Interdepartmental letterhead

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M E M O R A N D U M

To: Distribution

From: M. Glinsky MEG

Subject: Revised ROCKIT Documentation

Attached is the most recent documentation for the program ROCKIT, a program to calculate crystal rocking curves. Several new crystal structures have been added and a version of the program called CROCKIT has been compiled to run on the CRAY.

MG:lr

Distribution:

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X-ray Measurements Group
R-Project Group

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National Laboratory

ROCKIT USER'S GUIDE (Version 1.1)

Description of Program

ROCKIT is a program to calculate single and double crystal rocking curves -- diffraction of X-rays by crystals. Both transmission and reflection of the X-rays by the crystal can be calculated. The thickness of the crystals can be varied, as well as the angle between the crystal plane and the surface of the crystal. For two crystals, the transmission/reflection of the second crystal as a function of crystal angle is calculated along with the energy dispersion. All parameters of the two crystals are independent (i.e., type of crystal, crystal plane, photons transmitted or reflected, angle of crystal plane with respect to the surface, and the thickness of the crystal). Both parallel and anti-parallel orientation of the crystals are allowed. In addition, a card image file can be created that can be used as an input deck for the program COG to draw the crystal structure with the diffraction plane indicated.

The crystal structures are kept in a file in the ROCKIT library called XTAL. This file can be added to or modified by the user. If a file called XTAL is in the user's working file space, the program will use those crystal structures, not the ones in the library. The list of structures in the library has been compiled from various sources {1,2,3}.

The atomic structure factors for energies between 100 and 2000 eV are taken from the Henke tables {4}. The sin(theta)/lamda dependence of the real part of the form factor is taken from the ENDL tables {5}. The Cromer-Liberman relativistic correction is then made {6}. For energies above 2 keV the structure factors are calculated from the ENDL tables. In this energy region, it should be noted that no attempt is made to estimate the anomalous dispersion contribution to the real part of the form factor, hence the real part of the form factors will be in error close to an absorption edge. The program does warn the user when the energy is within 5% of an absorption edge of one of the elements in the crystal.

The expressions for the crystal reflection and transmission of the X-rays are taken from the book by Zachariasen {7}. In this derivation, a infinite flat slab of material is assumed with a complex dielectric constant and finite thickness. Two wave components are allowed in the crystal -- the incident and the diffracted wave. Appropriate boundary conditions are then applied to obtain the solution for case of the reflected and the transmitted wave.

Input Deck

A. Order of Deck

XTAL 1	(**required**)
PLANE 1	(**required**)
XTAL 2	(optional)
PLANE 2	(optional)
INPUT	(**required**)
OUTPUT	(**required**)
COGWRT	(optional)

(note: all fields separated by blanks)

B. Description of Cards

Field	Name	Description
==> XTAL Card <==		
1	xnbr	Number of crystal (1 or 2). Integer.
2	nmxtal	Name of crystal QUARTZ CALCITE SAPH = Sapphire (Rhombohedral) KAP SI = Silicon GE = Germanium MICA = Muscovite BERYL LIF = Lithium flouride CLNCLR = Clinochlore
3	typdff	Type of diffraction BRAGG = Reflection LAUE = Transmission (see figure 1)
4	thick	Thickness of crystal (in mm). Real.
5	errthk	Error in thickness (in mm). Real.
==>PLANE Card<==		
1	xnbr	Number of crystal (1 or 2). Integer.
2	h	First Miller index of plane. Integer.
3	k	Second Miller index. Integer.
4	l	Third Miller index. Integer.
5	alpha	Angle between crystal plane and surface of crystal (in degrees) (see figure 1). Real.

==>INPUT Card<==

1	energy	Energy of incomming photon (keV). Real.
2	crygeo	Crystal geometry ==> with one crystal ROTATE = vary angle of crystal LAUE = vary energy of photon ==> with two crystals PLUS = anti-parallel position MINUS = parallel position (see figure 2)

==>OUTPUT Card<==

1	xmin	==> if crygeo ≠ LAUE Minimum theta to output (in radians) referenced with respect to the bragg angle. ==> if crygeo = LAUE Minimum d(lamda)/lamda to output. Real.
2	xmax	Maximum theta or d(lamda)/lamda to output. Real.
3	numdt	Number of points to output (1<numx<2049). Integer.

==>COGWRT Card<==

1	thtnot	First theta of viewer (in degrees). Real.
2	phinot	First phi of viewer (in degrees). Real.
3	numtht	Number of theta to draw. Integer.
4	numphi	Number of phi to draw. Integer.

(Note: The viewer will be rotated 360 degrees starting at phinot, theta held constant. Then, the viewer will be rotated 360 degrees starting at thtnot, phi held constant. Angles phi and theta are defined in figure 3.)

Output Decks

Name of file	Contents of file
LROCKIT	Listing containing input parameters, crystal structures, bragg angles, two-d spacings, form factors, integrated reflectivities, and dispersion of the two crystal system.
SCURV1N	I/Io (Normal polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #1 (SOCKITTOME compatible card image format)
SCURV1P	I/Io (Parallel polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #1 (SOCKITTOME compatible card image format)
SCURV1T	I/Io (No polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #1 (SOCKITTOME compatible card image format)
SCURV2N	I/Io (Normal polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #2 (SOCKITTOME compatible card image format)
SCURV2P	I/Io (Parallel polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #2 (SOCKITTOME compatible card image format)
SCURV2T	I/Io (No polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #2 (SOCKITTOME compatible card image format)
DCURVN	I/Io (Normal polarization) as a function of angle (in rad) for crystal #2 off of crystal #1 (SOCKITTOME compatible card image format)
DCURVP	I/Io (Parallel polarization) as a function of angle (in rad) for crystal #2 off of crystal #1 (SOCKITTOME compatible card image format)
DCURVT	I/Io (No polarization) as a function of angle (in rad) for crystal #2 off of crystal #1 (SOCKITTOME compatible card image format)
COGX1	COG input deck to draw crystal structure for crystal #1
COGX2	COG input deck to draw crystal structure for crystal #2

Crystal Structure File Format

A. Order of deck

XTAL
UNIT
ATOM
ATOM
.
.
XTAL
UNIT
ATOM
.
.

B. Description of Cards

Field	Name	Description
==>XTAL Card<==		
1	nmxtal	Name of Crystal (Up to 8 characters)
==>UNIT Card<==		
1	**a**	length of first primative vector
2	**b**	Length of second primative vector
3	**c**	Length of third primative vector
4	alpha	Angle between **b**-**c** (in Degrees)
5	beta	Angle between **a**-**c** (in Degrees)
6	gamma	Angle between **a**-**b** (in Degrees)
==>ATOM Card<==	(200 allowed per crystal)	
1	z	Number of protons in atom
2	xatom	**a** coordinate of atom
3	yatom	**b** coordinate of atom
4	zatom	**c** coordinate of atom

Program Operation

To run ROCKIT type:

ROCKIT nameinputfile / t v

The only thing necessary to do before running the program is to access the ROCKIT library file. This file currently resides on mass storage as .886450:ROCKIT (CDC 7600) and .886450:CROCKIT (CRAY).

The program will extract three files from the library if they do not exist on the users account.

HXSEC	Henke cross-section data file
XSEC	ENDL cross-section data file
XTAL	Crystal structure data file

The time required to run the program is approximately one to three minutes depending on the information required and the complexity of the crystal structure.

To generate packing diagrams of the crystal structures from the COGX1 and COGX2 files the program COG must be executed on one of the CRAY-machines. To do this type the command:

COG K nameinputfile / t v

On program completion a DLI file will exist on the user's account and will contain the packing diagrams. The computer time required to draw these pictures is approximately 1/40 of a minute for each atom drawn.

The program COG can also generate DICOMED shaded color pictures of the crystal structures. The computer time required to do this is at least 1/25 of a minute per atom. The user will need to make minor modifications to the COG input decks. Intructions on how to do this can be obtained from Ed Lent.

References

1. Wyckoff, R. W. G.: Crystal Structures, Wiley New York, 1968.

2. Bertin, E. P.: Principles and Practice of X-Ray Spectrometric Analysis, Plenum New York, 1975.

3. Burek, A. J.: Crystals for Astronomical X-Ray Spectroscopy, LA-UR-75-1593, 1975.

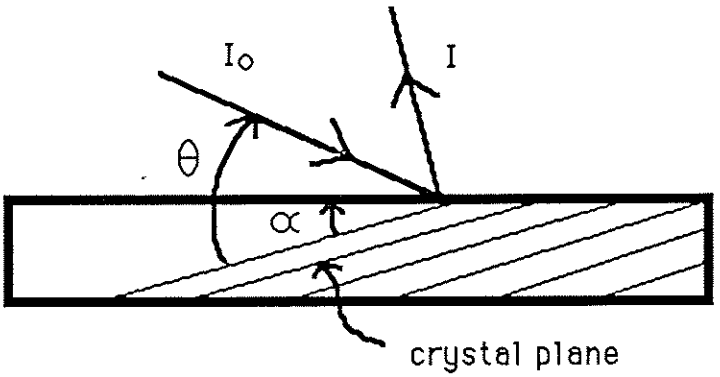
4. Henke, B. L., Lee, P., Tanaka, T. J., Shimabukuro, R. L., Fujikawa, B. K.: Atomic Data and Nuclear Data Tables **27**, 1-144 (1982).

5. Plechaty, E. F., Cullen, D. E., Howerton, R. J.: Tables and Graphs of Photon-Interaction Cross Sections From 0.1 keV to 100 Mev Derived From the LLL Evaluated-Nuclear-Data Library, UCRL-50400, Vol. 6, Rev. 3 (1981).

6. Cromer, D. T., Liberman, D.: J. Chem. Phys. **53**, 1891 (1970).

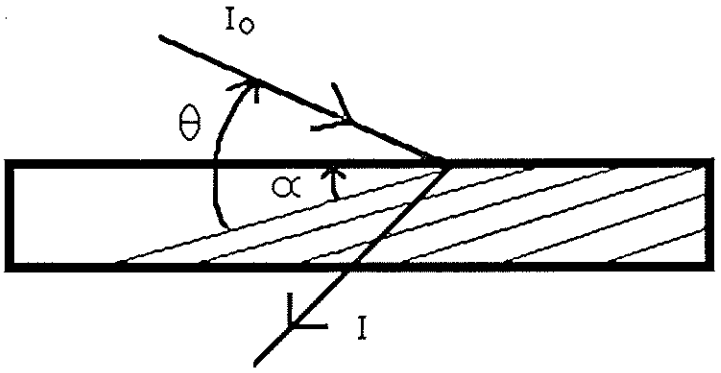
7. Zachariasen, W. H.: Theory of X-Ray Diffraction in Crystals, Wiley New York, 1945, pp. 82-155.

Figure 1a.



Type of diffraction = BRAGG = reflection

Figure 1b.



Type of diffraction = LAUE = transmission

Figure 2a.

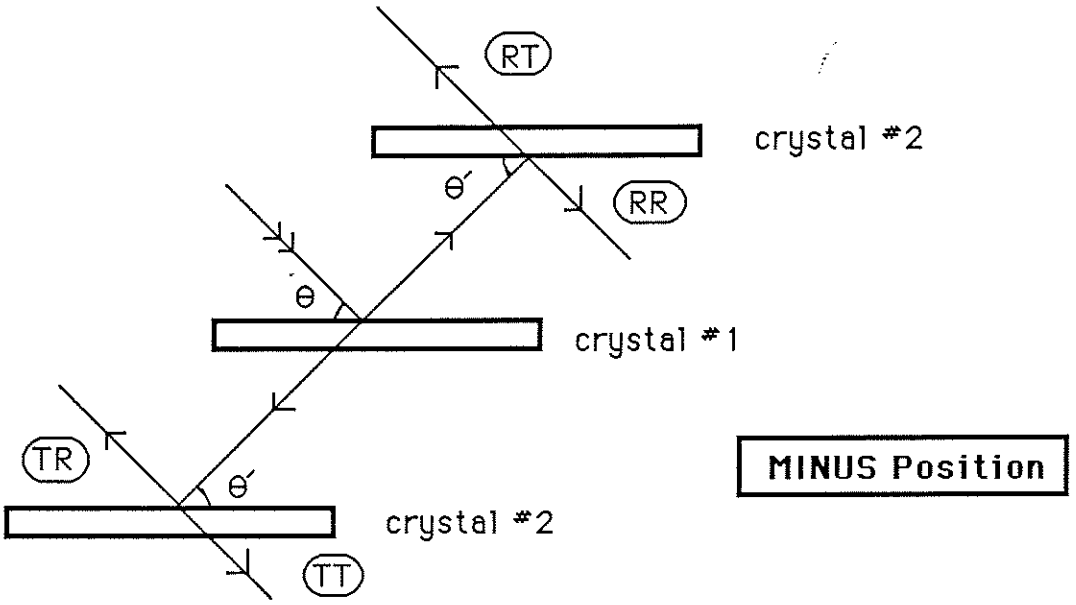


Figure 2b.

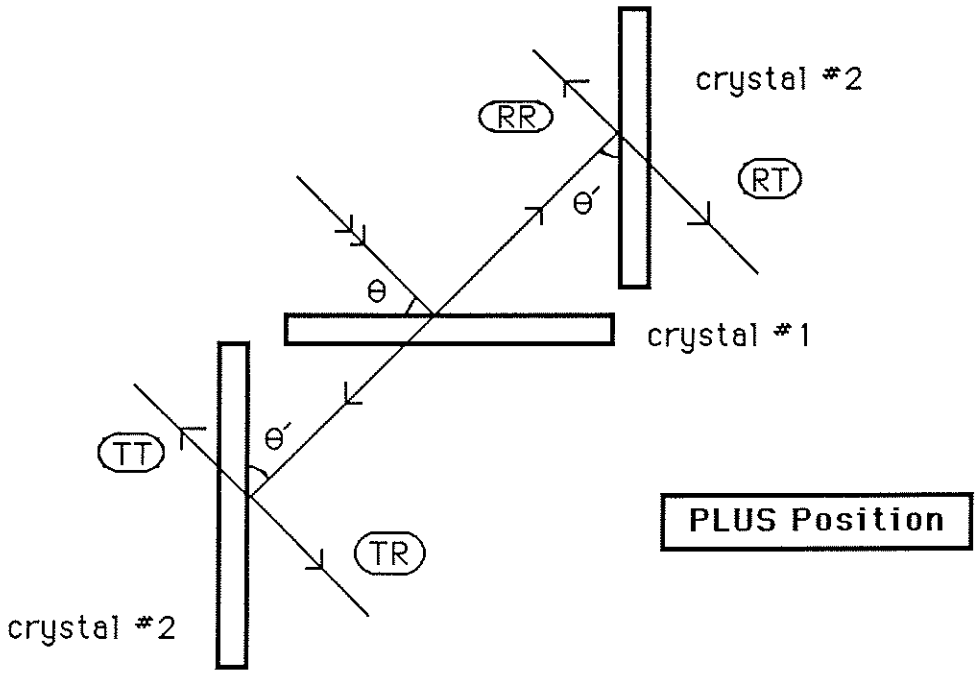
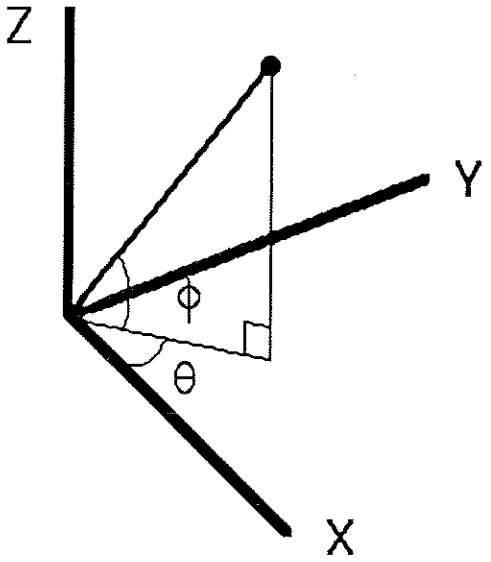


Figure 3.



Sample Run of ROCKIT

Input file = BERMIC

```
XTAL    1       BERYL       BRAGG       1.ØØ      Ø.Ø
PLANE   1           1           Ø           Ø     ØØ.ØØØ
XTAL    2        MICA       BRAGG       1.ØØ      Ø.Ø
PLANE   2           Ø           Ø           2     ØØ.ØØØ
INPUT          Ø1.ØØØ       MINUS
OUTPUT        -ØØ.ØØ4Ø    ØØ.ØØ6Ø    ØØ2ØØ3
COGWRT        Ø.Ø 2Ø.Ø 1 1
```

PROGRAM ROCKIT (VERSION 1)

```
CONTROL FILE = BERMIC
ENERGY INCIDENT OF PHOTON =  1.ØØØØE+ØØ KEV
CALCULATE FROM -4.ØØØE-Ø3 TO  6.ØØØE-Ø3 RADIANS
          2Ø48 TIMES
ROTATE THE CRYSTAL
MINUS POSITION
OUTPUT COG DECK
    WITH VIEW THETA =      Ø.    (DEG) INCREMENTED      1 TIMES
              PHI   =     2Ø.ØØØ (DEG) INCREMENTED      1 TIMES

CRYSTAL NUMBER  1 IS BERYL
REFLECTION
THICKNESS IS  1.ØØØØE+ØØ MM  +-  Ø.
PLANE IS   1    Ø    Ø
ANGLE BETWEEN PLANE/SURFACE  Ø.          (DEG)

CRYSTAL NUMBER  2 IS MICA
REFLECTION
THICKNESS IS  1.ØØØØE+ØØ MM  +-  Ø.
PLANE IS   Ø    Ø    2
ANGLE BETWEEN PLANE/SURFACE  Ø.          (DEG)


    STRUCTURE FOR CRYSTAL   1  (BERYL     )

UNIT CELL IS  (  9.2Ø6Ø,  9.2Ø6Ø,  9.2Ø5Ø) A
              ( 9Ø.ØØØØ, 9Ø.ØØØØ,12Ø.ØØØØ) DEG
```

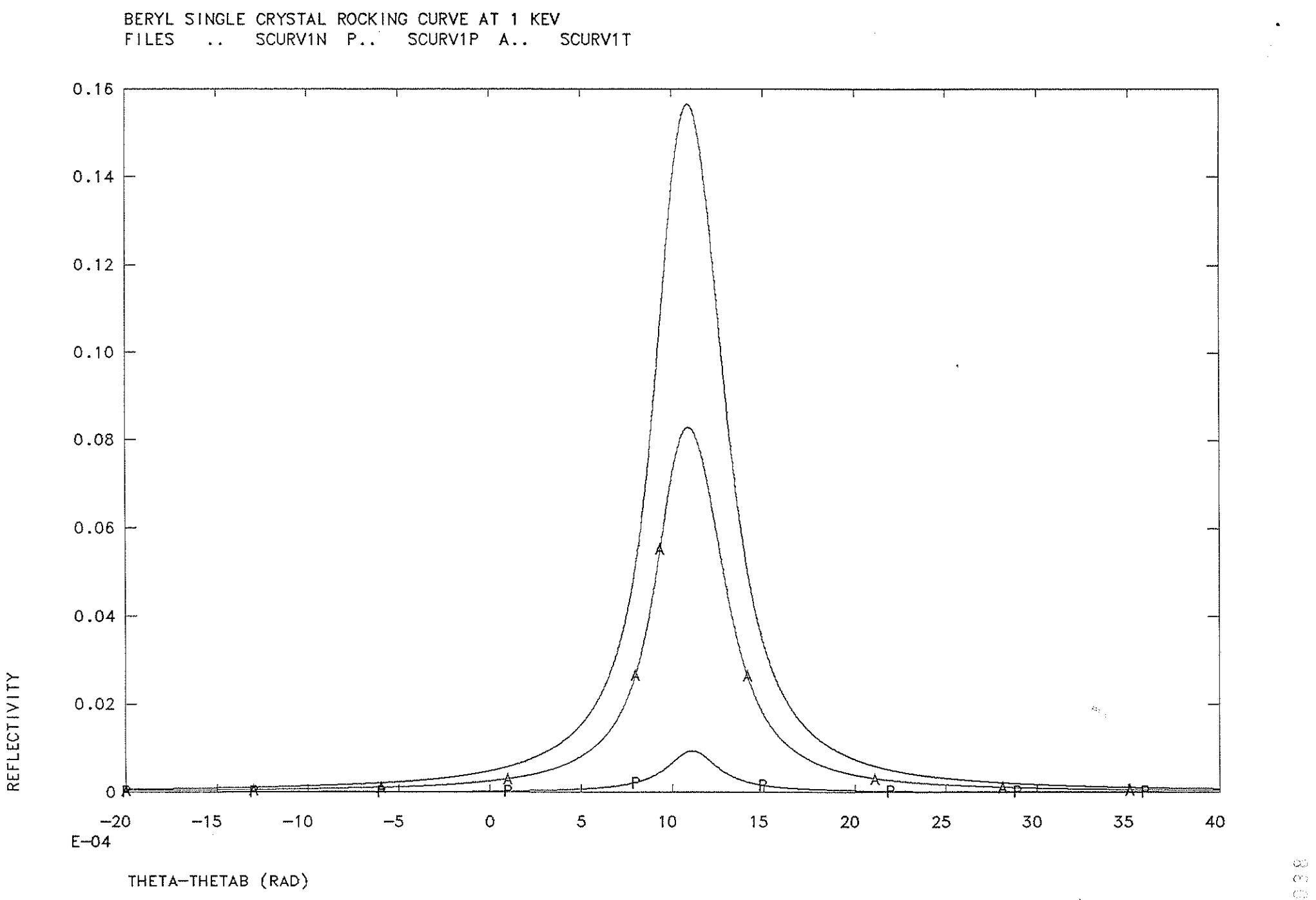
PROTONS	X	Y	Z
13	Ø.3333	Ø.6667	Ø.25ØØ
13	Ø.6667	Ø.3333	Ø.75ØØ
13	Ø.6667	Ø.3333	Ø.25ØØ
13	Ø.3333	Ø.6667	Ø.75ØØ
4	Ø.5ØØØ	Ø.5ØØØ	Ø.75ØØ
4	Ø.5ØØØ	Ø.5ØØØ	Ø.25ØØ
4	Ø.5ØØØ	Ø.	Ø.75ØØ
4	Ø.5ØØØ	Ø.	Ø.25ØØ
4	Ø.	Ø.5ØØØ	Ø.75ØØ
4	Ø.	Ø.5ØØØ	Ø.25ØØ
14	Ø.382Ø	Ø.118Ø	Ø.
14	Ø.618Ø	Ø.882Ø	Ø.
14	Ø.264Ø	Ø.382Ø	Ø.
14	Ø.736Ø	Ø.618Ø	Ø.
14	Ø.118Ø	Ø.736Ø	Ø.
14	Ø.882Ø	Ø.264Ø	Ø.
14	Ø.118Ø	Ø.382Ø	Ø.5ØØØ
14	Ø.882Ø	Ø.618Ø	Ø.5ØØØ
14	Ø.382Ø	Ø.264Ø	Ø.5ØØØ
14	Ø.618Ø	Ø.736Ø	Ø.5ØØØ
14	Ø.736Ø	Ø.118Ø	Ø.5ØØØ
14	Ø.264Ø	Ø.882Ø	Ø.5ØØØ
8	Ø.294Ø	Ø.242Ø	Ø.
8	Ø.7Ø6Ø	Ø.758Ø	Ø.
8	Ø.Ø52Ø	Ø.294Ø	Ø.
8	Ø.948Ø	Ø.7Ø6Ø	Ø.
8	Ø.242Ø	Ø.948Ø	Ø.

File = LROCKIT

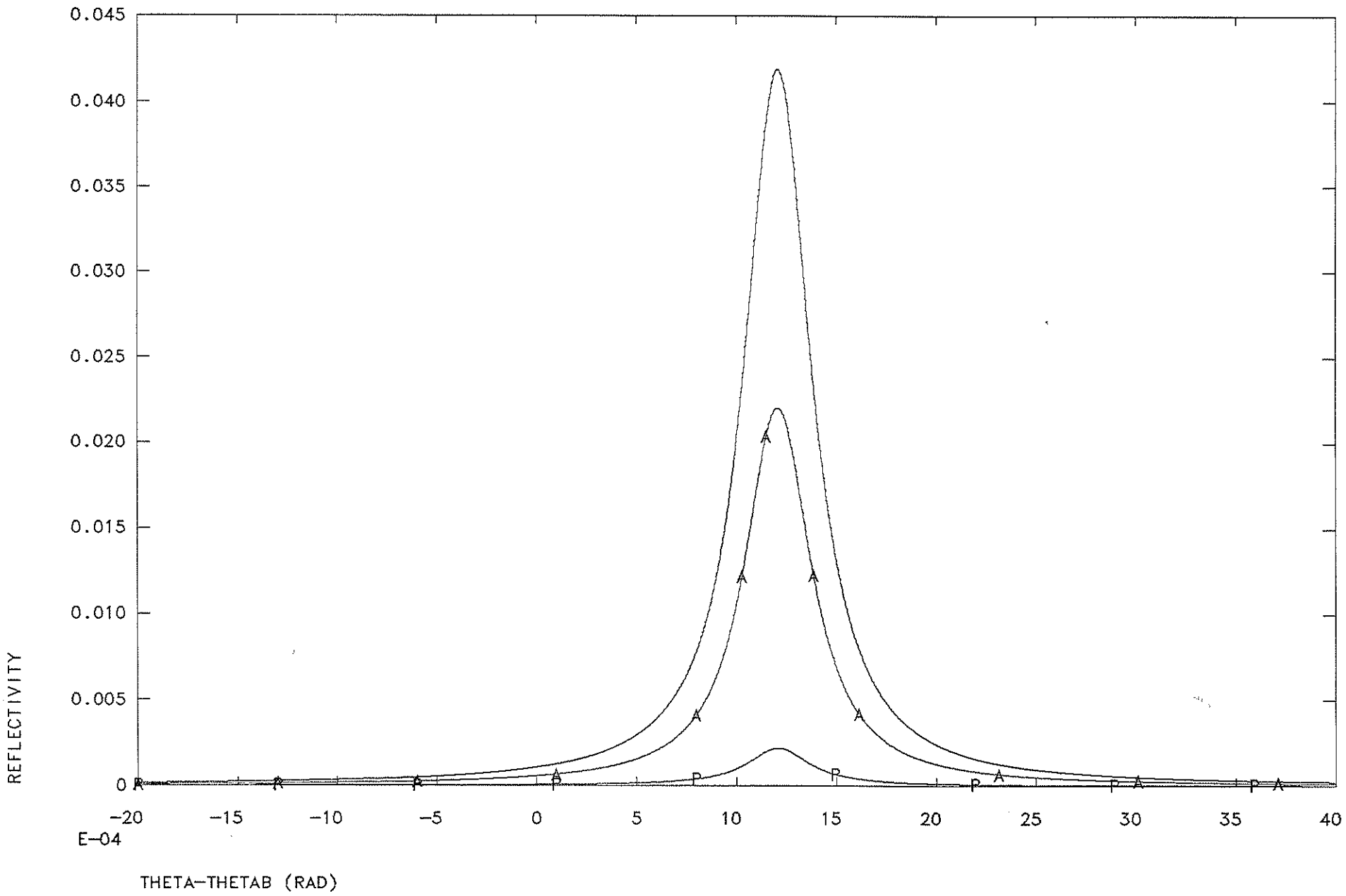
```
       8     Ø.758Ø     Ø.Ø52Ø     Ø.
       8     Ø.242Ø     Ø.294Ø     Ø.5ØØØ
       8     Ø.758Ø     Ø.7Ø6Ø     Ø.5ØØØ
       8     Ø.294Ø     Ø.Ø52Ø     Ø.5ØØØ
       8     Ø.7Ø6Ø     Ø.948Ø     Ø.5ØØØ
       8     Ø.948Ø     Ø.242Ø     Ø.5ØØØ
       8     Ø.Ø52Ø     Ø.758Ø     Ø.5ØØØ
       8     Ø.499Ø     Ø.143Ø     Ø.138Ø
       8     Ø.5Ø1Ø     Ø.857Ø     Ø.862Ø
       8     Ø.143Ø     Ø.644Ø     Ø.138Ø
       8     Ø.857Ø     Ø.356Ø     Ø.862Ø
       8     Ø.356Ø     Ø.499Ø     Ø.138Ø
       8     Ø.644Ø     Ø.5Ø1Ø     Ø.862Ø
       8     Ø.499Ø     Ø.143Ø     Ø.862Ø
       8     Ø.5Ø1Ø     Ø.857Ø     Ø.138Ø
       8     Ø.143Ø     Ø.644Ø     Ø.862Ø
       8     Ø.857Ø     Ø.356Ø     Ø.138Ø
       8     Ø.356Ø     Ø.499Ø     Ø.862Ø
       8     Ø.644Ø     Ø.5Ø1Ø     Ø.138Ø
       8     Ø.143Ø     Ø.499Ø     Ø.638Ø
       8     Ø.857Ø     Ø.5Ø1Ø     Ø.362Ø
       8     Ø.499Ø     Ø.356Ø     Ø.638Ø
       8     Ø.5Ø1Ø     Ø.644Ø     Ø.362Ø
       8     Ø.644Ø     Ø.143Ø     Ø.638Ø
       8     Ø.356Ø     Ø.857Ø     Ø.362Ø
       8     Ø.857Ø     Ø.5Ø1Ø     Ø.638Ø
       8     Ø.143Ø     Ø.499Ø     Ø.362Ø
       8     Ø.5Ø1Ø     Ø.644Ø     Ø.638Ø
       8     Ø.499Ø     Ø.356Ø     Ø.362Ø
       8     Ø.356Ø     Ø.857Ø     Ø.638Ø
       8     Ø.644Ø     Ø.143Ø     Ø.362Ø
Z =   13    FF =   1.Ø755E+Ø1   +    7.6291E-Ø1   I
Z =    4    FF =   3.7Ø44E+ØØ   +    1.2827E-Ø1   I
Z =   14    FF =   1.2ØØØE+Ø1   +    1.Ø428E+ØØ   I
Z =    8    FF =   7.8957E+ØØ   +    1.7558E+ØØ   I
NORMAL FF = -7.31Ø2E+Ø1 + -1.1Ø37E+Ø1 I
DIRECT FF =  5.32ØØE+Ø2 +  7.9542E+Ø1 I
BRAGG ANGLE =    51.Ø297 (DEG)
TWO D SPACING =    15.9453 (ANGSTROMS)
MASS ATTENUATION =  8.2259E+Ø3 (1/CM)


    STRUCTURE FOR CRYSTAL   2  (MICA      )

UNIT CELL IS  (  5.189Ø,  8.995Ø, 19.921Ø) A
              ( 9Ø.ØØØØ, 95.1833, 9Ø.ØØØØ) DEG

PROTONS          X          Y          Z
      19     Ø.         Ø.1Ø16     Ø.25ØØ
      19     Ø.         Ø.8984     Ø.75ØØ
      19     Ø.5ØØØ     Ø.6Ø16     Ø.25ØØ
      19     Ø.5ØØØ     Ø.3984     Ø.75ØØ
      13     Ø.2484     Ø.Ø871     Ø.Ø516
      13     Ø.7516     Ø.9129     Ø.9984
      13     Ø.2484     Ø.9129     Ø.5Ø16
      13     Ø.7516     Ø.Ø871     Ø.4984
      13     Ø.7484     Ø.5871     Ø.Ø016
      13     Ø.2516     Ø.4129     Ø.9984
      13     Ø.7484     Ø.4129     Ø.5Ø16
      13     Ø.2516     Ø.5871     Ø.4984
```

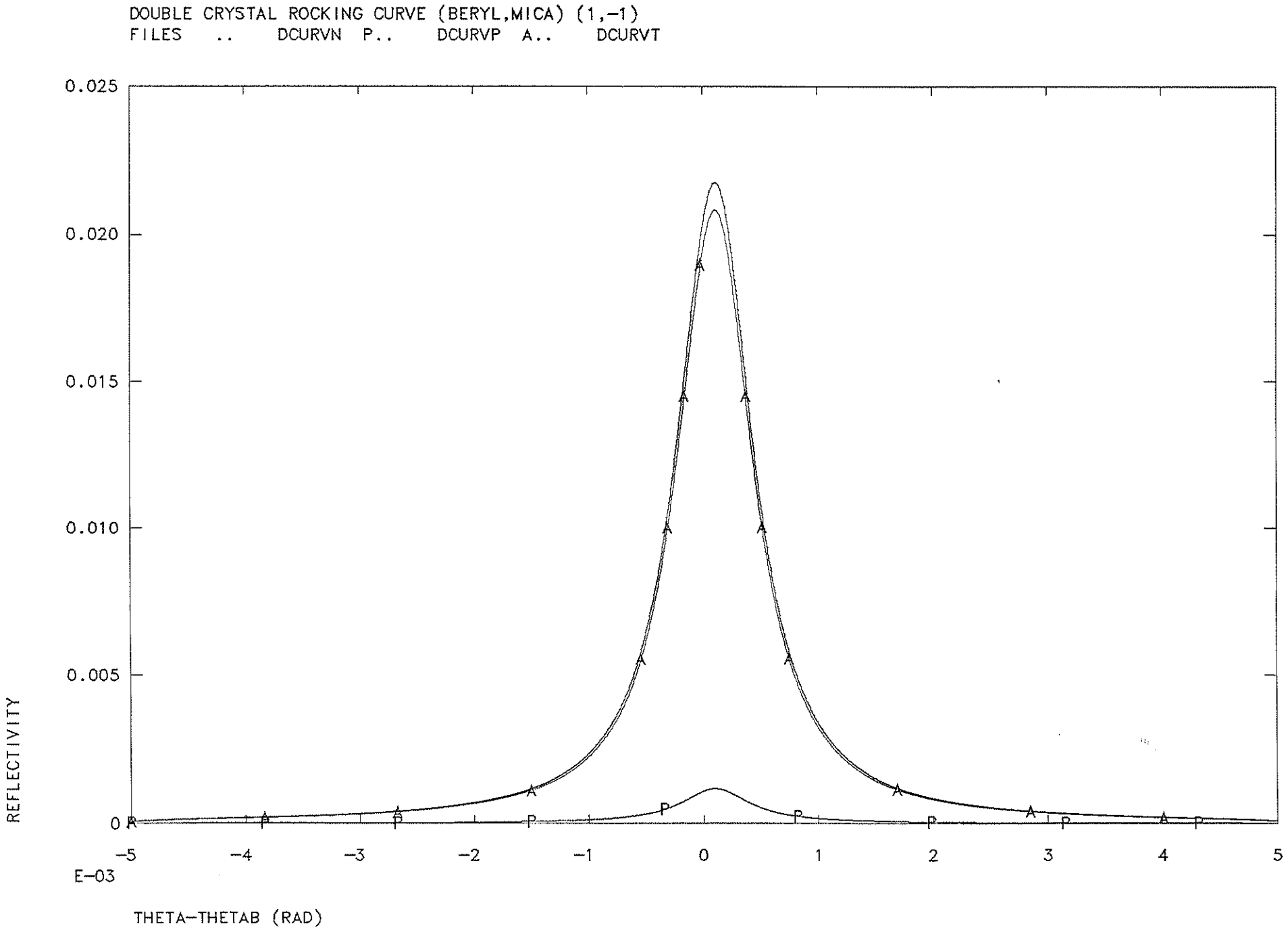
14	Ø.4625	Ø.9242	Ø.1372
13	Ø.5375	Ø.Ø758	Ø.8628
13	Ø.4625	Ø.Ø758	Ø.6372
14	Ø.5375	Ø.9242	Ø.3628
14	Ø.9625	Ø.4242	Ø.1372
14	Ø.ØØ375	Ø.5758	Ø.8628
13	Ø.9625	Ø.5758	Ø.6372
14	Ø.ØØ375	Ø.4242	Ø.3628
14	Ø.4593	Ø.2550	Ø.1365
14	Ø.5407	Ø.7450	Ø.8635
13	Ø.4593	Ø.7450	Ø.6365
14	Ø.5407	Ø.2550	Ø.3635
14	Ø.9593	Ø.7550	Ø.1365
14	Ø.ØØ407	Ø.2450	Ø.8635
14	Ø.9593	Ø.2450	Ø.6365
14	Ø.ØØ407	Ø.7550	Ø.3635
8	Ø.2629	Ø.3713	Ø.1674
8	Ø.7371	Ø.6287	Ø.8326
8	Ø.2629	Ø.6287	Ø.6674
8	Ø.7371	Ø.3713	Ø.3326
8	Ø.7629	Ø.8713	Ø.1674
8	Ø.2371	Ø.1287	Ø.8326
8	Ø.7629	Ø.1287	Ø.6674
8	Ø.2371	Ø.8713	Ø.3326
8	Ø.2450	Ø.8Ø2Ø	Ø.162Ø
8	Ø.7550	Ø.198Ø	Ø.838Ø
8	Ø.2450	Ø.198Ø	Ø.662Ø
8	Ø.7550	Ø.8Ø2Ø	Ø.338Ø
8	Ø.7450	Ø.3Ø2Ø	Ø.162Ø
8	Ø.2550	Ø.698Ø	Ø.838Ø
8	Ø.7450	Ø.698Ø	Ø.662Ø
8	Ø.2550	Ø.3Ø2Ø	Ø.338Ø
8	Ø.4Ø8Ø	Ø.ØØ96Ø	Ø.168Ø
8	Ø.592Ø	Ø.9Ø4Ø	Ø.832Ø
8	Ø.4Ø8Ø	Ø.9Ø4Ø	Ø.668Ø
8	Ø.592Ø	Ø.ØØ96Ø	Ø.332Ø
8	Ø.9Ø8Ø	Ø.596Ø	Ø.168Ø
8	Ø.ØØ92Ø	Ø.4Ø4Ø	Ø.832Ø
8	Ø.9Ø8Ø	Ø.4Ø4Ø	Ø.668Ø
8	Ø.ØØ92Ø	Ø.596Ø	Ø.332Ø
8	Ø.465Ø	Ø.945Ø	Ø.ØØ527
8	Ø.535Ø	Ø.ØØ55Ø	Ø.9473
8	Ø.465Ø	Ø.ØØ55Ø	Ø.5527
8	Ø.535Ø	Ø.945Ø	Ø.4473
8	Ø.965Ø	Ø.445Ø	Ø.ØØ527
8	Ø.ØØ35Ø	Ø.555Ø	Ø.9473
8	Ø.965Ø	Ø.555Ø	Ø.5527
8	Ø.ØØ35Ø	Ø.445Ø	Ø.4473
8	Ø.425Ø	Ø.26ØØ	Ø.ØØ542
8	Ø.575Ø	Ø.74ØØ	Ø.9458
8	Ø.425Ø	Ø.74ØØ	Ø.5542
8	Ø.575Ø	Ø.26ØØ	Ø.4458
8	Ø.925Ø	Ø.76ØØ	Ø.ØØ542
8	Ø.ØØ75Ø	Ø.24ØØ	Ø.9458
8	Ø.925Ø	Ø.24ØØ	Ø.5542
8	Ø.ØØ75Ø	Ø.76ØØ	Ø.4458
8	Ø.453Ø	Ø.558Ø	Ø.ØØ52Ø
8	Ø.547Ø	Ø.442Ø	Ø.948Ø
8	Ø.453Ø	Ø.442Ø	Ø.552Ø
8	Ø.547Ø	Ø.558Ø	Ø.448Ø

```
       8     Ø.953Ø     Ø.Ø58Ø     Ø.Ø52Ø
       8     Ø.Ø47Ø     Ø.942Ø     Ø.948Ø
       8     Ø.953Ø     Ø.942Ø     Ø.552Ø
       8     Ø.Ø47Ø     Ø.Ø58Ø     Ø.448Ø
       1     Ø.453Ø     Ø.558Ø     Ø.Ø52Ø
       1     Ø.547Ø     Ø.442Ø     Ø.948Ø
       1     Ø.453Ø     Ø.442Ø     Ø.552Ø
       1     Ø.547Ø     Ø.558Ø     Ø.448Ø
       1     Ø.953Ø     Ø.Ø58Ø     Ø.Ø52Ø
       1     Ø.Ø47Ø     Ø.942Ø     Ø.948Ø
       1     Ø.953Ø     Ø.942Ø     Ø.552Ø
       1     Ø.Ø47Ø     Ø.Ø58Ø     Ø.448Ø
Z =   19    FF =   1.79Ø2E+Ø1   +    3.9Ø71E+ØØ   I
Z =   13    FF =   1.1Ø52E+Ø1   +    7.6291E-Ø1   I
Z =   14    FF =   1.23Ø9E+Ø1   +    1.Ø428E+ØØ   I
Z =    8    FF =   8.Ø166E+ØØ   +    1.7558E+ØØ   I
Z =    1    FF =   9.4621E-Ø1   +    1.6657E-Ø4   I
NORMAL FF =   5.1886E+Ø1 + -1.8356E+ØØ I
DIRECT FF =   7.92ØØE+Ø2 +  1.2158E+Ø2 I
BRAGG ANGLE =    38.6722 (DEG)
TWO D SPACING =    19.8395 (ANGSTROMS)
MASS ATTENUATION =  9.1729E+Ø3 (1/CM)


INTEGRATED REFLECTIVITY (XTAL #1) =    5.2832E-Ø5


INTEGRATED REFLECTIVITY (XTAL #2) =    1.3312E-Ø5


DOUBLE INTEGRATED REFLECTIVITY =    2.4286E-Ø5
  DISPERSION =   -4.3585E-Ø1   (RAD/LAMDA)
```


BERYL SINGLE CRYSTAL ROCKING CURVE AT 1 KEV
FILES .. SCURV1N P.. SCURV1P A.. SCURV1T
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0
REFLECTIVITY
-20
-15
-10
-5
0
5
10
15
20
25
30
35
40
E-04
THETA-THETAB (RAD)

MICA SINGLE CRYSTAL ROCKING CURVE AT 1 KEV
FILES .. SCURV2N P.. SCURV2P A.. SCURV2T




DOUBLE CRYSTAL ROCKING CURVE (BERYL,MICA) (1,-1)
FILES .. DCURVN P.. DCURVP A.. DCURVT
0.025
0.020
0.015
0.010
0.005
0
REFLECTIVITY
-5
-4
-3
-2
-1
0
1
2
3
4
5
E-03
THETA-THETAB (RAD)

mica crystal structure --- plane 0 0 2

07/24/85 01:54:06 d

viewer orientation

center at x= 1.687e+00
y= 4.497e+00
z= 1.001e+01
radius viewed 1.886e+01
dist. to viewer 1.886e+03