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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 $P_{\ell}^{mn}(\Phi)$ 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.[7] 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 ℓ, 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[2] as follows:

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

where

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

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

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

${}_2F_1(\alpha,\beta;\gamma;t)$ is Gauss' hypergeometric series (see Appendix). The ${}_2F_1$ is generated easily as shown in Figure 1, where k and ε are pointer and allowance error, respectively. The symbol (:=) 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 $Z_{\ell 00}(\xi)$ and normalized associated Legendre polynomials $Z_{\ell m0}(\xi)$, and proved by numerical integration that the polynomials $Z_{\ell mn}(\xi)$ generated by this program satisfy the orthogonal relation[2]

$$\int_{-1}^{1} Z_{\ell mn}(\xi)\, Z_{\ell' mn}(\xi)\, d\xi = \delta_{\ell,\ell'} \ . \qquad (2)$$

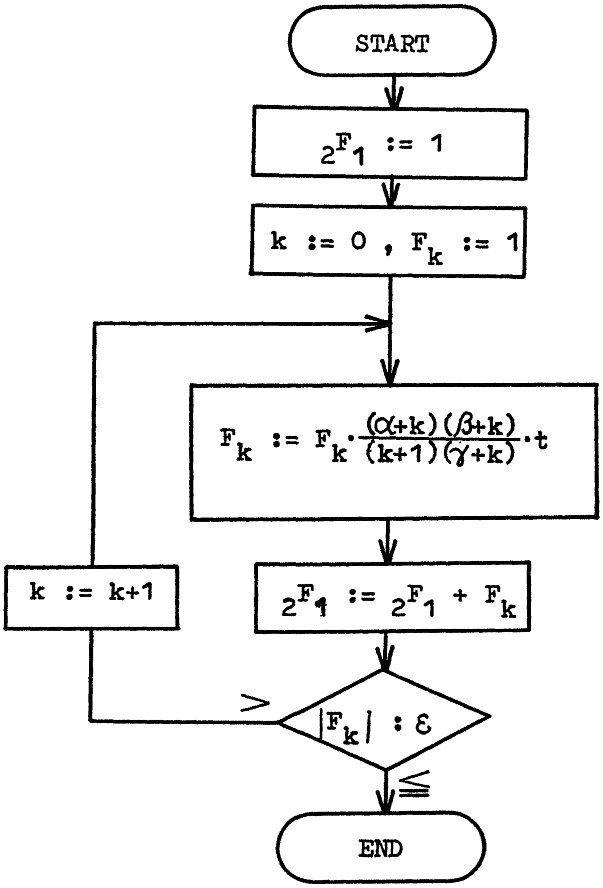


Figure 1. Algorithm to generate $_2F_1(\alpha,\beta;\gamma;t)$.

PRODUCTION OF SPATIAL ORIENTATION DISTRIBUTION OF CRYSTALLITES

In setting up our library program by using the coefficients of ODF given by Hu,[8] 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 ph (ϕ = 45°) 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 (ϕ = 45°), which is produced by using coefficients of ODF determined from our library of $Z_{\ell mn}(\xi)$. 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.

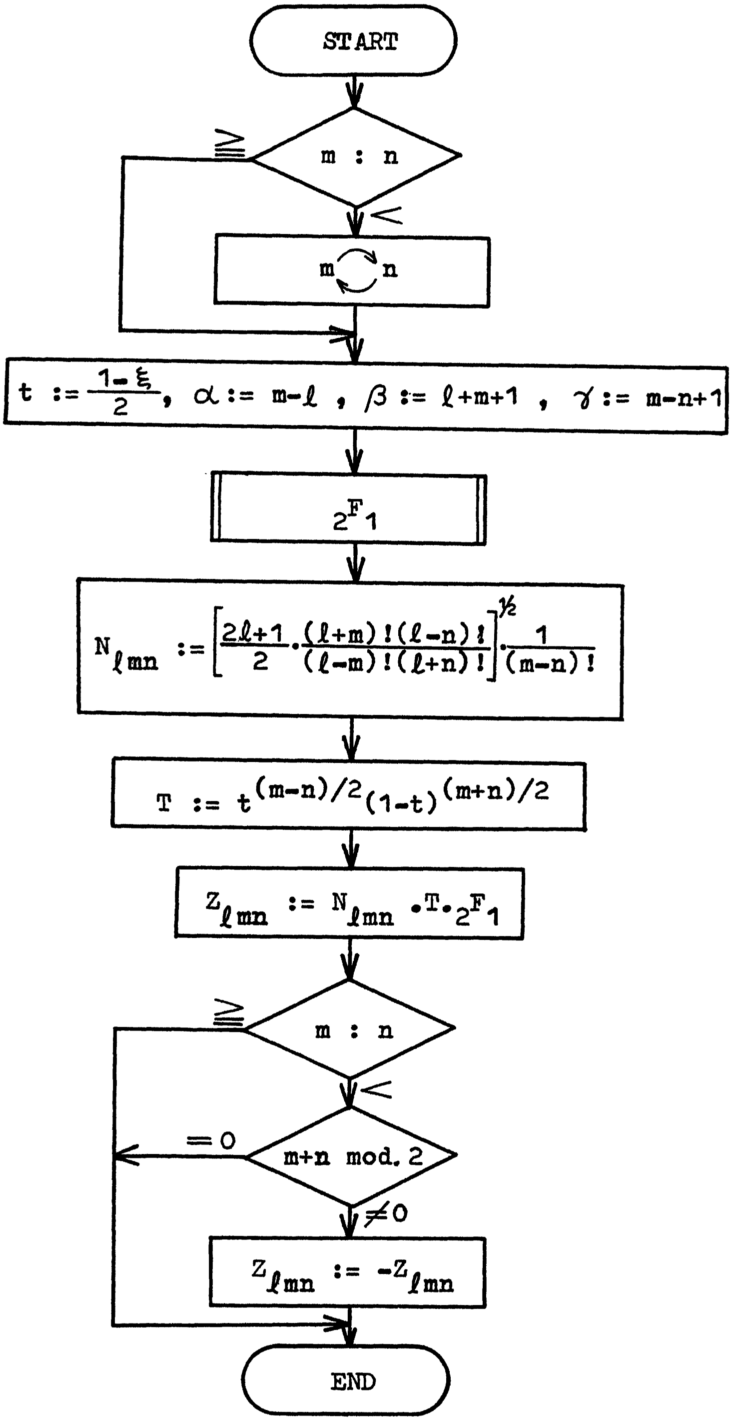
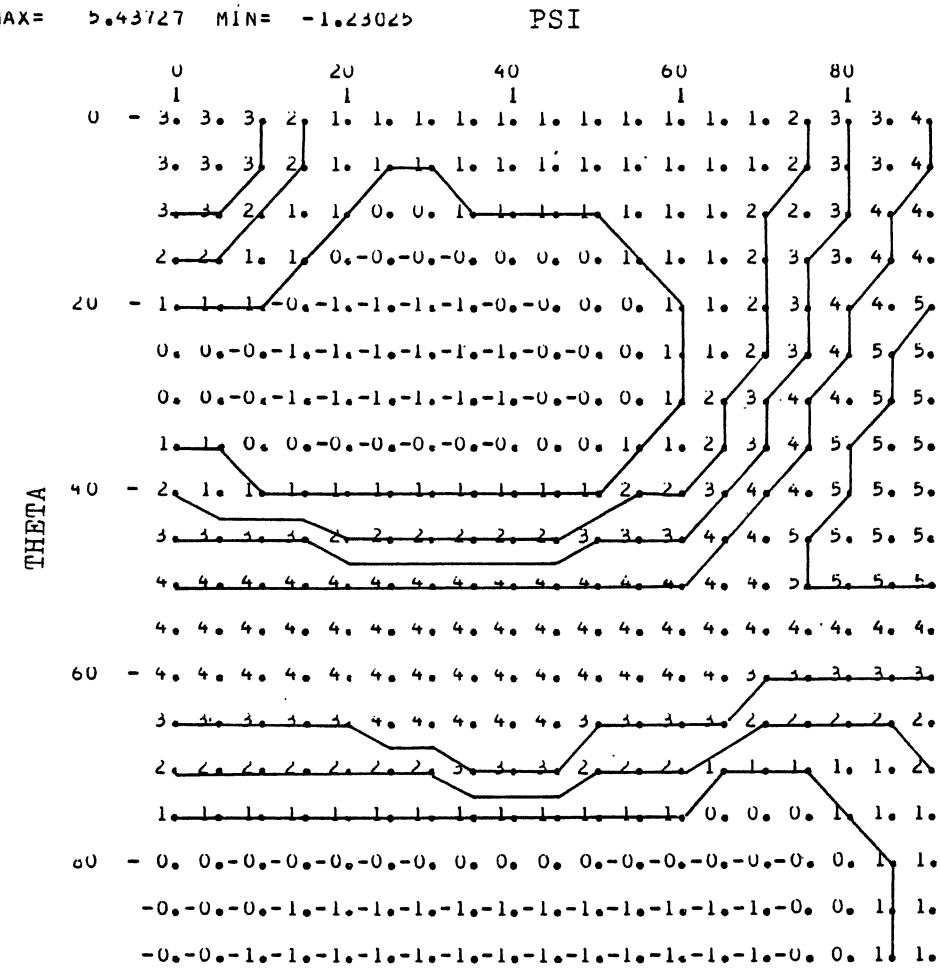


Figure 2. Algorithm to generate $Z_{\ell mn}(\xi)$, m n means interchanging m and n.

*** FIGURE OF ODF FOR PHI = 45.0 ***

MAX= 5.43727 MIN= -1.23025



RANDOM INTENSITY = 1

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..

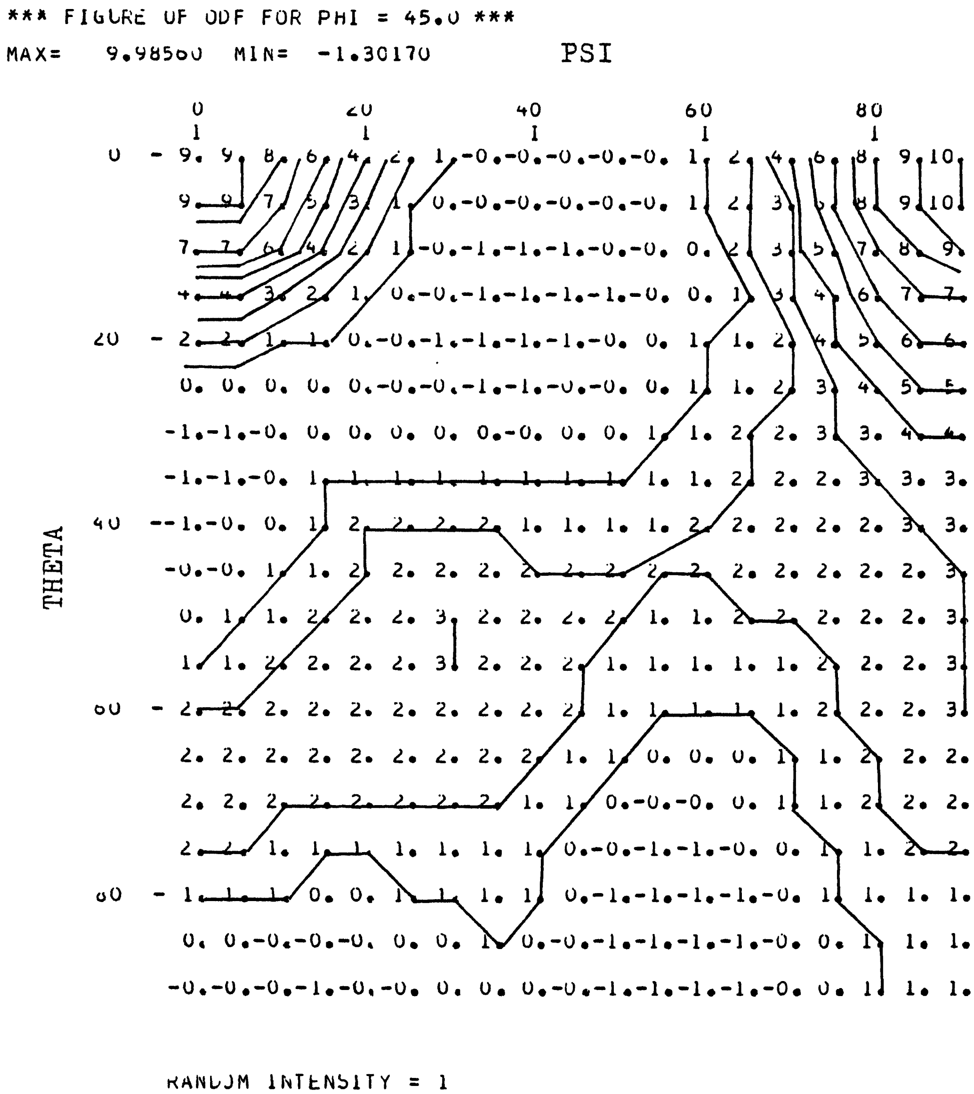


Figure 4. Spatial orientation distribution map of crystallites in the as-rolled molybdenum TZM-sheet, psi (ψ) vs theta (θ) at constant phi (ϕ = 45°) section, produced by using coefficients of ODF determined from our library.

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 ${}_2F_1(\alpha,\beta;\gamma;t)$ is known as Gauss' hypergeometric series.[9] This series has been generalized by the introduction of parameters p and q as follows:[10]

$$ {}_pF_q(\alpha_i;\gamma_j;t) = \sum_{n=1}^{\infty} \frac{(\alpha_1)_n(\alpha_2)_n \cdots (\alpha_p)_n}{(\gamma_1)_n(\gamma_2)_n \cdots (\gamma_q)_n} \cdot \frac{t^n}{n!} $$

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 αs, 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."[11]

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.[12,13] 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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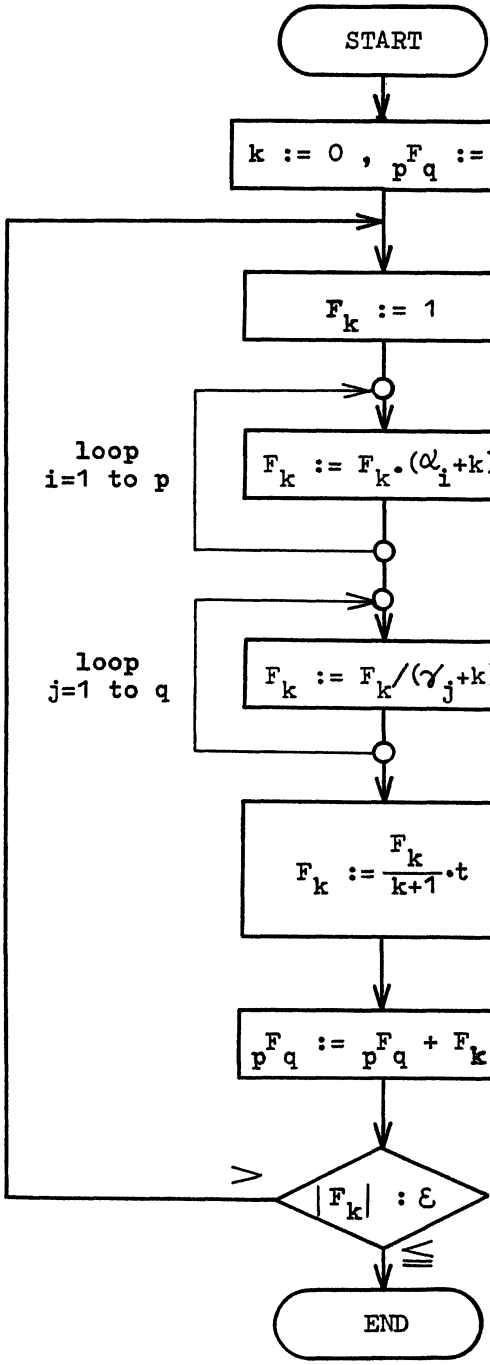

Figure 5. Algorithm to generate $_pF_q(\alpha_i;\gamma_j;t)$.

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11. *Ibid.*, Vol. 1, Chap. 6, pp. 248-293.
12. *Ibid.*, Vol. 2, Chap. 10, pp. 153-228.
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