

MINIMAL POLE FIGURE RANGES FOR QUANTITATIVE TEXTURE ANALYSIS

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Abstract

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.

1 REPRODUCTION PROBLEM

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) $f(g)$

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

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.

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)

$$\begin{aligned} \tilde{P}_{\bar{h}_i}(\bar{y}_i) &= \left[P_{\bar{h}_i}(\bar{y}_i) + P_{-\bar{h}_i}(\bar{y}_i) \right] / 2, \\ \text{with } P_{\bar{h}_i}(\bar{y}_i) &= \frac{1}{2\pi} \int_{\bar{\phi}_i=0}^{2\pi} f(\{\bar{h}_i, \bar{\phi}_i\}^{-1}\{\bar{y}_i, 0\}) d\bar{\phi}_i. \end{aligned} \quad (2)$$

are determined. The number of normals of net planes $\bar{h}_i, i = 1, \dots, I$ "visible" for the experiment and the quantity of measured pole directions $\bar{y}_i, l = 1, \dots, L(i)$ is restricted by manifold experimental conditions. Under all circumstances it is necessary to know are the measured data 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 modeled ODF of a olivin sample is reproduced from such MPR using a new (geometrical) approach to QTA¹.

2 DETERMINATION OF A SINGLE ORIENTATION

Crystal symmetry and normal scattering effect that all crystal directions

$$\vec{h}_i^j = \tilde{g}_{b,j}^{-1} \vec{h}_i, \quad \tilde{g}_{b,j} \in \tilde{G}_B = C_i \times G_B, j' = 1 \dots \tilde{N}_b, j = 1 \dots J(\tilde{G}_B, \vec{h}_i) \quad (3)$$

are equivalent in regard to the Laue group $\tilde{G}_B = C_i \times G_B$ (G_B - crystal class), i.e. we are not able to distinguish between them. The number of all equivalent but not parallel directions \vec{h}_i^j is given by $J(\tilde{G}_B, \vec{h}_i)$. 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 G_B are equivalent too². To determine $g_{B,j}, g$ the equation system

$$(\vec{y}_1, \vec{y}_2, \vec{y}_3) = (g_{B,j}, g)^{-1} (\vec{h}_1^{j_1}, \vec{h}_2^{j_2}, \vec{h}_3^{j_3}) \quad g_{B,j} \in G_B(G_B) \quad (4)$$

must be solved. It seems to be difficult to find out all conditions for the uniqueness of the solution in an analytical manner². Another "computational" approach is based on the following condition of the invariancy of correlation and uniqueness (CICU, sign $\overset{c}{\rightleftharpoons} \overset{u}{\rightleftharpoons}$):

The orientation $g_{B,j}, g$ may be found uniquely if all sets of net planes $(\pm \vec{h}_1, \vec{h}_2^{j_2}, \vec{h}_3^{j_3})$ 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.

With the help of a computer program (called UNIQUE) this condition (CICU) may be proved for all Laue groups $\tilde{G}_B = G_B \times C_i$. Starting from a arbitrary set of three (or two) net planes $(\vec{h}_1, \vec{h}_2, \vec{h}_3)$ all sets $(\pm \vec{h}_1, \vec{h}_2^{j_2}, \vec{h}_3^{j_3})$ possessing the same correlation are determined and are 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

$$(\vec{h}_1, \vec{h}_2, \vec{h}_3) \overset{c}{\rightleftharpoons} \overset{u}{\rightleftharpoons} (\pm \vec{h}_1, \vec{h}_2^{j_2}, \vec{h}_3^{j_3}) \quad j = 1 \dots J(\tilde{G}_B, \vec{h}_i) \quad (5)$$

for providing one equivalent solution $g_{B,j}, g$. One ore more \vec{h}_i have to be exchanged if the CICU is not satisfied.

3 NECESSARY CONDITION FOR QTA

I pole figures $\tilde{P}_{\vec{h}_i}(\vec{y})$ ($i = 1 \dots I$) 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 descripton the Y_i .

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

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

With other words the equation system

$$(\dots, \bar{y}_m, \dots) = (g_{B_i}, g)^{-1}(\dots, \bar{h}_{i_m}^j, \dots) \quad (6)$$

must satisfy the CICU $(\dots, \bar{y}_m, \dots) \xleftrightarrow{g} (\dots, \bar{h}_{i_m}^j, \dots)$ for each $g \in G$. Using the program UNIQUE this can be proved for a given set of Y_i in a simple manner.

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 MPDS⁴. Their ranges are described by ϑ_i^R with $\bar{y} = (\vartheta_y, \varphi_y) \in Y_i$, $0 \leq \vartheta_y \leq \vartheta_i^R$. For the transition case we have $\vartheta_i^T \leq \vartheta_y \leq \pi/2$ (see ²). 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 \bar{n} , that means they always appear in form of zones or calottes on the pole sphere possessing a common centre given by \bar{n} .

Therefore the calculation of MPR is confined to the calculation of the range of the latitude ϑ_y

$$\vartheta_s \leq \vartheta_y \leq \vartheta_e, \quad \vartheta_y \leq \pi/2 \quad (7)$$

with

$$\vartheta_y = \angle(\bar{g}^*, \bar{h}), \quad \bar{g}^* = (\beta, \pi - \gamma) \quad (8)$$

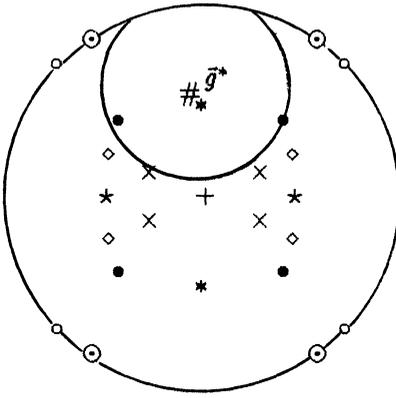
Commonly one of the limits ϑ_s or ϑ_e is given by the conditions of the experiment (e.g. $\vartheta_s = 0$ for reflection, $\vartheta_e = \pi/2$ for transmission measurement, cf. fig.1). The determination of the other limit for all possible \bar{g}^* can be done in a numerical manner using (8).

5 AN EXAMPLE

We consider a polycrystalline sample of olivin (crystal class $\mathcal{G}_B = D_{2h}$, 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 $\vartheta_s = 0$. 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 \bar{h}_i and it's equivalent directions are shown in regard to K_B in Fig.1. We computed the latitudes ϑ_y for all possible \bar{g}^* to determine the extremal values ϑ_e ($\Delta\bar{g}^* \approx 1.5^\circ$):



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 $\vec{g}^* = (55^\circ, 96.1^\circ)$) the $\vec{h}_i = (021), (121)$ are situated which are sufficient for the unambiguous determination of all orientations :
 $g = \{ \dots, 55^\circ, 83.9^\circ \}$.

Figure 1: Computation of MPR

hkl	021	101	111	120	002	121	130	112
ϑ_e	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 $\vec{g}^* = (55^\circ, 96.1^\circ)$. Within the plotted circle (radius 44.5° , centre \vec{g}^*) in fig.1 the directions $\vec{h}_i = (021), (121)$ are situated which are sufficient for the unambiguous determination of all orientations : $g = \{ \dots, 55^\circ, 83.9^\circ \}$.

By means of Gauss and Lorentz shaped standard functions⁵ $f_k^G, f_k^L, \tilde{P}_k^G, \tilde{P}_k^L$ an olivin-ODF consisting of two components

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

$$G_k + L_k = 1, \quad \int f(g) dg = 8\pi^2 \quad (9)$$

and the corresponding diffraction pole figures

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

$$\sum_i^I q_{ij} = 1, \quad \int_{Y_i} \tilde{P}_{\vec{h}_i}(\vec{y}) d\vec{y} = 4\pi \quad (10)$$

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 $\beta_k = 55^\circ$ and $\gamma_k = 83.9^\circ$ a mostly "unfavourable" orientation for the MPR calculated above. For reconstructing the ODF (all parameters of the table 1 are unknown now) a new approach¹ 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 ($\Delta\vec{y} \approx 5^\circ$) within the range Y_i^* : $0^\circ \leq \vartheta_y \leq 45^\circ$, $0^\circ \leq \varphi_y \leq 360^\circ$ (Fig. 2). Starting from this data the ODF was determined. All recalculated parameters are given in the table 1 (case refl.). The figures of the recalculated PF are not distinguishable from those of the experimental PF.

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

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

Table 1: Parameters of simulated and recalculated ODF and PF

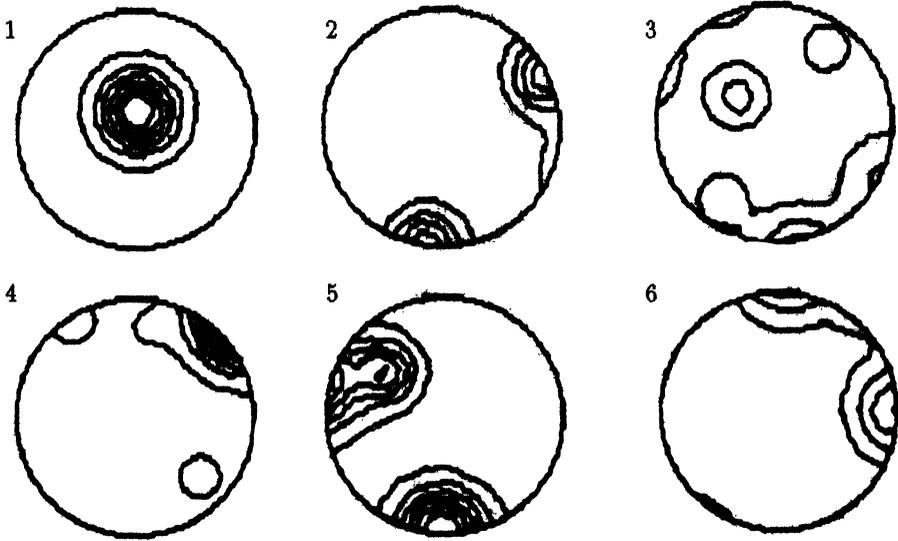


Figure 2: Experimental PF of the modeled sample. Contour lines : 1, 2, ...
 Y_i^+ : $0 \leq \vartheta_y \leq 45^\circ$, $0^\circ \leq \varphi_y \leq 360^\circ$.

Considering the case of transmission measurement ($\vartheta_e = 90^\circ$) for MPR we get:

hkl	021	101	111	120	002	121	130	112
ϑ_s	71.2	78.3	76.4	73.9	73.0	72.0	74.2	73.1

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

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 \bar{y}_i). 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 \bar{y}_i ⁵. If the maximal angular distance of the measured points \bar{y}_i is given by $\Delta\bar{y}$ the attainable resolution is approximately given by $2\Delta\bar{y}$. 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.

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