Texture of Crystalline Solids, 1980, Vol. 4, pp. 93-97
0390-7951/80/0402-0093$04.50/0

CALCULATION OF AUGMENTED JACOBI POLYNOMIALS BY MEANS OF A RECURRENCE RELATION

ZHI-DE LIANG, JIA-ZHENG XU and FU WANG
Northeast Institute of Technology
Shenyang, China

(Received February 16, 1980)

Abstract: A recurrence relation for $Z_{\ell mn}(\xi)$ is deduced from the recurrence relations for Jacobi polynomials. Based on this relation an ALGOL-60 program has been written for efficiently calculating the $Z_{\ell mn}(\xi)$ required in ODF analysis.

In the program of three-dimensional texture analysis it is necessary to calculate numerical values of the augmented Jacobi polynomials $Z_{\ell mn}(\xi)$ or the generalized Legendre polynomials $P_\ell^{mn}(\Phi)$. Bunge,[1,2] Morris and Heckler,[3,4] Morris,[5] Pospiech and Jura[6] have developed methods for numerical calculations of these polynomials by expanding in Fourier series. These methods have been universally adopted in the computer program for ODF analysis.

In this paper a recurrence relation for $Z_{\ell mn}(\xi)$ has been deduced. Using this relation, for any ℓ the elements of the whole array $Z_{\ell mn}(\xi)$ may be calculated easily. The computer program to be used is written in ALGOL-60.

DEDUCTION OF RECURRENCE RELATION

The augmented Jacobi polynomials, designated $Z_{\ell mn}(\xi)$ by Roe,[7] have the form

$$Z_{\ell mn}(\xi) = Nt^{(m-n)/2}(1-t)^{(m+n)/2}f(t), \tag{1}$$

where

$$t = \frac{1-\xi}{2};$$

$$N = \left[\frac{(2\ell+1)}{2}\cdot\frac{(\ell+m)!(\ell-n)!}{(\ell-m)!(\ell+n)!}\right]^{\frac{1}{2}}\cdot\frac{1}{(m-n)!};$$

$$f(t) = {}_2F_1(\alpha,\beta;\gamma;t).$$

${}_2F_1(\alpha,\beta;\gamma;t)$ is the hypergeometric function defined by

$$ {}_2F_1(\alpha,\beta;\gamma;t) = 1 + \frac{\alpha\cdot\beta}{1\cdot\gamma}\, t + \frac{\alpha(\alpha+1)\beta(\beta+1)}{2!\gamma(\gamma+1)}\, t^2 + \ldots \quad . \tag{1} $$

When α is a negative integer, the series terminates after a finite number of terms, and the resulting polynomial is called a Jacobi polynomial. Following Roe,[7] we set $\alpha = -\ell+m$, $\beta = \ell+m+1$ and $\gamma = m-n+1$.

Jacobi polynomials have the following recurrence relations[8]:

$$ {}_2F_1(\alpha,\beta+1;\gamma+1;t) - {}_2F_1(\alpha,\beta;\gamma;t) = \frac{\alpha(\gamma-\beta)}{\gamma(\gamma+1)} \cdot t\,{}_2F_1(\alpha+1,\beta+1;\gamma+2;t), \tag{2} $$

$$ (\alpha-\beta)\,{}_2F_1(\alpha,\beta;\gamma;t) = \alpha\,{}_2F_1(\alpha+1,\beta;\gamma;t) - \beta\,{}_2F_1(\alpha,\beta+1;\gamma;t) \tag{3} $$

and

$$ \alpha\,{}_2F_1(\alpha+1,\beta;\gamma;t) - (\gamma-1)\,{}_2F_1(\alpha,\beta;\gamma-1;t) = (\alpha+1-\gamma)\,{}_2F_1(\alpha,\beta;\gamma;t). \tag{4} $$

From these relations another one can be obtained

$$ {}_2F_1(\alpha,\beta;\gamma-1;t) = {}_2F_1(\alpha,\beta;\gamma;t) + \frac{\alpha\beta}{\gamma(\gamma-1)}\, t\,{}_2F_1(\alpha+1,\beta+1;\gamma+1;t). \tag{5} $$

By substituting equation (1) into equation (5) the following recurrence relation for $Z_{\ell mn}(\xi)$ is deduced:

$$ Z_{\ell m(n+1)}(\xi) = \frac{(m-n)}{[(\ell-n)(\ell+n+1)]^{\frac{1}{2}}} \cdot \left(\frac{1+\xi}{1-\xi}\right)^{\frac{1}{2}} \cdot Z_{\ell mn}(\xi) - \left[\frac{(\ell-m)(\ell+m+1)}{(\ell-n)(\ell+n+1)}\right]^{\frac{1}{2}} \cdot Z_{\ell(m+1)n}(\xi). \tag{6} $$

Equation (6) is valid for $\xi \neq 1$.

CALCULATION OF ARRAY $Z_{\ell mn}(\xi)$ BY THE RECURRENCE RELATION

Roe[7] has derived the equation

$$ Z_{\ell mn}(\xi) = Z_{\ell\bar{n}\bar{m}}(\xi), \tag{7} $$

and adopted the convention that

$$ Z_{\ell mn}(\xi) = (-1)^{m+n}\, Z_{\ell nm}(\xi) \tag{8} $$

to provide a unique determination of the sign of $Z_{\ell mn}(\xi)$ when m is less than n. Owing to equations (7) and (8), it is found that for any ℓ the numberical values of $Z_{\ell mn}(\xi)$ necessary to be calculated are tabulated in Table I.

TABLE I

$Z_{\ell mn}(\xi)$ to Be Calculated

$Z_{\ell\ell\bar{\ell}}(\xi)$				
$Z_{\ell\ell(\overline{\ell-1})}(\xi)$	$Z_{\ell(\ell-1)(\overline{\ell-1})}(\xi)$			
$Z_{\ell\ell(\overline{\ell-2})}(\xi)$	$Z_{\ell(\ell-1)(\overline{\ell-2})}(\xi)$			
·	·	·		
·	·	·	$Z_{\ell 1\bar{1}}(\xi)$	
·	·	·		
$Z_{\ell\ell 0}(\xi)$	$Z_{\ell(\ell-1)0}(\xi)$	·	$Z_{\ell 10}(\xi)$	$Z_{\ell 00}(\xi)$
·	·	·		
·	·	·	$Z_{\ell 11}(\xi)$	
·	·	·		
$Z_{\ell\ell(\ell-2)}(\xi)$	$Z_{\ell(\ell-1)(\ell-2)}(\xi)$			
$Z_{\ell\ell(\ell-1)}(\xi)$	$Z_{\ell(\ell-1)(\ell-1)}(\xi)$			
$Z_{\ell\ell\ell}(\xi)$				

From Equation (1), the first element of Table I takes the form

$$Z_{\ell\ell\bar{\ell}}(\xi) = \left(\frac{2\ell+1}{2}\right)^{\frac{1}{2}} \cdot \left(\frac{1-\xi}{2}\right)^{\ell} . \tag{9}$$

Putting m= ℓ [hence, the second term of the right side of equation (6) equals zero], n = $-\ell$ and substituting the value of $Z_{\ell\ell\bar{\ell}}(\xi)$ into equation (6) the value of $Z_{\ell\ell(\overline{\ell-1})}(\xi)$ is obtained. In a similar manner the remaining elements of the first column in Table I are obtained one by one. As for the second column, according to equation (7), $Z_{\ell(\ell-1)\bar{\ell}}(\xi)$ equals $Z_{\ell\ell(\overline{\ell-1})}(\xi)$, putting m = $(\ell-1)$, n = $-\ell$ and substituting $Z_{\ell\ell\bar{\ell}}(\xi)$ of the first column and $Z_{\ell(\ell-1)\bar{\ell}}(\xi)$ into equation (6) the value of $Z_{\ell(\ell-1)(\overline{\ell-1})}(\xi)$ is then derived and the remaining elements of this column are derived similarly. This process is repeated for the remaining elements of Table I.

For the exceptional case $\xi = 1$, $Z_{\ell mn}(1)$ deduced from equation (1) has the form

$$Z_{\ell mn}(\xi)_{\xi\to 1} = \begin{cases} \left(\frac{2\ell+1}{2}\right)^{\frac{1}{2}} , & m = n = 0,\ 1,\ 2,\ \ldots,\ \ell; \\ 0 , & m \neq n. \end{cases} \qquad (10)$$

Hence, the values of the whole $Z_{\ell mn}(1)$ are obtained readily by equation (10) without using the recurrence relation.

Finally, it should be noted that errors of $Z_{\ell mn}(\xi)$ generated by successive application of the recurrence relation would be greater than by Fourier series expansion; especially for large value of ℓ. However, in texture analysis the accuracy of measured pole figure data would be much lower than the accuracy of $Z_{\ell mn}(\xi)$ obtained by either method. So, errors of $Z_{\ell mn}(\xi)$ have no significant influence on ODF computation.

CONCLUSION

An ALGOL-60 program has been written for the calculation of an array of $Z_{\ell mn}(\xi)$ by means of a recurrence relation. The calculation is simpler, the program shorter, and the running time less in comparison with previously available algorithms.

Use of a recurrence relation requires the generation of values of the complete array of $Z_{\ell mn}(\xi)$. The program is therefore most suitable for the three-dimensional analysis of materials of low symmetry systems.

ACKNOWLEDGEMENTS

We acknowledge our gratitude to Dr. H. Hu of the U.S. Steel Corp., and Dr. P. R. Morris of Armco, Inc. They have read our manuscript and offered helpful advice. Dr. P. R. Morris proposed these equations[9]

$$Z_{\ell m\bar{n}}(\xi) = (-1)^{\ell+m} \cdot Z_{\ell mn}(-\xi)$$

and

$$Z_{\ell\bar{m}n}(\xi) = (-1)^{\ell+n} \cdot Z_{\ell mn}(-\xi)$$

to improve our computing program, and we shall try to test this idea with great pleasure in the near future.

REFERENCES

1. H-J. Bunge, *Mathematische Methoden der Texturanalyse* (Akademie-Verlag, Berlin, 1969).
2. H-J. Bunge, *Kristall und Technik*, 9, 939 (1974).
3. P. R. Morris and A. J. Heckler, *Advances in X-Ray Analysis*, 11, 454 (1968).
4. P. R. Morris and A. J. Heckler, *Trans. TMS-AIME*, 245, 1877 (1969).
5. P. R. Morris, *Texture Cryst. Sol.*, 2, 57 (1976).

6. J. Pospiech and J. Jura, *Kristall und Technik.*, 10, 783 (1975).
7. R-J. Roe, *J. Appl. Phys.*, 36, 2024 (1965).
8. I. N. Sneddon, *Special Functions of Mathematical Physics and Chemistry* (Oliver and Boyd, Edinburgh, 1956).
9. P. R. Morris and D. C. Koskenmaki, *Texture Cryst. Sol.*, 2, 253 (1977).