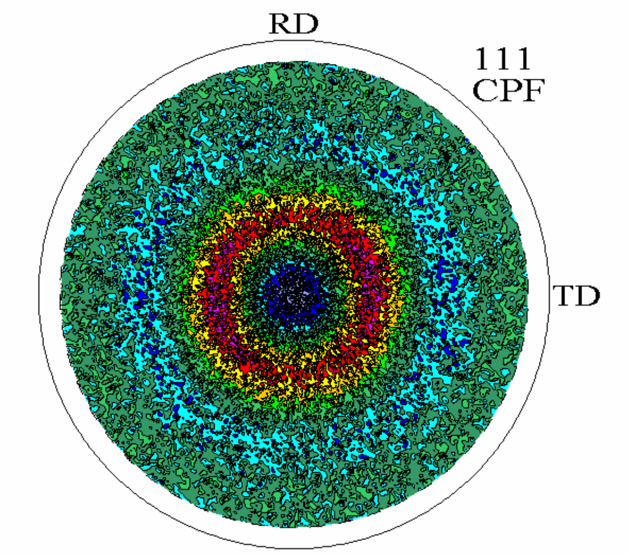
L
A
B
SOFT

LaboTex

Version 3.0

The Texture Analysis Software for Windows



Fundamentals of 3-D Texture Analysis. Symmetry aspects of 3-D texture analysis.

Krzysztof Pawlik

LaboSoft s.c.
Telephone: +48-502-311838
Telefax: +48-12-3953891
E-mail: office@labosoft.com.pl

Fundamentals of 3-D Texture Analysis

1. Orientation

The crystallographic texture is a quantity describing statistically orientation of objects called crystallites. A crystallite can be defined as a region of common crystallographic orientation *g*. If we desire to describe completely *i.e.* statistically the orientations of crystallites in polycrystalline material, we have to specify the relevant orientation *g* for each crystallite. In order to define the orientation *g* it is necessary to fix two Cartesian coordinate systems. The first one K_S is fixed to the sample and the second one K_C is fixed to each individual crystallite. The orientation *g* is defined as a proper rotation (excluding translations and inversion transformations) which transforms the K_S system into the K_C system:

$$K_C = g\ K_S \tag{1}$$

The rotation g can be described in different sets of three angular parameters. The most frequently applied parameterization is the set of Euler angles:

$$g = g(\varphi_1, \Phi, \varphi_2) \tag{2}$$

2. Orientation Distribution Function (ODF), Pole Figure (PF), Inverse Pole Figure (IPF).

The main quantity describing the texture is three dimensional (3-D) function (function of orientation g in three parameters) - Orientation Distribution Function (ODF). ODF is also called *texture function.* The ODF is defined as a probability density function of orientations. If we denote by *dV* a volume of a crystal element *i.e.* crystallites, which possess orientations in the range *dg* and by *V* the total volume of a sample consisting of all crystallites then the Orientation Distribution Function *f*(*g*) is defined as:

$$\frac{dV}{V} = f(g)\,dg \tag{3}$$

The ODF characterizes the polycrystalline state of the material from the point of view of the distribution of its crystallographic orientations. The ODF can be obtained in two ways. The first one is based on measurements (using electronomicroscope diffraction) of statistically large number of so-called individual orientations of crystallites. The second method requires measurement of the so-called Pole Figures (PF) by means of X-ray or neutron diffraction. In the first case the ODF is calculated directly from the quantity of single orientations. In the second case the ODF is calculated by solution of the set of integration equations of the form:

$$PF_h(y) = \frac{1}{2\pi}\int f(g)\,d\gamma \tag{4}$$

The above formula is a mathematical representation the distribution of the crystal direction *h* (vector in the crystal coordinate system K_C) measured in sample direction *y* (vector in the sample coordinate system K_S).

It can be defined second 2-D distribution on the base of ODF. It is called Inverse Pole Figure (IPF):

$$IPF_y(h) = \frac{1}{2\pi}\int f(g)\,d\gamma \tag{5}$$

IPF represents distribution of the sample direction y (vector in the sample coordinate system K_S) measured in crystal direction h (vector in the crystal coordinate system K_C).

3. ODF calculation - Algorithm of the ADC method

The solution of the system of integral equations (4) is not a trivial problem. There are two groups of methods allowing to calculate the ODF *i.e.* indirect methods using the Fourier series analysis and the direct methods.

In the ADC (Arbitrarily Defined Cells) method the ODF calculation proceeds directly in the orientation space (hence the name - the direct method) and distinguishes it from the series expansion method (the Fourier analysis) where the process takes place in the Fourier space and then is transformed to the orientation space. The orientation space is three-dimensional space of Euler angles. According to the principles of the ADC method (Pawlik 1986), both the pole figure and the orientation space are discretized. The orientation space is discretized to cells C_a (where a is the number of a cell). Pole figures are discretized to the domains D_{kie} (where k - numbers the domains, i - numbers the pole figures, e - numbers the symmetrically equivalent poles on the i-th pole figure). Pole figure values P_{kie} correspond to discrete elements (domains D_{kie}) of pole figures. The domains D_{kie} are represented through the projection tubes T_{kie} in the orientation space. The ODF values $f(g)$ correspond to the cells C_a which are discrete elements of the orientation space. Projection tubes T_{kie} are integration tubes (for the above integration equation) in the orientation space. In general, the division of PFs into domains and that of the orientation space into cells are independent of each other hence the Arbitrarily Defined Cells and the ADC method. The projection tubes T_{kie} and the cells C_a are intersecting in the orientation space. Geometrical intersections are quantitatively represented by the weight factors U_{akie} *i.e.* volume fractions of the tubes T_{kie} intersecting C_a cells. The iteration operators of the ADC method based on the above described discretizations are shown below.

The structure of this operator and the principles of the iteration process in the ADC method have been described by Pawlik (1986) and extended by Pawlik *et al.* (1990). A complete process of ODF approximation by the ADC method comprises of the three iteration stages:

1st iteration stage

The ODF calculation by averaging (geometrical) the PF (P_{kie}) values over the pole figures (i = 1, I) and the symmetrically equivalent poles (e = 1, E_i) on each pole figure:

$${}_I f_a^{(1)} = \left\langle \left\langle \left[\sum_{T_{kie}|C_a} U_{akie} P_{kie} \right] \right\rangle_{e=1,E_i} \right\rangle_{i=1,I} \tag{6}$$

$${}_I f_a^{(n+1)} = {}_I f_a^{(n)} \left\langle \left\langle \left[\sum_{T_{kie}|C_a} U_{akie} \frac{P_{kie}}{{}_I P_{kie}^{(n)}} \right] \right\rangle_{e=1,E_i} \right\rangle_{i=1,I} \tag{7}$$

where: $f_a^{(n)}$ - ODF values ascribed to the cell C_a calculated in nth iteration step, $T_{kie}|C_a$ - all T_{kie} tubes intersecting the cell C_a, P_{kie} - experimental PF values, $P_{kie}^{(n)}$ - PF values calculated in nth iteration step from $f_a^{(n)}$ values using discrete form of shown above integral equation:

$$P_{kie}^{(n)} = \frac{1}{V_{kie}} \sum_{T_{kie}|C_a} V_{akie} f_a^{(n)} \tag{8}$$

where: V_{kie} - volume of the tube T_{kie}, V_{akie} - volume of the cell C_a inside a tube T_{kie}.

2nd iteration stage

Ghost correction by selecting a minimal value for each of $f_a^{(n)}$ values:

$${}_{II}P_{kie} = {}_{I}P_{kie}^{(n)} \tag{9}$$

$${}_{II}f_a^{(1)} = \mathrm{Min}\left[\sum_{T_{kie}|C_a} U_{akie}\ {}_{II}P_{kie}\right] \Rightarrow i = i_m,\ e = e_m$$

(10)

$${}_{II}f_a^{(n+1)} = \begin{cases} {}_{II}f_a^{(n)} \text{ if } Q_{II}^{(n)} \geq 1 \\ {}_{II}f_a^{(n)}\ {}_{II}Q_{II}^{(n)} \text{ if } Q_{II}^{(n)} < 1 \end{cases}$$

(11)

$$Qf_{II}^{(n)} = \left[\sum_{T_{kie}|C_a} U_{akie} \frac{{}_{II}P_{kie}}{{}_{II}P_{kie}^{(n)}}\right] \tag{12}$$

3rd iteration stage

The final procedure for the ghost correction and smoothing:

$${}_{III}P_{kie} = {}_{II}P_{kie}^{(n)} \tag{13}$$

$${}_{III}f_a^{(1)} = \begin{cases} {}_{I}f_a^{(n)} \text{ if } {}_{II}f_a^{(n)} \geq 1 \\ {}_{II}f_a^{(n)} \text{ if } {}_{II}f_a^{(n)} < 1 \end{cases} \tag{14}$$

$${}_{III}f_a^{(n+1)} = \begin{cases} {}_{III}f_a^{(n)} Q_{III}^{(n)} \text{ if } {}_{III}f_a^{(n)} \geq 1 \\ {}_{III}f_a^{(n)} \text{ if } {}_{III}f_a^{(n)} < 1 \end{cases} \tag{15}$$

$$Q_{III}^{(n)} = \left\langle \left\langle \left[\sum_{T_{kie}|C_a} U_{akie} \frac{{}_{III}P_{kie}}{{}_{III}P_{kie}^{(n)}}\right] \right\rangle_{e=1,E_i} \right\rangle_{i=1,I} \tag{16}$$

During the iteration process both ODF and the pole figures undergo normalization. The structure of the iteration operator ensures in a natural way the non-negativity of the ODF. In the successive iteration stages the statistical error of the experimental pole figures become averaged, the so-called "ghosts" are corrected basing on the lowest values of the pole figures and finally smoothing of ODF is performed.

From the generality of above formulae it follows that the ODF may be approximated:

- for materials of arbitrary symmetry of the crystal lattice,
- for pole figures of arbitrary symmetry (arbitrary sample symmetry),
- for complete pole figures and incomplete ones (*i.e.* measured using only one diffraction method - reflection or transmission, which simplifies the measurement but gives PF values in incomplete region),
- from one or many pole figures (the number of pole figures is the result of MPDS (Minimal Pole Density Set) criteria

Symmetry aspects of 3-D texture analysis

For defining of the orientation g it is necessary to fix the Cartesian coordinate system K_c to the crystallite. It can be done using elements of the known structure of the corresponding crystal lattice.

These elements may be parts of the elementary cell of the crystal, such as directions of the elementary translations and the lengths of the corresponding basic vectors, directions of rotation axes. The prescription for the orientation of the crystal coordinate system K_c in dependence to the crystal system (CS) may be defined as shown below:

Crystal System(CS) (Crystal Symmetry)	Basic Vectors – lengths $\lvert\mathbf{a}_1\rvert$ $\lvert\mathbf{a}_2\rvert$ $\lvert\mathbf{a}_3\rvert$	Basic Vectors – angles $\lvert\alpha_{23}\rvert$ $\lvert\alpha_{31}\rvert$ $\lvert\alpha_{12}\rvert$	K_c starting set	Space group G_c
Cubic	a a a	$\pi/2$ $\pi/2$ $\pi/2$	$\mathbf{e}_x \parallel \mathbf{a}_1$ $\mathbf{e}_y \parallel \mathbf{a}_2$ $\mathbf{e}_z \parallel \mathbf{a}_3$	O , T
tetragonal	a a c $(a \neq c)$	$\pi/2$ $\pi/2$ $\pi/2$	$\mathbf{e}_x \parallel \mathbf{a}_1$ $\mathbf{e}_y \parallel \mathbf{a}_2$ $\mathbf{e}_z \parallel \mathbf{a}_3$	D_4 , C_4 , D_2 , C_2
orthorhombic	a b c $(a < b < c)$	$\pi/2$ $\pi/2$ $\pi/2$	$\mathbf{e}_x \parallel \mathbf{a}_1$ $\mathbf{e}_y \parallel \mathbf{a}_2$ $\mathbf{e}_z \parallel \mathbf{a}_3$	D_2 , C_2
monoclinic	a b c $(a < b)$	$\pi/2$ $\pi/2$ γ $(\gamma < \pi/2)$	$\mathbf{e}_x \parallel \mathbf{a}_1$ $\mathbf{e}_y = \mathbf{e}_z \mathrm{x}\, \mathbf{e}_x$ $\mathbf{e}_z \parallel \mathbf{a}_3$	C_2 , C_1
triclinic	a b c $(a < b < c)$	α β γ $(\alpha,\beta,\gamma < \pi/2)$	$\mathbf{e}_x = \mathbf{e}_y \mathrm{x}\, \mathbf{e}_z$ $\mathbf{e}_y \parallel \mathbf{a}_3 \mathrm{\ x\ } \mathbf{a}_1$ $\mathbf{e}_z \parallel \mathbf{a}_3$	C_1
hexagonal	a a c	$\pi/2$ $\pi/2$ $2\pi/3$	$\mathbf{e}_x \parallel \mathbf{a}_1$ $\mathbf{e}_y = \mathbf{e}_z \mathrm{x}\, \mathbf{e}_x$ $\mathbf{e}_z \parallel \mathbf{a}_3$	D_6 , C_6 , D_3 , C_3
trigonal	a a a	α α α $(\alpha < 2\pi/3)$	$\mathbf{e}_x \parallel (\mathbf{a}_1 - \mathbf{a}_2)$ $\mathbf{e}_y = \mathbf{e}_z \mathrm{x}\, \mathbf{e}_x$ $\mathbf{e}_z \parallel (\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)$	D_3 , C_3

$\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ - unit vectors of the Cartesian coordinate system K_c
$\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ – unit vectors of the elementary cell
$\lvert\alpha_{23}\rvert$ $\lvert\alpha_{31}\rvert$ $\lvert\alpha_{12}\rvert$ - angles defined between $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ vectors respectively:
$\alpha_{12}=\mathrm{angle}(\mathbf{e}_x, \mathbf{e}_y)$, $\alpha_{23}=\mathrm{angle}(\mathbf{e}_y,\mathbf{e}_z)$, $\lvert\alpha_{31}\rvert=\mathrm{angle}(\mathbf{e}_z,\mathbf{e}_x)$

There exist 32 crystal classes. The properties of symmetry of a given crystal lattice (from these 32 crystal classes) are completely described by one of the 230 possible space groups. A space group contains all symmetry elements (symmetry operations) transforming every (infinite) crystal lattice into itself. From the point of view of orientation g defined as a proper rotation (excluding translation and inversion elements), only 11 possible rotation groups are taken into consideration.

Inside those 11 rotation groups can be defined equivalent sets of 31 independent symmetry elements (31 rotation axes) which exists in each of group in different subset respectively. One of possible sets of symmetry elements is defined in the table below. Group symbols and corresponding crystal system (CS) are the same like in the table above. It corresponds to Schoenfliess symbols..

Symmetry elements for space groups G_c of crystal system (CS) (crystal symmetry):

	$g_c \in G_c$	Space group - G_c										
	symmetry elements	O	T	D_4,	C_4	D_2	C_2	C_1	D_6,	C_6	D_3	C_3
1	E	+	+	+	+	+	+	+	+	+	+	+
2	-1 1 1 C_3	+	+									
3	-1 1 1 C_3^2	+	+									
4	1 1 0 C_2	+		+								
5	0 -1 1 C_2	+										
6	1 0 1 C_2	+										
7	0 0 1 C_4	+		+	+							
8	0 1 1 C_2	+										
9	0 1 0 C_4^3	+										
10	1 0 0 C_2	+	+	+		+			+		+	
11	1 1 -1 C_3	+	+									
12	1 -1 1 C_3^2	+	+									
13	0 0 1 C_2	+	+	+	+	+	+		+	+		
14	1 1 1 C_3^2	+	+									
15	1 1 -1 C_3^2	+	+									
16	1 -1 0 C_2	+		+								
17	1 0 0 C_4	+	+									
18	0 1 0 C_4	+	+									
19	0 0 1 C_4^3	+		+	+							
20	1 0 0 C_4^3	+										
21	-1 0 1 C_2	+										
22	0 1 0 C_2	+	+	+		+			+			
23	1 -1 1 C_3	+	+									
24	1 1 1 C_3	+	+									
25	0 0 1 C_6								+	+		
26	0 0 1 C_3								+	+	+	+
27	0 0 1 C_3^2								+	+	+	+
28	0 0 1 C_6^5								+	+		
29	1-$\sqrt{3}$ 0 C_2								+		+	
30	$\sqrt{3}$-1 0 C_2								+			
31	$\sqrt{3}$ 1 0 C_2								+			
32	1 $\sqrt{3}$ 0 C_2								+		+	

E – means basic orientation
C_i^k – means rotation axis where: i-th fold axis, j-th step (substep) in rotation around i-th axis (i-th=blank means 1st step in rotation)
Numbers before C_i^k mean vector units of the rotation axis C_i^k

ODF describes a statistical distribution of crystallites in a sample, so there may additionally exist an another type of symmetry, so called "sample symmetry" (SS). So there are possible three types of sample symmetry (point groups: C_1, C_2, D_2).
In general when the crystal symmetry is C_1 and the sample symmetry is also C_1 ODF space (Euler angles space - φ_1 , Φ , φ_2) has the following range:

$$0^\circ \leq \varphi_1 \leq 360^\circ \ , \quad 0^\circ \leq \Phi \leq 180^\circ \ , \quad 0^\circ \leq \varphi_2 \leq 360^\circ$$

Making all possible operations on orientation g according to the formula

$$f(g^{ik}) = f(g); \qquad g^{ik} \equiv g_{ci} \bullet g \bullet g_{sk}$$

(i,k - indicate all possibile symmetrical elements of symmetry group of crystal and sample),

ODF space splits into ik equivalent regions all containing the complete information on the ODF.
Each of that region we call “elementary region”. To make complete analysis of the ODF for established crystal system (crystal symmetry) and sample (sample symmetry) it is sufficient to chose one such elementary region (basic region) instead of full ODF space.

The elementary regions - basic regions (theirs ranges) of ODF space (Euler angles space – φ_1 , Φ , φ_2) for the groups G_c of crystal system (CS) (crystal symmetry) and groups G_s of sample symmetry (SS) (pole figure symmetry) are shown in table:

G_c	φ_1			Φ	φ_2
	$G_s=C_1$	$G_s=C_2$	$G_s=D_2$		
O	0°-360°	0°-180°	0°-90°	threefold region in 0°-90°	0°-90°
T				threefold region in 0°-90°	0°-180°
D_4				0°-90°	0°-90°
C_4				0°-180°	0°-90°
D_2				0°-90°	0°-180°
C_2				0°-180°	0°-180°
C_1				0°-180°	0°-360°
D_6				0°-90°	0°-60°
C_6				0°-180°	0°-60°
D_3				0°-90°	0°-120°
C_3				0°-180°	0°-120°

References

1) K.Pawlik - phys.stat.sol.(b) 134 (1986), p.477, "Determination of the Orientation Distribution Function from Pole Figures in Arbitrarily Defined Cells" .
2) K.Pawlik, J.Pospiech, K.Lucke - Proc. of ICOTOM-9, Avignon , France, (1990), p25, "The ODF approximation from pole figures with the aid of the ADC-method".