A NEW LIBRARY PROGRAM FOR TEXTURE CALCULATIONS

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Abstract: A new library program which allows the calculation and storage of the numerical tables necessary for a three-dimensional texture analysis is proposed. Its main characteristics are:

- possibility of selecting the values to be stored according to the desired microscopic and macroscopic symmetries as well as to the step of exploration of the pole figures;
- possibility of choosing the quantity of information to be stored for obtaining, in the further three-dimensional analysis, a good agreement between the computing time and the memory space; and
- great precision of the stored values and short time of calculation due to the use of new and optimized algorithms.

INTRODUCTION

The computation chains used for the three-dimensional texture analysis (according to works of Bunge¹ and of Roe²) generally call upon numerical data previously stored.³⁻⁵

The choice of the numerical data to be stored is essentially governed by two considerations:

- adjustment of these data to microscopic and macroscopic symmetries of the samples the texture of which will be studied, and adjustment to the step of exploration used for pole figures.
- adjustment of the number of stored data to the possibilities of the computer used for their later processing in analysis programmes. In fact, minimal times are required, and it is an advantage to have large data tables if there is enough space in the main storage unit. This is not necessarily true with very powerful computers whose times of access to peripheral units (disk or magnetic tape) and computing times necessary to restore the data tables must be compared.

Finally, the precision of these values must be such that the errors which are necessarily introduced are very small in comparison with other causes of errors.⁶ This latter demand requires the use of highly performant algorithms, especially when the development into series of texture functions and intensity functions used for analysis must reach high orders. It is, therefore, believed that to present a library program which best satisfies the aforementioned considerations would be of interest and usefulness.

I. GENERALITIES AND DEFINITIONS

The library program which we present is written in FORTRAN IV. The numerical data tables which are computed may be stored on a disk or a magnetic tape (sequential form). All the intermediate calculations are executed in double precision; final results are transferred to tables in simple precision form, and they are stored. One of the possibilities offered by our program is the establishment of a library which will be later called "standard library" and which is suited to the three-dimensional analysis chain proposed by Jura, Pospiech and Bunge.⁴

We define hereafter, according to the notations used by Bunge,⁷ the quantities which can be calculated and stored by our program.

i. Coefficients Q_{ℓ}^{mn} defined by:

$$Q_{\ell}^{mn} = i^{m+n} P_{\ell}^{mn}(\pi/2) \quad (1)$$

where the functions $P_{\ell}^{mn}(\phi)$ are polynomials associated to the Jacobi polynomials^{8,9} with

$$\begin{array}{lll} \ell = 2, \text{ LMAX}, 2 & \text{and} & 2 \leq \text{LMAX} \leq 34 \quad (\text{the third index is} \\ m = 0, \ell, \text{ IDN} & & \text{IDN} = 1 \text{ or } 2 \quad \text{the step of pro-} \\ n = 0, m, \text{ IDN} & & \text{gression}) \end{array}$$

The limits fixed for LMAX are the same in all the following definitions. These Q_{ℓ}^{mn} coefficients, proposed by Bunge, lead to a good compromise between the storage space and the computing time necessary to build up the functions used in texture analysis.⁹ They are always real. We use for their calculation a very performant algorithm which is described elsewhere.⁸

These coefficients which are calculated at the beginning of the program are used in all the following calculations.

ii. Functions $\overline{P}_{\ell}^m(\phi)$ defined by:

$$\overline{P}_{\ell}^m(\phi) = i^{-m} (2\ell + 1)^{1/2} P_{\ell}^{m0}(\phi) \quad (2)$$

where $P_{\ell}^{m0}(\phi)$ always represents a polynomial associated with the Jacobi polynomial, with

$$\begin{aligned} \ell &= 2, \text{ LMAX}, 2 \quad \text{and} \quad \text{IDN} = 1 \text{ or } 2 \\ m &= 0, \ell, \text{IDN} \quad 1.25^\circ \leq \Delta\phi \leq 90^\circ \\ \phi &= 0, 90^\circ, \Delta\phi \end{aligned}$$

These functions $\overline{P}_\ell^m(\phi)$ are calculated in our program by using their development into Fourier sums.

iii. *Symmetrized harmonic functions* $\dot{k}_\ell^\mu(h_i)$

with $\ell = 2, \text{ LMAX}, 2$
 $\mu = 1, M(\ell), 1$ where $M(\ell)$ is dependent on the microscopic symmetry considered;
 $h_i = \{\phi_i, \beta_i\} =$ angles characterizing the normal to the (hkl) plane required

These functions are linear combinations of the harmonic functions $k_\ell^m(\phi, \beta)$.⁷ The most general expression for them is:

$$\begin{aligned} \dot{k}_\ell^\mu(\phi_i, \beta_i) &= \dot{A}_\ell^{\text{O}\mu} k_\ell^{\text{O}}(\phi_i, \beta_i) + \sum_{m=1}^{\ell} \dot{A}_\ell^{m\mu} (2\pi)^{-1/2} \overline{P}_\ell^m(\phi_i) \cos m\beta_i \\ &+ \sum_{m=1}^{\ell} \dot{A}_\ell^{m\mu} (2\pi)^{-1/2} \overline{P}_\ell^m(\phi_i) \sin m\beta_i \quad (3) \end{aligned}$$

where the coefficients $\dot{A}_\ell^{\text{O}\mu}$, $\dot{A}_\ell^{m\mu}$ and $\dot{A}_\ell^{m\mu}$ are symmetry coefficients, which are real ($\dot{A}_\ell^{\text{O}\mu}$, $\dot{A}_\ell^{m\mu}$) or imaginary ($\dot{A}_\ell^{m\mu}$).

They have very simple expressions except in the case of cubic symmetry which will be considered in a later section.

Our program allows the calculation of these functions $\dot{k}_\ell^\mu(h_i)$ for all the symmetry cases where the $\dot{A}_\ell^{m\mu}$ coefficients are zero, i.e. for real $\dot{k}_\ell^\mu(h_i)$ functions, so that the definition expression can be written:

$$\dot{k}_\ell^\mu(h_i) = \sum_{m=0}^{\ell} \dot{B}_\ell^{m\mu} \overline{P}_\ell^m(\phi_i) \cos m\beta_i \quad \text{with} \quad \begin{cases} \dot{B}_\ell^{\text{O}\mu} = (2\pi)^{-1/2} \dot{A}_\ell^{\text{O}\mu} \\ \dot{B}_\ell^{m\mu} = (2\pi)^{-1/2} \dot{A}_\ell^{m\mu} \end{cases} \quad (4)$$

These symmetry cases correspond to all the Laue classes including the holoedry of crystalline systems except the triclinic system.

The case of the monoclinic system is rather different, because it requires an unusual choice of the microscopic reference axis (Z axis in the mirror plane) for the definition

(4) to be appropriate.

These functions can be calculated for 8 (hkl) planes at most in the case of cubic symmetry without data reading and/or for 12 (hkl) planes at most in the case of any other microscopic symmetry (except the triclinic). When a non-cubic symmetry is asked one has to specify the values of angles ϕ_i, β_i characterizing the (hkl) planes required as input values (by card reader).

For the cubic symmetry the 8 possible (hkl) planes are: (100), (110), (111), (102), (112), (122), (103), (113).

iv. Coefficients a_{ℓ}^{ms}

$$a_{\ell}^{ms} = \epsilon (4\ell + 2)^{1/2} Q_{\ell}^{ms} Q_{\ell}^{so} \quad (5)$$

where the coefficients Q_{ℓ}^{mn} are those defined in i. and where

$$\begin{aligned} \epsilon &= (-1/2)^{m/2} \quad \text{if } s = 0 \\ \epsilon &= (-1)^{m/2} \quad \text{if } m \text{ is even} \\ \epsilon &= (-1)^{(m-1)/2} \quad \text{if } m \text{ is odd} \end{aligned}$$

with $\ell = 2, LMAX, 2$

$m = 0, \ell, IDN$ IDN is an integer

$s = 0, \ell, 2$

These coefficients are real numbers.

v. Coefficients of cubic symmetry $B_{\ell}^{m\mu}$

with $\ell = 2, LMAX, 2$

$m = 0, \ell, 4$

$\mu = 1, M(\ell), 1$

In the case of cubic symmetry, it is not possible to give a simple analytical expression which defines these coefficients. As a matter of fact, they are obtained during the search for linear combinations of harmonic functions $k_{\ell}^m(\phi, \beta)$ leading to the invariant functions $k_{\ell}^{\mu}(h_i)$ for this symmetry. We use for the calculation of cubic symmetry coefficients $B_{\ell}^{m\mu}$ a very efficient subroutine which was conceived after the work of Esling et al.¹⁰ concerning the use of projectors in the problems of symmetrisation.¹¹

vi. Coefficients a_{ℓ}^{mns}

$$a_{\ell}^{mns} = \epsilon Q_{\ell}^{ms} Q_{\ell}^{sn} \quad (6)$$

where $\epsilon = 1$ if $s = 0$ with $\ell = 2, LMAX, 2$
 $\epsilon = 2$ if $m + n$ even $m = 0, \ell, IDM$
 $\epsilon = 2i$ if $m + n$ odd $n = 0, \ell, IDN$
 $s = 0, \ell, 1$

For s being different from zero and $m + n$ being odd these coefficients are imaginary numbers, i.e., of the ib form. In these cases, the value b alone is stored.

II. ORGANIZATION

Two main possibilities are offered by our program. The first one consists of the storing of the Q_{ℓ}^{mn} coefficients, the $k_{\ell}^{\mu}(h_1)$ symmetrized functions and the $B_{\ell}^{m\mu}$ coefficients if cubic symmetry is of interest.

The second one allows us to constitute a library which includes the $\overline{P}_{\ell}^m(\phi)$ functions, the a_{ℓ}^{ms} and a_{ℓ}^{mns} coefficients as well as the $k_{\ell}^{\mu}(h_1)$ functions, and eventually the $B_{\ell}^{m\mu}$ coefficients.

In both cases, the LMAX value can be chosen, and so can be the step of progression of all the indices and of the angles included in the study.

The "standard library" answers a special choice of the different indices within the second possibility previously mentioned. Indeed, we have here LMAX = 34, $\Delta\phi = 5^\circ$, IDN = 2 and IDM = 4, the microscopic symmetry required being the cubic symmetry.

Figure 1 shows the ordinogram of our library program. The three parameters ISTOK, IST, ISYM are respectively used to test the choice between the two main possibilities, the possible choice of the "standard library," and the desired microscopic symmetries. The parameter ISYM allows three options: cubic symmetry (ISYM = 1), a symmetry other than cubic (ISYM = 0), or cubic and another non-cubic symmetry (ISYM = -1).

The listing of the library program is given in Annex I. Some information about the necessary data cards (only one for "standard library") are given in Annex II. Lastly, explanations for reading again the stored values will be found in Annex III.

III. RESULTS

1. Memory space used by the program

The described library program requires 25 K words in the main storage unit, with words of 32 bits (4 bytes). This necessary memory space can be reduced by reducing the size of some arrays, when the maximum possibilities of the program are not used (for example LMAX < 34 or only one microscopic symmetry asked). The classical methods of overlay or of the storage of intermediate results outside the main memory also allow the use of this program with computers having less than 25 K words available.

2. Computing time

The whole execution time of the program depends, of course, on the configuration of the computer used. Therefore, let us give for guidance only some computing times obtained with various equipments.

To create the "standard library" 13 minutes are necessary with an IBM 370/135 computer, and 84 minutes with an IBM 370/11

Figure 1. Ordinogram of the library program.

computer using virtual memory. By using overlay with a PDP 11/70 computer having an available central memory of 32 K words of 16 bits, setting up a library where LMAX = 22 takes 6.67 minutes. We must remark that the printing of all the results reduces considerably the speed of the carrying out

of the program, the time necessary being approximately halved when the output instruction PRINT is cut out.

3. Accuracy

By using a computer which needs 32 bits to represent a real value in simple precision (64 bits in double precision) i.e. with about 7.2 decimal digits (16.8 in double precision), the error in the stored values is always smaller than one on the seventh significant digit.

A very detailed analysis of the errors on the Q_l^{mn} coefficients⁸ on which our program is based has shown that the calculation algorithm used gives at least 9 significant figures at order $l = 34$. Therefore, it becomes obvious that for these coefficients as well as for the other stored values, the accuracy achieved is not determined by the calculation stages (in double precision), but by the size of the computer word (7.2 decimals in simple precision) used for the storage of the values.

CONCLUSION

The "library program" described here allows a coherent construction of all the data tables generally required for texture calculations. Thanks to the accuracy obtained for the stored values, it succeeds in reducing as much as possible the causes of errors, a constant subject of care in texture analysis. Because of its numerous possibilities, especially for that concerning symmetries, the development of the present program has taken these variables into consideration to enable the study of materials with diverse microscopic symmetries.

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ANNEX I - LIBRARY PROGRAM

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1  C
2  C
3  C      ****LIBRARY PROGRAM****
4  C
5  C
6      DOUBLE PRECISION IQLMN(4046),DANG(2,12),DEB(16,3,9),PI,PI2,SI,CX,
7      *CT,CF,CF,C
8      DIMENSION BB(16,3,9),RES(73),XK(16,3,8),YK(17,12,12),NOMB(16),
9      *HKL(15)
10     COMMON/FREM/IQLMN,PI,LMAX
11     COMMON/DEUS/DEB
12     DATA HKL/' CU', 'BIQU','E', '100','110','111','102','112',
13     *'122','103','113',4*'0'/
14     DATA NOMB/1,1,1,1,2,1,2,2,2,2,3,2,3,3,3,3/
15     DATA LEC,IMP,LIE/1,3,8/
16     DATA DANG/0.157079632679490D01,0.D0,0.157079632679490D01,
17     *0.785398163397448D0,0.955316618124509D0,0.785398163397448D0,
18     *0.463647609000806D0,0.D0,0.615479708670387D0,0.785398163397448D0,
19     *0.841068670567930D0,0.110714871779409D01,0.321750554396642D0,
20     *0.D0,0.440510663004699D0,0.785398163397448D0,8*0.D0/
21     PI = 3.141592653589793 D0
22     PI2=1.570796326794897D0
23     READ(LEC,10) IST
24     LMAX = 34
25     IDM = 4
26     IDN = 2
27     ISYM = 1
28     JV = 40
29     IPAS=500
30     IF(IST) 100,100,101
31     100 READ (LEC,10) LMAX,IDN,IDM
32     101 CALL DLMNR1
33     IF(IST) 102,102,103
34     102 READ (LEC,10) ISTOK
35     IF (ISTOK) 103, 103, 104
36  C
37  C      ***STORAGE OF COEFFICIENTS Q(L,M,N)***
38  C
39     104 WRITE(IMP,11) LMAX, IDN, IDN
40     DO 106 L = 2, LMAX,2
41     WRITE (IMP,12)L
42     J1=(L*L*L/2+3*L*L/4-L/2)/6
43     IL=L+1
44     DO 106 IM=1,IL,IDN
45     M= IM-1
46     J2=M*(M+1)/2
47     JI= J1+J2
48     I=M/IDN+1
49     DO 105 N=1,IM,IDN
50     J=(N-1)/IDN+1
51     105 RES(J)=DQLMN(JI+N-1)
52     WRITE(LIB) (RES(J),J=1,I)
53     106 WRITE(IMP,13)M,(RES(J),J=1,I)
54     103 IF(IST)118,118,119
55     118 IF(ISTOK)107, 107, 125
56  C
57  C      ***CALCULATION AND STORAGE OF FUNCTIONS P(L,M,PHI)***
58  C
59     107 READ (LEC,10) IPAS
60     119 CF=DFLOAT(IPAS)*PI/18.D03
61     JF = 9000/IPAS + 1
62     IF((IPAS-250).LT.0) JV = JF

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63     RES(1) = FLOAT(IPAS)/100.
64     WRITE(IMP,14) LMAX,IDN,RES(1)
65     DO 120 L=2,LMAX,2
66     WRITE(IMP,12)L
67     CT=DSQRT(DFLOAT(4*L+2))
68     IL = L+1
69     J1=(L*L*L/2+3*L*L/4-L/2)/6
70     DO 120 IM = 1,IL,IDN
71     M = IM-1
72     CX=0.DO
73     SI=1.DO
74     IF (M/2*2-M) 109,110,110
75     109 CX=PI2
76     IF ((M-1)/4*4-M+1) 111,112,112
77     110 IF (M/4*4-M) 111,112,112
78     111 SI=-1.DO
79     112 J2=J1+(M+1)*M/2
80     DO 123 J=1,JF
81     CF=DGLMN(J1)*DGLMN(J2)*SI*CT/2.DO
82     DO 124 IS = 2,L,2
83     I=(IS+1)*IS/2
84     IF (M-IS) 113,114,114
85     114 JI=J2+IS
86     GO TO 124
87     113 JI=J1+I+M
88     124 CF=CF+DGLMN(JI)*DGLMN(J1+I)*SI*CT*DCOS(CF*DFLOAT((J-1)*IS)-CX)
89     123 RES(J)=CF
90     WRITE(IMP,13)M,(RES(I),I=1,JF)
91     WRITE(LIB) (RES(J), J = 1,JV)
92     120 CONTINUE
93     JV = 40
94     125 JF= 8
95     IF (IST) 126,126,127
96     126 READ(LEC,10) ISYM,JF
97     127 IF (ISYM) 128,129,128
98     C
99     C ***CALCULATION OF CUBIC SYMMETRY'S COEFFICIENTS B(L,M,MU)***
100    C
101    128 CALL CSYM
102    C
103    C ***CALCULATION AND STORAGE OF FUNCTIONS K(L,MU,PHI)-CUBIC SYMMETRY***
104    C
105    WRITE(IMP,17) (HKL(J),J=1,3),LMAX
106    DO 130 J=1,JF
107    WRITE(IMP,18) HKL(J+3)
108    DO 130 L=4,LMAX,2
109    I = NOMB(L/2-1)
110    JI=L/4+1
111    L2=L/2-1
112    CT=DSQRT(DFLOAT(4*L+2))
113    J1=(L*L*L/2+3*L*L/4-L/2)/6
114    DO 131 MU=1,I
115    C=0.DO
116    DO 132 IM= 1,JI
117    M = 4*(IM-1)
118    J2=J1+(M+1)*M/2
119    CF=DGLMN(J1)*DGLMN(J2)*CT/2.DO
120    DO 133 IS = 2,L,2
121    IN=(IS+1)*IS/2
122    IF (M-IS) 115,116,116
123    115 N=IN+M+J1
124    GO TO 133
125    116 N=J2+IS
126    133 CF=CF+DGLMN(N)*DGLMN(J1+IN)*CT*DCOS(DFLOAT(IS)*DANG(1,J))
127    132 C=C+DCOS(DFLOAT(M)*DANG(2,J))*CF*DBB(L2,MU,IM)
128    131 XK(L2,MU,J) = C
129    130 WRITE(IMP,19) L, (XK(L2,MU,J),MU=1,I)
130    WRITE(LIB)XK
131    DO 158 J=1,JV
132    158 RES(J)=0.
133    DO 159 J=1,17
134    159 WRITE(LIB)RES
135    129 IF (ISYM) 134, 134, 135

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136 C
137 C   ***CALCULATION AND STORAGE OF FUNCTIONS K(L,MU,PHI)-NON CUBIC SYMMETRY**
138 C
139   134 READ(LEC,10) I,JF,J
140       IF (J.EQ.1) I=1
141       JF=JF+3
142       READ(LEC,20) (HKL(J), J=1,JF)
143       READ(LEC,21) DANG
144       C=1.DO/DSQRT(PI)
145       WRITE(IMP,25) (HKL(J), J=1,3), LMAX, I
146       JF=JF-3
147       DO 136 J=1, JF
148       WRITE(IMP,26) HKL(J+3), DANG(1,J), DANG(2,J)
149       DO 136 L=2, LMAX, 2
150       JT = L/I+1
151       L2 = L/2
152       CT=DSQRT(DFLOAT(4*L+2))
153       J1=(L*L*L/2+3*L*L/4-L/2)/6
154       DO 137 MU = 1, JT
155       M = (MU-1)*I
156       CX=C
157       IF (M) 121,121,122
158   121 CX=C/DSQRT(2.DO)
159   122 CF=0.DO
160       SI=1.DO
161       J2=J1+(M+1)*M/2
162       IF (M/2-M) 117,138,138
163   117 CX=-C
164       CF=PI2
165       IF ((M-1)/4-M) 139,108,108
166   138 IF (M/4-M) 139,108,108
167   139 SI=-1.DO
168   108 CF=DQLMN(J1)*DQLMN(J2)*CT*SI/2.DO
169       DO 140 IS = 2, L, 2
170       IM=(IS+1)*IS/2
171       IF (M-IS) 160,161,161
172   160 N=J1+M+IM
173       GO TO 140
174   161 N=J2+IS
175   140 CF=CF+DQLMN(N)*DQLMN(J1+IM)*CT*SI* DCOS(DFLOAT(IS)*DANG(1,J)-CF)
176   137 YK(L2,MU,J)=CF*CX*DCOS(DFLOAT(M)*DANG(2,J))
177   136 WRITE(IMP,19) L, (YK(L2,MU),0), MU=1, JT
178       WRITE(LIB) YK
179   135 IF (IST.EQ.1) ISTOK=0
180       IF (ISTOK) 142,142,141
181 C
182 C   ***CALCULATION AND STORAGE OF COEFFICIENTS APRIM(L,M,S)***
183 C
184   142 WRITE(IMP,23) LMAX, IDN
185       DO 143 L=2, LMAX, 2
186       WRITE(IMP,12) L
187       J1=(L*L*L/2+3*L*L/4-L/2)/6
188       CT=DSQRT(DFLOAT(4*L+2))
189       IL = L + 1
190       JF=L/2+1
191       DO 143 IM = 1, IL, IDN
192       M = IM - 1
193       J2=J1+(M+1)*M/2
194       SI=1.DO
195       IF (M/2-M) 162,163,163
196   163 IF (M/4-M) 164,165,165
197   162 IF ((M-1)/4-M) 164,165,165
198   164 SI=-1.DO
199   165 RES(1)=DQLMN(J1)*DQLMN(J2)*CT*SI/2.DO
200       DO 144 IS=2, L, 2
201       I=(IS+1)*IS/2
202       IF (M-IS) 167,166,166
203   166 JI=J2+IS
204       GO TO 144
205   167 JI=J1+I+M
206   144 RES(IS/2+1)=DQLMN(JI)*DQLMN(J1+I)*CT*SI
207       WRITE (IMP,13) M, (RES(I), J = 1,JF)
208   143 WRITE(LIB) (RES(J), J = 1,JF)
209   141 IF (ISYM) 145, 146, 145

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210 C
211 C      ***STORAGE OF CUBIC SYMMETRY'S COEFFICIENTS B(L,M,MU)***
212 C
213 145 WRITE (IMP,15) LMAX
214 DO 147 L=4,LMAX,2
215   WRITE (IMP,12) L
216   L2 = L/2-1
217   JJ = L/4+1
218   JF = NOMB(L2)
219   DO 147 MU = 1,JF
220   DO 148 IM=1,JI
221   148 BB(L2,MU,IM)=DBB(L2,MU,IM)
222 147 WRITE (IMP,16) MU, (BB(L2,MU,IM), IM=1,JI)
223   WRITE (LIB) BB
224 146 IF (ISTOK) 149,149,157
225 C
226 C      ***CALCULATION AND STORAGE OF COEFFICIENTS APRIM(L,M,N,S)***
227 C
228 149 WRITE (IMP,22) LMAX, JIM, IDN
229 DO 150 L=2,LMAX,2
230   WRITE (IMP,12) L
231   IL = L+1
232   J1=(L*L*L/2+3*L*L/4-L/2)/6
233   DO 150 IM = 1,IL, IDM
234   M = IM-1
235   JI=(M+1)*M/2+J1
236   DO 150 IN=1,IL, IDN
237   N = IN-1
238   JF=(N+1)*N/2+J1
239   RES(1)=DQLMN(JI)*DQLMN(JF)
240   DO 151 IS=1,L
241   IF (M-IS) 152, 153, 153
242 152 I=(IS+1)*IS/2+M+J1
243   GO TO 154
244 153 I=JI+IS
245 154 IF (N-IS) 155, 156, 156
246 155 J=(IS+1)*IS/2+N+J1
247   GO TO 151
248 156 J=JF+IS
249 151 RES(IS+1)=DQLMN(I)*DQLMN(J)*2.DO
250   WRITE (LIB) (RES(I), I = 1, JV)
251 150 WRITE (IMP,24) M,N, (RES(J), J=1,IL)
252 157 REWIND LIB
253 STOP
254 10 FORMAT(3I3)
255 11 FORMAT(1H1,54X,21HCoefficients G(L,M,N),10X,4HL=2,,I2,4H( 2)/54X,
256   *23(1H*),9X,7HM=0, L(,I2,1H)/86X,7HN=0, M(,I2,1H)///)
257 12 FORMAT(1X/,64X,2HL=,I2/63X,6(1H+)/)
258 13 FORMAT(1X/2X,2HM=,I2,4X,10F12.8/7(10X,10F12.8//)
259 14 FORMAT(1H1,49X,32HFonctions de Legendre P(L,M,Phi),10X,4HL=2,,I2,4
260   *H( 2)/49X,34(1H*),9X,7HM=0, L(,I2,1H)/90X,9HPhi=0,90(,F5.2,1H)///)
261 15 FORMAT(1H1,43X,44HCoefficients de Symetrie (Cubique) B(L,M,MU),10X
262   *,4HL=4,,I2,3H(2)/43X,46(1H*),9X,9HM=0, L(4)/97X,9HMu=1,M(L)///)
263 16 FORMAT(1X/1X,3HMu=,I2,4X,10F12.8/2(10X,10F12.8//)
264 17 FORMAT(1H1,36X,34HFonctions Harmoniques Symetrisees(,3A4,11H)K(L,M
265   *U,HI),10X,4HL=2,,I2,3H(2)/36X,59(1H*),8X,9HMu=1,M(L)/103X,18HHI=AN
266   *GLES POUR HKL///)
267 18 FORMAT(1X///61X,5HHKL=(,A4,1H)/60X,12(1H=)//)
268 19 FORMAT(1X/2X,2HL=,I2,4X,10F12.8/2(10X,10F12.8//)
269 20 FORMAT(16(A4,1X))
270 21 FORMAT(4I20,13)
271 22 FORMAT(1H1,52X,27HCoefficients APRIM(L,M,N,S),10X,4HL=2,,I2,4H( 2)
272   */52X,29(1H*),9X,7HM=0, L(,I2,1H)/90X,7HN=0, L(,I2,1H)/90X,10HS=0,
273   *L( 1)///)
274 23 FORMAT(1H1, 52X ,25HCoefficients APRIM(L,M,S),10X,4HL=2,,I2,4H( 2)
275   */52X,27(1H*),9X,7HM=0, L(,I2,1H)/88X,10HS=0, L( 2)///)
276 24 FORMAT(1X/,1X,2HM=,I2,3H N=,I2,10F12.8/(10X,10F12.8//)
277 25 FORMAT(1H1,36X,34HFonctions Harmoniques Symetrisees(,3A4,11H)K(L,M
278   *U,HI),10X,4HL=2,,I2,3H(2)/36X,59(1H*),8X,9HMu=1,M(L)/103X,18HHI=AN
279   *GLES POUR HKL//49X,33HL'AXE Z DE KB EST UN AXE D'ORDRE ,I2///)
280 26 FORMAT(1X///61X,5HHKL=(,A4,1H)/60X,12(1H=)//33X,4HPhi=,I20,13,
281   *4HRAD.,10X,5HBETA=,I20,13,4HRAD.//)
282 END

```

```

1 C
2 C
3 C   THIS SUBROUTINE CALCULATES THE Q(L,M,N) COEFFICIENTS
4 C
5 C
6     SUBROUTINE DLMNR1
7     DOUBLE PRECISION DGLMN(4046)
8     DOUBLE PRECISION DDPI(35,35),DIB ,DIPSJ,PI
9     DOUBLE PRECISION DALPHA
10    COMMON/PRM/DGLMN,PI,LMAX
11    ALPHA(M,K)=DSQRT(DFLOAT((M+K)*(M+1-K)))
12    DO 116 L=2,LMAX,2
13    J1=(L*L*L/2+3*L*L/4-L/2)/6
14    LPS1=L+1
15    DDPI(LPS1,LPS1)=1.D0/2.D0**L
16    IN=L
17    CALL IRIN(L,IN,DIB)
18    DDPI(LPS1,1)=DSQRT(DIB)*DDPI(LPS1,LPS1)
19    DDPI(L,1)=0.D0
20    DO 101 J=2,L
21    IP=LPS1-J
22    CALL IRIN (IP,IN,DIB)
23    DDPI(LPS1,J)=DSQRT(DIB)*DDPI(LPS1,LPS1)
24    IF ((IP/2*2-IP) .NE. 0) DDPI(LPS1,J)=-DDPI(LPS1,J)
25    DDPI(L,J)=DDPI(LPS1,J)*DFLOAT(J-1)*DSQRT(2.D0/DFLOAT(L))
26 101 CONTINUE
27    I=LPS1
28 105 I=I-1
29    DO 110 J=2,I
30    DIPSJ=DFLOAT(I+J-2)
31    DDPI(I-1,J-1)=(-DIPSJ*2.D0*DFLOAT(J-2)*DDPI(I,J)+2.D0*DIPSJ*DALPHA
32    1(L,I)*DDPI(I+1,J)+DALPHA(L,I)*DALPHA(L,J)*DDPI(I+1,J+1))/(DALPHA(
33    2L,I-1)*DALPHA(L,J-1))
34 110 CONTINUE
35    IF (I-2)115,115,105
36 115 LMS2=L-2
37    IF (LMS2.EQ.0) GO TO 114
38    DO 113 I=2,LMS2+2
39    DDPI(I,1)=0.D0
40 113 CONTINUE
41 114 DO 116 I=1,LPS1
42    DO 116 J=1,I
43    IF ((I-1)/2*2-(I-1) .NE. 0) DDPI(I,J)=-DDPI(I,J)
44    KLIN=J1+I*(I-1)/2+J-1
45    DGLMN(KLIN)=DDPI(I,J)
46 116 CONTINUE
47    RETURN
48    END

```

```

1 C
2 C
3 C   THIS SUBROUTINE CALCULATES THE B(L,M,MU) COEFFICIENTS
4 C
5 C
6     SUBROUTINE CSYM
7     DOUBLE PRECISION DGLMN(4046)
8     DOUBLE PRECISION DDPI(35,35),DPROJ(9,9),DREDUC(9,9),DBB(16,3,9),
9     *PI,DFISQ,DDIMS,DNORM,DFISQD
10    COMMON/PRM/DGLMN,PI,LMAX
11    COMMON/DEUS/DBB
12    DFISQ=DSQRT(PI)
13    DFISQD=DFISQ*DSQRT(2.D0)
14    DO 120 L=4,LMAX,2
15    IDIMH=L/4+1
16    LL=L/2-1
17    J1=(L*L*L/2+3*L*L/4-L/2)/6
18    LPS1=L+1
19    DO 205 I=1,LPS1,4
20    DO 205 J=1,I,4
21    KLIN=J1+I*(I-1)/2+J-1
22    II=(I-1)/4+1

```

```

23      JJ=(J-1)/4+1
24      IF (J.EQ.1) GO TO 200
25      IF (I.EQ.J) DPROJ(II,JJ)=(1.DO+4.DO*DGLMN(KLIN))/3.DO
26      IF (I.NE.J) DPROJ(II,JJ)=4.DO*DGLMN(KLIN)/3.DO
27      GO TO 204
28      200 IF (I.EQ.1) DPROJ(II,JJ)=(1.DO+2.DO*DGLMN(KLIN))/3.DO
29      IF (I.NE.1) DPROJ(II,JJ)=2.DO*DSQRT(2.DO)*DGLMN(KLIN)/3.DO
30      204 DPROJ(JJ,II)=DPROJ(II,JJ)
31      205 CONTINUE
32      DDIMS=0.DO
33      DO 220 I=1, IDIMH
34      DDIMS=DDIMS+DPROJ(I,I)
35      220 CONTINUE
36      IDIMS=IFIX(SNGL(DDIMS+0.5IDO))
37      IMINS=IDIMH+1-IDIMS
38      I=IDIMH+1
39      I=I-1
40      IF (DPROJ(I,I).GT.1.D-4) GO TO 170
41      IF (I-1) 210,210,160
42      170 DNORM=DSQRT(DPROJ(I,I))
43      DO 250 J=1, IDIMH
44      DREDUC(I,J)=DPROJ(I,J)/DNORM
45      DPROJ(I,J)=DPROJ(I,J)/DPROJ(I,I)
46      250 CONTINUE
47      IF (I-1) 210,210,180
48      180 IMS1=I-1
49      DO 300 ILINE=1,IMS1
50      DO 300 JCOLON=1,I
51      DPROJ(ILINE,JCOLON)=DPROJ(ILINE,JCOLON)-DPROJ(I,JCOLON)*DPROJ(ILIN
52      I,I)
53      300 CONTINUE
54      IF (I-IMINS) 210,210,160
55      210 DO 650 I=IMINS, IDIMH
56      II=IDIMH-I+1
57      DREDUC(I,1)=DREDUC(I,1)/DFISQD
58      DBB(LL,II,1)=DREDUC(I,1)
59      DO 650 J=2, IDIMH
60      DREDUC(I,J)=DREDUC(I,J)/DFISQ
61      DBB(LL,II,J)=DREDUC(I,J)
62      650 CONTINUE
63      120 CONTINUE
64      RETURN
65      END

```

```

1  C
2  C
3  C      THIS SUBROUTINE CALCULATES A BINOMIAL COEFFICIENT
4  C
5  C
6  C      SUBROUTINE IBIN(IP,N,BI)
7  C      DOUBLE PRECISION BI,XM,XI
8  C      BI=1.DO
9  C      IF (2*IP-N) 630,630,640
10 C      630 JP=IP
11 C      GO TO 650
12 C      640 JP=N-IP
13 C      650 IF (JP) 699,680,660
14 C      660 XM=DFLOAT(N-JP)
15 C      DO 670 I=1,JP
16 C      XI=DFLOAT(I)
17 C      670 BI=(BI*(XM+XI))/XI
18 C      680 RETURN
19 C      699 WRITE(3,611) IP,N
20 C      BI=0.DO
21 C      611 FORMAT(1X,3I3)
22 C      END

```

ANNEX II - DATA CARDS

If the "standard library" is asked, only one data card is necessary with the value 1 in column 3 (value of parameter IST). To create any other library, the data cards must be presented in the order specified. All the cards settling the values of integer variables are read with a 3I3 format.

- 1) 0 in column 3 (value of parameter IST)
- 2) Values of LMAX, IDN, IDM (see definitions in paragraph I and ordinogram for the signification of those parameters).
- 3) Value of ISTOK (0 or 1 according to the chosen option)
- *4) Value of IPAS expressed in hundredths of degree. This card must be present only when ISTOK = 0
- 5) Value of ISYM and JF where JF is the required number of (hkl) planes. When ISYM is equal to 0 or -1 (i.e. when a non-cubic symmetry is required) the following cards must be added:
- *6) Values of I, JF and J where I is the class of the highest symmetry axis (ex. 6 for hexagonal), JF is the number of (hkl) lattice planes required, J is a parameter characterizing the monoclinic symmetry (J = 1 when this symmetry is asked, J = 0 in the opposite case).
- *7) Information about the symmetry asked and (hkl) lattice planes used. The reading is done with the help of a 15(A4, 1X) format. The data are classified in a 15 position array HKL (15). The first three array positions are reserved for the alphanumeric characters describing the required symmetry, the other twelve contain the (hkl) indices.

We give here an example of this data card:

```
column : 1   5   10   15   20
          HEXA GONA  LE      10.0 11.0...and so on.
```

- *8) Values of ϕ_i and β_i angles characterizing the previously described (hkl) lattice planes. These values in radians must be given in double precision. They are read with a 4D20.13 format. Therefore, we have two pairs on each card; the maximum number of pairs is fixed to be 12 (i.e. 6 data cards here for angles ϕ_i and β_i).

Besides the "standard library" case, we must have at least 4 data cards. The stars (*) show the additional cards which must be added when some options are chosen.

ANNEX III

CALLING THE STORED VALUES OF THE LIBRARY PROGRAM

The library's values are stored in a sequential file on a magnetic band or a disk. Each time a WRITE statement is executed by the library program a logical record is created. The total number of records is, of course, dependent on the chosen library.

The writing is made in binary mode without format. So reading again the library must be made without format according to the order used to store it.

To reach a table of numerical data it is necessary to know the number of records which precede this table and to jump over them. For example, jumping over the 323 records containing the coefficients Q_{ℓ}^{mn} (with, in this case, $\ell = 2$, LMAX, 2; $m = 0, \ell, 1$; $n = 0, m, 1$) can be achieved by the following statements:

```
10 | DO 10 I = 1,323
    | READ (LIB)      where LIB specifies the logical
                        input-output unit for the library
```

For the coefficients Q_{ℓ}^{mn} , a_{ℓ}^{ms} and the functions $\overline{P}_{\ell}^m(\phi)$ the reading as well as the writing is made for fixed values of ℓ and m , with an implicit DO statement involving the third "parameter" (index n , index s and value of angle ϕ respectively). So, an array is filled up whose dimension must be at least equal to the number, let's say IMAX, of coefficients or functions obtained when the third "parameter" varies throughout. Then a READ statement will be of the form:

```
| READ (LIB) (RES(I), I = 1,IMAX)
```

where RES is an array in which the coefficients or functions are placed. This statement will be given in two loops in which ℓ ($\ell = 2, \text{LMAX}, 2$) then m ($m = 0, \ell, \text{IDN}$) are successively fixed.

For the coefficients a_{ℓ}^{mns} the READ statement is the same. However, it is made in three loops settling in this case ℓ , m and n .

The functions $\dot{k}_{\ell}^{\mu}(h_i)$ for cubic symmetry, $\dot{k}_{\ell}^{\mu}(h_i)$ for non-cubic symmetry and the coefficients $\dot{B}_{\ell}^{m\mu}$ are placed within arrays with three indices (these arrays are named, in the library program, XK, YK and BB). Each of these arrays is stored as a lump, i.e. with one WRITE statement, and therefore must be read again in the same way. For example, all the functions $\dot{k}_{\ell}^{\mu}(h_i)$ for cubic symmetry can be read with the statement:


```

| | READ (LIB) XK

```

The dimensions of these arrays are as follow:

```

| | DIMENSION XK(16,3,8), YK(17,12,12), BB(16,3,9)

```

The two first indices in the previous arrays correspond to the indices l and μ . The third is correlated with h_i or m according as the functions $k_l^\mu(h_i)$ or the coefficients B_l^{μ} are involved.

It is important also to note that, after the array XK, 17 empty records are stored; this is only made so as to have a "standard library" which can be used directly in existing analysis programs.

For example we give hereafter a short program which allows to read again all the stored values in the "standard library" (let us remember that for this library $LMAX = 34$, $IDN = 2$, $IDM = 4$, $\Delta\phi = 5^\circ$).

```

C      DIMENSION RES(35), XK(16,3,8), BB(16,3,9)
      DATA LIB /1/
      DATA LMAX, IDN, IDM, IDPHI /34,2,4,500/
C      READING OF FUNCTIONS P(L,M,PHI)
      IMAX = 9000/IDPHI
      DO 10 L = 2,LMAX,2
      IL = L+1
      DO 10 IM = 1,IL,IDN
10      READ (LIB) (RES(I), I = 1,IMAX)
C      READING OF FUNCTIONS K(L,MU,HI)
      READ (LIB) XK
C      READING OF COEFFICIENTS APRIM(L,M,S)
      DO 20 L = 2,LMAX,2
      IL = L+1
      IMAX = L/2+1
      DO 20 IM = 1,IL,IDN
20      READ (LIB) (RES(I), I = 1,IMAX)
C      READING OF COEFFICIENTS B(L,M,MU)
      READ (LIB) BB
      READING OF COEFFICIENTS APRIM (L,M,N,IS)
      DO 30 L = 2,LMAX,2
      IL = L+1
      DO 30 IM = 1,IL,IDM
      DO 30 IN = 1,IL,IDN
30      READ (LIB) (RES(I), I = 1,IL)
      END

```