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A Method of Orienting Hexagonal Crystal Surfaces from Surface Trace Observations

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Manual methods employing the Wulff net and stereographic projections are used to determine the crystallographic orientation of hexagonal crystal or grain surfaces from observations of traces of crystallographic planes. Equations are developed which enable such determinations to be carried out easily and precisely with computers for many kinds and combinations of traces observed. A method of this nature should reduce considerably the labour in the single-surface trace analysis of hexagonal crystals or grains.

Introduction

A well-known method of orienting the surface of a crystal or grain is to utilize traces of known crystallographic planes on the surface such as slip lines, twin boundaries, edges of plate-shaped precipitates and etch pits, *etc.* Given traces on the surface of a crystal or grain one may proceed to orient the surface by operating a stereographic plot containing the trace information, a Wulff net, and a standard stereographic plot in the manner described by Barrett (1952) or that described by Reed-Hill & Baldwin (1965). These manual procedures require some amount of labour and practised skill and can be tedious if many orientation determinations are to be made.

More appealing is the analytical or mathematical approach such as that of Tucker & Murphy (1953) for $\{100\}$ traces on cubic crystals or those of Drazin & Otte (1963) and Fong (1973) developed for $\{111\}$ traces also for cubic crystals. The attractiveness of this type of approach is that in it are derived equations and mathematical relationships which, although complex for some cases, are readily programmed on a computer so that thereafter the business of obtaining crystal or grain surface orientations from trace observations becomes simply a matter of feeding in trace data to the computer. Precise results are obtained and a multitude of orientation determinations may be performed effortlessly in a short space of time.

In this paper we will develop an analytical or mathematical method of deriving the orientatioo of a hexagonal crystal or grain surface given data on three trace directions on the surface all of $\{h0\bar{h}k\}$ or all of $\{hh\bar{2}hk\}$ and usually two other trace directions of any type. It is felt that such a method would be useful as it provides for a labour-saving computerized approach to the problem of orienting the surface of hexagonal crystals, particularly metals, using traces such as twins, slip lines, and basal planes revealed by polarized light.

Preliminary considerations

In Fig. 1 the regular hexagon $A_1A_2A_3A_4A_5A_6$, with centre O, represents the basal plane of a hexagonal crystal. The six planes of $\{h0\bar{h}k\}$ or of $\{hh\bar{2}hk\}$ are shown as A_1A_2K, A_2A_3K, A_3A_4K, A_4A_5K, A_5A_6K, and A_6A_1K. We will work in terms of a rectangular coordinate system $OXYZ$ with axis OX parallel to OA_3, axis OY perpendicular to OA_3, and axis OZ in the direction of OK. Thus, in the case of $\{h0\bar{h}k\}$ planes OX, OY, and OZ will be in the directions of $[\bar{1}2\bar{1}0]$, $[\bar{1}010]$, and $[0001]$; in the case of $\{hh\bar{2}hk\}$ planes they will be parallel to $[01\bar{1}0]$, $[\bar{2}110]$, and $[0001]$ respectively. We will also refer to crystallographic directions in terms of vectors referred to the $OXYZ$ system; in the case of planes vectors expressing the directions of their normals will be used. So the six planes A_1A_2K, A_2A_3K, A_3A_4K, A_4A_5K, A_5A_6K, and A_6A_1K are given by $0,2/\sqrt{3},g)$,

$(1,1/\sqrt{3},g)$, $(1,-1/\sqrt{3},g)$, $(0,2/\sqrt{3},-g)$, $(1,1/\sqrt{3},-g)$, and $(1,-1/\sqrt{3},-g)$ respectively in the $OXYZ$ system where

$$\left.\begin{array}{ll} g=(k/h)/(c/a) & \text{for } \{h0\bar{h}k\} \text{ traces} \\ g=(k/\sqrt{3}h)/(c/a) & \text{for } \{hh\bar{2}\bar{h}k\} \text{ traces}, \end{array}\right\} \quad (1)$$

c/a being the crystal axial ratio.

Our approach will be to consider firstly only three $\{h0\bar{h}k\}$ or three $\{hh\bar{2}\bar{h}k\}$ trace directions (preferably the most distinct and precise looking ones), obtain the limited number of surface orientations which could give rise to these three trace directions, and then use the other observed trace directions to identify the correct surface orientation.

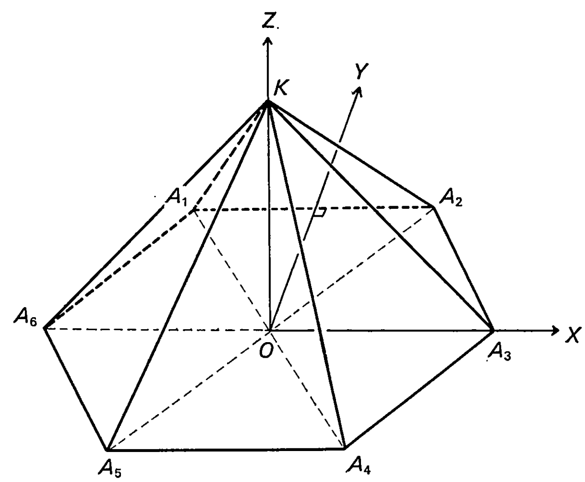

Fig. 1. Planes A_1A_2K, A_2A_3K, A_3A_4K, A_4A_5K, A_5A_6K, and A_6A_1K of $\{h0\bar{h}k\}$ or of $\{hh\bar{2}\bar{h}k\}$ whose normals referred to the rectangular coordinate system $OXYZ$ shown are given by the vectors $(0,2/\sqrt{3},g)$, $(1,1/\sqrt{3},g)$, $(1,-1/\sqrt{3},g)$, $(0,2/\sqrt{3},-g)$, $(1,1/\sqrt{3},-g)$, and $(1,-1/\sqrt{3},-g)$ respectively where $A_1A_2A_3A_4A_5A_6$ is a basal plane.

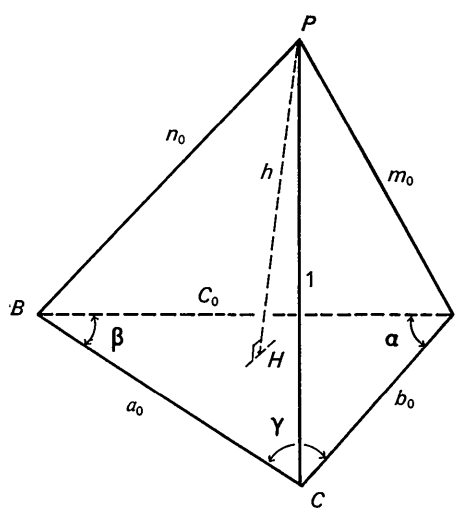

Fig. 2. Three traces AB, BC, and CA on the crystal surface ABC produced by planes ABP, BCP, and CAP of $\{h0\bar{h}k\}$ or of $\{hh\bar{2}\bar{h}k\}$. HP is a perpendicular to the plane ABC.

In Fig. 2 AB, BC, and CA represent the three initially considered trace directions observed on the crystal surface ABC. ABP, BCP, and CAP are the crystal planes producing these traces. There are three distinct geometrical arrangements of planes ABP, BCP, and CAP which we shall hereafter refer to as

Arrangement I: ABP, BCP, and CAP are oriented as the planes A_1A_2K, A_2A_3K, and A_4A_5K in Fig. 1.

Arrangement II: ABP, BCP, and CAP are oriented as A_1A_2K, A_2A_3K, and A_3A_4K.

Arrangement III: ABP, BCP, and CAP are oriented as A_1A_2K, A_3A_4K, and A_5A_6K.

For each of these Arrangements I, II, and III we shall choose the outward normals to the planes CAP, ABP, and BCP to be the crystal directions shown in Table 1 where $j_1,j_3=\pm 1$ provide for the fact that within each arrangement the pyramid $ABCP$ may have as many as four distinct configurations corresponding to the various ways the crystal surface ABC may intersect the planes ABP, BCP, and CAP. The crystallographic directions of $\overrightarrow{AP}$, $\overrightarrow{BP}$, and $\overrightarrow{CP}$ and the cosines (c_1, c_2, and c_3 respectively) of the angles $\widehat{BPC}$, $\widehat{APC}$, and $\widehat{APB}$ have been worked out and are also displayed in Table 1 where $j_2=j_1j_3$.

In Fig. 2 HP is perpendicular to the plane ABC with H situated in ABC. We shall take the lengths of HP, BC, CA, AB, AP, BP, and CP to be h, a_0, b_0, c_0, m_0, n_0, and 1 respectively. We shall also let the angles the three trace directions make with each other be α, β, and γ as shown in Fig. 2. We now obtain quite readily:

$$a_0^2=p_1n^2-n+1 \quad (2)$$

$$b_0^2=p_2m^2-m+1 \quad (3)$$

$$c_0^2=p_2m^2-qmn+p_1n^2 \quad (4)$$

where

$$p_1=1/4c_1^2,\ p_2=1/4c_2^2,\ q=c_3/2c_1c_2,\ m=2c_2m_0,\ n=2c_1n_0\,. \quad (5)$$

From equations (2) and (3),

$$p_1n^2=\frac{\sin^2\alpha}{\sin^2\beta}(p_2m^2-m+1)+n-1 \quad (6)$$

$$n=\frac{1}{2p_1}\left\{1\pm\sqrt{\left[\frac{4p_1\sin^2\alpha}{\sin^2\beta}(p_2m^2-m+1)+1-4p_1\right]}\right\}. \quad (7)$$

From equations (3), (4), and (6) we get

$$\left(1+\frac{\sin^2\alpha-\sin^2\gamma}{\sin^2\beta}\right)(p_2m^2-m+1)+m-2=(qm-1)n\,. \quad (8)$$

Some simplification follows if we now work in terms of:

$$\left.\begin{aligned} r&=1+\frac{\sin^2\alpha-\sin^2\gamma}{\sin^2\beta}=\frac{2\sin\alpha\cos\gamma}{\sin\beta}\\ x&=qm-1\\ p_0&=\frac{2p_1p_2}{q^2}=\frac{1}{2c_3^2}\\ q_0&=\frac{2p_1}{q}=\frac{c_2}{c_1c_3}\,. \end{aligned}\right\} \quad (9)$$

With these substitutions we obtain from equations (7) and (8):

$$n=\frac{1}{2p_1}\left\{1\pm\sqrt{\left[\frac{2\sin^2\alpha}{\sin^2\beta}(p_0x^2+(2p_0-q_0)x+p_0-q_0+2p_1)+1-4p_1\right]}\right\} \quad (10)$$

$$\frac{1}{2p_1}[rp_0x^2+(2rp_0-rq_0+q_0)x+r(p_0-q_0+2p_1)+q_0-4p_1]=xn\,. \quad (11)$$

Substituting in equation (11) the value of n given by equation (10) and re-arranging,

$$rp_0x^2+S_1x+S_2=\pm x\sqrt{\left\{\frac{2\sin^2\alpha}{\sin^2\beta}\times[p_0x^2+(2p_0-q_0)x]+S_3\right\}} \quad (12)$$

where

$$\left.\begin{aligned} S_1&=2rp_0+q_0(1-r)-1\\ S_2&=r(p_0-q_0+2p_1)+q_0-4p_1\\ S_3&=\frac{2\sin^2\alpha}{\sin^2\beta}(p_0-q_0+2p_1)+1-4p_1\,. \end{aligned}\right\} \quad (13)$$

On squaring equation (12) and gathering like terms together we obtain:

$$p_0\left(r^2p_0-\frac{2\sin^2\alpha}{\sin^2\beta}\right)x^4+2\left[rp_0S_1-\frac{(2p_0-q_0)\sin^2\alpha}{\sin^2\beta}\right]x^3+(S_1^2+2rp_0S_2-S_3)x^2+2S_1S_2x+S_2^2=0\,, \quad (14)$$

This is a polynomial equation in x whose coefficients and constant term are known for each of the Arrangements I, II, and III since α, β, and γ are measured values and p_1, p_0, and q_0 are known crystal lattice constants shown in Table 1. Hence equation (14), which is at most and in most cases a quartic equation, may be solved for x using established methods.

Table 1. *Crystallography defined in the derivation*

Note: $j_1=\pm1$, $j_3=\pm1$, $j_2=j_1j_3$

	Arrangement I	Arrangement II	Arrangement III
Crystal direction of outward normal to CAP	$\left(0,\frac{2}{\sqrt{3}},g\right)$	$\left(0,\frac{2}{\sqrt{3}},g\right)$	$\left(0,\frac{2}{\sqrt{3}},g\right)$
Crystal direction of outward normal to ABP	$j_1\left(1,\frac{1}{\sqrt{3}},g\right)$	$j_1\left(1,\frac{1}{\sqrt{3}},g\right)$	$j_1\left(1,-\frac{1}{\sqrt{3}},g\right)$
Crystal direction of outward normal to BCP	$j_3\left(0,\frac{2}{\sqrt{3}},-g\right)$	$j_3\left(1,-\frac{1}{\sqrt{3}},g\right)$	$j_3\left(1,\frac{1}{\sqrt{3}},-g\right)$
Crystal direction of $\overrightarrow{AP}$ (as a unit vector)	$\frac{j_1(g,\sqrt{3}g,-2)}{2\sqrt{(g^2+1)}}$	$\frac{j_1(g,\sqrt{3}g,-2)}{2\sqrt{(g^2+1)}}$	$\frac{j_1(3g,\sqrt{3}g,-2)}{2\sqrt{(3g^2+1)}}$
Crystal direction of $\overrightarrow{BP}$ (as a unit vector)	$\frac{j_2(-3g,\sqrt{3}g,2)}{2\sqrt{(3g^2+1)}}$	$\frac{j_2(g,0,-1)}{\sqrt{(g^2+1)}}$	$\frac{j_2(0,\sqrt{3}g,1)}{\sqrt{(3g^2+1)}}$
Crystal direction of $\overrightarrow{CP}$ (as a unit vector)	$j_3(1,0,0)$	$\frac{j_3(-3g,-\sqrt{3}g,2)}{2\sqrt{(3g^2+1)}}$	$\frac{j_3(3g,-\sqrt{3}g,2)}{2\sqrt{(3g^2+1)}}$
$\cos\widehat{BPC}=c_1$	$-\frac{3j_1g}{2\sqrt{(3g^2+1)}}$	$-\frac{j_1(3g^2+2)}{2\sqrt{[(g^2+1)(3g^2+1)]}}$	$-\frac{j_1(3g^2-2)}{2(3g^2+1)}$
$\cos\widehat{APC}=c_2$	$\frac{j_2g}{2\sqrt{(g^2+1)}}$	$-\frac{j_2(3g^2+2)}{2\sqrt{[(g^2+1)(3g^2+1)]}}$	$\frac{j_2(3g^2-2)}{2(3g^2+1)}$
$\cos\widehat{APB}=c_3$	$-\frac{j_3}{\sqrt{[(g^2+1)(3g^2+1)]}}$	$\frac{j_3(g^2+2)}{2(g^2+1)}$	$\frac{j_3(3g^2-2)}{2(3g^2+1)}$
$p_1=\frac{1}{4c_1^2}$	$\frac{3g^2+1}{9g^2}$	$\frac{(g^2+1)(3g^2+1)}{(3g^2+2)^2}$	$\frac{(3g^2+1)^2}{(3g^2-2)^2}$
$p_0=\frac{1}{2c_3^2}$	$\frac{(g^2+1)(3g^2+1)}{2}$	$\frac{2(g^2+1)^2}{(g^2+2)^2}$	$\frac{2(3g^2+1)^2}{(3g^2-2)^2}$
$q_0=\frac{c_2}{c_1c_3}$	$\frac{3g^2+1}{3}$	$\frac{2(g^2+1)}{g^2+2}$	$-\frac{2(3g^2+1)}{3g^2-2}$

When the various values of x have been obtained for the Arrangements I, II, and III the corresponding values of m and n may next be found using equations (9) and (11) which give:

$$m=\frac{x+1}{q}=\frac{q_0(x+1)}{2p_1} \tag{15}$$

$$n=\frac{1}{2p_1x}\,[rp_0x^2+(1+S_1)x+S_2]\,. \tag{16}$$

If $x=0$ (this occurs as a repeated root) the two corresponding n values should be obtained through equation (10) which gives:

$$n=(1\pm\sqrt{S_3})/2p_1\,. \tag{17}$$

We shall let the normal $\overrightarrow{HP}$ to the plane ABC, which gives the crystal-surface orientation, be given by the unit vector (v_1,v_2,v_3). After the various possible values of m and n for the three Arrangements I, II, and III have been obtained the corresponding crystal-surface orientations may next be determined.

Surface orientations under Arrangement I

The crystallographic directions of $\overrightarrow{AP}$, $\overrightarrow{BP}$, and $\overrightarrow{CP}$ for Arrangement I is given in Table 1. Taking the scalar product of (v_1,v_2,v_3) and these directions and equating the products to the cosines of $\widehat{HPA}$, $\widehat{HPB}$, and $\widehat{HPC}$ we get:

$$\begin{aligned} gv_1+\sqrt{3}gv_2-2v_3 &= 2j_3hg/m\\ -3gv_1+\sqrt{3}gv_2+2v_3 &= -6j_3hg/n\\ v_1 &= j_3h\,. \end{aligned}$$

From these equations we get (except for an uncertainty in sign):

$$(v_1,v_2,v_3)=\frac{\left[1,\ \frac{1}{\sqrt{3}}\left(1+\frac{1}{m}-\frac{3}{n}\right),\ \frac{g}{2}\left(2-\frac{1}{m}-\frac{3}{n}\right)\right]}{\left|\left[1,\ \frac{1}{\sqrt{3}}\left(1+\frac{1}{m}-\frac{3}{n}\right),\ \frac{g}{2}\left(2-\frac{1}{m}-\frac{3}{n}\right)\right]\right|}\,. \tag{18}$$

We now have (v_1,v_2,v_3) in terms of known or determinable quantities g, m, and n so that we may evaluate it. Since equation (14) may give as many as four real values of x we may find up to four possible values of (v_1,v_2,v_3) for Arrangement I. There will however be, in general, six ways of assigning observed inter-trace angles δ_1, δ_2, and δ_3 to α, β, and γ so that there are in fact six equations like (14) to consider. There could therefore be up to 24 possibilities of surface orientation (v_1,v_2,v_3) under Arrangement I in accord with the three traces AB, BC, and CA in Fig. 2.

Surface orientations under Arrangement II

Proceeding as for Arrangement I we will obtain for Arrangement II (but for the proper sign):

$$(v_1,v_2,v_3)=\frac{\left[\frac{1}{m}-\frac{3g^2+1}{3g^2+2},\ \frac{1}{\sqrt{3}}\left(-\frac{1}{m}+\frac{2}{n}-\frac{3g^2+1}{3g^2+2}\right),\ g\left(\frac{1}{m}+\frac{1}{n}-\frac{3g^2+1}{3g^2+2}\right)\right]}{\left|\left[\frac{1}{m}-\frac{3g^2+1}{3g^2+2},\ \frac{1}{\sqrt{3}}\left(-\frac{1}{m}+\frac{2}{n}-\frac{3g^2+1}{3g^2+2}\right),\ g\left(\frac{1}{m}+\frac{1}{n}-\frac{3g^2+1}{3g^2+2}\right)\right]\right|}\,. \tag{19}$$

In Arrangement II planes BCP and CAP are symmetrically located about plane ABP so that when γ is made equal to observed inter-trace angles δ_1, δ_2, and δ_3 in turn it does not matter how the remaining two observed intertrace angles are assigned to α and β. There are thus only three distinct ways of assigning δ_1, δ_2, and δ_3 to α, β, and γ and therefore only three equations like (14) to solve. Therefore, under Arrangement II, only up to twelve surface orientations will be found to be in accord with three $\{h0\bar{h}k\}$ or $\{hh\bar{2}\bar{h}k\}$ trace directions.

Surface orientations under Arrangement III

In the case of Arrangement III it will be found that but for an uncertainty in sign

$$(v_1,v_2,v_3)=\frac{\left[\frac{1}{m}+\frac{3g^2+1}{3g^2-2},\ \frac{1}{\sqrt{3}}\left(\frac{1}{m}-\frac{2}{n}-\frac{3g^2+1}{3g^2-2}\right),\ -g\left(\frac{1}{m}+\frac{1}{n}-\frac{3g^2+1}{3g^2-2}\right)\right]}{\left|\left[\frac{1}{m}+\frac{3g^2+1}{3g^2-2},\ \frac{1}{\sqrt{3}}\left(\frac{1}{m}-\frac{2}{n}-\frac{3g^2+1}{3g^2-2}\right),\ -g\left(\frac{1}{m}+\frac{1}{n}-\frac{3g^2+1}{3g^2-2}\right)\right]\right|}\,. \tag{20}$$

In Arrangement III the planes ABP, BCP, and CAP are similarly oriented to one another so it does not matter how a set of observed inter-trace angles δ_1, δ_2, and δ_3 are allocated to α, β, and γ. There will therefore be in this case only one equation of the type (14) to contend with so that no more than four surface orientations in keeping with three $\{h0\bar{h}k\}$ or $\{hh\bar{2}\bar{h}k\}$ trace directions could arise.

Identification of the correct surface orientation

With up to as many as forty possibilities of surface orientations applicable to the three trace directions in

Fig. 2 (in practice the number of possible orientations is frequently around twenty) the problem now is to identify the correct one. This can be done by checking the compatibility of the various possible surface orientations with other observed trace directions.

If we have a plane given by the vector (u_1, u_2, u_3) then from a consideration of the geometry of the situation it will be found that the angle θ between the trace of the plane and the direction $\overrightarrow{CA}$ in Fig. 2 is given by:

$$\theta = 90° + \tan^{-1}\left[\frac{(2v_2 + \sqrt{3}gv_3)(u_1v_1 + u_2v_2 + u_3v_3) - 2u_2 - \sqrt{3}gu_3}{u_1(\sqrt{3}gv_2 - 2v_3) + v_1(2u_3 - \sqrt{3}gu_2)}\right]. \tag{21}$$

For the sake of convenience and simplicity we have not cared about the proper sign of (v_1, v_2, v_3). Further as we permute the observed trace angles δ_1, δ_2, and δ_3 among α, β, and γ we will for some permutations effect a 180° rotation of the crystal about HP in Fig. 2. Consequently, at this point, we are not certain whether θ should be measured from $\overrightarrow{CA}$ in the same sense as γ (see Fig. 2) or in the opposite direction. The correct direction can be ascertained however by determining, using equation (21), the angle θ_{CB} which the trace of the plane BCP makes with $\overrightarrow{CA}$, assuming $\gamma \neq 90°$. If θ_{CB} turns out to be equal to γ then θ should be measured in the same sense as γ. If θ_{CB} works out to be $180° - \gamma$ then θ should be measured in the opposite direction to γ. If $\gamma = 90°$, we could consider in the same way θ_{AB} instead where θ_{AB} is the angle made by the trace of the plane ABP with $\overrightarrow{CA}$ as evaluated from equation (21) and should be equal to $180° - \alpha$ for θ to have the same sense as γ.

With a means to resolve the sense of θ we may use equation (21) to compute the location of other observed trace directions on letting (u_1, u_2, u_3) be the planes for these traces. This is to be done for all possibilities of surface orientation and that surface orientation for which the computed directions of the additional traces are reasonably close to the actual observed directions will be the right one.

Discussion

Reed-Hill & Baldwin (1965) produced an example of a zirconium grain with four $\{10\bar{1}2\}$ twins three of which may be taken to form a triangle ABC with angles α, β, and γ equal to 42, 117, and 21° respectively and the fourth makes an angle of 127° with $\overrightarrow{CA}$ (angles made with $\overrightarrow{CA}$ will now be taken to be measured in the same direction as γ). Using the equations derived in this paper the various possible orientations of the zirconium grain surface consistent with the first three twin traces and the corresponding angles θ_4, θ_5, θ_6, and θ_0 the other $\{10\bar{1}2\}$ twin boundaries and the basal plane trace should respectively make with $\overrightarrow{CA}$ have been worked out and are displayed in Table 2 where ξ is the angle the grain surface normal makes with [0001] and η the angle the projection of the normal onto (0001) makes with $[\bar{1}2\bar{1}0]$.

There are altogether sixteen possible surface orientations and it is clear that, allowing for reasonable errors in the data, it is difficult to differentiate between possibilities 1, 8, and 13 as the correct orientation as all three provide a $\{10\bar{1}2\}$ trace direction close to the fourth observed twin boundary. However, in the example, the basal plane trace was also observed with polarized light to make 157° with $\overrightarrow{CA}$ and this fifth trace observation completely identifies the No. 1 possibility as the right orientation. (This orientation agrees with Reed-Hill & Baldwin's result obtained by Wulff-net operations).

Table 2. *Possible orientations* (ξ, η) *of a zirconium grain surface with three* $\{10\bar{1}2\}$ *twin traces forming a triangle* ABC *with angles* α, β, *and* γ *of* 42, 117 *and* 21° *respectively and the corresponding angles* θ_4, θ_5, θ_6 *and* θ_0 *made by the remaining three* $\{10\bar{1}2\}$ *trace directions and the basal plane trace with* $\overrightarrow{CA}$.

	Surface orientation		Remaining $\{10\bar{1}2\}$ trace directions			Basal plane trace
No.	ξ(°)	η(°)	θ_4(°)	θ_5(°)	θ_6(°)	θ_0(°)
1	86	6	129	116	6	158
2	51	21	177	104	85	145
3	31	22	99	83	41	174
4	48	27	163	81	58	19
5	74	8	138	119	26	164
6	20	2	119	92	46	68
7	65	21	147	54	38	6
8	10	5	126	74	65	96
9	71	6	135	118	26	163
10	34	5	154	100	59	83
11	31	22	122	83	41	46
12	33	16	140	100	59	90
13	46	9	125	94	55	69
14	71	5	119	113	6	156
15	52	29	144	107	85	143
16	41	27	107	69	30	71

If Table 2 were to be inspected in detail it will be found that the chances are high of two observed additional trace directions being met by one orientation possibility only and by no other. Examination of other cases of α, β, and γ values leads to the conclusion that after the first three traces only two further trace observations will generally suffice to distinguish the correct orientation possibility. Any further trace information should completely mark out the correct orientation.

While the first three traces need to be of $\{h0\bar{h}k\}$ or of $\{hh\overline{2h}k\}$, there is no restriction whatsoever as to the nature of further traces which could be used. These further traces may be of the same planes as the first three or they may be of other planes such as $\{10\bar{1}0\}$ produced by slip and (0001) in the crystal and its twins revealed by polarized light. There should therefore be a good possibility of finding at least five suitable trace directions. It is also to be noted that the basal planes in twins of one type are all parallel to particular $\{h0\bar{h}k\}$ or $\{hh\bar{2}hk\}$ planes in the crystal so that their traces may also be used for the initial three trace directions.

In h.c.p. metals $\{h0\bar{h}k\}$ and $\{hh\bar{2}hk\}$ traces usually arise from twins. If twins of different types exist then there is uncertainty as to the planes to be specified for the various observed twin boundaries. Fortunately, in such cases, one twin type, say $\{10\bar{1}2\}$, usually predominates. By considering then that a few likely choices of three twin traces are of $\{10\bar{1}2\}$, working out the possible orientations with these choices, and checking to see whether there is an orientation for which the remaining observed traces are in acceptable directions, one should on many occasions discover the correct orientation. There have also been reports that twins of one type may be distinguished from another by their width and shape characteristics. For example, in yttrium (Carnahan & Scott, 1973), hafnium (Seelinger & Stoloff, 1971), and zirconium (Reed-Hill, Slippy & Buteau, 1963) $\{10\bar{1}2\}$ twins are generally broad lenticular shapes whilst the accompanying $\{11\bar{2}1\}$ twins are narrow and parallel-sided.

The initial three traces of $\{h0\bar{h}k\}$ or $\{hh\bar{2}hk\}$ employed in the current method strictly refer to pyramidal planes. They may however also be taken to be of prismatic $\{10\bar{1}0\}$ or $\{11\bar{2}0\}$ planes if k is made very small; for example, with $g=0{\cdot}001$ the method is found to give orientations within 1° of values actually applying to $\{10\bar{1}0\}$ or $\{11\bar{2}0\}$ traces. In applying the method to $\{10\bar{1}0\}$ or $\{11\bar{2}0\}$ traces Arrangement I should be discarded for we see in Fig. 1 that when OK becomes very large planes A_1A_2K and A_4A_5K tend to parallelism so that one of the three $\{10\bar{1}0\}$ or $\{11\bar{2}0\}$ planes is not accounted for in Arrangement I. Further, as OK becomes very large Arrangement II approximates to Arrangement III so we need only consider solutions for Arrangement III. There will of course be multiple orientations because of the quartic equation (14), but these will be very nearly identical and will all be very close to the only orientation which can apply to three $\{10\bar{1}0\}$ or $\{11\bar{2}0\}$ traces. (When we deal with $\{10\bar{1}0\}$ or $\{11\bar{2}0\}$ traces unique orientations are obtained without consideration of further traces).

Conclusion

A set of equations and mathematical relationships have been derived from which given three trace directions all of $\{h0\bar{h}k\}$ or all of $\{hh\bar{2}hk\}$ on the surface of a hexagonal crystal or grain and usually two other trace directions of any type the crystallographic orientation of the surface may be precisely evaluated. The case of three observed trace directions all of $\{10\bar{1}0\}$ or all of $\{11\bar{2}0\}$ fall within the framework of this treatment to a high degree of approximation. The explicitness of the equations and mathematical relationships allow a computer program to be readily written and thus full advantage may be taken of the speed, precision, and ease provided by computers. Because of the near-general nature of the traces which may be considered, the orientation-determination method developed here should be applicable to many kinds of trace observations made of hexagonal crystals, particularly metals.

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