the elements of the T and L tensors and their standard deviations.

Test of the program

TEERRIG has been critically tested for each one of the seventeen examples of BFM. In some of these examples a perfect parallelism was obtained. Major discrepancies were seen to exist for some of the examples and these have been reported by Armagan & Yücel (1982).

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References


A generalized library program for texture calculations with even and odd coefficients. By F. WAGNER, E. BECHLER-FERRY, C. ESLING and R. BARO, Laboratoire de Métallurgie Structurale, Faculté des Sciences, 57045 Metz CEDEX, France

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Abstract

A previously published library program [Wagner, Esling & Baro (1977). Texture Cryst. Solids, 2, 225–241] allowed the creation and storage of the set of numerical values necessary for three-dimensional texture analysis, with the even ranks in the spherical harmonics expansion. To take into account the recent developments in texture analysis, a more general version of this program is proposed, including, besides the calculation for even ranks, its extension to the odd ones. In addition, the formulae and the general analytical expressions, valid whatever the rank l, are given for the set of the calculated constants and functions.

Introduction

Three-dimensional texture analysis requires many numerical calculations. These calculations can be greatly facilitated if the user has at his disposal a library program able to generate and store the necessary numerical data with a view to further use in three-dimensional texture analysis.

This paper represents the extension to odd ranks l of the previously published library program (Wagner, Esling & Baro, 1977). Recent works have established (Matthies, 1979; Bunge & Esling, 1979; Bunge, Esling & Muller, 1980; Wenk, Wagner, Esling & Bunge, 1981) the necessity of including odd ranks in the three-dimensional texture analysis. Both the terminology and the notations are chosen according to the preceding paper (Wagner et al., 1977) and to the reference book of H. J. Bunge (1969). The analytical expressions, valid whatever the rank l, are given for all the calculated constants, polynomials and functions. Moreover, this program offers the same fundamental characteristics as the previous one (Wagner et al., 1977).

(1) Numerical calculations are based on the accurate determination of the fundamental constants Q_l^m (Bunge, 1974).

(2) The numerical values are all generated in the computer; thus, no preliminary data have to be read on punched cards – except some parameters of organization indicating the alternative library which is to be created.

(3) The program offers good characteristics of generality and adaptability. Indeed, according to the choice of the user, it gives the numerical constants and functions adapted to most of the microscopic symmetries (especially cubic, hexagonal and trigonal) and macroscopic symmetries (especially orthorhombic and triclinic).

Lastly, the algorithms for the main calculations are original (Esling, 1981a) and are optimized for precision as well as for computation time.

1. Mathematical foundations

We recall hereafter the analytical expressions of the various mathematical quantities which can be calculated and stored by the proposed library program. The notations are those used by Bunge (1969) and all the given formulas hold for both even and odd values of the integer index l, which is the rank of the series expansion. For these mathematical quantities, l can vary between chosen limits LMIN and LMAX with a chosen step LP with the following limitations:

1 ≤ LMIN ≤ 4, 1 ≤ LMAX ≤ 34, LMIN ≤ LMAX and 1 ≤ LP ≤ 2.

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However, for the symmetry coefficients and symmetry-adapted functions of the cubic case, the calculation starts only at the rank \( l \) at which a value different from zero first appears, i.e., \( l = 9 \) when the calculations concern only odd ranks \( l \) and \( l = 4 \) in the other cases (see § v). The above-mentioned limitations for LMIN and LP can be transgressed without any change except in the parts of the program which calculate these cubic coefficients or functions.

(i) \( Q_l^m \) coefficients

These are defined by the relation

\[
Q_l^m = i^{m+n} P_l^m (\pi/2),
\]

where the function \( P_l^m (\Phi) \) denotes a polynomial associated with the Jacobi polynomial as defined by Bunge (1969). These real coefficients verify the relations

\[
Q_l^m = 0 \text{ if } l + m \text{ is odd}
\]

and

\[
Q_l^m = (-1)^m Q_l^m.
\]

They are always calculated at the beginning of the program and can be stored for the following indices (the third term is always the step of progression of the corresponding index):

\[
\begin{align*}
&l = \text{LMIN, LMAX, (LP)} \\
&m = 0, l, \text{(IDN)} \\
&n = 0, m, \text{(IDN)} \\
&\text{IDN} = 1 \text{ or } 2.
\end{align*}
\]

(ii) \( a_l^m \) coefficients

These are defined by the relation

\[
a_l^m = \varepsilon Q_l^m Q_l^m
\]

with

\[
\varepsilon = 1 \text{ if } s = 0, \\
\varepsilon = 2 \text{ if } m + n \text{ is even} \\
\varepsilon = 2i \text{ if } m + n \text{ is odd}.
\]

They are real or pure imaginary numbers. In this last case \( s \neq 0 \) and \( m + n \) odd, the stored values are in fact \( a_l^m \) coefficients are calculated for

\[
\begin{align*}
&l = \text{LMIN, LMAX, (LP)} \\
&m = 0, l, \text{(IDM)} \text{ with } 1 \leq \text{IDM} \leq 6 \\
&n = 0, l, \text{(IDN)} \text{ with } 1 \leq \text{IDN} \leq 2 \\
&s = 0, l, (1).
\end{align*}
\]

These coefficients are used for calculating the \( P_l^m (\Phi) \) polynomials with the relation

\[
P_l^m (\Phi) = \sum_{s=0}^{l} a_l^m \cos \left( s \Phi - \frac{\pi}{2} \right)
\]

with

\[
\delta = 0 \text{ if } m + n \text{ even} \\
\delta = 1 \text{ if } m + n \text{ odd}.
\]

(iii) \( a_l^m \) coefficients

These coefficients are calculated with the formula

\[
a_l^m = \varepsilon (4l + 2)^{1/2} Q_l^m Q_l^0,
\]

with

\[
\varepsilon = \frac{1}{2} (-1)^{n+1} \text{ if } s = 0.
\]

They verify the condition \( a_l^m = 0 \) if \( l - s \) is odd so that these coefficients are only calculated for even values of \( s \) when \( l \) is even and only for odd values of \( s \) when \( l \) is odd. The indices \( l, m, s \) vary then in the following manners:

\[
\begin{align*}
l &= \text{LMIN, LMAX, (LP)} \\
m &= 0, l, \text{(IDN)} \text{ with } \text{IDN} = 1 \text{ or } 2 \\
s &= t, l, (2) \text{ with } t = 0 \text{ if } l \text{ is even} \\
&= 1 \text{ for odd } l.
\end{align*}
\]

(iv) \( P_l^m (\Phi) \) polynomials

These polynomials, associated with the Legendre polynomials, which enter in the analytical expression of the spherical harmonics \( k_l^n (\Phi, \beta) \), are given by

\[
P_l^m (\Phi) = i^{m} (2l+1)^{1/2} P_l^m (\Phi).
\]

An equivalent definition, which offers an easy way to calculate them reads

\[
P_l^m (\Phi) = \sum_{s=0}^{l} a_l^m \cos \left( s \Phi - \frac{\pi}{2} \right)
\]

with

\[
\delta = 0 \text{ if } m \text{ is even} \\
\delta = 1 \text{ if } m \text{ is odd}.
\]

These polynomials can be calculated and stored in the library program for

\[
\begin{align*}
l &= \text{LMIN, LMAX, (LP)} \\
m &= 0, l, \text{(IDN)} \\
\Phi &= 0, 90^\circ, (\Delta \Phi) \text{ with } 1.25 \leq \Delta \Phi \leq 90^\circ.
\end{align*}
\]

(v) \( B_l^m \) coefficients

These coefficients are necessary to build up the simple or generalized spherical harmonic functions for cubic symmetry. These symmetrized functions can be determined by applying mathematical operators, which are called projection operators or projectors, to the ordinary functions (Esling, 1981b). In the case of cubic symmetry, which is the most complicated, the use of these projectors leads to a set of functions from which one can extract a set of orthogonal and normalized functions which are the searched symmetrized ones (Esling, 1981b).

It is tedious, and not the right place in this paper, to give an analytical expression of the cubic coefficients \( B_l^m \), although it would be mathematically possible. In the proposed library program, they can be calculated and stored for

\[
\begin{align*}
l &= \text{lm}_1, \text{ LMAX, (LP)} \\
\mu &= 1, M(l), (1) \\
m &= 0, l, (4),
\end{align*}
\]

where \( M(l) \) is the number of independent symmetrized functions at a given rank \( l \) and \( \text{lm}_1 \) is the first value of \( l \) at which a coefficient \( B_l^m \) different from zero appears (it is well known that \( \text{lm}_1 = 4 \) when coefficients with even \( l \) are of interest; \( \text{lm}_1 = 9 \) when the coefficients with only odd \( l \) are investigated). These coefficients are used, for example, to calculate the cubic generalized spherical harmonics \( T_l^m (\varphi_1, \Phi, \varphi_2) \) which are given by

\[
T_l^m (\varphi_1, \Phi, \varphi_2) = \sum_{s=0}^{l} B_l^m \cos \left( s \Phi - \frac{\pi}{2} \right)
\]
The spherical harmonics, symmetrized for cubic symmetry, \( k_\ell^m(h_i) \), are defined by

\[
\hat{k}_\ell^m(h_i) = \sum_{m'=0}^{\ell} B_{\ell m'}^m (\Phi) \cos \left( m\beta - \frac{\pi}{2} \right)
\]

with \( \delta = 0 \) for even \( \ell \) and \( \delta = 1 \) for odd \( \ell \) values.

These real functions are calculated and stored for eight different and independent \((hkl)\) planes. The significance of \( \ell m \) and \( M(l) \) is exactly the same as in § v.

(vii) \( \hat{k}_\ell^m(h_i) \) for other symmetries

The application of projectors leads to very simple analytical expressions for the symmetrized spherical harmonics \( \hat{k}_\ell^m(h_i) \) when the considered symmetry is not the cubic one. The library program allows the calculation of these functions for the rotational subgroups of the holohedries of all crystalline systems (except the triclinic one). Indeed, only rotational symmetries are to be taken into account in the program the calculation holds then for the following point-group symmetries 6mm, 6/m, 6, 3m, 3, 3mm, 4/m, 4, m, a symmetrized function \( \hat{k}_\ell^m(h_i) \) appears as a particular \( k_\ell^m(h_i) \) harmonic which fulfills, for this \( m' \) index, the selection rule imposed by the symmetry axis along \( Z \). In these cases the section of the library program where these \( \hat{k}_\ell^m(h_i) \) functions are calculated should be changed; formula (11) should be replaced by

\[
\hat{k}_\ell^m(h_i) = k_\ell^m(\Phi, \beta) = (2\pi)^{-1/2} P_\ell^m(\Phi) \exp(i m' \beta)
\]

with, as usual, \( m' = J (\mu - 1) \), but now \( -l \leq m' \leq l \). (The point groups 6m2 and 4m2 have the same rotational subgroups as 32 and 222 respectively.)

### II. Characteristics of the library program

(1) Generalities

The program is written in Fortran IV.* The ordinogram is exactly the same as for the previous version (Wagner et al., 1977) except that to the input parameter LMAX, IDN, IDM must be added the parameters LMIN and LP as defined in the previous section. So the organization of the program is preserved with the two main possibilities:

(i) storage of the \( Q_{\ell m}^m \) coefficients and of the symmetry function \( \hat{k}_\ell^m(h_i) \) and additionally the symmetry coefficients \( \hat{B}_\ell^m \) if cubic symmetry is required;

(ii) storage of the following coefficients and functions:

\[
\hat{B}_\ell^m(\Phi, h_i), \ a_{\ell m}^m,
\]

Within option (ii) it is always possible to generate a 'standard library' (Wagner et al., 1977) adapted to the published programs of texture analysis for cubic-orthorhombic symmetries (Jura, Pospiech & Bunge, 1974, 1976), working only with even \( l \). To obtain this 'standard library' it is necessary to reduce the size of the arrays \( \mathbf{XY} \) and \( \mathbf{BB} \) of the actual version to respectively \( \mathbf{XY} (16,3,8) \) and \( \mathbf{BB} (16,3,9) \) as in the previous publication. With just this modification the 'standard library' is obtained by having just one data card with the value 1 [value of the parameter IST (Wagner et al., 1977)].

We also wish to underline that, in the present version, the functions \( \hat{k}_\ell^m(h_i) \) and the coefficients \( \hat{B}_\ell^m \) are stored, whatever the parameter LP, in arrays \( \mathbf{XY}, \mathbf{YK} \) and \( \mathbf{BB} \) in a compact form characterizing the normal to a \((hkl)\) plane and \( 1 \leq l \leq 12 \) (12 planes at the most).

The existence of the twofold axis along \( Y \) implies that a function \( k_\ell^m(h_i) \) is defined as the sum of two ordinary harmonics \( k_\ell^m(h_i) \), with opposite \( m' \) values, thus leading to the cosine factor in (11). Furthermore, the axis of multiplicity \( J \) along \( Z \) introduces the selection rule: \( m' = J \). When there is no twofold axis along \( Y \), as is the case for point-group symmetries 6mm, 6/m, 6, 3m, 3, 3mm, 4/m, 4, m, a symmetrized function \( \hat{k}_\ell^m(h_i) \) appears as a particular \( k_\ell^m(h_i) \) harmonic which fulfills, for this \( m' \) index, the selection rule imposed by the symmetry axis along \( Z \).

For this condition the symmetrized harmonics \( \hat{k}_\ell^m(h_i) \) are given by

\[
\hat{k}_\ell^m(h_i) = \hat{k}_\ell^m(\Phi, \beta) = (2\pi)^{-1/2} P_\ell^m(\Phi) \exp(i m' \beta)
\]

with \( \delta = 0 \) for even \( \ell \) and \( \delta = 1 \) for odd \( \ell \) values.
manner. This means that when, for example, only odd ranks \( l \) are calculated and stored, the first index of the arrays \( XK, YK \) and \( BB \) is calculated to take on the values 1, 2, 3, ... successively, so that there is no empty 'line' in these arrays. It is obvious that the exploitation of these stored functions or coefficients must take this setting into account.

(2) **Memory space used by the program and computing time**

This program was tested with a Univac 1110 computer. It requires 38035 words (a word is 36 bits), which corresponds approximately to 150 kbytes for a computer working with words of 4 bytes. In the presented version the array \( YK \), in which the functions \( k_l^s(h_i) \) are stored for non-cubic symmetry, has the dimensions \( YK (35,12,12) \). These dimensions allow the calculation of the \( k_l^s(h_i) \) for \( l=0 \) to 34, and for 12 \((hkl)\) planes at most, for the symmetry cases including the hexagonal, quadratic and trigonal symmetries. For the other symmetries (orthorhombic or monoclinic), the dimensions of this array \( YK \) must be extended if the maximal value of \( l \) is always fixed to 34. For example, when monoclinic symmetry is required, the array \( YK \) has the dimensions \( YK (35,35,12) \). When only some of the possibilities of this program are to be used (\( LMAX \leq 34 \) or \( LP = 2 \) or no cubic symmetry wanted, for example), it is easy to reduce the necessary memory space by reducing the dimensions of the various arrays. It is also possible to 'cut' the program for working in overlay mode or to use peripheral memories to write and read \( Q_{lm}^n \) coefficients when the available central memory space is not sufficient for this library program.

The computing time of this program depends obviously on the number of data to be calculated and stored. To give an idea of the computing time we will give two examples: on a Univac 1100 computer it takes 1 min 32 s (including 32.2 s for the input/output operations) to create a 'standard library' and on a PDP 11/70 computer a library up to \( LMAX=21 \) for only odd \( l \) values, including \( P_l^s(\Phi), a_l^m, k_l^s(h_i) \) for trigonal symmetry, \( a_l^{mn} \), necessitates 42.56 s.

**Conclusion**

The necessity of including the odd-\( l \) orders in the series expansion method of texture analysis is now well established (Matthies, 1979; Bunge et al., 1980) and several methods (Bunge & Esling, 1979; Wenk, Wagner, Esling & Bunge, 1981; Wagner, Wenk, Esling & Bunge, 1981; Hirsch, Virnich & Lücke, 1980; Esling, Bechler-Ferry & Bunge, 1981) have been proposed to calculate the odd part of the orientation distribution function (ODF), which cannot be deduced directly from the pole figures. It is then clear that in the future most texture analysis will be performed with the odd-\( l \) orders in order to avoid the so-called 'ghosts' (Pospiech, 1974) in the ODF and thus to determine the true density distribution. The library program presented here allows one to generate results with great precision and to store all the mathematical quantities which are necessary for such calculations. The numerous possibilities for the symmetries (microscopic and macroscopic symmetries) which are included in this program permit all the usual texture studies in metallurgy as well as in geology.

**References**


