52	.1613467E+01	-.7804677E+00	-.6883520E+00
53	-.5327672E-01	.1919442E+01	-.7122008E+00
54	-.5660612E-01	.3315453E+00	.2063794E+01
55	-.1363024E+01	-.9579605E+00	-.1705629E+01
56	-.1483518E+01	-.1832305E+01	-.4003913E+00
57	-.2324718E+01	-.4477878E+00	-.2060256E+00
58	.1378434E+01	-.1038785E+01	-.1612607E+01
59	.1393848E+01	-.1726983E+01	-.8897992E+00
60	.2316008E+01	-.2730557E+00	-.2304989E+00
61	.1172531E+00	.1594587E+01	-.1682998E+01
62	-.1160266E+01	.1958527E+01	-.1603868E+00
63	.1175806E+01	.1907548E+01	-.1674181E+00
64	-.3516758E-01	-.2040049E+01	.8872391E+00
65	-.1087514E+01	.2836724E+00	.2011218E+01
66	.9802335E+00	.3116941E+00	.2039919E+01

In Table 1 structural information is given in terms of B_n and r_n (for lists (a) and (b)) and in terms of coordinate positions (for the particular compound in (c)). The lattice parameters a for the FCC microcrystal and c and a for the hexagonal microcrystallites can be given any reasonable values from the literature or particular values for definite materials. The example given

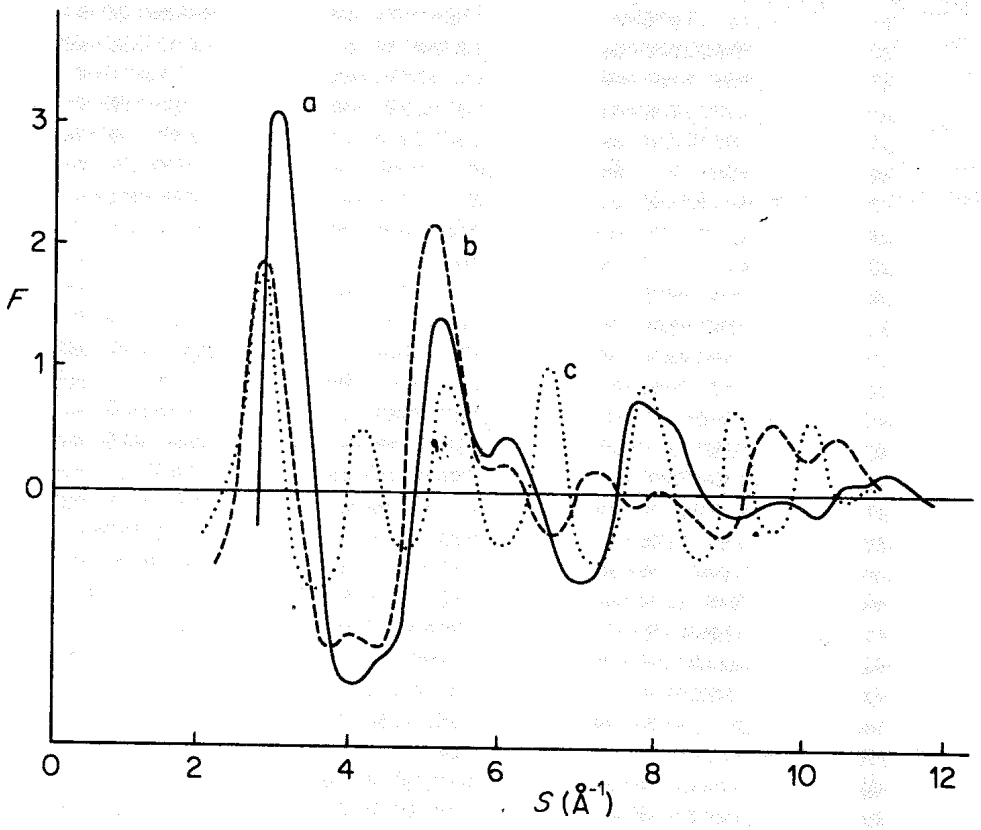


Figure 3. Interference functions for: (a) an experimental $Gd_{10}Co_{90}$ alloy thin film; (b) a calculation for a random assembly of 77 atom Gd_2Co_{17} microcrystallites; and (c) a calculation for a similar assembly of 17 atom $GdCo_5$ microcrystallites

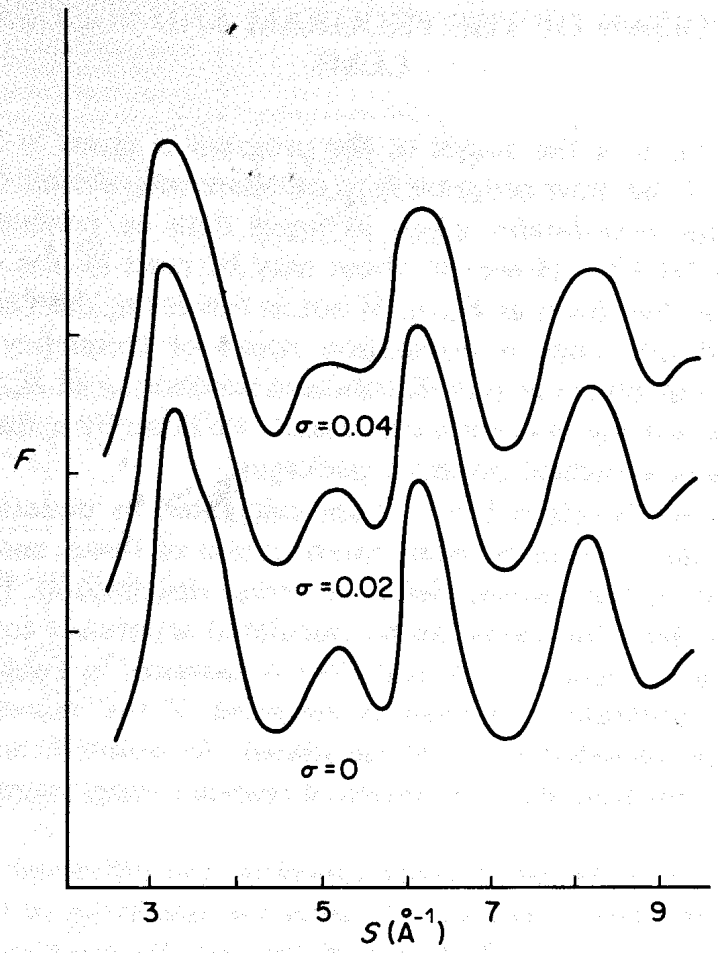


Figure 4. Curves showing the calculated effect of different strain levels on the interference function for 55-atom FCC microcrystallites

in (c) is for $GdCo_5$. Such structural details can be obtained from drawings, constructed models (e.g. 'ball and spoke' models) as in Table 2 and tabulated crystallographic data.[6,7]

Calculated $F(S)$ functions using these and other data are superimposed on those obtained from the experimental $I(S)$ (using equations (4) and (4a)) for particular thin films in Figure 3. The effect of strain on interference functions calculated via equations (9) and (10) are illustrated in Figure 4. Inspection of these curves and the experimental $F(S)$ curve of Figure 2a suggests that strained microcrystalline assemblies are not responsible for the observed diffraction pattern from the specimen.

Although the agreement, or lack of it, between experimental and model functions is not of importance here, computational exercises of this kind are of significance in showing that these materials are not composed of simple microcrystalline atomic arrangements.

4. A BREAKDOWN OF THE PROGRAM AND SUGGESTED PROBLEMS

A specimen outline of the stages of the program is given in Figure 5. The first operation of the main program is to calculate interatomic distances from values of atomic coordinates given as input data or generated in a subroutine (e.g. MODEL). However, these may be read in, for example from Table 1, in a 'sorted' form as B_n, r_n. If not in this form, the values of r_n may be then sorted into such a population count or frequency spectrum. If required such a spectrum or pair distribution function, ρ of B_n against r_n can be plotted. The sorting operation can usually be done by a standard routine available in most statistical program packages.

The interference function $F(S)$ is then calculated by equations (5) or (6) (depending on the data) or by some modification of these, such as equation (10), incorporating a particular defect or strain distribution. For multicomponent systems these functions can be calculated separately for the different correlations, e.g. Gd–Gd, Gd–Co and Co–Co distances in Table 1c, and then summed. This separate treatment is essential if the relevant scattering factors are to be included and $I(S)$ calculated. As pointed out earlier, such curves can be compared with the results of relevant experimental determinations.

A computation of the interference functions and diffracted intensities for the data given in Table 3 will serve to show the sensitivity of the calculation to small structural changes. Both sets of data are for random assemblies of clusters containing 13 atoms. The set in (a) is for atoms packed in a close-packed structure of 12 atoms, showing 6 membered rings, round a central atom. That in (b) is for a 13-atom icosahedron in which 12 atoms are evenly spaced round and in contact with the centre atom. These atoms do not touch each other and form 5 membered rings in section. The first model can fill space to form an ordered crystalline structure, the second cannot and would produce an extremely disordered structure. In the table d is the atomic diameter (this can usually be taken as the Goldschmidt diameter for 12-fold close packing[6]). For the crystalline packing d could be taken as the closest distance of approach which is usually very close to the Goldschmidt diameter,[6] e.g. for FCC nickel the lattice parameter a is 3.524 Å and the closest distance of approach is 2.49 Å which is very near to the Goldschmidt diameter of 2.50 Å. In the comparative calculation the data of Table 1a could be used for the crystal or that of Table 3 given in terms of the lattice parameter or atomic diameter in hard packing (for which $a \simeq \sqrt{2}d$). The two interference functions of Figure 6 are clearly different and this distinction is reflected fairly clearly in the diffracted intensity. Hence it is evident that with careful measurement such packings in experimental specimens could be distinguished with interference functions calculated from experimental $I(S)$ data obtained out to large S values.

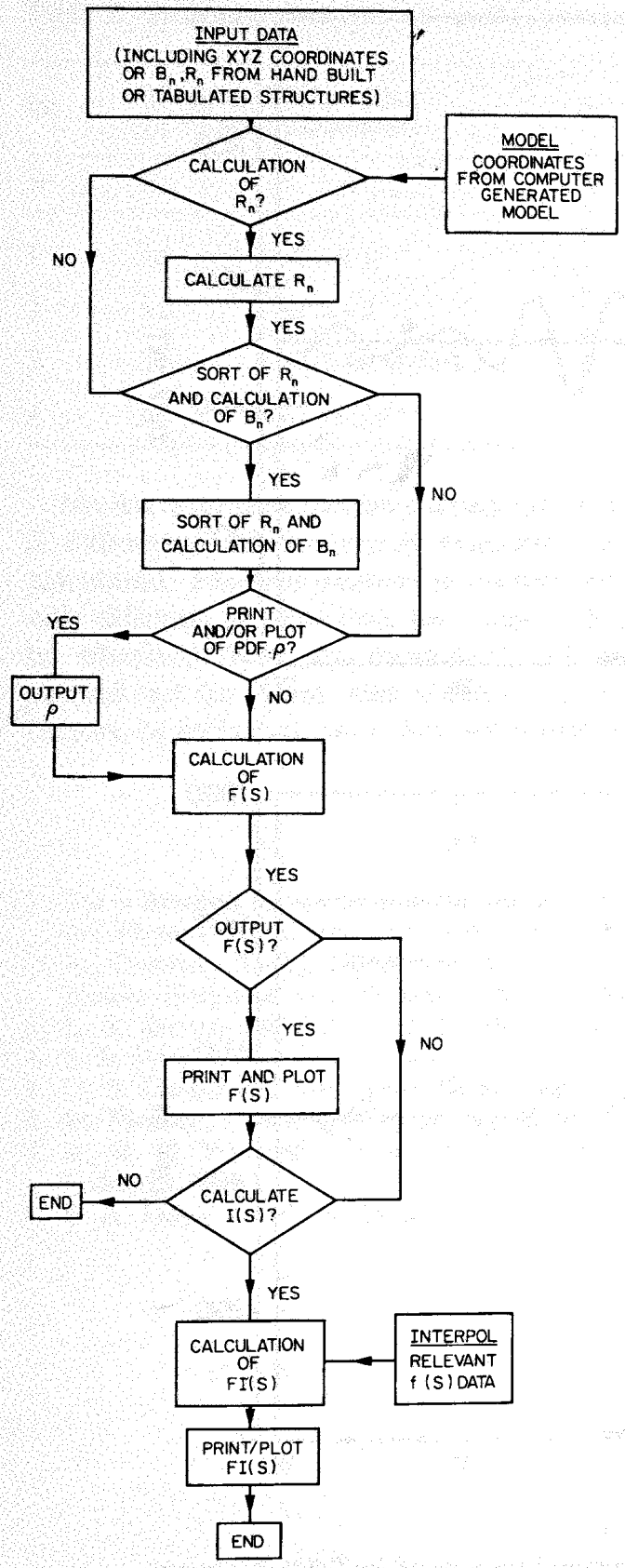
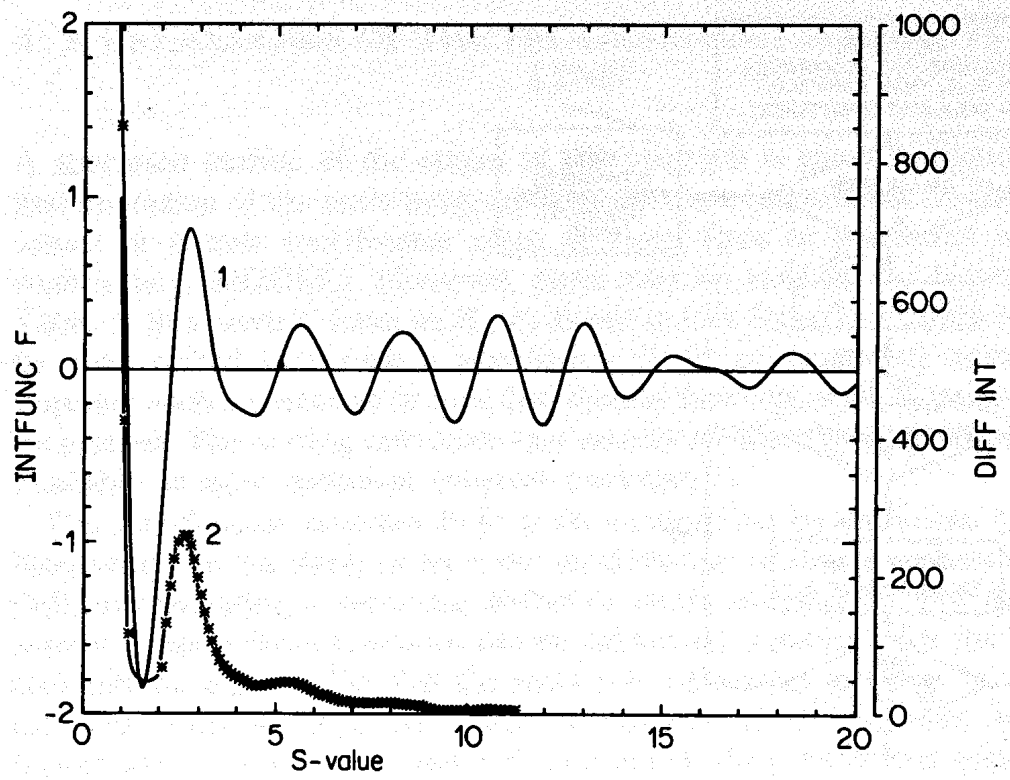


Figure 5. A schematic layout of the program given in section 5



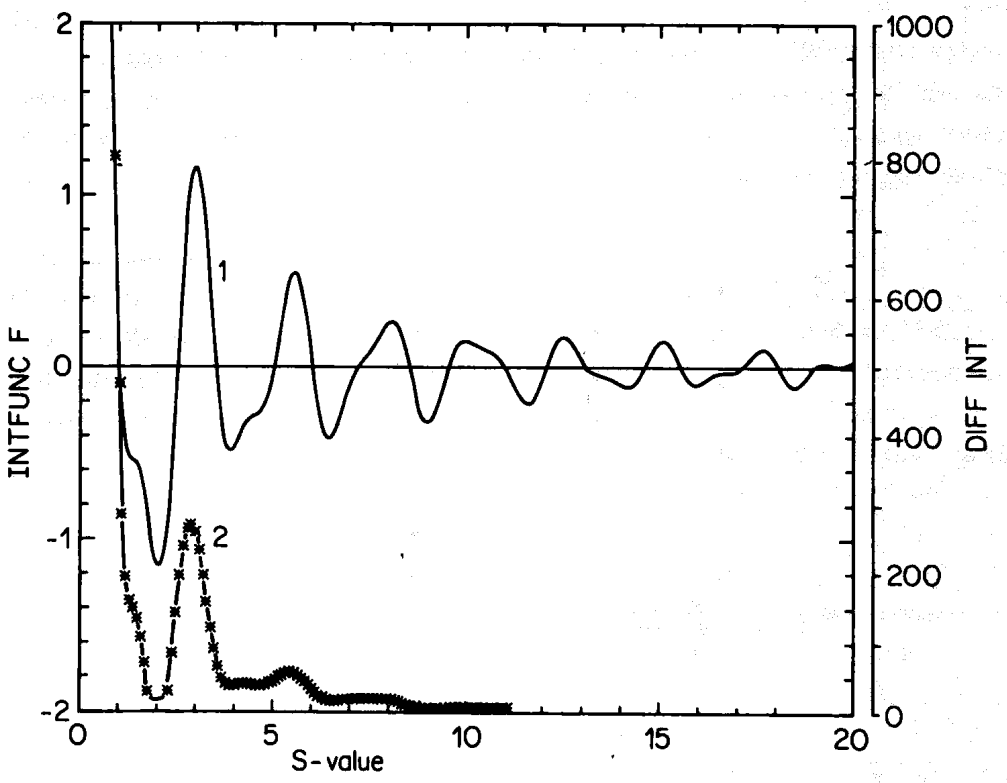


Figure 6. Typical output for the structural data given in Table 3. Curves (1) are the interference functions and curves (2) are the diffracted intensity (neglecting any inelastic contribution); (a) is for the FCC cluster and (b) is for the icosahedral packing.

Table 3. Structural data for two similar atomic arrangements

(a)	13-atom FCC packing (a = lattice parameter)		(b)	13-atom icosahedron (d = atomic diameter)	
n	B_n	r_n	n	B_n	r_n
1	36	$a/\sqrt{2}$ or d	1	12	$1.0d$
2	12	a or $d\sqrt{2}$	2	6	$2.0d$
3	24	$a\sqrt{3}/2$ or $d\sqrt{3/2}$	3	20	$1.868d$
4	6	$a\sqrt{2}$ or $2d$	4	30	$1.052d$
			5	10	$1.902d$

Similar exercises can be carried out with other packings and models, and if diffraction information is available pair distribution functions could be calculated. Electron-scattering factors have the same form for all atoms, only differing in value over the range of S (details for use in the program can be obtained from the literature[8]). Of course, these calculations can be carried out for X-ray and neutron scattering; in these cases the scattering factors, or form factors as they are sometimes called, have different forms.

REFERENCES

1. For a detailed review of general diffraction theory see D. H. Martin, *Contemporary Physics*, **18,** 81 and 193 (1977) and reference 2.
2. A. Guinier, *X-ray Diffraction in Crystals, Imperfect Crystals and Amorphous Bodies* (Freeman, San Francisco and London, 1963).
3. L. B. Davies and P. J. Grundy, *Physica Status Solidi* (a), **8,** 189 (1971).
4. S. S. Nandra and P. J. Grundy, *J. Phys. F*, **7,** 207 (1977).
5. G. S. Cargill III, *Solid State Physics*, **30,** 227 (Academic Press, London, 1975).
6. M. Hansen, *Constitution of Binary Alloys* (McGraw-Hill, New York, 1958).
7. R. W. G. Wyckoff, *Crystal Structures* (Interscience/Wiley, New York, London, Sydney, 1960).
8. P. A. Doyle and P. S. Turner, *Acta Cryst.*, **A24,** 390 (1968).

DIFFRACTION PATTERN SIMULATION

```
C THIS PROGRAM CALCULATES THE INTERFERENCE FUNCTION,A PAIR DISTRIBUTION
C FUNCTION (IF REQUIRED) AND THE COHERENTLY DIFFRACTED INTENSITY FOR AN
C ATOMIC ARRANGEMENT GIVEN EITHER THE COORDINATES X Y Z OF THE ATOMS OR
C A FREQUENCY COUNT BN OF ATOMIC SPACINGS RN AS INPUT DATA.
C ALTERNATIVELY DATA MAY BE INPUT FROM A ROUTINE GENERATING A COMPUTED MODEL
C
C IN THIS PROGRAM F IS THE INTERFERENCE FUNCTION. S AND SS ARE USED FOR
C THE SCATTERING PARAMETER. RHO IS THE PAIR DISTRIBUTION FUNCTION. R IS
C THE SCALE OF THE INTERATOMIC DISTANCES. FS IS THE ELECTRON SCATTERING
C FACTOR, X Y AND Z ARE ATOMIC COORDINATES. FI IS THE COHERENTLY
C DIFFRACTED INTENSITY. NB REPRESENTS THE FREQUENCY OF SORTED CORRELAT-
C IONS RN. NA AND NS ARE POINTERS TO THE ARRAYS X,Y,Z,NB AND RN. RNEW IS
C USED AS A WORKING ARRAY FOR ATOMIC CORRELATIONS. IARR AND IST ARE USED
C FOR POINTERS AND WORK SPACE. ITF,ITP AND ITI ARE ARRAYS FOR GRAPHS
C
      DIMENSION F(200),FI(200),S(200),RHO(100),R(100),RNEW(100),FS(200)
      DIMENSION NA(100),X(100),Y(100),Z(100),IARR(5000),IST(5000)
      DIMENSION SS(200)
      DIMENSION NS(100),NB(100),RN(100)
      DIMENSION A1(20),A2(20),B1(20),B2(20),FSS(200),SIS(200),AM(20)
      DIMENSION D(20)
      COMMON/SCDTA/RV(2000)
      DIMENSION ITF(13),ITI(12),ITP(13)
C
C HERE WE HAVE CHOSEN CONVENIENT SIZES FOR THE VARIABLE ARRAYS
C
      DATA ITF/21,21HINTERFERENCE FUNCTION,7,7HS-VALUE,7,7HINTFUNC/
      DATA ITI/20,20HDIFFRACTED INTENSITY,7,7HS-VALUE,8,8HDIFF INT/
      DATA ITP/26,26HPAIR DISTRIBUTION FUNCTION,8,8HRN-VALUE,3,3HPDF/
C
C THESE ENTRIES GIVE THE GRAPH TITLES AND ORDINATE AND ABSCISSA
C DESCRIPTIONS FOR GRAPHICAL OUTPUT OF THE CHOSEN EXAMPLES
C
      READ(1,100)N,M
      WRITE(2,44)
      WRITE(2,101)N,M
C
C N IS THE NUMBER OF ATOMS IN THE MODEL
C M/10 IS THE UPPER LIMIT TO S (THIS IS JUST A CONVENIENT CHOICE IN
C THIS EXAMPLE BUT IF FI IS SUBSEQUENTLY CALCULATED IT WILL DEPEND ON
C THE AVAILABLE DATA ON FS WHICH SHOULD BE KNOWN UP TO THE UPPER LIMIT
C CHOSEN FOR S)
C
      NN=(N*(N-1))/2
C
C NN IS THE TOTAL NUMBER OF INTERATOMIC DISTANCES
C
      READ(1,102)IA,IC
      WRITE(2,55)
      WRITE(2,103)IA,IC
      IF(IA-2)1,2,3
C
C IA ACCOUNTS FOR THE DIFFERENT DATA INPUTS. IC CHOOSES THE ALTERNATIVE
C CALCULATION FOR F IF A PAIR DISTRIBUTION FUNCTION IS NOT REQUIRED
C FOR THE CHOICE IA=1 READ IN ATOMIC COORDINATES
C
```

```
DIFFRACTION PATTERN SIMULATION
    1 READ(1,104)(NA(I),X(I),Y(I),Z(I),I=1,N)
      WRITE(2,66)
      WRITE(2,104)(NA(I),X(I),Y(I),Z(I),I=1,N)
C
C NOW CALCULATE THE INTERATOMIC DISTANCES R FROM THIS DATA
C
      K=0
      IN=N-1
      DO 4 I=1,IN
      JN=I+1
      DO 5 J=JN,N
      F1=(X(J)-X(I))**2
      F2=(Y(J)-Y(I))**2
      F3=(Z(J)-Z(I))**2
      K=K+1
    5 R(K)=SQRT(F1+F2+F3)
    4 CONTINUE
      IF(IC.GT.1)GO TO 9
C
C R(K) MAY BE SORTED INTO A 'FREQUENCY SPECTRUM' NB OF CORRELATIONS RN
C VIA SOME SUITABLE SORTING ROUTINE. THESE ARE USUALLY AVAILABLE IN
C STATISTICAL LIBRARY ROUTINES. THIS SORTING IS ASKED FOR OF IC=1 AND
C SHOULD BE IN A FORM SUITABLE FOR PLOTTING A PAIR DISTRIBUTION FCTN
C
C CALL 'SORT'
C
C
C HERE IS AN ALTERNATIVE INPUT AF DATA - READ IN NB AND RN VALUES FROM
C TABULATED STRUCTURE OR HAND BUILT MODEL AND PLOT THE PDF
C L IS THE NUMBER OF VALUES OF NB
C
    2 READ(1,107)L
      WRITE(2,107)L
      READ(1,105)(NB(I),RN(I),I=1,L)
      WRITE(2,77)
      WRITE(2,105)(NB(I),RN(I),I=1,L)
C IF THE PDF IS NOT REQUIRED THEN
      GO TO 6
      CALL NARROW
      CALL FGPLT(RN,NB,L,2,0,1,0,ITP,2)
C
C NARROW REQUESTS A PARTICULAR OUTPUTMEDIUM AND FGPLT IS A LIBRARY GRAPH
C PLOTTING ROUTINE
C
C ANOTHER ALTERNATIVE INPUT - VALUES OF X,Y,Z OP NB AND RN GIVEN BY A
C ROUTINE GENERATING A COMPUTER BUILT STRUCTURAL MODEL MAY REPLACE THE
C FOLLOWING CONTINUE COMMAND
C
    3 CONTINUE
C
C CALCULATE, WRITE AND PLOT THE INTERFERENCE FUNCTION. OF COURSE,
C SEPERATE FUNCTIONS MAY BE CALCULATED FOR A-A, A-B,AND B-B CORRELATIONS
C IF A BINARY MODEL COMPOSED OF A AND B ATOMS IS CONSIDERED
C
    6 DO 7 IX=1,M
      SX=FLOAT(IX)/10.0
```

```
DIFFRACTION PATTERN SIMULATION

      SUM=0.0
      DO 8 IK=1,L
      IF(RN(IK).EQ.0.0)GO TO 8
      PROD=SIN(SX*RN(IK))/(SX*RN(IK))
      RES=PROD*NB(IK)
      SUM=SUM+RES
    8 CONTINUE
      F(IX)=(2.0*SUM)/N
      S(IX)=SX
    7 CONTINUE
      GO TO 12
    9 DO 10 IX=1,M
      SX=FLOAT(IX)/10.0
      SUM=0.0
      DO 11 IK=1,NN
      IF(R(IK).EQ.0.0)GO TO  1
      PROD=SIN(SX*R(IK))/(SX*R(IK))
      SUM=SUM+PROD
   11 CONTINUE
      F(IX)=SUM/N
      S(IX)=SX
   10 CONTINUE
C
C NOW WRITE THE INTERFERENCE FUNCTION
C
   12 WRITE(2,88)
      WRITE(2,106)(F(IX),S(IX),IX=1,M)
C
C IF THE COHERENTLY DIFFRACTED INTENSITY IS REQUIRED VALUES OF THE
C ELECTRON SCATTERING FACTOR AT THE S VALUES FOR WHICH F HAS BEEN
C CALCULATED ARE NEEDED. THESE CAN BE OBTAINED BY INTERPOLATING FACTORS
C OBTAINED FROM THE PUBLISHED LITERATURE. IF WANTED THE INTERPOLATED
C FACTORS MAY BE PRINTED
C
      CALL INTERPOL(FS,SS)
      WRITE(2,99)
      WRITE(2,106)(FS(I),SS(I),I=1,M)
C
C USE THESE VALUES OF S TO CALCULATE WHAT IS IN EFFECT THE DIFFRACTION
C PATTERN EXPECTED FROM THE MODEL
C
      DO 13 I=1,M
      SUM=1.0+F(I)
      FACT=FS(I)**2
      FI(I)=N*FACT*SUM
      SUM=0.0
      FACT=0.0
   13 CONTINUE
      WRITE(2,144)
      WRITE(2,106)(FI(I),S(I),I=1,M)
C PLOT THE INTERFERENCE FUNCTION AND THE DIFFRACTED INTENSITY
      CALL NARROW
      CALL FIXAXS(0.0,20.0,-2.0,2.0)
C FIXAXS IS A LIBRARY ROUTINE FOR SETTING THE LIMITS OF THE
C ORDINATE AND ABSCISSA
      CALL FGPLT(S,F,M,2,0,1,0,ITF,2)
```

```
DIFFRACTION PATTERN SIMULATION ,
      CALL FIXAXS(0.0,20.0,0.0 1000.0)
      CALL FGPLT(S,FI,M,1,8,1,2,ITI,2)
      CALL DEVFIN
  999 CONTINUE
C
C DEVFIN CLOSES DOWN THE GRAPHICAL OUTPUT DEVICE
C
   44 FORMAT(1X,15HNUMBER OF ATOMS,5X,13HLIMIT TO 5X10)
   55 FORMAT(1X,18HWHICH INPUT SCHEME,5X,16HWHICH CALC FOR F)
   66 FORMAT(5X,11HATOM NUMBER,10X,5HX VAL,10X,5HY VAL,10X,5HZ VAL)
   77 FORMAT(1X,18HBN FREQUENCY OF RN,5X,11HVALUE OF RN)
   88 FORMAT(1X,21HINTERFERENCE FUNCTION,15X,7HS VALUE)
   99 FORMAT(1X,17HSCATTERING FACTOR,15X,7HS VALUE)
  144 FORMAT(1X,20HDIFFRACTED INTENSITY,15X,7HS VALUE)
  100 FORMAT(2I4)
  101 FORMAT(6X,I4,15X,I4)
  102 FORMAT(2I3)
  103 FORMAT(8X,I3,20X,I3)
  104 FORMAT(10X,I5,5X,E14.7,5X,E14.7,5X,E14.7)
  105 FORMAT(10X,I4,10X,F14.7)
  106 FORMAT(5X,E14.7,10X,E14.7)
  107 FORMAT(1I4
      STOP
      END
C
      SUBROUTINE INTERPOL(FSS,SIS)
      DIMENSION A1(20),A2(20),B1(20),B2(20),FSS(200),SIS(200),AM(20)
      DIMENSION D(20)
C
C THIS ROUTINE RETURNS VALUES OF SCATTERING FACTOR FS AND THE RELEVANT
C VALUES OF SCATTERING PARAMETER SS TO THE MAIN PROGRAM INTERPOLATED
C FROM TABULATED INPUT VALUES OF FSS (AS B2) AND SIS (AS A2). N1 IS THE
C NUMBER OF STARTING VALUES OF FSS AND SIS. IR1 IS THE
C STARTING VALUE(*1000) OFSIS. IH IS THE INCREMENT(*1000) IN SIS AT
C WHICH INTERPOLATION IS REQUIRED. IN THE USE OF THE PARTICULAR
C INTERPOLATION ROUTINE E01ADF THE INPUT ARRAYS ARE REASSIGNED FOR EACH
C ITERATION. AM AND D APE WORKING SPACE.
C
C FIRST READ IN VALUES OF NV,IR1 AND IH. CONVENIENT VALUES OF IR1 AND
C IH ARE 100.
C
      READ(1,200)NV,IR1,IH
      WRITE(2,200)NV,IR1,IH
      N1=NV+1
C
C NOW READ IN STARTING VALUES OF FSS AND SIS;CONVENIENTLY 20 VALUES IF
C KNOWN.
C
      READ(1,201)A2
      WRITE(2,202)A2
      READ(1,201)B2
      WRITE(2,202)B2
      IX=1
   40 X=FLOAT(IR1)/1000
C
C REASSIGN THE ARRAYS AND CALL E01ADF
```

```
DIFFRACTION PATTERN SIMULATION

C
   30 DO 16 I=1,20
      B1(I)=B2(I)
   16 A1(I)=A2(I)
      CALL E01ADF(NV,X,A1 B1,AM,D,N1,VAL)
C
C BUILD THE OUTPUT ARRAYS SIS AND FSS AND INCREMENT AND LIMIT THEIR SIZE.
C
      SIS(IX)=X
      FSS(IX)=VAL
      IX=IX+1
      IR1=IR1+IH
      IF(IX.GT.200)GO TO 20
      GO TO 40
   20 CONTINUE
  200 FORMAT(3I4)
  201 FORMAT(20F0.0)
  202 FORMAT(20F7.4)
      RETURN
      END
      FINISH
C
C
C ENTER THE DATA FOR THE PROGRAM IN THIS SPACE
C
C
ENDJOB
```

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