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MINIMAL POLE FIGURE RANGES FOR QUANTITATIVE TEXTURE ANALYSIS

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The use of only a small number of incomplete pole figures for texture determinations is of practical interest for reducing the effort of texture measurement. The determination of minimal pole figure ranges (MPR) is explained and the use of MPR is demonstrated on an example.

KEY WORDS Crystal orientation, Poles of lattice planes, Incomplete pole figures, Minimal ranges.

1. INTRODUCTION

During the last years the quantitative texture analysis (QTA) has been more and more established in its traditional field of metal research as well as in geosciences and other applied fields. Polycrystalline samples are investigated consisting of some crystalline phases which may possess low crystal symmetry. The texture of a polycrystalline phase will be described quantitatively by the orientation distribution function (ODF) $f(g)$

$$\int_G f(g)\,dg = 8\pi^2, \qquad dg = \sin\alpha\,d\alpha\,d\beta\,d\gamma, \qquad f(g) \geq 0. \tag{1}$$

with $G: 0 \leq \alpha,\ \gamma < 2\pi,\ 0 \leq \beta \leq \pi$. At this $\{\alpha, \beta, \gamma\} \equiv g$ are three Eulerian angles describing the orientation of two right-handed cartesian coordinate systems relatively to each other (cf. appendix (24)–(26)).

Starting points for the calculation of the ODF are mostly diffraction patterns (X-ray, thermal neutrons, electrons). From this so called reduced pole figures (PF)

$$\tilde{P}_{\vec{h}_i}(\vec{y}_r) = [P_{\vec{h}_i}(\vec{y}_r) + P_{-\vec{h}_i}(\vec{y}_r)]/2,$$

with

$$P_{\vec{h}_i}(\vec{y}_r) = \frac{1}{2\pi}\int_{\tilde{\phi}_i=0}^{2\pi} f(\{\vec{h}_i, \tilde{\phi}_i\}^{-1}\{\vec{y}_r, 0\})\,d\tilde{\phi}_i. \tag{2}$$

are determined. The number of normals of net planes $\vec{h}_i$, $i = 1, \cdots, I$ "visible" for the experiment and the quantity of measured pole directions $\vec{y}_l$, $r = 1, \cdots, R(i)$ is restricted by manifold experimental conditions. Under all circumstances it is necessary to know if the measured data are sufficient for QTA. Moreover the knowledge of the minimal expense of measurement i.e. of the minimal pole figure ranges (MPR) is important for optimizations of texture measurements. Starting only from principles of crystal geometry the determination of MPR is demonstrated in this paper. As an example the modelized ODF of an olivin sample is reproduced from such MPR using a new (geometrical) approach to QTA (Helming and Eschner 1990).

2. DETERMINATION OF A SINGLE ORIENTATION

2.1. *Triclinic case*

We describe an orientation g (cf. appendix) by two longitudes ($0 \leq \alpha, \gamma < 2\pi$) and one latitude ($0 \leq \beta \leq \pi$). In order to determine g therefore two poles $\vec{y}_1$, $\vec{y}_2$ of normales of the net planes $\vec{h}_1$, $\vec{h}_2$ satisfying the equations

$$\vec{y}_1 = g^{-1}\vec{h}_1, \qquad \vec{y}_2 = g^{-1}\vec{h}_2 \quad \text{or} \quad (\vec{y}_1, \vec{y}_2) = g^{-1}(\vec{h}_1, \vec{h}_2) \tag{3}$$

have to be known at least. Because they provide two longitudinal and two latitudinal angles one latitude angle has to be an invariant.

The searched solution g is given by the point of intersection of two PF-threads (cf. (37))

$$g = \{\vec{h}_1, \tilde{\phi}_1\}^{-1}\{\vec{y}_1, 0\} = \{\vec{h}_2, \tilde{\phi}_2\}^{-1}\{\vec{y}_2, 0\} \tag{4}$$

which follow from the equation system (3). It follows that (cf. (27)-(30))

$$\begin{aligned} &\{\vec{h}_1, \vec{h}_2\}\{\tilde{\phi}_1\}^{-1} = \{\tilde{\phi}_2\}^{-1}\{\vec{y}_1, \vec{y}_2\} \\ &= \{\alpha_h - \tilde{\phi}_1, \beta_h, \gamma_h\} = \{\alpha_y, \beta_y, \gamma_y - \tilde{\phi}_2\} \end{aligned} \tag{5}$$

with $\tilde{\phi}_1 = \alpha_h - \alpha_y$, $\tilde{\phi}_2 = \gamma_y - \gamma_h$ and hence

$$\beta_h = \angle(\vec{h}_1, \vec{h}_2) = \beta_y = \angle(\vec{y}_1, \vec{y}_2) \equiv \beta_{12}^* \tag{6}$$

must be true (cf. (28)). The angle β_{12}^* describes the "correlation" of the net planes $\vec{h}_1$, $\vec{h}_2$ and provides the invariant mentioned above.

Further on the invariancy of the correlation of two or more net planes will be described by the sign $\overset{c}{\Longleftrightarrow}$. From

$$(\vec{y}_1, \vec{y}_2) \overset{c}{\Longleftrightarrow} g^{-1}(\vec{h}_1, \vec{h}_2) \overset{c}{\Longleftrightarrow} (\vec{h}_1, \vec{h}_2) \tag{7}$$

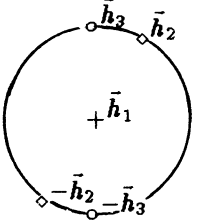
then follows (3) together with (6).

Beside this common condition of the invariancy of the correlation (CIC) special conditions may exist. In our case $\beta_{12}^* \neq 0, \pi$ must be valid for determining g uniquely by using (4) and (5).

Normal scattering causes an additional centrosymmetric symmetry (a "measured" $\vec{y}_i$ may correspond to $\vec{h}_i$ or $-\vec{h}_i$). Then from

$$g = \{-\vec{h}_1, \tilde{\phi}_1\}^{-1}\{\vec{y}_1, 0\} = \{-\vec{h}_2, \tilde{\phi}_2\}^{-1}\{\vec{y}_2, 0\} \tag{8}$$

a second (but false) solution follows where $\tilde{\phi}_1 = \pi - \alpha_h - \alpha_y$, $\tilde{\phi}_2 = \gamma_y - \gamma_h - \pi$ (cf. (27)–(31)). For an unambiguous determination the orientation g by means of diffraction patterns therefore at least three poles $\vec{y}_i$ ($i = 1, \cdots, 3$) belonging to the net planes $\vec{h}_i$ must be known. Their correlation is given completely by the



If the correlation of a vector triple $(\vec{h}_1, \vec{h}_2, \vec{h}_3)$ is given by $\beta^*_{12} = \beta^*_{13} = \pi/2 \neq \beta^*_{13}$ the triple $(\vec{h}_1, -\vec{h}_2, -\vec{h}_3)$ has the same correlation. From this triple a wrong orientation would be determined.

Figure 1 Special condition of correlation

three latitudinal angles $\beta^*_{ij} = \angle(\vec{y}_i, \vec{y}_j)$, $(i, j = 1, \cdots, 3,\ i \neq j)$ and the sign of spatial product $v_{123} = (\vec{y}_1(\vec{y}_2 \times \vec{y}_3))$. Solving the equation of intersection (5)

$$g = \{\pm\vec{h}_i, \tilde{\phi}_i\}^{-1}\{\vec{y}_i, 0\} = \{\pm\vec{h}_j, \tilde{\phi}_j\}^{-1}\{\vec{y}_j, 0\}, \qquad i \neq j \tag{9}$$

only for such net planes which satisfy the CIC

$$(\vec{y}_1, \vec{y}_2, \vec{y}_3) \overset{c}{\Longleftrightarrow} (\pm\vec{h}_1, \pm\vec{h}_2, \pm\vec{h}_3) \tag{10}$$

the searched orientation g may be found uniquely. Obviously, as a special condition $v_{123} \neq 0$ has to be true. Another special condition is explained in Figure 1 which shows that two β^*_{ij} must be unequal to $\pi/2$ at least.

2.2. *Common case*

Crystal symmetry and normal scattering effect that all crystal directions

$$\vec{h}^j_i = g^{-1}_{b_{j'}}\vec{h}_i, \qquad g_{b_{j'}} \in \tilde{\mathscr{G}}_B = C_i \times \mathscr{G}_B,$$
$$j' = 1, \cdots, \tilde{N}_b, j = 1, \cdots, J(\tilde{\mathscr{G}}_B, \vec{h}_i) \tag{11}$$

are equivalent in regard to the Laue group $\tilde{\mathscr{G}}_B$, i.e. we are not able to distinguish between them. The number of all equivalent but not parallel directions $\vec{h}^j_i$ is given by $J(\tilde{\mathscr{G}}_B, \vec{h}_i)$. On the other hand all orientations $g_{B_{j'}}g$ given by the rotational part $G_B(g_{B_{j'}} \in G_B)$ of the crystal class $\mathscr{G}_B$ are equivalent, too. The equation of correlation (7) then reads as follows

$$(\vec{y}_1, \vec{y}_2, \vec{y}_3) \overset{c}{\Longleftrightarrow} (g_{B_{j'}}g)^{-1}(\vec{h}^{j_1}_1, \vec{h}^{j_2}_2, \vec{h}^{j_3}_3)$$
$$\overset{c}{\Longleftrightarrow} (\vec{h}^{j_1}_1, \vec{h}^{j_2}_2, \vec{h}^{j_3}_3) \qquad g_{B_{j'}} \in G_B(\mathscr{G}_B). \tag{12}$$

Special conditions of correlations depend on $\mathscr{G}_B$ and the given set of $\vec{h}_i$. It seems to be difficult to find out all of them. (Helming 1985).

Another "computational" approach is based on the following statement:

> The orientation $g_{B_{j'}}g$ may be found uniquely if all sets of net planes $(\pm\vec{h}_1, \vec{h}^{j_2}_2, \vec{h}^{j_3}_3)$ possessing the same correlation as the set $(\vec{h}_1, \vec{h}_2, \vec{h}_3)$ (or its poles $(\vec{y}_1, \vec{y}_2, \vec{y}_3)$) may be transferred into each other by pure rotations $g_{B_{j'}} \in G_B$ only.

However, this is impossible for crystal classes of the type III (C_s, C_{2v}, . . . , T_d) as shown (Matthies and Helming 1982). In these cases the half of all sets provide false solution although they satisfy the CIC. On the other hand in some cases two net planes are sufficient for the determination of g, namely, if $\vec{h}_1 \times \vec{h}_2$ is parallel to a C_2-axis of the crystal class. E.g. for $\mathscr{G}_B = O_h$ and $\vec{h}_i^1 = [111]$, $\vec{h}_i^2 = [\bar{1}11]$ the equations (4) and (8) give equivalent orientations because $\vec{h}_i^1 \times \vec{h}_i^2$ is parallel to the direction [011] describing a C_2-axis $\in O_h$.

With the help of a computer program (called UNIQUE), developed on the basis of the statement given above, the CIC and the uniqueness of the solution (CICU, sign $\overset{cu}{\Longleftrightarrow}$) may be proved for all Laue groups $\bar{\mathscr{G}}_B = \mathscr{G}_B \times C_i$. Starting from an arbitrary set of three (or two) net planes $(\vec{h}_1, \vec{h}_2, \vec{h}_3)$ all sets $(\pm\vec{h}_1, \vec{h}_2^{j_2}, \vec{h}_3^{j_3})$ satisfying the CIC can be determined and must be tested if they may be transferred into $(\vec{h}_1, \vec{h}_2, \vec{h}_3)$ by a rotational element $g_{B_j'} \in G_B$. That means the program checks the CICU

$$(\vec{h}_1, \vec{h}_2, \vec{h}_3) \overset{cu}{\Longleftrightarrow} (\pm\vec{h}_1, \vec{h}_2^{j_2}, \vec{h}_3^{j_3}) \qquad j = 1, \cdots, J(\bar{\mathscr{G}}_B, \vec{h}_i) \tag{13}$$

for providing one equivalent solution $g_{B_j'}g$. One or more $\vec{h}_i$ have to be exchanged if the CICU is not satisfied. In the other case a searched orientation $g_{B_j'}g$ can be determined taking two $\vec{h}_i^j$ from a possible set and solving the corresponding equation of intersection (4, 5).

3. NECESSARY CONDITION FOR QTA

I pole figures $\tilde{P}_{\vec{h}_i}(\vec{y})$ $(i = 1, \cdots, I)$ may be given in the pole figure ranges Y_i to determine $f(g)$. The Y_i could have a complex form, but mostly they are described by simple zones or calottes of the pole sphere. Considering the inversion symmetry caused by the normal scattering we use only one half sphere for the description the Y_i.

Following the conclusions of section 2 we postulate a necessary condition for the QTA:

> Starting from I pole figures $\tilde{P}_{\vec{h}_i}(\vec{y})$ the ODF may be recalculated only if all poles $\vec{y}_m = g^{-1}\vec{h}_i^j$ with $\vec{y}_m \in Y_i$, $m = 1, \cdots, M(g)$ are sufficient for an unique determination of every orientation $g \in G$ (or $g_{B_j'}g$).

With other words the equation system

$$(\ldots, \vec{y}_m, \ldots) = (g_{B_j'}g)^{-1}(\ldots, \vec{h}_{i_m}^{j_m}, \ldots) \tag{14}$$

must satisfy the CICU $(\ldots, \vec{y}_m, \ldots) \overset{cu}{\Longleftrightarrow} (\ldots, \vec{h}_{i_m}^{j_m}, \ldots)$ for each $g \in G$. Using the program UNIQUE this can be proved for a given set of Y_i in a simple manner.

In the case of a sample symmetry G_A, $(g_{A_k} \in G_A)$ instead of $\vec{y}$ we "see" $\vec{y}_k = g_{A_k}\vec{y}$ or because of the Friedels law $-\vec{y}_k$. Then the Y_i may be "completed" by $g_{A_k} \in G_A$ and by the inversion to get the corresponding $Y_i^{C_i}$ for triclinic sample symmetry. This Y_i will be checked for satisfying the CICU as described above.

4. MINIMAL POLE FIGURE RANGES

For optimizing texture measurements it is necessary to find MPR satisfying CICU. Starting from only one pole figure these ranges were calculated by Vadon for the reflection case of scattering and called minimal pole density sets MPDS (Vadon 1981). Their ranges are described by θ_i^R with $\vec{y}=(\theta_y, \phi_y)\in Y_i$, $0\le\theta_y\le\theta_i^R$. For the transmition case we have $\theta_i^T\le\theta_y\le\pi/2$ (see Helming 1982). MPDS only may be found for a small set of net planes and crystal classes (cubic, hexagonal, tetragonal). For determining the more general MPR Y_i^* the following statement may be used:

> For the case of triclinic sample symmetry all MPR Y_i^* have to be symmetrical to a sample fixed axis $\vec{n}$, that means they always appear in form of zones or calottes on the pole sphere possessing a common centre given by $\vec{n}$.

Taking $\vec{n}\parallel\vec{z}_A$ the angle α turns all poles $\vec{y}$ (or all Ranges Y_i) about the $\vec{n}$-axis

$$\vec{h}=g\vec{y}=\{\alpha, \beta, \gamma\}(\theta_y, \phi_y)=\{0, \beta, \gamma\}(\theta_y, \phi_y^*) \tag{15}$$

and because for triclinic sample symmetry we have $0\le\alpha<2\pi$. For the longitude $\phi_y^*=\phi_y-\alpha$ follows $0\le\phi_y^*<2\pi$. Therefore the calculation of MPR is confined to the calculation of the range of the latitude θ_y

$$\theta_s\le\theta_y\le\theta_e,\ \theta_y\le\pi/2 \tag{16}$$

with (see app. (35))

$$\theta_y=\angle(\vec{g}^*, \vec{h}),\ \vec{g}^*=(\beta, \pi-\gamma) \tag{17}$$

Commonly one of the limits θ_s or θ_e is given by the conditions of the experiment (e.g. $\theta_s=0$ for reflection, $\theta_e=\pi/2$ for transmission measurement). The algorithm for the determination of the other limit reads as follows. For a given $\vec{g}^*$ all angles $\Delta\theta_i^j(\vec{g}^*)$ are determined by

$$\Delta\theta_i^j(\vec{g}^*)=\angle(\vec{g}^*, \vec{h}_i^j)-\theta_s, \qquad \theta_s\text{-fixed}$$

or

$$\Delta\theta_i^j(\vec{g}^*)=\theta_e-\angle(\vec{g}^*, \vec{h}_i^j), \qquad \theta_e\text{-fixed}$$

$$i=1,\cdots,I,\ j=1,\cdots,J(\mathscr{G}_B, \vec{h}_i) \tag{18}$$

and sorted

$$\Delta\theta_{i_1}^{j_1}(\vec{g}_1^*)\le\Delta\theta_{i_2}^{j_2}(\vec{g}_2^*)\le\cdots\le\Delta\theta_{i_M}^{j_M}(\vec{g}_M^*) \tag{19}$$

with $M=M(g)=M(\vec{g}^*)$ (cf. section 3). For a great M the sorting may be stopped after $M'\le M$ (we used $M'=7$). Taking the corresponding net planes of the first three (or two) $\Delta\theta_i^j(\vec{g}^*)$ the CICU has to be proved:

$$(\vec{h}_{i_1}, \vec{h}_{i_2}, \vec{h}_{i_3})\overset{cu}{\Longleftrightarrow}(\pm\vec{h}_{i_1}, \vec{h}_{i_2}^{j_2}, \vec{h}_{i_3}^{j_3}) \tag{20}$$

One or more net planes in (20) have to be exchanged by others (following from (19)) to satisfy CICU. The corresponding $\Delta\theta_{i_m}^{j_m}(\vec{g}_m^*)$ are saved if they are greater than the value $\Delta\theta_i$ saved before

$$\Delta\theta_{i_m}^{j_m}(\vec{g}_m^*)\ge\Delta\theta_i\Rightarrow\Delta\theta_i:=\Delta\theta_{i_m}^{j_m}(\vec{g}_m^*) \tag{21}$$

At last we return to the beginning of the algorithm with another $\vec{g}^*\Rightarrow\vec{g}^*+\Delta\vec{g}^*$. $\vec{g}^*$ has to run through all β- and γ-values of the elementary region (Matthies, Vinel and Helming 1987) of the corresponding crystal symmetry.

5. AN EXAMPLE

We consider a polycrystalline sample of olivin (crystal class $\mathscr{G}_B = D_{2h}$, lattice parameter relations $c/a = 5.99/4.76$ and $c/b = 5.99/10.21$). Its texture shall be measured in reflection arrangement with $\theta_s = 0$. Eight Bragg reflections may be analysed considered in six pole figures:

1. (021) 2. (101) 3. (111)/(120)
4. (002)/(121) 5. (130) 6. (112).

The third and fourth pole figure both include two closed together reflections. The corresponding normals of net planes $\vec{h}_i$ and it's equivalent directions are shown in regard to K_B in Figure 2. We computed the latitudes $\Delta\theta_i^j(\vec{g}^*)$ for all possible $\vec{g}^*$ to determine the extremal values $\Delta\theta_i(\Delta\vec{g}^* \approx 1.5°)$:

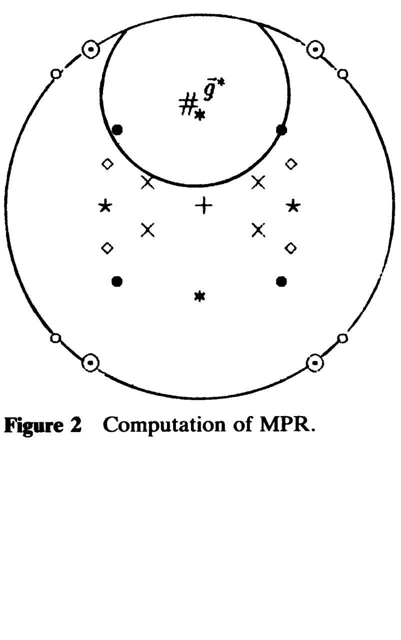
hkl	*021*	*101*	*111*	*120*	*002*	*121*	*130*	*112*
$\theta_e = \Delta\theta_i$	40.8	40.5	41.1	42.1	38.0	**44.5**	43.8	43.8

The maximum of 44.5° is provided by the (121)-reflection of the fourth PF and may be found at $\vec{g}^* = (55°, 96.1°)$. Within the plotted circle (radius 44.5°, centre $\vec{g}^*$) in Fig. 2 the directions $\vec{h}_i = (021)$, $(\bar{1}21)$ and (121) are situated which are sufficient for the unambiguous determination of all orientations: $g = \{\ldots, 55°, 83.9°\}$.

By means of Gauss and Lorentz shaped standard functions (Matthies, Vinel and Helming 1987) f_k^G, f_k^L, $\tilde{P}_k^G$, $\tilde{P}_k^L$ an olivin-ODF consisting of two components

$$f(g) = \sum_k^{K=2} [G_k f_k^G(g_k, b_k) + L_k f_k^L(g_k, b_k)] + F,$$

$$G_k + L_k = 1, \int f(g)dg = 8\pi^2 \qquad (22)$$



The arrangement of the eight net planes $\vec{h}_i$ ($\vec{x}_B$ points to the right, $\vec{y}_B$ upward) of the described example:
∗-(021) ★-(101) ◇-(111)
○-(120) +-(002) ●-(121)
⊙-(130) ×-(112)
Within the plotted circle (radius 44.5°, centre # at $\vec{g}^* = (55°, 96.1)$) the $\vec{h}_i = (021)$, (121) are situated which are sufficient for the unambiguous determination of all orientations: $g = \{\ldots, 55°, 83.9°\}$.

Figure 2 Computation of MPR.

and the corresponding diffraction pole figures

$$\tilde{D}_j(\vec{y}) = n_j\left(\sum_i^I q_{ij} \sum_k^{K=2} [G_k \tilde{P}_k^G(g_k, b_k, \vec{h}_i) + L_k(\tilde{P}_k^L(g_k, b_k, \vec{h}_i)] + F\right),$$

$$\sum_i^I q_{ij} = 1, \quad \int_{Y_i} \tilde{P}_{\vec{h}_i}(\vec{y})\, d\vec{y} = 4\pi \tag{23}$$

were constructed. The parameters of the texture: G_k/L_k (Gauss/Lorentz part), g_k (component position), b_k (halfwidth), F (background) and of the pole figures: n_j (PF-norm), q_{ij} (PF-part) are given in Table 1. For one component we have $\beta_k = 55°$ and $\gamma_k = 83.9°$ a mostly "unfavourable" orientation for the MPR calculated above. For reconstructing the ODF (all parameters of the Table 1 are unknown now) a new approach (Helmig and Eschner 1990) was used basing on an optimization by means of standard functions with a direct treatment of the pole figures. All "experimental" pole figures were calculated for a "thinned" grid of measurement ($\Delta\vec{y} \approx 5°$) within the range Y_i^*: $0° \leq \theta_y \leq 45°$, $0° \leq \phi_y \leq 360°$ (Figure 3). Starting from this data the ODF was determined. All recalculated parameters are given in Table 1 (case refl.). The figures of the recalculated PF are not distinguishable from those of the experimental PF.

Considering the case of transmission measurement ($\theta_e = 90°$) for MPR we get:

hkl	*021*	*101*	*111*	*120*	*002*	*121*	*130*	*112*
$\theta_s = (90° - \Delta\theta_i)$	**71.2**	78.3	76.4	73.9	73.0	72.0	74.2	73.1

The maximal $\Delta\theta_i$ is given by the (021) reflex in the first PF. Starting from PF within the ranges: Y_i^*: $70° \leq \theta_y \leq 90°$, $0° \leq \Phi_y \leq 360°$ we reproduced the ODF described in Table 1 (case trans.).

Table 1 Parameters of simulated and recalculated ODF and PF

Texture	g_k	b_k	G_k/L_k	*F*
model	{43.39, 55.0, 83.90} {53.86, 90.00, 25.90}	23.00° 18.00°	0.332/0.263 0.134/0.095	0.176
refl.	{43.40, 55.00, 83.89} {53.85, 89.99, 25.03}	23.22° 18.23°	0.341/0.250 0.140/0.083	0.186
trans.	{43.37, 54.98, 83.93} {53.84, 90.00, 25.05}	23.27° 18.17°	0.344/0.244 0.138/0.087	0.187

Pole figures	n_1	n_2	$n_3(q_{33})$	$n_4(q_{54})$	n_5	n_6
model	2220	798	1540(0.5077)	2184(0.7408)	6848	4588
refl.	2235	805	1552(0.5084)	2195(0.7403)	6897	4626
trans.	2237	804	1551(0.5087)	2201(0.7409)	6890	4630

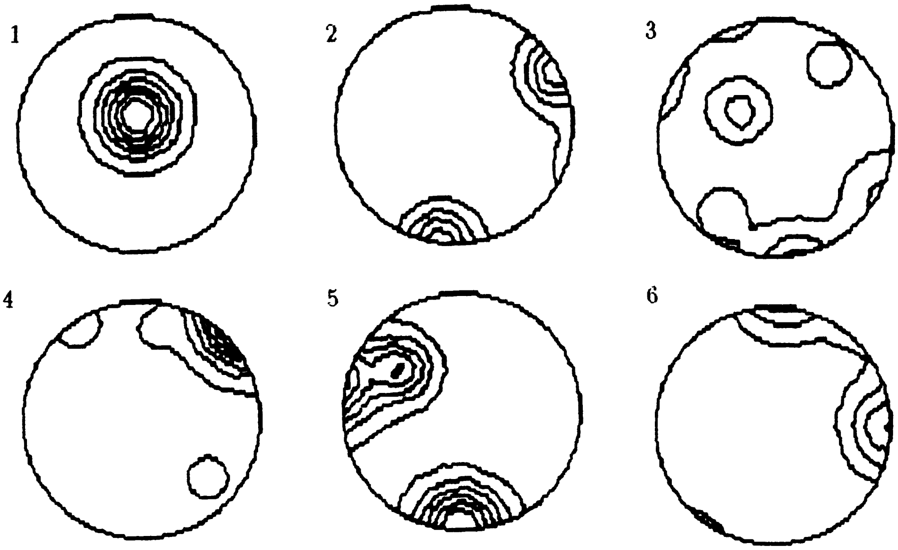


Figure 3 Experimental PF of the modelized sample. Contour lines: 1, 2, ... $Y_i^*: 0 \leq \theta_y \leq 45°$, $0 \leq \phi_y \leq 360°$.

6. CONCLUSIONS

The determination of MPR follows from the necessary condition that every single orientation $g \in G$ must be determinable at least. On the other hand special, sufficient conditions may exist for various reproduction methods (e.g. minimal number of pole figures or pole directions $\vec{y}_r$). For this cases MPR may not be sufficient for determining the ODF.

The *resolution* of the ODF-determination is connected with the density of the measured pole directions $\vec{y}_r$ (Matthies, Vinel and Helming 1987). If the maximal angular distance of the measured points $\vec{y}_r$ is given by $\Delta\vec{y}$ the attainable resolution is approximately given by $2\Delta\vec{y}$. For an optimized measurement an equidistant grid is preferred. The smaller the expected halfwidth of the components of the searched ODF the higher the density of the measured grid has to be. Considering this rules ODF's may be determined from MPR with minimal effort. The quality of a result may be tested taking larger and/or more pole figures in a more densed grid of measurement and repeating the ODF-reproduction with this extended pole figure ranges.

APPENDIX

An orientation g of a crystal fixed coordinate system K_B in regard to the sample fixed one K_A may be described by three Eulerian angles α, β and γ. Two of them are longitudes ($0 \leq \alpha, \gamma < 2\pi$), one angle is a latitude ($0 \leq \beta \leq \pi$). They describe three successive rotations about the topical $\vec{z}$-, $\vec{y}$- and $\vec{z}$-axis turning K_A parallel to K_B. Combining β and α to a formal direction $\vec{g} = (\beta, \alpha)$ we have

$$g = \{\alpha, \beta, \gamma\} = \{\vec{g}, \gamma\} \tag{24}$$

and for the inverse orientation

$$g^{-1} = \{-\gamma, -\beta, -\alpha\} = \{\pi - \gamma, \beta, \pi - \alpha\} = \{\vec{g}^*, \pi - \alpha\} \tag{25}$$

For $\beta = 0$ only one rotation about the $\vec{z}_A$-axis is used

$$\{\alpha, 0, \gamma\} = \{\alpha + \gamma, 0, 0\} = \{\alpha + \gamma\} \tag{26}$$

We define an "elementary product" of rotations by

$$g = \{\vec{g}_2, 0\}\{\vec{g}_1, 0\}^{-1} = \{\alpha_g, \beta_g, \gamma_g\} = \{\vec{g}_1, \vec{g}_2\} \tag{27}$$

The latitudinal angle β_g is given by the angle between $\vec{g}_1$ and $\vec{g}_2$

$$\beta_g = \angle(\vec{g}_1, \vec{g}_2), \cos\beta g = \cos(\alpha_2 - \alpha_1)\sin\beta_1\sin\beta_2 + \cos\beta_1\cos\beta_2. \tag{28}$$

Hence we have for α_g and γ_g

$$\begin{aligned}
\sin\beta_g \sin\alpha_g &= \sin(\alpha_2 - \alpha_1)\sin\beta_2,\\
\sin\beta_g \cos\alpha_g &= \cos(\alpha_2 - \alpha_1)\cos\beta_1\sin\beta_2 - \sin\beta_1\cos\beta_2;\\
\sin\beta_g \sin\gamma_g &= -\sin(\alpha_2 - \alpha_1)\sin\beta_1,\\
\sin\beta_g \cos\gamma_g &= -\cos(\alpha_2 - \alpha_1)\sin\beta_1\cos\beta_2 + \cos\beta_1\sin\beta_2.
\end{aligned} \tag{29}$$

For $\beta_g = 0$ (upper sign) or $\beta_g = \pi$ (lower sign) we obtain

$$\begin{aligned}
\pm\sin(\alpha_g \pm \gamma_g) &= \sin(\alpha_2 - \alpha_1)\cos\beta_2,\\
\pm\cos(\alpha_g \pm \gamma_g) &= \cos(\alpha_2 - \alpha_1)\cos\beta_1\cos\beta_2 + \sin\beta_1\sin\beta_2.
\end{aligned} \tag{30}$$

Some useful relations for the elementary product are

$$\begin{aligned}
\{\vec{g}_1, \vec{g}_2\}^{-1} &= \{\vec{g}_2, \vec{g}_1\},\\
\{-\vec{g}_1, -\vec{g}_2\}^{-1} &= \{\pi - \alpha_g, \beta_g, \pi - \gamma_g\},\\
\{-\vec{g}, \vec{g}\} = \{\vec{g}, -\vec{g}\} &= \{\pi, \pi, 0\}.
\end{aligned} \tag{31}$$

The common product of two rotations (rotation of an orientation) thus

$$\begin{aligned}
\{\alpha_2, \beta_2, \gamma_2\}\{\alpha_1, \beta_1, \gamma_1\} &= \{\alpha_2, \beta_2, \gamma_2\}\{\pi - \gamma_1, \beta_1, \pi - \alpha_1\}^{-1}\\
&= \{\gamma_2\}\{\vec{g}_2, 0\}\{\vec{g}_1^*, 0\}^{-1}\{\pi - \alpha_1\}^{-1}\\
&= \{\gamma_2\}\{\vec{g}_1^*, \vec{g}_2\}\{\alpha_1 - \pi\}.
\end{aligned} \tag{32}$$

For a fixed orientation g the direction $\vec{y}$ in regard to K_A is given in K_B by the direction $\vec{h}$

$$\vec{h} = (\theta_h, \phi_h) = g\vec{y} = g(\theta_y, \phi_y). \tag{33}$$

With (24) and (25) we have for the latitudes θ_h and θ_y

$$\theta_h = \angle(\vec{g}, \vec{y}), \tag{34}$$

and

$$\theta_y = \angle(\vec{g}^*, \vec{h}). \tag{35}$$

If a direction is given in K_A as well as in K_B because $\vec{y} \parallel \vec{h}$ from

$$(0, 0) = \{\vec{y}, \phi'\}\vec{y} = \{\vec{h}, \phi''\}\vec{h}, \qquad 0 \leq \phi', \phi'' < 2\pi \tag{36}$$

we obtain all orientations

$$g(\tilde{\phi}) = \{\vec{h}, \tilde{\phi}\}^{-1}\{\vec{y}, 0\}, \qquad 0 \leq \tilde{\phi} \leq 2\pi \tag{37}$$

satisfying the eq. (33). The orientations $g(\tilde{\phi})$ describe a closed "thread" in the space of orientations to be in possession of the property

$$\{\vec{h}, \tilde{\phi}\}^{-1}\{\vec{y}, 0\} = \{-\vec{h}, \tilde{\phi}\}^{-1}\{-\vec{y}, 0\} \tag{38}$$

follows from (31), (37) and

$$(\pi, 0) = \{-\vec{y}, \phi'\}\vec{y} = \{-\vec{h}, \phi''\}\vec{h}. \tag{39}$$

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