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CRYSTAL GEOMETRY COMPUTER PROGRAM

by

Lawrence P. Bush and Lowell T. Lloyd

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ARGONNE NATIONAL LABORATORY
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Lawrence P. Bush* and Lowell T. Lloyd**

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**Metallurgy Division

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ABSTRACT

A program which calculates various relationships of crystal geometry has been prepared in FORTRAN notation for use with the IBM-704 computer. The primary outputs are the angles between planes, and the angles between directions, that are required to construct standard stereographic projections for any of the seven crystal systems. Also, values are tabulated for interplanar spacing, area of the unit parallelogram on a lattice plane, and the distance between identical points along a lattice direction. The relations can be evaluated for permutations of Miller indices whose absolute values are less than, or equal to, 22. Redundant indices are omitted from the output. The program has been made available for listing by the computer committee of the American Crystallographic Association.

I. INTRODUCTION

When using single crystals in experimental studies, it is necessary to know their spatial orientation. One of the most convenient and moderately accurate methods of determining the orientation of a single crystal, or of an individual grain in an aggregate, is the back-reflection Laue X-ray diffraction technique.[1,2] Laue photograms can be readily solved by using a Greninger chart[3,4] together with a stereographic net and a standard projection for the crystal structure of the material. The latter graphically represents the angles between the crystallographic planes. Standard projections for cubic structures, regardless of the material, are identical. But standard projections for crystal systems of lower symmetry must be prepared for each material because the angles between planes involve the values of the lattice dimensions as well as the angles between the principal crystallographic directions. As the crystal system becomes less symmetrical, the equation for calculating the angle between planes becomes more complex, and the number of computations required to construct the complete standard projection increases. These calculations for the crystal systems with low symmetry are quite laborious and time consuming.

This report describes a computer program which can be used to calculate various relations of crystal geometry for all of the seven possible crystal systems. In addition to calculating the angles between crystallographic planes, the program also computes the angles between directions. Other geometrical relations, which are developed during the calculation of the angles, and an additional relation, which is occasionally of interest, are tabulated in the output.

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ABSTRACT

A program which calculates various relationships of crystal geometry has been prepared for FORTRAN solution for use with the IBM-704 computer. The primary outputs are the angles between planes, and the angles between directions that are required to construct standard stereographic projections for any of the seven crystal systems. Also, values are tabulated for interplanar spacing, area of the unit parallelogram on a lattice plane, and the distance between identical points along a lattice direction. The relations can be evaluated for permutations of Miller indices whose absolute values are less than, or equal to, 25. Reciprocal indices are accepted from the output. The programs have been made available for distribution by the crystal committee of the American Crystallographic Association.

I. INTRODUCTION

When using single crystals in experimental studies, it is necessary to know their spatial orientation. One of the most convenient and moderately accurate methods of determining the orientation of a single crystal, or of an individual grain in an aggregate, is the back-reflection Laue X-ray diffraction technique.[1,2] Laue photograms can be readily solved by using a Greninger chart[3,4] together with a stereographic net and a standard projection for the crystal structure of the material. The latter graphically represents the angles between the crystallographic planes, standard projections, for cubic structures, regardless of the material are identical. But standard projections for crystal systems of lower symmetry must be prepared for each material because the angles between planes involve the values of the lattice dimensions as well as the angles between the principal crystallographic directions. As the crystal system becomes less symmetrical, the equation for calculating the angle between planes becomes more complex, and the number of computations required to construct the complete standard projection increases. These calculations for the crystal systems with low symmetry are quite laborious and time consuming.

This report describes a computer program which can be used to calculate various relations of crystal geometry for all of the seven possible crystal systems. In addition to calculating the angles between crystallographic planes, the program also computes the angles between directions. Other geometrical relations, which are developed during the calculation of the angles, and an additional relation, which is occasionally of interest, are tabulated in the output.

II. MATHEMATICAL RELATIONS

The formulas for computing the more important relations of crystal geometry have been compiled by Barrett.[5] These equations for the most complex crystal system, the triclinic system, are given below. The equations for the other crystal systems are simplifications of these.

The volume of the unit cell, V, is given by the equation

$$V = abc\,[1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma]^{1/2} \quad , \quad (1)$$

where a, b, c, α, β, and γ have the usual meanings of the lattice constants. The equation for the distance d_i between adjacent lattice planes is

$$d_i = V[S_{11}h_i^2 + S_{22}k_i^2 + S_{33}\ell_i^2 + 2\,S_{12}h_ik_i + 2\,S_{23}k_i\ell_i + 2\,S_{13}h_i\ell_i]^{-1/2} \quad , (2)$$

where h_i, k_i, and ℓ_i are the Miller indices of a plane and

$$S_{11} = b^2c^2\sin^2\alpha \quad ; \qquad S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma) \quad ;$$

$$S_{22} = a^2c^2\sin^2\beta \quad ; \qquad S_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha) \quad ;$$

$$S_{33} = a^2b^2\sin^2\gamma \quad ; \qquad S_{13} = ab^2c(\cos\gamma\cos\alpha - \cos\beta) \quad ;$$

The angle ϕ between two crystal planes with indices $(h_1k_1\ell_1)$ and $(h_2k_2\ell_2)$ is given by the relation

$$\cos\phi = d_1d_2V^{-2}[S_{11}h_1h_2 + S_{22}k_1k_2 + S_{33}\ell_1\ell_2 + S_{12}(h_1k_2 + h_2k_1)$$
$$+ S_{23}(k_1\ell_2 + k_2\ell_2) + S_{13}(\ell_1h_2 + \ell_2h_1)] \quad . \quad (3)$$

The shortest distance I_i between identical points in a crystal lattice along a direction with indices $[u_iv_iw_i]$ is given by the equation

$$I = [a^2u_i^2 + b^2v_i^2 + c^2w_i^2 + 2\,bcv_iw_i\cos\alpha + 2\,caw_iu_i\cos\beta$$
$$+ 2\,abu_iv_i\cos\gamma]^{1/2} \quad . \quad (4)$$

The angle ρ between the lattice directions $[u_1v_1w_1]$ and $[u_2v_2w_2]$ is given by the relation

$$\cos\rho = [I_1I_2]^{-1}[a^2u_1u_2 + b^2v_1v_2 + c^2w_1w_2 + bc(v_1w_2 + v_2w_1)\cos\alpha$$
$$+ ac(w_1u_2 + w_2u_1)\cos\beta + ab(u_1v_2 + u_2v_1)\cos\gamma] \quad . \quad (5)$$

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$$d_i = V[S_{11}h_i^2 + S_{22}k_i^2 + S_{33}l_i^2 + 2\,S_{12}h_ik_i + 2\,S_{23}k_il_i + 2\,S_{13}h_il_i]^{-1/2} \quad . \tag{2}$$

where h_i, k_i, and l_i are the Miller indices of a plane and

$$S_{11} = b^2c^2\sin^2\alpha \quad ; \qquad S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma) \quad ;$$

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The angle φ between two crystal planes with indices $(h_1k_1l_1)$ and $(h_2k_2l_2)$ is given by the relation

$$\cos\phi = d_1d_2V^{-2}\,[S_{11}h_1h_2 + S_{22}k_1k_2 + S_{33}l_1l_2 + S_{12}(h_1k_2 + h_2k_1)$$

$$+ S_{23}(k_1l_2 + k_2l_1) + S_{13}(l_1h_2 + l_2h_1)] \quad . \tag{3}$$

The shortest distance l_i between identical points in a crystal lattice along a direction with indices $[u_iv_iw_i]$ is given by the equation

$$l_i = [a^2u_i^2 + b^2v_i^2 + c^2w_i^2 + 2\,bcv_iw_i\cos\alpha + 2\,cauw_i\cos\beta$$

$$+ 2\,abu_iv_i\cos\gamma]^{1/2} \quad . \tag{4}$$

The angle ρ between the lattice directions $[u_1v_1w_1]$ and $[u_2v_2w_2]$ is given by the relation

$$\cos\rho = [l_1l_2]^{-1}\,[a^2u_1u_2 + b^2v_1v_2 + c^2w_1w_2 + bc(v_1w_2 + v_2w_1)\cos\alpha$$

$$+ ac(w_1u_2 + w_2u_1)\cos\beta + ab(u_1v_2 + u_2v_1)\cos\gamma] \quad . \tag{5}$$

The area A_i of the smallest unit parallelogram on the lattice plane $(h_i k_i \ell_i)$ is given by

$$A_i = [S_{11}h_i^2 + S_{22}k_i^2 + S_{33}\ell_i^2 + 2\,S_{12}h_ik_i + 2\,S_{23}k_i\ell_i + 2\,S_{13}h_i\ell_i]^{1/2} \quad .(6)$$

Finally, the angle δ between the direction $[u_iv_iw_i]$ and the plane $(h_ik_i\ell_i)$ is given by the relation

$$\sin\delta = V^2[A_iI_i]^{-1}[u_ih_i + v_ik_i + w_i\ell_i] \quad . \qquad (7)$$

III. COMPUTER PROGRAM

A. Discussion:

The computer program is written in FORTRAN notation. Input data consist of the unit cell constants for the crystal structure, and some choice of output can be exercised by control parameters. Values are tabulated for the relations given by equations 1 through 6. Although A_i is not required to calculate ϕ or ρ, it is convenient to have these values for further considerations of the crystal structure. The angles δ (see Eq. 7) are not calculated by the program because the possible permutations are extremely large, and normally only a few values of δ are of interest. Since values of A_i, I_i, and V are available from the computer output, it is simple to calculate manually those values of δ which are required.

The angles ϕ and ρ are calculated between the principal crystallographic planes or directions, respectively, and the plane or direction of interest. Since only two angles are required to locate the plane pole, or direction, with respect to the principal crystallographic elements on a standard stereographic projection, the two principal elements which are used can be selected with a control parameter M as follows:

M	Principal Crystallographic Elements $(h_1k_1\ell_1)$ or $[u_1v_1w_1]$
1	1 0 0 and 0 1 0
2	1 0 0 and 0 0 1
3	0 1 0 and 0 0 1

Miller indices h, k, and ℓ are varied in the order ℓ, then k, then h.* The maximum values which are considered by the program for each one of the indices are selected as additional control parameters. As the

*For the purposes of calculation by the program, the indices for directions, $[u_iv_iw_i]$, are replaced by the respective indices for planes, $(h_ik_i\ell_i)$.

The area A_i of the smallest unit parallelogram on the lattice plane $(h_i k_i \ell_i)$ is given by

$$A_i = [S_{11} h_i^2 + S_{22} k_i^2 + S_{33} \ell_i^2 + 2\, S_{12} h_i k_i + 2\, S_{23} k_i \ell_i + 2\, S_{13} h_i \ell_i]^{1/2} \quad . \tag{6}$$

Finally, the angle δ between the direction $[u_i v_i w_i]$ and the plane $(h_i k_i \ell_i)$ is given by the relation

$$\sin \delta = V^2 [A_i \ell_i]^{-1} [u_i h_i + v_i k_i + w_i \ell_i] \quad . \tag{7}$$

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The angles δ and σ are calculated between the principal crystallographic planes or directions, respectively, and the plane or direction of interest. Since only two angles are required to locate the plane pole, or direction, with respect to the principal crystallographic elements on a standard stereographic projection, the two principal elements which are used can be selected with a control parameter M as follows:

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1	1 0 0 and 0 1 0
2	1 0 0 and 0 0 1
3	0 1 0 and 0 0 1

Miller indices h, k, and ℓ are varied in the order ℓ, then k, then h.* The maximum values which are considered by the program for each one of the indices are selected as additional control parameters. As the

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*For the purposes of calculation by the program, the indices for directions, $[u_i v_i w_i]$ are replaced by the respective indices for planes, $(h_i k_i \ell_i)$.

program is currently written, the maximum permissible value for the indices is 22; however, it could be changed easily to extend the maximum value to any integer which is desired. For the triclinic and rhombohedral crystal systems the program generates all possible combinations of positive and negative indices. Positive and negative values are generated for only one of the indices which pertain to the axes bounding the non-ninety degree angle in the case of the monoclinic crystal system. Only positive indices are generated for the other crystal systems.

Redundant indices are omitted by the program: i.e., (111) is calculated, but (222), (333), etc., are eliminated; also, (321) is calculated, but (642), (963), etc., are eliminated; etc. Further elimination of redundant indices can be accomplished with the control parameters h, k, and ℓ. For the hexagonal and tetragonal crystal systems, the maximum value of one of the two indices which refer to the axes with equal length is set equal to 1, and the other is set equal to the maximum index which is desired. The maximum value of two of the indices are set equal to 1 for the cubic system, and the third is set equal to the maximum index which is of interest.

The angles that are computed by the program for the cubic, hexagonal, tetragonal, and orthorhombic crystal systems are used directly to construct the unit portions of the standard stereographic projections. But this is not always true in the cases of the other crystal systems, for which permutations are made of negative as well as positive indices. Since the cosine is an even function, it goes through its range of values between 0° and 180°, and all computed angles are in this range. The permutation of negative Miller indices results in some angles which are greater than 180° in the true crystal structure. For those angles, the computer tabulates values which are equal to 360° minus the true angle. The angles that are greater than 180° become obvious in the process of plotting the standard stereographic projection, and, in reality, they can be plotted as the tabulated value but in the opposite sense to that which is used for plotting the angles less than 180°.

B. FORTRAN Notation:

The following FORTRAN notations are used for the various input data and computed functions:

Input	FORTRAN Symbol	Functions	FORTRAN Symbol(s)
a	A	V	V
b	B	d_i	DP, DQ, WD
c	C	I_i	SIP, SIQ, WI
α	GA	A_i	AP, AQ, WA
β	GB	ϕ	UU11, UU12
γ	GG	ρ	VV11, VV12
M	M		
h, u	JH		
k, v	JK		
ℓ, w	JL		

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B. FORTRAN Notation:

The following FORTRAN notations are used for the various input data and computed functions:

C. Source Deck:

A listing of the source deck for the crystal geometry computer program is given below. The program makes use of the following subroutines from the computer library: square root, cosine, sine, arc sine, absolute value, minimum value, and maximum value.

```
C      1482/MET143   LARRY BUSH   X3658
     1 FORMAT(6E12.5/4I6)
     2 FORMAT(//69H      A            B            C          ALPHA      BETA
      1  GAMMA        V)
     3 FORMAT(1P3E12.5,0P3F9.4,1PE12.5)
     4 FORMAT(/43H  H1  K1  L1      D1           I1           A1)
     5 FORMAT(3I4,1P3E12.5)
     6 FORMAT(/81H  H2  K2  L2      D2           I2           A2          PHI
      1      RHO       PHI       RHO)
     7 FORMAT(3I4,1P3E12.5,0P4F9.4)
     9 FORMAT(72H
      1                    )
       DIMENSION P(8)
       D11F(TH,TK,TL)=SQRTF(S11*TH*TH+S22*TK*TK+S33*TL*TL
      1+2.*S12*TH*TK+2.*S23*TK*TL+2.*S13*TH*TL)
       W122F(TH,TK,TL)=SQRTF((A*TH)**2+(B*TK)**2+(C*TL)**2
      1+2.*B*C*TK*TL*A123+2.*C*A*TL*TH*B123
      2+2.*A*B*TH*TK*G123)
       A33F(TH,TK,TL)=SQRTF(S11*TH*TH+S22*TK*TK+S33*TL*TL
      1+2.*S12*TH*TK+2.*S13*TH*TL+2.*S23*TK*TL)
       P(1)=2.
       P(2)=3.
       P(3)=5.
       P(4)=7.
       P(5)=11.
       P(6)=13.
       P(7)=17.
       P(8)=19.
     8 READ 9
       READ 1, (A,B,C,GA,GB,GG,M,JH,JK,JL)
       RGA=.0174532925*GA
       RGB=.0174532925*GB
       RGG=.0174532925*GG
       A123=COSF(RGA)
       B123=COSF(RGB)
       G123=COSF(RGG)
       BCSINA=B*C*SINF(RGA)
       ACSINB=A*C*SINF(RGB)
       ABSING=A*B*SINF(RGG)
       S11=BCSINA**2
       S22=ACSINB**2
       S33=ABSING**2
       S12=A*B*(C**2)*(A123*B123-G123)
       S23=(A**2)*B*C*(B123*G123-A123)
       S13=A*(B**2)*C*(G123*A123-B123)
       V=A*B*C*SQRTF(1.-A123**2-B123**2
      1-G123**2+2.*A123*B123*G123)
       AA=A*A
       BB=B*B
       CC=C*C
       ABCOSG=A*B*COSF(RGG)
       ACCOSB=A*C*COSF(RGB)
       BCCOSA=B*C*COSF(RGA)
       WRITE OUTPUT TAPE 6,9
       WRITE OUTPUT TAPE 6,2
       WRITE OUTPUT TAPE 6,3,(A,B,C,GA,GB,GG,V)
       IF(M-2)50,60,70
    50 DP=V/BCSINA
       DQ=V/ACSINB
       SIP=A
       SIQ=B
```

C. Source Deck:

A listing of the source deck for the crystal geometry computer program is given below. The program makes use of the following subroutines from the computer library: square root, cosine, sine, arc sine, absolute value, minimum value, and maximum value.

```
      AP=BCSINA
      AQ=ACSINB
      IPH=1
      IPK=0
      IPL=0
      IPHH=0
      IPKK=1
      IPLL=0
      GOTO80
   60 DP=V/BCSINA
      DQ=V/ABSING
      SIP=A
      SIQ=C
      AP=BCSINA
      AQ=ABSING
      IPH=1
      IPK=0
      IPL=0
      IPHH=0
      IPKK=0
      IPLL=1
      GOTO80
   70 DP=V/ACSINB
      DQ=V/ABSING
      SIP=B
      SIQ=C
      AP=ACSINB
      AQ=ABSING
      IPH=0
      IPK=1
      IPL=0
      IPHH=0
      IPKK=0
      IPLL=1
   80 WRITE OUTPUT TAPE 6,4
      WRITE OUTPUT TAPE 6,5,(IPH,IPK,IPL,DP,SIP,AP)
      WRITE OUTPUT TAPE 6,5,(IPHH,IPKK,IPLL,DQ,SIQ,AQ)
      WRITE OUTPUT TAPE 6,6
      IF (ABSF(GA-90.)+ABSF(GB-90.)+ABSF(GG-90.)) 100,90,100
   90 IHH=JH+1
      JH=0
      IKK=JK+1
      JK=0
      ILL=JL+1
      JL=0
      GOTO110
  100 IF (ABSF(GA-90.)+ABSF(GB-90.)) 101,91,101
   91 IF (GG-120.) 191,90,191
  191 IHH=JH+1
      JH=0
      IKK=JK*2+1
      ILL=JL+1
      JL=0
      GO TO 110
  101 IF (ABSF(GA-90.)+ABSF(GG-90.)) 102,92,102
   92 IF (GB-120.) 192,90,192
  192 IHH=JH+1
      JH=0
      IKK=JK+1
      JK=0
      ILL=JL*2+1
      GO TO 110
  102 IF(ABSF(GB-90.)+ABSF(GG-90.)) 66,93,66
   93 IF (GA-120.) 193,90,193
  193 IHH=JH+1
      JH=0
      IKK=JK+1
      JK=0
      ILL=JL*2+1
      GO TO 110
   66 IHH=JH*2+1
      IKK=JK*2+1
      ILL=JL*2+1
```

```
  110 DO150IH=1,IHH
      TH=IH-JH-1
      DO150IK=1,IKK
      TK=IK-JK-1
      DO150IL=1,ILL
      TL=IL-JL-1
      ATH=ABSF(TH)
      ATK=ABSF(TK)
      ATL=ABSF(TL)
      IF (ATH-1.) 21,1022,21
   21 IF (ATK-1.) 22,1022,22
   22 IF (ATL-1.) 23,1022,23
   23 ABC=MIN1F(ATH,ATK,ATL)
      DO 55 I=1,8
      IF (ABC) 31,32,31
   31 IF (ABC-P(I)) 1022,51,51
   32 IF (MAX1F(ATH,ATK,ATL)-P(I)) 1022,51,51
   51 IATH=ATH/P(I)
      IATK=ATK/P(I)
      IATL=ATL/P(I)
      AIH=IATH
      AIK=IATK
      AIL=IATL
      IF ((ATH+ATK+ATL)-P(I)*(AIH+AIK+AIL)) 55,150,55
   55 CONTINUE
 1022 WAIT=D11F(TH,TK,TL)
      WD=V/WAIT
      WI=WI22F(TH,TK,TL)
      WA=A33F(TH,TK,TL)
      IF(M-2)71,72,73
   71 U11=(S11*TH+S13*TL+S12*TK)/(WAIT*AP)
      U12=(S22*TK+S23*TL+S12*TH)/(WAIT*AQ)
      V11=(AA*TH+TL*ACCOSB+TK*ABCOSG)/(SIP*WI)
      V12=(BB*TK+TL*BCCOSA+TH*ABCOSG)/(SIQ*WI)
      GO TO 79
   72 U11=(S11*TH+S13*TL+S12*TK)/(WAIT*AP)
      U12=(S33*TL+S23*TK+S13*TH)/(WAIT*AQ)
      V11=(AA*TH+TL*ACCOSB+TK*ABCOSG)/(SIP*WI)
      V12=(CC*TL+TK*BCCOSA+TH*ACCOSB)/(SIQ*WI)
      GO TO 79
   73 U11=(S22*TK+S23*TL+S12*TH)/(WAIT*AP)
      U12=(S33*TL+S23*TK+S13*TH)/(WAIT*AQ)
      V11=(BB*TK+TL*BCCOSA+TH*ABCOSG)/(SIP*WI)
      V12=(CC*TL+TK*BCCOSA+TH*ACCOSB)/(SIQ*WI)
   79 UU11=90.-57.2957795*ASINF(U11)
      UU12=90.-57.2957795*ASINF(U12)
      VV11=90.-57.2957795*ASINF(V11)
      VV12=90.-57.2957795*ASINF(V12)
      ITH=TH
      ITK=TK
      ITL=TL
      WRITEOUTPUTTAPE6,7,(ITH,ITK,ITL,WD,WI,WA,UU11,VV11,UU12,VV12)
  150 CONTINUE
      GOTO 8
      END(0,1,0,0,0)
```

```
118 DO150IH=1,IHM
    IH=IH-IH-1
    DO150IK=1,IKM
    IK=IK-IK-1
    DO150IL=1,ILL
    IL=IL-IL-1
    ATH=ABS(F(IH)
    ATK=ABS(F(IK)
    ATL=ABS(F(IL)
    IF (ATH-1.) 21,1022,21
21  IF (ATK-1.) 22,1022,22
22  IF (ATL-1.) 23,1022,23
23  ABC=MIN1F(ATH,ATK,ATL)
    DO 55 I=1,8
    IF (ABC) 31,32,31
31  IF (ABC-F(I)) 1022,51,51
32  IF (MAX1F(ATH,ATK,ATL)-F(I)) 1022,51,51
51  IATH=ATH\F(I)
    IATK=ATK\F(I)
    IATL=ATL\F(I)
    AIH=IATH
    AIK=IATK
    AIL=IATL
    IF (IATH+ATK+ATL)-F(I)*(AIH+AIK+AIL)) 55,150,55
55  CONTINUE
1022 WAIT=DIIFIT(H,TK,IL)
    WD=V\WAIT
    WI=WI2F(IH,TK,IL)
    WA=A3E(IH,TK,IL)
    IFIN=SIZI(IZ,IZ)
71  U1I=(SIZ+IH+SIZ*IL+SIZ*TK)\(WAIT*AP)
    U12=(SZZ*TK+SZZ*IL+SIZ*IH)\(WAIT*AD)
    V11=IAA*IH+IL*ABCCOSB+TK*ABCOSD)\(SIP*WI)
    V12=IBB*TK+TK*IL*BCCOSA+IH*ABCOSD)\(SID*WI)
    GO TO 79
72  U1I=(SIZ+IH+SIZ*IL+SIZ*TK)\(WAIT*AP)
    U12=(SZZ*IL+SZZ*TK+SIZ*IH)\(WAIT*AD)
    V11=(AA*IH+IL*ABCCOSB+TK*ABCOSD)\(SIP*WI)
    V12=(CC*IL+TK*BCCOSA+IH*ACCOSB)\(SID*WI)
    GO TO 79
73  U1I=(SZZ*TK+SZZ*IL+SIZ*IH)\(WAIT*AP)
    U12=(SZZ*IL+SZZ*TK+SIZ*IH)\(WAIT*AD)
    V11=(BB*TK+TL*ABCCOSA+IH*ABCOSD)\(SIP*WI)
    V12=(CC*IL+TK*BCCOSA+IH*ACCOSB)\(SID*WI)
79  UU11=90.-SZ.*ZPS/ZPS*ASIN(U1I)
    UU12=90.-SZ.*ZPS/ZPS*ASIN(U12)
    VV11=90.-SZ.*ZPS/ZPS*ASIN(V11)
    VV12=90.-SZ.*ZPS/ZPS*ASIN(V12)
    ITH=TH
    ITK=TK
    ITL=TL
    WRITE(UU7)UU11,UU12,VV11,VV12,WAIT,WD,WI,WA,IH,IK,IL,X,IIH,IIK,IIL
150 CONTINUE
    GOTO 8
    END(0,1,0,0,0)
```

D. Input Cards:

Input information for a problem consists of three cards with the following form:

Card	Columns	Variable	Description
1	1 to 72	-	Hollerith title card. A "1" in column 1 restores output sheet for successive problems; otherwise it should be left vacant.
2	1 to 12	a	Lattice constants. Each value is given with a floating-point decimal which can appear at any position in the respective fields. Five digits may be given after the decimal point. (Format 6E12.5)
	13 to 24	b	
	25 to 36	c	
	37 to 48	α	
	49 to 60	β	
	61 to 72	γ	
3	1 to 6	M	Control parameter, as described above, to select indices of reference lattice elements.
	7 to 12	h	Maximum values of indices. Each of these and M is given as an integer, and they must be at the far right of their respective fields. (Format 4I6)
	13 to 18	k	
	19 to 24	ℓ	

E. Card-deck Arrangement:

The card deck is arranged in the following order:

Crystal geometry binary program deck

Three data cards for each problem:

Card 1 - Problem title
Card 2 - Lattice constants
Card 3 - Control parameters

F. Operating Instructions:

The general operating instructions for the program are as follows:

D. Input Cards:

Input information for a problem consists of three cards with the following form:

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	13 to 24	b	
	25 to 36	c	
	37 to 48	α	
	49 to 60	β	
	61 to 72	γ	
3	1 to 6	M	Control parameter, as described above, to select indices of reference lattice elements.
	7 to 12	h	Maximum values of indices. Each of these and M is given as an integer, and they must be at the far right of their respective fields. (Format 4I6)
	13 to 18	k	
	19 to 24	ℓ	

E. Card-deck Arrangement:

The card deck is arranged in the following order:

Crystal geometry binary program deck

Three data cards for each problem:

Card 1 - Problem title
Card 2 - Lattice constants
Card 3 - Control parameters

F. Operating Instructions:

The general operating instructions for the program are as follows:

1482/MET 143
704 PROGRAM

Programmer L. Bush *Date* 7/27/62

GENERAL OPERATING INSTRUCTIONS

	USED	NOT USED
DRUM:		X
UF SWITCH:	X	

READER: 72 x 72 board

PUNCH: Not used

PRINTER: Not used

SENSE SWITCH SETTINGS: All up

TAPES:

Input: FORTRAN Library Subroutine tape No. 1

Scratch: None

Output - Printed 6
- Punched None
To Be Saved None

Rewound by Program Prior to Calculation None After None
Manual EOF Needed Tape 6

TIME BEFORE OUTPUT: Negligible NORMAL RUNNING TIME: Subject to values of h, k, ℓ, α, β, and RUN NO LONGER THAN: γ.

RUNNING PROCEDURE: *(Indicate both regular and restart)*

1. READY tapes 1 and 6
2. Set UF switch on
3. Raise sense switches
4. CLEAR and LOAD CARDS (binary deck followed by data cards)
5. Final stop HPR 0,1. Write EOF on Tape 6, remove the print under program control.

STOPS (OCTAL): FORTRAN error stops

G. Running Time:

The running time of a problem depends upon the lattice system and the maximum values chosen for h, k, and ℓ. The sample problem given below required 15 sec. The largest problem encountered thus far pertained to the monoclinic system with maximum values of h, k, and ℓ equal to 15. A total of 6,482 sets of output were obtained in 14 min on the IBM-704 computer.

H. Output Form:

The form of the output is as follows:

Printed Line	Description
1	Problem title
2	Identification of input data a, b, c, α, β, and γ are given as A, B, C, ALPHA, BETA, and GAMMA. V labels the unit cell volume which is computed from the unit cell constants.
3	Values of a, b, c, α, β, γ, and V.
4	Identification of the output pertaining to the reference principal lattice elements selected by the control parameter M is given as follows: H1, K1 plus L1 designate the indices, and D1, I1, and A1 are the functions d_i, I_i, and A_i, respectively.
5 and 6	Values of h_i, k_i, ℓ_i, d_i, I_i, and A_i for the reference lattice elements.
7	Identification of the output generated by permutations of h_i, k_i, and ℓ_i is given as follows: H2, K2, and L2 identify indices, D2, I2, and A2 identify the functions d_i, I_i, and A_i for the indices, the first PHI and RHO refer to the functions ϕ and ρ for the indices with respect to the first of the reference lattice elements, and the second PHI and RHO identify the same angles with respect to the second.
8, etc.	Values of h_i, k_i, ℓ_i, d_i, I_i, A_i, ϕ_1, ρ_1, ϕ_2, and ρ_2.

G. Running Time:

The running time of a problem depends upon the lattice system and the *maximum* values chosen for h, k, and ℓ. The sample problem given below required 15 sec. The largest problem encountered thus far pertained to the monoclinic system with maximum values of h, k, and ℓ equal to 15. A total of 6,182 sets of output were obtained in 14 min on the IBM-704 computer.

H. Output Form:

The form of the output is as follows:

Printed Line	Description
1	Problem title.
2	Identification of input data a, b, c, α, β, and γ are given as A, B, C, ALPHA, BETA, and GAMMA. V labels the unit cell volume which is computed from the unit cell constants.
3	Values of a, b, c, α, β, γ, and V.
4	Identification of the output pertaining to the reference principal lattice elements selected by the control parameter M is given as follows: HI, KI plus LI designate the indices, and DI, II, and AI are the functions d_i, I_i, and A_i, respectively.
5 and 6	Values of h_i, k_i, ℓ_i, d_i, I_i, and A_i for the reference lattice elements.
7	Identification of the output generated by permutations of h_i, k_i, and ℓ_i is given as follows: H2, K2, and L2 identify indices, D2, I2, and A2 identify the functions d_i, I_i, and A_i for the indices, the first PHI and RHO refer to the functions φ and ρ for the indices with respect to the first of the reference lattice elements, and the second PHI and RHO identify the same angles with respect to the second.
8, etc.	Values of h_i, k_i, ℓ_i, d_i, I_i, A_i, φ_1, ρ_1, φ_2, and ρ_2.

IV. SAMPLE PROBLEM

The program has successfully run test problems for all of the possible space lattices. Alpha uranium was selected as a suitable sample problem for the purposes of this report. This metal has an orthorhombic crystal structure with the following lattice constants at 24.6°C.[6]

$a = 2.85360$ Å $\qquad c = 4.95552$ Å

$b = 5.86984$ Å $\qquad \alpha = \beta = \gamma = 90°$

The form of the data sheet, which is used for punching the three input cards, is shown in Figure 1. The maximum values for h, k and ℓ were selected equal to 3 in order to limit the quantity of the output which is shown in Figure 2.

704 INPUT DATA

FORM II

COST CODE 148

PROGRAM MET 143 PROBLEM ALPHA URANIUM ORIGINATOR L. T. LLOYD DATE 8/1/62 PAGE 1 OF 1

1	2	3	4	5	6	7	8
1 1 4 8 2 /	M E T 1 4 3	A L P H A	U R A N I	U M (2 4	. 6 C) S	A M P L E	P R O G R A
2	. 8 5 3 6 0	5	. 8 6 9 8 4	4	. 9 5 5 5 2	9 0	. 0 0
2	3	3	3				

5	6	7	8
M L . T .	L L O Y D	X 2 2 4 9	8 / 1 / 6 2
9 0	. 0 0	9 0	. 0 0

AMD-9 (9-60)

Figure 1. Data Sheet - Alpha Uranium Sample Program

Figure 1. Data Sheet - Alpha Literature Sample Program

PROGRAM NETWORK	PROGRAM ALPHA NETWORK	ORIGINATOR L.T.LLOYD	DATE 8/1/62	PAGE 1 OF 1

1	2	3	4	5	6	7	8
1234567890123456789012345678901234567890123456789012345678901234567890							
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Figure 2. Output Sheet - Alpha Uranium Sample Program

1482/MET143 ALPHA URANIUM (24.6C) SAMPLE PROGRAM L.T.LLOYD X2249 8/1/62

A	B	C	ALPHA	BETA	GAMMA	V
2.85360E 00	5.86984E 00	4.95552E 00	90.0000	90.0000	90.0000	8.30058E 01

H1	K1	L1	D1	I1	A1
1	0	0	2.85360E 00	2.85360E 00	2.90881E 01
0	0	1	4.95552E 00	4.95552E 00	1.67502E 01

H2	K2	L2	D2	I2	A2	PHI	RHO	PHI	RHO
0	0	0	0.00000E-40	0.	0.	90.0000	90.0000	90.0000	90.0000
0	0	1	4.95552E 00	4.95552E 00	1.67502E 01	90.0000	90.0000	0.0000	0.0000
0	1	0	5.86984E 00	5.86984E 00	1.41411E 01	90.0000	90.0000	90.0000	90.0000
0	1	1	3.78656E 00	7.68194E 00	2.19212E 01	90.0000	90.0000	40.1722	49.8278
0	1	2	2.28272E 00	1.15188E 01	3.63627E 01	90.0000	90.0000	22.8854	30.6363
0	1	3	1.59008E 00	1.59834E 01	5.22023E 01	90.0000	90.0000	15.7172	21.5458
0	2	1	2.52526E 00	1.27427E 01	3.28702E 01	90.0000	90.0000	59.3637	67.1146
0	2	3	1.43950E 00	1.89429E 01	5.76628E 01	90.0000	90.0000	29.3718	38.2971
0	3	1	1.81989E 00	1.82935E 01	4.56103E 01	90.0000	90.0000	68.4542	74.2828
0	3	2	1.53557E 00	2.02070E 01	5.40556E 01	90.0000	90.0000	51.7029	60.6282
1	0	0	2.85360E 00	2.85360E 00	2.90881E 01	0.0000	0.0000	90.0000	90.0000
1	0	1	2.47290E 00	5.71841E 00	3.35662E 01	29.9352	60.0648	60.0648	29.9352
1	0	2	1.87091E 00	1.03137E 01	4.43666E 01	49.0325	73.9378	40.9675	16.0622
1	0	3	1.42960E 00	1.51380E 01	5.80623E 01	59.9351	79.1344	30.0649	10.8656
1	1	0	2.56640E 00	6.52672E 00	3.23433E 01	25.9265	64.0735	90.0000	90.0000
1	1	1	2.27892E 00	8.19483E 00	3.64233E 01	37.0022	69.6215	62.6209	52.7918
1	1	2	1.78255E 00	1.18670E 01	4.65657E 01	51.3421	76.0861	43.9932	33.3661
1	1	3	1.38900E 00	1.62362E 01	5.97595E 01	60.8726	79.8773	32.7670	23.7024
1	2	0	2.04595E 00	1.20815E 01	4.05709E 01	44.1951	76.3379	90.0000	90.0000
1	2	1	1.89111E 00	1.30583E 01	4.38927E 01	48.4931	77.3775	67.5661	67.6979
1	2	2	1.57765E 00	1.56266E 01	5.26144E 01	56.4369	79.4781	50.4527	50.6364
1	2	3	1.28524E 00	1.91567E 01	6.45842E 01	63.2312	81.4333	38.9165	39.0995
1	3	0	1.61371E 00	1.78392E 01	5.14378E 01	55.5629	80.7953	90.0000	90.0000
1	3	1	1.53441E 00	1.85147E 01	5.40964E 01	57.4722	81.1339	71.9627	74.4754
1	3	2	1.35222E 00	2.04075E 01	6.13850E 01	61.7146	81.9619	56.9247	60.9445
1	3	3	1.15431E 00	2.32218E 01	7.19094E 01	66.1395	82.9414	45.6689	50.1934
2	0	1	1.37110E 00	7.55839E 00	6.05396E 01	16.0622	40.9675	73.9378	49.0325
2	0	3	1.07977E 00	1.59244E 01	7.68738E 01	40.8193	68.9984	49.1807	21.0016
2	1	0	1.38643E 00	8.18701E 00	5.98702E 01	13.6621	45.8049	90.0000	90.0000
2	1	1	1.33516E 00	9.56997E 00	6.21692E 01	20.6467	53.3900	74.3697	58.8139
2	1	2	1.20990E 00	1.28552E 01	6.86055E 01	32.0072	63.6431	60.7708	39.5584
2	1	3	1.06195E 00	1.69718E 01	7.81637E 01	41.9021	70.3499	49.9924	28.8416
2	2	1	1.24223E 00	1.39624E 01	6.68201E 01	29.4669	65.8734	75.4825	69.2116
2	2	3	1.01336E 00	1.97840E 01	8.19113E 01	44.7460	73.2333	52.1588	41.2844
2	3	0	1.15284E 00	1.85113E 01	7.20014E 01	36.1002	72.0426	90.0000	90.0000
2	3	1	1.12285E 00	1.91631E 01	7.39241E 01	38.0965	72.6731	76.9038	75.0132
2	3	2	1.04524E 00	2.09975E 01	7.94133E 01	42.8973	74.2284	65.0487	61.8352
2	3	3	9.45367E-01	2.37420E 01	8.78027E 01	48.5032	76.0908	55.0884	51.2318
3	0	1	9.34147E-01	9.89164E 00	8.88574E 01	10.8656	30.0649	79.1344	59.9351
3	0	2	8.88012E-01	1.30964E 01	9.34737E 01	21.0016	49.1807	68.9984	40.8193
3	1	0	9.38952E-01	1.03799E 01	8.84027E 01	9.2047	34.4371	90.0000	90.0000
3	1	1	9.22538E-01	1.15022E 01	8.99756E 01	14.1012	41.9029	79.2710	64.4795
3	1	2	8.78022E-01	1.43517E 01	9.45373E 01	22.6213	53.3803	69.2457	46.3237
3	1	3	8.16291E-01	1.81317E 01	1.01687E 02	30.8883	61.8263	60.3849	34.9229
3	2	0	9.04863E-01	1.45295E 01	9.17330E 01	17.9574	53.8998	90.0000	90.0000
3	2	1	8.90146E-01	1.53514E 01	9.32497E 01	20.6401	56.1061	79.6520	71.1673
3	2	2	8.49959E-01	1.75880E 01	9.76587E 01	26.6754	60.8733	69.9381	55.7009
3	2	3	7.93595E-01	2.07875E 01	1.04595E 02	33.4560	65.6806	61.2865	44.3431
3	3	1	8.42998E-01	2.01975E 01	9.84650E 01	27.5946	64.9218	80.2056	75.7973
3	3	2	8.08628E-01	2.19456E 01	1.02650E 02	31.7760	67.0398	70.9523	63.1525

V. ACKNOWLEDGEMENTS

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