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An Analytical Method of Determining Cubic Crystal Orientation from {111} Surface Traces

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An alternative analytical treatment to that of Drazin & Otte is given for the determination of the orientation of a cubic crystal from three non-parallel {111} trace directions on a surface of the crystal. The treatment allows considerable simplification in the orientation determination if a fourth {111} trace direction is also known.

Introduction

The orientation of a cubic crystal may be determined from {111} traces on a surface of the crystal by graphic methods (Barrett, 1952; Mykura, 1958; Drazin & Otte, 1963), with the aid of charts such as that devised by Takeuchi, Honma & Ikeda (1959), or with the assistance of tables such as those produced by Drazin & Otte (1964). Drazin & Otte (1963) have also given a thorough analytical treatment for the determination of crystal orientation from three non-parallel {111} traces. The determination hinges around the solution of a quartic equation which was not however given in its explicit form because of its awkwardness.

The purpose of the present paper is to present an alternative treatment to that of Drazin & Otte for the analytical determination of the orientation of a cubic crystal from three non-parallel {111} traces on a surface of the crystal. In the treatment given here, the orientation determination also depends on the prior solution of a quartic equation which will in this case be developed to its complete form and its solutions expressed. The more valuable aspect of the treatment however is that, given a fourth distinct {111} trace direction, it will permit the quartic equation to be replaced by a linear equation which is of course readily solved and makes the overall orientation determination much simpler.

Preliminary considerations

In Fig. 1 plane *ABC* represents the crystal surface on which are observed {111} traces *AB*, *BC* and *CA* making angles α, β, and γ with one another as indicated. α and β are measurable quantities; γ is simply 180° less the sum of α and β. It is our intention to work out the crystal orientation from these quantities. Imagine, in Fig. 1, {111} planes *ABP*, *BCP*, and *CAP* which intersect at a point *P* outside the crystal and which make the traces *AB*, *BC*, and *CA*. *AP*, *BP*, and *CP* will be [110] directions and since they lie in pairs in {111} planes the angles ϱ_1, ϱ_2, and ϱ_3 between them as shown in Fig. 1 will be 60 or 120° but not 90°. ϱ_1, ϱ_2, and ϱ_3 are, however, restricted to all being 60°, or one being 60° and the other two 120°. This is explained in Appendix I. If we define the quantities j_1, j_2, and j_3 to be such that

$$j_i=+1 \text{ when } \varrho_i=60^\circ$$
$$j_i=-1 \text{ when } \varrho_i=120^\circ \text{ for } i=1, 2, \text{ or } 3$$

then it would follow from the possible values of ϱ_1, ϱ_2, and ϱ_3 in conjunction that

$$j_1j_2j_3=+1\,,\quad j_1j_2=j_3\,,\quad j_2j_3=j_1\,,\quad \text{and}\quad j_1j_3=j_2\,.$$

The [110] directions *AP*, *BP*, and *CP* in Fig. 1 may be taken to be represented by the unit vectors $\sqrt{\tfrac{1}{2}}(0,j_2,1)$ $\sqrt{\tfrac{1}{2}}(j_1,0,j_3)$ and $\sqrt{\tfrac{1}{2}}(1,1,0)$, as it can be readily checked that the angles between these vectors are ϱ_1, ϱ_2, and ϱ_3. The outward normals to the planes *ABP*, *BCP*, and *CAP* in Fig. 1 are then given respectively by the vectors

$$(0,j_2,1)\wedge(j_1,0,j_3)=j_1(1,1,-j_2)$$
$$(j_1,0,j_3)\wedge(1,1,0)=j_3(-1,1,j_2)$$

and

$$(1,1,0)\wedge(0,j_2,1)=(1,-1,j_2)\,.$$

Thus *ABP*, *BCP*, and *CAP* are the crystallographic planes $(11\bar{j}_2)$, $(\bar{1}1j_2)$ and $(1\bar{1}j_2)$ respectively.

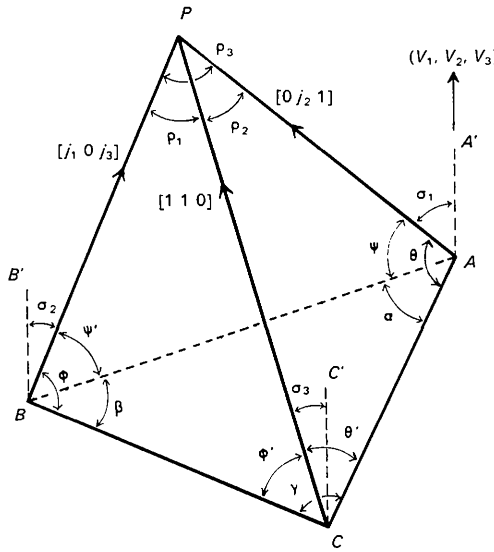

Fig. 1. The pyramidal figure *ABCP* formed by {111} planes *ABP*, *BCP*, and *CAP* through {111} traces *AB*, *BC*, and *CA* on crystal surface *ABC*. *AA'*, *BB'*, and *CC'* are outward normals to crystal surface *ABC*.

The crystallographic plane constituting the crystal surface with the {111} traces may be determined once the cosines of the angles σ_1, σ_2, and σ_3 made by AP, BP, and CP with the normal to the crystal surface (see Fig. 1) are found along with the actual values for j_1 and j_2. For if this crystallographic plane is taken to be given by the unit vector (v_1,v_2,v_3) directed towards P then

$$(v_1,v_2,v_3)\,.\,\sqrt{\tfrac{1}{2}}(0,j_2,1)=\sqrt{\tfrac{1}{2}}(j_2v_2+v_3)=\cos\sigma_1$$
$$(v_1,v_2,v_3)\,.\,\sqrt{\tfrac{1}{2}}(j_1,0,j_3)=\sqrt{\tfrac{1}{2}}(j_1v_1+j_3v_3)=\cos\sigma_2$$
$$(v_1,v_2,v_3)\,.\,\sqrt{\tfrac{1}{2}}(1,1,0)=\sqrt{\tfrac{1}{2}}(v_1+v_2)=\cos\sigma_3\,.$$

From these equations v_1, v_2, and v_3 emerge as:

$$v_1=\sqrt{\tfrac{1}{2}}(-j_2\cos\sigma_1+j_1\cos\sigma_2+\cos\sigma_3)$$
$$v_2=\sqrt{\tfrac{1}{2}}(j_2\cos\sigma_1-j_1\cos\sigma_2+\cos\sigma_3)$$
$$v_3=\sqrt{\tfrac{1}{2}}(\cos\sigma_1+j_1j_2\cos\sigma_2-j_2\cos\sigma_3)\,.$$

In their turn $\cos\sigma_1$, $\cos\sigma_2$, and $\cos\sigma_3$ are known in terms of the angles θ,θ', φ,φ', ψ, and ψ' shown in Fig. 1 as follows:

$$\cos\sigma_1=\sqrt{\left\{1-\frac{\cos^2\theta+\cos^2\psi-2\cos\theta\cos\psi\cos\alpha}{\sin^2\alpha}\right\}}$$
$$\cos\sigma_2=\sqrt{\left\{1-\frac{\cos^2\varphi+\cos^2\psi'-2\cos\varphi\cos\psi'\cos\beta}{\sin^2\beta}\right\}}$$
$$\cos\sigma_3=\sqrt{\left\{1-\frac{\cos^2\varphi'+\cos^2\theta'-2\cos\varphi'\cos\theta'\cos\gamma}{\sin^2\gamma}\right\}}.$$

The proof of these relations is given in Appendix II. Thus (v_1,v_2,v_3) may be determined if θ, θ', φ, φ', ψ, ψ', j_1, and j_2 can first be obtained from the inter-trace angles α, β, and γ.

Once (v_1,v_2,v_3) is found the crystallographic direction on the crystal parallel to the trace BC becomes known since it is given by the unit vector

$$\frac{(v_1,v_2,v_3)\wedge(-1,1,j_2)}{|(v_1,v_2,v_3)\wedge(-1,1,j_2)|}=\frac{(j_2v_2-v_3,\,-j_2v_1-v_3,\,v_1+v_2)}{\sqrt{\{2(1+v_1v_2+j_2v_1v_3-j_2v_2v_3)\}}}\,.$$

We will take for our frame of reference the right-handed rectangular coordinate system $OXYZ$ which has axis OX parallel to the trace BC and axis OZ parallel to the outward normal to the crystal surface ABC. Then the crystallographic direction parallel to OX is given by the unit vector

$$\frac{(j_2v_2-v_3,\,-j_2v_1-v_3,\,v_1+v_2)}{\sqrt{[2(1+v_1v_2+j_2v_1v_3-j_2v_2v_3)]}}\,.$$

That parallel to OZ is given by the unit vector

$$(v_1,v_2,v_3)\,,$$

and that parallel to OY is given by the unit vector

$$(v_1,v_2,v_3)\wedge\frac{(j_2v_2-v_3,\,-j_2v_1-v_3,\,v_1+v_2)}{\sqrt{[2(1+v_1v_2+j_2v_1v_3-j_2v_2v_3)]}}$$
$$=\frac{[1+v_1(j_2v_3+v_2-v_1),\,-1+v_2(j_2v_3+v_2-v_1),\,-j_2+v_3(j_2v_3+v_2-v_1)]}{\sqrt{[2(1+v_1v_2+j_2v_1v_3-j_2v_2v_3)]}}\,.$$

Consider now the matrix M whose rows are the above unit vectors:

$$\mathsf{M}=\begin{pmatrix}\dfrac{j_2v_2-v_3}{w_1} & \dfrac{-j_2v_1-v_3}{w_1} & \dfrac{v_1+v_2}{w_1}\\[2ex] \dfrac{1+v_1w_2}{w_1} & \dfrac{-1+v_2w_2}{w_1} & \dfrac{-j_2+v_3w_2}{w_1}\\[2ex] v_1 & v_2 & v_3\end{pmatrix}$$

where

$$w_1=\sqrt{[2(1+v_1v_2+j_2v_1v_3-j_2v_2v_3)]}$$
$$w_2=j_2v_3+v_2-v_1\,.$$

The product of M and any crystallographic direction of the crystal expressed as a unit vector will give the direction cosines of that crystallographic direction with respect to the $OXYZ$ coordinate system. M is therefore the so-called rotation matrix which will transform directions in the crystal system to directions in the chosen frame of reference $OXYZ$. The orientation of the crystal is therefore known with M which in turn can be found from θ, θ', φ, φ', ψ, ψ', j_1 and j_2 through v_1, v_2 and v_3.

Looking at Fig. 1 again we will see that the location selected for P (outside the crystal) is not the only possibility. Another possible geometry of {111} planes in accord with the disposition of the traces AB, BC, and CA is that where P is located in an analogous position on the other side of the crystal surface ABC, that is, within the crystal. This geometry would constitute an orientation which is a mirror image of that where P is outside the crystal, the crystal surface ABC acting as a mirror. Thus there are to be derived from the quantities θ, θ', φ, φ', ψ, ψ', j_1 and j_2, which define the correct shape of the pyramidal figure $ABCP$, not one but a pair of mirror image orientations, that is a pair of orientations with z coordinates of opposite signs, and these orientations will be given by the rotation matrices

$$\mathsf{M}_j=\begin{pmatrix}\dfrac{j_2v_2-v_3}{w_1} & \dfrac{-j_2v_1-v_3}{w_1} & \dfrac{v_1+v_2}{w_1}\\[2ex] \dfrac{1+v_1w_2}{w_1} & \dfrac{-1+v_2w_2}{w_1} & \dfrac{-j_2+v_3w_2}{w_1}\\[2ex] jv_1 & jv_2 & jv_3\end{pmatrix}$$

where $j=\pm1$.

Determination of θ, θ', φ, φ', ψ, ψ', j_1 and j_2

The preceding considerations show that if the quantities θ, θ', φ, φ', ψ, ψ', j_1 and j_2 can be worked out from the inter-trace angles α, β, and γ then the crystal orientation becomes determinable. The determination of θ, θ', φ, φ', ψ, ψ', j_1 and j_2 from α, β, and γ will now be discussed.

Referring to Fig. 1 and using standard trigonometric relationships the equations (1) to (4) below are readily obtained:

$$BC=\frac{\sqrt{3}CP}{2\sin\varphi} \quad (1)$$

$$AC=\frac{\sqrt{3}CP}{2\sin\theta} \quad (2)$$

$$BP=\frac{CP\sin\varphi'}{\sin\varphi}=\frac{CP\sin(\varrho_1+\varphi)}{\sin\varphi} \quad (3)$$

$$AP=\frac{CP\sin\theta'}{\sin\theta}=\frac{CP\sin(\varrho_2+\theta)}{\sin\theta}. \quad (4)$$

Equations (1) and (2) give

$$\frac{BC}{AC}=\frac{\sin\theta}{\sin\varphi}. \quad (5)$$

At the same time

$$\frac{BC}{AC}=\frac{\sin\alpha}{\sin\beta}. \quad (6)$$

Hence

$$\sin\varphi=\frac{\sin\theta}{k} \quad (7)$$

where

$$k=\frac{\sin\alpha}{\sin\beta}; \quad (8)$$

also,

$$\begin{aligned}AB^2&=AP^2+BP^2-2AP\,.\,BP\cos\varrho_3\\ &=CP^2\left\{\frac{\sin^2(\varrho_2+\theta)}{\sin^2\theta}+\frac{\sin^2(\varrho_1+\varphi)}{\sin^2\varphi}-\frac{j_3\sin(\varrho_2+\theta)\sin(\varrho_1+\varphi)}{\sin\theta\sin\varphi}\right\}\\ &=\frac{CP^2}{\sin^2\theta}\{\sin^2(\varrho_2+\theta)+k^2\sin^2(\varrho_1+\varphi)\\ &\quad -j_3k\sin(\varrho_2+\theta)\sin(\varrho_1+\varphi)\}. \quad (9)\end{aligned}$$

Equations (10) to (14) below are readily obtained by trigonometric expansion and by applying equation (7):

$$\sin(\varrho_2+\theta)=\tfrac{1}{2}(\sqrt{3}\cos\theta+j_2\sin\theta) \quad (10)$$

$$\sin^2(\varrho_2+\theta)=\tfrac{1}{4}(3-2\sin^2\theta+2\sqrt{3}j_2\sin\theta\cos\theta) \quad (11)$$

$$\sin(\varrho_1+\varphi)=\tfrac{1}{2}\left(\sqrt{3}\cos\varphi+\frac{j_1\sin\theta}{k}\right) \quad (12)$$

$$\sin^2(\varrho_1+\varphi)=\tfrac{1}{4}\left(3-\frac{2\sin^2\theta}{k^2}+\frac{2\sqrt{3}j_1\sin\theta\cos\varphi}{k}\right) \quad (13)$$

$$\sin(\varrho_2+\theta)\sin(\varrho_1+\varphi)=\tfrac{1}{4}\left\{3\cos\theta\cos\varphi+\sqrt{3}\sin\theta\left(\frac{j_1\cos\theta}{k}+j_2\cos\varphi\right)+\frac{j_1j_2\sin^2\theta}{k}\right\}. \quad (14)$$

Substituting into equation (9)

$$\begin{aligned}AB^2&=\frac{CP^2}{4\sin^2\theta}\{3-2\sin^2\theta+2\sqrt{3}j_2\sin\theta\cos\theta+3k^2\\ &\quad -2\sin^2\theta+2\sqrt{3}kj_1\sin\theta\cos\varphi-3j_3k\cos\theta\cos\varphi\\ &\quad -\sqrt{3}j_3\sin\theta(j_1\cos\theta+j_2k\cos\varphi)-j_1j_2j_3\sin^2\theta\}\\ &=\frac{CP^2}{4\sin^2\theta}\{3(1+k^2)-5\sin^2\theta\\ &\quad +\sqrt{3}\sin\theta(j_2\cos\theta+j_1k\cos\varphi)-3j_1j_2k\cos\theta\cos\varphi\}. \quad (15)\end{aligned}$$

From triangle ABC in Fig. 1 and using equation (2),

$$AB^2=\frac{\sin^2\alpha}{\sin^2\beta}\,.\,AC^2=\frac{3\sin^2\gamma\,.\,CP^2}{4\sin^2\beta\sin^2\theta}. \quad (16)$$

Substituting into equation (15),

$$\begin{aligned}\frac{3\sin^2\gamma}{\sin^2\beta}&=3(1+k^2)-5\sin^2\theta\\ &\quad +\sqrt{3}\sin\theta(j_2\cos\theta+j_1k\cos\varphi)-3j_1j_2k\cos\theta\cos\varphi,\end{aligned}$$

i.e.

$$\begin{aligned}&\sqrt{3}\sin\theta(j_2\cos\theta+j_1k\cos\varphi)\\ &\quad =5\sin^2\theta-r+3j_1j_2k\cos\theta\cos\varphi \quad (17)\end{aligned}$$

where

$$r=3\left(1+k^2-\frac{\sin^2\gamma}{\sin^2\beta}\right)=3\left(1+\frac{\sin^2\alpha-\sin^2\gamma}{\sin^2\beta}\right). \quad (18)$$

On squaring, equation (17) becomes

$$\begin{aligned}&3\sin^2\theta(\cos^2\theta+k^2\cos^2\varphi+2j_1j_2k\cos\theta\cos\varphi)\\ &\quad=(5\sin^2\theta-r)^2+9k^2\cos^2\theta\cos^2\varphi\\ &\quad+6j_1j_2k(5\sin^2\theta-r)\cos\theta\cos\varphi\end{aligned}$$

$$\begin{aligned}&3\sin^2\theta\{1-\sin^2\theta+k^2(1-\sin^2\varphi)+2j_1j_2k\cos\theta\cos\varphi\}\\ &\quad=25\sin^4\theta-10r\sin^2\theta+r^2\\ &\quad+9k^2(1-\sin^2\theta)(1-\sin^2\varphi)\\ &\quad+6j_1j_2k(5\sin^2\theta-r)\cos\theta\cos\varphi.\end{aligned}$$

Putting $\sin\varphi=\sin\theta/k$ and gathering like terms together,

$$\begin{aligned}&40\sin^4\theta-2(5r+6k^2+6)\sin^2\theta+r^2+9k^2\\ &\quad=6j_1j_2k(r-4\sin^2\theta)\cos\theta\cos\varphi. \quad (19)\end{aligned}$$

Squaring again,

$$\begin{aligned}&[40\sin^4\theta-2(5r+6k^2+6)\sin^2\theta+r^2+9k^2]^2\\ &\quad=36k^2(r^2-8r\sin^2\theta+16\sin^4\theta)\\ &\quad\times(1-\sin^2\theta)(1-\sin^2\varphi).\end{aligned}$$

Multiplying through by 4 and putting $\sin\varphi=\sin\theta/k$ and

$$y = 4\sin^2\theta \quad (20)$$

$$q = 3k^2 \quad (21)$$

we get

$$[5y^2-(5r+2q+6)y+2(r^2+3q)]^2 = 3(r^2-2ry+y^2)(4-y)(4q-3y)\,. \quad (22)$$

This, on expanding and gathering like terms together, gives

$$4y^4-2(4r+q+3)y^3+(9r^2+q^2-rq-3r+9q+9)y^2 - (5r^3-r^2q-3r^2-9rq+6q^2+18q)y+(r^2-3q)^2 = 0\,, \quad (23)$$

which for convenience of further discussion may be written as

$$y^4+4by^3+6cy^2+4dy+e=0 \quad (24)$$

where

$$b=-\tfrac{1}{8}(4r+q+3)$$
$$c=\tfrac{1}{24}(9r^2+q^2-rq-3r+9q+9)$$
$$d=-\tfrac{1}{16}(5r^3-r^2q-3r^2-9rq+6q^2+18q)$$
$$e=\tfrac{1}{4}(r^2-3q)^2.$$

The solution of the quartic equation (24) is discussed in various mathematical texts, for example Briggs & Bryan (1960). The solution may be written as

$$y=-(b+m)\pm\sqrt{(b+m)^2-c-n-2z\}} \quad (25)$$

where with

$$H=\tfrac{1}{12}(4bd-e-3c^2)$$
$$G=\tfrac{1}{4}(ce+2bcd-d^2-eb^2-c^3)$$

and

$$F=G^2+4H^3$$

$$z=\left(\frac{\sqrt{F}-G}{2}\right)^{1/3}-H/\left(\frac{\sqrt{F}-G}{2}\right)^{1/3} \text{ if } F>0$$
$$=2\sqrt{(-H)}\cos\{\tfrac{1}{3}\cos^{-1}[-G/2\sqrt{(-H^3)}]\} \text{ if } F\leqslant 0$$
$$m=\pm\sqrt{(b^2-c+z)}$$
$$n=(bc-d+2bz)/m\,.$$

There are therefore four possible values for $y=4\sin^2\theta$ which may be obtained from the angles α, β, and γ between three non-parallel {111} traces but values which are imaginary, negative, or greater than 4 are of course inadmissible.

For each acceptable solution for y there may be two possible values for θ and φ:

$$\theta=\sin^{-1}(\sqrt{y}/2) \text{ or } 180°-\sin^{-1}(\sqrt{y}/2) \quad (26)$$

$$\varphi=\sin^{-1}\left(\frac{\sqrt{y}\sin\beta}{2\sin\alpha}\right) \text{ or } 180°-\sin^{-1}\left(\frac{\sqrt{y}\sin\beta}{2\sin\alpha}\right) \quad (27)$$

[referring to equations (7) and (8)].
$\theta=180°-\sin^{-1}(\sqrt{y}/2)$ is inadmissible however if $\sin^{-1}(\sqrt{y}/2)<60°$ for then $\theta>120°$ so that $\varrho_2+\theta>180°$. Similarly $\varphi=180°-\sin^{-1}\left(\frac{\sqrt{y}\sin\beta}{2\sin\alpha}\right)$ is not permissible if $\sin^{-1}\left(\frac{\sqrt{y}\sin\beta}{2\sin\alpha}\right)<60°$.

Of the various combinations of the possible values of θ, φ, j_1 and j_2, however, only one is correct, the one which is consistent with the geometry of Fig. 1, that is, permits the equating of the right-hand sides of equations (9) and (16). The correct combination is therefore found on substituting the various possible values of θ, φ, j_1 and j_2 into equation (17) noting that if $\theta>60°$ j_2 cannot be -1 since ϱ_2 in this case cannot be 120° and similarly if $\varphi>60°$ j_1 can only be $+1$. That set of values of θ, φ, j_1 and j_2 which satisfies equation (17) will be the correct set. Knowing j_1 and j_2 and therefore $j_3=j_1j_2$, ϱ_1, ϱ_2, and ϱ_3 may be deduced. θ' and φ' may then be determined from

$$\theta'=180°-\varrho_2-\theta \quad (28)$$

$$\varphi'=180°-\varrho_1-\varphi\,. \quad (29)$$

ψ and ψ' may now be obtained from Fig. 1:

$$\frac{AP}{BP}=\frac{\sin\psi'}{\sin\psi}=\frac{\sin(\psi+\varrho_3)}{\sin\psi} = \frac{\sin\psi\cos\varrho_3+\cos\psi\sin\varrho_3}{\sin\psi} = \frac{j_1j_2}{2}+\frac{\sqrt{3}\cot\psi}{2}\,. \quad (30)$$

From equations (3) and (4)

$$\frac{AP}{BP}=\frac{\sin\theta'\sin\varphi}{\sin\theta\sin\varphi'}\,.$$

This and equation (30) gives

$$\cot\psi=\frac{1}{\sqrt{3}}\left(\frac{2\sin\theta'\sin\varphi}{\sin\theta\sin\varphi'}-j_1j_2\right)\,. \quad (31)$$

Whence the value of ψ between 0 and 180° and $\psi'=180°-\varrho_3-\psi$ may be evaluated.

All the quantities θ, θ', φ, φ', ψ, ψ', j_1 and j_2 are therefore determinable given the values of the inter-trace angles α, β, and γ. From these quantities, as discussed above, a pair of mirror-image crystal orientations may be worked out. Because $y=4\sin^2\theta$ may have as many as four possible values there are as many as four possible sets of values of θ, θ', φ, φ', ψ, ψ', j_1 and j_2. There are thus arising from the consideration of three non-parallel {111} traces as many as four possible pairs of mirror-image crystal orientations, as has been pointed out by Mykura (1958) and Drazin & Otte (1963).

Solution of crystal orientation with four available trace directions

Each possible pair of mirror-image crystal orientations determined from three non-parallel {111} traces will have a particular pair of mirror-image orientations of the fourth {111} plane which will produce a fourth distinct {111} trace in a particular direction on the crystal surface containing the traces. If then a fourth non-parallel {111} trace is also observed, the number of possible crystal orientations compatible with all four traces is narrowed down to one pair of mirror-image orientations (see also Mykura, 1958, and Takeuchi, Honma & Ikeda, 1959). This correct pair of orientations may be ascertained by the method given below.

It was shown above that if the directions *AP*, *BP*, and *CP* in Fig. 1 are taken to be $[0j_21]$, $[j_10j_3]$, and $[110]$ then the planes *ABP*, *BCP* and *CAP* are respectively $(11j_2)$, $(\bar{1}1j_2)$, and $(1\bar{1}j_2)$. $(\bar{1}1j_2)$ and $(1\bar{1}j_2)$ always account for the two octahedral planes $(\bar{1}11)$ and $(1\bar{1}1)$ whereas $(11j_2)$ accounts for one of the other two octahedral planes which will be either $(11\bar{1})$ or (111) depending on whether $j_2=1$ or -1. It follows that the fourth {111} plane producing a fourth distinct trace direction is representable by $(11j_2)$.

The crystallographic direction of the fourth trace if seen on the surface of the crystal will therefore, on the above basis, be given by the unit vector

$$\frac{(v_1,v_2,v_3)\wedge(1,1,j_2)}{|(v_1,v_2,v_3)\wedge(1,1,j_2)|} = \frac{(j_2v_2-v_3,\ -j_2v_1+v_3,\ v_1-v_2)}{\sqrt{\{2(1-v_1v_2-j_2v_1v_3-j_2v_2v_3)\}}}\ . \tag{32}$$

That for the trace *BC* in Fig. 1 has been shown to be

$$=\frac{(j_2v_2-v_3,\ -j_2v_1-v_3,\ v_1+v_2)}{\sqrt{\{2(1+v_1v_2+j_2v_1v_3-j_2v_2v_3)\}}} \tag{33}$$

and that for the trace *CA* is

$$\frac{(v_1,v_2,v_3)\wedge(1,-1,j_2)}{|(v_1,v_2,v_3)\wedge(1,-1,j_2)|} = \frac{(j_2v_2+v_3,\ -j_2v_1+v_3,\ -v_1-v_2)}{\sqrt{\{2(1+v_1v_2-j_2v_1v_3+j_2v_2v_3)\}}}\ . \tag{34}$$

The smaller angle η which the fourth trace makes with *BC* is obtainable from the dot product of the vectors in equations (32) and (33) and works out to be

$$\eta=\cos^{-1}\left[\frac{|v_1^2-j_2v_2v_3|}{\sqrt{[1-2j_2v_2v_3(1+v_1^2)-v_1^2v_2^2+v_2^2v_3^2-v_3^2v_1^2]}}\right]. \tag{35}$$

Similarly the smaller angle ζ made by the fourth trace with *CA* is given by the dot product of the vectors in equations (32) and (34) and is

$$\zeta=\cos^{-1}\left[\frac{|v_2^2-j_2v_1v_3|}{\sqrt{[1-2j_2v_1v_3(1+v_2^2)-v_1^2v_2^2-v_2^2v_3^2+v_3^2v_1^2]}}\right]. \tag{36}$$

By employing equations (35) and (36) the direction of the fourth {111} trace relative to traces *BC* and *CA* may be computed for each possible pair of mirror-image crystal orientations derived from three {111} traces *AB*, *BC*, and *CA* and the only pair of crystal orientations that can exist for four traces ascertained by comparing the computed directions of the fourth trace with its actually observed direction. The correct pair of orientations will be that for which the computed and observed directions of the fourth trace tally.

Alternatively, the fourth trace may be substituted for say *BC* to give a new set of inter-trace angles α, β^* and γ^* whereupon another set of possible crystal orientations may be obtained as already discussed. One pair of crystal orientations of this second set will be identical (or nearly identical in the practical situation) with a pair in the first set arising from the inter-trace angles α, β, and γ. This is then the correct pair of crystal orientations applicable to the four observed traces.

Indeed, the angle α being maintained in the second set of inter-trace angles, '$y=4\sin^2\theta$' should be the same for both sets of inter-trace angles, as will be clear from Fig. 2, which shows the two alternative arrangements of the pyramidal figure AB^*CP^* formed by the {111}

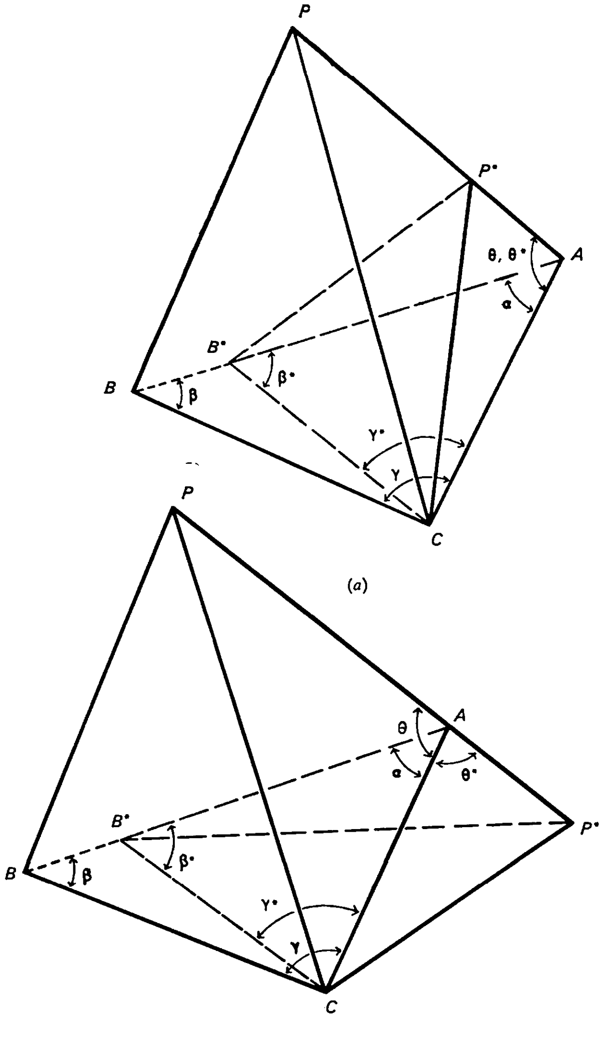

Fig. 2. The two imaginable arrangements of the pyramidal figure AB^*CP^* formed by (111) planes through {111} traces *AB*, B^*C, and *CA* relative to the pyramidal figure *ABCP* formed by (111) planes through {111} traces *AB*, *BC*, and *CA*.

planes through traces AB, CA, and the fourth trace B^*C. From these figures the angle θ^* between AP^* and AC is seen to be either equal to θ of the pyramidal figure $ABCP$ for the set of traces AB, BC, and CA or equal to $180°-\theta$. Hence $\sin\theta^*=\sin\theta$ so that '$y=4\sin^2\theta$' should be the same for both sets of three traces for the right pair of crystal orientations. It would therefore be enough, and more convenient in practice, to obtain the values for '$y=4\sin^2\theta$' for both sets of three traces and select the value of y common to both as the one from which the correct pair of crystal orientations may be determined. This manner of consideration gives rise to another approach for obtaining the correct value of $y=4\sin^2\theta$ when four trace directions are available without having to solve a quartic equation and then attempting to pick the correct solution from as many as four possibilities. This approach is next discussed.

If x is taken to be the common value of y contained in the set of values of $y=4\sin^2\theta$ and that of $y=4\sin^2\theta^*$ arising respectively from the traces AB, BC, and CA and the traces AB^*, B^*C, and CA in Fig. 2 then on referring to equation (23)

$$x^4+a_3x^3+a_2x^2+a_1x+a_0=0 \quad (37)$$

$$x^4+b_3x^3+b_2x^2+b_1x+b_0=0 \quad (38)$$

where

$$a_3=-\tfrac{1}{2}(4r+q+3)$$
$$a_2=\tfrac{1}{4}(9r^2+q^2-rq-3r+9q+9)$$
$$a_1=-\tfrac{1}{4}(5r^3-r^2q-3r^2-9rq+6q^2+18q)$$
$$a_0=\tfrac{1}{4}(r^2-3q)^2$$
$$r=3\left(1+\frac{\sin^2\alpha-\sin^2\gamma}{\sin^2\beta}\right)$$
$$q=\frac{3\sin^2\alpha}{\sin^2\beta}.$$

b_3, b_2, b_1, and b_0 are identical with a_3, a_2, a_1, and a_0 respectively except that for them

$$r=3\left(1+\frac{\sin^2\alpha-\sin^2\gamma^*}{\sin^2\beta^*}\right) \text{ and } q=\frac{3\sin^2\alpha}{\sin^2\beta^*}.$$

Equation (38) minus equation (37) gives

$$(b_3-a_3)x^3+(b_2-a_2)x^2+(b_1-a_1)x+(b_0-a_0)=0 \quad (39)$$

$[b_0\times\text{equation (37)}]-[a_0\times\text{equation (38)}]$ gives

$$(b_0-a_0)x^4+(b_0a_3-a_0b_3)x^3+(b_0a_2-a_0b_2)x^2 +(b_0a_1-a_0b_1)x=0\,. \quad (40)$$

Putting aside the case where $x=0$ (this corresponds to a crystal orientation where the crystal surface with the traces is a $\{111\}$ plane and would be obvious from all traces being 60° to one another and in any case would not apply to the present consideration since only three trace directions at most would be present) equation (40) is reducible to

$$(b_0-a_0)x^3+(b_0a_3-a_0b_3)x^2+(b_0a_2-a_0b_2)x +(b_0a_1-a_0b_1)=0\,. \quad (41)$$

Thus equations (37) and (38) of the fourth degree in x have been replaced by equations (39) and (41) of the third degree in x. In a similar fashion equations (39) and (41) may be reduced to two equations of the second degree in x:

$$c_2x^2+c_1x+c_0=0 \quad (42)$$

$$d_2x^2+d_1x+d_0=0 \quad (43)$$

where

$$c_2=(b_0-a_0)(b_2-a_2)-(b_3-a_3)(b_0a_3-a_0b_3)$$
$$c_1=(b_0-a_0)(b_1-a_1)-(b_3-a_3)(b_0a_2-a_0b_2)$$
$$c_0=(b_0-a_0)^2-(b_3-a_3)(b_0a_1-a_0b_1)$$
$$d_2=-c_0$$
$$d_1=(b_0a_1-a_0b_1)(b_2-a_2)-(b_0-a_0)(b_0a_3-a_0b_3)$$
$$d_0=(b_0a_1-a_0b_1)(b_1-a_1)-(b_0-a_0)(b_0a_2-a_0b_2)\,.$$

Equations (42) and (43) will by the same process yield two equations in x of the first degree:

$$(c_2d_1-d_2c_1)x+c_2d_0-d_2c_0=0 \quad (44)$$

$$(c_0d_2-d_0c_2)x+c_0d_1-d_0c_1=0\,. \quad (45)$$

Whence

$$x=\frac{c_0d_2-d_0c_2}{c_2d_1-d_2c_1}\,; \quad (46)$$

or equivalently

$$x=\frac{c_1d_0-d_1c_0}{c_0d_2-d_0c_2}\,. \quad (47)$$

If the $\{111\}$ trace directions are precisely known then equations (46) and (47) will be perfectly identical. If not, either because of inherent errors or errors of measurement, the two values of x will not be the same. The difference will clearly be small if small errors are involved and generally large if large errors are involved. $x=4\sin^2\theta$ computed from either equations (46) or (47) may now be used to determine in the manner already discussed the correct set of values of θ, θ', φ, φ', ψ, ψ', j_1 and j_2 and the only pair of crystal orientations possible for four trace directions with an uncertainty (if there is a error in the measured trace dispositions) the qualitative extent of which is usually indicated by the disparity in the values of x given by equations (46) and (47).

Concluding remarks

A series of equations and expressions have therefore been established relating the orientation of a crystal to the angles between $\{111\}$ traces on a surface of the crystal enabling the possibilities of crystal orientation to be determined analytically once the angles between the traces have been measured. The determination is based on the prior evaluation of the inclinations of the $\langle 110\rangle$ edges of the pyramidal figure formed by the $\{111\}$ planes producing the traces. These inclinations are obtained through the solution of a quartic equation (23) or from relations essentially expressing the inclinations explicitly in terms of the angles between the traces [equations (46) and (47)]. When one or more of four non-parallel traces are not well defined it is obvious that the method of solving through the quartic equation is the better since the angles between the best three traces may then be used to establish the quartic equation and the most doubtful last trace employed only for indicating which of up to four possible solutions is the correct one; in this way errors are minimized. Otherwise the method of solving through equations (46) or (47) would be the neater and more expeditious. Where only three trace directions are found the method of solving through the quartic equation has to be adopted, yielding as many as four possible pairs of mirror-image crystal orientations. It is clear that the methods discussed readily lend themselves to being programmed on a computer.

APPENDIX I

In the situation as given in Fig. 1 and described in the text it is clear that angles ϱ_1, ϱ_2, and ϱ_3 cannot all be 120° at the same time; otherwise *AP*, *BP*, and *CP* would be coplanar. Thus at least one of these angles is 60°. Without loss of generality take ϱ_1 to be 60° and *CP* and *BP* to be the directions [110] and [101] respectively. *AP* is a ⟨110⟩ type direction making 60 or 120° with *CP* and *BP*, *i.e.* with [110] and [101] and is therefore representable by the direction $[0j_2j_3]$ where $j_2,j_3 = \pm 1$. The following relations should hold:

$$\sqrt{\tfrac{1}{2}}(0,j_2,j_3)\,.\,\sqrt{\tfrac{1}{2}}(1,1,0)=\cos\varrho_2\,,$$

i.e.

$$j_2=2\cos\varrho_2\,;$$

and

$$\sqrt{\tfrac{1}{2}}(0,j_2,j_3)\,.\,\sqrt{\tfrac{1}{2}}(1,0,1)=\cos\varrho_3\,,$$

i.e.

$$j_3=2\cos\varrho_3\,.$$

AP, *BP*, and *CP* are coplanar if

$$(0,j_2,j_3)\,.\,(1,0,1)\wedge(1,1,0)=0$$

which gives

$$j_2+j_3=0$$

i.e.

$$\cos\varrho_2+\cos\varrho_3=0\,.$$

Thus *AP*, *BP*, and *CP* are coplanar if one of ϱ_2 and ϱ_3 is 60° and the other 120°. Hence in Fig. 1 ϱ_1, ϱ_2, ϱ_3 are all 60° or one of them 60° and the other two 120°.

APPENDIX II

In Fig. 3 the direction *OP* makes angles of θ, ψ, and σ with *OW*, *OX* and *OZ* respectively where *OXYZ* constitute a set of rectangular coordinate axes and *OW* lies in the *OXY* plane at an angle α to *OX*. The unit vector for the direction *OW* is $(\cos\alpha, \sin\alpha, 0)$. Let that for *OP* be $(\cos\psi, p, \cos\sigma)$. Then

$$(\cos\psi,\ p,\ \cos\sigma)\,.\,(\cos\alpha,\ \sin\alpha,\ 0)=\cos\theta$$

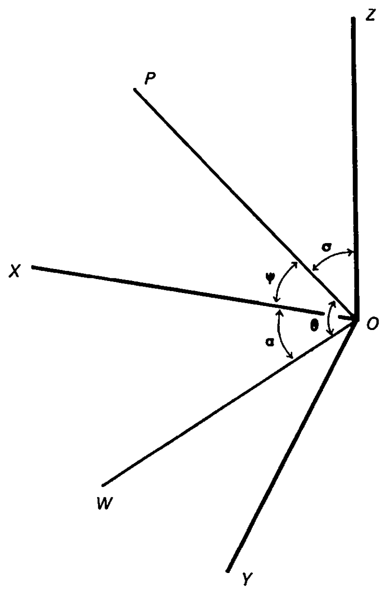

Fig. 3. The direction *OP* relative to rectangular coordinate axes *OX*, *OY*, and *OZ* and direction *OW* in the *OXY* plane.

i.e.

$$\cos\psi\cos\alpha+p\sin\alpha=\cos\theta$$

giving

$$p^2=\frac{\cos^2\theta+\cos^2\psi\cos^2\alpha-2\cos\theta\cos\psi\cos\alpha}{\sin^2\alpha}\,.$$

But because $(\cos\psi, p, \cos\sigma)$ is a unit vector we also have

$$p^2=1-\cos^2\psi-\cos^2\sigma\,.$$

Hence

$$\frac{\cos^2\theta+\cos^2\psi\cos^2\alpha-2\cos\theta\cos\psi\cos\alpha}{\sin^2\alpha}=1-\cos^2\psi-\cos^2\sigma\,.$$

This gives

$$\cos^2\sigma=1-\frac{\cos^2\theta+\cos^2\psi-2\cos\theta\cos\psi\cos\alpha}{\sin^2\alpha}\,.$$

If *OP* is limited to lying on the same side of *OXY* as *OZ* then σ is always acute and is related to θ, ψ, and α by

$$\cos\sigma=\sqrt{\left[1-\frac{\cos^2\theta+\cos^2\psi-2\cos\theta\cos\psi\cos\alpha}{\sin^2\alpha}\right]}\,.$$

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