CALCULATION OF AUGMENTED JACOBI POLYNOMIALS
BY MEANS OF A RECURRANCE RELATION

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

In the program of three-dimensional texture analysis it
is necessary to calculate numerical values of the augmented
Jacobi polynomials $Z_{lmn}(\xi)$ or the generalized Legendre poly-
nomials $P_{m}^{\alpha}(\phi)$. Bunge,1,2 Morris and Heckler,3,4 Morris,5
Pospiech and Jura6 have developed methods for numerical cal-
culations of these polynomials by expanding in Fourier ser-
ries. These methods have been universally adopted in the
computer program for ODF analysis.

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

DEDUCTION OF RECURRANCE RELATION

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

$$Z_{lmn}(\xi) = N t^{(m-n)/2}(1-t)^{(m+n)/2}f(t),$$

where

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

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

$$f(t) = {}_2F_1(\alpha, \beta; \gamma; t).$$
$\,_{2}F_{1}(\alpha, \beta; \gamma; t)$ is the hypergeometric function defined by

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

When $\alpha$ 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$^8:$

$$\,_{2}F_{1}(\alpha, \beta+1; \gamma+1; t) - \,_{2}F_{1}(\alpha, \beta; \gamma; t) = \frac{\alpha(\gamma - \beta)}{\gamma(\gamma+1)} \cdot \,_{2}F_{1}(\alpha+1, \beta+1; \gamma+2; t), \quad (2)$$

$$(\alpha - \beta) \,_{2}F_{1}(\alpha, \beta; \gamma; t) = \alpha \,_{2}F_{1}(\alpha+1, \beta; \gamma; t) - \beta \,_{2}F_{1}(\alpha, \beta+1; \gamma; t) \quad (3)$$

and

$$\alpha \,_{2}F_{1}(\alpha+1, \beta; \gamma; t) - (\gamma - 1) \,_{2}F_{1}(\alpha, \beta; \gamma-1; t) = (\alpha+1 - \gamma) \,_{2}F_{1}(\alpha, \beta; \gamma-1; t). \quad (4)$$

From these relations another one can be obtained

$$\,_{2}F_{1}(\alpha, \beta; \gamma-1; t) = \,_{2}F_{1}(\alpha, \beta; \gamma; t)$$

$$+ \frac{\alpha \beta}{\gamma(\gamma-1)} t \,_{2}F_{1}(\alpha+1, \beta+1; \gamma+1; t). \quad (5)$$

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

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

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

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

$$Z_{\ell mn}(\xi) = Z_{\ell, m-n}(\xi), \quad (7)$$

and adopted the convention that

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

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 $\lambda$ the numberical values of $Z_{\lambda mn}(\xi)$ necessary to be calculated are tabulated in Table I.

**TABLE I**

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

<table>
<thead>
<tr>
<th>$Z_{\lambda m}(\xi)$</th>
<th>$Z_{\lambda m}(\xi-1)$</th>
<th>$Z_{\lambda m}(\xi-2)$</th>
<th>$Z_{\lambda m}(\xi-3)$</th>
<th>$Z_{\lambda m}(\xi-4)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Z_{\lambda m}(\xi)$</td>
<td>$Z_{\lambda m}(\xi-1)$</td>
<td>$Z_{\lambda m}(\xi-2)$</td>
<td>$Z_{\lambda m}(\xi-3)$</td>
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</table>

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

$$Z_{\lambda m}(\xi) = \left(\frac{2\lambda+1}{2}\right)^{\lambda} \cdot \left(1-\xi\right)^{\lambda}.$$  \(\text{(9)}\)

Putting $m = \lambda$ [hence, the second term of the right side of equation (6) equals zero], $n = -\lambda$ and substituting the value of $Z_{\lambda m}(\xi)$ into equation (6) the value of $Z_{\lambda m}(\xi-1)$ 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), $Z_{\lambda m}(\xi-1)$ equals

$Z_{\lambda m}(\xi-1)(\xi)$, putting $m = (\lambda-1)$, $n = -\lambda$ and substituting $Z_{\lambda m}(\xi)$ of the first column and $Z_{\lambda m}(\xi-1)(\xi)$ into equation (6) the value of $Z_{\lambda m}(\xi-1)(\xi-1)$ 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 $\xi = 1$, $Z_{l m n}(l)$ deduced from equation (1) has the form

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

Hence, the values of the whole $Z_{l m n}(l)$ are obtained readily by equation (10) without using the recurrence relation.

Finally, it should be noted that errors of $Z_{l m n}(\xi)$ 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 $Z_{l m n}(\xi)$ obtained by either method. So, errors of $Z_{l m n}(\xi)$ have no significant influence on ODF computation.

CONCLUSION

An ALGOL-60 program has been written for the calculation of an array of $Z_{l m n}(\xi)$ 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 $Z_{l m n}(\xi)$. The program is therefore most suitable for the three-dimensional analysis of materials of low symmetry systems.

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

and

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

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

REFERENCES