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The Determination of the Crystallographic Directions of Paths in Crystals

By J. W. Davisson

United States Naval Research Laboratory, Washington, D.C., U.S.A.

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Linear transformation equations are derived which relate the crystallographic directions of paths uniquely to their angles of inclination and azimuth in any crystal plate of known orientation.

Whenever linear arrays of any type that occur within or on the surface of crystals, such as electrical breakdown paths, crystal intergrowths, slip lines, etc., are to be correlated with the atomic structure of the crystal or with the crystal morphology, it is necessary to determine their crystallographic directions. More generally, problems in crystal geometry sometimes arise wherein it is desired to relate the crystallographic directions uniquely to certain reference angles, as, for example, the determination of all directions lying in a given plane that deviate by the variable angle φ from some reference direction in that plane. In this paper linear transformation equations are derived which yield the crystallographic directions of paths uniquely from their angles of inclination and azimuth in any crystal plate of known orientation, but the equations are directly applicable to many general problems of crystal geometry.

The orientation of a path observed in a crystal plate is usually specified by the two angles θ and φ which measure its inclination and its azimuth respectively. The inclination θ, Fig. 1, is the angle between the path direction $\mathbf{R}_2$ and the normal to the crystal plate $\mathbf{R}_0$, while the azimuth φ is the angle, measured counterclockwise, between the surface projection $\mathbf{S}_1$ of a known reference direction $\mathbf{R}_1$, and the surface projection $\mathbf{S}_2$ of the path. The angles θ and φ thus refer the orientation of the path to a secondary set of orthogonal axes consisting of the directions specified by the vectors $\mathbf{R}_0$, $\mathbf{S}_1$ and $\mathbf{R}_3$, where $\mathbf{R}_3 = \mathbf{R}_0 \times \mathbf{S}_1$. The crystallographic direction of a path $\mathbf{R}_2$ is specified by the parameters $[u_2v_2w_2]$ which are the components of the path upon the coordinate axes of the crystal in units of the basic lattice vectors **a**, **b** and **c**.

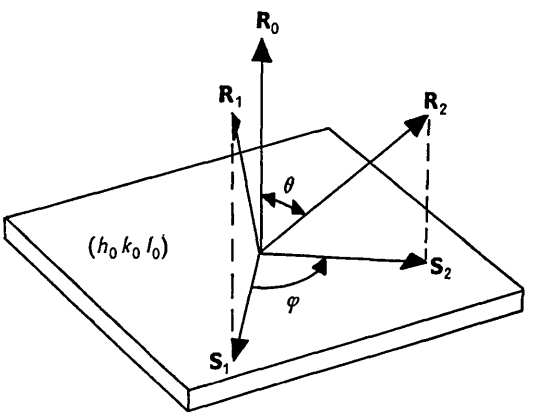

Fig. 1. The orientation of a path $\mathbf{R}_2$ observed in a $(h_0k_0l_0)$ crystal plate is specified by the two angles θ and φ, which measure its inclination and its azimuth respectively. The inclination θ is the angle between the path direction $\mathbf{R}_2$ and the normal to the crystal plate $\mathbf{R}_0$, while the azimuth φ is the angle, measured counterclockwise, between the surface projection $\mathbf{S}_1$ of a known reference direction $\mathbf{R}_1$, and the surface projection $\mathbf{S}_2$ of the path. The problem is to refer the orientation of the path to the crystallographic axes.

The problem is to determine the crystallographic direction $[u_2v_2w_2]$ of a path $\mathbf{R}_2$ when the following information is given: (1) morphological information: (*a*) the system of symmetry, (*b*) the interaxial angles, and (*c*) the axial ratios, of the crystal; (2) specific information: (*a*) the Miller indices $(h_0k_0l_0)$ of the surface plane of the crystal slice, which specify its orientation, (*b*) the parameters $[u_1v_1w_1]$ which specify the crystallographic direction of the reference vector $\mathbf{R}_1$, and (*c*) the angles θ and φ. The solution is as follows.

A unit vector specifying the path direction has components in the secondary reference system given by

$$\frac{\mathbf{R}_2}{|\mathbf{R}_2|} = \frac{\mathbf{R}_0}{|\mathbf{R}_0|}\cos\theta + \frac{\mathbf{S}_1}{|\mathbf{S}_1|}\sin\theta\cos\varphi + \frac{\mathbf{R}_3}{|\mathbf{R}_3|}\sin\theta\sin\varphi\,, \quad (1)$$

where

$$\mathbf{S}_1 = \mathbf{R}_1 - (\mathbf{R}_1\cdot\mathbf{R}_0)\mathbf{R}_0/|\mathbf{R}_0|^2 \quad (2)$$

and

$$\mathbf{R}_3 = \mathbf{R}_0\times\mathbf{S}_1 = \mathbf{R}_0\times\mathbf{R}_1\,.$$

Since any vector $\mathbf{R}_p$ has components upon the crystallographic axes given by†

† **abc** and **a*b*c*** are the basic lattice vectors in the direct and the reciprocal lattice respectively; the parameters $[u_pv_pw_p]$ are the components of the vector $\mathbf{R}_p$ in the direct lattice which specify its crystallographic direction; the parameters $(h_pk_pl_p)$ are the components of $\mathbf{R}_p$ in the reciprocal lattice and are the Miller indices of the planes in the direct lattice that are perpendicular to $\mathbf{R}_p$. For convenience these parameters and indices are expressed in the notation $\alpha_{pi}\mathbf{a}_i$ where the convention is used that a repeated dummy index occurring in a product implies the summation over the index, viz:

$$\mathbf{R}_p = \alpha_{pi}\mathbf{a}_i = \alpha_{p1}\mathbf{a}_1+\alpha_{p2}\mathbf{a}_2+\alpha_{p3}\mathbf{a}_3 = u_p\mathbf{a}+v_p\mathbf{b}+w_p\mathbf{c}\,.$$

The (projection) vectors $\mathbf{S}_p$ are distinguished from the (parent) vectors $\mathbf{R}_p$ by being primed. Thus

$$\mathbf{S}_p = \alpha'_{pi}\mathbf{a}_i = u'_p\mathbf{a}+v'_p\mathbf{b}+w'_p\mathbf{c}\,.$$

$$\left.\begin{aligned}\mathbf{R}_p &= u_p\mathbf{a}+v_p\mathbf{b}+w_p\mathbf{c} = \alpha_{pi}\mathbf{a}_i \\ &\qquad\text{direct lattice} \\ \mathbf{R}_p &= h_p\mathbf{a}^*+k_p\mathbf{b}^*+l_p\mathbf{c}^* = \alpha^*_{pi}\mathbf{a}^*_i \\ &\qquad\text{reciprocal lattice}\end{aligned}\right\} \quad (3)$$

equation (1) can be written

$$\frac{\alpha_{2i}\mathbf{a}_i}{|\mathbf{R}_2|} = \frac{\alpha_{0i}\mathbf{a}_i}{|\mathbf{R}_0|}\cos\theta + \frac{\alpha'_{1i}\mathbf{a}_i}{|\mathbf{S}_1|}\sin\theta\cos\varphi + \frac{\alpha_{3i}\mathbf{a}_i}{|\mathbf{R}_3|}\sin\theta\sin\varphi\,. \quad (4)$$

Since $\mathbf{R}_3 = \mathbf{R}_0\times\mathbf{S}_1 = \mathbf{R}_0\times\mathbf{R}_1$ and $\mathbf{R}_0 \perp \mathbf{S}_1$ we have

$$\alpha_{3i}\mathbf{a}_i = \frac{1}{\Delta}\,\mathrm{Det}\,(\mathbf{a}_i,\ \alpha^*_{0i},\ \alpha^*_{1i})\,, \quad (5)$$

where $\Delta = \mathbf{a}\cdot\mathbf{b}\times\mathbf{c}$ and

$$|\mathbf{R}_3| = |\mathbf{R}_0||\mathbf{S}_1| = 1/\{(\alpha_{0i}\alpha^*_{0i})(\alpha'_{1i}\alpha'^*_{1i})\}\,. \quad (6)$$

Substituting (5) and (6) into (4) and setting $|\mathbf{R}_2| = |\mathbf{R}_0|$, which is acceptable since we are interested only in relative values of the components of $\mathbf{R}_2$, we obtain the crystallographic direction of the path as

$$\alpha_{2i} = \alpha_{0i}\cos\theta + \frac{|\mathbf{R}_0|}{|\mathbf{S}_1|}\sin\theta\cos\varphi\alpha'_{1i} + \frac{\sin\theta\sin\varphi}{\Delta|\mathbf{S}_1|}(\alpha^*_{0j}\alpha^*_{1k}-\alpha^*_{0k}\alpha^*_{1j})\,, \quad (7)$$

where i, j and k maintain the cyclical order or 1, 2, and 3. Transposing to parameter form by means of equation (3), equation (7) becomes

$$\left.\begin{aligned}u_2 &= Au_0+Bu'_1+C(k_0l_1-k_1l_0)\,, \\ v_2 &= Av_0+Bv'_1+C(l_0h_1-l_1h_0)\,, \\ w_2 &= Aw_0+Bw'_1+C(h_0k_1-h_1k_0)\,,\end{aligned}\right\} \quad (8)$$

where

$$A = \cos\theta;\quad B = \sin\theta\cos\varphi\,\sqrt{\frac{h_0u_0+k_0v_0+l_0w_0}{h'_1u'_1+k'_1v'_1+l'_1w'_1}};$$

and

$$C = \sin\theta\sin\varphi/\Delta\sqrt{(h'_1u'_1+k'_1v'_1+l'_1w'_1)}\,.$$

The parameters that are primed in equation (8) relate to the projection vector $\mathbf{S}_1$ and not to the reference vector $\mathbf{R}_1$. However, equation (2) shows that the parameters of $\mathbf{S}_1$ and $\mathbf{R}_1$ are identical for the usual case where $\mathbf{R}_1$ lies in the surface of the crystal plate. When $\mathbf{R}_1$ does not lie in the surface the values of the parameters of $\mathbf{S}_1$ are given in terms of the parameters of $\mathbf{R}_1$ and $\mathbf{R}_0$ by the solution of equation (2), which yields

$$\left.\begin{aligned}u'_1 &= u_1-Du_0, & h'_1 &= h_1-Dh_0\,, \\ v'_1 &= v_1-Dv_0, & k'_1 &= k_1-Dk_0\,, \\ w'_1 &= w_1-Dw_0, & l'_1 &= l_1-Dl_0\,,\end{aligned}\right\} \quad (9)$$

where

$$D = \frac{h_0u_1+k_0v_1+l_0w_1}{h_0u_0+k_0v_0+l_0w_0}\,.$$

The transformation equations are applied to any crystal as follows: We are given the parameters $(h_0k_0l_0)$ and $[u_1v_1w_1]$ of the vectors $\mathbf{R}_0$ and $\mathbf{R}_1$ but must determine the related parameters $[u_0v_0w_0]$ of $\mathbf{R}_0$ and $(h_1k_1l_1)$ of $\mathbf{R}_1$ which also enter the transformation equations. These are obtained by solving the equations

$$\alpha^*_{pj} = \mathbf{a}_j\cdot\alpha_{pi}\mathbf{a}_i \quad (10)$$

in the appropriate symmetry system. The transformation equations are then solved by straightforward substitution of the parameters and the evaluation of Δ. For example, let us determine the crystallographic direction of a path observed in a (010) slice of a monoclinic crystal. We are given that the inclination of the path is θ degrees and that its azimuth, measured from the reference [100] direction is φ degrees. The parameters $(h_0k_0l_0)$ and $[u_1v_1w_1]$ are therefore given as (010) and [100]. To obtain the parameters $[u_0v_0w_0]$ and $(h_1k_1l_1)$ we must solve equations (10) in the monoclinic system. Since for monoclinic crystals $\mathbf{a}\cdot\mathbf{b} = \mathbf{b}\cdot\mathbf{c} = 0$ and $\mathbf{a}\cdot\mathbf{c} = ac\cos\beta$, where β is the monoclinic angle and $a = |\mathbf{a}|$ etc., equations (10) yield

$$\left.\begin{aligned}h_p &= u_pa^2+w_pac\cos\beta\,, \\ k_p &= v_pb^2\,, \\ l_p &= w_pc^2+u_pac\cos\beta\,.\end{aligned}\right\} \quad (11)$$

Thus the parameters that relate to the orientation of the crystal slice $(h_0k_0l_0)$; $[u_0v_0w_0]$ become (010); $[0\ 1/b^2\ 0]$ and those relating to the datum direction $(h_1k_1l_1)$; $[u_1v_1w_1]$ become $(a^2\ 0\ ac\cos\beta)$; [100]. Upon substituting these values into equations (9) we find that $D = 0$; thus the parameters of $\mathbf{S}_1$ and $\mathbf{R}_1$ are identical in this case. Hence the parameters of $\mathbf{R}_1$ and $\mathbf{R}_0$ can be applied directly to the transformation equations (8). Since the value of $\Delta = \mathbf{a}\cdot\mathbf{b}\times\mathbf{c}$ for monoclinic crystals is $abc\sin\beta$, equations (8) yield the crystallographic direction of the path $\mathbf{R}_2$ as

$$\left.\begin{aligned}u_2 &= (c/a)(\sin\beta\cot\varphi+\cos\beta)\,, \\ v_2 &= (c/b)(\sin\beta/\tan\theta\sin\varphi)\,, \\ w_2 &= -1\,.\end{aligned}\right\} \quad (12)$$

In a similar manner the crystallographic direction of any path in any crystal plate of known orientation can be obtained uniquely. More explicitely, equations (8) and (9) uniquely transform the specification of directions in crystals from two secondary reference directions $\mathbf{R}_0$ and $\mathbf{R}_1$ to the crystallographic axes. The transformation equations presented above do not entail any consideration of the angular relationships between the axes of the two coordinate systems. Thus they are not subject to the errors that can occur whenever the problem is solved by methods that demand a three-dimensional visualization of the coordinate systems and the calculation of direction cosines.

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