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OPTIMIZATION OF TEXTURE MEASUREMENTS. FURTHER APPLICATIONS: OPTIMAL SMOOTHING

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1. INTRODUCTION

The problem of the optimal texture experiment was formulated by the author in his other article (Luzin, 1997). It was shown that the optimal texture experiment can be conducted if the texture is known. When the texture can not be initially estimated the standard or an overabundant measurement grid is used to prevent loss of information.

How should the data from this experiment be processed? The one possible answer is to smooth the directional data. Some successful attempts have been made to apply this procedure for processing the probability density functions on the sphere (Traas *et al.*, 1993; Schaeben, 1996; Nikolayev *et al.*, 1996). In this paper the smoothing procedure in the form used by Nikolayev *et al.* (1996) is applied

$$P_{h_i}^{smooth}(\vec{y}_k)=\frac{\sum_{j=1}^{J} w_j P_{h_i}^{e}(\vec{y}_j)}{\sum_{j=1}^{J} w_j},\quad w_j=exp\left\{-\frac{\omega_j^2}{\omega^2}\right\},\quad \omega_j=arccos(\vec{y}_j,\vec{y}_k),$$

where ω is the smoothing parameter.

Usually raw pole figures (PFs) contain statistical noise. High degree of smoothing however leads to loss of information. Only optimal smoothing provides proper smoothing when statistical noise is eliminated and, at the same time, oversmoothing is avoided. In this paper, the main attention is paid to the fact that the optimal smoothing parameter (degree of smoothing) depends on the size of the investigated sample (or the number of grains) in the texture experiment and the sharpness of the texture. Both facts are built into the consideration in the same way as it was done in (Luzin, 1997).

As a result the solution of the optimal smoothing problem is directly connected with the solution of the optimal measurement problem when the texture is known (Section 2). Optimal smoothing can also be carried out in a self-contained way even if the texture is not initially known (Section 3).

2. THE OPTIMAL SMOOTHING PROCEDURE

Let us take a sampling of size N from the sample multitude of orientations described by some true ODF $f^{t}(g)$ and the corresponding PFs $P_{h_i}^{t}(\vec{y})$. The actual distributions can be written as

$$f^{s}(g,N)=\frac{1}{V}\sum_{n=1}^{N}V_n\delta(gg_n^{-1}),\quad g\in SO(3),\qquad V=\sum_{n=1}^{N}V_n,$$

and

$$P_{h_i}^{s}(\vec{y},N)=\frac{1}{V}\sum_{n=1}^{N}V_n\delta(\vec{y}-\vec{y}_n),\qquad \vec{y},\vec{y}_n\in S^2.$$

They yield the observed (experimental) distributions determined on a certain measurement grid $\Gamma=\{\vec{y}_j\}$, $j=1,\dots,J$:

$$P_{h_i}^{e}(\vec{y}_j,N)=\int_{\Omega_j}P_{h_i}^{s}(\vec{y},N)K(\vec{y},\vec{y}_j)d\omega(\vec{y}),\qquad \vec{y},\vec{y}_j\in S^2,$$

where $K(\vec{y},\vec{y}_n)$ is the integral kernel which reflects the conditions of the texture experiment.

The recipe for chosing the grid parameter for the given N in the optimal way was already reported (Luzin, 1997). Next, the following problem is of particular interest. Let us assume the experimental PFs $P_{h_i}^{e}(\vec{y}_j,N)$ are measured for the given number of grains N and the fixed measurement grid $\Gamma=\{\vec{y}_j\}$. Can one improve the obtained data (in the sense of RP-value) by the smoothing procedure? In this article the problem is investigated directly by plotting quantitative dependencies of RP-value on the variables of interest. The simplest texture model of the Gaussian distribution with the center at $g=\{0,0,0\}$ and HWHM=19.7° is used for further calculations.

The most informative is the behavior of the RP-value on the smoothing parameter ω and the equiangular grid parameter $\Delta\varphi$ when the number of grains N is fixed for the given texture. This dependence is presented as the surface and sections of this surface in Fig. 1. It should be emphasized that the minimum RP-value achieved by smoothing is

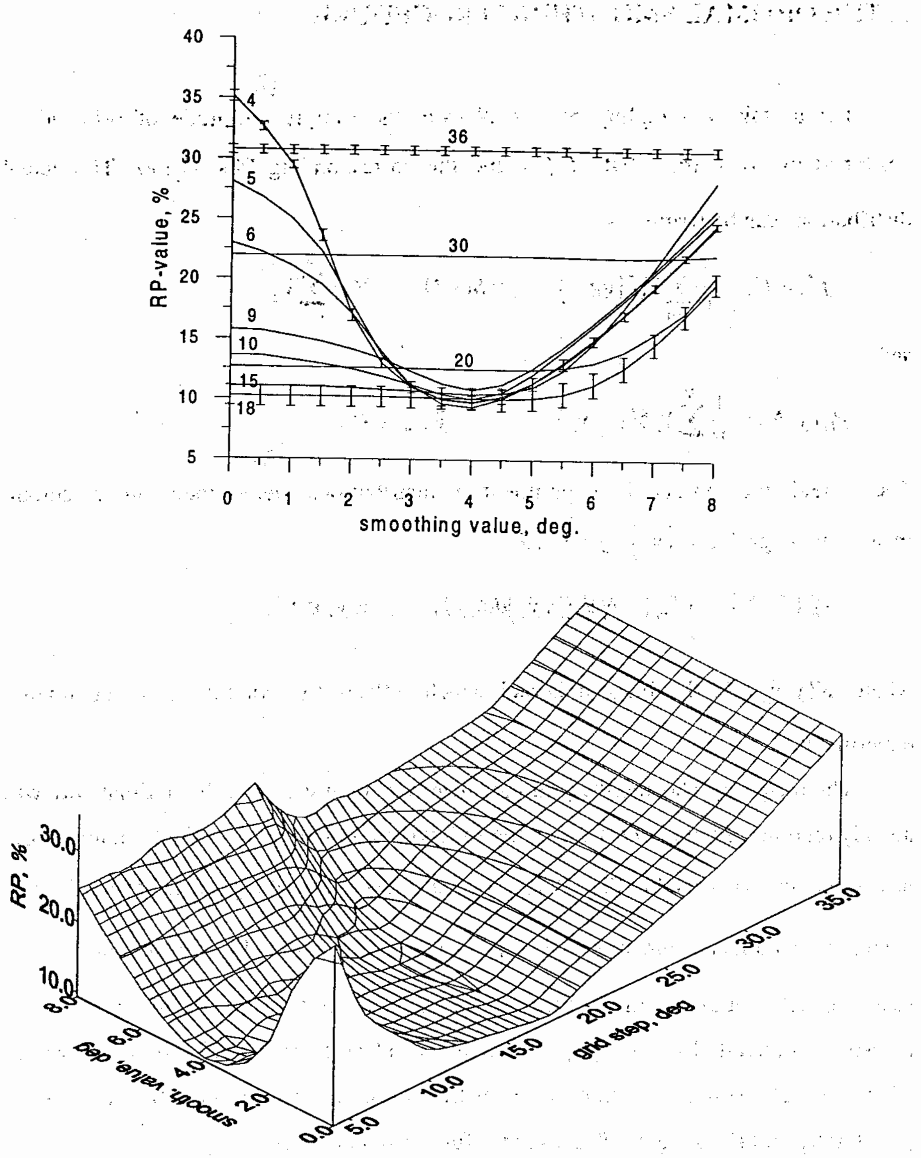

Fig.1. The dependence of the RP-value on the smoothing parameter and the grid parameter plotted as a surface (bottom) and as its sections (top).

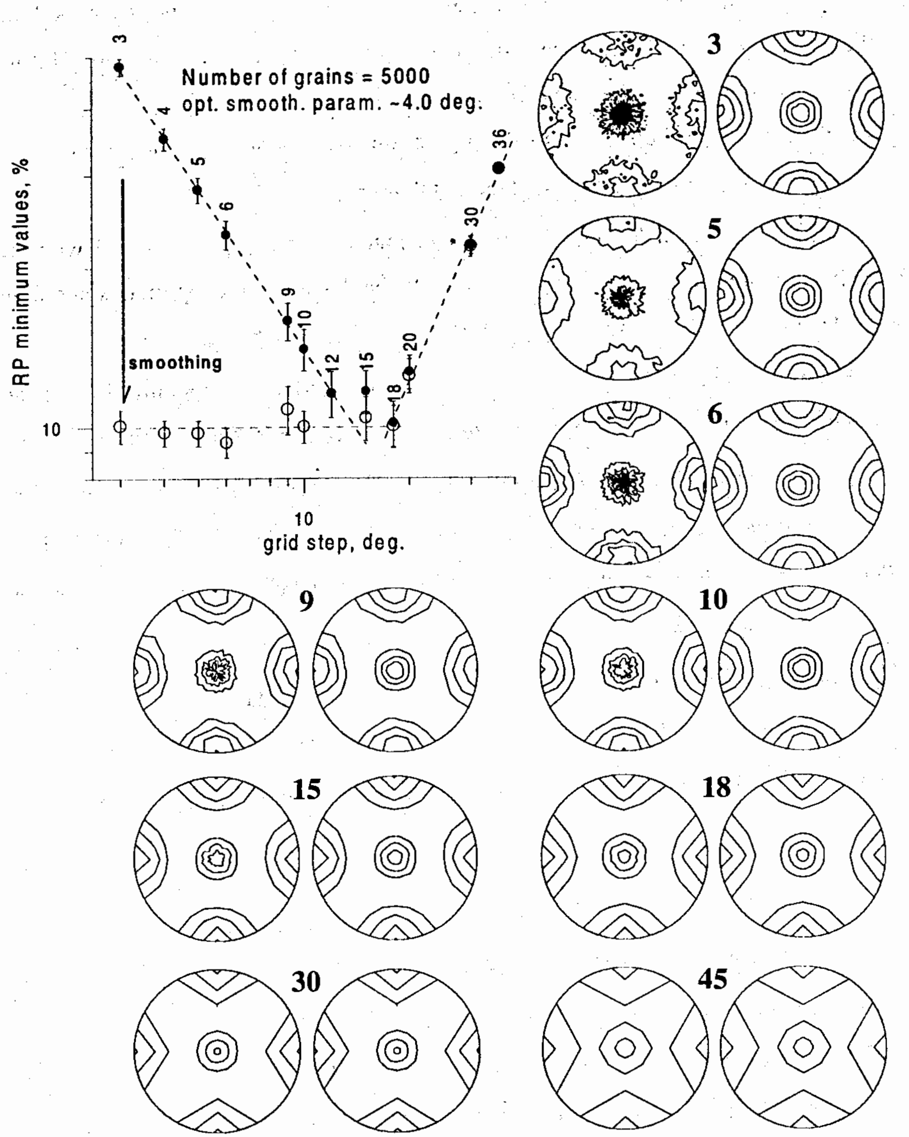

Fig.2. The dependencies of the RP-value before pole figures smoothing (dashed circles) and the minimum achived RP-value after optimal smoothing (clear circles) on the grid parameter of the net used. As an illustration, the pairs unsmoothed-smoothed pole figures (100) are plotted.

precisely the limit achieved in the optimal experiment. So the use of optimal smoothing on the fixed grid leads to the same result as the optimal experiment with optimal grid. This is actual only for grid parameters less than the optimal one. For grid parameters greater than the optimal one the smoothing procedure can not decrease the resultant RP-value. Figure 2 illustrates the aforesaid (N=5000 grains, $\Delta\varphi = 5^\circ$).

Different values of N produce surfaces analogous to the surface in Fig. 1 with the following features. The greater the number N the lesser is the optimal smoothing parameter ω_{opt} and the minimal achieved RP-value $RP_{min} = RP(\omega_{opt})$.

From the multitude of the above-mentioned surfaces (scanning by N) an information about the dependence of ω_{opt} and $RP_{min} = RP(\omega_{opt})$ on N can be extracted. It turns out that these quantities have a very expressed behavior shown in Fig. 3 for the grid parameters $\Delta\varphi = 5^\circ, 15^\circ, 30^\circ$ and the grain numbers in the range N=100-50000. Due to the fact that the optimal smoothing parameter ω_{opt} and the minimal achieved RP-value, $RP_{min} = RP(\omega_{opt})$, are directly connected with the optimal parameters of the optimal grid problem, in the range of the smallest values the curves $\omega_{opt} = \omega_{opt}(N)$ and $RP_{min} = RP_{min}(N)$ coincide and are independent of the grid parameter $\Delta\varphi$. This branch appears as line in double logarithmic scale and is described by

$$\omega_{opt} = \frac{A_1}{N^q}, \qquad RP_{\min} = \frac{A_2}{N^p},$$

where the coefficients A_1 and A_2 depend only on the sharpness of texture and numerically determined constants p and q are $p \approx 0.3$, $q \approx 0.17$.

The N-range where the linear law holds determined by the grid parameter. As N is getting larger and larger and statistical errors decrease, the dependence on N deviates from the linear behavior and tends to some limit. This limit corresponds to approximation errors and is specific for the chosen grid. For the given grid parameter $\Delta\varphi$ the dependence on N begins to deflect when N achieves the value N_{opt} for which the given grid parameter $\Delta\varphi$ is close to the optimal one. Then in the limit $N > N_{opt}$, the

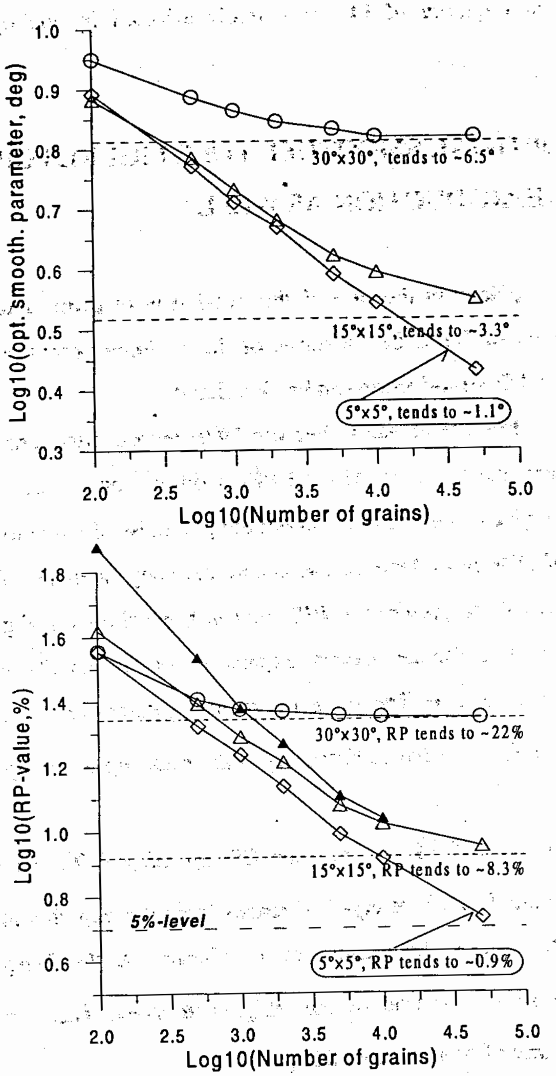

Fig.3. The dependencies of the optimal smoothing parameter (top) and minimum RP-value (bottom) on the number of grains in the sample. (Dashed points are unsmoothed data).

optimal smoothing parameter ω_{opt} and the minimal RP-value RP_{min} achieve their lowest level so and quality of PFs is scarcely affected by the optimal smoothing procedure.

3. ARE THE OPTIMAL SMOOTHED POLE FIGURES OPTIMAL FOR THE ODF REPRODUCTION AS WELL?

The question placed in the title of this section is of prime interest for anybody working in the field of QTA. In the frame of the outlined approach the influence of smoothing on the ODF reproduction can be elucidated.

Three sets of PFs are at hand after the ODF reproduction procedure: the exact (true), experimental and the reconstructed PFs. Comparison of these sets for various smoothing degrees gives us information about the goodness of the smoothing procedure for the purposes of ODF reproduction. The quantitative dependencies of all possible RP-values (*RP(exp,true)*, *RP(exp,calc)* and *RP(calc,true)*) are shown in Fig. 4 for the above mentioned texture. The Bunge (series expansion up to L=22) method and the component method were used. The optimal smoothing parameter ω_{opt} is described as the position of the $RP_{min}(exp, true)$. From Fig. 4 the meaning of the optimal smoothing parameter follows.

In the component method ω_{opt} is when *RP(exp,calc)=RP(calc,true)*. This means that the set of calculated PFs is at equal distances from the experimental PFs and true PFs sets and the RP-value is the measure of the distance. In the Bunge method, ω_{opt} coincides with the actual position of the $RP_{min}(calc, true)$. These results show the advantages and validity of optimal smoothing.

4. SMOOTHING OF THE REAL EXPERIMENTAL DATA

Relatively simple dependencies of the optimal smoothing parameter ω_{opt} and the minimum RP-value give us a hint as to how to apply the smoothing procedure to the real

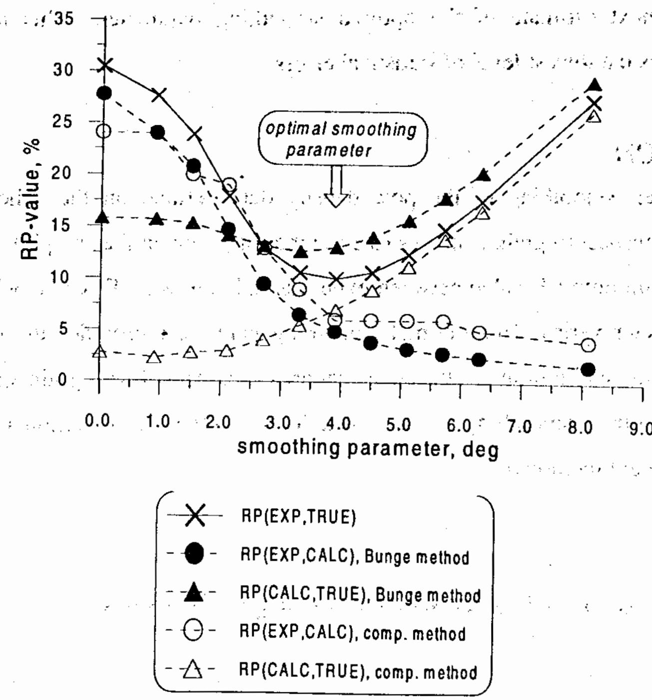

Fig.4. The comparison of reconstructed PFs and experimental PFs with respect to the true ones. (N=5000 grains, 5°H5° measurement grid).

texture data. Since the optimal values can not be evaluated without knowledge of the texture, i.e. before the experiment, the following alternative can be proposed.

Let the number of grains be known and the grid be fixed. The first approximation of the texture can be done by the component method of ODF reproduction. Then, the optimal values can be evaluated and the procedure of optimal smoothing can be performed. After that the smoothed PFs can be used for the second approximation of the texture and the next estimate of the optimal smoothing parameters. This iterative procedure provides the lowest level of statistical errors.

5. CONCLUSION

In this paper, smoothing of the pole density data defined on the sphere was investigated with respect to grain statistics (the number of grains in the sample). It turns out that for the minimum RP-value between experimental and true PFs exists when the smoothing parameter varies. This optimal smoothing parameter provides the optimal smoothing procedure and minimizes the statistical errors connected with grain statistics. The validity of optimal smoothing is confirmed for two ODF reproduction methods (Bung and component methods).

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Оптимизация текстурных измерений.
Оптимальное сглаживание

Ранее нами были изложены основные принципы количественного подхода к решению задачи оптимизации текстурных измерений. В настоящей работе изложены дальнейшие продвижения в данном направлении.

Развитый количественный подход здесь применен для решения задачи оптимального сглаживания. Показано, как параметр оптимального сглаживания зависит от статистики зерен, т.е. от числа зерен в образце. Предложена схема для оптимального сглаживания реальных данных текстурного эксперимента (полюсных фигур).

Также обсуждается применение процедуры оптимального сглаживания по отношению к основной задаче количественного текстурного анализа (восстановлению функции распределения ориентаций).

Работа выполнена в Лаборатории нейтронной физики им. И.М.Франка ОИЯИ.

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Luzin V. E3-98-330

Optimization of Texture Measurements.
Further Applications: Optimal Smoothing

In our previous paper (Luzin, 1997) the basic principles of the quantitative approach to optimize the texture measurements were obtained. This paper is the report of advances in this.

The quantitative approach is used to solve the smoothing problem. Smoothing by singular integrals with an integral kernel used by Nikolayev et al. (1996) is used in this paper. It is shown how the optimal smoothing parameter depends on the grain statistics, i.e. the number of grains in the sample. The algorithm for optimal smoothing of real pole density data (pole figures) is proposed.

Also, the application of optimal smoothing for solving the central problem of quantitative texture analysis (QTA), i.e. orientation distribution function (ODF) reproduction, is discussed.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR.

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