VECTOR FORMULAS FOR IDENTIFICATION OF TWINNED LATTICES

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When the reciprocal lattice vectors for planes in a lattice are known, the reciprocal lattice vectors for the twins of these planes (by reflection, rotation or inversion) may be found with the aid of simple vector formulas which are derived in the following report. The vectors are often (as in the case of location by Laue diagrams) most easily designated in terms of spherical coordinates. The transformation equations necessary for such cases are given in the fourth section of this paper.

Twinning by Reflection Across a Lattice Plane

Consider the reflection in a plane $(h_0k_0l_0)$ of another plane (hkl). In Fig. 1, $\boldsymbol{B}^*$ represents the vector[1] from the origin to the reciprocal lattice point $(h_0k_0l_0)$, and i s,therefore, normal to the $(h_0k_0l_0)$ plane. Similarly, $\boldsymbol{A}^*$ is the reciprocal lattice vector for the plane (hkl). The reflection of $\boldsymbol{A}^*$ in the plane $(h_0k_0l_0)$ is the reciprocal lattice vector $\boldsymbol{X}^*$ of $(\underline{hkl})$, i.e. (hkl) in twinned position.

$$\boldsymbol{X}^* = \boldsymbol{A}^* + \boldsymbol{M}^*$$

$$\boldsymbol{M}^* = -2\frac{\boldsymbol{A}^*\cdot\boldsymbol{B}^*}{|\boldsymbol{B}^*|}\frac{\boldsymbol{B}^*}{|\boldsymbol{B}^*|} = -2\frac{\boldsymbol{A}^*\cdot\boldsymbol{B}^*}{B^{*2}}\boldsymbol{B}^*.$$

Therefore,

$$\boldsymbol{X}^* = \boldsymbol{A}^* - 2\frac{\boldsymbol{A}^*\cdot\boldsymbol{B}^*}{B^{*2}}\boldsymbol{B}^*.$$

In terms of the indices and the fundamental reciprocal lattice vectors $\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*$,

$$\boldsymbol{A}^* = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$$

$$\boldsymbol{B}^* = h_0\boldsymbol{a}^* + k_0\boldsymbol{b}^* + l_0\boldsymbol{c}^*.$$

$$\boldsymbol{A}^*\cdot\boldsymbol{B}^* = hh_0a_0^{*2} + kk_0b_0^{*2} + ll_0c_0^{*2} + (hk_0 + kh_0)\boldsymbol{a}^*\cdot\boldsymbol{b}^* + (hl_0 + lh_0)\boldsymbol{a}^*\cdot\boldsymbol{c}^* + (kl_0 + lk_0)\boldsymbol{b}^*\cdot\boldsymbol{c}^*.$$

$$B^{*2} = h_0^2a_0^{*2} + k_0^2b_0^{*2} + l_0^2c_0^{*2} + 2h_0k_0\boldsymbol{a}^*\cdot\boldsymbol{b}^* + 2h_0l_0\boldsymbol{a}^*\cdot\boldsymbol{c}^* + 2k_0l_0\boldsymbol{b}^*\cdot\boldsymbol{c}^*.$$

If the lattice is cubic, these expressions will simplify to

$$\boldsymbol{A}^*\cdot\boldsymbol{B}^* = (hh_0 + kk_0 + ll_0)a_0^{*2},$$

$$B^{*2} = (h_0^2 + k_0^2 + l_0^2)a_0^{*2}$$

and

$$\boldsymbol{X}^* = \boldsymbol{A}^* - 2\frac{hh_0 + kk_0 + ll_0}{h_0^2 + k_0^2 + l_0^2}\boldsymbol{B}^*.$$

[1] All starred vectors are vectors which are most conveniently expressed in terms of reciprocal lattice coordinates.

Since only the direction of $\boldsymbol{X}^*$ is of interest and not its actual length, the unit cell edge in the reciprocal lattice may be taken as unity ($a_0^*=1$), in which case the reciprocal lattice components of $\boldsymbol{A}^*$, $\boldsymbol{B}^*$ and $\boldsymbol{X}^*$ are the corresponding indices. (This holds only for the cubic case. The "indices" of $\boldsymbol{X}^*$ are not necessarily integers.)

Written in terms of components along the axes of any Cartesian coordinate system, the expression for $\boldsymbol{X}^*$ becomes

$$X_x^* = A_x^* - 2\,\frac{hh_0 + kk_0 + ll_0}{h_0^2 + k_0^2 + l_0^2}\,B_x^*$$

with similar expressions for X_y^* and X_z^*.

Twinning by Rotation Around a Lattice Row

Consider the rotation of a plane (hkl) around the row $[u_0v_0w_0]$ as axis of rotation. In Fig. 2, $\boldsymbol{B}$ represents the vector from the origin to the point $[\,[u_0v_0w_0]\,]$ and is therefore directed along the axis of rotation. $\boldsymbol{A}^*$ is the reciprocal lattice vector for the plane (hkl) and is therefore perpendicular to that plane. $\boldsymbol{X}^*$ is the reciprocal lattice vector for $(\underline{hkl})$ ((hkl) in twinned position) and is located by rotating $\boldsymbol{A}^*$ through an angle, α, around $\boldsymbol{B}$. From the figure

$$\boldsymbol{X}^* = \boldsymbol{N}^* + \boldsymbol{L}^*$$

$$\boldsymbol{N}^* = \frac{\boldsymbol{A}^*\cdot\boldsymbol{B}}{|\boldsymbol{B}|}\,\frac{\boldsymbol{B}}{|\boldsymbol{B}|} = \frac{\boldsymbol{A}^*\cdot\boldsymbol{B}}{B^2}\,\boldsymbol{B}$$

$$\boldsymbol{L}^* = \boldsymbol{S}^* + \boldsymbol{T}^*.$$

But $|\boldsymbol{L}^*| = |\boldsymbol{K}^*|$, so

$$\boldsymbol{S}^* = \boldsymbol{K}^* \cos\alpha$$

$$\boldsymbol{T}^* = |\boldsymbol{K}^*|\ \sin\alpha\,\frac{\boldsymbol{B}\times\boldsymbol{K}^*}{|\boldsymbol{B}\times\boldsymbol{K}^*|}\cdot$$

But

$$\boldsymbol{K}^* = \boldsymbol{A}^* - \boldsymbol{N}^* = \boldsymbol{A}^* - \frac{\boldsymbol{A}^*\cdot\boldsymbol{B}}{B^2}\,\boldsymbol{B}$$

and so

$$\boldsymbol{B}\times\boldsymbol{K}^* = \boldsymbol{B}\times\boldsymbol{A}^*$$

$$|\boldsymbol{B}\times\boldsymbol{K}^*| = |\boldsymbol{B}|\,|\boldsymbol{A}^*|\ \sin\beta.$$

Also

$$|\boldsymbol{K}^*| = |\boldsymbol{A}^*|\ \sin\beta.$$

Therefore,

$$\boldsymbol{S}^* = \boldsymbol{A}^*\cos\alpha - \frac{\boldsymbol{A}^*\cdot\boldsymbol{B}}{B^2}\boldsymbol{B}\cos\alpha$$

$$\boldsymbol{T}^* = \frac{\sin\alpha}{|\boldsymbol{B}|}\boldsymbol{B}\times\boldsymbol{A}^*$$

and

$$X^* = \frac{A^* \cdot B}{B^2} B(1 - \cos\alpha) + A^* \cos\alpha + \frac{\sin\alpha}{|B|} B \times A^*.$$

In terms of the indices h, k, l, the coordinates u_0, v_0, w_0, fundamental reciprocal lattice vectors $\boldsymbol{a}^*$, $\boldsymbol{b}^*$, $\boldsymbol{c}^*$ and fundamental crystal lattice vectors $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$,

$$\begin{aligned} A^* &= h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^* \\ B &= u_0\boldsymbol{a} + v_0\boldsymbol{b} + w_0\boldsymbol{c} \\ A^* \cdot B &= hu_0 + kv_0 + lw_0 \\ B^2 &= u_0^2a_0^2 + v_0^2b_0^2 + w_0^2c_0^2 + 2u_0v_0\boldsymbol{a}\cdot\boldsymbol{b} + 2u_0w_0\boldsymbol{a}\cdot\boldsymbol{c} + 2v_0w_0\boldsymbol{b}\cdot\boldsymbol{c}. \\ |B| &= +\sqrt{B^2}. \end{aligned}$$

If the lattice is cubic

$$B^2 = (u_0^2 + v_0^2 + w_0^2)a_0^2$$

and the expression for X^* may be written

$$X^* = \frac{hu_0 + kv_0 + lw_0}{u_0^2 + v_0^2 + w_0^2} \frac{1}{a_0^2} (1 - \cos\alpha)B + A^* \cos\alpha + \frac{\sin\alpha}{\sqrt{u_0^2 + v_0^2 + w_0^2}} \frac{1}{a_0} B \times A^*.$$

Since in the cubic system every row of the crystal lattice is coincident with its corresponding row in the reciprocal lattice, u_0, v_0, w_0 may be replaced by h_0, k_0, l_0, and B by the reciprocal lattice vector $a_0^2 B^*$. Then

$$X^* = \frac{hh_0 + kk_0 + ll_0}{h_0^2 + k_0^2 + l_0^2} (1 - \cos\alpha)B^* + A^* \cos\alpha + \frac{\sin\alpha}{\sqrt{h_0^2 + k_0^2 + l_0^2}} a_0 B^* \times A^*.$$

Again, only the direction of X^* is of interest so that a_0^* (and also a_0) may be made equal to unity which eliminates the factor a_0 in the last term of X^*, and

$$X^* = \frac{hh_0 + kk_0 + ll_0}{h_0^2 + k_0^2 + l_0^2} (1 - \cos\alpha)B^* + A^* \cos\alpha + \frac{\sin\alpha}{\sqrt{h_0^2 + k_0^2 + l_0^2}} B^* \times A^*.$$

in which the reciprocal lattice components of A^*, B^*, and X^* are the corresponding indices. (This also holds only for the cubic case. The "indices" of X^* are not necessarily integers.)

Written in terms of components along the axes of any Cartesian coordinate system, this expression for X^* becomes

$$X_x^* = \frac{hh_0 + kk_0 + ll_0}{h_0^2 + k_0^2 + l_0^2}(1 - \cos\alpha)B_x^* + A_x^* \cos\alpha + \frac{\sin\alpha}{\sqrt{h_0^2 + k_0^2 + l_0^2}}(B_y^*A_z^* - B_z^*A_y^*)$$

$$X_y^* = \frac{hh_0 + kk_0 + ll_0}{h_0^2 + k_0^2 + l_0^2}(1 - \cos\alpha)B_y^* + A_y^* \cos\alpha + \frac{\sin\alpha}{\sqrt{h_0^2 + k_0^2 + l_0^2}}(B_z^*A_x^* - B_x^*A_z^*)$$

$$X_z^* = \frac{hh_0 + kk_0 + ll_0}{h_0^2 + k_0^2 + l_0^2}(1 - \cos\alpha)B_z^* + A_z^* \cos\alpha + \frac{\sin\alpha}{\sqrt{h_0^2 + k_0^2 + l_0^2}}(B_x^*A_y^* - B_y^*A_x^*)$$

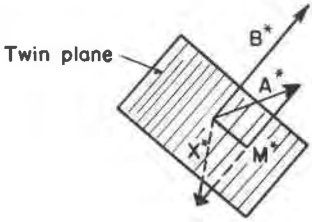

Figure 1

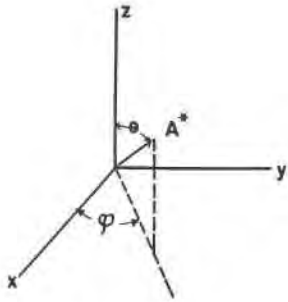

Figure 3

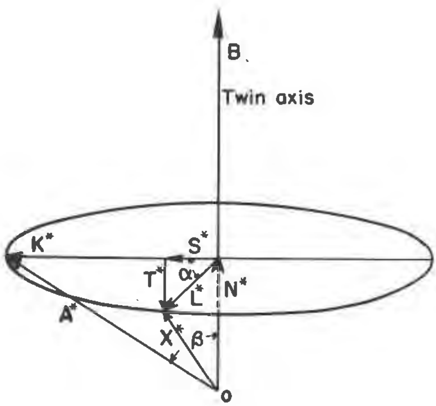

Figure 2

For the most common case of twinning by rotation, $\alpha = \pi$, and the formula for $\boldsymbol{X}^*$ reduces to

$$\boldsymbol{X}^* = 2\,\frac{\boldsymbol{A}^* \cdot \boldsymbol{B}}{B^2}\,\boldsymbol{B} - \boldsymbol{A}^*$$

or, for a cubic lattice,

$$\boldsymbol{X}^* = 2\,\frac{hh_0 + kk_0 + ll_0}{h_0^2 + k_0^2 + l_0^2}\,\boldsymbol{B}^* - \boldsymbol{A}^*$$

and the Cartesian components are of the form

$$X_x^* = 2\,\frac{hh_0 + kk_0 + ll_0}{h_0^2 + k_0^2 + l_0^2}\,B_x^* - A_x^*,$$

Twinning by Inversion Through a Lattice Point

Twinning by inversion through a point is merely a reversal of the sense of the reciprocal lattice vector. Therefore, if $\mathbf{A}^*$ is the reciprocal lattice vector for the plane (hkl) and $\mathbf{X}^*$ the reciprocal lattice vector for $(\underline{hkl})$,

$$\mathbf{X}^* = -\mathbf{A}^*$$

with Cartesian components of the form

$$X_x^* = -A_x^*.$$

Transformation Equations in Terms of Spherical Coordinates

Let the reciprocal lattice vector $\mathbf{A}^*$ for the point (hkl) be located by θ and ϕ in some arbitrary Cartesian system xyz, as shown in Fig. 3. (For a grain in a rolled sheet, x may be the rolling direction, y the cross-rolling direction and z the normal to the rolling plane.) The following relations may be set up:

$$\begin{aligned}
\mathbf{A}^* &= h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \\
|\mathbf{A}^*| &= \sqrt{h^2a_0^{*2} + k^2b_0^{*2} + l^2c_0^{*2} + 2hk\mathbf{a}^*\cdot\mathbf{b}^* + 2hl\mathbf{a}^*\cdot\mathbf{c}^* + 2kl\mathbf{b}^*\cdot\mathbf{c}^*} \\
&= \sqrt{A_x^{*2} + A_y^{*2} + A_z^{*2}}. \\
A_x^* &= |\mathbf{A}^*| \sin\theta\cos\phi \\
A_y^* &= |\mathbf{A}^*| \sin\theta\sin\phi \\
A_z^* &= |\mathbf{A}^*| \cos\theta.
\end{aligned}$$

Thus if hkl, and θ, ϕ are known, A_x^*, A_y^* and A_z^* may be found; also if A_x^*, A_y^* and A_z^* are known, θ and ϕ may be found.

For the cubic lattice the expression for $|\mathbf{A}^*|$ simplifies to

$$|\mathbf{A}^*| = \sqrt{h^2 + k^2 + l^2}\; a_0^*$$

and again if a_0^* is made unity

$$|\mathbf{A}^*| = \sqrt{h^2 + k^2 + l^2} = \sqrt{A_x^{*2} + A_y^{*2} + A_z^{*2}}.$$

Examples

I. Consider the case of twinning by reflection across the (112) plane of a cubic crystal. Let the orientation of the initial crystal be given by the full line gnomonic projection of the (hkl) net shown in Fig. 4.

The "indices," in terms of the initial lattice, of points on the lattice of the twin may be found by the formula

$$\mathbf{X}^* = \mathbf{A}^* - 2\,\frac{hh_0 + kk_0 + ll_0}{h_0^2 + k_0^2 + l_0^2}\,\mathbf{B}^*$$

where the components of $\mathbf{A}^*$ and $\mathbf{B}^*$ are the reciprocal lattice components, i.e. the indices. Then, since $(h_0k_0l_0)$ is (112),

$$\begin{aligned}
X_h^* &= h - \tfrac{1}{3}(h + k + 2l) \\
X_k^* &= k - \tfrac{1}{3}(h + k + 2l) \\
X_l^* &= l - \tfrac{2}{3}(h + k + 2l).
\end{aligned}$$

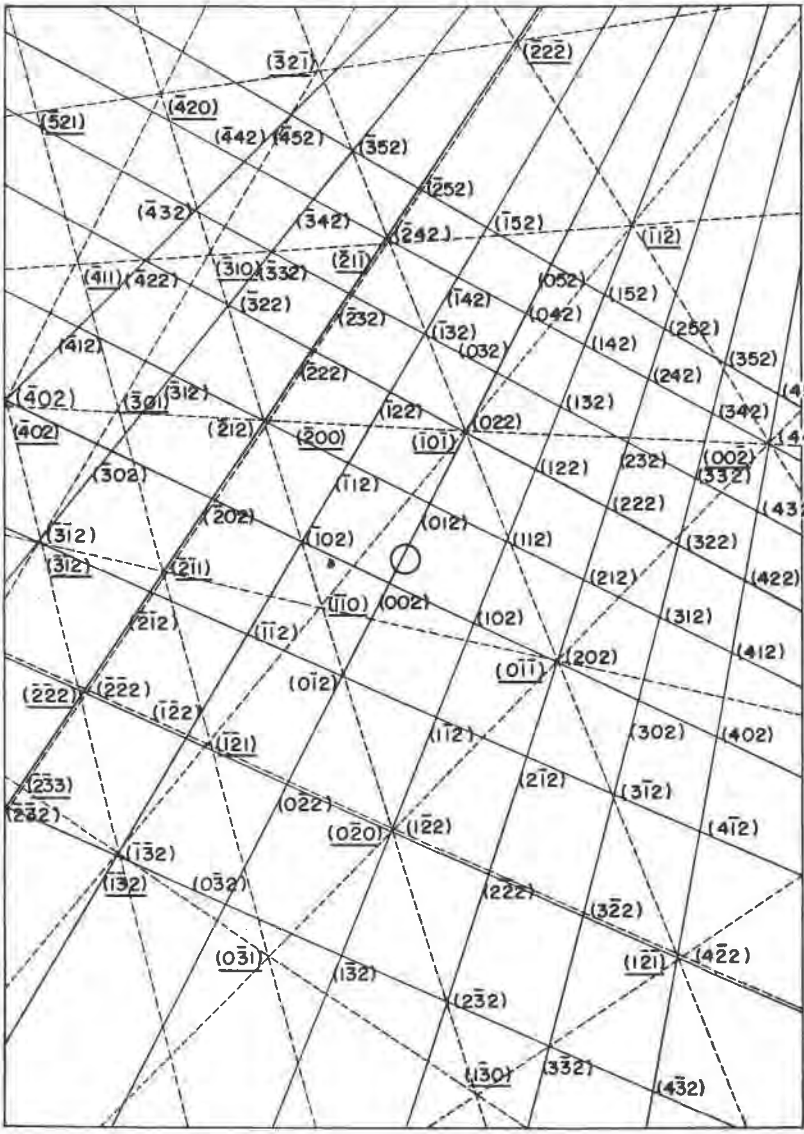

Figure 4

Using these relations, the twins (represented by $\boldsymbol{X}^*$) of various planes (represented by $\boldsymbol{A}^*$) may be found:

A*	X*
$(\bar{2}00)$	$\left(\frac{\bar{4}}{3}\ \frac{2}{3}\ \frac{4}{3}\right)$
$(0\bar{2}0)$	$\left(\frac{2}{3}\ \frac{\bar{4}}{3}\ \frac{4}{3}\right)$
$(00\bar{2})$	$\left(\frac{4}{3}\ \frac{4}{3}\ \frac{2}{3}\right)$
$(0\bar{1}\bar{1})$	$(1\ 0\ 1)$
$(\bar{2}\bar{2}2)$	$(\bar{2}\ \bar{2}\ 2)$

Therefore, on the projection

$(\bar{2}00)$ coincides with $(\bar{2}12)$
$(0\bar{2}0)$ coincides with $(1\bar{2}2)$
$(00\bar{2})$ coincides with (442)
$(0\bar{1}\bar{1})$ coincides with (202)
$(\bar{2}\bar{2}2)$ coincides with $(\bar{2}\bar{2}2)$

From these points the gnomonic projection of the twin can be constructed, as shown by the broken lines in Fig. 4, which make up the (hkl) net with $h+k+l=-2$.

II. Consider the case of twinning by reflection across the $(10\cdot 2)$ plane of a hexagonal crystal. In the hexagonal system

$$a_0^* = b_0^* = \frac{2}{\sqrt{3}a_0} \qquad (\text{or } a_0 = b_0)$$
$$c_0^* = 1/c_0$$
$$\boldsymbol{a}^* \cdot \boldsymbol{c}^* = 0$$
$$\boldsymbol{b}^* \cdot \boldsymbol{c}^* = 0$$
$$\boldsymbol{a}^* \cdot \boldsymbol{b}^* = 1/2a_0^{*2}.$$

From these relations and the general formulas in the first section of this paper

$$\boldsymbol{A}^* = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$$
$$\boldsymbol{B}^* = 1\boldsymbol{a}^* + 0\boldsymbol{b}^* + 2\boldsymbol{c}^*$$
$$\boldsymbol{A}^* \cdot \boldsymbol{B}^* = ha_0^{*2} + 2lc_0^{*2} + \tfrac{1}{2}ka_0^{*2}$$
$$= \frac{2}{3a_0^2}(2h + k) + \frac{1}{c_0^2}2l$$
$$B^{*2} = a_0^{*2} + 4c_0^{*2}$$
$$= 4\left(\frac{1}{3a_0^2} + \frac{1}{c_0^2}\right)$$
$$\boldsymbol{X}^* = \boldsymbol{A}^* - 2\frac{\boldsymbol{A}^* \cdot \boldsymbol{B}^*}{\boldsymbol{B}^{*2}}\boldsymbol{B}^*.$$

Putting in the values found above for $A^* \cdot B^*$ and B^{*2}

$$X^* = A^* - \frac{(2h+k)\left(\frac{c}{a}\right)^2 + 3l}{\left(\frac{c}{a}\right)^2 + 3} B^*.$$

The "indices," in terms of the initial lattice, of points on the lattice of the twin may be found from the formula just derived by substituting the components of A^* and B^* along the reciprocal lattice axes, i.e. the indices:

$$X_h^* = h - \frac{(2h+k)\left(\frac{c}{a}\right)^2 + 3l}{\left(\frac{c}{a}\right)^2 + 3}$$

$$X_k^* = k$$

$$X_l^* = l - 2\frac{(2h+k)\left(\frac{c}{a}\right)^2 + 3l}{\left(\frac{c}{a}\right)^2 + 3}.$$

III. The example just given may also be considered as a case of twinning by rotation of 180° about the row $(21\cdot\bar{1})$. In the hexagonal system

$$a_0 = b_0$$
$$\boldsymbol{a}\cdot\boldsymbol{c} = 0$$
$$\boldsymbol{b}\cdot\boldsymbol{c} = 0$$
$$\boldsymbol{a}\cdot\boldsymbol{b} = -\tfrac{1}{2}a_0^2.$$

From these relations and the general formulas in the second section of this paper

$$\boldsymbol{A}^* = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$$
$$\boldsymbol{B} = 2\boldsymbol{a} + 1\boldsymbol{b} + (-1)\boldsymbol{c}$$
$$\boldsymbol{A}^*\cdot\boldsymbol{B} = 2h + k - l$$
$$B^2 = 4a_0^2 + b_0^2 + c_0^2 - 2a_0^2$$
$$= 3a_0^2 + c_0^2$$
$$\boldsymbol{X}^* = 2\,\frac{\boldsymbol{A}^*\cdot\boldsymbol{B}}{B^2}\,\boldsymbol{B} - \boldsymbol{A}^*$$

or, putting in the values found for $\boldsymbol{A}^*\cdot\boldsymbol{B}$ and B^2

$$\boldsymbol{X}^* = 2\,\frac{2h+k-l}{3a_0^2 + c_0^2}\,\boldsymbol{B} - \boldsymbol{A}^*$$

The "indices," in terms of the initial lattice, of points on the lattice of the twin may be found from this formula by substituting the components of $\boldsymbol{A}^*$ and $\boldsymbol{B}$ along the reciprocal lattice axes. For $\boldsymbol{A}^*$ these will be the indices, but an expression must be found for $\boldsymbol{B}$ in terms of $\boldsymbol{a}^*$, $\boldsymbol{b}^*$, $\boldsymbol{c}^*$ instead of $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$. In the hexagonal system

$$\mathbf{a} = a_0^2\mathbf{a}^* - \tfrac{1}{2}a_0^2\mathbf{b}^*$$
$$\mathbf{b} = -\tfrac{1}{2}a_0^2\mathbf{a}^* + a_0^2\mathbf{b}^*$$
$$\mathbf{c} = c_0^2\mathbf{c}^*.$$

Therefore

$$\mathbf{B} = \tfrac{3}{2}a_0^2\mathbf{a}^* - c_0^2\mathbf{c}^*$$

and

$$X_h^* = 3\,\frac{2h+k-l}{3+\left(\frac{c}{a}\right)^2} - h$$
$$X_k^* = -k$$
$$X_l^* = -2\,\frac{(2h+k-l)\left(\frac{c}{a}\right)^2}{3+\left(\frac{c}{a}\right)^2} - l.$$

These "indices" are not identical with those of example I, but may be derived from them by symmetry operations of the lattice.

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