Materials Science Forum Vols. 495-497 (2005) pp 267-272
Online available since 2005/Sep/15 at www.scientific.net

doi:10.4028/www.scientific.net/MSF.495-497.267

Determination of an ODF from diffraction measurements based on optimal smoothing splines

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Keywords:
ODF, PDF, Splines, Geostatistics, optimal linear inversion

Abstract

A long time has past since the introduction of the harmonic method for the reconstruction of the ODF from polefigure measurements, and it has been replaced by discrete methods of inversion, because of its incapability with respect to ghost effects. The harmonic method is still not in its best possible state: it disregards the high order harmonics; it disregards measurement errors and therefore gives suboptimal results; it does not provide standard errors, neither for the C-coefficients nor for the ODF; and there are the ghost effects.

However, the harmonic method is a well established inversion method and it can improved at these points. Statistical considerations based on geostatistics and a model of the unknown ODF as a random function in a Baysian approach yields an inversion method, which can be characterized as a smoothing spline method. This new method is statistically optimal among all linear methods and resembles favorable features of the harmonic method in an improved way. It provides an optimal linear reconstruction of the even part of the ODF. It does not truncate the harmonic series expansion at a fixed level, but accounts for every even harmonic space in an optimal way with respect to its signal to noise ratio in the polefigure measurements. The method applies for irregularly sampled and incomplete pole figures. The method accomplishes standard errors for the ODF and the C-coefficients.

Discrete inversion methods, explicitly or not, reconstruct the odd harmonic part of the function based on the principle of maximum entropy. Based on the theory of exponential families a continuous odd part (and the truncated even part) can be computed based on the entropy principle and the C-coefficients estimated by the spline method.

Motivation

The determination of the ODF from arbitrary diffraction measurements essentially splits into two parts: The determination of the even part of the ODF, which is linearly solvable problem (e.g. by the harmonic method) and the determination of the odd part, which is merely a matter of a good guess based on more or less justified assumptions about the true ODF e.g. zero regions, small texture index or high entropy. This paper is essentially concerned with the first part of the problem, which only drew small attention during the years, since a satisfactory solution was early available through the harmonic method[3]. However the harmonic method

does not achieve some interesting goals, we promise to reach through the method sketched in this extended abstract:

- *Usage of non-PDF diffraction data*: Often data obtained from the various diffraction experiment especially with area detectors can not be seen as pole figure data, but are integrals over more or less irregularly spaced patches of the axial distribution function. While the harmonic method demands a transformation of the data to F-coefficients of polefigures, our method can use any set of measured intensities and even integral intensity measurements.

- *Optimal linear reconstruction*: With a realistic covariance model our method optimally weights the different measurements to achieve minimal expected reconstruction error under all linear method, of which the harmonic method is one.

- *Completeness:* The harmonic method does not use the information on high order harmonic spaces available in the pole-figures. Until [1] this was even considered impossible. Our methods reconstructs even the determined subspaces of the high order harmonic spaces.

- *Optimal Smoothing:* Due to the noise introduced by the measurement error any reconstruction of the ODF needs to apply some smoothing. The harmonic method damps errors in the different harmonic space either not at all (in the lower spaces) or totally (in the not reconstructed high order spaces). We use an optimal smoothing adapted to the roughness of the ODF and the relative amount of measurement errors, based on the signal to noise ratio observed in the data.

- *Known Precision:* Our methods automatically provides the expected squared difference between the true and the estimated ODF or PDF.

Linear reconstruction with minimum error variance

The basic problem is to infer the ODF $f(g)$ or respectively its even part $f_e(g)$ or an unmeasured polefigure $P_h(r)$, which are considered as unknown, from a set of measured reflection intensities

$$I_i = A(\mathbf{h}_i, \mathbf{r}_i) + \varepsilon_i$$

Where $A(\mathbf{h}, \mathbf{r})$ denotes the axial distribution density function (cf. [3]) corresponding to the ODF $f(g)$.

$$A(\mathbf{h}, \mathbf{r}) = \frac{1}{4\pi} \int_{\pm g\mathbf{h}=\mathbf{r}} f(g)dg = P_{\mathbf{h}}(\mathbf{r})$$

Alternatively the measurements can be seen as integral densities over small patches of $A(\mathbf{h}, \mathbf{r})$

$$I_i = \int_{A_i} m_i(\mathbf{r}) A(\mathbf{h}_i, \mathbf{r}) d\mathbf{r} + \varepsilon_i$$

with some detection patch A_i and some angle dependent detection efficiency function $m_i(\mathbf{r})$.

Since the true $f(g)$ is unknown, we consider it as randomly selected from a statistical population of suggestive ODFs. This Bayesian assumption is primarily not an assumption about the odf or the texture forming process itself[5], but an assumption on the structure of our prior knowledge or suspicion about the odf. We will first explain that assumption and the implied

reconstruction method and then show that it is essentially an assumption on the roughness of the odf and which can itself be estimated from the observed diffraction data.

We restrict ourself to a linear reconstruction method:

$$\hat{f}(g) = \sum_{i=1}^{n} w_i(g) I_i + w_0 \tag{1}$$

with arbitrary weights w_i depending on g. Since we do not want to overestimate or underestimate the odf we assert:

$$E[\hat{f}(g) - f(g)] = 0, \text{ for all g} \tag{2}$$

The expected squared reconstruction error of any linear reconstruction with that property of any random object $f(g)$ from observations I_i given by [7]:

$$\begin{aligned} & E[(\hat{f}(g) - f(g))^2] \\ = \; & \operatorname{var}(\hat{f}(g) - f(g)) \\ = \; & \begin{pmatrix} w_1(g) \\ \vdots \\ w_n(g) \\ -1 \end{pmatrix}^t \begin{pmatrix} \operatorname{cov}(I_1, I_1) & \cdots & \operatorname{cov}(I_1, I_n) & \operatorname{cov}(I_1, f(g)) \\ \vdots & \ddots & \vdots & \vdots \\ \operatorname{cov}(I_n, I_1) & \cdots & \operatorname{cov}(I_n, I_n) & \operatorname{cov}(I_n, f(g)) \\ \operatorname{cov}(f(g), I_1) & \cdots & \operatorname{cov}(f(g), I_n) & \operatorname{cov}(f(g), f(g)) \end{pmatrix} \begin{pmatrix} w_1(g) \\ \vdots \\ w_n(g) \\ -1 \end{pmatrix} \end{aligned} \tag{3}$$

Thus to we only need to know the covariances of $f(g)$ and I_i with respect to our prior distribution to calculate the Bayesian prediction variance. According to the formulas of simple kriging [7] this variance is minimized by the setting:

$$\begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} \operatorname{cov}(I_1, I_1) & \cdots & \operatorname{cov}(I_1, I_n) \\ \vdots & \ddots & \vdots \\ \operatorname{cov}(I_n, I_1) & \cdots & \operatorname{cov}(I_n, I_n) \end{pmatrix}^{-1} \begin{pmatrix} \operatorname{cov}(I_1, f(g)) \\ \vdots \\ \operatorname{cov}(I_n, f(g)) \end{pmatrix}$$

Equation (2) is ensured by $w_0 = 1 - \sum_{i=1}^{n} w_i$ The the resulting estimate:

$$\hat{f}(g) = \begin{pmatrix} I_1 - 1 \\ \vdots \\ I_n - 1 \end{pmatrix}^t \begin{pmatrix} \operatorname{cov}(I_1, I_1) & \cdots & \operatorname{cov}(I_1, I_n) \\ \vdots & \ddots & \vdots \\ \operatorname{cov}(I_n, I_1) & \cdots & \operatorname{cov}(I_n, I_n) \end{pmatrix}^{-1} \begin{pmatrix} \operatorname{cov}(I_1, f(g)) \\ \vdots \\ \operatorname{cov}(I_n, f(g)) \end{pmatrix}$$

is a spline in a Hilbert space (cf. [8]) of orientation density functions with reproducing kernel $c(g_1, g_2) = \operatorname{cov}(f(g_1), f(g_2))$ interpolating the measured data, when the measurement error $\operatorname{var}(\varepsilon_i) = 0$ is set to zero. Otherwise it is a smoothing spline. Generally speaking splines are very good approximating functions. Thus even if our assumed covariance is not in some sense "correct" the method remains a solid numerical approximation procedure with regularization and a radial basis function inversion method. But when the assumed covariance is "correct" the procedure given here is the one with smallest expected mean squared error among all linear methods (including the harmonic method).

Finding a covariance model for $f(g)$

Since we truly don't know anything about the ODF before the measurements, we should somehow try to find the covariance model itself from the observed data. One could imagine different ways to do so, but I would like to propose the method well established in the geostatistical community[7]: The first assumption is that we don't know the orientation of the ODF beforehand, such that all rotated ODFs are seen as equally probable. This assumption of ignorance might not be valid, however it simplifies things dramatically and anybody should feel free to invent a better method incorporating all his prior knowledge. The important implication of that assumption is that the covariance is a function of the relative rotation only (G=Laue Group)

$$\mathrm{cov}(f(g_i), f(g_j)) =: c(g_i, g_j) = c_K(Gg_i^{-1}g_jG) = c(GgG) =: \sum_l \sum_{m,n} V_l^{mn} T_l^{mn}(g), \text{ with } g = g_i^{-1}g_j$$

Further as a covariance function the function has to be positive semidefinite [7], which is due to a generalisation of Bochners theorem [7] to the sperical case equivalent to have only real nonnegative V_l^{mn}-coefficients[3] in the given harmonic expansion. To give models for such a function it is most easy to start from a unimodal positive semidefinite kernel function $c_R(g)$, which will later serve as a radial basis function in the sense of [4] and to apply symmetrization:

$$c_K(g) = \frac{1}{|G|^2} \sum_{\sigma \in G} \sum_{\tau \in G} c_R(\sigma g \tau)$$

Let us for one moment assume, that $c(g_i, g_j)$, were the true covariance of a random function $f(g)$, then the covariance with the of the observations I_i would be given by:

$$\mathrm{cov}(f(g), I_j) = \frac{1}{4\pi} \int_{\pm g \mathbf{h_i} = \mathbf{r_i}} c_K(g_i^{-1}g_j) dg_i$$

correspondingly the covariance with pole figures:

$$\mathrm{cov}(P_{\mathbf{h}}(\mathbf{r}), I_j) = \frac{1}{16\pi^2} \int_{\pm g_j \mathbf{h_j} = \mathbf{r_j}} \int_{\pm g \mathbf{h} = \mathbf{r}} c_K(g^{-1}g_j) dg dg_j$$

and the covariance between the observations by:

$$\mathrm{cov}(I_i, I_j) = \frac{1}{16\pi^2} \int_{\pm g_j \mathbf{h_j} = \mathbf{r_j}} \int_{\pm g \mathbf{h_i} = \mathbf{r_i}} c_K(g_i^{-1}g_j) dg_i dg_j + \delta_{ij} \mathrm{var}(\varepsilon_i)$$

since covariances of linear transformations are given by the correspondingly transformed covariances [2]. When the observations are seen as integral densities of small patches in sample directions a similar integration should be applied to the covariance function.

Example calculations

We will now demonstrate the presented method on a simple example. In order to simulate some experimental data we choose the Abel-Poisson-kernel

$$K(\omega) = \frac{1}{2}\left[\frac{1-\chi^2}{(1-2\chi\cos(\omega/2)+\kappa^2)^2} + \frac{1-\chi^2}{(1+2\chi\cos(\omega/2)+\kappa^2)^2}\right] \tag{4}$$

and define a multimodal test ODF as the superposition

$$\tilde{f}(g) = \sum_{i=1}^{3} \lambda_i K(\omega(g_i^{-1}g)). \tag{5}$$

[3] setting here additionally $V_0^{00} = 0$ ensures later $\int \hat{f}(g) dg = 1$

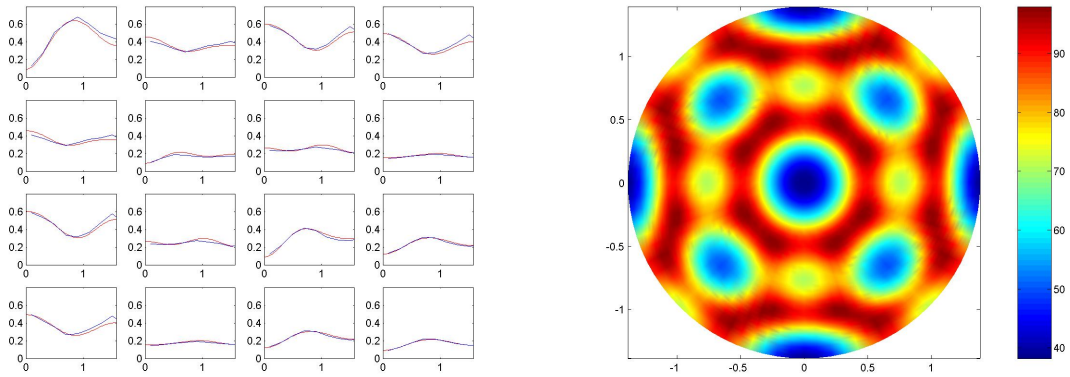

Figure 1: The variogram of the test data described in the text (left picture) and the ratio of uncertainty of the reconstructed inverse pole figure with respect to the x-axis specimen direction (right picture).

Here the first component should be centered in $g_1 = \mathbf{Id}$ and has the parameter $\kappa_1 = 0.8$ whereas the two other components has centers in $g_{2/3} = (\pm 0.1, 0, 0)$ (Euler angles) respectively and parameter $\kappa_{2/3} = 0.9$. The coefficients are set to $\lambda_1 = 0.9$ and $\lambda_{2/3} = 0.05$. Hence the ODF $\tilde{f}$ is nearly unimodal distributed with none radial symmetric peak in the identical rotation. Finely we obtain a cubic symmetric ODF

$$f(g) = \sum_{\hat{g} \in T} \tilde{f}(g\hat{g}) \tag{6}$$

by summation of $\tilde{f}$ over the cubic point group T. Using the fact that

$$(\mathcal{R}K)(g, h, r) = \frac{1 - \kappa^4}{(1 - 2\kappa^2 \cos\omega + \kappa^4)^{3/2}} \tag{7}$$

the PDF of f can be easily calculated. In order to simulate a X-ray diffraction experiment we calculate the pole figures to the crystal directions $\{100\}$, $\{110\}$, $\{111\}$ and $\{221\}$ and a set of 160 approximately equidistant distributed specimen directions and adding to them some $\mathcal{N}(0, 0.2^2)$-distributed noise.

Fitting the covariance function

Under the given assumption for fixed $\mathbf{h}_i, \mathbf{h}_j$ the $\mathrm{cov}(I_i, I_j)$ only depends on the angle between $\mathbf{r}_i$ and $\mathbf{r}_j$. However the I_i's are observed and thus there covariance can be estimated and used to check and fit a model function c_K representing the true covariation structure in the data. In Fig. 1 this comparison of a fitted covariance model with the empirical covariation from a example texture is done in a variogram and crosscovariogram like fashion used in geostatistics (see [7]).

Since the covariance depends in a unknown way on both the differences between crystal directions and the difference between specimen directions it is actually a function in two variables. Fixing the differences between the crystal directions to every pair $(h_i, h_j)_{i,j=1}^4$ we obtain 16 combinations of pairs of polefigures which are plotted in Fig. 1. To this variogram we adapted by hand a covariance function, which we generated based on a von-Mises-Fisher distributed with

parameter $\chi = 8$ and nugget effect 0.3. The corresponding variogram function are plotted as the red graph in figure 1.

Since the theoretical and the empirical functions agree very well we would assume, that the chosen model function well represents the true covariation structure for the even part of the ODF.

Assessing Uncertainty

In Fig. 1 is also plotted the ratio of uncertainty of the reconstructed inverse pole figure with respect to the x-axis specimen direction. This picture would look very similar for any other specimen direction. The figure shows that the error of the inverse pole figure is minimal in regions of crystal directions we have measured and that the rate of reliability we get in these region is bigger when the crystal direction is invariant under some of the crystal symmetries. In direction {123} the IPDF and thus the ODF is nearly undefined by the measurements. We need to recognize that this is not the fault of the method, which makes the most out of the available data, but a problem of the configuration of polefigures measured. The graphic suggests a measurement of the {123} polefigure to overcome that problem. Thus the possibility to compute the expected squared error is an valuable tool to detect problems in the reconstruction process and to decide which additional polefigures should be measured.

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Textures of Materials - ICOTOM 14
doi:10.4028/www.scientific.net/MSF.495-497

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