in the change of this displacement field component. This change we can calculate as a directional derivative defined as:

$$\begin{aligned} D_{\boldsymbol{v}} f(x,y,z) &= \frac{\partial f(x,y,z)}{\partial x} v_x + \frac{\partial f(x,y,z)}{\partial y} v_y + \frac{\partial f(x,y,z)}{\partial z} v_z \\ &= \boldsymbol{\nabla} f \cdot \boldsymbol{v} \end{aligned}$$

Such that the second term in (2) becomes:

$$|\boldsymbol{g}| \frac{\partial u_g}{\partial r_{inc}} = |\boldsymbol{g}| \, D_{r_{inc}}(\boldsymbol{u} \cdot \hat{\boldsymbol{g}})$$

Similarly, the last term in (2) is:

$$\theta_B |\boldsymbol{g}| \frac{\partial u_g}{\partial r_g} = |\boldsymbol{g}| \, D_{r_g}(\boldsymbol{u} \cdot \hat{\boldsymbol{g}})$$

In the above derivation $\mathbf{g}$ is expressed in Cartesian coordinates (x, y, z) in real space. However, $\boldsymbol{g} = \boldsymbol{g}_{hkl} = h\boldsymbol{a^*} + k\boldsymbol{b^*} + l\boldsymbol{c^*}$ is usually given in the reciprocal space coordinates system of the crystal structure. We need to make a coordinate transformation to the Cartesian reference frame. We choose this approach rather than making the computation in the crystal coordinate system since results will be viewed in the Cartesian system of 2D media (screen, paper).

The g vector must be the same regardless of the chosen coordinate system:

$$\boldsymbol{g} = g_i \boldsymbol{e}_i = k_j \boldsymbol{a}^*_j$$

where we can relate the reciprocal space vector components k_j with respect to the reciprocal basis vector $\boldsymbol{a^*}$ to the Cartesian components g_i by the reciprocal structure matrix b_{ij}.

$$g_i = b_{ij} k_j$$

where

$$b_{ij} = a_{il} g^*_{lj}$$

with a_{il} is the direct structure matrix and g^*_{lj} is the reciprocal metric tensor. For a hexagonal crystal (a, a, c, 90°, 90°, 120°) the direct structure matrix looks like:

$$a^{hex}_{ij} = \begin{pmatrix} a & \frac{-a}{2} & 0 \\ 0 & \frac{\sqrt{3}a}{2} & 0 \\ 0 & 0 & c \end{pmatrix}$$

and the reciprocal metric tensor is:

$$g^{*hex}_{lj} = \begin{bmatrix} \frac{4}{3a^2} & \frac{2}{3a^2} & a \\ \frac{2}{3a^2} & \frac{4}{3a^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{bmatrix}$$

The incident beam direction r_{inc} must also be defined in the Cartesian system.

$$x_i = a_{ij} * r_j$$

where x_i are the components of r_{inc} in the Cartesian reference frame and r_j are the components in the crystal reference frame.

References