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THE EFFECT OF SMOOTHING ON ODF REPRODUCTION

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Although the smoothing of experimental pole-density data modifies the primary data set, the effect of such a procedure on the Orientation Distribution Function and on the interpretation of the texture was not considered until recently. The influence of smoothing on texture reproduction will be derived for the case, that the Orientation Distribution Function is approximated by a linear combination of normal distributions (ideal orientation components) and smoothing is carried out with normal distributions, too. The characteristic component parameters are well-suited to indicate changes of the Orientation Distribution Function. The observed texture variations as a consequence of smoothing lead to the conclusion, that moderate smoothing does not falsify the texture. Several possibilities to control the effect of smoothing will be discussed. Based on the visual comparison of smoothed and unsmoothed pole-figures it is argued, that even extreme smoothing may be useful for some purposes.

KEY WORDS: Smoothing, texture approximation by ideal orientation components, normal distribution function, ODF-variation.

INTRODUCTION

Smoothing of experimental pole-density data may be applied for several purposes, *e.g.* to speed up numerical calculations, to reduce statistical noise or to minimize the influence of outliers (high intensity gradients) on Quantitative Texture Analysis (QTA). Since smoothing is carried out independently for each pole-figure (PF), some negative influence on the resulting Orientation Distribution Function (ODF) may not be excluded. One well-known effect is the accentuation of the most prominent features of the texture, which is accepted to be a useful property of smoothing. On the other hand, the loss of substantial details may influence the interpretation of the texture in a negative manner.

Several attempts of pole-figure smoothing were made and its influence on the pole-density distributions was discussed (Welch, 1984, Andonov *et al.*, 1987, Nikolayev and Ullemeyer, 1994, Traas *et al.*, 1994). However, the effect of smoothing on the ODF and on the interpretation of the texture was not considered until recently. This paper tries to derive this influence and to characterize it by suitable indicators. In order to obtain clear and instructive parameters for the description of texture modifications, the ODF is represented as a linear combination of normal distributions, i.e. by a finite number of ideal orientation components (Grewen and Wassermann, 1955). The changes of the component characteristics 'orientation' and 'dispersion of intensity' represent excellent and easy to visualize parameters to describe the effect of smoothing on the ODF.

As an example for such an approach a quartzite sample with a mean grain size of 500 μm (50–5000 μm) was selected. TOF-spectra were recorded for a regular 7.2° – grid at the neutron diffractometer NSHR, which is situated at the pulsed reactor IBR-2 in Dubna, Russia. Details about the applied method and the experimental equipment are given by Feldmann (1989) and Helming *et al.* (1992). From the measured spectra PFs $P_{\vec{h}_i}(\vec{y})$; $i = 1,...,N$ were extracted as a basis for QTA and the ODF $f(g)$ was reproduced from this data set by means of component deconvolution. Subsequently, the PFs were smoothed and the ODF $f^s(g)$ was calculated from the smoothed PFs $P^s_{\vec{h}_i}(\vec{y})$; $i = 1,...,N$ (the unit vector $\vec{h}_i$ represents a direction in the crystal coordinate system, $\vec{y}$ is a sample direction in the sample coordinate system). What is the connection between $f(g)$ and $f^s(g)$, supposing the connection between $P_{\vec{h}_i}(\vec{y})$ and $P^s_{\vec{h}_i}(\vec{y})$ is known? On which scale are the changes of the ODF in dependence upon the amount of smoothing?

For QTA the algorithm developed by Helming and Eschner (1990) was applied. The texture modifications are described by the changes of the component parameters 'orientation' and 'half-width' (g^c and b^c, respectively). In addition, the global error parameter *RP0* (Matthies *et al.*, 1988) is used to characterize the differences between smoothed and unsmoothed PFs and the effect of smoothing as well.

FUNDAMENTALS

ODF approximation by means of normal distributions

The method is based on the *a priori* suggestion, that the ODF may be represented as a linear combination of normal distributions (Bukharova *et al.*, 1988, Helming, 1992, Nikolayev *et al.*, 1992, Eschner, 1993)

$$f(g) \sum_{k=1}^{K} A_k N(g_k,\ \varepsilon_k,\ g), \tag{1a}$$

where A_k are weights. The central normal distribution has the form

$$N(g_k,\ \varepsilon_k,\ g) = \sum_{l=0}^{\infty} (2l+1)\exp(-l(l+1)\,\varepsilon_k^2)\ \frac{\sin[(l+1/2)\,t_k]}{\sin[t_k/2]} \tag{1b}$$

with $\cos t_k = (Tr[g_k^{-1}g]-1)/2$. The parameters g_k and ε_k possess a clear geometrical sense, namely, g_k is the position of the peak in orientation space, ε_k describes the dispersion of the intensity with increasing distance from the central position.

From the relation between the ODF and the PFs we obtain

$$(4\pi)^{-1} P_{\vec{h}_i}(\vec{y}) = (8\pi^2)^{-1} \int_{SO(3)} \{\delta(\vec{h}_i - g\vec{y}) + \delta(\vec{h}_i + g\vec{y})\} f(g)dg, \tag{2}$$

here $SO(3)$ describes the rotation group. The expression for the PFs is

$$P_{\vec{h}_i}(\vec{y}) = \sum_{k=1}^{K} A_k P^N_{\vec{h}_i}(g_k,\ \varepsilon_k,\ \vec{y}). \tag{3}$$

The PF for the central normal distribution may be written as

$$P^N_{\vec{h}_i}(g_k,\ \varepsilon_k,\ \vec{y}) = \sum_{l=0}^{\infty} (2l+1)\exp(-l(l+1)\varepsilon_k^2)\, P_l(\cos\tau), \tag{4}$$

where $P_l(\cos\tau)$ are Legendre polynomials with $\cos\tau = \cos\theta\cos\chi_k - \sin\theta\sin\chi_k\cdot\cos(\eta_k - \varphi)$ and θ, φ; χ_k, η_k $(0 \le \varphi, \eta_k < 2\pi,\ 0 \le \theta, \chi_k \le \pi)$ are the spherical coordinates of vectors $\vec{h}_i$ and $g_k\vec{y}'$, respectively.

From experimental PFs the parameters A_k, ε_k, g_k of the linear combination (3) are determined and the ODF (1) is computed. The ODF is always positive because of the positivity of functions $N(g_k, \varepsilon_k, g)$. The 'odd' part of the ODF is assumed to be the 'odd' part of the functions $N(g_k, \varepsilon_k, g)$.

Smoothing by means of normal distributions

It is suggested to smooth the experimental data according to

$$P^{s}_{\vec{h}_i}(\vec{y}) = \int_{S^2} P_{\vec{h}_i}(\vec{y}')\, w((\vec{y}\vec{y}'))\, d\vec{y}', \tag{5a}$$

here $w((\vec{y}\vec{y}'))$ is a function of type (4) with parameters ε_0 and cost $\tau = (\vec{y}\vec{y}'), (\vec{y}\vec{y}')$: scalar product. S^2 denotes the two-dimensional unit sphere. Such a procedure is suggested for smoothing, since the coefficients of the expansion of $P^{s}_{\vec{h}_i}(\vec{y})$ over spherical harmonics are the product of the coefficients of $P^{s}_{\vec{h}_i}(\vec{y})$ and $w((\vec{y}\vec{y}'))$. Considering the relation

$$w((\vec{y}\vec{y}')) = \sum_{l=0}^{\infty} w_l P_l((\vec{y}\vec{y}')) = \sum_{l=0}^{\infty} w_l \sum_{m=-l}^{l} Y_l^m(\vec{y})\, Y_l^{m*}(\vec{y}') \tag{5b}$$

one can see that

$$F_l^{ms} = F_l^m w_l. \tag{5c}$$

It follows

$$P^{NS}_{\vec{h}_i}(g_k, \varepsilon_k + \varepsilon_0, \vec{y}) = \int_{S^2} P^{N}_{\vec{h}_i}(g_k, \varepsilon_k, \vec{y}')\, P^{N}_{\vec{h}_i}((\vec{y}\vec{y}'), \varepsilon_0)\, d\vec{y}', \tag{6}$$

where $P^{N}_{\vec{h}_i}((\vec{y}\vec{y}'), \varepsilon_0)$ is a function of type (4) with $\cos\tau = (\vec{y}\vec{y}')$. Relation (6) allows conclusions about the influence of smoothing on the reconstructed ODF. If unsmoothed PFs are approximated by means of the linear combination (3) with parameters A_k, ε_k; $k = 1, \ldots, K$, then the smoothed PFs will be approximated with parameters A_k, $\varepsilon_k + \varepsilon_0$; $k = 1, \ldots, K$. In other words, smoothing of the experimental data leads to an increase of the parameter, which describes the dispersion of the normal distributions.

Numerical realization

As a numerical realization of (6) the following formula was applied:

$$P^{s}_{\vec{h}_i}(\vec{y}^*) = \frac{\sum_{j=1}^{J} w_j P_{\vec{h}_i}(\vec{y}_j)}{\sum_{j=1}^{J} w_j} \tag{7a}$$

This function for smoothing is concentrated close to its maximum with weights

$$w_j = \exp\left(-\frac{\omega_j^2}{\omega_0^2}\right), \tag{7b}$$

where ω_0 is the half-width of the weight function and ω_j is the angular distance between vectors $\vec{y}^*$ and $\vec{y}_j$. Function (7a) and function (4) are almost indistinguishable (Matthies *et al.*, 1988).

RESULTS

QTA on the basis of unsmoothed PFs leads to 15 components with intensities $I^c > 1\%$ ($1.7\% \le I^c \le 12.7\%$, mean: 4.9%, see Table 1). The existing type of the texture requires such a large number of components with quite small intensities for satisfactory texture description. Half-widths b^c range from 16.7° to 36.9° (mean: 21.5°), *RP0* of the PFs from 9% to 25% (*RP0*(texture): 19%, see Table 2). After moderate smoothing ($\omega_0 = 7.2°$) the component parameters b^c and g^c change to some extent ($-1.5° \le \Delta b^c \le 5.0°$; $0.5° \le \Delta g^c \le 7.3°$; see Table 1). Neglecting the only negative value, b^c generally increases. One can see, that after smoothing better agreement between experimental and recalculated PFs has been achieved ($5\% \le RP0 \le 19\%$; *RP0*(texture): 11%; see Table 2). More extensive smoothing ($\omega_0 = 14.4°$) leads to greater changes of the significant component parameters ($0.7° \le \Delta b^c \le 13.7°$; $2.7° \le \Delta g^c \le 29.5°$; see Table 1) and the disappearing of two components, whereas the changes of *RP0* are smaller compared to the values of *RP0* after moderate smoothing ($3\% \le RP0 \le 17\%$; *RP0* (texture): 8%, see Table 2).

The visual comparison of smoothed and unsmoothed PFs also offers an impression of the effect of smoothing. Some selected PFs are plotted in Figure 1. As has been expected, smoother contour lines are one result and the maximum intensity in the PFs decreases. Moderate smoothing with ω_0 equal to grid step size preserves most details

Table 1 Results of component deconvolution, based on unsmoothed (X) and smoothed (7.2° and 14.4°) data. Each component c is represented by its intensity I^c and half-width b^c. Component 0 corresponds to the random part of the texture. The parameters Δb^c and Δg^c describe the changes of b^c and g^c compared to the unsmoothed data.

	X		7.2°				14.4°			
c	I^c	b^c	I^c	b^c	Δb^c	Δg^c	I^c	b^c	Δb^c	Δg^c
0	26.0		31.2				34.0			
1	12.7	19.0	11.0	21.6	2.6	1.3	11.0	31.7	12.7	3.6
2	8.3	20.0	6.8	21.9	1.9	0.5	5.4	29.2	9.2	3.6
3	7.8	18.1	6.5	20.4	2.3	0.8	5.5	30.3	12.2	4.5
4	7.5	18.2	6.7	20.4	2.2	2.5	4.6	28.0	9.8	5.4
5	6.4	16.7	5.2	19.1	2.4	1.7	4.0	26.5	9.8	6.1
6	6.3	28.7	8.3	32.4	3.7	6.6	11.8	40.8	12.1	12.2
7	5.7	23.2	4.5	24.2	1.0	5.2	3.1	25.9	2.7	10.6
8	3.3	25.4	3.3	27.3	1.9	7.3	3.5	31.4	6.0	16.4
9	2.8	21.8	2.0	22.0	0.2	1.5				
10	2.7	24.4	3.2	29.4	5.0	7.1	3.9	35.8	11.4	21.3
11	2.5	17.6	3.1	20.8	3.2	2.5	4.1	30.4	12.8	2.7
12	2.3	36.9	2.5	35.4	−1.5	3.2	3.9	37.6	0.7	4.1
13	2.0	17.9	2.4	21.7	3.8	2.8	2.9	31.6	13.7	10.4
14	2.0	17.1	1.6	18.5	1.4	1.1	2.3	26.5	9.4	29.5
15	1.7	17.6	1.7	20.6	3.0	4.5				

Table 2 Difference between smoothed and unsmoothed PFs (columns *e.o.s.* = effect of smoothing). Columns *RP0* indicate the quality of texture reproduction. At the bottom mean values of the parameters *e.o.s.* and *RP0* (texture) are given. *n*: index of the PF. For discussion see text.

		e.o.s.		*RP0*		
n	*(hkl)*	7.2°	14.4°	X	7.2°	14.4°
1	(011)(101)	16	31	25	19	17
2	(110)	28	62	23	12	10
3	(012)(102)	19	37	24	16	12
4	(111)	17	27	18	8	4
5	(201)(021)	19	38	24	14	8
6	(112)	15	26	16	8	6
7	(011)(013) (101)(103)	11	20	15	11	7
8	(210)	21	35	23	11	7
9	(121)(211)	15	23	18	9	5
10	(113)	17	28	18	9	7
11	(031)(203) (122)(212) (301)	10	18	11	7	5
12	(213)(310) (114)(221) (123)	8	13	9	5	3
		16	30	19	11	8

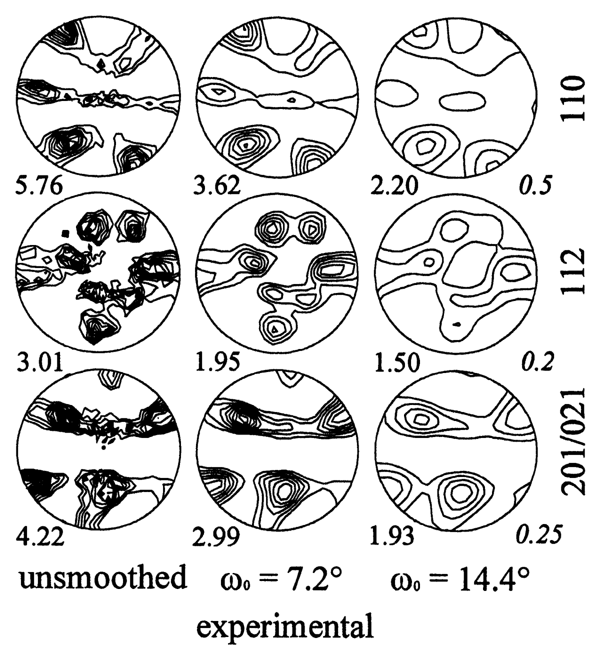

Figure 1 Comparison of some selected experimental PFs, unsmoothed and smoothed with different half-widths of the weight function (ω_0 = 7.2° and ω_0 = 14.4°). Contouring starts at one time random, the distance between contour lines is given in italics. At the bottom left of each PF the maximum intensity is indicated.

of the intensity distributions, however, more extensive smoothing may suppress significant aspects of the intensity distributions. Examples are the disappearing of the horizontal girdle in the (110) PF and the restraining of several submaxima in the (112) PF (see Figure 1).

From the difference between smoothed and unsmoothed PFs information on the effect of smoothing is obtained (see Table 2). In case of a greater number of overlapping Bragg reflections the differences are generally small, whereas PFs comprising only one Bragg reflection show much larger values (Table 2). This observation is also valid for the parameter *RP0*, which describes the quality of texture reproduction (Table 2).

In Figure 2 some recalculated PFs are presented to demonstrate the influence of smoothing on ODF reproduction. An additional simplification of the recalculated PFs is observed as a consequence of the smoothing effect, which is introduced by the applied method of QTA. After extreme smoothing the simplification of the recalculated PFs is quite strong. The (110) PF may serve as an example: the unsmoothed PF contains a characteristic rotational element about a vertical axis, which is no longer visible in the recalculated PF after extensive smoothing. The influence of smoothing is also visible in orientation space, in Figure 3 the ODF is presented in sections γ = constant. As well as in the PFs, extreme simplification of the intensity distribution is obvious after extensive smoothing. In Figure 4 the section $\gamma = 0°$, $\beta = 30°$ is

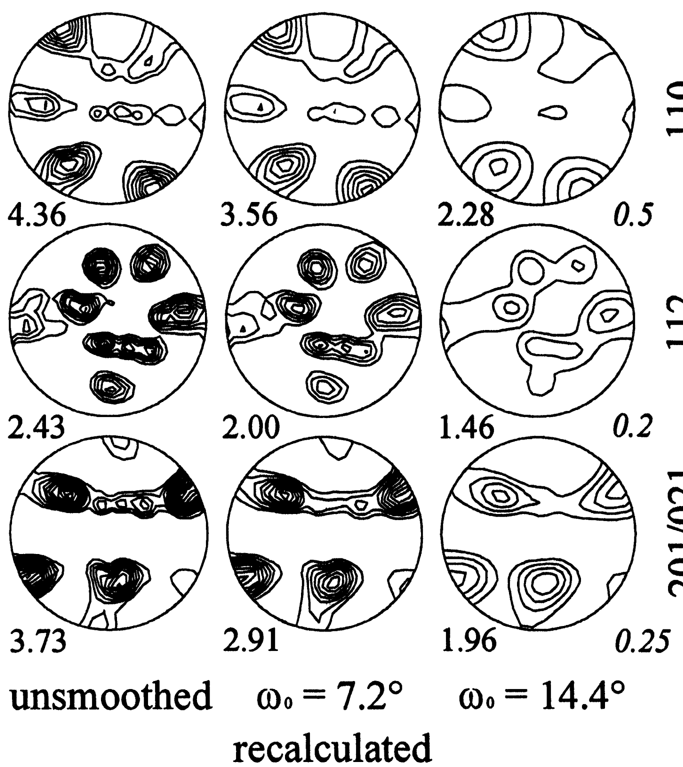

Figure 2 Comparison of recalculated PFs for different amounts of smoothing. For further explanations see Figure 1.

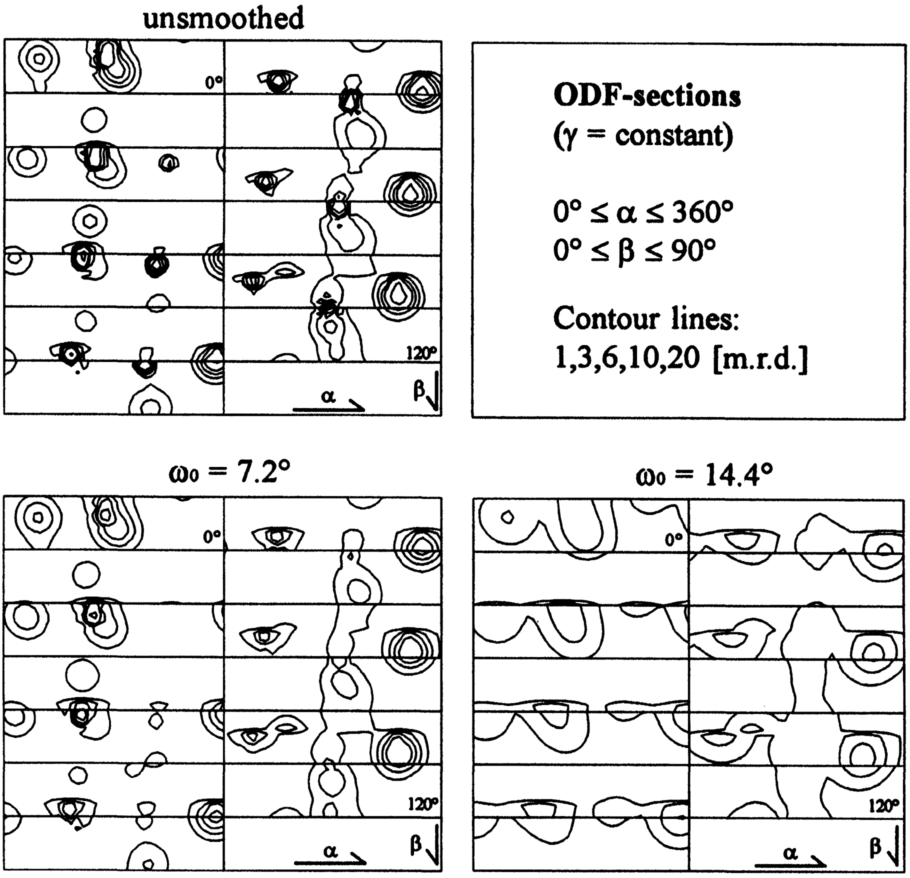

Figure 3 γ = constant sections for the three ODFs, unsmoothed and smoothed with $\omega_0 = 7.2°$ and $\omega_0 = 14.4°$, respectively.

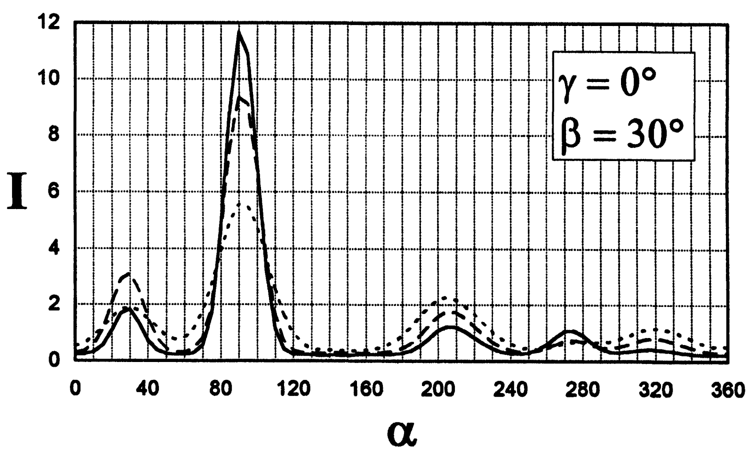

Figure 4 One dimensional section ($\gamma = 0°$, $\beta = 30°$) of the orientation space. Solid line: unsmoothed, dashed line: smoothed with $\omega_0 = 7.2°$, dotted line: smoothed with $\omega_0 = 14.4°$.

additionally plotted to demonstrate, that smoothing also causes an intensity increase in the low intensity ranges of the Euler space. Since all visual observations also depend on feeling, some reflections on possible falsifications of the texture are essential and it is desirable to find an objective criterion, which allows accurate determination of the critical parameter ω_0.

DISCUSSION AND CONCLUSIONS

Concerning the changes of g^c after moderate smoothing ($\omega_0 = 7.2°$), the orientation of the components is interpreted to be stable, because the shift is less than grid step size. In contrast, more extensive smoothing ($\omega_0 = 14.4°$) leads to orientation changes up to $\Delta g^c = 29.5°$ (almost four times grid step size). The quality of a texture measurement also depends on the density of the measuring grid. If the density of the grid points is assumed to be sufficient for correct texture description, the observed large shift of some orientations indicates significant modifications of the ODF as a consequence of the smoothing. The behavior of the half width b^c corresponds to the predicted one from theoretical considerations. An increase is observed, which is smaller than grid step size after moderate smoothing and sometimes much larger after extensive smoothing (up to two times grid step size). Since the components depend from each other due to overlappings, no interdependence of b^c and I^c is noticed. The dependence of components may also explain the observed decrease of b^c.

The quality parameter *RP0* should be interpreted with care. Since low intensities contribute much more to the value of *RP0* (for discussion see Matthies *et al.*, 1988), it depends also on the texture itself and therefore is not very instructive, but its variation allows some conclusion. The alteration of *RP0* is non-linear in dependence upon the amount of smoothing (see Table 2), this trend may be interpreted in the following way: moderate smoothing ($\omega_0 = 7.2°$) mainly removes statistical noise from the PFs and therefore results in relatively large changes of the value of *RP0*. Extreme smoothing ($\omega_0 = 14.4°$) modifies the texture, but the texture modification causes only small changes of *RP0*, since it is compensated by an increase of the component parameter b^c. The trend of the parameter 'effect of smoothing' supports this interpretation: its increase is linear (mean values: 16% and 30%, see Table 2) and therefore indicates significant changes of the PFs after extreme smoothing, but the modifications do not effect the value of *RP0* due to the increase of b^c.

The reduction of the number of components after extensive smoothing also indicates significant simplification of the texture. In our opinion, this phenomenon may be used as a further criterion, that smoothing is too effective. However, such an application is related to the purpose of smoothing. If the best possible texture reproduction is desired, any simplication after smoothing must be avoided. On the other hand, smoothing may be applied to create a simplified texture. It was postulated, that a reduced texture description by a small number of components may be sufficient for several purposes (Ullemeyer *et al.*, 1994, Helming *et al.*, this volume), but a criterion to control possible misinterpretation of the ODF was not mentioned. Smoothing of experimental PFs may serve as a test, whether a reduced texture description is possible or not. The number of components which is really required for texture reproduction should significantly decrease after extreme smoothing, otherwise the existing type of texture does not allow data reduction. The examined quartizite sample confirms, that a reduced texture description is not possible in each case, only minor reduction of the number of components is obtained.

It is concluded, that especially for qualitative texture analysis smoothing may be applied to simplify ODF reconstruction. If QTA is realized by deconvolution into a linear combination of normal distributions, the influence of smoothing may be predicted theoretically. Furthermore, the approximation by means of components provides excellent parameters to indicate changes of the ODF. The latter are the basis to control the effect of smoothing and to determine the critical parameter ω_0.

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References

Andonov, P., Dervin, P. and Esling, C. (1987). *Revue Phys. Appl.*, **22**, 603–612.

Bukharova, T. I., Karcherin, A. S., Nikolayev, D. I., Papirov, I. I., Savyolova, T. I. and Shkuropatenko, V. A. (1988). A new method of reconstructing the grain orientation distribution function, axial texture. *Phys. Met. Metall.*, **65**, 94–99.

Eschner, T. (1993). Texture analysis by means of model functions. *Textures and Microstructures*, **21**, 139–146.

Feldmann, K. (1989). Texture Investigations by Neutron Time-of-Flight Diffraction. *Textures and Microstructures*, **10**, 309–323.

Grewen, J. and Wassermann, G. (1955). *Acta Met.*, **3**, 354.

Helming, K. (1992). Minimal Pole Figure Ranges for Quantitative Texture Analysis. *Textures and Microstructures*, **19**, 45–54.

Helming, K. and Eschner, T. (1990) A new approach to texture analysis of multiphase materials using a texture component model. *Cryst. Res. Technol.*, **25**, K203–K208.

Helming, K., Voitus, W. and Walther, K. (1992). Progress in texture investigations at the pulsed reactor IBR-2. *Physica B*, **180 & 181**, 1025–1028.

Helming, K., Schmidt, D. and Ullemeyer, K. (1995). Preferred Orientations of Mica Bearing Rocks Described by Texture Components (this volume).

Matthies, S., Wenk, H.-R. and Vinel, G. W. (1988). Some basic concepts of texture analysis and comparison of three methods to calculate orientation distributions from pole figures. *J. App. Cryst.*, **21**, 285–304.

Nikolayev, D. I., Savyolova, T. I. and Feldmann, K. (1992). *Textures and Microstructures*, **19**, 9–27.

Nikolayev, D. I. and Ullemeyer, K. (1994). A Note on Preprocessing of Diffraction Pole-Density Data. *J. Appl. Cryst.*, **27**, 517–520.

Traas, C., Siemens, H. and Schaeben, H. (1994). Smoothing Pole Figures using Tensor Products of Trigonometric and Polynomial Splines. *Materials Science Forum*, **157–162**, 453–458.

Ullemeyer, K., Helming, K. and Siegesmund, S. (1994). Quantitative texture analysis of plagioclase. In *Textures of Geological Materials*, edited by H. J. Bunge, S. Siegesmund, W. Skrotzki and K. Weber, pp. 93–108. Oberursel: DGM Informationsgesellschaft-Verlag.

Welch, P. I. (1984). A new Method of Smoothing Polefigure Data. *Proceedings of ICOTOM 7*, 863–868.

Will, G., Schäfer, W. and Merz, P. (1989). Texture analysis by neutron diffraction using a linear position sensitive detector. *Textures and Microstructures*, **10**, 375–387.