DETERMINATION OF THE ORIENTATION DISTRIBUTION FUNCTION FROM ISOLATED AXIS DENSITY VALUES

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INTRODUCTION

The orientation distribution of the crystallites in a polycrystalline specimen, the texture, is described by a distribution function using three parameters, e.g. the three Euler angles. This function can be calculated from experimentally determined pole-figures. Two different approaches to effectuate these calculations have been developed, of which the series expansion method has assumed the broader application.[1] In its original form the method starts with pole density values covering the whole assymmetric unit of the pole-figures densely enough to calculate the coefficients of the series by integration.[2] This allows one to make use of the orthogonality relations of the surface spherical harmonics. If one wants to start only from the more easily determined back-reflection parts of the pole-figures alone, then one has to neglect the orthogonality and to determine the coefficients by integration only over the available range of the pole-figures. This leads to a single large-system of equations containing all the coefficients, rather than smaller separate systems for every order of ℓ. Hence, a simplification of the experimental procedure is obtained at the expense of more sophisticated calculations. This principle can be followed by even another step further. Recently energy dispersive X-ray and neutron diffraction methods have been developed and their application to texture analysis has been proposed.[3] These methods allow the determination of pole-density values at the same point of a great number of pole figures simultaneously (much more

than are generally used for the calculation of orienta-
tion distribution functions). In compensation one would
like to reduce the number of points in the pole-figure.
This, however, would lead to larger integration intervals,
and hence to larger errors. Therefore, it is desirable
to employ a method which does not use integration at all.
A method of this type can be obtained if one does not
postulate a least-squares-fit between an experimental and
a theoretical function, leading to integration, but rather
a least-squares-fit of the theoretical function to iso-
lated experimental values. A method of this type is quite
general. It can start from pole-density or axis-density
values at points deliberately chosen in the pole-figure.
Hence, the points can be chosen in the back-reflection
region only; and they can also be chosen so as to cover
the available range with about equal distances (usually
pole-density values are measured on a grid of equiangular
steps leading to an accumulation of the points in the
center of the grid). When using evenly distributed points
then the experimental effort can be reduced by about a
factor of two without loss of accuracy.

Calculation of the Coefficients $C_\ell^{\mu\nu}$

We assume that the reflected intensity P_{ij} is
measured at a point i of the pole-figure j. Then $P_{ij} \cdot N_j$
is the normalized pole density value expressed in mul-
tiples of the random density. The normalization factors
N_j need not be known. The angular coordinates of the
point i in the pole-figure j may depend also on the index
j of the pole-figure, ϕ_{ij} β_{ij}. An orientation distribu-
tion function f(g) is assumed to be represented by a
series

$$f(g) = 1 + \sum_{\ell=2}^{L} \sum_{\mu=1}^{M(\ell)} \sum_{\nu=1}^{N(\ell)} C_\ell^{\mu\nu} \; \ddot{T}_\ell^{\mu\nu}(g) \tag{1}$$

From this function a theoretical pole-density is obtained,

$$P_{ij}^{(th)} = 1 + \sum_{\ell=2}^{L} \sum_{\mu=1}^{M(\ell)} \sum_{\nu=1}^{N(\ell)} \frac{4\pi}{2\ell+1} \; C_\ell^{\mu\nu} \; \dot{k}_\ell^\mu(j) \; \dot{k}_\ell^\nu(ij) \tag{2}$$

where $\ddot{T}_\ell^{\mu\nu}(g)$ are the generalized spherical functions of
crystal and specimen symmetry, $\dot{k}_\ell^\mu(j)$ are the surface
spherical

harmonics of crystal symmetry at a point θ_i ρ_i corresponding to the normal direction of the reflecting lattice plane j and $\dot{k}_\ell^\nu(ij)$ are the spherical harmonics of specimen symmetry at the point ϕ_{ij} β_{ij} at which the pole density has been measured. The coefficients $C_\ell^{\mu\nu}$ and the normalization factors N_j are determined according to the least squares condition

$$\sum_i \sum_j \left[P_{ij} N_j - P_{ij}^{(th)} \right]^2 \cdot W_{ij} = \text{Min} \tag{3}$$

where W_{ij} is a weight factor that might be put to unity for the simplest case. Minimization of equation (3) with respect to $N_{j'}$ and $C_{\ell'}^{\mu'\nu'}$ yields the relations

$$\sum_i \left[P_{ij'} N_{j'} - 1 - \sum_{\ell\mu\nu} \frac{4\pi}{2\ell+1} C_\ell^{\mu\nu} \dot{k}_\ell^\nu(ij') \ddot{k}_\ell^\mu(j') \right] P_{ij'} \cdot W_{ij'} = 0 \tag{4}$$

$$\sum_i \sum_j \left[P_{ij} N_j - 1 - \sum_{\ell\mu\nu} \frac{4\pi}{2\ell+1} C_\ell^{\mu\nu} \dot{k}_\ell^\nu(ij) \ddot{k}_\ell^\mu(j) \right] \dot{k}_{\ell'}^{\nu'}(ij) \ddot{k}_{\ell'}^{\mu'}(j) \cdot W_{ij} = 0 \tag{5}$$

with the abbreviations

$$A_j = \sum_i W_{ij} P_{ij}^2 \tag{6}$$

$$B_{\ell(j)}^{\mu\nu} = \sum_i W_{ij} P_{ij} \dot{k}_\ell^\nu(ij) \ddot{k}_\ell^\mu(j) \tag{7}$$

$$D_j = \sum_i W_{ij} P_{ij} \tag{8}$$

$$E_{\ell\ell'}^{\mu\mu'\nu\nu'} = \sum_i \sum_j W_{ij} \dot{k}_\ell^\nu(ij) \dot{k}_{\ell'}^{\nu'}(ij) \ddot{k}_\ell^\mu(j) \ddot{k}_{\ell'}^{\mu'}(j) \tag{9}$$

$$G_\ell^{\mu\nu} = \sum_i \sum_j W_{ij} \dot{k}_\ell^\nu(ij) \ddot{k}_\ell^\mu(j) \tag{10}$$

equations (4) and (5) read

$$N_{j'} A_{j'} - \sum_{\ell\mu\nu} C_\ell^{\mu\nu} \frac{4\pi}{2\ell+1} B_{\ell(j')}^{\mu\nu} = D_{j'} \tag{11}$$

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$$\sum_j N_j \, B_{\ell'(j)}^{\mu'\nu'} - \sum_{\ell\mu\nu} C_\ell^{\mu\nu} \frac{4\pi}{2\ell+1} E_{\ell\ell'}^{\mu\mu'\nu\nu'} = G_{\ell'}^{\mu'\nu'} \tag{12}$$

Equation (11) can be solved for N_j and this can be sub-stituted for N_j in equation (12). With the abbreviations

$$a_{\ell\ell'}^{\mu\mu'\nu\nu'} = \frac{4\pi}{2\ell+1} \left[E_{\ell\ell'}^{\mu\mu'\nu\nu'} - \sum_j \frac{B_{\ell(j)}^{\mu\nu} \, B_{\ell'(j)}^{\mu'\nu'}}{A_j} \right] \tag{13}$$

$$b_\ell^{\mu\nu} = - G_\ell^{\mu\nu} + \sum_j B_{\ell(j)}^{\mu\nu} \frac{D_j}{A_j} \tag{14}$$

$$c_{\ell(j)}^{\mu\nu} = \frac{4\pi}{2\ell+1} \frac{B_{\ell(j)}^{\mu\nu}}{A_j} \tag{15}$$

$$d_j = \frac{D_j}{A_j} \tag{16}$$

this yields

$$\sum_{\ell=2}^{L} \sum_{\mu=1}^{M(\ell)} \sum_{\nu=1}^{N(\ell)} C_\ell^{\mu\nu} \, a_{\ell\ell'}^{\mu\mu'\nu\nu'} = b_{\ell'}^{\mu'\nu'} \tag{17}$$

and for the normalization factors

$$N_j = d_j + \sum_{\ell=2}^{L} \sum_{\mu=1}^{M(\ell)} \sum_{\nu=1}^{N(\ell)} C_\ell^{\mu\nu} \, c_{\ell(j)}^{\mu\nu} \tag{18}$$

Equation (17) is a system of linear equations for the coefficients $C_\ell^{\mu\nu}$ with the quantities a and b depending on the experimental density values P_{ij}, and from equation (18) the normalization factors N_j are obtained. The equations (17) and (18) represent the most general method of fitting a distribution function to pole-density values measured at angular values arbitrarily chosen. When the coefficients $C_\ell^{\mu\nu}$ are known then the calculation of the distribution function equation (1) or other functions, such as the complete pole-figures or the inverse pole-figures, can be carried out using standard methods.[2]

Applications

In the Equations (6) to (10) and (13) to (16) which define the coefficients of the general system of Equations (17) and (18), no presumptions have been made as to the angular coordinates ϕ_{ij} β_{ij} at which experimental density measurements are to be carried out. This allows one to use always the most convenient experimental method. For example, certain texture goniometers are constructed to measure pole densities at a helical path. Then the simple expression

$$\phi_{ij} = i \cdot \Delta\phi \ , \quad \beta_{ij} = i \cdot \Delta\beta \tag{19}$$

is obtained for the angular coordinates indpendent of the index j of the pole figure.

Another possibility is to chose the points ϕ_{ij} β_{ij} along the equidensity lines of the pole-figures.

$$P(\phi_{ij} \ \beta_{ij}) = \text{const.} \tag{20}$$

This method may be convenient if pole-figures plotted by a pole-figure plotter in terms equidensity lines are to be used. Then one needs not to interpolate density values between the given density lines, which is always a source of error. One simply has to read the coordinates ϕ_{ij} β_{ij} of certain points chosen somehow along the equidensity lines. As a special case of this latter method the exact maximum density values

$$P(\phi_m \ \beta_m) = \text{Max.} \tag{21}$$

can be included in the calculations which is generally not possible when only predetermined angular positions are being used. The incorporation of the maximum density values is especially desirable when the highest possible accuracy is to be obtained.

For the sake of minimum measuring time an equi-area set of points ϕ_{ij} β_{ij} is to be chosen rather than an equiangular set, because the angular resolving power depends on the largest angular distances between neighbouring points of the set. If the points are crowded together in the vicinity of the pole $\phi = 0$ as is the case in the equiangular set, then an unfavourable ratio between the number of points and the resolving power is obtained. Hence, an equi-area set of points is to be preferred which leads however to uneven values of the angular coordinates ϕ_{ij} β_{ij}. But this does not matter in the present method

of calculation. Finally, there is, of course, no objection against applying the formulae (17) and (18) also to equiangular measurements as they are obtained with a conventional step-operated texture goniometer. Hence the present method is easily applicable to any kind of pole-density measurements whatsoever. Of course this versatility is being achieved at the expense of more sophisticated computational methods, but this is a general trend in the experimental technique since larger and larger computers have become available.

REFERENCES

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