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The Determination of the Crystallographic Orientation of the Surface of a Hexagonal Crystal from Data on Traces on the Surface all of $\{10\bar{1}0\}$ or all of $\{11\bar{2}0\}$

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An analytical method is developed for evaluating the orientation of a hexagonal crystal surface from traces on the surface which are all of $\{10\bar{1}0\}$ or all of $\{11\bar{2}0\}$. A chart showing this surface orientation for various inter-trace angles is produced.

Introduction

Features on a crystal surface such as slip lines, twin boundaries and edges of plate-shaped precipitates and etch pits, which are referred to as traces and which mark out the intersections of particular crystallographic planes with the crystal surface may be conveniently employed to indicate the orientation of the crystal. Barrett & Massalski (1966) describe a graphic method of determining crystal orientation from surface traces which consists of rotating relevant poles on a standard stereographic projection with the aid of a Wulff net, such that they all move into position on diameters of an underlying basic circle which are perpendicular to the observed trace directions, the new position of the poles giving the crystal orientation. The method is in principle applicable to any type of crystallographic plane which the traces delineate but in practice becomes impossibly cumbersome with other than low-multiplicity planes. Even when dealing with planes of simple form the method is quite laborious and inaccurate as it involves a trial-and-error process of pinpointing the correct rotation of poles. Thus for the more frequently encountered types of traces particular procedures have been devised to simplify and also to improve the accuracy of the orientation evaluation.

Table 1. *Methods devised for evaluating crystal orientation*

Trace type	Method
{100}	Analytical and Table (Tucker & Murphy, 1953); Chart (Takeuchi, Honma & Ikeda, 1959).
{111}	Analytical, Semi-Graphic, and Iterative Computer Process (Drazin & Otte, 1963); Table (Drazin & Otte, 1964); Chart (Takeuchi, Honma & Ikeda, 1959).
Mixture of {100} and {111}	Chart (Takeuchi, Honma & Ikeda, 1959).
{110}	Chart (Tsubaki & Nishiyama, 1960).

These special procedures consist of either solving for the orientation analytically, producing tables or charts from which the crystal surface orientation may be read off for relevant values of the angles between the trace directions, a semi-graphic treatment where the loci of relevant poles consistent with the observed traces are computed and mapped out on a stereographic plot, or employing a computer to work out the orientation by an iterative process of successive approximations beginning with some initial approximate solution. They are all for the case of cubic crystals and for delineated planes of simple form. A summary is given in Table 1.

The concern of this paper is the analytical evaluation of crystal orientation from observations of surface traces either all of $\{10\bar{1}0\}$ or all of $\{11\bar{2}0\}$ in hexagonal crystals. $\{10\bar{1}0\}$ traces are known to be produced by slip in some hexagonal crystals, *e.g.* titanium and zirconium (Honeycombe, 1968). $\{11\bar{2}0\}$ traces, to our knowledge, have not yet been reported but are nevertheless considered here as the treatment for this case is essentially identical with that for $\{10\bar{1}0\}$ traces.

We shall however be content to show only how the orientation of the crystal surface carrying the traces (*i.e.* the crystallographic plane constituting this surface) may be determined. This is because the crystal-surface orientation constitutes the basic information for determining the complete crystal orientation. Given the former the procedure for determining the latter is straightforward and need not be discussed in this paper. A chart of crystal-surface orientation against inter-trace angles will also be produced.

Preliminary considerations

In Fig. 1 plane ABC represents the surface of a hexagonal crystal on which are found traces with directions AB, BC, and CA making angles α, β, and γ with one another. It is assumed that neither α, β, nor γ is 0 or 180°. The traces are all of $\{10\bar{1}0\}$ or all of $\{11\bar{2}0\}$. In either case AED is a basal plane of the crystal and EB

and DC are [0001] directions. AED is therefore an equilateral triangle whose sides may, for simplicity, be taken to be of unit length.

Let

$$EB=s\,,\quad DC=r\,,$$

$$f=\sin^2\beta/\sin^2\gamma\,,\quad g=\sin^2\alpha/\sin^2\gamma\,, \tag{1}$$

$$h=f-g+1=(\sin^2\beta+\sin^2\gamma-\sin^2\alpha)/\sin^2\gamma\,, \tag{2}$$

$$x=1+s^2\,. \tag{3}$$

We have

$$\frac{CA^2}{AB^2}=\frac{1+r^2}{x}=f,\quad 1+r^2=fx\,. \tag{4}$$

Also

$$\frac{BC^2}{AB^2}=\frac{1+(s-r)^2}{x}=g\,,\quad x-2rs+r^2=gx\,. \tag{5}$$

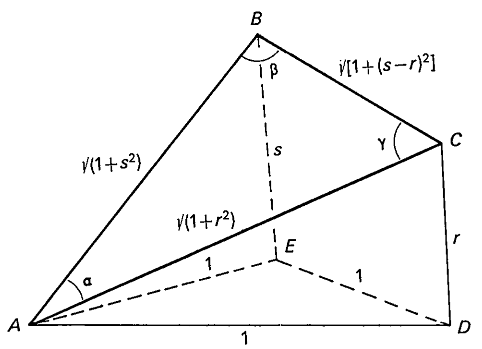

Fig. 1. ABC represents the crystal surface with observed traces AB, BC, and CA. AED is a basal plane of the crystal and EB and DC are perpendicular to AED.

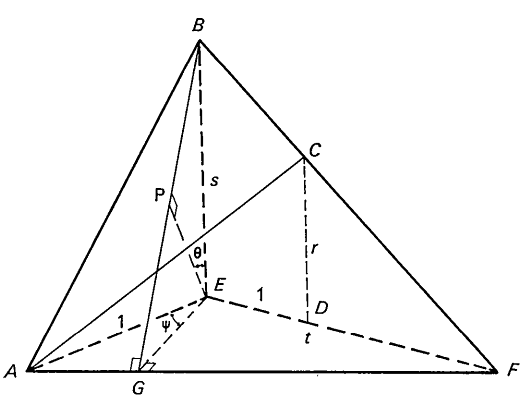

Fig. 2. Same as Fig. 1 but with plane ABC extended to meet the basal plane AED along AF and to intersect ED extended in F. EP is a normal to the crystal surface ABF.

Equation (4) minus equation (5) gives

$$1-x+2rs=(f-g)x\,,$$

$$2rs=hx-1\,. \tag{6}$$

Squaring equation (6) and substituting in the values of s^2 and r^2 given by equations (3) and (4) gives

$$4(fx-1)\,(x-1)=h^2x^2-2hx+1\,,$$

$$(4f-h^2)x^2-2(2f+2-h)x+3=0\,. \tag{7}$$

On reference to Blakey (1965) h given in equation (2) may also be written as

$$h=2\sin\beta\cos\alpha/\sin\gamma\,.$$

With this value of h and with f given by equation (1)

$$4f-h^2=4\sin^2\alpha\sin^2\beta/\sin^2\gamma\,. \tag{8}$$

Also, with the help of equations (1) and (2)

$$2f+2-h=f+g+1$$

$$=(\sin^2\alpha+\sin^2\beta+\sin^2\gamma)/\sin^2\gamma\,. \tag{9}$$

Substituting equations (8) and (9) into (7)

$$4\sin^2\alpha\sin^2\beta\,.\,x^2$$

$$-2(\sin^2\alpha+\sin^2\beta+\sin^2\gamma)x+3\sin^2\gamma=0\,.$$

Solving this quadratic equation for x we obtain

$$x=\sin^2\gamma[S_1+j\sqrt{(S_1^2-3S_2)}]/S_2 \tag{10}$$

where

$$S_1=\sin^2\alpha+\sin^2\beta+\sin^2\gamma\,, \tag{10a}$$

$$S_2=4\sin^2\alpha\sin^2\beta\sin^2\gamma\,, \tag{10b}$$

$$j=\pm 1\,.$$

Evaluation of the crystal-surface orientation

It will be convenient to define the orientation of the crystal surface as (θ,φ) where θ is the angle between [0001] and the normal to the crystal surface and φ the angle (made in a clockwise direction about [0001]) between $[2\bar{1}\bar{1}0]$ and the projection of the normal onto the basal plane (0001).

Fig. 2 is Fig. 1 redrawn to show the extension of the plane ABC to meet ED in F and the basal plane along AF. BEG is a plane perpendicular to AF and meeting AF in G so that the normal from E to plane ABC lies in BEG being say EP in Fig. 2 where P is a point in ABF. By definition $B\hat{E}P=\theta$. Let $A\hat{E}G=\psi$. If we are dealing with $\{10\bar{1}0\}$ traces we may take EA to be $[2\bar{1}\bar{1}0]$ so that $\varphi=\psi$. On the other hand if we are dealing with $\{11\bar{2}0\}$ traces we could take EA to be $[10\bar{1}0]$ so that $\varphi=\psi+30°$. The crystal-surface orientation (θ,φ) can thus be found if we can put θ and ψ in terms of the experimentally measurable quantities α, β, and γ.

Letting $EF=t$ and noting that $A\hat{E}F=60°$, we have from triangle AEF

$$\sin E\hat{F}A=\sin A\hat{E}F \times \frac{1}{\sqrt{(t^2+1-2t\cos A\hat{E}F)}}=\frac{\sqrt{3}}{2\sqrt{(t^2-t+1)}}\,.$$

Considering now triangle EFG,

$$GE=t\,.\,\sin E\hat{F}A=\frac{\sqrt{3}t}{2\sqrt{(t^2-t+1)}}\,.$$

Now

$$t=s\,.\,\tan E\hat{B}F=s/(s-r)\,.$$

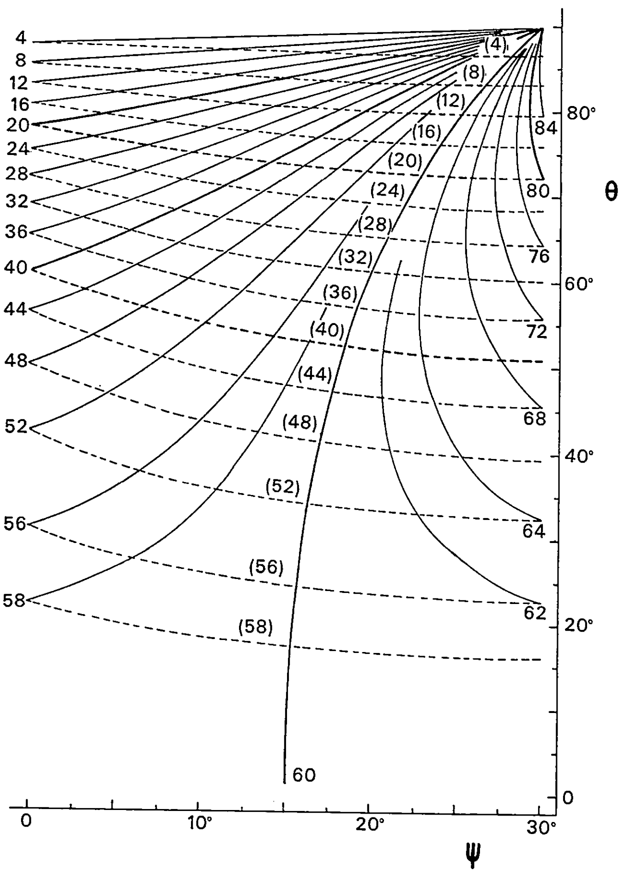

Fig. 3. Surface orientation–Inter-trace angle chart. The dashed curves are lines of constant α the value of which is given in degrees by the numbers in brackets. The solid curves are lines of constant β the value of which is given in degrees by the unbracketed numbers. The α and β curves are in intervals of 4° except for values between 56 and 64 °where they are in 2° intervals. To obtain the crystal-surface orientation (θ,φ) for inter-trace angles of $\alpha=\alpha_0$ and $\beta=\beta_0$ the point on the chart lying on both the $\alpha=\alpha_0$ and $\beta=\beta_0$ lines is first located and the θ and ψ values for this point (say θ_0 and ψ_0 respectively) read off from the vertical and horizontal scales. The crystal-surface orientation is then (θ_0,ψ_0) for $\{10\bar{1}0\}$ traces and $(\theta_0,\psi_0+30°)$ for $\{11\bar{2}0\}$ traces.

Hence

$$\cos\psi=GE=\frac{|s-r|}{s-r}\cdot\frac{\sqrt{3}\,.\,s}{2\sqrt{(s^2-sr+r^2)}}\,. \qquad (11)$$

Also,

$$\tan\theta=\tan B\hat{G}E=s/GE=\frac{|s-r|}{s-r}\cdot\frac{2\sqrt{(s^2-sr+r^2)}}{\sqrt{3}}\,. \qquad (12)$$

The factor $|s-r|/(s-r)$ may be dropped from equations (11) and (12). This is clear when $\beta\le\gamma$ for then $\sqrt{(1+s^2)}/\sqrt{(1+r^2)}=AB/CA\ge 1$ so that $s\ge r$ and $|s-r|/(s-r)=+1$. If $\beta>\gamma$ then, reasoning similarly, $|s-r|/(s-r)=-1$. In this case omitting the factor $|s-r|/(s-r)$ would give rise to θ and ψ values which are supplements of the actual values so that the crystallographic form of the surface orientation remains unchanged.

Substituting into equation (12) the values of s^2, r^2, and sr as given by equations (3), (4), and (6) and dropping $|s-r|/(s-r)$ we get

$$\tan\theta=(2/\sqrt{3})\sqrt{[x-1-\tfrac{1}{2}(hx-1)+fx-1]}=\sqrt{\{(\tfrac{2}{3})\,[(2f+2-h)x-3]\}}\,. \qquad (13)$$

On putting in the values of $2f+2-h$ and x as given by equations (9) and (10)

$$\tan\theta=\sqrt{\left\{\tfrac{2}{3}\left[\frac{S_1[S_1+j\sqrt{(S_1^2-3S_2)}]}{S_2}-3\right]\right\}}=\sqrt{\{(2/3S_2)\,[S_1^2-3S_2+jS_1\sqrt{(S_1^2-3S_2)}]\}}\,. \qquad (14)$$

In the same way from equation (11)

$$\cos\psi=\sqrt{\left\{\tfrac{3}{2}\cdot\frac{\sin^2\gamma[S_1+j\sqrt{(S_1^2-3S_2)}]-S_2}{S_1^2-3S_2+jS_1\sqrt{(S_1^2-3S_2)}}\right\}}\,. \qquad (15)$$

$\tan\theta$ may be rewritten as

$$\tan\theta=\sqrt{\left\{\frac{2\sqrt{(S_1^2-3S_2)}}{3S_2}\,[\sqrt{(S_1^2-3S_2)}+jS_1]\right\}}\,.$$

When $j=-1$ $\sqrt{(S_1^2-3S_2)}+jS_1$ is negative so that $\tan\theta$ becomes imaginary. $j=-1$ is therefore unacceptable and j may therefore be dropped from equations (14) and (15).

We therefore have now θ and ψ expressible in terms of α, β, and γ so that the crystal-surface orientation may be determined analytically from data on the angles between surface traces.

Discussion

θ and hence also ψ will not exist only for those values of α, β, and γ for which $S_1^2-3S_2$ is negative. Such values of the inter-trace angles will therefore not be observed in practice. Now

$$S_1^2-3S_2=[S_1+\sqrt{(3S_2)}]\,[S_1-\sqrt{(3S_2)}]$$

$$=\tfrac{1}{2}\sqrt{S_2}[S_1+\sqrt{(3S_2)}]\left(\frac{\sin\alpha}{\sin\beta\sin\gamma}+\frac{\sin\beta}{\sin\alpha\sin\gamma}+\frac{\sin\gamma}{\sin\alpha\sin\beta}-2\sqrt{3}\right).$$

But

$$\frac{\sin\alpha}{\sin\beta\sin\gamma}=\frac{\sin\beta\cos\gamma+\cos\beta\sin\gamma}{\sin\beta\sin\gamma}=\cot\beta+\cot\gamma\,.$$

Similarly

$$\frac{\sin\beta}{\sin\alpha\sin\gamma}=\cot\alpha+\cot\gamma\,,$$

$$\frac{\sin\gamma}{\sin\alpha\sin\beta}=\cot\alpha+\cot\beta\,.$$

Therefore

$$S_1^2-3S_2=\sqrt{S_2}[S_1+\sqrt{(3S_2)}]\times(\cot\alpha+\cot\beta+\cot\gamma-\sqrt{3})\,.$$

It is known that $\cot\alpha+\cot\beta+\cot\gamma$ is never less than $\sqrt{3}$ (Hall & Knight, 1952). $S_1^2-3S_2$ is therefore never negative whatever the values of α, β, and γ. Hence all values of the inter-trace angles between 0 and 180° can be found in practice.

Further, if two inter-trace angles say α and β are equal then θ and ψ may be very simply expressed:

$$\theta=\tan^{-1}\sqrt{(\tfrac{1}{3}\tan^2\beta-1)}\,,\quad \psi=90^\circ \text{ if } \beta>60^\circ\,,$$

$$\theta=0^\circ,\ \psi=\text{indeterminate value if } \beta=60^\circ\,,$$

$$\theta=\tan^{-1}\sqrt{(3\cot^2\beta-1)}\,,\quad \psi=0^\circ \text{ if } \beta<60^\circ\,.$$

This is shown in the Appendix.

Using equations (14) and (15) θ and ψ may be computed for various values of α and β (note that $\gamma=180^\circ-\alpha-\beta$) and a chart then drawn showing θ and ψ for the whole range of inter-trace angles. This has been done and the chart is produced in Fig. 3 where the α and β curves are in 4° intervals except for values between 56 and 64° where 2° intervals are employed. Since we can always select our inter-trace angles such that $\alpha\le\beta\le\gamma$ the complete range of inter-trace angles will be covered by taking α from 0 to 60° and β from α to $90^\circ-\alpha/2$ as has been done in Fig. 3.

The chart in Fig. 3 serves not only as a quick means of obtaining an approximate orientation from surface traces but also to indicate the possible magnitude of the uncertainty in the orientation for inaccurate trace-angle data. It will be seen from the chart that errors in α or β will cause more than a fourfold error in the surface orientation for orientations within about 30° of $\theta=0^\circ$ (the basal orientation) and for orientations close to $\theta=90^\circ$, $\psi=0^\circ$ (which would be $\{11\bar{2}0\}$ for $\{10\bar{1}0\}$ traces and $\{10\bar{1}0\}$ for $\{11\bar{2}0\}$ traces). Near $\theta=90^\circ$, $\psi=30^\circ$ ($\{10\bar{1}0\}$ and $\{11\bar{2}0\}$ orientations for $\{10\bar{1}0\}$ and $\{11\bar{2}0\}$ traces respectively) errors in β have small effect on the accuracy of the evaluated surface orientation. The error in the case of the other evaluated surface orientations are more or less of the same order as the error in the trace angles.

As mentioned earlier, the determination of the complete crystal orientation after finding the surface orientation is a straightforward process. It should however be pointed out that although a unique crystal-surface orientation is found to arise from a given set of trace-angle values the complete crystal orientation is not unique. This may be understood on referring to Fig. 1 where it will be seen that if we relocate D and E on the other side of the plane ABC in positions which are reflexions of their initial positions in the plane ABC the geometry of the resulting figure $ABCDE$ remains unchanged so that our solutions for θ and ψ do not differentiate between this and the original configuration. It follows that for an obtained surface orientation one will derive two possible complete crystal orientations which are reflexions of each other as seen in the crystal-surface plane. This is the general consequence of a single-surface trace analysis.

Conclusion

If on a surface of a hexagonal crystal a complete set of traces all of $\{10\bar{1}0\}$ or all of $\{11\bar{2}0\}$ are observed and if α and β are the angles one of the trace directions make with the other two as in Fig. 1 then the orientation (θ,φ) of this crystal surface {where θ is the angle between the normal to the surface and [0001] and φ the angle between $[2\bar{1}\bar{1}0]$ and the projection of the normal onto (0001)} may be computed from

$$\theta=\tan^{-1}\sqrt{\left\{\frac{2[S_1^2-S_3+S_1\sqrt{(S_1^2-S_3)}]}{S_3}\right\}}\,,$$

$$\varphi=\xi+\cos^{-1}\sqrt{\left\{\frac{3\sin^2(\alpha+\beta)\,[S_1+\sqrt{(S_1^2-S_3)}]-S_3}{2[S_1^2-S_3+S_1\sqrt{(S_1^2-S_3)}]}\right\}}$$

where

$$S_1=\sin^2\alpha+\sin^2\beta+\sin^2(\alpha+\beta)\,,$$

$$S_3=12\sin^2\alpha\sin^2\beta\sin^2(\alpha+\beta)\,,$$

$$\xi=\ 0^\circ \text{ if traces delineate } \{10\bar{1}0\}\,,$$

$$\xi=30^\circ \text{ if traces delineate } \{11\bar{2}0\}\,.$$

APPENDIX

When two inter-trace angles are equal the expressions for $\tan\theta$ and $\cos\psi$ take on very simple forms. Let $\alpha=\beta$. Then from equations (10a) and (10b)

$$S_1=2\sin^2\beta(1+2\cos^2\beta)\,,$$

$$S_2=16\sin^6\beta\cos^2\beta\,,$$

$$S_1^2-3S_2=4\sin^4\beta(1+4\cos^2\beta+4\cos^4\beta-12\sin^2\beta\cos^2\beta)$$

$$=4\sin^4\beta(1-8\cos^2\beta+16\cos^4\beta)\,,$$

$$\surd(S_1^2-3S_2)=2\sin^2\beta|1-4\cos^2\beta|\,.$$

Hence equation (10) with $j=1$ gives

$$x=\frac{1+2\cos^2\beta+|1-4\cos^2\beta|}{2\sin^2\beta}$$

$$=1 \text{ if } \beta\geq 60°$$

$$=3\cot^2\beta \text{ if } \beta\leq 60°\,.$$

We thus have from equation (13)

$$\tan\theta=\surd\left\{\tfrac{2}{3}\left[\frac{S_1x}{\sin^2\gamma}-3\right]\right\}$$

$$=\surd\left\{\tfrac{2}{3}\left[\left(\frac{1+2\cos^2\beta}{2\cos^2\beta}\right)x-3\right]\right\}$$

$$=\surd(\tfrac{1}{3}\tan^2\beta-1) \text{ if } \beta\geq 60°$$

$$=\surd(3\cot^2\beta-1) \text{ if } \beta\leq 60°\,.$$

Also

$$\cos\psi=s/\tan\theta=\surd(x-1)/\tan\theta$$

$$=0 \text{ if } \beta>60°$$

$$=1 \text{ if } \beta<60°$$

$$=\text{indeterminate value if } \beta=60°\,.$$

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