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A REVISED FORTRAN IV PROGRAM TO CALCULATE
CRYSTALLOGRAPHIC FUNCTIONS

George J. Werkema

THE DOW CHEMICAL COMPANY
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A REVISED FORTRAN IV PROGRAM TO CALCULATE CRYSTALLOGRAPHIC FUNCTIONS

George J. Werkema

Abstract. This program is a revision of one written earlier (USAEC Report RFP-326, August 1963) for a small computer. The availability of a computer having a medium-to-large memory permits various improvements in operating convenience to be made. The present program has been written in IBM 360 E-level FORTRAN IV. Values of the interplanar spacing 'd,' $\sin^2\theta$, and 2θ are calculated for the crystallographic planes hkl . Planes that are found to be systematically nonreflecting by virtue of the space group symmetry elements coded in the data are omitted from the output list. The calculated results are sorted on increasing 2θ in blocks of 2000 before listing.

INTRODUCTION

The identification of a polycrystalline material by means of x-ray diffraction relies upon the proper indexing of the x-ray diffractogram of that compound. For many materials, only the unit cell parameters, density, and perhaps a proposed space group have been reported in the literature. In these cases, identification of the material depends solely upon matching the observed diffraction angles or interplanar spacings of the unknown material with those values which may be calculated from known unit cell parameters. Although the algorithm for these calculations is trivial, the results frequently constitute a "last resort" in the identification of unknown materials.

MATHEMATICAL EXPRESSIONS

Values of the interplanar spacing $d(hkl)$ are calculated using the expression

$$d(hkl) = [V^2 / (S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl)]^{1/2},$$

where $V^2 = a^2b^2c^2 (1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)$,

$$S_{11} = b^2c^2\sin^2\alpha,$$

$$S_{22} = a^2c^2\sin^2\beta,$$

$$S_{33} = a^2b^2\sin^2\gamma,$$

$$S_{12} = abc^2 (\cos\alpha\cos\beta - \cos\gamma),$$

$$S_{23} = a^2bc (\cos\beta\cos\gamma - \cos\alpha),$$

$$S_{13} = ab^2c (\cos\alpha\cos\gamma - \cos\beta).$$

Using the Bragg equation, values of $\sin\theta_{hkl}$ are computed from values of $d(hkl)$. Hastings arcsine approximation, sheet 37,¹ is used to compute values of $2\theta_{hkl}$. This approximation is of the form:

$$2\theta_{hkl} = 180.0 - 114.5916 (\sqrt{1 - \sin^2\theta_{hkl}}) \Psi, \text{ where}$$

$$\Psi = 1.570795207 - 0.214512362 \sin\theta_{hkl} + 0.087876311 \sin^2\theta_{hkl} - 0.044958884 \sin^3\theta_{hkl} + 0.019349939 \sin^4\theta_{hkl} - 0.004337769 \sin^5\theta_{hkl}.$$

FEATURES

Miller Index Generation:

The order of Miller Index generation within the program is $\overline{hkl}$. The sets $\pm(hkl)$ are generated by means of a three-level nested loop, one level for each index. As a set (hkl) is generated, it is tested first for systematic extinction, and then its corresponding $d(hkl)$ is calculated and tested for containment within the chosen sphere (as determined from the value of the input datum $2\theta_{\max}$). A systematically extinct set (hkl) lying within the chosen sphere is discarded and the inferior index, h , is incremented to produce a new set. When a set (hkl) is found to lie outside the chosen sphere, that set is discarded, and program control is transferred to the next loop level. Finally, a set $(00l)$ with $|l|$ greater than any previous value is found to lie outside the chosen sphere, which signals an exit from the index generation routine.

Sorting of Output:

For each set (hkl) , the program calculates $d(hkl)$, $\sin^2\theta_{hkl}$ and $2\theta_{hkl}$. These results are then sorted

¹ Cecil B. Hastings, *Approximations for Digital Computers*, (Princeton University Press, 1955), page 161.

on increasing $2\theta_{hkl}$ in blocks of 2000. Sorting is accomplished by the "step-ladder" technique, while preserving the association among the computed values for each set. There is no limit to the number of sets that may be computed. If the input data permit the generation of more than 2000 sets, the first 2000 are sorted and listed, after which the program returns to the index generation routine and the process continues.

Total Planes Count:

The last record of the output is a fixed point number equal to the total number of sets generated.

Multijob Operation:

Upon completion of output, the program has an option which directs the computer to process immediately the next set of input data and to repeat the calculations for the material defined by those data.

INPUT INSTRUCTIONS

Card 1: Control Card 1 (4X, 14)
col. 1-4 blank
5-8 NJOB
Number of data sets to be processed.
Only one card of this type is needed for each program use.

Card 2: Title Card (4X, 17A4)
col. 1-4 blank
5-72 TITLE
Any Hollerith characters, e.g., name of material.

Card 3: Unit Cell Constants (4X, 6F10.5)
col. 1-4 blank
5-14 A unit cell constant a in Angstroms
15-24 B unit cell constant b in Angstroms
25-34 C unit cell constant c in Angstroms
35-44 ALF unit cell constant α in degrees
45-54 BET unit cell constant β in degrees
55-64 GAM unit cell constant γ in degrees

Card 4: Calculation Control Card (4X, 2F10.5, 2I1)
col. 1-4 blank
5-14 TTHMAX maximum limit of 2θ to be calculated
15-24 WAVE wavelength of radiation used in Angstroms

25 KSW1 external program control indicator
KSW1=0, program generates four octants (hkl), ($h\bar{k}l$), ($h\bar{k}\bar{l}$), and ($\bar{h}kl$), sorts, and outputs automatically.
KSW1=1, program generates all positive (hkl) only, then looks for "INDIC" control cards (Card 6) for further instructions.
Note: With this option in effect, the program will not list output unless it is instructed to do so with an "INDIC" = 4 control card.
26 KSW2 Output control character
KSW2=0, output routine lists only non-redundant crystallographic planes plus one representative of any redundant set. For example, in the cubic system, (200), (020), and (002) are redundant, and only one of these three would be listed.
KSW2=1, output routine lists all planes that have passed extinction and limitation tests.

Card 5: Space Group Systematic Extinction Card (4X, 16I4)

col. 1-4 blank
5-8 KTYPE(1) code number for first reflection class suffering conditional extinction.
9-12 MCOND(1) code number of extinction condition for first class.
13-16 KTYPE(2) code number for second reflection class suffering conditional extinction.
17-20 MCOND(2) code number of extinction condition for second class.
.
.
.
.
.
.
61-64 KTYPE(8)
65-68 MCOND(8)

Each of the 230 three-dimensional space groups is defined by a unique set of symmetry operators. The presence of certain of these operators in crystals imposes conditions on the appearance of various zones or classes of x-ray reflections which may be observed in the diffractometry of those crystals. The same conditions obtain for polycrystalline diffractometry as well. Provision is made in this program to specify up to eight reflection classes and their corresponding extinction conditions in order to produce a list which contains only those reflections which are theoretically possible. Table I lists the codes which are recognized by this program. A zero

Table I. Systematic absence words.

Reflection Class	Nonextinction Condition	Extinction Code (214) KTYPE(N), MCOND(N)
hk l	$h + k + l = 2n$	9 1
	$h + k = 2n$	9 2
	$h + l = 2n$	9 3
	$k + l = 2n$	9 4
	$h - k = 3n$	9 5
	$-h + k + l = 3n$	9 6
	$h - k + l = 3n$	9 7
	$h + k + l = 3n$	9 8
Ok l	$k = 2n$	8 1
	$l = 2n$	8 2
	$k + l = 2n$	8 3
	$k + l = 4n$	8 4
hh l	$l = 2n$	7 1
	$h = 2n$	7 2
	$h + l = 2n$	7 3
	$2h + l = 4n$	7 4
hOl	$h = 2n$	6 1
	$l = 2n$	6 2
	$h + l = 2n$	6 3
	$h + l = 4n$	6 4
OO l	$l = 2n$	5 1
	$l = 3n$	5 2
	$l = 4n$	5 3
	$l = 6n$	5 4
hkO	$h = 2n$	4 1
	$k = 2n$	4 2
	$h + k = 2n$	4 3
	$h + k = 4n$	4 4
OkO	$k = 2n$	3 1
	$k = 4n$	3 2
hhO	$h = 2n$	2 1
hOO	$h = 2n$	1 1
	$h = 4n$	1 2

or blank field instructs the computer to exit the extinction routine, and therefore, any non-zero extinction codes must appear to the left of the unused fields on this card. A completely blank card simply inactivates the extinction routine. The order of code pairs on this card is not important; the order within a code pair must list class code first and condition code second, i.e., KTYPE(N), MCOND(N).

Cards 6, and on. External Program Control Cards (4X, II)

col. 1-4 blank

5 INDIC, external program control character.

This option permits the user to control the course of the program if it is not desired to generate all four octants. For example, in an orthogonal crystal system, all of the lines on a powder diffractogram can be indexed using (hk l) all positive. The other three octants are redundant. In the monoclinic system, powder diffractograms may be indexed using (hk l) and ($\bar{h}$ k l). The other two octants are redundant.

The INDIC control cards are interrogated by the program only if KSW1=1 on card 4. If this option is chosen, the course of the program is under the control of the user, user, who must supply the proper sequence of INDIC cards to obtain the desired output. The program generates (hk l) all positive and computes the associated values of d , $\sin^2\theta$, and 2θ before interrogating the first INDIC control card.

INDIC=1 The program generates (hk l) and computes the associated values of d , $\sin^2\theta$, and 2θ .

INDIC=2 The program generates ($\bar{h}$ k l) and computes associated values of d , $\sin^2\theta$, and 2θ .

INDIC=3 The program generates ($\bar{h}$ k l) and computes associated values of d , $\sin^2\theta$, and 2θ .

INDIC=4 The program sorts and lists all the stored values of $\pm(hk\bar{l})$, d , $\sin^2\theta$, and 2θ , then tests NJOB for additional computations. If NJOB is satisfied, the program terminates via a normal exit.

PROGRAM LISTING

```

C DRFXR.1
C THIS PROGRAM CALCULATES D-SPACING AND TWO THETA FOR
C CRYSTALLOGRAPHIC PLANES (HKL) AND NOTES SPACE GROUP
C SYSTEMATIC ABSENCES.
      DIMENSION DBL(2000),TBL(2000),SNBL(2000)
      DIMENSION NH(2000),NK(2000),NL(2000)
      DIMENSION TITLE(17),KTYPE(8),MCOND(8)
      INPT = 1
      LIST = 3
91  READ(INPT,2001)NJOB
2001 FORMAT(4X,I4)
      DO 222 JOB = 1,NJOB
      READ(INPT,2002)TITLE
2002 FORMAT(4X,17A4)
      READ(INPT,2003)A,B,C,ALF,BET,GAM
2003 FORMAT(4X,6F10.5)
      READ(INPT,2004)TTHMAX,WAVE,KSU1,KSU2
2004 FORMAT(4X,2F10.5,2I2)
      READ(INPT,2005)(KTYPE(N),MCOND(N),N = 1,8)
2005 FORMAT(4X,16I4)
      ALF = ALF*0.017453292
      BET = BET*0.017453292
      GAM = GAM*0.017453292
      CSA = COS(ALF)
      CSB = COS(BET)
      CSG = COS(GAM)
      SNA = (1.0-CSA*CSA)**0.5
      SNB = (1.0-CSB*CSB)**0.5
      SNG = (1.0-CSG*CSG)**0.5
      WAVBY2 = WAVE/2.0
      THMAX = TTHMAX*0.008726646
      DLIM = WAVBY2/SIN(THMAX)
      ASQ=A*A
      BSQ=B*B
      CSQ=C*C
      ANGFAC=1.0-CSA*CSA-CSB*CSB-CSG*CSG
      ANGFAC=ANGFAC+2.0*CSA*CSB*CSG
      VSQ=ASQ*BSQ*CSQ*ANGFAC
      S11=BSQ*CSQ*SNA*SNA
      S22=ASQ*CSQ*SNB*SNB
      S33=ASQ*BSQ*SNG*SNG
      S12=A*B*CSQ*((CSA*CSB)-CSG)
      S23=ASQ*B*C*((CSB*CSG)-CSA)
      S13=A*BSQ*C*((CSG*CSA)-CSB)
      INDIC=1
      INCRH=1
      INCRK=1
      INCRL=1

```

```

NC=0
M=1
144  IH=0
      IK=0
      IL=0
147  IH=IH+INCRH
      MARKER=1
212  KCLASS=0
      IF(IH) 240,241,240
240  KCLASS=KCLASS+1
241  IF(IK) 242,243,242
242  KCLASS=KCLASS+3
243  IF(IL) 244,245,244
244  KCLASS=KCLASS+5
245  IF(IH+IK) 246,248,246
246  IF(IH-IK) 248,247,248
247  KCLASS=KCLASS-2
248  DO 340 N=1,8,1
      IF(KTYPE(N)) 249,50,249
249  IF(KCLASS-KTYPE(N)) 340,250,340
250  K=MCOND(N)
      KB=KCLASS-4
      IF(KB) 251,251,252
251  GO TO (401,402,403,404),KCLASS
252  GO TO (405,406,407,408,409),KB
401  JFNHKL=IH
      GO TO (9,29),K
402  JFNHKL=IH
      GO TO 9
403  JFNHKL=IK
      GO TO (9,29),K
404  GO TO (414,424,434,444),K
414  JFNHKL=IH
      GO TO 9
424  JFNHKL=IK
      GO TO 9
434  JFNHKL=IH+IK
      GO TO 9
444  JFNHKL=IH+IK
      GO TO 29
405  JFNHKL=IL
      GO TO (9,19,29,39),K
406  GO TO (416,426,436,446),K
416  JFNHKL=IH
      GO TO 9
426  JFNHKL=IL
      GO TO 9
436  JFNHKL=IH+IL

```

```

GO TO 9
446 JFNHKL=IH+I6
GO TO 29
407 GO TO (417,427,437,447),K
417 JFNHKL=IL
GO TO 9
427 JFNHKL=IH
GO TO 9
437 JFNHKL=IH+IL
GO TO 9
447 JFNHKL=(IH*2)+IL
GO TO 29
408 GO TO (418,428,438,448),K
418 JFNHKL=IK
GO TO 9
428 JFNHKL=IL
GO TO 9
438 JFNHKL = IK + IL
GO TO 9
448 JFNHKL=IK+IL
GO TO 29
409 GO TO (419,429,439,449,459,469,479,489),K
419 JFNHKL=IH+IK+IL
GO TO 9
429 JFNHKL=IH+IK
GO TO 9
439 JFNHKL=IH+IL
GO TO 9
449 JFNHKL=IK+IL
GO TO 9
459 JFNHKL=IH-IK
GO TO 19
469 JFNHKL=IK+IL-IH
GO TO 19
479 JFNHKL=IH-IK+IL
GO TO 19
489 JFNHKL=IH+IK+IL
GO TO 19
9 IF(JFNHKL)3,340,1
1 JFNHKL=JFNHKL-4
IF(JFNHKL)2,340,1
2 JFNHKL=JFNHKL+2
IF(JFNHKL)55,340,55
3 JFNHKL=JFNHKL+4
IF(JFNHKL)3,340,4
4 JFNHKL=JFNHKL-2
IF(JFNHKL)55,340,55
19 IF(JFNHKL)13,55,11

```

```

11  JFNHKL=JFNHKL-6
    IF(JFNHKL)12,340,11
12  JFNHKL=JFNHKL+3
    IF(JFNHKL)55,340,55
13  JFNHKL=JFNHKL+6
    IF(JFNHKL)13,340,14
14  JFNHKL=JFNHKL-3
    IF(JFNHKL)55,340,55
29  IF(JFNHKL)23,55,21
21  JFNHKL=JFNHKL-8
    IF(JFNHKL)22,340,21
22  JFNHKL=JFNHKL+4
    IF(JFNHKL)55,340,55
23  JFNHKL=JFNHKL+8
    IF(JFNHKL)23,340,24
24  JFNHKL=JFNHKL-4
    IF(JFNHKL)55,340,55
39  IF(JFNHKL)37,340,38
38  JFNHKL=JFNHKL-6
    IF(JFNHKL)55,340,38
37  JFNHKL=JFNHKL+6
    IF(JFNHKL)37,340,55
55  MARKER=2
    GO TO 51
340 CONTINUE
    GO TO 50
177 IF(IH)191,179,191
179 IF(IK)193,180,193
180 IF(KSW1)222,181,101
101 READ(INPT,2007)INDIC
2007 FORMAT(4X,I1)
181 GO TO (111,112,121,211),INDIC
191 IK=IK+INCRK
    IH=0
    GO TO 212
193 IL=IL+INCRL
    IK=0
    IH=0
    GO TO 212
111 INCRH=1
    INCRK=1
    INCRL = -1
    GO TO 124
112 INCRH=1
    INCRK=-1
    INCRL = 1
    GO TO 124
121 INCRH=-1

```

```

        INCRK=1
        INCRL=1
124      INDIC=INDIC+1
        GO TO 144
50      MARKER=1
51      FH=IH
        FK=IK
        FL=IL
        DENOM=S11*FH*FH+S22*FK*FK
        DENOM=DENOM+S33*FL*FL+2.0*S12*FH*FK
        DENOM=DENOM+2.0*S23*FK*FL+2.0*S13*FH*FL
7000    D = SQRT(VSQ/DENOM)
7003    IF(D-DLIM)177,177,53
53      GO TO (313,147),MARKER
313     GO TO(56,314,315,316),INDIC
314     IF(IL)56,147,56
315     IF(IK)56,147,56
316     IF(IH)56,147,56
56      IF(KSW2)222,57,61
57      KR=M-1
58      IF(KR)61,61,59
59      IF(DBL(KR)-D)60,147,60
60      KR=KR-1
        GO TO 58
61      STH=WAVBY2/D
        STH2 = STH*STH
        STH4=STH2*STH2
        PSI=1.570795207-0.214512362*STH
        PSI=PSI+0.087876311*STH2
        PSI=PSI-0.044958884*STH2*STH
        PSI=PSI+0.019349939*STH4
        PSI=PSI-0.004337769*STH4*STH
7001    TWOTH=180.0-PSI*114.5916*SQRT(1.0-STH)
7002    MSW=1
        NH(M)=IH
        NK(M)=IK
        NL(M) = IL
        DBL(M)=D
        TBL(M)=TWOTH
        SNBL(M)=STH2
        M=M+1
        IF(M-2001)147,800,800
800     MD2=M-2
        DO 850 I=1,MD2,1
        MD1=M-1
        I11=I+1
        DO 849 J=I11,MD1,1
        IF(TBL(I)-TBL(J))849,849,803

```

```

803  TEMT=TBL(I)
      TEMD=DBL(I)
      TEMS=SNBL(I)
      IHT=NH(I)
      IKT=NK(I)
      ILT=NL(I)
      TBL(I)=TBL(J)
      DBL(I)=DBL(J)
      SNBL(I)=SNBL(J)
      NH(I)=NH(J)
      NK(I)=NK(J)
      NL(I)=NL(J)
      TBL(J)=TEMT
      DBL(J)=TEMD
      SNBL(J)=TEMS
      NH(J)=IHT
      NK(J)=IKT
      NL(J)=ILT
849  CONTINUE
850  CONTINUE
      WRITE(LIST,2006)
2006  FORMAT(4H1DSP)
      WRITE(LIST,2008)TITLE
2008  FORMAT(4H0    ,16A4)
      FLAM = 2.0*WAVBY2
      WRITE(LIST,2009)FLAM
2009  FORMAT(13H0    LAMBDA = ,F10.5)
      WRITE(LIST,2010)
2010  FORMAT(49H1    H    K    L    D,ANGSTROMS    TWO THETA    SIN2 THETA)
      WRITE(LIST,2011)
2011  FORMAT(1H0)
      I = 0
      LBOX = 0
860  I = I + 1
      LBOX = LBOX + 1
      WRITE(LIST,2012)NH(I),NK(I),NL(I),DBL(I),TBL(I),SNBL(I)
2012  FORMAT(1X,3I4,3F12.5)
      IF(I-MD1)862,872,222
862  IF(LBOX-50)860,868,222
868  WRITE(LIST,2010)
      WRITE(LIST,2011)
      LBOX = 0
      GO TO 860
872  NC = NC + MD1
      M=1
      GO TO (147,221),MSW
211  MSW=2
      GO TO 800

```



```
221  WRITE(LIST,2013)NC
2013  FORMAT(36H0 THE NUMBER OF PLANES GENERATED IS ,I4)
222  CONTINUE
      CALL EXIT
      STOP
      END
```