

Appendix

Application of the Δg 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 $\mathbf{A}_{i|}^*$, 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 , α , β , γ 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

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

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. $|\text{T}$ 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}_{MT} and \mathbf{S}_{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}_{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}_{MT} is a 3×3 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}_{PL} is a 3×3 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}_{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}_{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^c unit cell can be calculated from \mathbf{S}_{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}_{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^{c} unit cell only slightly differs from the unit cell of unconstrained magnetite.