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A FORTRAN IV COMPUTER PROGRAM FOR CALCULATING INTERPLANAR SPACINGS

A. L. Coffey, Jr.

UNION CARBIDE CORPORATION
NUCLEAR DIVISION
OAK RIDGE Y-12 PLANT

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ABSTRACT

A time-share FORTRAN computer program has been developed which reliably calculates values of interplanar spacings d, $\sin^2\theta$, 2θ, and the crystallographic planes, hkl, for materials whose unit cell parameters and extinction conditions are known. Calculated reflections that are systematically absent because of space group or translational symmetry are eliminated from the output list.

CONTENTS

SUMMARY

For materials whose unit cell parameters and extinction conditions are known, interplanar spacings d, $\sin^2\theta$, and 2θ values can be calculated for the crystallographic planes, hkl. Preexisting BASIC language programs for these calculations were found to be unsuitable for present needs; therefore, a fast, flexible, and easy-to-use FORTRAN program was developed. This program is a reliable revision of the one reported earlier.(1) Originally written for IBM 360 equipment, the program, now on a time-share system, contains a major modification in the extinction subroutine that systematically eliminates calculated reflections which are absent due to space group or translational symmetries.

The use of this FORTRAN program made a vast improvement in time requirements and in the integrity of results over the time-share programs previously available for these calculations.

INTRODUCTION

Analysis of polycrystalline materials by X rays and electron diffraction relies on the proper indexing of the diffraction pattern. Often this program requires information not found in the X-ray powder diffraction data file. For materials whose unit cell parameters and extinction conditions are known, however, identification is possible by matching the observed interplanar spacings of the unknown with values which may be calculated.

An available BASIC language computer program for the calculation of interplanar spacings,[2] although useful, was limited by the confusing practice of ordering the reflections on increasing hkl instead of on decreasing d values and by the lengthy operator time requirements. Modifications by this author, and subsequently by Sjodahl, et al,[3] rearranged the interplanar spacings in decreasing order and decreased operation time, respectively. However, the lack of any provision for supplying extinction information directly, and the necessity for combining two subprograms for the successful operation of the code were additional factors limiting the usefulness of this program.

In a search for a more suitable program, an X-ray powder diffraction trace simulation program, POWD2,[4] was considered. But, even when modified[5] to generate interplanar spacings only, the program was much too large for the available time-share systems.

A smaller FORTRAN IV program was then found in the literature;[1] but, this program, though fast and reasonably flexible, listed d-spacings which should have been absent. However, a check of the program revealed that eliminating the error would probably be more time consuming than replacing the entire extinction routine with one that was previously determined to be reliable. An extra bonus resulting from the exchange of extinction subroutines was that the extinction data for this program and POWD2 would be identical. The substitution was accomplished, the input and output format revised, and the program performed as anticipated.

Since the program is written in FORTRAN, an option has been employed which allows the program to be saved and run in object code instead of source code. This option cuts drastically the time required for the program to run and for the information to be printed. The source program is listed in Appendix A.

CALCULATING INTERPLANAR SPACINGS

PROGRAM DESCRIPTION

Main Program

Miller index generation within the main program is in the order of h, k, l. The sets ± (hkl) are generated by means of a three-level nested loop. As a set of hkl is generated, it is tested first for systematic extinction (subroutine EXTN), and then its corresponding d_{hkl} is calculated and tested for containment within a sphere of reflection as determined by 2θ max.

For each allowed set (hkl), the program calculates d_{hkl}, $\sin^2\theta_{hkl}$, and $2\theta_{hkl}$ which are then sorted on increasing $2\theta_{hkl}$ in blocks of 200. If the input data permit the generation of more than 200 sets, the first 200 are sorted and tested, after which the program returns to the index generation routine and the process continues.

Extinction Conditions

Each of 230 three-dimensional space groups is defined by a unique set of symmetry operations. These operations impose, on a single crystal, conditions affecting the appearance of various zones of X-ray reflections. The same conditions also pertain to polycrystalline diffractometry.

In the subroutine EXTN, the Miller indices are examined for the extinction conditions defined in the input data. Those reflections passing all the tests for nonextinction are accepted. Translational symmetry extinctions as well as lattice extinctions can be considered by the subroutine.

The subroutine tests a reflection by comparing the condition [ie, (h+k)/2n] with its integral equivalent (ie, decimal portion truncated). If the two values are not the same, the reflection does not pass the test and is eliminated.

Mathematical Expressions

Interplanar spacings d_{hkl} are calculated, as in the original program,[1] using the expression:

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

where:

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

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

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

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

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

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

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

Values of $\sin\theta_{hkl}$ are computed from d_{hkl} using Bragg's equation:

$$\sin\theta_{hkl} = \frac{\lambda}{2d_{hkl}}.$$

The Hastings arcsine approximation is used to compute $2\theta_{hkl}$ values in the form:

$$2\theta_{hkl} = 180.0 - 114.5916\left(\sqrt{1 - \sin\theta_{hkl}}\right)\psi,$$

where:

$$\psi = 1.570795207 - 0.214512362\sin\theta_{hkl} + 0.087876311\sin^2\theta_{hkl} - 0.049958884\sin^3\theta_{hkl} + 0.019349939\sin^4\theta_{hkl} - 0.004337769\sin^5\theta_{hkl}.$$

Input Information

The input format required in the original program has been eliminated in favor of a free-field input to facilitate operation on a time-share system. The input must be placed in a data file named CRDATA in the following order:

Data 1. NJOB

Number of data sets to be processed. This information is needed only once.

Data 2. TITLE

Any Hollerith character (30 spaces allowed) for identification.

Data 3. A Cell parameter a in angstroms

B Cell parameter b in angstroms

C Cell parameter c in angstroms

ALF Cell parameter α in degrees

BET Cell parameter β in degrees

GAM Cell parameter γ in degrees

Data 4. TTMAX Maximum 2θ to be calculated in degrees

WAVE Wavelength of radiation used in angstroms

KSW1 External Program Control Indicator

KSW1=0, program generates four octants (hkl), (hk$\bar{l}$), (h$\bar{k}$l), and ($\bar{h}$kl), and outputs automatically

KSW1=1, program generates all positive (hkl) only, then looks for INDIC controls for further instructions

NOTE: With this option in effect, KSW1=1, the program will not list output unless it is instructed to do so with an INDIC = 4 control data.

KSW2-Output Control Character

KSW2=0, output routine lists only nonredundant 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.

Data 5. IXXX (14) or I1, I2, I3, . . . I14

SPACE GROUP EXTINCTION CODES

I1. Nonextinction indicator for lattice type as follows:

I1=1 A-centered (k+l = 2n)
I1=2 B-centered (h+l = 2n)
I1=3 C-centered (h+k = 2n)
I1=4 F-centered (h+k = 2n, h+l = 2n, k+l = 2n)
I1=5 I-centered (h+k+l = 2n)
I1=6 R-obverse (-h+k+l = 3n)
I1=7 R-reverse (h-k+l = 3n)
I1=8 Hexagonal (h-k = 3n)
I1=9 or 0 Primitive (no conditions).

I2. Nonextinction indicator for (hk0) zone as follows:

I2=0 no conditions
I2=1 a-glide (h=2n)
I2=2 b-glide (k=2n)
I2=3 n-glide (h+k=2n)
I2=4 d-glide (h+k=4n, h=2n, k=2n).

I3. Nonextinction indicator for (h0l) zone as follows:

I3=0 no conditions
I3=1 a-glide (h=2n)
I3=2 c-glide (l=2n)
I3=3 n-glide (h+l=2n)
I3=4 d-glide (h+l=4n, h=2n, l=2n).

I4. Nonextinction indicator for (0kl) zone as follows:

I4=0 no conditions
I4=1 b-glide (k=2n)
I4=2 c-glide (l=2n)
I4=3 n-glide (k+l=2n)
I4=4 d-glide (k+l=4n, k=2n, l=2n).

I5. Nonextinction indicator for (hhl) zone as follows:

I5=0 no conditions
I5=1 c(n)-glide (l=2n)
I5=2 d-glide (2h+l=4n)
I5=3 h+l=2n.

16. Nonextinction indicator for ($\bar{h}$hl) zone as follows:

16=0 no conditions
16=1 c(n)-glide (l=2n)
16=2 d-glide (2h+l=4n).

17. Nonextinction indicator for (hkh) zone as follows:

17=0 no conditions
17=1 b(n)-glide (k=2n)
17=2 c-glide (2h+k=4n).

18. Nonextinction indicator for (hk$\bar{h}$) zone as follows:

18=0 no conditions
18=1 b(n)-glide (k=2n)
18=2 d-glide (2h+k=4n).

19. Nonextinction indicator for (hkk) zone as follows:

19=0 no conditions
19=1 a(n)-glide (h=2n)
19=2 d-glide (2k+h=4n).

110. Nonextinction indicator for (hk$\bar{k}$) zone as follows:

110=0 no conditions
110=1 a(n)-glide (h=2n)
110=2 d-glide (2k+h=4n).

111. Nonextinction indicator for (h00) row as follows:

111=0 no conditions
111=1 2_1 or 4_2 screw (h=2n)
111=2 4_1 or 4_3 screw (h=4n).

112. Nonextinction indicator for (0k0) row as follows:

112=0 no conditions
112=1 2_1 or 4_2 screw (k=2n)
112=2 4_1 or 4_3 screw (k=4n).

I13. Nonextinction indicator for (00l) row as follows:

I13=0 no conditions
I13=1 2_1, 4_2, or 6_3 screw (l=2n)
I13=2 3_1, 3_2, 6_2, or 6_4 screw (l=3n)
I13=3 4_1 or 4_3 screw (l=4n)
I13=4 6_1 or 6_5 screw (l=6n).

I14. EXTRA Nonextinction indicators for (hkl) as follows:

I14=0 no conditions
I14=1 h=2n
I14=2 l=2n
I14=3 h+k+l=4n
I14=4 2h+l+4n
I14=5 If h-k=3n, then l=2n
I14=6 h=4n, k=4n, l=4n.

Data 6. 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 (hkl) all positive. The other three octants are redundant. In the monoclinic system, powder diffractograms may be indexed using (hkl) and $(\bar{h}kl)$. The other two octants are redundant.

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

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

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

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

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

The usual values of KSW1, KSW2, and INDIC are, respectively, 1, 0, and 4. For high-symmetry groups, where permutations of Miller indices are allowed, the conditions for each arrangement of indices must be defined separately if KSW2=1; however, for KSW2=0, the nonredundancy option will automatically eliminate permutable systems, such as 200, 020, or 002.

The lattice type for the material is chosen from the I1 list. Base-centered lattices will be given by I1=1, 2, or 3; face centered by I1=4; body centered by I1=5; rhombohedral or rhombohedral on hexagonal axes by I1=6 or 7, respectively; triply primative hexagonal by I1=8; and all simple or primative lattices by I1=9 or 0. Translational symmetry indicators I2 - I14, may also be input data if available. Typical code indicators are listed in Appendix B.

DISCUSSION

For general use, the object code (CF0B) offers the most efficient operation. However, to list or to modify the program, the source code (CRSFCN) must be used. Changes in the program are automatically placed in object code upon operation of the source program. Size requirements of the object code are about 85 percent of that of the source code, and the time required for the example job to run in object code is about 20 percent of that required by the source version.

The printout of the lattice type and parameters, the extinction codes, and other relevant data are a check for the operator on the input data. The agreement between the calculated lines and the experimentally determined values is quite good, as can be seen in a typical example output and the corresponding ASTM file card listed in Appendix C.

APPENDIX A

SOURCE PROGRAM LIST

```
01$SAV
02$NDM
10C  SAVED BY A.L.COFFEY,JR. 2/16/70   Y-12  3-5415
20C
3C THIS PROGRAM CALCULATES D-SPACINGS AND TWO THETA VALUES
40C  FOR CRYSTALLOGRAPHIC PLANES(HKL) AND UTILIZES SPACE GROUP
50C  AND TRANSLATIONAL SYMMETRY CONDITIONS FOR SYSTEMATIC ABSENCES.
60C
70C THIS PROGRAM IS SAVED IN OBJECT CODE AS "CFOB".
80C
90C THIS PROGRAM USES DATA FILE "CRDATA" FOR DATA INPUT.
100C
110C DATA INPUT IS IN FREE FIELD FORMAT:
120C
130C  1ST DATA---NUMBER OF JOBS
140C  2ND DATA---TITLE(30 SPACES AVAILABLE IN A3 FORMAT)
150C  3RD DATA---LATTICE PARAMETERS
160C  4TH DATA---MAX.TWO THETA,WAVELENGTH,KSW1,KSW2
170C  5TH DATA---EXTINCTION CODES
180C  6TH DATA---INDIC CONTROL
190C
200C  DETAILED DESCRIPTION OF PROGRAM AND INPUT DATA IS AVAILABLE
210C  FROM THE AUTHOR.
220C
230     COMMON LFLAG,IH,IK,IL,IXXX
240     DIMENSION DBL(200),TBL(200),SNBL(200),NH(200),NK(200),NL(200)
250 DIMENSION IXXX(14)
260      CALL OPENF(1,"CRDATA")
270  91  READ(1,)NJOB
280 7070 DO 222 JOB=1,NJOB
290 PRINT,"JOB NUMBER",JOB
300 PRINT,†
310 READ(1,5005)A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
320 5005 FORMAT(10A3)
330      READ(1,)A,B,C,ALF,BET,GAM
340 PRINT5006,A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
350 5006 FORMAT(20X,10A3)
360 PRINT,†
370 PRINT,"      A         B         C          ALF        BET        GAM"
380 PRINT145,A,B,C,ALF,BET,GAM
390 1045 FORMAT(3F10.5,3F10.3)
400      READ(1,)TTHMAX,WAVE,KSW1,KSW2
410 PRINT,†
420 READ(1,) (IXXX(N),N=1,14)
430 PRINT2009,WAVE,TTHMAX
440 2009 FORMAT(2X,"LAMBDA=",F10.5,10X,"TWO THETA MAX.=",F7.2)
450 PRINT,†
460 PRINT,"                    EXTINCTION CONDITIONS"
470 PRINT,"   I1  I2  I3  I4  I5  I6  I7  I8  I9  I10 I11 I12 I13 I14"
480 PRINT1009, (IXXX(N),N=1,14)
490 1009 FORMAT(14I4)
500 PRINT,††
510 CALL DETSYS
520   ALF=ALF*0.017453292
```

```
530    BET=BET*0.017453292
540    GAM=GAM*0.017453292
550    CSA=COS(ALF)
560    CSB=COS(BET)
570    CSG=COS(GAM)
580    SNA=(1.0-CSA*CSA)**0.5
590    SNB=(1.0-CSB*CSB)**0.5
600    SNG=(1.0-CSG*CSG)**0.5
610    WAVBY2=WAVE/2
620    THMAX=TTHMAX*0.008726646
630    DLIM=WAVBY2/SIN(THMAX)
60    ASQ=A*A
650    BSQ=B*B
660    CSQ=C*C
670    ANGFAC=1.0-CSA*CSA-CSB*CSB-CSG*CSG
680 ANGFAC=ANGFAC+2.0*CSA*CSB*CSG
690    VSQ=ASQ*BSQ*CSQ*ANGFAC
700    S11=BSQ*CSQ*SNA*SNA
710    S22=ASQ*CSQ*SNB*SNB
720    S33=ASQ*BSQ*SNG*SNG
730    S12=A*B*CSQ*((CSA*CSB)-CSG)
740    S23=ASQ*B*C*((CSB*CSG)-CSA)
750    S13=A*BSQ*C*((CSG*CSA)-CSB)
760    INDIC=1
770    INCRH=1
780    INCRK=1
790    INCRL=1
800    NC=0
810    M=1
820 144   IH=0
830    IK=0
840    IL=0
850 147   IH=IH+INCRH
860    MARKER=1
870 212   KLASS=0
880       CALL EXTN
890      IF(LFLAG.GT.0) GO TO 50
900 55    MARKER=2
910       GO TO 51
920 177   IF(IH)191,179,191
930 179   IFIK)193,180,193
940 180 IF(KSW1)222,181,101
950 101     READ(1,)INDIC
960 181 GO TO (111,112,121,211),INDIC
970 191 IK=IK+INCRK
980       IH=0
990       GO TO 212
1000 193   IL=IL+INCRL
1010       IK=0
1020       IH=0
1030       GO TO 212
1040 111   INCRH=1
1050       INCRK=1
1060       INCRL=-1
1070      GO TO 124
1080 112   INCRH=1
1090       INCRK=-1
1100       INCRL=1
1110      GO TO 124
1120 121   INCRH=-1
1130       INCRK=1
1140       INCRL=1
```

```
1150 124  INDIC=INDIC+1
1160      GO TO 144
1170 50   MARKER=1
1180 51   FH=IH
1190      FK=IK
1200      FL=IL
1210      DENOM=S11*FH*FH+S22*FK*FK
1220      DENOM=DENOM+S33*FL*FL+2.0*S12*FH*FK
1230      DENOM=DENOM+2.0*S23*FK*FL+2.0*S13*FH*FL
1240 7000   D=SQRT(VSQ/DENOM)
1250 7003   IF(D-DLIM)177,177,53
1260 53   GO TO (313,147),MARKER
1270 313   GO TO (56,314,315,316),INDIC
1280 314   IF(IL)56,147,56
1290 315   IF(IK)56,147,56
1300 316   IF(IH)56,147,56
1310 56   IF(KSW2)222,57,61
1320 57   KR=M-1
1330 58   IF(KR)61,61,59
1340 59  IF(DBL(KR)-D)60,147,60
1350 60   KR=KR-1
1360      GO TO 58
1370 61   STH=WAVBY2/D
1380      STH2=STH*STH
1390      STH4=STH2*STH2
1400      PSI=1.570795207-0.214512362*STH
1410      PSI=PSI+0.087876311*STH2
1420      PSI=PSI-0.044958884*STH2*STH
1430      PSI=PSI+0.01939939*STH4
1440      PSI=PSI-0.004337769*STH4*STH
1450 7001   TWOTH=180.0-PSI*114.5916*SQRT(1.0-STH)
1460 7002   MSW=1
1470      NH(M)=IH
1480      NK(M)=IK
1490      NL(M)=IL
1500      DBL(M)=D
1510      TBL(M)=TWOTH
1520      SNBL(M)=STH2
1530      M=M+1
1540     IF(M-201)147,800,800
1550 800   MD2=M-2
1560      DO 850 I=1,MD2,1
1570      MD1=M-1
1580      II1=I+1
1590      DO 849J=II1,MD1,1
160      IF(TBL(I)-TBL(J))849,849,803
1610 803   TEMT=TBL(I)
1620     TEMD=DBL(I)
1630      TEMS=SNBL(I)
1640      IHT=NH(I)
1650      IKT=NK(I)
1660      ILT=NL(I)
1670      TBL(I)=TBL(J)
1680      DBL(I)=DBL(J)
1690      SNBL(I)=SNBL(J)
1700      NH(I)=NH(J)
1710      NK(I)=NK(J)
1720      NL(I)=NL(J)
1730      TBL(J)=TEMT
1740      DBL(J)=TEMD
1750      SNBL(J)=TEMS
1760      NH(J)=IHT
```

```
1770      NK(J)=IKT
1780      NL(J)=ILT
1790  849  CONTINUE
1800  850  CONTINUE
1810      FLAM=2.0*WAVBY2
1820      PRINT,†
1830     PRINT,"     H    K    L         D        TWO THETA     SIN2 THETA"
1840      PRINT,"    ----------------------------------------------------"
1850      PRINT,†
1860      I=0
1870     LBOX=0
1880  860   I=I+1
1890      LBOX=LBOX+1
1900      PRINT2012,NH(I),NK(I),NL(I),DBL(I),TBL(I),SNBL(I)
1910  2012  FORMAT(1X,3I4,3F12.5)
1920      IF(I-MD1)862,872,222
1930  862 IF(LBOX-50)860,868,222
1940  868 PRINT,†
1950      LBOX=0
1960      GO TO 860
1970  872  NC=NC+MD1
1980      M=1
1990      GO TO (147,221),MSW
2000  211  MSW=2
2010      GO TO 800
2020  221 PRINT,††,"     THE NUMBER OF PLANES GENERATED IS",NC
2030      PRINT,†
2040  222 CONTINUE
2050    STOP
2060     END
2070 SUBROUTINE EXTN
2080 COMMON LFLAG,IH,IK,IL,I1,I2,I3,I4,I5,I6,I7,I8,I9,I10,I11,I12,I13,I4
2090 LFLAG=1
2100 AH=IH
2110 AK=IK
2120 AL=IL
2130 IF(I1.GT.9.OR.I1.LT.1) I1=9
2140 GO TO (1,2,3,4,5,6,7,8,9),I1
2150      1 XIX=(AK+AL)/2.0
2160 IXI=XIX
2170 XII=IXI
2180    990 IF (XIX-XII) 999,9,999
2190    999 LFLAG=-1
2200 RETURN
2210      2 XIX=(AH+AL)/2.0
2220 IXI=XIX
2230 XII=IXI
2240 GO TO 990
2250      3 XIX=(AH+AK)/2.0
2260 IXI=XIX
2270 XII=IXI
2280 GO TO 990
2290      4 XIX=(AH*AK*AL)/2.0
2300 IXI=XIX
2310 XII=IXI
2320 IF (XIX-XII) 9,400,9
2330    400 XIX=AH/2.0
2340 IXI=XIX
2350 XII=IXI
2360 IF (XIX-XII) 999,401,999
2370    401 XIX=AK/2.0
2380 IXI=XIX
```

```
2390 XII=IXI
2400 IF (XIX-XII) 999,402,999
2410   402 XIX=AL/2.0
2420 IXI=XIX
2430 XII=IXI
2440 GO TO 990
2450     5 XIX=(AH+AK+AL)/2.0
2460 IXI=XIX
2470 XII=IXI
2480 GO TO 990
2490     6 XIX=(-AH+AK+AL)/3.0
2500 IXI=XIX
2510 XII=IXI
2520 GO TO 990
2530     7 XIX=(AH-AK+AL)/3.0
2540 IXI=XIX
2550 XII=IXI
2560 GO TO 990
2570     8 XIX=(AH-AK)/3.0
2580 IXI=XIX
2590 XII=IXI
2600 GO TO 990
2610 9 IF(AL) 14,91,14
2620    91 IN=I2+1
2630 GO TO (14,10,11,12,13),IN
2640    10 XIX=AH/2.0
2650 GO TO 131
2660    11 XIX=AK/2.0
2670 GO TO 131
2680    12 XIX=(AH+AK)/2.0
2690 GO TO 131
2700    13 XIX=(AH+AK)/4.0
2710 IXI=XIX
2720 XII=IXI
2730 IF (XIX-XII) 999,11,999
2740   131 IXI=XIX
2750 XII=IXI
2760 IF (XIX-XII) 999,14,999
2770    14 IF (AK) 19,141,19
2780   141 IN=I3+1
2790 GO TO (19,15,16,17,18),IN
2800    15 XIX=AH/2.0
2810 GO TO 181
2820    16 XIX=AL/2.0
2830 GO TO 181
2840    17 XIX=(AH+AL)/2.0
2850 GO TO 181
2860    18 XIX=(AH+AL)/4.0
2870 IXI=XIX
2880 XII=IXI
2890 IF (XIX-XII) 999,16,999
2900   181 IXI=XIX
2910 XII=IXI
2920 IF (XIX-XII) 999,19,999
2930    19 IF (AH) 24,191,24
2940   191 IN=I4+1
2950 GO TO (24,20,21,22,23),IN
2960    20 XIX=AK/2.0
2970 GO TO 231
2980    21 XIX=AL/2.0
2990 GO TO 231
3000    22 XIX=(AK+AL)/2.0
```

```
3010 GO TO 231
3020    23 XIX=(AK+AL)/4.0
3030 IXI=XIX
3040 XII=IXI
3050 IF (XIX-XII) 999,21,999
3060   231 IXI=XIX
3070 XII=IXI
3080 IF (XIX-XII) 999,24,999
3090    24 IF (AH-AK) 124,25,124
3100    25 IN=I5+1
3110    GO TO(124,26,27,2711),IN
3120    26 XIX=AL/2.0
3130GO TO 271
3140    27 XIX=(2.0*AH+AL)/4.0
3150     GO TO 271
3160 2711  XIX=(AH+AL)/2.0
3170   271 IXI=XIX
3180 XII=IXI
3190 IF (XIX-XII) 999,124,999
3200   124 IF (AK-AL) 224,125,224
3210   125 IN=I9+1
3220 GO TO (224,126,127),IN
3230   126 XIX=AH/2.0
3240 GO TO 1271
3250   127 XIX=(AH+2.0*AL)/4.0
3260  1271 IXI=XIX
3270 XII=IXI
3280 IF (XIX-XII) 999,224,999
3290   224 IF (AH-AL) 28,225,28
3300   225 IN=I7+1
3310 GO TO (28,226,227),IN
3320   226 XIX=AK/2.0
3330 GO TO 2271
3340   227 XIX=(2.0*AH+AK)/4.0
3350  2271 IXI=XIX
3360 XII=IXI
3370 IF (XIX-XII) 999,28,999
3380    28 IF (AH+AK) 128,29,128
3390    29 IN=I6+1
3400 GO TO (31,30,301),IN
3410    30 XIX=AL/2.0
3420 GO TO 302
3430   301 XIX=(2.0*AH+AL)/4.0
3440   302 IXI=XIX
3450 XII=IXI
3460 IF (XIX-XII) 999,128,999
3470   128 IF(AK+AL) 228,129,228
3480   129 IN=I10+1
3490 GO TO (228,130,132),IN
3500   130 XIX=AH/2.0
3510 GO TO 1311
3520   132 XIX=(AH+2.0*AK)/4.0
3530  1311 IXI=XIX
3540 XII=IXI
3550 IF (XIX-XII) 999,228,999
3560   228 IF (AH+AL) 31,229,31
3570   229 IN=I8+1
3580 GO TO (31,230,232),IN
3590   230 XIX=AK/2.0
3600 GO TO 2311
3610   232 XIX=(2.0*AH+AK)/4.
3620  2311 IXI=XIX
```

```
3630 XII=IXI
3640 IF (XIX-XII) 999,31,999
3650    31 IF (AK) 34,311,34
3660   311 IF (AL) 34,312,34
3670   312 IN=I11+1
3680 GO TO (34,32,33),IN
3690    32 XIX=AH/2.0
3700   331 IXI=XIX
3710 XII=IXI
3720 IF (XIX-XII) 999,34,999
3730    33 XIX=AH/4.0
3740 GO TO 331
3750    34 IF (AH) 37,341,37
3760   341 IF (AL) 37,342,37
3770   342 IN=I12+1
3780 GO TO (37,35,36),IN
3790    35 XIX=AK/2.0
380 GO TO 361
3810    36 XIX=AK/4.0
3820 361 IXI=XIX
3830 XII=IXI
3840 F (XIX-XII) 999,37,999
3850    37 IF (AH) 42,371,42
3860   371 IF AK) 42,372,42
3870   372 IN=I13+1
3880 GO TO (42,38,39,40,41),IN
3890    38 XIX=AL/2.0
3900 GO TO 411
3910    39 XIX=AL/3.0
3920 GO TO 411
3930    40 XIX=AL/4.0
3940 GO TO 411
390    41 XIX=AL/6.0
3960   411 IXI=XIX
3970 XII=IXI
3980 IF (XIX-XII) 999,42,999
3990 42 IN=I14+1
4000 GO TO(6153,6001,6002,6003,6004,6005,6006),IN
4010 6001 XIX=AH/2.0
4020 GO TO 6152
4030 6002  XIX=AL/2.0
4040  GO TO 6152
4050 6003  XIX=(AH+AK+AL)/4.0
4060  GO TO 6152
470 6004 XIX=(2*AH+AL)/4.0
4080  GO TO 6152
4090 6005 XIX=(AH-AK)/3.0
4100  IXI=XIX
4110  XII=IXI
4120 IF(XIX-XII)999,6012,6153
4130 6012 XIX=AL/2.0
4140  GO TO 6152
4150 6006  XIX=AH/4.0
4160 IXI=XIX
4170 XII=IXI
4180  IF(XIX-XII)999,6013,999
4190 6013 XIX=AK/4.0
4200  IXI=XIX
4210 XII=IXI
4220 IF(XIX-XII)999,6014,999
4230 6014 XIX=AL/4.0
4240 6152 IXI=XIX
```

```
4250 XII=IXI
4260  IF(XIX-XII)999,6153,999
4270 6153  RETURN
4280 END
4290 SUBROUTINE DETSYS
4300 COMMON LFLAG,IH,IK,IL,I1
4310 GO TO(1,2,3,4,5,6,7,8,9),I1
4320 1 PRINT,"                    A-CENTERED LATTICE"
4330 RETURN
4340 2 PRINT,"                    B-CENTERED LATTICE"
4350 RETURN
4360 3 PRINT,"                    C-CENTEREDLATTICE"
4370 RETURN
4380 4 PRINT,"                    F-CENTERED LATTICE"
4390 RETURN
4400 5 PRINT,"               BODY-CENTERED LATTICE"
4410 RETURN
4420 6 PRINT,"                     R-OBVERSE LATTICE"
4430 RETURN
4440 7 PRINT,"                     R-REVERSE LATTICE"
4450 RETURN
4460 8 PRINT,"                      HEXAGONAL LATTICE"
4470 RETURN
4480 9 PRINT,"                       PRIMATIVE LATTICE"
4490 RETURN
4500 END
```

APPENDIX B

EXTINCTION CODE TABULATION

The appropriate extinction codes for a crystal structure can be obtained from the International Tables for X-ray Crystallography[7] by knowing the space group, the number of equivalent positions, and the Wyckoff notation for the set of equivalent positions. Pearson[6] lists the necessary data for each structure according to Strukturbericht type. The extinction codes for some of the more common Strukturbericht types are as follows:

STRUKTURBERICHT TYPE	SPACE GROUP NUMBER	EXTINCTION CODES													
		I1	I2	I3	I4	I5	I6	I7	I8	I9	I10	I11	I12	I13	I14
A1	225	4	0	0	4	3	0	0	0	0	0	0	0	0	0
A2	229	5	0	0	3	1	0	0	0	0	0	0	0	0	0
A3	194	9	0	0	0	1	0	0	0	0	0	0	0	0	5
A12	217	5	*												
A15	223	5				1									
A20	63	3		2											
B1	225	4			4	3									
B2	221	9													
B3	216	4				3									
B4	184	9				1									5
$B8_1$	194	9				1									2
$B8_2$	194	9				1									5
B20	198	9										1			
B27	62	9	1		3										
B31	62	9	1		3										
B32	227	4			3										
C1	225	4			4	3									1
$C1_b$	216	4				0									
C2	205	4	1	2	1										
C4	136	5			3										
C6	164	9													
$C11_a$	139	5	3		3	1									
C14	194	9				1									2
C15	227	4			4	3									6
C16	140	5	3		2	1									2
C18	58	5		3	3										
C32	191	9													
C36	194	9				1									2
C38	129	3	3												
C_c	141	5	1			2									3
$D0_3$	225	4			4	3									1
$D0_{18}$	194	9				1									2
$D0_{19}$	194	9				1									5
$D2_1$	221	9													2
$D2_3$	226	4			1	1									1
$D2_d$	191	9													
$D5_1$	167	5				1									
$D5_2$	164	9													
$D5_3$	206	5			1										1
$D5_8$	62	9	1		3										
$D5_{13}$	164	9													
$D7_3$	220	5				2									6
$D7_b$	71	5													
$D8_{1-3}$	229	5			3	1									
$D8_8$	193	9					1								2
$D8_b$	136	5			3										
$D8_m$	140	5	3		2	1									2
$E1_1$	122	5				2									
E3	82	5													
$L1_0$	123	3													
$L1_2$	221	9													
$L2_1$	225	4													1
L_3'	194	9				1									2

*Note: All blanks should be zeros but are omitted for ease of reading.

APPENDIX C

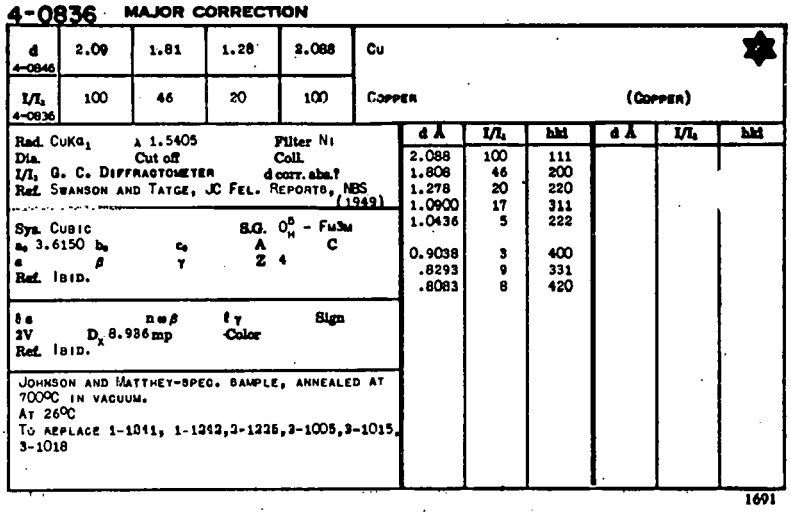
INPUT AND OUTPUT EXAMPLES

An example of the data in CRDATA is:

```
10  1
20          COPPER
30  3.615,3.615,3.615,90,90,90
40  165,1.54178,1,0
50  4
60  4
```

NOTE: If the data are for a run of the source code (CRSFCN), all zeros must be included in the extinction code data.

The ASTM powder diffraction card for copper is:



4-0836 MAJOR CORRECTION

d 4-0846	2.09	1.81	1.28	0.088	Cu
I/I$_1$ 4-0836	100	46	20	100	COPPER (COPPER)

Rad. CuKα$_1$ λ 1.5405 Filter Ni
Dia. Cut off Coll.
I/I$_1$ G. C. DIFFRACTOMETER d corr. abs.?
Ref. SWANSON AND TATGE, JC FEL. REPORTS, NBS (1949)

Sys. CUBIC S.G. O_h^5 - Fm3m
a_o 3.6150 b_o c_o A C
α β γ Z 4
Ref. IBID.

εα nωβ εγ Sign
2V D_x 8.936mp Color
Ref. IBID.

JOHNSON AND MATTHEY-SPEC. SAMPLE, ANNEALED AT 700°C IN VACUUM.
AT 26°C
TO REPLACE 1-1011, 1-1242, 3-1225, 3-1005, 3-1015, 3-1018

d Å	I/I$_1$	hkl	d Å	I/I$_1$	hkl
2.088	100	111			
1.808	46	200			
1.278	20	220			
1.0900	17	311			
1.0436	5	222			
0.9038	3	400			
.8293	9	331			
.8083	8	420			

1691

The output from CF0B for the data just given is:

JOB NUMBER 1

COPPER

A	B	C	ALF	BET	GAM
3.61500	3.61500	3.61500	90.000	90.000	90.000

LAMBDA= 1.54178 TWO THETA MAX.= 165.00

EXTINCTION CONDITIONS

I1	I2	I3	I4	I5	I6	I7	I8	I9	I10	I11	I12	I13	I14
4	0	0	0	0	0	0	0	0	0	0	0	0	0

F-CENTERED LATTICE

H	K	L	D	TWO THETA	SIN2 THETA
1	1	1	2.08712	43.35161	0.13642
2	0	0	1.80750	50.49041	0.18190
2	2	0	1.27810	74.19190	0.36380
3	1	1	1.08996	90.02445	0.50022
2	2	2	1.04356	95.24267	0.54569
4	0	0	0.90375	117.07566	0.72759
3	3	1	0.82934	136.72049	0.86402
4	2	0	0.80834	144.98189	0.90949

THE NUMBER OF PLANES GENERATED IS 8

REFERENCES

(1) Werkema, G. J.; A Revised FORTRAN IV Program to Calculate Crystallographic Functions, RFP-1329; The Dow Chemical Company, Rocky Flats Division, Golden, Colorado; May 14, 1969.

(2) Budelov, P. R. and Cullipher, J. R.; A Basic Language Computer Program for Calculating Interplanar Spacings, Y-1603; Union Carbide Corporation-Nuclear Division, Oak Ridge Y-12 Plant, Oak Ridge, Tennessee, February 15, 1968.

(3) Bartram, S. F., Rau, R. C., and Sjodahl, L. J.; DSPACE, A Program to Calculate Interplanar Spacings from Lattice Parameters, GEMP-680; General Electric, Missile and Space Division, Nuclear Systems Programs, Cincinnati, Ohio; March 11, 1969.

(4) Smith, D. K.; A Revised Program for Calculating X-Ray Powder Diffraction Patterns, UCRL-50264; Lawrence Radiation Laboratory, University of California, Livermore, California; June 12, 1967.

(5) Hermann, O. W.; MILIN - A FORTRAN Computer Program for Generating Interplanar Spacings, Unpublished; Union Carbide Corporation-Nuclear Division, Oak Ridge Gaseous Diffusion Plant, Oak Ridge, Tennessee.

(6) Pearson, W. B.; Handbook of Lattice Spacings and Structures of Metals, 1 (1958); 2 (1967); Pergamon Press, London, England.

(7) The International Union of Crystallography; International Tables for X-Ray Crystallography, 1, N. F. M. Henry and K. Lunsdale, Editors; the Kynoch Press, Birmingham, England (1965).