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OPTIMIZATION OF TEXTURE MEASUREMENTS. IV. THE INFLUENCE OF THE GRAIN-SIZE DISTRIBUTION ON THE QUALITY OF TEXTURE MEASUREMENTS

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It is the focus of attention that texture experiments deal with real samples which consist of a finite number of crystallites of different size. Because of this the main sample-induced statistics (grain statistics and grain-size statistics) have essential influence on the quality of experimental data. This article quantitatively analyzes the dependence of the integral error on the parameters of the mentioned statistics and the approximation goodness.

Keywords: Statistical errors; Grain statistics; Grain-size distribution; Gamma distribution

1. INTRODUCTION

In texture measurements there exist several sources of statistical errors induced by the investigated sample. This article concentrates on two sources as the most interesting ones from the viewpoint of the author and Mucklich and Klimanek (1994):

- Grain statistics arising when a sample with finite number of grains is taken for texture measurements from the sample multitude (e.g., a geological sample taken from a rock).
- Grain-size statistics related to the distribution of grains over size or volume.

They influence the experimental results during texture measurements increasing the total statistical errors of pole figures (PFs) or the orientation distribution function (ODF).

The aim of this article is to show the impact of these two statistics on the quality of the measured texture data and reveal their relationship with an earlier introduced concept of an "optimal" texture measurement (Luzin, 1997a), which provides the best feasible quality of experimental data.

2. FUNDAMENTALS

To analyze the quality of experimental PF, one needs to compare quantitatively the true PF

$$P^{\mathrm{t}}_{h_i}(\vec{y}): \quad \frac{1}{4\pi}\int_{S^2} P^{\mathrm{t}}_{h_i}(\vec{y})\,\mathrm{d}\omega(\vec{y}) = 1 \tag{1}$$

related to the sample multitude and the experimental PF

$$P^{\mathrm{e}}_{h_i}(\vec{y}_j, N) = \int_{\Omega_j} P^{\mathrm{s}}_{h_i}(\vec{y}, N) K(\vec{y}, \vec{y}_j, \{\rho\})\,\mathrm{d}\omega(\vec{y}), \quad \vec{y}_j \in \Gamma,\ j = 1, \ldots, \#\Gamma \tag{2}$$

determined on the measurement grid $\Gamma \equiv \{y_j\}$ with the number of grid points $J = \#\Gamma$. Experimental PF is expressed in the form of a sampling PF:

$$P^{\mathrm{s}}_{h_i}(\vec{y}, N) = \frac{1}{V}\sum_{n=1}^{N} V_n \delta(\vec{y} - \vec{y}_n),$$
$$\frac{1}{4\pi}\int_{S^2} \delta(\vec{y} - \vec{y}_n)\,\mathrm{d}\omega(\vec{y}) = 1, \quad V = \sum_{n=1}^{N} V_n. \tag{3}$$

$P^{\mathrm{s}}_{h_i}(\vec{y}, N)$ represents a sample with N grains (individual orientations). It is assumed that each grain is represented by the δ-function. The integral kernel $K(\vec{y}, \vec{y}_j, \{\rho\})$, system of local supports $\{\Omega_j\}$ together with the measurement grid $\Gamma \equiv \{y_j\}$ reflect the experimental conditions of the given texture experiment. For the sake of simplicity, $\{\Omega_j\}$ can be referred to the system of elementary patches on PF produced by the detector window and $K(\vec{y}, \vec{y}_j, \{\rho\})$ to the detector sensitivity.

The quantitative characteristic of the PF quality is the R-value

$$R = \frac{1}{J'} \sum_{j=1}^{J'} \sqrt{E\left\{ \left(\frac{P^{\mathrm{t}}_{h_i}(\vec{y}_j) - P^{\mathrm{e}}_{h_i}(\vec{y}_j, N)}{P^{\mathrm{t}}_{h_i}(\vec{y}_j)} \right)^2 \right\}}. \tag{4}$$

It is the sum of expectation of local weighted errors obtained by conventional summing (sensitivity level $\varepsilon = 0.1$). It can be reduced to

$$R \approx \frac{1}{J'} \sum_{j=1}^{J'} \sqrt{\frac{\left(P^{\mathrm{t}}_{h_i}(\vec{y}_j) - P^{\mathrm{i}}_{h_i}(\vec{y}_j)\right)^2}{\left(P^{\mathrm{t}}_{h_i}(\vec{y}_j)\right)^2} + \frac{E\left\{(p_j - w_j)^2\right\}}{p_j^2}},$$

$$P^{\mathrm{i}}_{h_i}(\vec{y}_j) = \int_{\Omega_j} P^{\mathrm{t}}_{h_i}(\vec{y}) K(\vec{y}, \vec{y}_n, \{\rho\})\, \mathrm{d}\omega(\vec{y}) = \frac{1}{\|\Omega_j\|} \int_{\Omega_j} P^{\mathrm{t}}_{h_i}(\vec{y})\, \mathrm{d}\omega(\vec{y}) \equiv \frac{4\pi}{\|\Omega_j\|} p_j, \tag{5}$$

where

$$p_j = \frac{1}{4\pi} \int_{\Omega_j} P^{\mathrm{t}}_{h_i}(\vec{y})\, \mathrm{d}\omega(\vec{y}) = \mathrm{Prob}\{\vec{y} \in \Omega_j\} \tag{6}$$

and the random variable

$$w_j(N) = \frac{\sum_{\vec{y}_n \in \Omega_j} V_n}{V} \tag{7}$$

is the volume fraction of grains with the poles $\vec{y}_n \in \Omega_j$. The first term in (5) does not depend on the sample statistics and represents the approximation errors. The second term appears due to sample statistics. In the framework of an equal grain model ($V_n = V_0, n = 1, \ldots, N, V = NV_0$) for a sample consisting of N grains we get (Luzin, 1997a)

$$R \approx \frac{1}{J'} \sum_{j=1}^{J'} \sqrt{\left[\int_{\Omega_j} \left(1 - \frac{P^{\mathrm{t}}_{h_i}(\vec{y})}{P^{\mathrm{t}}_{h_i}(\vec{y}_j)}\right) \mathrm{d}\omega(\vec{y})\right]^2 + \frac{1}{N} \frac{1 - p_j}{p_j}}, \tag{8}$$

under the assumption that

$$K(\vec{y}, \vec{y}_j, \{\rho\}) = \begin{cases} 1/\|\Omega_j\|, & \vec{y} \in \Omega_j, \\ 0, & \vec{y} \notin \Omega_j. \end{cases} \tag{9}$$

Further, we assume that the grain volumes do not have constant value and are distributed with some distribution density

$$p(V): \quad \int p(V)\,\mathrm{d}V = 1. \tag{10}$$

Next, the purpose is to show how this assumption changes formula (8).

3. CALCULATION OF THE *R*-VALUE IN THE CASE OF THE GRAIN-VOLUME DISTRIBUTION

Ensuing analysis is connected with the distribution of the random variable

$$\xi_n = \frac{\eta_1 + \eta_2 + \cdots + \eta_n}{\eta_1 + \eta_2 + \cdots + \eta_N} = \frac{\Sigma_n}{\Sigma_n + \Sigma_{N-n}}, \tag{11}$$

where

$$\Sigma_n = \eta_1 + \eta_2 + \cdots + \eta_n, \quad \Sigma_{N-n} = \Sigma_N - \Sigma_n = \eta_{n+1} + \eta_{n+2} + \cdots + \eta_N. \tag{12}$$

Here n is the integer number ($n = 1, \ldots, N$) and $\eta_1, \eta_2, \ldots, \eta_N$ are the independent random quantities identically distributed with the density $p(x)$. For definiteness sake we take as this η-distribution the gamma distribution

$$p_{\alpha,\nu}(x) = \frac{1}{\Gamma(\nu)} \alpha^{\nu} x^{\nu-1} \mathrm{e}^{-\alpha x}, \quad \nu > 0, \ 0 \le x < \infty, \tag{13}$$

($\Gamma(\nu)$ is the gamma function) with the following properties. The expectation and dispersion of this distribution are

$$E\{\eta\} = \frac{\nu}{\alpha}, \qquad D\{\eta\} = \frac{\nu}{\alpha^2}, \tag{14}$$

and the parameter

$$\nu = \frac{E^2\{\eta\}}{D\{\eta\}} = \left(\frac{V_0}{\Delta V}\right)^2 \tag{15}$$

can be interpreted, in the sense of the grain-volume distribution, as the squared ratio of the average grain volume V_0 to the spread parameter ΔV of grain volumes around the average value. The gamma distribution is chosen because it is good with respect to convolution

$$p_{\alpha,\nu_1} * p_{\alpha,\nu_2} = p_{\alpha,\nu_1+\nu_2}. \tag{16}$$

So, the quantities Σ_n and Σ_{N-n} have similar gamma distributions,

$$\begin{aligned} \Sigma_n: \quad & \varphi_1(x) = \frac{1}{\Gamma(n\nu)} \alpha^{n\nu} x^{n\nu-1} \mathrm{e}^{-\alpha x}, \\ \Sigma_{N-n}: \quad & \varphi_2(x) = \frac{1}{\Gamma((N-n)\nu)} \alpha^{(N-n)\nu} x^{(N-n)\nu-1} \mathrm{e}^{-\alpha x}. \end{aligned} \tag{17}$$

After intermediate calculations it turns out that the distribution $\varphi(x)$ of the quantity ξ_n is

$$\xi_n: \quad \varphi(x) = \frac{1}{B(n\nu, (N-n)\nu)} x^{n\nu-1}(1-x)^{(N-n)\nu-1}, \quad 0 \le x \le 1, \tag{18}$$

i.e. it is the beta distribution $B(x, s, t)$ with the parameters $s = n\nu$ and $t = (N-n)\nu$ ($B(s, t)$ is the beta function). For ξ_n it is valid that

$$E\{\xi_n\} = \frac{s}{s+t} = \frac{n}{N}, \qquad D\{\xi_n\} = \frac{st}{(s+t)^2(s+t+1)} = \frac{n(N-n)}{N^2(Nn+1)}. \tag{19}$$

Using the obtained relations we can analyze formula (5) and calculate $E\{(p_j - w_j)^2\}$. First, we note that

$$\begin{aligned} E\{w_j\} &= \sum_k E\{\xi_{n_j} \mid n_j = k\} \cdot \mathrm{Prob}(n_j = k) \\ &= \frac{1}{N} \sum_k k \cdot \mathrm{Prob}(n_j = k) = \frac{1}{N} E\{n_j\}. \end{aligned} \tag{20}$$

Taking into account that $E\{n_j\} = Np_j$, $D\{n_j\} = Np_j(1 - p_j)$ it can be written that

$$E\{(p_j - w_j)^2\} = D\{w_j\}, \tag{21}$$

and the formula for the R-value (1) has the form

$$R \approx \frac{1}{J'}\sum_{j=1}^{J'}\sqrt{\left[\int_{\Omega_j}\left(1 - \frac{P^{\mathrm{t}}_{h_i}(\vec{y})}{P^{\mathrm{t}}_{h_i}(\vec{y}_j)}\right)\mathrm{d}\omega(\vec{y})\right]^2 + \frac{D\{w_j\}}{p_j^2}}. \tag{22}$$

Calculations analogous to the calculation of $E\{w_j\}$ give

$$D\{w_j\} = E\{w_j^2\} - E^2\{w_j\} = p_j(1 - p_j)\frac{1 + 1/\nu}{N + 1/\nu} \tag{23}$$

and, finally,

$$R \approx \frac{1}{J'}\sum_{j=1}^{J'}\sqrt{\left[\int_{\Omega_j}\left(1 - \frac{P^{\mathrm{t}}_{h_i}(\vec{y})}{P^{\mathrm{t}}_{h_i}(\vec{y}_j)}\right)\mathrm{d}\omega(\vec{y})\right]^2 + \frac{1 - p_j}{p_j}\cdot\frac{1 + \delta}{N + \delta}},$$

$$\delta = \frac{1}{\nu} = \left(\frac{\Delta V}{V_0}\right)^2. \tag{24}$$

This equation can be reduced to (8) simply putting $\Delta \mathrm{V} = 0$. When $N \gg \delta$, Eq. (24) gives the sample statistical error

$$\frac{1 - p_j}{p_j}\frac{1}{N}(1 + \delta). \tag{25}$$

It means that the sample statistical error in (24) is greater than a similar one in (8) by the factor $(1 + \delta)$. Thus, the influence of grain-volume distribution on the PF statistical errors can be interpreted as a decrease in the grain number $(1 + \delta)$ times. The main point of (24) is that the result does not depend on the grain-volume distribution features: it depends only on the first two moments of the distribution (expectation and dispersion). It should be emphasized that this is valid for the gamma distribution considered as the grain-volume distribution.

Such a probabilistic approach allows us to generalize easily formula (24) (which describes the statistical errors of PF) to conduct the error analysis of ODF (cf. Luzin, 1997c):

$$R_{\mathrm{ODF}} \approx \frac{1}{J'}\sum_{j=1}^{J'}\sqrt{\left[\int_{W_j}\left(1-\frac{f^{\mathrm{t}}(g)}{f^{\mathrm{t}}(g_j)}\right)\mathrm{d}g\right]^2+\frac{1-p_j}{p_j}\cdot\frac{1+\delta}{N+\delta}}, \tag{26}$$

where $\{W_j\}$ is a system of local supports in the orientational space.

4. AN EXAMPLE

The results obtained in the previous section can be applied for the evaluation of an optimal grid parameter (Luzin, 1997a) which minimizes the R-value when all other parameters are given. An equidistant measurement grid is taken and the system of local supports is chosen so that it makes the Dirichlet tesselation of the hemisphere related to the equidistant grid.

The grain-volume distribution is the gamma distribution with the parameters $\alpha = 0.8$, $\nu = 1.28$ and, consequently, $\delta = 0.781$. The distribution density of this distribution is shown in Fig. 1 and is used in further numerical calculations.

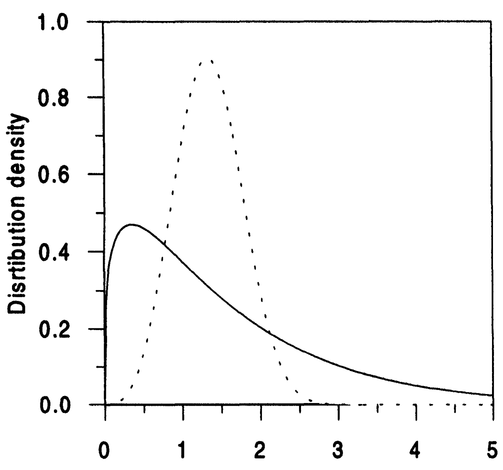

FIGURE 1 The grain-volume (solid line) and the grain-size (dashed line) distributions.

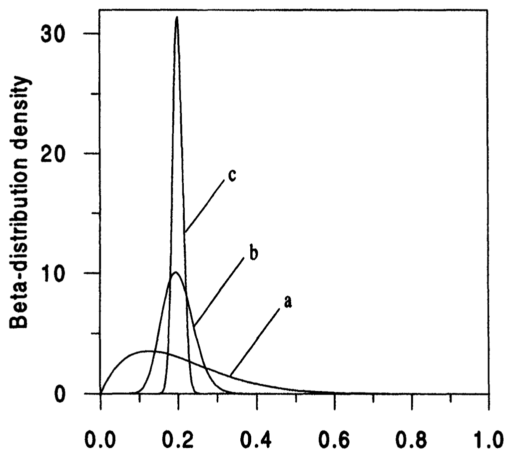

FIGURE 2 The beta-distribution $B(x, n\nu, (N-n)\nu)$: (a) $N=10$, $n=2$; (b) $N=100$, $n=20$; (c) $N=1000$, $n=200$. $\nu=1$.

It is conventional to work mainly with the grain-size distribution. It can be recalculated from the grain-volume distribution with the help of the relation $\nu = as^3$, where v is the grain volume, s is the grain size, a is the constant which depends on the grain shape. Thus recalculated grain-size distribution is also shown in Fig. 1 for $a=0.5$ (a is equal to 0.52 for a spherical grain). It looks like a typical distribution of the grain size.

To illustrate the statistical properties of ξ_n, in Fig. 2 its distribution density (beta distribution) is plotted for several sets of parameters. It can be clearly seen how the dispersion of ξ_n changes as the number of grains in the sample N increases.

For the described conditions the dependence of the R-value (for $P_{\{100\}}$, cubic crystal symmetry) on the grid parameter $\Delta\varphi$ is presented in Fig. 3 for different numbers of grains. The texture model is quite simple (Luzin, 1997a), it is the one Gauss component $\{0°, 0°, 0°\}$ with HWHM $= 19.7°$. Two types of R-value curves are plotted: with and without taking into consideration the grain-volume distribution.

5. CONCLUDING REMARKS

1. The gamma distribution is very convenient for solving the posed problem and it provides the possibility of an analytical description of

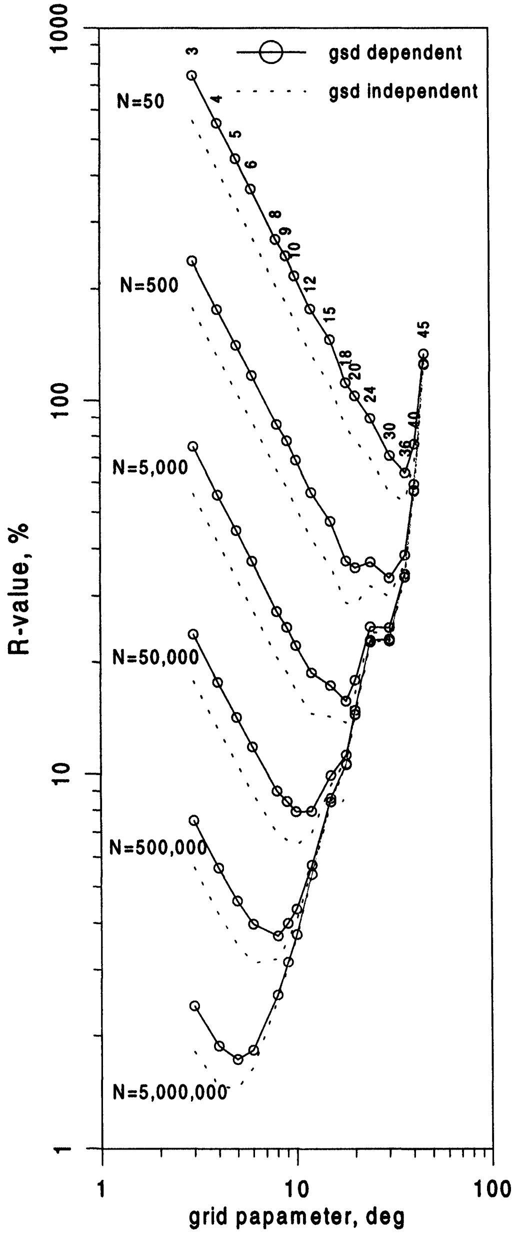

FIGURE 3 The dependences of R-value on the grid parameter for different number of grains. (gsd, grain-size distribution).

the influence of the grain-volume distribution on the PF statistical errors. The other candidates (Lognormal, Maxwell, Weibull distributions, etc.) do not provide the simple analytical description.

2. Dispersion of grain volumes leads to an increase in the statistical error of experimental PF (ODF) and is described by rather simple formulas (24) and (26). So, the quality of experimental PF for a sample with the finite number of grains N decreases because of the spreading of grain volumes.
3. Introducing the grain-volume distribution shifts the value of the optimal grid parameter to greater values and the minimal achieved R-value becomes higher. It is safe to assume that the optimal smoothing procedure (Luzin, 1997b) guarantees attainment of this minimal R-value (for the left branch of the R-value curves in Fig. 3).
4. When the grain-volume (-size) distribution is experimentally found, in (24) and (26) the mean (value) and the standard deviation can be used instead of the expectation and the dispersion, respectively.

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