

Introducing a conditional ghost correction into the vector method

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The concept of conditional ghost correction is introduced into the vector method of quantitative texture analysis. The mathematical model actually chosen here reduces the texture problem to one of quadratic programming. Thus, a well defined optimization problem has to be solved, the singular system of linear equations governing the correspondence between pole and orientation distribution being reduced to a set of equality constraints of the restated texture problem. This new mathematical approach in terms of the vector method reveals the modeling character of the solution of the texture problem provided by the vector method completely.

INTRODUCTION

The vector method of quantitative texture analysis was first introduced by Ruer (1976) and later generalized and optimized by Vadon (1981). They have chosen a discrete approach to tackle the texture problem, i.e. to reproduce an orientation distribution function (ODF) from pole figures measured in x-ray or neutron diffraction experiments. Thus the problem was stated as to solve the system of linear equations

$$\tilde{X} = \tilde{\sigma} Y \quad (1)$$

where \tilde{X} denotes the discrete pole distribution (pole figure), $\tilde{\sigma}$ denotes the $(P \times N)$ -matrix to establish the correspondence between the discrete pole and orientation distribution, with $N \leq P$, and Y denotes the discrete orientation distribution, the texture vector.

The discrete pole figure \tilde{X} is related to the experimentally measured intensities $I_{hkl}(\eta, \xi)$ by

$$\tilde{x}_p(hkl) = \int_{Z_p} I_{hkl}(\eta, \xi) \sin \eta \, d\eta \, d\xi \quad p = 1, \dots, P \quad (2)$$

where Z_p is a surface element of the unit sphere. However, in most practical problems the quantities \tilde{x}_p are associated with the measured intensities directly.

Quite analogously, the texture vector Y is related to the ODF $f(g)$ by

$$y_n = \int_{G_n} f(g) dg \quad n = 1, \dots, N \quad (3)$$

where G_n is a volume element of the orientation space.

For a more detailed introduction the reader is referred to Ruer and Vadon (1982) or Schaeben *et al.* (1984).

Introducing constraints on Y being a (step) distribution function

$$0 \leq y_n \leq 1 \quad n = 1, \dots, N \quad (4)$$

$$\text{and } \sum_{n=1}^N y_n = 1 \quad (5)$$

the system (1) of linear equations was claimed to possess a unique solution (Ruer, 1976) and was solved by iteratively applying the gradient method of steepest descent to the corresponding system of normal equations

$$\tilde{\sigma}' \tilde{\sigma} Y = \tilde{\sigma}' X \quad (6)$$

equivalent to the least squares problem corresponding to (1).

Additionally the fact was used that $\tilde{x}_{p_0} = 0$ implies $y_n = 0$ for all $n = 1, \dots, N$ with $\tilde{\sigma}_{p_0 n} \neq 0$, and account was taken of (4) by replacing any negative values of $y_n^{(l)}$ in the l -th step of iteration by zero.

Considering that the vector method requires much less data than the harmonic method, the results obtained were surprisingly good, especially when applied to analyze pole figures sufficiently different from uniformity and with large ranges of zero intensities (Ruer, 1976; Vadon, 1981; Pospiech *et al.*, 1981; Ruer and Vadon, 1982).

experiments in a series of pioneering papers by Matthies (1979; 1980; 1981) it was understood that ambiguity enters the texture problem through the diffraction experiment itself. Any pole figure measured in a polycrystalline diffraction experiment is centrosymmetric, independent of any crystal or specimen symmetry of the true ODF of the texturized sample, or to be more specific, positive and negative directions cannot be identified by normal diffraction techniques though they are geometrically different in the common case. Thus pole figures measured in diffraction experiments are in general of higher symmetry than their corresponding true ODF. Consequently, they provide reduced information concerning the true ODF, which in turn means, that any reproduction method to solve the texture problem is afflicted with this ambiguity. But this does not mean, that ghost phenomena in reproduced ODFs are independent of the reproduction method actually used; it rather suggests the possibility of introducing some kind of ghost correction in genuine terms of each method, except of course for those cases, where any correction is impossible (Matthies and Helming, 1982).

Though it was stated earlier, that the vector method cannot be free of ghost phenomena (Matthies 1979; 1980; 1981; Tani et al., 1981), it was only recently explicitly shown by the author (Schaeben, 1984) that in general

$$\tilde{\rho} = rg(\tilde{\sigma}) \leq \frac{N}{2} \quad (7)$$

holds. Thus, system (1) respectively (6) has in general $N - \tilde{\rho} + 1$, or more than $N/2$ different solutions.

As it was shown in the same paper (Schaeben, 1984) after a thorough investigation of the numerical procedure involved in the vector method and referred to as "Durand's algorithm" (Durand, 1961) by its authors (Ruer, 1976; Vadon, 1981), the mystery about the uniqueness of the solution provided by the vector method is caused by the replacement of negative $y_n^{(i)}$ by zero. It is exactly this strategy of replacement which seems to make the kernel of the map $\tilde{\sigma}$ vanish and the solution given by the algorithm unique (cf Tani *et al.*, 1981). It may be concluded that this rule of replacement defines the modelling characteristics of the solution given by the vector method in its original form.

As stated earlier, problems concerning the non-uniqueness of (6) may not be found when analyzing pole figures of sharply texturized samples with large ranges of zero intensities, because the number N' of unknowns in (6) different from zero may be considerably smaller than N .

In cases when a ghost correction is possible, the ambiguity of the texture problem needs to be met in general by additional modelling assumptions favoring one solution out of the set of all solutions of (6). The mathematical modelling assumptions to be introduced in a reproduction method should be physically reasonable and mathematically efficient, i.e. such that the new mathematical problem of texture analysis has a unique solution. This kind of ghost correction was called conditional by Matthies (1981).

PHYSICALLY REASONABLE CONSTRAINTS

By physical reasoning it can be argued that from all solutions Y to describe a given texture or preferred orientation, the one with maximum background is preferred. This solution corresponds to the case that a given pattern of preferred orientation is materially realized by the least number of preferred orientated grains or single crystallites necessary to constitute the given pattern. In the same way, the solution is favored with the least number of local maxima and is preferred to be as smooth as compatible with all other constraints. Large contiguous areas of weak intensities in the pole figure \tilde{X} should correspond to large contiguous volumes of almost uniform weak densities in the ODF Y rather than in steep local minima. High and narrow peaks in the pole figure \tilde{X} should correspond to a minimum number of high and narrow peaks in the ODF Y . Furthermore, this solution should approximate best local maxima of high intensities in the pole figure \tilde{X} , as measurements of high intensities are considered to be much more accurate than those of weak intensities.

Similar modelling assumptions have been used by Matthies and Vinel (1982) to define a new reproduction method.

THE TEXTURE PROBLEM IN PROPER MATHEMATICAL TERMS

Actually all three of the constraints introduced in the previous section add up to a criterion of maximum smoothness to choose one particular out of the set of all solutions of (6). As a mathematical measure for the smoothness of a texture vector we define the variational sum

$$V(Y) = \sum_{n=1}^N \sum_{j \in J(n)} s_{nj} (y_n - y_j)^2 \quad (8)$$

where the inner sum of densities in (8) has to be taken over all neighboring volume elements G_j , $j \in J(n)$, of volume element G_n , weighted by the common surface area s_{nj} of G_j and G_n . The set of neighbors $J(n)$ of n is given by crystallographic and symmetry relations and the actually chosen partition of the orientation space G into orientation classes or more figurative boxes G_n .

Hence the mathematical model chosen here to find the smoothest solution is to minimize (8) subject to the set of equality constraints (6) and (5), and the inequality constraints (4).

To put more emphasis on the third of the above constraints in some situations (6) may be replaced by the more general approach

$$\tilde{\sigma}^t W \tilde{\sigma} Y = \tilde{\sigma}^t W \tilde{X} \quad (9)$$

where W denotes the diagonal matrix of weighting factors w_{pp} , $p = 1, \dots, P$. When using the weighted least squares method (9) we may choose elements w_{pp} of W to be proportional to \tilde{x}_p , the p -th entry in the discrete pole point distribution itself.

Rewriting (8) in matrix notation

$$V(Y) = Y^t A Y \quad (10)$$

where A denotes a $(N \times N)$ -matrix, the elements a_{kl} of which are given by

$$\begin{aligned} a_{kk} &= 2 \sum_{l \in J(k)} s_{kl} & k &= 1, \dots, N \\ a_{kl} &= a_{lk} = -2 \sum_{l \in J(k)} s_{kl} \chi_{J(k)}(l) & k &= 1, \dots, N; \\ & & l &= 1, \dots, k \end{aligned}$$

$\chi_{J(k)}(l) = 1$, if $l \in J(k)$; 0 otherwise; $V(Y)$ is recognized as a symmetric positive semidefinite quadratic form.

Thus introducing the conditional ghost correction (10) into the vector method means to state the texture problem now as a problem of quadratic programming. More specifically, instead of solving a singular system of linear equations, a well defined optimization problem has to be solved, the linear equations being reduced to be constraints of the new problem. This problem should have a unique solution in most practical applications.

For computational convenience to match the requirements of some standard procedures of quadratic programming, in most practical problems it should be possible to set a unique upper bound for all y_n , $n = 1, \dots, N$, empirically from the preferred orientation apparent in the

pole figure data. When doing so it should always be borne in mind, that a non-uniform ODF may have uniform pole figures (Matthies, 1981), and consequently the upper bound is chosen sufficiently large from the pole figures with the most distinguished patterns of preferred orientation.

Taking account of the singularity and sparsity of the $(P \times N)$ -matrix $\tilde{\sigma}$, the texture problem may now be numerically treated by any standard algorithm of quadratic programming.

CONCLUSIONS

The ambiguity of the texture problem is mathematically met by introducing a simple criterion into the vector method to choose the smoothest feasible solution. Thus the model character of the solution provided by both the original and the vector method with conditional ghost correction is completely revealed. In mathematical terms, the texture problem is properly restated as a problem of quadratic programming. This new approach should open a wider range of applications of the vector method, especially within the frame of structural geology, as the main advantage of the vector method, its small requirement of experimental pole figure data, is preserved.

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