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An inversion formula expressing the texture function in terms of angular distribution functions

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Abstract. — The determination of the orientation distribution function of crystallites in a polycrystalline material from experimental pole figures leads to an integral equation which is usually solved by a series expansion method. Recently S. Matthies [4] has proposed, without proof, an inversion formula which is not based on series expansion. Such a direct formula is being deduced by efficient group theoretical methods. The solution can further be expressed in terms of the angular distribution function \( W_b(\cos \theta) \) which had been introduced earlier [3]. Both methods are being compared with regard to the obtainable experimental data and the required computational efforts.

1. Notations and formulation of the inversion problem. — As it has been shown in [1, 2], in most cases of centrosymmetry, the texture can be described by a positive function on the space of rotations

\[
\text{SO}(3) \to \mathbb{R}^+
\]

\[
g \mapsto f(g) .
\]

The group \( \text{SO}(3) \), denoted by \( G \), is the group of rotation matrices (determinant + 1). If \( (XYZ) \) denotes the sample coordinate system and \( (xyz) \) the one fixed to a crystallite, the orientation of this crystallite will be defined by the rotation \( g \) which transforms \( (XYZ) \) into \( (xyz) \); thus \( g \) is the transformation matrix of the macroscopic reference frame to the microscopic one :

\[
(XYZ) \mapsto (xyz) .
\]

(2)

One shall denote by

\[
\text{Tr}(g) = g_{11} + g_{22} + g_{33} = 2 \cos \omega + 1
\]

the trace of the matrix \( g \), where \( \omega \) is the rotation angle of \( g \). If \( g \) runs through \( G \), the trace varies within the range \(-1, +3\). A function \( f(g) \) is central when the conjugaison relation holds :

\[
f(g') = f(g g' g^{-1}) \quad \forall g' \in G .
\]

(4)

In this case, \( f(g) \) only depends on \( \text{Tr}(g) \), through a function \( h \) defined on the interval \([-1, +3]\) :

\[
f(g) = h(\text{Tr}(g)) = h(2 \cos \omega + 1) .
\]

(5)

\( K \) denotes the subgroup of the \( Z \) axis rotations :

\[
K = \{ R_z(\Psi) \mid \Psi \in [0, 2\pi] \} .
\]
S₂ denotes the unit sphere of the R³ space, the north pole [001] of which is denoted by N.

It is possible to associate to any function \( f(g) \) its biaxial function \( A^f \) defined as following [3]. Being \( y, h \) two points on \( S_2 \) and \( g_1, g_2 \) two rotations such as:
\[
y = g_1 N \\
h = g_2 N
\]
then \(^{(1)}\)
\[
A^f(g_2, g_1) = \frac{1}{2\pi} \int_0^{2\pi} f(g_1, R_{\Psi}(g_2^{-1})) \, d\Psi = A^f(h, y).
\]

If \( h \) is the normal to a reflecting lattice plane and \( y \) a sample direction, then because of Friedel's law, only the symmetrized pole figure:
\[
\hat{P}_h(y) = \frac{1}{2} [A^f(+h, y) + A^f(-h, y)] = A^f(h, y)
\]
is attainable by polycrystal diffraction measurements.

The serial expansion of such a function contains only terms of even order [4, 5].

If \( \tilde{f}(g) \) similarly denotes the even part of the expansion of \( f(g) \) on the spherical harmonics:
\[
\tilde{f}(g) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} C^{mn}_l T_l^{mn}(g)
\]
it follows immediately [2]
\[
\tilde{A}^f = A^f = \frac{1}{2\pi} \int_0^{2\pi} \tilde{f}(g_1, R_{\Psi}(g_2^{-1})) \, d\Psi.
\]
Thus the solution of the integral equation (8), i.e. the computation of \( f \) from \( A^f \), will allow to determine only the even part \( \tilde{f} \) of the texture function, out of experimental pole figures.

2. Solution of the integral equation: inversion formula. — The computation of \( f(g) \) can be reduced to the calculation of the value at \( g = 1 \) (identity) for a centralized function [6].

2.1 Reduction to the calculation of the value at the identity of a function \( f^\phi \). — We put:
\[
f^\phi(g') = f(gg')
\]
then
\[
A^{f^\phi}(g_2, g_1) = \frac{1}{2\pi} \int_0^{2\pi} f^\phi(g_1, R_{\Psi}(g_2^{-1})) \, d\Psi = \frac{1}{2\pi} \int_0^{2\pi} f(gg_1, R_{\Psi}(g_2^{-1})) \, d\Psi = A^f(g_2, gg_1).\]

In other words, a rotation \( g \) of the sample coordinate system transforms \( f(1) \) into \( f(g) \):
\[
f^\phi(1) = f(g) \\
A^{f^\phi}(h, y) = A^f(h, gy).
\]

2.2 Reduction to the calculation of a centralized function. — We define a centralized function by
\[
f^\phi(g') = \int_G f(gy'g^{-1}) \, dg; \quad \int_G dg = 1
\]
which is a central function according to equation (4) with the following properties:
\[
f^\phi(1) = f(1)\]
\[
A^{f^\phi}(g_2, g_1) = A^{f^\phi}(h, y) = \int_G A^f(gh, gy) \, dg.
\]
Indeed:
\[
A^{f^\phi}(g_2, g_1) = \frac{1}{2\pi} \int_0^{2\pi} f^\phi(g_1, R_{\Psi}(g_2^{-1})) \, d\Psi = \frac{1}{2\pi} \int_0^{2\pi} d\Psi \int_G f(gg_1, R_{\Psi}(g_2^{-1}g^{-1})) \, dg =
\]
\[
= \int_G \frac{1}{2\pi} \int_0^{2\pi} f(gg_1, R_{\Psi}(g_2^{-1})) \, d\Psi = \int_G dg \int_G A^f(gg_2, gg_1).
\]

\(^{(1)}\) It should be noted that in the present work, in order to be in accordance with the usual convention in group theory, the rotations are described in fixed reference frame. This permutes the product of rotations with regard to the mobile reference frame, used in the reference book [3].
From equation (17) it follows

\[ A^f(h, y) = A^f(gh, gy) \forall g \in G. \tag{19} \]

For \( h = N \), one obtains the (001) pole figure:

\[ A^f(N, y) = P_N(y). \tag{20} \]

If in equation (19) \( g \) is a rotation about the north pole \( N \) then it follows

\[ P_N(R_x(\Psi) y) = P_N(y) = P(\cos \theta) \tag{21} \]

where \( \theta \) denotes the angle between \( y \) and the north pole \( N \). (For the explicit dependence of \( P \) on \( \theta \) in form of \( \cos \theta \) see equation (25).) This pole figure is axially symmetric.

From equation (19) it follows

\[ P_{\phi^N}(y) = P_N(g^{-1} y) \tag{22} \]

i.e. the pole figure of the north pole determines all the other pole figures, by the change of the sample reference frame. (This last property results from the centralization; it is of course wrong on the starting texture function.) Since \( f^c \) is central there exists according to the equation (5) a function \( h : [-1, 3] \to \mathbb{R} \) such as:

\[ f^c(g) = h(\text{Tr} g) = h(2 \cos \omega + 1) \]
\[ f(1) = f^c(1) = h(\text{Tr} 1) = h(3) \tag{23} \]

with \( g_2 = 1 \) and \( g_1 = R_x(\theta) \) it follows from equations (7) and (8):

By multiplying the matrices \( R_x(\theta) \) and \( R_z(\Psi) \) one obtains:

\[ P(\cos \theta) = \frac{1}{2 \pi} \int_0^{2\pi} h(\cos \theta \cos \Psi + \cos \theta + \cos \Psi) \, d\Psi. \tag{25} \]

Thus, the problem consists in determining \( h \) from \( P \).

With the variable transformation

\[
\begin{align*}
  u &= 1 + \cos \theta \\
  2v - 1 &= \cos \theta \cos \Psi + \cos \theta + \cos \Psi
\end{align*}
\]

one obtains:

\[ P(u - 1) = \frac{1}{\pi} \int_0^\infty \frac{h(2v - 1)}{\sqrt{v}} \, dv. \tag{26} \]

Thus, \( P(u - 1) \) is the Abel transform of \( \frac{1}{\sqrt{v}} h(2v - 1) \).

Let us recall that the Abel transform \( Af(u) \) of a function \( f(v) \) is defined by [7]

\[ Af(u) = \int_0^u \frac{f(v)}{\sqrt{u - v}} \, dv. \tag{28} \]

Its well known inversion is given by:

\[ f(v) = \frac{d}{dv} \frac{1}{\pi} \int_0^v Af(u) \, du. \tag{29} \]

\[ 2.3 \text{ The inverse Abel transform. — The application of the inversion formula (17) yields:} \]

\[ f(g) = P^q(-1) + 2 \int_0^\pi d\theta \cos \frac{\theta}{2} \frac{d}{d\cos \frac{\theta}{2}} P^q(\cos \theta) \tag{33} \]
where $P^q(\cos \theta)$ is given by the successive expressions:

\[ P^q(\cos \theta) = A_f^{(g)}(N, R_2(\theta) N) \]
\[ = \int_G A_f^{(g')}(N, g' R_2(\theta) N) \, dg' \]
\[ = \int_G A_f^{(g')}(N, g' R_2(\theta) N) \, dg' \]

obtained by taking into account successively the equations (24), (17), and (13).

3. Relationship between the function $P^q(\cos \theta)$ and the angular distribution functions $W_{by}(\cos \theta)$.  

In order to use the inversion formula, it is necessary to calculate the function $P^q(\cos \theta)$. This latter calculation is largely simplified by the preliminary calculation of the angular distribution functions $W_{by}(\cos \theta)$, which had been introduced in 1969 by Bunge [3].

$W_{by}$ is the mean value of the $P_h$ pole figure on circles with colatitude $\theta$, centred on $y$ (Fig. 1, after Bunge [3]).

![Fig. 1.](image)

Thus, the inversion formula reads:

\[ f(g) = \int_{S_2} P_h(- g h) \, dh + \]
\[ + 2 \int_0^{\pi_2} d\theta \cos \theta \frac{\partial}{\partial \cos \theta} \int_{S_2} dh \, W_{by}(\cos \theta) \]  

This quite general formula still holds if one considers the even part of the texture function according to the relation $\tilde{A} = A^f$ (see eq. (11)):

\[ \tilde{f}(g) = \int_{S_2} \tilde{P}_h(g h) \, dh + \]
\[ + 2 \int_0^{\pi_2} d\theta \cos \theta \frac{\partial}{\partial \cos \theta} \int_{S_2} dh \, W_{by}(\cos \theta) \]  

As the function $\tilde{W}_{by}(\cos \theta)$ is even in $\cos \theta$, this latter formula also reads:

\[ \tilde{f}(g) = \int_{S_2} \tilde{P}_h(g h) \, dh + 2^{3/2} \int_0^{\pi_2} d\theta \sin \frac{\pi}{4} - \theta \]
\[ \times \frac{\partial}{\partial \cos \theta} \int_{S_2} dh \, \tilde{W}_{by}(\cos \theta) \]  

analogous to that given, without proof, by S. Matthies [4].

The inversion formula is of great theoretical interest since it offers an exact solution to the fundamental integral relation, without truncation error. Indeed, it shows that if one would have disposal of the continuum of pole figures:

\[ \{ P_{by} , h \in S_2 \} \]  

it would be possible to calculate $\tilde{f}(g)$, by a triple integration. However, experimental measurements by X-rays or neutrons allow only to determine a very limited number of pole figures. So, in the case of polycrystals with cubic structure, only three to five pole figures are measured in the standard experimental procedures, and even the use of sophisticated experimental techniques (synchrotron radiation, energy dispersive analysis, etc.) do not permit the measurement of more than ten to twelve diffraction lines, quite insufficient to provide a satisfactory sampling in $h$.

Moreover, even if one could measure the biaxial function $A(h, y)$ as a continuous function of $h$, to make use of the inversion formula would require:

- the determination of the angular distribution functions $W_{by}(\cos \theta)$, curvilinear integrals along circles on the pole sphere;
- the calculation of $\frac{\partial}{\partial \cos \theta}$ through a numerical differentiation, the drastic sensitivity of which to the errors is well known.
In the case of continuously variable $h$ the series expansion method offers a much easier way of how to calculate $f(g)$. The biaxial function is expressed by the coefficients $C_i^{mn}$ by [3]:

$$A(h, y) = 4\pi \sum_{i=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} \frac{C_i^{mn}}{2l+1} k_i^m(h) k_i^n(y)$$  

from which it follows immediately by a double integration

$$C_i^{mn} = \frac{2l+1}{4\pi} \int_h \int_y A(h, y) k_i^m(h) k_i^n(y) \, dh \, dy. \tag{46}$$

The function $f(g)$ can then be obtained by

$$f(g) = \sum_{i=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} C_i^{mn} T_i^{mn}(g). \tag{47}$$

As far as numerical calculations are concerned the time consuming integration equation (46) has to be carried out only for a limited number of indices $imn$ from which the function $f(g)$ can be obtained for any value of $g$. In the inversion formula, on the other hand, the integration (eq. (42)) has to be carried out for any value of $g$ separately which is extremely ineffective from the standpoint of computer time.

However, the series expansion method is concerned with numerical problems too. For great $l$ the integrant equation (46) contains strong oscillating functions, which influence the correctness of the numerical integrations. For time consuming calculations in equation (46) and equation (47) the functions $k_i^m$ and $T_i^{mn}$ usually are given in form of tables, which require a relative great computing memory [8].

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References

[8] This last paragraph was added specifically by the referee (S. Matthies, private communication).