# Computational techniques for grain-orientation determinations using surface traces of crystal planes of any indices 

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#### Abstract

An analysis is given which permits a computer program to be written for the determination of the orientation of a grain of cubic lattice from measured directions on its surface of traces of crystallographic planes of any known indices. An application of the analysis to grain orientation with $\{112\}$ traces is given as an illustration, showing how such complex determinations are made feasible and easy with computers.


## 1. Introduction

During a metallographic examination, traces of crystallographic planes such as slip lines, Widmanstatten precipitates, edges of etch pits, and twin boundaries are commonly seen. Fig. 1 shows $\{112\}$ deformation twins in a ferrite grain in a mild steel specimen aligned along the six different directions shown in Fig. 2. Traces such as these provide a ready and convenient means of obtaining the orientation of grains as an alternative to more elaborate and costly techniques such as X-ray and electron diffraction. The orientation determination is taken here to mean the identification of the crystallographic plane constituting the surface of the grain under observation. Using these trace directions, it is possible to deduce the orientation of even small grains in polycrystalline specimens, as well as grains of phases which have completely transformed, e.g. austenite in steels.

The determination of grain orientations from crystallographic trace directions can be done by Wulff net manipulations [1], but this is tedious and impractical if the traces are of planes of relatively high order indices and, therefore, of high multiplicity, because many poles will have to be rotated into position. Charts and tables have been produced for specific trace types, namely $\{100\},\left\{\begin{array}{lll}11\end{array}\right\}$, and $\{110\}[2-5]$ for cubic lattices. These are necessarily limited to considerations of three or four trace directions at a time. The task of producing charts or tables for traces of planes of higher indices seems formidable because of the many combinations of variants which could produce a set of three or four observed trace directions. For example, for the $\{110\}$ case, three charts have to be used in combination [5]. The use of Wulff net, tables, or charts is subject to inaccuracies because of errors in manipulation in the case of the Wulff net, and because of the degree of divisioning employed in the tables or charts.

Analytical expressions and equations have also been derived for the determination of grain orientations from surface crystallographic traces. These are
simple for $\{100\}$ traces on grains of cubic lattice [2], but complex for $\left\{\begin{array}{lll}1 & 1 & 1\end{array}\right\}$ traces $[6,7]$. However, much simpler expressions have been established recently, not only for $\left\{\begin{array}{lll}1 & 1 & 1\end{array}\right\}$ traces [8], but also for $\left\{\begin{array}{lll}1 & 1 & 0\end{array}\right\}$ traces [9]. These analytical expressions and equations enable the grain orientation to be ascertained as accurately as the trace data will permit, without introduction of further errors. The principal advantage is, however, that they enable the grain-orientation determination process to be easily computerized, thus allowing for rapid, convenient, and accurate orientation determinations, and if required, for other computations to be performed at the same time, such as obtaining the orientation of other crystallographic planes or directions relative to the grain surface.

At present, analytical expressions and equations have not been established for higher order index planes in cubic systems than those mentioned above, such as $\{112\}$ planes, or for the more complex situation of mixed crystallographic traces, e.g. a combined observation of $\{111\}$ and $\{110\}$ traces. The purpose of this paper is, therefore, to develop analytical expressions and equations which will allow grainorientation determinations for cubic lattices for the general case, where the traces on a grain surface are of planes of any known type. With such expressions and equations, one should be able to write a computer program to deal with trace observations of planes of any type and combination, and thus render feasible orientation determinations which were hitherto not possible because of their complexity.

## 2. Derivation of equations for grain orientation

Consider three traces $\mathrm{BC}, \mathrm{CA}$, and AB on a grain surface ABC at angles of $\alpha, \beta$, and $\gamma$ to each other as shown in Fig. 3. Suppose they are produced by planes $\left(h_{1} k_{1} l_{1}\right),\left(h_{2} k_{2} l_{2}\right)$, and ( $\left.h_{3} k_{3} l_{3}\right)$, respectively. These planes may be imagined to form a pyramid ABCP as shown, with apex angles $\varrho_{1}, \varrho_{2}$, and $\varrho_{3}$, whose values are readily derived from the indices of the planes BCP ,


Figure 1 Deformation twins in ferrite in a mild steel specimen.

CAP, and ABP. Four sets of values of $\varrho_{1}, \varrho_{2}$, and $\varrho_{3}$ are possible because the planes $\left(h_{1} k_{1} l_{1}\right),\left(h_{2} k_{2} l_{2}\right)$, and $\left(h_{3} k_{3} l_{3}\right)$ can produce four pyramidal shapes. Given one pyramidal shape as in Fig. 3, a second pyramidal shape will have edges $\mathrm{AP}, \mathrm{BP}$, and CP reversed (i.e. $\mathrm{C}^{\prime} \mathrm{P}$ ), with apex angles $\left(\pi-\varrho_{1}\right),\left(\pi-\varrho_{2}\right)$, and $\varrho_{3}$. A third pyramidal shape results if the edge AP is reversed instead, the apex angles being now $\varrho_{1},\left(\pi-\varrho_{2}\right)$, and $\left(\pi-\varrho_{3}\right)$. Had the edge BP been reversed, instead, the fourth pyramidal shape with apex angles $\left(\pi-\varrho_{1}\right), \varrho_{2}$ and $\left(\pi-\varrho_{3}\right)$, would have been formed. We note that, excluding the case of any apex angle being $\pi / 2$, the sign of the product of the cosines of the three apex angles is the same for all these four possibilities, i.e. the sign is unique for a set of planes $\left(h_{1} k_{1} l_{1}\right),\left(h_{2} k_{2} l_{2}\right)$, and ( $h_{3} k_{3} l_{3}$ ) producing traces $\mathrm{AB}, \mathrm{BC}$, and CA .

The orientation of the grain can be deduced, once the relative lengths of the edges $\mathrm{AP}, \mathrm{BP}$, and CP have been obtained, as these control the inclination of the pyramidal faces to the grain surface plane ABC. For simplicity, CP shall be taken of unit length, whilst AP, $\mathrm{BP}, \mathrm{BC}, \mathrm{CA}$, and AB shall be taken to have lengths $k_{0}$, $t_{0}, a, b$ and $c$ respectively.


Figure 2 Stereographic plot showing the dispositions of the six $\{112\}$ twin boundary trace directions in the ferrite grain in Fig. 1. The small circles denote the locations of the $\{112\}$ poles of the twin boundary planes rotated $90^{\circ}$ about the vertical axis. The $\left\{\begin{array}{lll}1 & 1 & 2\end{array}\right\}$ pole positions were computed using the analysis of this paper.


Figure 3 Surface traces $\mathrm{AB}, \mathrm{BC}$, and CA produced by planes ABP, $B C P$, and CAP, respectively, which form a pyramid ABCP.

Applying the cosine rule to Fig. 3,

$$
\begin{align*}
& a^{2}=t_{0}^{2}-2 t_{0} j_{1} c_{1}+1  \tag{1}\\
& b^{2}=k_{0}^{2}-2 k_{0} j_{2} c_{2}+1  \tag{2}\\
& c^{2}=k_{0}^{2}-2 k_{0} t_{0} j_{3} c_{3}+t_{0}^{2} \tag{3}
\end{align*}
$$

where, for $m=1,2$, and 3 ,

$$
\begin{align*}
c_{\mathrm{m}} & =\left|\cos \varrho_{\mathrm{m}}\right|  \tag{4}\\
j_{\mathrm{m}} & =1 \text { or }-1 \tag{5}
\end{align*}
$$

according to whether $\varrho_{\mathrm{m}}$ is $\leqslant \pi / 2$ or $>\pi / 2$, respectively. Let

$$
\begin{align*}
k & =j_{2} k_{0}  \tag{6a}\\
t & =j_{1} t_{0} \tag{6b}
\end{align*}
$$

Then, Equations 1 to 3 may be written

$$
\begin{align*}
& a^{2}=t^{2}-2 c_{1} t+1  \tag{7}\\
& b^{2}=k^{2}-2 c_{2} k+1  \tag{8}\\
& c^{2}=k^{2}-2 c_{4} k t+t^{2} \tag{9}
\end{align*}
$$

where

$$
\begin{equation*}
c_{4}=j_{1} j_{2} j_{3} c_{3} \tag{10}
\end{equation*}
$$

We note that $j_{1} j_{2} j_{3}$ is a known quantity, being equal to 1 or -1 , giving, in fact, the sign of the product of the cosines of the apex angles of the pyramid in Fig. 3. (If at least one apex angle is $\pi / 2$, we shall choose it to be $\varrho_{3}$, so that $c_{4}=c_{3}=0$, and $j_{1} j_{2} j_{3}$ becomes irrelevant.) Because in Equations 7 to 9 we are using only the absolute values of the cosines of $\varrho_{1}$, $\varrho_{2}$, and $\varrho_{3}$, these equations apply to any of the four possible sets of values of $\varrho_{1}, \varrho_{2}$, and $\varrho_{3}$.

Dividing Equation 7 by 8 and using the sine rule,
$(\sin \alpha / \sin \beta)^{2}=\left(t^{2}-2 c_{1} t+1\right) /\left(k^{2}-2 c_{2} k+1\right)$
This gives
$t^{2}-2 c_{1} t+1-(\sin \alpha / \sin \beta)^{2}\left(k^{2}-2 c_{2} k+1\right)=0$

$$
\begin{equation*}
t=c_{1} \pm\left\{(\sin \alpha / \sin \beta)^{2}\left(k^{2}-2 c_{2} k+1\right)-s_{1}^{2}\right\}^{1 / 2} \tag{11}
\end{equation*}
$$

where

$$
\begin{equation*}
s_{1}=\sin \varrho_{1} \tag{13}
\end{equation*}
$$

Also from Equation 11,

$$
\begin{equation*}
t^{2}=(\sin \alpha / \sin \beta)^{2}\left(k^{2}-2 c_{2} k+1\right)-1+2 c_{1} t \tag{14}
\end{equation*}
$$

Dividing Equation 9 by Equation 8,

$$
\begin{equation*}
(\sin \gamma / \sin \beta)^{2}=\left(k^{2}-2 c_{4} k t+t^{2}\right) /\left(k^{2}-2 c_{2} k+1\right) \tag{15}
\end{equation*}
$$

Putting in for $t^{2}$ the expression in Equation 14 and rearranging,

$$
\begin{gather*}
k^{2}+\left[\left(\sin ^{2} \alpha-\sin ^{2} \gamma\right) / \sin ^{2} \beta\right]\left(k^{2}-2 c_{2} k+1\right)-1 \\
=2\left(c_{4} k-c_{1}\right) t \tag{16}
\end{gather*}
$$

Substituting for $t$ its expression in Equation 12 and, after some manipulation,

$$
\begin{align*}
&(\sin \alpha \cos \gamma / \sin \beta) k^{2}-\left[c_{1} c_{4}+c_{2} \sin (\alpha-\gamma) / \sin \beta\right] k \\
&+\sin \alpha \cos \gamma / \sin \beta-s_{1}^{2} \\
&= \pm\left(c_{4} k-c_{1}\right)\left[(\sin \alpha / \sin \beta)^{2}\right. \\
&\left.\times\left(k^{2}-2 c_{2} k+1\right)-s_{1}^{2}\right]^{1 / 2} \tag{17}
\end{align*}
$$

Squaring and collecting like powers of $k$ together, we obtain

$$
\begin{equation*}
b_{4} k^{4}+b_{3} k^{3}+b_{2} k^{2}+b_{1} k+b_{0}=0 \tag{18}
\end{equation*}
$$

where

$$
\begin{align*}
b_{4}= & \sin ^{2} \alpha\left(\cos ^{2} \gamma-c_{4}^{2}\right) \\
b_{3}= & 2 \sin \alpha\left\{c_{4}\left(c_{1}+c_{2} c_{4}\right) \sin \alpha\right. \\
& \left.-\cos \gamma\left[c_{1} c_{4} \sin \beta+c_{2} \sin (\alpha-\gamma)\right]\right\} \\
b_{2}= & 2 \sin \alpha \cos \gamma\left(\sin \alpha \cos \gamma-s_{1}^{2} \sin \beta\right) \\
& +\left[c_{1} c_{4} \sin \beta+c_{2} \sin (\alpha-\gamma)\right]^{2}  \tag{19}\\
& -\left(c_{1}^{2}+c_{4}^{2}+4 c_{1} c_{2} c_{4}\right) \sin ^{2} \alpha+c_{4}^{2} s_{1}^{2} \sin ^{2} \beta \\
b_{1}= & 2\left\{c_{1}\left[\left(c_{4}+c_{1} c_{2}\right) \sin ^{2} \alpha-c_{4} s_{1}^{2} \sin ^{2} \beta\right]\right. \\
& -\left[c_{1} c_{4} \sin \beta+c_{2} \sin (\alpha-\gamma)\right]
\end{align*}
$$

$$
\begin{equation*}
\boldsymbol{n}_{2}=\frac{\left[z_{\mathrm{p}} \sin \beta, z_{\mathrm{p}}(a / c-\cos \beta),\left(a-x_{\mathrm{p}}\right) \sin \beta+y_{\mathrm{p}}(\cos \beta-a / c)\right]}{\left\{z_{\mathrm{p}}^{2}\left[1+(a / c)^{2}-2 a \cos \beta / c\right]+\left[\left(a-x_{\mathrm{p}}\right) \sin \beta+y_{\mathrm{p}}(\cos \beta-a / c)\right]^{2}\right\}^{1 / 2}} \tag{20}
\end{equation*}
$$

will indicate that their corresponding apex angles are acute, and, if negative, indicate that they are obtuse (see Equations 1 to 5). Referring to Equation 6, $j_{2}=1$ or -1 according to whether $k$ is positive or negative; similarly, $j_{1}=1$ or -1 depending on the sign of $t$. Knowing $j_{1}$ and $j_{2}$, the value of $j_{3}$ follows from the fact that $j_{1} j_{2} j_{3}=1$ or -1 according to whether the product of the cosines of $\varrho_{1}, \varrho_{2}$, and $\varrho_{3}$ is positive or negative, respectively. Thus if $\varrho_{3}$ is not $\pi / 2$, it can be established whether it is acute or obtuse. Hence, for each solution for $k$, the values of $k_{0}, t_{0}, \varrho_{1}, \varrho_{2}$, and $\varrho_{3}$ giving the orientation of the pyramid in Fig. 3 may be found. From these the corresponding grain orientation may be deduced. With as many as four solutions for $k$, there will be as many as four grain orientations for the three observed traces $\mathrm{AB}, \mathrm{BC}$, and CA in Fig. 3.

Once specific values have been obtained for $k_{0}, t_{0}$, $\varrho_{1}$, and $\varrho_{3}$, the grain orientation, as a unit vector ( $v_{1}$, $v_{2}, v_{3}$, may be obtained as follows. Relative to a Cartesian coordinate system $0 X Y Z$ set up as in Fig. 3 with 0 coinciding with $B$, and with $0 Z$ perpendicular to the plane ABC , the coordinates of the vertices $\mathrm{A}, \mathrm{B}$, and C of the pyramid ABCP are, respectively, $(c \cos \beta, c \sin \beta, 0),(0,0,0)$ and $(a, 0,0)$. The coordinates of the vertex $P$ shall be taken to be ( $x_{\mathrm{p}}, y_{\mathrm{p}}, z_{\mathrm{p}}$ ). The values of $a, c$, and $\left(x_{\mathrm{p}}, y_{\mathrm{p}}, z_{\mathrm{p}}\right)$ can be put in terms of $k_{0}, t_{0}, \varrho_{1}$, and $\varrho_{3}$ as shown in the Appendix.

The vectors for the direction $\mathbf{A P}, \mathbf{B P}$, and $\mathbf{C P}$ are respectively $\left(x_{\mathrm{p}}-c \cos \beta, y_{\mathrm{p}}-c \sin \beta, z_{\mathrm{p}}\right)$, ( $x_{\mathrm{p}}, y_{\mathrm{p}}, z_{\mathrm{p}}$ ), and ( $x_{\mathrm{p}}-a, y_{\mathrm{p}}, z_{\mathrm{p}}$ ). By considering the cross product $\mathbf{B P} \times \mathbf{C P}$ we obtain the unit vector for the direction of the outward normal to the face BCP as

$$
\boldsymbol{n}_{1}=\frac{\left(0,-z_{\mathrm{p}}, y_{\mathrm{p}}\right)}{\left(y_{\mathrm{p}}^{2}+z_{\mathrm{p}}^{2}\right)^{1 / 2}}
$$

In the same way, the unit vectors $\boldsymbol{n}_{\mathbf{2}}$ and $\boldsymbol{n}_{3}$ for the outward normals to the faces ACP and ABP, respectively, will be found to be

$$
\left.\times\left[\sin \alpha \cos \gamma-s_{1}^{2} \sin \beta\right]\right\}
$$

$$
b_{0}=\left(\sin \alpha \cos \gamma-s_{1}^{2} \sin \beta\right)^{2}
$$

$$
\boldsymbol{n}_{3}=\frac{\left(-z_{\mathrm{p}} \sin \beta, z_{\mathrm{p}} \cos \beta, x_{\mathrm{p}} \sin \beta-y_{\mathrm{p}} \cos \beta\right)}{\left[z_{\mathrm{p}}^{2}+\left(x_{\mathrm{p}} \sin \beta-y_{\mathrm{p}} \cos \beta\right)^{2}\right]^{1 / 2}}
$$

$$
\begin{equation*}
-c_{1}^{2}\left(\sin ^{2} \alpha-s_{1}^{2} \sin ^{2} \beta\right) \tag{21}
\end{equation*}
$$

This is a quartic equation in $k$ which can be solved analytically (refer to a suitable mathematical text e.g. [10]). There could be up to four real solutions.

For each solution for $k$, the corresponding value for

$$
\begin{equation*}
d_{2}=\frac{\left(a-x_{\mathrm{p}}\right) \sin \beta+y_{\mathrm{p}}(\cos \beta-a / c)}{\left\{z_{\mathrm{p}}^{2}\left[1+(a / c)^{2}-2 a \cos \beta / c\right]+\left[\left(a-x_{\mathrm{p}}\right) \sin \beta+y_{\mathrm{p}}(\cos \beta-a / c)\right]^{2}\right\}^{1 / 2}} \tag{23}
\end{equation*}
$$

$t$ may be found from Equation 16. $k_{0}$ and $t_{0}$ are just the absolute values of $k$ and $t$ respectively. When an apex angle is $\pi / 2$, there is no ambiguity, but other than this, it will not be obvious whether the apex angle has its acute or obtuse form. This can be ascertained by referring to the signs of $j_{1}, j_{2}$, and $j_{3}$, which if positive,
$d_{3}=\frac{x_{\mathrm{p}} \sin \beta-y_{\mathrm{p}} \cos \beta}{\left\{z_{\mathrm{p}}^{2}+\left(x_{\mathrm{p}} \sin \beta-y_{\mathrm{p}} \cos \beta\right)^{2}\right\}^{1 / 2}}$
Let ( $n_{11}, n_{12}, n_{13}$ ), ( $n_{21}, n_{22}, n_{23}$ ), and ( $n_{31}, n_{32}, n_{33}$ ) give the unit vectors $\boldsymbol{n}_{\mathbf{1}}, \boldsymbol{n}_{\mathbf{2}}$, and $\boldsymbol{n}_{\mathbf{3}}$ in the crystal axes system, i.e.

$$
\begin{align*}
& \left(n_{11}, n_{12}, n_{13}\right)=\left(h_{1}, k_{1}, l_{1}\right) /\left(h_{1}^{2}+k_{1}^{2}+l_{1}^{2}\right)^{1 / 2} \\
& \left(n_{21}, n_{22}, n_{23}\right)=j_{12}\left(h_{2}, k_{2}, l_{2}\right) /\left(h_{2}^{2}+k_{2}^{2}+l_{2}^{2}\right)^{1 / 2} \tag{26}
\end{align*}
$$

$$
\begin{equation*}
\left(n_{31}, n_{32}, n_{33}\right)=j_{13}\left(h_{3}, k_{3}, l_{3}\right) /\left(h_{3}^{2}+k_{3}^{2}+l_{3}^{2}\right)^{1 / 2} \tag{27}
\end{equation*}
$$

where $j_{12}$ and $j_{13}= \pm 1$, the correct signs being those satisfying

$$
\begin{align*}
& \left(n_{11}, n_{12}, n_{13}\right)\left(n_{21}, n_{22}, n_{23}\right)=\boldsymbol{n}_{1} \boldsymbol{n}_{\mathbf{2}} \\
& \left(n_{11}, n_{12}, n_{13}\right)\left(n_{31}, n_{32}, n_{33}\right)=\boldsymbol{n}_{1} \boldsymbol{n}_{3}  \tag{28}\\
& \left(n_{21}, n_{22}, n_{23}\right)\left(n_{31}, n_{32}, n_{33}\right)=\boldsymbol{n}_{2} \boldsymbol{n}_{3}
\end{align*}
$$

Then,

$$
\begin{align*}
& n_{11} v_{1}+n_{12} v_{2}+n_{13} v_{3}=d_{1}  \tag{29}\\
& n_{21} v_{1}+n_{22} v_{2}+n_{23} v_{3}=d_{2}  \tag{30}\\
& n_{31} v_{1}+n_{32} v_{2}+n_{33} v_{3}=d_{3} \tag{31}
\end{align*}
$$

Solving Equations 29 to 31 for $v_{1}, v_{2}$, and $v_{3}$ we will obtain

$$
\begin{align*}
v_{1}= & {\left[d_{1}\left(n_{22} n_{33}-n_{32} n_{23}\right)+d_{2}\left(n_{32} n_{13}-n_{12} n_{33}\right)\right.} \\
& \left.+d_{3}\left(n_{12} n_{23}-n_{22} n_{13}\right)\right] / N  \tag{32}\\
v_{2}= & {\left[d_{1}\left(n_{31} n_{23}-n_{21} n_{33}\right)+d_{2}\left(n_{11} n_{33}-n_{31} n_{13}\right)\right.} \\
& \left.+d_{3}\left(n_{21} n_{13}-n_{11} n_{23}\right)\right] / N  \tag{33}\\
v_{3}= & {\left[d_{1}\left(n_{21} n_{32}-n_{31} n_{22}\right)+d_{2}\left(n_{31} n_{12}-n_{11} n_{32}\right)\right.} \\
& \left.+d_{3}\left(n_{11} n_{22}-n_{21} n_{12}\right)\right] / N  \tag{34}\\
N= & n_{11}\left(n_{22} n_{33}-n_{23} n_{32}\right)+n_{12}\left(n_{23} n_{31}-n_{21} n_{33}\right) \\
& +n_{13}\left(n_{21} n_{32}-n_{22} n_{31}\right) \tag{35}
\end{align*}
$$

Equations 32 to 34 allow the grain orientation $\left(v_{1}, v_{2}, v_{3}\right)$ to be obtained from the observed values of the angles $\alpha, \beta$, and $\gamma$ between the traces $\mathrm{AB}, \mathrm{BC}$ and CA in Fig. 3, produced by planes $\left(h_{1} k_{1} l_{1}\right),\left(h_{2} k_{2} l_{2}\right)$, and $\left(h_{3} k_{3} l_{3}\right)$, respectively. Because of the quartic Equation 18 there may be as many as four solutions. The correct solution wil be the one which will provide for other observed trace directions.

## 3. Application of the analysis to $\{112\}$ traces

The use of the equations and expressions developed above in determining a grain orientation is best illustrated by obtaining a solution for a specific case, e.g. the ferrite grain in Fig. 1. There are on the grain surface six $\{112\}$ twin boundary directions at angles which were measured to be as in Table I.

The first step in the orientation determination consists of selecting three trace directions, e.g. 1, 2, and 3 in Fig. 1 or 2, and noting the angles $\alpha, \beta, \gamma$ between them, when they are arranged to form a triangle ABC in the manner of Fig. 3.

Next, all the possible planes $\left(h_{1} k_{1} l_{1}\right),\left(h_{2} k_{2} l_{2}\right)$, and $\left(h_{3} k_{3} l_{3}\right)$, which could have produced these traces, are considered. For $\{112\}$ traces, there are twelve possibilities, as shown in Table II. Other combinations of $\{112\}$ planes will be found to be equivalent to one of these. The apex angles of the pyramid of the type in

TABLE I Directions of traces in Fig. 1

| Trace direction | Angle made with direction (1) <br> measured counter-clockwise <br> (degrees) |
| :--- | :---: |
| (1) | 0.0 |
| $(2)$ | 112.8 |
| $(3)$ | 84.3 |
| $(4)$ | 20.5 |
| $(5)$ | 21.1 |
| $(6)$ | 73.0 |

Fig. 3 are next to be ascertained. They work out to be the values shown in Table II.

For each combination of a $\{112\}$ triplet in Table II, we now have the basic data to compute, from Equations 1 to 34, the grain orientation of which, as we saw earlier, there may be as many as four possibilities (although it is usually found that there are two). The computation will have to be done for all the $12\{112\}$ combinations in Table II, producing many possible solutions which could have given rise to the three trace directions 1, 2, and 3. Further solutions arise because, for each combination in Table II, it is not known which particular planes should actually represent the trace directions 1,2 , and 3 . One will have to consider all possibilities of assigning the directions $\mathrm{AB}, \mathrm{BC}$, and CA in Fig. 3 to these three trace directions. This is tantamount to assigning the three $\left\{\begin{array}{lll}1 & 1 & 2\end{array}\right\}$ planes to these trace directions in all possible ways, there being six ways of doing this. In some cases where a pair of apex angles are similar, or the supplement of the other, the number of ways reduces to three, e.g. combination 11 in Table II. In the case of combination 12 , where all the apex angles are equal, there is only one way of assigning the $\{112\}$ planes to the trace directions 1,2 , and 3 . Any other way would be equivalent.

Such a vast number of computations is clearly not humanly possible, but is readily done with a computer. A program was written to perform such computations on the IBM 3081. The program, on execution, first accepts the data in Tables I and II. It next computes the values of $\alpha, \beta$, and $\gamma$ which are initially the angles between traces 2 and 3,3 and 1 , and 1 and 2 , respectively. It then performs the solution of the quartic Equation 18, and obtains the corresponding grainorientation possibilities. This is done for the various triplets of $\{112\}$ in Table II and assignments of AB, BC , and CA to the trace directions 1,2 , and 3. The program also computes, for each orientation possibility, the directions of the other $\{112\}$ trace directions, and compares them with the actually observed directions of other $\{112\}$ traces, i.e. 4,5 , and 6 in Fig. 2. It identifies the solution whose computed $\{112\}$ trace directions best match with these observed directions, and prints out this solution in the manner illustrated in Fig. 4. The printout shows the observed trace directions and the angles between traces 1, 2, and 3 , the correct orientation possibility ( $v_{1}, v_{2}, v_{3}$ ), the computed trace directions for this orientation, and the corresponding computed azimuthal elevations of the $\left\{\begin{array}{lll}1 & 1 & 2\end{array}\right\}$ planes. The apex angles for this orientation solution as well as which inter-trace angles served for

TABLE II The 12 possible sets of $\{112\}$ triplets for the trace planes in Fig. 3 and the corresponding pyramid apex angles*

|  | $\left(h_{1} k_{1} l_{1}\right)$ | $\left(h_{2} k_{2} l_{2}\right)$ | $\left(h_{3} k_{3} l_{3}\right)$ | $\varrho_{1}(\mathrm{deg})$ | $Q_{2}(\mathrm{deg})$ | $Q_{3}(\mathrm{deg})$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1. | (112) | (121) | ( $\mathrm{I}_{1} 1$ ) | 48.50602029 | 121.48215411 | 151.43917478 |
| 2. | (112) | (121) | (112) | 82.25063362 | 121.48215411 | 140.76847952 |
| 3. | (112) | (121) | (172) | 31.48215411 | 150.04297932 | 162.97613382 |
| 4. | (112) | (121) | ( $\overline{1} \overline{1} 1)$ | 14.45828792 | 160.71367459 | 169.32930473 |
| 5. | (112) | ( $\overline{1} 11$ ) | (1] 12) | 146.25538667 | 151.43917478 | 39.23152048 |
| 6. | (112) | (21]) | (121) | 107.02386618 | 122.87834956 | 72.97613382 |
| 7. | (112) | ( $\overline{1} \overline{1}$ ) | ( $\overline{1} 11)$ | 135.58469140 | 112.20765430 | 67.79234570 |
| 8. | (112) | ( $\overline{1} \overline{1}$ ) | (121) | 101.53695903 | 101.53695903 | 78.46304097 |
| 9. | (112) | ( $\overline{\mathrm{T}} \mathrm{T}$ ) | (2T1) | 72.97613382 | 118.56082522 | 90.00000000 |
| 10. | (112) | (11 2) | (IT 1 ) | 129.23152048 | 78.46304097 | 129.23152048 |
| 11. | (112) | (121) | (211) | 92.92132889 | 92.92132889 | 145.95226763 |
| 12. | (112) | (121) | (211) | 117.03569179 | 117.03569179 | 117.03569179 |

*For each triplet, three further sets of apex angles may be obtained by replacing a pair of the apex angles by their supplementary angles.
$\alpha, \beta$, and $\gamma$ are also shown. The information has been used to plot stereographically in Fig. 2 the $\{112\}$ poles pertaining to the observed trace directions 1 to 6. In this plot the $\{112\}$ poles have been rotated $90^{\circ}$ about $\left(v_{1}, v_{2}, v_{3}\right)$ so that they should lie on their respective trace directions. It is seen that the poles are on or very near their relevant trace directions. The slight deviations are probably due to limitations in the accuracy to which the trace directions can be measured.
analysis which would allow for computerization of the process.

A listing of the computer program used above for obtaining grain orientations from $\{112\}$ traces will be made available on request.

## Appendix

For given values of $k_{0}, t_{0}, \varrho_{1}$, and $\varrho_{3}$ the corresponding values of $a$ and $c$ in Fig. 3 follow from the cosine rule:

$$
\begin{align*}
a & =\left(t_{0}^{2}+1-2 t_{0} \cos \varrho_{1}\right)^{1 / 2}  \tag{A1}\\
c & =\left(k_{0}^{2}+t_{0}^{2}-2 k_{0} t_{0} \cos \varrho_{3}\right)^{1 / 2} \tag{A2}
\end{align*}
$$

In Fig. 3, $H$ is the vertical projection of $P$ on to the plane $A B C$. We see that

$$
\begin{array}{r}
x_{\mathrm{p}}^{2}+y_{\mathrm{p}}^{2}=\mathrm{BH}^{2}=t_{0}^{2}-z_{\mathrm{p}}^{2} \\
\left(x_{\mathrm{p}}-a\right)^{2}+y_{\mathrm{p}}^{2}=\mathrm{CH}^{2}=1-z_{\mathrm{p}}^{2}  \tag{A4}\\
\left(x_{\mathrm{p}}-c \cos \beta\right)^{2}+\left(y_{\mathrm{p}}-c \sin \beta\right)^{2}=\mathrm{AH}^{2}=k_{0}^{2}-z_{\mathrm{p}}^{2}
\end{array}
$$

(A5)
(A) OBSERVED TRACE DIRECTIONS ARE IN DEGS:

| (1) | 0.0 | (2) | 112.8 | (3) | 84.3 |
| :--- | ---: | ---: | ---: | ---: | ---: |
| (4) | 20.5 | (5) | 21.1 | (6) | 73.0 |

(B) ANGLES BETWEEN TRACES (1) \& (2), (2) \& (3), (3) \& (1)

$$
=\quad 67.2 \quad 28.5 \quad 84.3 \text { DEGS }
$$

(C) CORRECT ORIENTATION POSSIBILITY:


Figure 4 Computer printout showing the results of the application of the analysis of this paper to the ferrite grain in Fig. 1.

From Equations A3 to A5 one will be able to obtain
$x_{\mathrm{p}}=\left(a^{2}+t_{0}^{2}-1\right) / 2 a$
$y_{\mathrm{p}}=\left(c^{2}+t_{0}^{2}-k_{0}^{2}-2 c x_{\mathrm{p}} \cos \beta\right) / 2 c \sin \beta$
$z_{\mathrm{p}}=\left(t_{0}^{2}-x_{\mathrm{p}}^{2}-y_{\mathrm{p}}^{2}\right)^{1 / 2}$
Equations A6 to A8 enable us to obtain $x_{\mathrm{p}}, y_{\mathrm{p}}$, and $z_{\mathrm{p}}$ from a given set of values of $k_{0}, t_{0}, \varrho_{1}, \varrho_{3}$.

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