***Reflect - A Computer Program For The X-Ray Reflectivity
of Bent Perfect Crystals***

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1. Introduction

The design of monochromators for x-ray applications, using either standard laboratory sources or synchrotron radiation sources, requires a knowledge of the reflectivity of the crystals. The reflectivity depends on the crystals used, the geometry of the reflection, the energy range of the radiation, and, in the present case, the cylindrical bending radius of the optical device. This report is intended to allow the reader to become familiar with, and therefore use, a computer program called REFLECT which we have used in the design of a dual beam Laue monochromator for synchrotron angiography [1]. The results of REFLECT have been compared to measured reflectivities for both bent Bragg and Laue geometries [2]. The results are excellent and should give full confidence in the use of the program.

The program calculates the crystal reflectivities as a function of deviation angle from the Bragg condition using a lamellar model introduced by White [3] and the formulae given by Zachariasen [4] and Wilkins [5]. The formalism is based on the work of Boeuf et al. [6]. The program is listed in Appendix A, with many of the steps referred to equations found in these references.

2. Lamellar Model

The lamellar model approximates a cylindrically bent perfect crystal by a stack of perfect crystal lamellae which have a gradually changing orientation [2]. Figure 1 shows the basic geometry of the crystal approximation. Each lamella is normal to the radius of curvature at the point an x-ray hits its entrance surface at the angle $\chi \pm \theta$. χ is the asymmetry angle of the crystal given by the angle between the reflecting planes of the lamella and the surface normal (radius of curvature) and θ is the angle between an x-ray and the reflecting planes (see Figure).

As a ray at a fixed angle to the crystal surface traverses the stack of lamellae, there is a change of angle between each successive lamella caused by the bending of the crystal. The basic decision to be made in this model is the thickness of the lamellae in a particular situation. Once the lamella thickness, T_0 , is determined, the problem reduces to one of summing the partial reflections from the lamella traversed at each angle. Most of the formalism involves the geometrical determination of the angles, orientations and thicknesses of the lamellae in order to calculate the

reflection and transmission ratios from the dynamical theory of diffraction. In the current program, the power of the reflected beam is corrected for absorption on its way out while the transmitted beam is the incident beam for the next lamella. Throughout, the Poisson ratio, ν , is assumed to be isotropic.

The basic assumption of the model is to take the thickness T_0 such that the angle between two successive lamellae is equal to the Darwin width of the reflection. As a result, only a few lamellae contribute to the reflection for each incident ray. When the direction of the incident beam changes, the layer of the reflecting lamellae moves through the crystal. This choice of the lamella thickness is arbitrary to a certain degree. The important thing is that T_0 be large enough so that the dynamical theory of diffraction can be applied to each lamella. The reflectivity for a narrow pencil beam at fixed incident angle to the crystal surface is

$$r_n(\theta) = \sum_{j=1}^n \left\{ r_j \exp(-\mu S_j) \left[\prod_{k=0}^{j-1} t_k \right] \right\} \quad (1)$$

where the crystal consists of n lamellae, r_j and t_j are the reflection and transmission ratios of the j th lamella, respectively, S_j is the absorption path length of the reflected beam, and μ the linear absorption coefficient. The integrated reflectivity for a finite beam is the sum over the reflectivities $r_n(\theta)$ for all incident angles θ near the Bragg condition.

The reflection and transmission ratios are calculated from the formulas given by Zachariasen [4], Wilkins [5], and Boeuf et al. [6]. Following the theory developed by Zachariasen, the geometrical angular scale is replaced by the y -scale. Much of the formalism of REFLECT is not immediately obvious due to this scaling. The y -scale replaces the incident beam direction with respect to the surface of the crystal by $y(0)$, and deviations from this are given by Δy . For example, the "angle" of incidence for the j th lamella would be $y(0) + j\Delta y_D$, where Δy_D is the change of y between successive lamella. The simplification in the original theory comes about because in the y -scale notation, the Darwin width of a Bragg reflection is $\Delta y_D = 2$ and for a Laue reflection it is $\Delta y_D = \pi/2$.

The thickness of one lamella, T_0 , is given in units of the extinction thickness $L_{ex} = V_c \left| \gamma_0 \gamma_H \right|^{1/2} / r_e \lambda K F_H$. This normalized thickness is called A and

given by $A = T_o/L_{ex}$. Here, V_c is the volume of the unit cell, $r_e = e^2/mc^2$ the classical electron radius, λ the x-ray wavelength, K the polarization factor, and F_H the structure factor. The directions of the incident and reflected beams are given by $\gamma_o = \sin \alpha$, $\gamma_H = \sin \beta$, where α and β are the angles between the beams and the surfaces of the crystal.

The Darwin width of an asymmetric Bragg reflection is

$$W_s M^{\frac{1}{2}} = W_a = (2\lambda/\pi\Lambda_s \sin 2\theta) \left| \gamma_H/\gamma_o \right|^{\frac{1}{2}} \quad (2)$$

where W_s is the width of the symmetrical reflection, $M = \left| \gamma_H/\gamma_o \right|$ is the lateral magnification of the beam, and $\Lambda_s = L_{ex} / \left| \gamma_o \gamma_H \right|^{\frac{1}{2}}$.

The thickness of each lamella is taken such that the change in the Bragg angle across the lamella is equal to W_a . For a bent crystal with bending radius ρ and Poisson ratio ν , the change in angle across a lamella at depth T from the surface is given by

$$\Delta\theta(T) = \left(\frac{T}{\rho} \right) \left[\tan(\chi \pm \theta) + \frac{1}{2}(1+\nu) \sin 2\chi + \tan\theta (\cos^2 \chi - \nu \sin^2 \chi) \right] \quad (3)$$

The change in Bragg angle across a lamella is due to the geometrical curvature of the crystal as well as the change in angle and lattice spacing due to the stretching (on compression) of the crystal.

In the formalism used here, the change in y across a lamella is related to the bending radius ρ and thickness A by the parameter $c = \Delta y/A$,

$$c = \frac{\pi \Lambda_s^2}{\lambda \rho} (b-1) \gamma_H \left[1 + b \gamma_H^2 (1+\nu) \right] \quad (4)$$

where $b = \gamma_o/\gamma_H$.

The reflectivities, integrated reflectivities, and reflection widths are calculated in quantities which are based on the y -scale. Conversion of each quantity to SI units is done within the program. The results are printed along with information on the input parameters, y scale conversion factors, and calculated parameters such as the number of reflecting lamellae and their thickness.

In summary, the program takes a set of parameters for a crystal which includes the bending radius and incident beam direction, calculates a lamellar thickness A based on ρ and the Darwin width for the desired reflection, and then calculates the reflectivity for a set of incident beam angles near the Bragg condition at the crystal surface. This results in the relectivity curve $R(\theta)$ which, when integrated, gives the integrated reflectivity. The program is written to account properly for the beam polarization. Each polarization, Sigma and Pi, is considered separately with a complete calculation and set of output files for each.

3. Users' Notes

3.A. Computing Time

The running time of the program depends on the computer used. The following numbers are based on the use of a VAX 750/11 at the University of Helsinki.

The CPU time goes roughly linearly with the number of lamellae. The number of lamellae is proportional to the thickness of the crystal and inversely proportional to the bending radius and x-ray wavelength. In the Bragg case the thickness is determined by the absorption if the crystal is totally absorbing. Typically, the CPU time per lamella and point of calculation is 1.5 msec in the Laue case and 0.5 msec to 0.7 msec in the Bragg case. The difference is due to the decreased computing time in the low intensity tails of the Bragg reflection. For example, calculation of the reflectivity curve at 100 points for one state of polarization with AgK-alpha radiation takes 25 sec for Si(220) from a crystal bent to 0.8 meters in the symmetrical Bragg case. The same calculation for reflection from a 0.5 mm thick wafer cut perpendicular to [111] in the Laue case takes 55 sec.

3.B. Angular Range

The number of points calculated (POINTS) is usually taken to be 100 to 200. The angular range (from TLOW to TUP) can be calculated from Eq. 3 in the Laue case. In the Bragg case, a preliminary calculation with a small value of POINTS is recommended, and then TLOW is set to correspond to a reflectivity of 0.01 to 0.001 of the maximum value.

If many bending radii, RHO , are included in the same run, these are ordered to increase monotonically, and $TLOW$ and TUP correspond to the smallest $RHO = RHO_{min}$. If $DISCON = 0$, $TLOW$ and TUP stay constant for all RHO . With $DISCON = 1$ the range $TUP-TLOW$ decreases proportionally to RHO_{min}/RHO . This ensures the same degree of precision throughout the calculation. If the reflectivity curves are plotted, the angular scale refers to the case $RHO = RHO_{min}$.

$TLOW$ and TUP can be calculated by the program, but it is recommended that $TLOW$ and TUP be given in the input data. This will avoid excessive computing time when the Darwin width (Eq. 2) is small.

3.C. Integrated Reflectivity

In the Bragg case, the integrated reflectivity increases monotonically with the thickness of the lamella, reaching the asymptotic value at a few extinction thicknesses. In the Laue case, the integrated reflectivity is an oscillatory function of A . The same oscillations are seen in the integrated reflectivity of the whole crystal, which is a computational artifact arising from the lamellar model. This can be avoided by using the asymptotic value of the reflectivity for lamellae with A larger than $\pi/2$. In the program, this is done by setting $RB = 1$ in subroutine `LAUE`.

4. Program Structure

The program `REFLECT` is written in Fortran with the version presented here running on a Micro Vax. The program reads an input file which is created separately for each crystal program desired. The input contains the crystal parameters, bending radii, and wavelength of radiation to be considered. Control of the output format is also an input parameter. The following is an outline of the program. Output files will be discussed separately. Since plotting is a machine dependent function, routines for plotting are not discussed. Plotting is done by accessing the output files `FOROXX.DAT` created by the program. The Main Program calls subroutines which are underlined and capitalized in the following outline.

PROGRAM REFLECT

INPUT FILE - crystal parameters
 reflection parameters
 bending radii

MAIN PROGRAM

- I. Read Input File
- II. Choose first crystal thickness
 - A. Choose Sigma Polarization
 1. Call CONSTANTS - calculate quantities based on the minimum bending radius considered (non θ dependent).
 2. Call LIMITS - either read input limits or calculate limits to be used in the calculation of $R(\theta)$.
 3. Call RCURVE - calculate reflectivity curve between limits.
 - a. Choose first bending radius ρ .
 - b. Call CONSTANTS.
 - c. For each angle step $\Delta\theta$, call REFLECTION to calculate $R(\theta)$
 - i. Call either BRAGG on LAUE to calculate the reflectivities at each lamella.
 - d. Call INTEGRALS - calculate integrated reflectivity, FWHM, maximum reflectivity.
 4. Call TABLE - creates output table containing the input, parameters, and integrated values of reflectivity.
 5. Call OUTPUT - creates an output file called FOROXX.DAT where XX is determined by the polarization and the bending radius.

B. Choose Pi Polarization and repeat the calculations

III. Choose the next crystal thickness and repeat until all thicknesses have been considered.

5. INPUT FILE

5.A. Input Parameters

The input data file can be named anything. The program asks the user what file to read, and has a default input file called BCR.DAT. The file is read in open format and contains the following data. Reference can be made to the sample input file listed in Section 5.B for actual values. The values for the structure factors for Si reflections are listed in Section 5.C.

Parameters (all units are SI, except FO and FH)

1. Title of the calculation	(HEAD)
2. Poisson Ratio	(SIG)
3. Unit Volume	(VC)
4. Linear Absorption Coefficient	(MY)
5. Wavelength	(LAMB)
6. Bragg Angle (Radians)	(THB)
7. Asymmetry Angle (Radians)	(CHI)
8. Structure Factor	(FO)
9. Structure Factor for Reflection	(FH)
10. Number of different bending radii	(NR)
11. Bending Radii	(RHOO (I))
12. Number of different thicknesses	(NT)
13. Thickness of crystals	(THICK (I))
14. Geometry: Bragg = 1	(GEO)
Laue = 0 (Default)	
15. Output Control - If ABS (OUT) = 10	(OUT)
the output file FORON.DAT is	
created with $10 \leq N < 30$	
16. Number of data points (angles)	(POINTS)
in each reflectivity curve	
17. Theta range control:	(DISCON)
If DISCON = 1 the theta range	

is not constant
 DISCON = 0 the theta range
 is the same for all RHOO (I)
 18./19. Theta limits:
 If TLOW $\geq$ TUP the program (TLOW, TUP)
 calculates limits. Otherwise it
 uses the input values.

The input file is read by the following lines of the Main Program:

READ THE INPUT DATA:

```

READ(1,*) HEAD
READ(1,*) SIG, VC,MY,LAMB,THB,CHI
READ(1,*) FO,FH
READ(1,*) NR,(RHOD(I),I=1,NR)
READ(1,*) NT,(THICK(I),I=1,NT)
READ(1,*) GEO,OUT
READ(1,*) POINTS,DISCON
READ(1,*) TLOW,TUP
CLOSE(1,STATUS='KEEP')
```

5.B. SAMPLE INPUT FILE

X17> TYPE LAUE.DAT

```

'(\bf Laue: Si(111) / #MoK_{\alpha_1}# / T=.5 mm '
.282352 1.601650E-28 1461.6000 0.7093000E-10
0.113440 0.955393
(112.2300,0.58560000) (60.265,0.4082)
2 2.0 5.0
1 .525-3
0 10
51 0
400E-6 100E-6
```

5.C. STRUCTURE FACTORS FOR Si

FO: (112.2300, 0.5856)

(hkl)	(FH', FH'')
111	(60.265, 0.4082)
220	(67.470, 0.5460)
400	(56.361, 0.5452)
440	(43.087, 0.5075)
311	(43.7970, 0.3936)
331	(38.367, 0.3826)
333	(33.043, 0.3656)
422	(49.405, 0.5253)
555	(16.149, 0.3017)
444	(33.504, 0.4898)

6. OUTPUT FILE

6.A. There are two sets of output created by REFLECT. The first is created by the Main Program and the subroutine TABLE and consists of the input parameters as well as values of parameters calculated by the program. The resulting table of information is printed on the screen. A file can also be created for printing and storage. We have done this by assigning the default output device to be a file called TABLES.DAT. An example of the output created using the LAUE.DAT Input File given above is reproduced here. It consists of the following main sections:

1. Heading

2. Crystal and Reflection Input File Parameters

3. SIGMA POLARIZATION Parameters

a. PSIO, FO, PSIH, FH, G, KAPPA, Energy of radiation

b. Scaling factors from y-scale

c. Theoretical reflecting values in kinematic and dynamical limits, as well as the calculated extinction thickness

d. Reflection Parameters:

RHO, RMAX, FWHM, REFLECTING POWER, T_0 # of layers reflecting,
C, A

4. PI POLARIZATION Parameters (Same set of data as for Sigma)

SAMPLE OUTPUT: TABLES.DAT

X17> type tables.dat

LAUE LAUE LAUE

<\bf Laue: Si(111) / \$MoK_{\alpha_1}\$ / T=.5 mm

CHI = 54.740 THICKNESS OF THE CRYSTAL 0.5250 mm

F01	F02	FH1	FH2	LAMBDA
112.2300	0.5856000	60.26500	0.4082000	0.7093000E-10

UNIT VOLUME	MY(1/M)	SIGMA	BRAGG ANGLE (RAD./DEG.)
0.1601650E-27	1461.600	0.2823520	0.1134400 6.499633

SIGMA-POLARIZATION: PSIO : -0.3162155E-05 -0.1649967E-07 F0 in SI-units
PSIH : -0.1698006E-05 -0.1150130E-07 FH in SI-units

G = 0.1586607E-02 ABSORPTION TERM
KAPPA = 0.6773418E-02 SAME AS FH2/FH1
E(KEV) = 17.479 ENERGY OF THE RADIATION

Scaling factor: CONSTANT WAVELENGTH: ANGLE/Y = 6.416 microrad
CONSTANT ANGLE: WAVELENGTH/Y = 39.947 micro Angstrom
ENERGY/Y = 0.984 eV

R Ideal Imperfect Crystal = 0.359 mrad
Extinction Length = 7.527 micron
Width of Perfect Crystal = 13.603 microrad

RHO (m)	Rmax	(mrad)	FWHM (mAngstrom)	(eV)	Reflecting Power (mrad)
2.00	0.2726	0.5220	3.2501	80.09	0.1205
5.00	0.2087	0.1984	1.2354	30.44	0.0309

To (micron)	Layers	C	A
10.3879	51	1.138	1.380
25.9697	20	0.455	3.450

PI-POLARIZATION: PSIO : -0.3162155E-05 -0.1649967E-07 FO in SI-units
 PSIH : -0.1654491E-05 -0.1120656E-07 FH in SI-units

G = 0.1628337E-02 ABSORPTION TERM
 KAPPA = 0.6773417E-02 SAME AS FH2/FH1
 E(KEV)= 17.479 ENERGY OF THE RADIATION

Scaling factor: CONSTANT WAVELENGTH: ANGLE/Y = 6.252 microrad
 CONSTANT ANGLE: WAVELENGTH/Y = 38.923 micro Angstrom
 ENERGY/Y = 0.959 eV

R Ideal Imperfect Crystal= 0.341 mrad
 Extinction Length = 7.725 micron
 Width of Perfect Crystal = 13.254 microrad

RHO (m)	Rmax		FWHM		Reflecting
		(mrad)	(mAngstrom)	(eV)	Power (mrad)
2.00	0.2828	0.5159	3.2118	79.15	0.1187
5.00	0.2059	0.1886	1.1743	28.94	0.0287

To (micron)	Layers	C	A
10.1217	52	1.199	1.310
25.3042	21	0.480	3.276

6.B. Reflection Curves $R(\theta)$ - FILES FOROXX.DAT

The subroutine OUTPUT creates a data file which lists sequentially the reflectivity calculated as a function of Δy , i.e. the deviation from $y(0)$. The file is automatically named by the following scheme:

The file is called FOR $\%\%\%$.DAT where $\%\%\%$ = OXX. The value of XX = NT + L - 1 with

NT = 1 for SIGMA - POLARIZATION

NT = 2 for PI - POLARIZATION

and L is the value corresponding to the bending radius. The number of bending radii allowed is 1-10 so that $10 \leq XX \leq 29$.

An example of the file FOR020.DAT, for the above examples and the SIGMA polarization, is given below. The output consists of the following data:

1. Number of a Δy steps in $R(\theta)$
2. Reflectivity as a function of Δy , sequentially tabulated from θ min
3. THETA MIN - starting angle (μ rad)
4. DELTA THETA - step size (μ rad)
5. BENDING RADIUS RHO (m)
6. HEADING FOR DATA
7. CRYSTAL THICKNESS (m)

OUTPUT FILE SAMPLE: FOR020.DAT

```
type for020.dat
{\bf Laue: Si(111) / $Mok_{\alpha_1}$ / T=.5 mm
Si
2.4989373E-03 2.8405904E-03 3.2638442E-03 3.7996608E-03 4.4969250E-03
5.4374984E-03 6.7695519E-03 8.7910667E-03 1.2200598E-02 1.9083599E-02
3.9085783E-02 0.1697551 0.2827620 0.2553147 0.2736019
0.2570170 0.2577614 0.2604751 0.2392485 0.2590142
0.2337731 0.2508168 0.2342493 0.2368134 0.2372509
0.2193280 0.2371198 0.2135363 0.2299415 0.2132230
0.2176171 0.2162550 0.2046761 0.2168686 0.1966156
0.2112449 0.1947646 0.2004799 0.1977715 0.1886737
0.1993292 0.1808315 0.1956197 0.1782272 0.1828254
2.3410393E-02 1.0940689E-02 7.2114551E-03 5.1773190E-03 4.1505736E-03
3.4726085E-03
```

THE FIRST DATA IS THE NUMBER OF POINTS
NEXT THE REFLECTIVITY VALUES

```
THETA: (MICRORAD) -676.1526
THETA STEP: 15.41020
BENDING RADIUS 2.000000
X17>
```

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References:

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- [2] E. Erola, V. Eteläniemi, P. Suortti, P. Pattison, and W. Thomlinson, to be published in J. Appl. Cryst.
- [3] J.E. White, J. Appl. Phys. 21, 855(1950).
- [4] W.H. Zachariasen, "Theory of X-ray Diffraction in Crystals", John Wiley & Sons, New York (1945).
- [5] S.W. Wilkins, Acta Cryst. A34, 343 (1978).
- [6] A. Boeuf, S. Lagomarsino, S. Mazkedian, S. Melone, P. Puliti and F. Rustichelli, J. Appl. Cryst. 11, 442 (1978).

APPENDIX

REFLECT

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AUGUST 1989

MAINPROGRAM

REFLECTION POWER FOR BENT CRYSTAL IN LAUE AND BRAGG GEOMETRY

REFERENCES:

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- A. BOELF, et al., J. APPL. CRYST. 11 (1978) pp. 442-449
- E. ALBERTINI, et al., PHYS. STAT. SOL. (a)44 (1979) 127

*****SUBROUTINE DESCRIPTIONS*****

THE SUBROUTINES USED DO THE FOLLOWING CALCULATIONS OR TASKS:

CONSTANTS(K,KL,RHO)--CALCULATES CONSTANTS AND TERMS IN EQUATIONS WHICH DO NOT DEPEND ON THE DEVIATION ANGLE Y FROM THE BRAGG CONDITION BUT CAN BE FUNCTIONS OF RADIUS, THICKNESS, ETC.

LIMITS(RHO,NR,POL)--CALCULATES THE ANGULAR (Y) LIMITS FOR THE CALCULATIONS AND INTEGRATIONS

RCURVE(SIGMA,DISCON,ALA,PU,RT,T,NK,CC,AA)--CALCULATES REFLECTION POWER FOR ALL Y (THETA) VALUES FOR GIVEN THICKNESS, RADIUS, AND POLARIZATION

TABLE(ALA,PU,RT,NK,CC,AA)--OUTPUTS THE VALUES FOR REFLECTIVITY, PHASE, RHO AS WELL AS THE INPUT DATA IN TABULAR FORM

OUTPUT(NT)--PLACES REFLECTIVITY VALUES IN TABLES FOR USE BY PLOTTING ROUTINE OR DECONVOLUTION PROGRAM

INTEGRALS(POINTS,TA,PLG,RHAI,ALA,YLOW,DY)--CALCULATES THE INTEGRATED REFLECTIVITY (ALL THETAS), RHAS, AND PHAS

RFL(RH,YY,N)--CALCULATES REFLECTIVITY FOR A SINGLE VALUE OF Y. IT SUMS OVER ALL LAYERS OF THE CRYSTAL, USING THE INDIVIDUAL LAYER REFLECTIVITIES CALCULATED BY BRAGG OR LAUE

BRAGG OR LAUE(R,T,Y)--CALCULATES REFLECTIVITY OF A SINGLE LAYER OF THE CRYSTAL FOR GIVEN VALUE OF Y (THETA)

IMPLICIT LOGICAL(A-Z)

INTEGER NR,1,DEO,IT,OUT,POINTS,NK(10)

REAL RHVALUES(10,500),RHO(10),THICK(10),ALA(10),PU(10),RH(10)

REAL T(10),CC(10),AA(10),DISCON

REAL CHI,RY,LAMB,KH,KP,VC,SIG,THB,PHHO,PA,SIGMA,PII,TLOW,TUP

COMPLEX FO,PH

CHARACTER *70 HEAD

CHARACTER *20 INFILE

COMMON/INPUT1/FO,PH,VC,RY,SIG

COMMON/INPUT2/LAMB,THB,CHI,PA

COMMON/VALUES/FAC,PHAS,NLAYERS,RY

COMMON/LAUEBRAGG/O,BA,SABA,PHBA,PHAS,II,ZIS,RC1,A

COMMON/SCALING/RC4,RCAL,RCAS

COMMON/VALUES/YO,C,AG

COMMON/VALUES/DEO

COMMON/VALUES/HEAD

COMMON/VALUES/RHO,NR,OUT

COMMON/INPUT10/YLOW,YUP,DY

COMMON/INPUT11/POINTS,RHVALUES

COMMON/THETA12/TLOW,TUP

COMMON/AREA:1-2 INPUT DATA, CONSTANTS

3 ABSORPTION FACTORS, NUMBER OF LAYERS

4 USE IN SUBPROGRAMS LAUE AND BRAGG AND LIMITS

5 SCALING FACTORS, Y --> ANGLE, LAMBDA, ENERGY

6 SELECT LAUE OR BRAGG

7-11 OUTPUT DATA

READ THE INPUT DATA FROM INFILE

READ BY FREE FORMAT

TYPE = 'WHAT INPUT FILE? SCR.DAT = CR.'

ACCEPT 11, INFILE

FORMAT (A20)

IF (INFILE.EQ.' ') INFILE = 'SCR.DAT'

OPEN(1,NAME=INFILE,TYPE = 'OLD')

PARAMETERS:

1. TITLE OF THE CALCULATIONS (HEAD)
2. POISSON RATIO (SIG)
3. UNIT VOLUME (VC)
4. LINEAR ABS. FACTOR (RY)
5. WAVELENGTH (LAMB)
6. BRAGG ANGLE (RAD) (THB)
7. DEVIATION FROM SYMMETRICAL REFLECTION (RAD) (CHI)
8. STRUCTURE FACTOR (FO)
9. STRUCTURE FACTOR FOR REFLECTION (PH)
10. NUMBER OF BENDING RADII (NR)
11. BENDING RADIUS (RHO(1))
12. NUMBER OF THICKNESSES (NT)
13. THICKNESS OF THE CRYSTAL (THICK(1))
14. GEOMETRY: BRAGG = 1 (DEO)
- LAUE = 0 (DEFAULT)
15. OUTPUT NUMBER IF ABS(OUT) = 10 YOU SET THE RHVALUES IN FILES FORN.DAT (10XN30)
16. NUMBER OF DATPOINTS (POINTS)
17. DISCON = 1 THETAMIN, THETAMAX ARE NOT CONSTANT
- 0 SAME THETA RANGE FOR ALL RHO(1)
- 18/19. YOUR OWN LIMITS TLOW,TUP
- IF TLOW = 0 TUP FIND THE PROGRAM LIMITS YLOW AND YUP
- YLOW AND YUP ARE IN PRINCIPAL THE SAME AS THETALOW AND THETAP

ALL THE VALUES ARE IN SI-UNIT
EXCEPT STRUCTURE FACTORS IN ELECTRON UNITS

NOTE:

7. CHI=0, SYMMETRICAL REFLECTION
11. DEFAULT: MINIMUM RHO AT FIRST

READ THE INPUT DATA:

```
READ(1,*) HEAD
READ(1,*) SIG,VC,RY,LAMB,THB,CHI
READ(1,*) FO,PH
READ(1,*) NR,(RHO(1),I=1,NR)
READ(1,*) NT,(THICK(1),I=1,NT)
READ(1,*) DEO,OUT
READ(1,*) POINTS,DISCON
READ(1,*) TLOW,TUP
CLOSE(1,STATUS='KEEP')
```

DETERMINE THE GEOMETRY

LAUE GEOMETRY: CHI > 0, SYMMETRICAL LAUE REFLECTION IS IMPOSSIBLE

IF (DEO.EQ.1) THEN

WRITE(6,95)

ELSE:

IF (CHI.LT.0.01) THEN

WRITE(6,96)

STOP

ELSE

WRITE(6,96)

END IF

END IF

POLARIZATION FACTORS:

SIGMA = 1.

PII = ABS(COS(2.*THB))

LIMITS YLOW AND YUP CHANGE LIKE 1/RHO

FIRST CALCULATION SETS LIMITS USING MIN RHO

```
RHO = RHO(1)
DO 10 I=1,NR
RHO = MIN(RHO,RHO(I))
CONTINUE
```

PROGRAM STARTS WITH FIRST THICKNESS AND CALCULATES ALL QUANTITIES LOOPING IN POLARIZATION AND RADIUS

SELECT THICKNESS

DO 50 IT=1,NT

PA = THICK(IT)

WRITE HEADINGS, ANGLE CHI AND THE THICKNESS OF THE CRYSTAL

WRITE(6,99) HEAD,CHI=57.29578,PA/1.E-3

SIGMA-POLARIZATION

CALL CONSTANTS(SIGMA,0.,RHO)

CALL LIMITS(RHO,NR,SIGMA)

CALL RCURVE(SIGMA,DISCON,ALA,PU,RT,T,NK,CC,AA)

CALL TABLE (ALA,PU,RT,T,NK,CC,AA)

IF (OUT.EQ.10) CALL OUTPUT (1)

PII-POLARIZATION

IF (PII.LT.1E-2) THEN

WRITE(6,*) 'NO PI-POLARIZATION, COS(2*THETA) < 1E-2'

GO TO 50

END IF

CALL CONSTANTS(PII,0.,RHO)

CALL LIMITS(RHO,NR,PII)

CALL RCURVE(PII,DISCON,ALA,PU,RT,T,NK,CC,AA)

CALL TABLE (ALA,PU,RT,T,NK,CC,AA)

IF (OUT.EQ.10) CALL OUTPUT (2)

CONTINUE

```
95 FORMAT(1X,31'BRAGG',10X1//)
96 FORMAT(1X,31'LAUE',10X1//)
99 FORMAT(1X,31' SYMMETRICAL LAUE IS IMPOSSIBLE',10X1//)
99 FORMAT(1X,470,11X,31,CHI = '57.3,2X,
6 'THICKNESS OF THE CRYSTAL',F9.4,' nm//)
```

STOP

END

SUBROUTINE CONSTANTS(K,KL,RHO)

CALCULATE CONSTANTS THAT ARE NOT A FUNCTION OF ANGLE Y
THEY MAY DEPEND ON THE BENDING RADIUS

RC4 - SCALING FACTOR BETWEEN Y AND ANGLE THETA

RCAL - CONVERTS Y TO WAVELENGTH

RCAS - CONVERTS Y TO ENERGY

NLAYERS - NUMBER OF LAYERS IN THE CRYSTAL

TO - THICKNESS OF ONE LAYER

PHAS = EXP(-RY*TO)/FAC EFFECTIVELY FAC=PHAS FOR LAUE CASE

FAC = EXP(-RY*TO) ABSORPTION IN ONE LAYER AFTER REFLECT

KAPPA=SIGMA*(PH)/REAL(PH)

PHO,PHK - FO AND PH IN SI-UNIT

S - SMO WHEN NO ABSORPTION OR SYMMETRICAL REFLECTION (CHI=0)

YHAI - ESTIMATE OF THE ANGLE WHERE REFLECTIVITY IS A MAXIMUM

LET - ESTIMATION LENGTH

PERFECTC-TOTAL REFLECTION AREA OF THE PERFECT CRYSTAL

LAUE GEOMETRY: TWO POSSIBILITIES

1. FOCUSING OR -GEOMETRY: THE OUTPUT ANGLE IS THB-CHI
2. DIVERGING OR -GEOMETRY: OUTPUT ANGLE IS CHI-THB WHERE THB IS NEGATIVE

IMPLICIT LOGICAL(A-Z)


```

      ZR=PSHRA+BSHR*Y      : ZACHARIASEN (3.181)
      Z=CMPLX(ZR,ZI)
      C1=Q1**2
      C2=CBRT(C1)          : ZACHARIASEN (3.182), WILKINS (3)
      V=REAL(C2)           : ZACHARIASEN (3.182)
      W=AIMAG(C2)           : "-"
      R1=CABS(C1)          : ZACHARIASEN (3.139)
      R2=IR**2+ZIS
      R3=R1+R2
      R4=R1-R2
      R5=4*W
      R7=4*V
      RB=(SIN(R7))**2
      CS=CONJG(ZI)*C2
C OVERFLOW WHEN ABS(R5) > 44 (OR EXP(2*ABS(R5)) TOO BIG)
C YOU MUST CHECK THE LIMIT IN YOUR OWN COMPUTER
C OVERFLOW HAPPENS WHEN THE CRYSTAL IS ALMOST FLAT AND
C -1 < Y < 1 (THAT IS TOTAL REFLECTION RANGE)

```

```

      IF (R5,ST,44.) THEN
        R = 3*PSHRA/(R3 + 2.*REAL(-C3))
        T = R1*EXP(1.05*RC1) - 2.*R5 / (R3 + 2.*REAL(-C3))
        RETURN
      ELSE IF (R5,LT,-44.) THEN
        R = 3*PSHRA/(R3 - 2.*REAL(-C3))
        T = R1*EXP(1.05*RC1)+2.*R5 / (R3 - 2.*REAL(-C3))
        RETURN
      END IF

```

```

      RB=ABS(DBSINH(R5))**2
      R = R1 + R3+R4 - R4*RB + REAL(-C3)*DBSINH(2*R5)
      S = AIMAG(C3)*SIN(2*R7)
      R=3*PSHRA*(RB+R4)/D      : BOEUF (13), ZACH. (3.139), WILK (2)
      T=R1*RC1/D              : BOEUF (16), WILK (15), (17)

```

```

      RETURN
      END

```

SUBROUTINE LAUE(R,T,Y)

```

*****
SAVE AS SUBPROGRAM BRAGG BUT IN THE LAUE-GEOMETRY
SELECT THE GEOMETRY BRAGG/LAUE ONLY ONCE IN SUBPROGRAM RFL
OTHERWISE, IT MUST BE SELECTED N TIMES (N=NUMBER OF LAYERS)

```

```

HERE WE USE THE ASYMMETRY FACTOR OF WILKINS IN OUR RC1
DIFFERENCES IN THE TRANSMISSION FACTOR BETWEEN WILKINS'S S-VALUE
AND OUR S-VALUE IS THE SIGN OF THE LAST TWO TERMS
REFLECTED POWER = PH/PO = (1H/10)/BA      BOEUF (15)

```

```

SYMMETRICAL LAUE REFLECTION IS NOT POSSIBLE SO THAT
USUALLY ABS(R5) < 44.
THERE MAY BE REFLECTIONS WHERE THAT IS NOT TRUE

```

```

      REAL R,T,Y,A,BA,BSHR,PSHRA,PSHRS,ZI,ZIS,ZR,RC1
      COMPLEX C1,C2,C3,0.1
      DOUBLE PRECISION RC,R4,R5,D
      COMMON/LAUEBRAGG/D,BA,BSHR,PSHRA,PSHRS,ZI,ZIS,RC1,A

```

```

      ZR=PSHRA+BSHR*Y      : ZACHARIASEN (3.181)
      Z=CMPLX(ZR,ZI)
      C1=Q1**2
      C2=CBRT(C1)          : ZACHARIASEN (3.182), WILKINS (3)
      V=REAL(C2)           : ZACHARIASEN (3.182)
      W=AIMAG(C2)           : "-"
      R1=CABS(C1)          : ZACHARIASEN (3.139)
      R2=IR**2+ZIS
      R3=R1+R2
      R4=R1-R2
      R5=4*W
      R7=4*V
      RB=(SIN(R7))**2
      CS=CONJG(ZI)*C2
      D=R1+R3+R4-R4*RB+REAL(-C3)*DBSINH(2*R5)-AIMAG(C3)*SIN(2*R7)
      R=3*PSHRA*(RB+R4)/D
      T=D/R1*RC1

```

```

      RETURN
      END

```

SUBROUTINE LIMITS(RND,NR,POL)

```

*****
INTERIOR REQ,NLAYERS,POINTS
REAL PA,CHI,LAMB,POL,YH

```

```

COMMON/INPUT2/LAMB,THI,CHI,PA
COMMON/BLUES/FAC,FABS,NLAYERS,YH
COMMON/SCALINES/RC4,REAL
COMMON/BLUES/REQ
COMMON/INPUT10/YLOW,YUP,DY
COMMON/INPUT11/POINTS,VALUES
COMMON/THETA12/TLOW,TUP

```

```

FIND THE MAXIMUM R AND THEN THE LIMITS WHERE R < RMAX/100
FIND THE MAXIMUM POINT YH = (1-B)/(S+IN(2THI)+ABS(REAL(PSD)))
THIS IS CALCULATED IN CONSTANTS

```

```

POL= POLARIZATION FACTOR
YH = ESTIMATE OF THE ANGLE WHERE R IS THE MAXIMUM(BRAGG)
YLOW= LOWER LIMIT OF THE ANGLE RANGE
YUP = UPPER LIMIT
DY = STEP = (YLOW-YUP)/PP.4
RMAX= MAXIMUM OF THE R
RLOW= LIMIT = RMAX/100
YAREA= ESTIMATE OF THE RANGE = YH*2 - YH*IN

```

```

LAUE: THE WIDTH OF THE REFLECTION CURVE IS
NUMBER OF THE LAYERS = AC = NLAYERS*PI/2 (AC SEE SUBP. RFL)

```

```

C THE LIMITS FOR P1-POLARIZATION ARE THE SAME AS IN
C SIGMA-POL DIVIDED BY PARAMETER POL

```

```

      IF (POL,LT,1.) THEN
        YLOW = YLOW/POL
        YUP = YUP/POL
        DY = (YUP - YLOW)/(POINTS-1)
        RETURN
      END IF

```

```

C IF YOU USE YOUR OWN LIMITS

```

```

      IF (TLOW,LT,TUP) THEN
        YLOW = TLOW/RC4
        YUP = TUP/RC4
        DY = (YUP-YLOW)/(POINTS-1)
        RETURN
      END IF

```

```

C FIND THE LIMITS WHERE R = RMAX/100
C FOR THE FLAT CRYSTAL BRAGG CASE, RND >> 1
C THEN, R = 1 AND ONE OBTAINS THE DARWIN CURVE.
C PL = WIDTH OF THE CURVE FROM GEOMETRICAL ESTIMATE

```

```

      IF (REQ,EQ,1) THEN
        PL = PA/(RND*TAN(THI+CHI))
        YAREA= PL/RC4
        YH=2-ABS(YH)/RC4
        YDS = YH*2
        IF (YDS,EQ,0) YDS = 2.

```

```

      IF (RND,ST,10.) THEN      : DARWIN CURVE
        RMAX = 1.
        DO 20 I=1,N
          END IF
      ELSE                        : LAUE
        YAREA= NLAYERS*2.0
        YH= -YAREA/2.
        YDS = YH*2/6.
        END IF

```

```

C LAUE: REFLECTION CURVE IS LIKE A "BOX"
C MAXIMUM IS OFTEN THE SAME AS THE FIRST VALUE --> S

```

```

      RMAX=0.0

```

```

      DO 30 I=1,N

```

```

        Y1=YH+YDS
        Y2=YH+YDS
        DYT=(Y2-Y1)/3
        Y=Y1
        S = 0.

```

```

        DO 20 J=1,6
          CALL RFL(R,Y,IN)
          IF (R,GE,RMAX) THEN
            YH=Y
            RMAX=R
          END IF
          Y=Y+DYT
          S = S + R
        20 CONTINUE

```

```

        SH=ABS(S/6.-RMAX)
        IF (S,LT,5.E-3).AND. (SSD,EQ,0) GO TO 40
        YDS=YDS/1.5

```

```

C 30 CONTINUE
C ANGLES YUP AND YLOW
C USUALLY RMAX > 0.1 AND R/100 > 1.E-3

```

```

      40 RLOW = RMAX/RMAX/100.,1E-3)

```

```

C YUP NEAR POINT Y = 0
C CRUDE ESTIMATE

```

```

      Y = 22.
      DYT = 10.
      45 CALL RFL(R,Y,IN)
      IF (R,ST,RLOW) THEN
        Y=Y+DYT
        DO 45
      END IF

```

```

C FIND POINT YUP: Y-DYT <= RLOW < Y
C DY IS APPROXIMATION OF THE STEP IN Y-SPACE
C (SEE THE END OF THIS SUBPROGRAM)

```

```

      DY = (Y + YAREA)/POINTS
      N = INT(DYT/DY)

```

```

      DO 60 I=1,N
        Y = Y - DY
        CALL RFL(R,Y,IN)
        IF (R,ST,RLOW) GO TO 70
      60 CONTINUE
      YUP = Y + DY

```

```

C FIND YLOW: YUP IS APPROX ZERO AND YAREA IS APPROX (YUP - YLOW)
C YH = -YAREA

```

```

C FIND THE POINT WHERE R > RLOW
C FIRST CHECK IF THE APPROX Y = -YAREA IS TOO BIG (BRAGG)

```

```

      75 CALL RFL(R,Y,IN)
      IF (R,LT,RLOW) THEN
        Y=Y/1.3
        GO TO 75
      END IF

```

```

C DYT = Y/5.
C Y = Y - DYT
C CALL RFL(R,Y,IN)
C IF (R,ST,RLOW) GO TO 80

```

```

C Y < YLOW < Y+DYT

```

```

      N = INT(DYT/DY)
      DO 90 I=1,N
        Y=Y+DY
        CALL RFL(R,Y,IN)
        IF (R,ST,RLOW) GO TO 100
      90 CONTINUE

```

```

100 YLOW = Y - DY
      DY = (YUP - YLOW)/(POINTS-1)      ! STEP IN Y-SPACE

      RETURN
      END

SUBROUTINE RFLVZ( POL,DISCON,ALA,PUO,RAJA,T,NK,CC,AA)
*****
CALCULATE THE REFLECTION POWER BETWEEN ANGLES YLOW AND YUP

REAL RVALUES - REFLECTING POWER AT ANGLE Y
ALA - INTEGRATED INTENSITY
PUO = PNOI (APPROX)
RAJA - MAXIMUM OF THE RVALUES
NK - NUMBER OF THE LAYERS (NOT ALWAYS THE SAME AS THE THICKNESS)
T - THICKNESS OF ONE LAYER ! BY COMMON AREA
POL - POLARIZATION FACTOR

REAL RVALUES(10,500),RHOD(10),APU(500),ALA(10),
PUO(10),RAJA(10),T(10),CC(10),AA(10),RAJA(10)
INTEGER NR,NK(10),POINTS,I
REAL TO,S,P,R,N,KK,Y,YLOW,YUP,DY,RHO,C,RC4,AG,POL,DISCON

COMMON/SCALINES/RC4,RCAL,RC4E
COMMON/ALUES/TO,C,AG
COMMON/ALUES/RHOD,NR,OUT
COMMON/INPUTIO/YLOW,YUP,DY
COMMON/INPUT11/POINTS,RVALUES

C
      DYT = DY
      YLN = YLOW - DYT      ! Y = YMIN + (I-1)*DYT + YLN + I*DYT

      DO 100 L=1,NR
        RHO = RHOD(L)
        CALL CONSTANTS (POL,1.,RHO) ! DEPENDS ON THE BENDING RADIUS

        T(L) = TO*1.E4      ! COMMON/ALUES
        CC(L) = C
        AA(L) = AG
        IF (L.NE.1) THEN
          YMIN = YLOW+(1-DISCON = DISCON+RHO(L)/RHOD(1))*1.5
          DYT = (YUP-YMIN)/(POINTS-1)
          YLN = YMIN - DYT
        END IF

C
      DO 10 I=1,POINTS
        APU(I) = 0.0
10      CONTINUE

C
      IN = 0
      DO 20 I=POINTS,1,-1
        Y = YLN + I*DYT
        CALL RFL(R,T,N)
        APU(I) = R
        IN = MAX(IN,N)
        IF (R.LT.1E-3).AND.(I.LT.POINTS*0.75) GO TO 25
20      CONTINUE

C THE EFFECTIVE THICKNESS OF THE CRYSTAL
C IN LAUE IS THE SAME AS THE GIVEN THICKNESS OF THE CRYSTAL
C
25      NK (L) = IN

C CALCULATE THE INTEGRATED REFLECTIVITY, PNOI, AND MAX R
      CALL INTEGRALS (POINTS,APU,P,R,S,YLOW,DYT)

      ALA(L) = S*RC4*1E3      ! Y-SPACE TO PNOI
      PUO(L) = P*RC4*1E3
      RAJA(L) = R

      DO 30 I=1,POINTS
        RVALUES(L,I) = APU(I)
30      CONTINUE

100      CONTINUE      ! NEXT RHO

      RETURN
      END

SUBROUTINE INTEGRALS (POINTS,TA,PUO,RAJA,ALA,YLOW,DY)
*****
CALCULATE THE REFLECTING POWER, FIND MAXIMUM AND THE
PNOI (APPROX)

REAL TA(500)
REAL RAJA,RAJA,LU1,LU2,ARVO1,ARVO2,PUO,DY,YLOW,ALA,BN
INTEGER POINTS

REFLECTING POWER = SUM RVALUES(I) * DELTA THETA
CALCULATE THE AREA AND MAX R
      BN = 0.0      ! SUM RVALUES(I)
      RAJA = 0.0
      DO 10 I=1,POINTS
        BN = BN + TA(I)
        RAJA = MAX(RAJA,TA(I)) ! MAXIMUM
10      CONTINUE
      RAJA = RAJA/2.0
      IF (RAJA.EQ.0.) RETURN

      FIND THE POINT WHERE RVALUES = MAXIMUM/2 (LEFT SIDE)

      I = 1
      I = I+1
      IF (TA(I).LT.RAJA) GO TO 15

```

```

      LINEAR APPROXIMATION BETWEEN TWO POINTS

      K=1
      LU1=RAJA - TA(K)
      LU2=TA(I) - TA(K)
      ARVO1=YLOW + K*DY + (LU1/LU2)*DY

      FIND THE POINT WHERE RVALUES = MAXIMUM/2 (RIGHT SIDE)

      I=POINTS
      I=I-1
      IF (TA(I).LT.RAJA) GO TO 20

      K=1
      LU1=RAJA - TA(I)
      LU2=TA(I) - TA(K)
      ARVO2=YLOW + I*DY - (LU1/LU2)*DY

      DEFINE THE PNOI AT THE VALUES RAJA/2
      PUO = (ARVO2-ARVO1)      ! PNOI
      ALA = BN*DY      ! AREA

      RETURN
      END

SUBROUTINE OUTPUT (NT)
*****
PUT THE RVALUES IN FILE FORXXX.DAT, WHERE XXX IS THE SAME
AS THE SCALIER VALUE 10<=XXX<=20
THE TABLE CAN BE ACCESSSED FOR PLOTTING OR THE DECONVOLUTION
PROGRAM
IF ULDS = -10 THEN NO OUTPUT IS CALLED

REAL RVALUES(10,500),RHOD(10)
REAL YLOW,DY,YUP,RC4
INTEGER OUT,NT,NR,L,POINTS
CHARACTER*70 HEAD

COMMON/SCALINES/RC4,RCAL,RC4E
COMMON/ALUES/HEAD
COMMON/ALUES/RHOD,NR,OUT
COMMON/INPUTIO/YLOW,YUP,DY
COMMON/INPUT11/POINTS,RVALUES

      DO 10 L=1,NR

        WRITE (10+NT-L-1,*)      HEAD
        WRITE (10+NT-L-1,*)      POINTS
        WRITE (10+NT-L-1,*)      (RVALUES(L,I),I=1,POINTS)
        WRITE (10+NT-L-1,*)      'THETA: (MICRORAD) ',YLOW+RC4*1E3
        WRITE (10+NT-L-1,*)      'THETA STEP: ',DY*RC4*1E3
        WRITE (10+NT-L-1,*)      'BENDING RADIUS ',RHOD(L)

10      CONTINUE

1      FORMAT(//5X,' THE FIRST DATA IS THE NUMBER OF POINTS',/,
        & 5X,' NEXT THE REFLECTIVITY VALUES',/)

      RETURN
      END

SUBROUTINE TABLE ( ALA,PU,RA,T,NK,CC,AA)
*****
REAL ALA(10),PU(10),RA(10),RHOD(10),T(10),CC(10),AA(10)
REAL RC4,RCAL,RC4E
INTEGER I,NR,NK(10)
CHARACTER*3 JA

COMMON/SCALINES/RC4,RCAL,RC4E
COMMON/ALUES/RHOD,NR,OUT

      WRITE(6,30)

      DO I=1,NR
        WRITE(6,35) RHOD(I),RA(I),PU(I),PU(I)+RCAL*1E-6/RC4,
        & PU(I)+RC4E*1E-3/RC4,ALA(I)
        IDDDD
      CONTINUE

      WRITE(6,31)

      DO I=1,NR
        WRITE(6,36) T(I),NK(I),CC(I),AA(I)
        IDDDD
      CONTINUE

30      FORMAT(//5X,' PNOI (a) ',5X,' PNOI ',10X,' PNOI ',10X,
        & ' Reflecting ',7.2F3,' (arcdeg) ',2X,' (arcdeg) ',2X,' (a.u) ',4X,
        & ' Power (arcdeg) ')

31      FORMAT(//5X,' Ta (micron) ',5X,' Layers ',8X,' C ',11X,' A ')
33      FORMAT(//3X,P7.2,X3,P7.4,X3,P7.2,X3,P8.4)
34      FORMAT(//7X,P8.4,X3,P7.2,X3,P8.3)

C
      WRITE(6,39)
      99      FORMAT(1X,////)

      RETURN
      END

```