

## Appendix

### Application of the $\Delta g$ method

We apply a transformation on the crystal lattice of magnetite (MT) to bring the selected nearly coincident diffraction spots of magnetite ( $\mathbf{g}_{MTi}$ ) into coincidence with the corresponding diffraction spots of plagioclase ( $\mathbf{g}_{PLi}$ ). This transformation is expressed as a transformation matrix  $\mathbf{A}_{\text{I}}^*$ , where  $|^*$  refers to reciprocal space. Prior to applying the transformation to the crystal lattice of magnetite, the magnetite and plagioclase unit cells need to be expressed in accordance with a common orthonormal coordinate system  $Oxyz$  in units of Å. The base vectors of the orthonormal coordinate system are  $\mathbf{i}$ ,  $\mathbf{j}$ ,  $\mathbf{k}$ , which are along the  $Ox$ -,  $Oy$ - and  $Oz$ -axes. The crystal coordinates of magnetite and plagioclase are defined by the lattice constants  $a, b, c, \alpha, \beta, \gamma$  with the base vectors  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ . The convention for aligning the crystal coordinate system to the orthonormal coordinate system is  $\mathbf{a} \parallel Ox$  and  $\mathbf{a} \times \mathbf{c} \parallel Oy$ . The crystal coordinate vectors  $\mathbf{a}$ ,  $\mathbf{b}$ , and  $\mathbf{c}$  can then be denoted in orthogonal coordinates  $\mathbf{i}, \mathbf{j}, \mathbf{k}$  by

$$\begin{aligned}\mathbf{a} &= i s_1^1 + j s_1^2 + k s_1^3 \\ \mathbf{b} &= i s_2^1 + j s_2^2 + k s_2^3 \\ \mathbf{c} &= i s_3^1 + j s_3^2 + k s_3^3\end{aligned}$$

and in matrix notation

$$\mathbf{u}^T = \mathbf{u}_{(\text{orth})}^T \cdot \mathbf{S}$$

where  $\mathbf{u}$  represents the array of the base vectors of the crystal coordinate and  $\mathbf{u}_{(\text{orth})}$  represents the array of the base vectors of the orthogonal coordinate system.  $|^T$  indicates a transpose operation over the array. Matrix  $\mathbf{S}$  is composed of three column vectors that are the unit vectors in the crystal coordinate system expressed as linear combinations of the base vectors of the orthonormal coordinate system,

$$\mathbf{S} = \begin{pmatrix} s_1^1 & s_2^1 & s_3^1 \\ s_1^2 & s_2^2 & s_3^2 \\ s_1^3 & s_2^3 & s_3^3 \end{pmatrix}$$

The coefficients of matrix  $\mathbf{S}$  can be obtained from the scalar products of the base vectors in crystal coordinates using the orthogonality of the base vectors in the orthonormal coordinate system (Bollmann & Nissen 1968), and are written as

$$\mathbf{S} = \begin{pmatrix} a & b \cdot \cos\gamma & c \cdot \cos\beta \\ 0 & (b/\sin\beta)(\sin^2\beta - \cos^2\alpha - \cos^2\gamma + \cos\alpha \cdot \cos\beta \cdot \cos\gamma)^{1/2} & 0 \\ 0 & (b/\sin\beta)(\cos\alpha - \cos\beta \cdot \cos\gamma) & c \cdot \sin\beta \end{pmatrix}$$

We inserted the lattice constants of magnetite and plagioclase from Fleet (1981) and Wenk et al. (1980), respectively, into the equation above to obtain  $\mathbf{S}_{\text{MT}}$  and  $\mathbf{S}_{\text{PL}}$ . The cubic magnetite has the lattice constant  $a_{\text{MT}} = 8.397 \text{ \AA}$ , and the triclinic plagioclase has the lattice constants  $a_{\text{PL}} = 8.1736 \text{ \AA}$ ,  $b_{\text{PL}} = 12.8736 \text{ \AA}$ ,  $c_{\text{PL}} = 7.1022 \text{ \AA}$ ,  $\alpha_{\text{PL}} = 93.462^\circ$ ,  $\beta_{\text{PL}} = 116.054^\circ$ ,  $\gamma_{\text{PL}} = 90.475^\circ$ . A column vector  $\mathbf{v}$  in the crystal coordinate system can thus be expressed in the orthonormal coordinate as  $\mathbf{v}_{(\text{orth})} = \mathbf{S} \cdot \mathbf{v}$ .

In the next step, the transformation matrix  $\mathbf{A}_{\text{II}}^*$  is applied to the magnetite to make the selected pairs of diffraction spots coincident, i.e.  $\mathbf{g}_{\text{MT}i}$  with the corresponding  $\mathbf{g}_{\text{PL}i}$ . The application can be described as

$$\mathbf{A}_{\text{II}}^* \cdot (\mathbf{S}_{\text{MT}}^* \cdot \mathbf{G}_{\text{MT}}) = \mathbf{S}_{\text{PL}}^* \cdot \mathbf{G}_{\text{PL}}$$

where  $\mathbf{S}^* = (\mathbf{S}^T)^{-1}$ , which corresponds to  $\mathbf{S}$  in reciprocal space.  $\mathbf{G}_{\text{MT}}$  is a  $3 \times 3$  matrix consisting of three non-coplanar magnetite lattice vectors in reciprocal space  $\mathbf{G}_{\text{MT}} = (\mathbf{g}_{\text{MTI}}, \mathbf{g}_{\text{MTII}}, \mathbf{g}_{\text{MTIII}})$ , where

$$\mathbf{g}_{\text{MTI}} = \begin{pmatrix} -1 \\ 1 \\ 3 \end{pmatrix}, \mathbf{g}_{\text{MTII}} = \begin{pmatrix} 2 \\ -2 \\ 2 \end{pmatrix}, \mathbf{g}_{\text{MTIII}} = \begin{pmatrix} 0.1667 \\ 0.1667 \\ 0 \end{pmatrix}$$

the third vector  $\mathbf{g}_{\text{MTIII}}$  corresponds to MT[330] expressed in reciprocal space by the following procedure: (i) express MT[110] in reciprocal space, which yields MT(0.5, 0.5, 0) holding the same direction and the same magnitude; (ii) the reciprocal vector MT(0.5, 0.5, 0) is then divided by 3 to adjust the length to MT[330]. Likewise,  $\mathbf{G}_{\text{PL}}$  is a  $3 \times 3$  matrix consisting of three plagioclase lattice vectors in reciprocal space.  $\mathbf{G}_{\text{PL}} = (\mathbf{g}_{\text{PLI}}, \mathbf{g}_{\text{PLII}}, \mathbf{g}_{\text{PLIII}})$ , where

$$\mathbf{g}_{\text{PLI}} = \begin{pmatrix} 3 \\ -1 \\ 0 \end{pmatrix}, \mathbf{g}_{\text{PLII}} = \begin{pmatrix} 1 \\ 5 \\ 0 \end{pmatrix}, \mathbf{g}_{\text{PLIII}} = \begin{pmatrix} -0.1010 \\ -0.0218 \\ 0.2000 \end{pmatrix}$$

The third vector  $\mathbf{g}_{\text{PLIII}}$  corresponds to PL[005] in reciprocal space, which is obtained by the same procedure as described for  $\mathbf{g}_{\text{MTIII}}$ . The transformation matrix  $\mathbf{A}_{\text{II}}^*$  is then obtained from

$$\mathbf{A}_{\text{II}}^* = \mathbf{S}_{\text{PL}}^* \cdot \mathbf{G}_{\text{PL}} \cdot (\mathbf{S}_{\text{MT}}^* \cdot \mathbf{G}_{\text{MT}})^{-1}$$

and lastly the transformation matrix  $\mathbf{A}_{\text{II}} = ((\mathbf{A}_{\text{II}}^*)^{-1})^T$ , which yields

$$\mathbf{A}_{\text{II}} = \begin{pmatrix} -0.4804 & -0.1390 & 0.8252 \\ 0.6693 & -0.6693 & 0.2869 \\ 0.5499 & 0.7170 & 0.4029 \end{pmatrix}$$

The matrix  $\mathbf{S}_{\text{MT}}^c$  of the constrained magnetite is obtained from

$$\mathbf{S}_{\text{MT}}^c = \mathbf{A}_{\text{II}} \cdot \mathbf{S}_{\text{MT}}$$

and the result reads

$$\mathbf{S}_{\text{MT}}^c = \begin{pmatrix} -4.0321 & -1.1669 & 6.9269 \\ 5.6185 & -5.6185 & 2.4079 \\ 4.6158 & 6.0184 & 3.3819 \end{pmatrix}$$

The lattice constants of the constrained magnetite MT<sup>c</sup> unit cell can be calculated from  $\mathbf{S}_{\text{MT}}^c$ . The constrained base vector  $\mathbf{a}_{\text{MT}}^c = \mathbf{S}_{\text{MT}}^c \cdot [100]'$ , which corresponds to the first column in  $\mathbf{S}_{\text{MT}}^c$ . The value of the base vector  $a_{\text{MT}}^c = 8.3145 \text{ \AA}$  is the new lattice constant

of the constrained magnetite. Similarly,  $\mathbf{b}_{\text{MT}}^{\text{c}} = \mathbf{S}_{\text{MT}}^{\text{c}} \cdot [010]'$  and  $\mathbf{c}_{\text{MT}}^{\text{c}} = \mathbf{S}_{\text{MT}}^{\text{c}} \cdot [001]'$ . The angle between the base vectors  $\mathbf{b}_{\text{MT}}^{\text{c}}$  and  $\mathbf{c}_{\text{MT}}^{\text{c}}$  of the constrained magnetite thus define the angle  $\alpha_{\text{MT}}^{\text{c}} = \angle(\mathbf{b}_{\text{MT}}^{\text{c}}, \mathbf{c}_{\text{MT}}^{\text{c}})$ , and is calculated from the inverse tangent formula  $\alpha_{\text{MT}}^{\text{c}} = \text{atan2}(|\mathbf{b}_{\text{MT}}^{\text{c}} \times \mathbf{c}_{\text{MT}}^{\text{c}}|, \mathbf{b}_{\text{MT}}^{\text{c}} \cdot \mathbf{c}_{\text{MT}}^{\text{c}})$ .  $\beta_{\text{MT}}^{\text{c}}$  and  $\gamma_{\text{MT}}^{\text{c}}$  are obtained following the same procedure. The lattice constants of the constrained magnetite are shown in Table 3. The MT<sup>c</sup> unit cell only slightly differs from the unit cell of unconstrained magnetite.