A NEW LIBRARY PROGRAM FOR GENERATING AUGMENTED JACOBI POLYNOMIALS FOR TEXTURE CALCULATIONS

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Abstract. A new library program for generating augmented Jacobi polynomials for texture analysis is presented. By using this program, the spatial orientation distribution maps for the three-dimensional texture analysis can be produced.

INTRODUCTION

In the three-dimensional texture analysis, numerical values of polynomials should be calculated by using generalized Legendre polynomials or augmented Jacobi polynomials.

These polynomials denoted $P^m_n(\theta)$ by Bunge\(^1\) and $Z_{\ell mn}(\xi)$ by Roe\(^2\) are identical with each other except for their normalization constants and, in some cases, sign.

However, the polynomials $Z_{\ell mn}(\xi)$ (we define hereafter, according to the notations used by Roe) have up to now been calculated in the form of Fourier series\(^3\)–\(^6\); the Fourier coefficients in tabular form have already been provided by Morris et al.\(^3\),\(^4\)

If the numerical values of polynomials expanded in Fourier series are adopted in the computer program for ODF analysis, the following disadvantages occur:

1. A computer with a large memory is required to store resident data.

2. Errors of numerical values in a table of Fourier coefficients cause errors in the calculation of the polynomials $Z_{\ell mn}(\xi)$.

To avoid these disadvantages, two methods have been considered feasible to calculate the numerical values of polynomials $Z_{\ell mn}(\xi)$: The first one is deducing $Z_{\ell mn}(\xi)$ from a
recurrence relation. The second is deducing $Z_{\ell mn}(\xi)$ from the hypergeometric series directly. Liang et al. suggested in the recent report the method of generating the polynomials $Z_{\ell mn}(\xi)$ by the first method. To apply this method, however, initial values for each $\ell$, $m$, $n$ must be given previously, which would inevitably lead to the increase in program size, required memory, and processing time.

The purposes of this report are to produce a library program for generating $Z_{\ell mn}(\xi)$ based on the second method; and by using this program to work out the orientation distribution maps for the rolled texture of b.c.c. metals, as an example, by use of a small computer (NEAC-3100).

DEFINITION OF $Z_{\ell mn}(\xi)$ AND ITS GENERATION

The augmented Jacobi polynomials is defined by Roe as follows:

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

where

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

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

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

${}_2F_1(\alpha, \beta; \gamma; t)$ is Gauss' hypergeometric series (see Appendix). The ${}_2F_1$ is generated easily as shown in Figure 1, where $k$ and $\varepsilon$ are pointer and allowance error, respectively. The symbol ($\Leftarrow$) shows that the calculation result on the right hand side should be substituted in the variable on the left hand side.

The polynomials $Z_{\ell mn}(\xi)$ are generated by using the ${}_2F_1$ as shown in Figure 2. According to Figure 1 and Figure 2, a library program for generating augmented Jacobi polynomials was formed in FORTRAN for small computer (NEAC-3100) and in BASIC for personal computer (PC-8001).

We verified the library program by calculating normalized Legendre polynomials $Z_{100}(\xi)$ and normalized associated Legendre polynomials $Z_{100}(\xi)$, and proved by numerical integration that the polynomials $Z_{\ell mn}(\xi)$ generated by this program satisfy the orthogonal relation

$$\int_{-1}^{1} Z_{\ell mn}(\xi) Z_{\ell', mn}(\xi) \, d\xi = \delta_{\ell, \ell'}, \quad (2)$$
PRODUCTION OF SPATIAL ORIENTATION DISTRIBUTION OF CRYSTALLITES

In setting up our library program by using the coefficients of ODF given by Hu, the spatial orientation distribution of crystallites in the as-cold-rolled phosphorus steel sheet can be obtained, as shown in Figure 3. The picture at constant phi ($\phi = 45^\circ$) is almost the same as that obtained by Hu.

Figure 4 shows the spatial orientation distribution of crystallites in the as-rolled molybdenum TZM-sheet at constant phi ($\phi = 45^\circ$), which is produced by using coefficients of ODF determined from our library of $Z_{l_{mn}}(\xi)$. For the spatial orientation distribution map, texture data from X-ray pole figure were used in the form of one of the incomplete pole figures obtained only by the Schulz back reflection technique.
Figure 2. Algorithm to generate $Z_{\lambda \mu \nu}(\xi)$, $\mu \nu$ means interchanging $m$ and $n$. 

$$t := \frac{1-\xi}{2}, \quad \alpha := m-l, \quad \beta := l+m+1, \quad \gamma := m-n+1$$

$$N_{\lambda \mu \nu} := \left[ \frac{2^{l+1} \cdot (l+m)! \cdot (l-n)! \cdot \gamma^2}{2 \cdot (l-m)! \cdot (l+n)! \cdot (m-n)!} \right]^{1/2}$$

$$T := t \cdot \frac{(m-n)/2 \cdot (1-t) \cdot (m+n)/2}{2}$$

$$Z_{\lambda \mu \nu} := N_{\lambda \mu \nu} \cdot T \cdot 2^F_1$$

$$Z_{\lambda \mu \nu} := -Z_{\lambda \mu \nu}$$

START

\[ m : n \]

\[ m \leq n \]

\[ m \sim n \]

END
Figure 3. Spatial orientation distribution map of crystallite in the as-cold-rolled phosphorus-sheet, psi (ψ) vs theta (θ) at constant phi (ϕ = 45°) section, produced by using coefficients of ODF given by Hu.
Figure 4. Spatial orientation distribution map of crystallites in the as-rolled molybdenum TZM-sheet, psi ($\psi$) vs theta ($\theta$) at constant phi ($\phi = 45^\circ$) section, produced by using coefficients of ODF determined from our library.

CONCLUSION

A new library program for generating augmented Jacobi polynomials for three-dimensional texture analysis has been carried out for the purpose of obtaining the spatial orientation distribution of crystallites by the use of a small computer (NEAC-3100) or a personal computer (PC-8001). The details of the program, the required memory capacity and the
accuracy in the computer calculation will be presented in a forthcoming paper.

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APPENDIX

The series \( _1F_1(\alpha; \beta; \gamma; t) \) is known as Gauss' hypergeometric series. This series has been generalized by the introduction of parameters \( p \) and \( q \) as follows:

\[
_pF_q(\alpha_1; \gamma_1; t) = \sum_{n=0}^{\infty} \frac{(\alpha_1)_n (\alpha_2)_n \ldots (\alpha_p)_n}{(\gamma_1)_n (\gamma_2)_n \ldots (\gamma_q)_n} \cdot \frac{t^n}{n!}
\]

where

\[
(x)_n = \frac{\Gamma(x+n)}{\Gamma(x)}
\]

and \( \Gamma(x) \) is Gamma function.

When \( x \) is integer,

\[
(x)_n = x(x+1) \ldots (x+n-1)
\]

The series \( _pF_q \) is known as Pochhammer's generalized hypergeometric series. This series is terminated by the negative integer \( \alpha \), in which case it is useful in the physical sciences. In the case of \( p = q = 1 \), the series is written as \( _1F_1(\alpha; \gamma; t) \) and called "Kummer's confluent hypergeometric series."

Moreover, Kummer's confluent hypergeometric series leads to Laguerre, associated Laguerre and Hermite polynomials. Also, Gauss' hypergeometric series leads to Legendre, associated Legendre, Jacobi, Gegenbauer and Tchebycheff polynomials. It is, therefore, very important to deduce the polynomials \( _pF_q \).

The series \( _pF_q \) is generated easily according to the algorithm as shown in Figure 5.

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