

H.-J. Bunge



Texture Analysis in Materials Science

Mathematical Methods



Butterworths



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Mathematical Methods

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Preface

By application of counting techniques it is possible to obtain quantitative information about the orientation distribution of crystallites in polycrystalline materials. This has created a need for the mathematical treatment of the orientation distribution function, and the relationships between various functions, such as pole figures, inverse pole figures, three-dimensional orientation distribution functions and directionally dependent physical properties. In the present book an effort will be made to give a unified presentation of these relationships. It is shown that the representation of the orientation distribution function as a series expansion is a very useful aid for its numerical calculation. The relations between the single crystal properties and texture and the corresponding polycrystal properties also follow particularly simply and logically in this representation. For these reasons I have restricted myself almost exclusively to this form of representation.

Textures have been studied chiefly in metallic materials. They are in principle of importance, not only for these, but also for all polycrystalline materials. The relationships between the various orientation distribution functions and the methods of their treatment are largely independent of the particular material. They are therefore applicable to ceramic materials or partially crystalline synthetics in a manner completely analogous with that for metals.

This book is intended for those who are concerned with the orientation distribution of crystallites. It seeks to provide some mathematical aids for the quantitative treatment of such problems.

At this point I should like to express my sincere thanks to several of my colleagues for their support during writing and correction of the manuscript. Professor BOLL-DORNBERGER has undertaken a critical review of the manuscript. Dr H. SCHMITTLER displayed particular interest in the writing of the book. She has contributed many valuable suggestions in numerous discussions during drafting of the manuscript and has called my attention to a number of errors. She has very intensively examined the manuscript and corrections. I should also like to thank Mr J. TOBISCH and Mrs U. SCHLÄFER for their help with the corrections.

HANS-JOACHIM BUNGE

Preface to the English Edition

Since the first appearance of this book in 1969 quantitative texture analysis has developed very rapidly. Since large enough computers have become easily accessible in recent years, the calculation of the orientation distribution function (ODF) from experimentally determined pole figures or even incomplete (back-reflection) pole figures can be regarded as a routine procedure which is carried out by available computer programs. The user of this method does not need to be concerned with the mathematics involved. Several brief reviews directed mainly towards the practical use of the ODF method are available^{51,52,57,59,62-64,171,233,236}.

The result obtained, the ODF, is much easier to interpret because it is an unambiguous representation of the texture data compared with pole figures which cannot distinguish by themselves between crystal orientations rotated about the normal of the reflecting lattice plane. Thus, in recent years a large number of texture investigations have been presented in the form of ODF, while in the first edition of this book reference could be made only to a very small number of actual numerical calculations. Chapter 11, dealing with some results of texture analysis, has therefore been completely rewritten. Changes have also been made in Section 2.1, which describes the various orientation parameters used by different authors and the relations between them.

Only very recently have the implications of the centre of inversion as a symmetry element been considered in greater detail. This has led to extending the considerations to polycrystalline materials containing right- and left-handed crystals which must thus be looked at as being two-phase materials which are to be described by two independent texture functions. The description of the sample symmetries thus requires black-white point groups instead of the ordinary ones. Also, in many cases the odd terms of the series expansion have to be taken into account. These problems have been considered in the additional Sections 4.11 for general textures and 5.10 for fibre textures. The implications of the odd part of the texture function have not yet been considered in most of the numerical calculations carried out thus far, but this particular aspect of ODF analysis is in a very effervescent state of development at present.

The concept of the texture transformation by means of an orientation relation function had been treated among other problems in the first edition, Section 10.1, in connection with the development of recrystallization textures from deformation textures. However, exactly the same formalism holds also for phase transformation if the product crystals have the same symmetry as the parent crystals, as

is the case, for example, in the $\gamma \rightarrow \alpha$ transformation in steels or the $\alpha \rightarrow \beta$ transformation in brasses. Because of its great importance in texture formation a special chapter has been devoted to texture transformation (Chapter 8), including also the general case of change of crystal symmetry.

In the first edition, Section 4.9, a system of ALGOL programs was mentioned by which ODF of cubic-orthorhombic symmetry had been calculated. These programs have been used for quite a number of ODF calculations but they have not been published in detail. On the basis of these programs, however, a set of FORTRAN programs has been developed which have been published in the full text.¹⁷¹ In Chapter 9 we therefore give these FORTRAN programs along with the library program by WAGNER, ESLING and BARO.²⁹²

Although a comprehensive error analysis of the mathematical procedure leading from pole figures with their experimental errors to ODF has not yet been developed, a number of different error estimations have been used. Some of them have been described in reference I, Chapter 7, along with the experimental examples. With increasing experimental accuracy, e.g. by the application of neutron diffraction, and with increasing demand for ODF's as accurate as possible, the error analysis becomes more and more important. Hence, a special section was devoted to the estimate of errors. In Chapter 13, dealing with the anisotropy of physical properties, some additions have been made, especially with respect to the plastic properties. In Chapter 14 on mathematical aids the sign convention of the associated LEGENDRE functions has been changed with respect to that used in reference I. Furthermore, Section 14.3 has been changed according to the FOURIER coefficients Q_l^{ms} , which seem to be the most economic way of representing the generalized spherical harmonics.

Finally, Chapter 15, the numerical tables, and Appendix A.4, the graphic representations, have been changed. The coefficients Q_l^{mn} and $B_l^{m\mu}$ are the fundamental quantities by which all the other quantities can easily be expressed. Tables of these quantities have therefore been given up to $l = 34$, which is assumed to be a reasonable upper limit for practical texture calculations. (The value $L = 100$ as given in some of the tables in reference I seems much too high compared with the experimental accuracy and the obtainable resolving power.) Tables of the deduced quantities are given only up to an l of much lower degree, just for checking purposes, since it is assumed that these quantities will never be used as primary data. The Q_l^{ms} and $B_l^{m\mu}$ of Tables 15.1.1 and 15.2.1 might be used as primary data for texture calculations (although it is recommendable to produce them by the library program inside the computer). The numerical tables have been calculated by Dr C. ESLING and Mme Ing. E. BECHLER, Metz. The computations were carried out in the computer centre IRSID, Maizières-les-Metz under the supervision of Mr J. C. FILLER, whose helpful support is gratefully acknowledged. The tables have been recalculated from the very beginning without making use of any primary numerical data. The tables given are photoreproductions of the computer outputs so that typing errors as they occurred in the hand-set tables in reference I have been avoided.

The main part of the book, Chapters 4 and 5, remained nearly unchanged. It should be mentioned that in equations (2.17) and (2.20) in reference I a symmetry assumption according to the cubic symmetry was made which is not correct for the lower symmetries. Thus, in equation (4.35) in the case of lower symmetries the complex conjugate notation is required. I am very much indebted to Dr C. ESLING for making me aware of this error. He also read carefully the whole manuscript and drew my attention to several mistakes. In numerous valuable discussions he contributed much to the finishing of the book.

I also wish to express my gratitude to P. R. MORRIS. He not only carried out the laborious task of the translation, but also as an experienced worker in ODF analysis made many valuable comments on the contents, especially Section 4.10, the comparison between the two notations used in the series expansion method.

Finally, I should like to acknowledge many helpful discussions with Dr J. POSPIECH, who especially contributed to the methods of numerical calculations and provided the numerical example given in Section 9.6.

List of Symbols Used

K_A	Sample fixed coordinate system
XYZ	Coordinate axes in K_A
xyz	Coordinates in K_A
y	Sample direction
$\Phi\gamma$	Spherical polar coordinates in K_A (pole figure)
$\alpha\beta$	Spherical polar coordinates of the crystal direction $[hkl]$ in K_A
γ	Orientation angle measured about $[hkl]$
K_B	Crystal fixed coordinate system
$X'Y'Z'$	Coordinate axes in K_B
$x'y'z'$	Coordinates in K_B
h	Crystal direction
h_i, hkl	Direction cosines of the crystal direction in K_B
$\Phi\beta$	Spherical polar coordinates in K_B (inverse pole figure)
$\alpha'\beta'$	Spherical polar coordinates of the sample direction y in K_B
γ'	Orientation angle measured about y
dh, dy	Element of solid angle
g	Rotation (particularly that which transforms K_A into K_B)
dg	Element of orientation
Δg	Orientation distance
a_{ij}	Components of g in matrix representation (transformation coefficients)
$\varphi_1\Phi\varphi_2$	EULER angles (first definition)
$\Psi\Theta\Phi$	EULER angles (second definition)
d	Rotation axis
$\vartheta\psi$	Polar coordinates of the rotation axis
ω	Rotation angle
$\rho\alpha\beta$	WILLIAMS' orientation parameters
$\omega\psi\varrho$	RUER's orientation parameters
$\varrho_1\varrho_2\varrho_3$	LÜCKE's orientation parameters
$(hkl) [uvw]$	MILLER indices of normal direction and rolling direction
ζ	Orientation parameter $\cos \Phi$
I	The invariant measure

g_A, g_B	Rotations of sample and crystal symmetries
G_A, G_B	Groups of rotations of sample and crystal symmetries
h_α, y_α	Symmetrically equivalent directions
g_α	Symmetrically equivalent orientations
Z	Number of symmetrically equivalent orientations (multiplicity)
$h_i, h_j, y_i, y_j, g_i, g_j$	Symmetrically non-equivalent directions and orientations
$f(g), R(h)$	Orientation distribution function in the case of general texture and fibre texture, respectively
$C_i^{\mu\nu}, C_i^\mu$	Coefficients of the orientation distribution function
$\Delta C_i^{\mu\nu}, \Delta C_i^\mu$	Errors of the coefficients $C_i^{\mu\nu}$ and C_i^μ , respectively
$A(h, y), A(h, \Phi)$	Generalized axis distribution function
$P_{h_i}(y), P_{h_i}(\Phi)$	The pole figure associated with the crystal direction h_i
$F_i^y(h_i), F_i(h_i)$	Coefficients of pole figures
$\Delta F_i^y(h_i), \Delta F_i(h_i)$	Errors of coefficients of pole figures
$\varepsilon_i^y(h_i), \varepsilon_i(h_i)$	Differences between measured and calculated coefficients
$R_{y_j}(h), R_{\Phi_j}(h)$	Inverse pole figure of the sample direction y_j and Φ_j , respectively
$H_i^\mu(y_j), H_i^\mu(\Phi_j)$	Coefficients of the inverse pole figure
$W_{h_i y_j}(\Theta)$	Angular distribution function
$G_i(h_i, y_j)$	Coefficients of the angular distribution function
r	(As index) random distribution
obs., cal.	(As index) observed and calculated quantities
\wedge	Unnormalized quantities
N_i	Normalization factor for the h_i pole figure
w_i	Weighting factor for the h_i pole figure
I_P, I_R	Number of pole figures and inverse pole figures respectively
$l_{\max.}$	Resolving power
ΔP	Difference integral of the pole figures
R, R_{hi}	Residual errors (R factors)
$A_L, A_L(h_i), A_L(y_j)$	Truncation error of the orientation distribution function, pole figure and inverse pole figure, respectively
J, J_{h_i}, J_{y_j}	Texture index (sharpness measure) of the orientation distribution function, pole figure and inverse pole figure, respectively
q_j	Weighting factor of coincident reflections
q_{ij}	Weighting factor of multi-phase coincident reflections
$f_0(g)$	Non-random distribution function with vanishing pole figure
ABDE, abde	Abbreviations used in connection with the generalized axis distribution function

$\Phi_A \Phi_B$	Limiting angles in incomplete figure
a	Matching factor for transmission and back-reflection range
Z_{lmn}	Augmented JACOBI polynomials
$w(\Psi\Theta\Phi)$	Orientation distribution function (ROE's notation)
W_{lmn}	Coefficients of the orientation distribution function (ROE's notation)
$q(\chi\eta)$	Pole figure (ROE's notation)
Q_{lm}	Coefficients of pole figures (ROE's notation)
$\chi\eta$	Spherical polar coordinates of the pole figure (ROE's notation)
$\Theta\Phi$	Spherical polar coordinates of the inverse pole figure (ROE's notation)
$S(\Phi)$	Scattering function in the neighbourhood of a preferred orientation (ideal orientation in a generalized sense)
a_λ, b_λ	Coefficients of the series expansion of the scattering function in the general case and in the case of fibre textures
S_0	Value of the scattering function for $\Phi = 0$
Φ_0	The value of the angle Φ , for which $S(\Phi)$ has fallen to 1/e of its maximum value
M_i	Proportion of the i th texture component (ideal orientation or fibre component)
$\Psi_1(\Phi_0), \Psi_2(\Phi_0)$	Proportion functions
$n(g)$	Orientation distribution function of crystal numbers
$v(g)$	Orientation distribution function of the average grain size
$r_{y_0}(\mathbf{h})$	Orientation distribution of the crystallographic planes in a section perpendicular to the sample direction \mathbf{y}_0
$r(\mathbf{h})$	Orientation distribution of the crystallographic planes in an arbitrarily bent section
$\varphi_i^r, \varphi_i'^\mu$	Coefficients of the series expansions of the functions $\varphi(\mathbf{y})$ and $\varphi'(\mathbf{h})$, respectively
$\varphi(\mathbf{y}), \varphi'(\mathbf{h})$	Orientation distribution of the grain boundary surfaces in the sample fixed and crystal fixed coordinate systems, respectively
$z(\mathbf{y}_0)$	Length of grain boundary lines per unit area for a section perpendicular to the sample direction \mathbf{y}_0
z_i^r	Coefficients of the series expansion of the function $z(\mathbf{y}_0)$
$z'(\mathbf{h})$	Length of grain boundary lines per unit area of grains in \mathbf{h} orientation of a spherical section
$z_i'^\mu$	Coefficients of the series expansion of the function $z'(\mathbf{h})$
$\psi(\mathbf{y}), \psi'(\mathbf{h})$	Orientation distribution of the grain boundary lines in sample fixed and crystal fixed coordinate systems

$\psi_l^v, \psi_l'^\mu$	Coefficients of the series expansion of the function $\psi(\mathbf{y})$ and $\psi'(\mathbf{h})$
$n(\mathbf{y}_0)$	Number of grain corner points per unit area of a section perpendicular to the sample direction \mathbf{y}_0
n_l^v	Coefficients of the series expansion of the function $n(\mathbf{y}_0)$
$n'(\mathbf{h})$	Number of grain corner points per unit area of grains in \mathbf{h} orientation of a spherical section
$n_l'^\mu$	Coefficients of the series expansion of the function $n'(\mathbf{h})$
\vdots	
$W(\Delta g)$	Texture transformation function (relating two textures of possibly different crystal symmetries $(:)$ and $(:)$)
$w(r, \Delta g)$	Orientation correlation function
$E(x)$	Physical properties of a material
\mathbf{E}	Property tensor
$E_{i_1 i_2 i_3 \dots}$	Components of the property tensors
$E(\mathbf{h}), E(\Phi\beta)$	Property function dependent on the direction \mathbf{h}
e_l^μ	Coefficients of the series expansion of the function $E(\mathbf{h})$
$E(g), E(\varphi_1\Phi\varphi_2)$	Property function dependent on the orientation g
$e_l^{\mu\nu}$	Coefficients of the series expansion of the function $E(g)$
\sim	Denotes a polycrystal value
$—$	Denotes a simple orientation averaged value
μ_{im}, ν_{jn}	Components of the series expansion of a_{ij}
$a_l^{mn}(i_1, \dots, i_r; j_1, \dots, j_r)$	Components of the series expansion of the transformation coefficients of a tensor of rank r
$\bar{a}(i_1, \dots, i_r; j_1, \dots, j_r)$	Averaging coefficients of a tensor of rank r
$a_l^{\mu\nu}(i_1, \dots, i_r; j_1, \dots, j_r)$	Coefficients of the series expansion of the averaging coefficients
K_2, K_4, K_6	Magnetic anisotropy constants
I_S	Saturation magnetization
I_R	Remanence
σ_{ij}	Stress tensor
ε_{ij}	Strain tensor
s_{ijkl}, c_{ijkl}	Elastic compliance, stiffness tensor
V, R, H	Approximation according to VOIGT, REUSS and HILL
s_a, c_a	Elastic anisotropy of cubic crystals
t_{ijkl}	Anisotropy tensor of cubic crystals
t_{ijkl}	Texture tensor of cubic materials
N	Number of counts in X-ray or neutron intensity measurements
M	Magnetic torque
P	Magnetic power losses
u_i	Displacement vector
e_{ij}	Deformation tensor
η	Amount of deformation

q	Contraction ratio
M	TAYLOR factor
$m_i^{\mu\nu}$	Coefficients of the series expansion of the TAYLOR factor
α	Angle towards the rolling direction
R	Measure of plastic anisotropy
E_i, E^i	Anisotropy coefficients
\mathfrak{R}_g	Representation matrix
$T_l^{mn}(g), S_l^{mn}(g)$	Generalized spherical harmonics
$Q_l^{mn}(x)$	Generalized spherical functions
Q_l^{mn}	FOURIER coefficients of generalized spherical functions
$\chi_i(\Phi)$	Trace of the generalized spherical harmonics
$\dot{T}_l^{\mu\nu}(g)$	Symmetric generalized spherical harmonics
$k_l^\mu(\mathbf{h})$	Spherical surface harmonics
$\dot{k}_l^\mu(\mathbf{h})$	Symmetric spherical surface harmonics
$P_l^{mn}(\Phi)$	Generalized LEGENDRE functions
$a_l^{mns}, a_l'^{mns}$	FOURIER coefficients of the $P_l^{mn}(\Phi)$
$\bar{P}_l^m(\Phi)$	Normalized associated LEGENDRE functions
$a_l^{ms}, a_l'^{ms}$	FOURIER coefficients of the $\bar{P}_l^m(\Phi)$
$\bar{P}_l^0(\Phi), \bar{P}_l(\Phi)$	Normalized LEGENDRE polynomials
$\dot{A}_l^{m\mu}, \dot{A}_l^{n\nu}, \dot{B}_l^{m\mu}, \dot{B}_l^{n\nu}$	Symmetry coefficients
$M(l), N(l)$	Number of linearly independent spherical surface harmonics of the crystal and sample symmetries, respectively
$\cdot : \cdot$	Symbols for various symmetries
ε_m	Normalization factor
*	Conjugate complex quantity
$\langle \rangle$	Angle between
$(l_1 l_2 m_1 m_2 lm)$	CLEBSCH—GORDAN coefficients
$((l_1 l_2 m_1 m_2 lm))$	Multiplication coefficients of the spherical surface harmonics
$(l_1 l_2 l)$	Multiplication coefficients of the LEGENDRE polynomials
$\{l_1 l_2 \mu_1 \mu_2 l\mu\}$	Symmetric CLEBSCH—GORDAN coefficients
$\{\{l_1 l_2 \mu_1 \mu_2 l\mu\}\}$	Multiplication coefficients of the symmetric spherical surface harmonics
A_l^{mn}, B_l^{mn}	Integrals with generalized LEGENDRE functions
D_l^μ	Integrals with symmetric spherical surface harmonics
φ_4, φ_6	Cubic invariants
n_4, n_6	Normalization factors for cubic spherical surface harmonics
e	Identical rotation
\mathbb{E}	Identity matrix

xx *Symbols*

\tilde{g}	Class of conjugate rotations
\oint	Integral over the total spherical surface or over the total orientation space
\oint	Integral over the elementary region of symmetry
\int_w	Integral over a specified path
$F(g', g''), F(g')$	Convolution integral
G_E	Symmetry group in EULER space

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