MEMORANDUM

To: Distribution

From: M. Glinsky

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:

L-Division Group Leaders
G. Chandler
X-ray Measurements Group
R-Project Group
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)/lambda dependence of the real part of the form factor is taken from the EN DL tables {5}. The Cromer-Liberman relativistic correction is then made {6}. For energies above 2 keV the structure factors are calculated from the EN DL 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, an 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

<table>
<thead>
<tr>
<th>Field</th>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>XTAL 1</td>
<td>xnbr</td>
<td>Number of crystal (1 or 2). Integer.</td>
</tr>
<tr>
<td>PLANE 1</td>
<td>nmxtal</td>
<td>Name of crystal</td>
</tr>
<tr>
<td>XTAL 2</td>
<td>typdff</td>
<td>Type of diffraction</td>
</tr>
<tr>
<td>PLANE 2</td>
<td>thick</td>
<td>Thickness of crystal (in mm). Real.</td>
</tr>
<tr>
<td>INPUT</td>
<td>errtk</td>
<td>Error in thickness (in mm). Real.</td>
</tr>
<tr>
<td>OUTPUT</td>
<td></td>
<td></td>
</tr>
<tr>
<td>COGWRT</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note: all fields separated by blanks

B. Description of Cards

<table>
<thead>
<tr>
<th>Field</th>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>xnbr</td>
<td>Number of crystal (1 or 2). Integer.</td>
</tr>
<tr>
<td>2</td>
<td>nmxtal</td>
<td>Name of crystal</td>
</tr>
<tr>
<td>3</td>
<td>typdff</td>
<td>Type of diffraction</td>
</tr>
<tr>
<td>4</td>
<td>thick</td>
<td>Thickness of crystal (in mm). Real.</td>
</tr>
<tr>
<td>5</td>
<td>errtk</td>
<td>Error in thickness (in mm). Real.</td>
</tr>
</tbody>
</table>

Note: all fields separated by blanks

Note: fields are separated by blanks.
**==>INPUT Card<==**

1  energy  Energy of incoming 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.

(Nota: 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

<table>
<thead>
<tr>
<th>Name of file</th>
<th>Contents of file</th>
</tr>
</thead>
<tbody>
<tr>
<td>LROCKIT</td>
<td>Listing containing input parameters, crystal structures, bragg angles, two-d spacings, form factors, integrated reflectivities, and dispersion of the two crystal system.</td>
</tr>
<tr>
<td>SCURV1N</td>
<td>I/lo (Normal polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #1 (SOCKITTOME compatible card image format)</td>
</tr>
<tr>
<td>SCURV1P</td>
<td>I/lo (Parallel polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #1 (SOCKITTOME compatible card image format)</td>
</tr>
<tr>
<td>SCURV1T</td>
<td>I/lo (No polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #1 (SOCKITTOME compatible card image format)</td>
</tr>
<tr>
<td>SCURV2N</td>
<td>I/lo (Normal polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #2 (SOCKITTOME compatible card image format)</td>
</tr>
<tr>
<td>SCURV2P</td>
<td>I/lo (Parallel polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #2 (SOCKITTOME compatible card image format)</td>
</tr>
<tr>
<td>SCURV2T</td>
<td>I/lo (No polarization) as a function of angle (in rad) or d(lamda)/lamda for crystal #2 (SOCKITTOME compatible card image format)</td>
</tr>
<tr>
<td>DCURV1N</td>
<td>I/lo (Normal polarization) as a function of angle (in rad) for crystal #2 off of crystal #1 (SOCKITTOME compatible card image format)</td>
</tr>
<tr>
<td>DCURV1P</td>
<td>I/lo (Parallel polarization) as a function of angle (in rad) for crystal #2 off of crystal #1 (SOCKITTOME compatible card image format)</td>
</tr>
<tr>
<td>DCURV1T</td>
<td>I/lo (No polarization) as a function of angle (in rad) for crystal #2 off of crystal #1 (SOCKITTOME compatible card image format)</td>
</tr>
<tr>
<td>COGX1</td>
<td>COG input deck to draw crystal structure for crystal #1</td>
</tr>
<tr>
<td>COGX2</td>
<td>COG input deck to draw crystal structure for crystal #2</td>
</tr>
</tbody>
</table>
Crystal Structure File Format

A. Order of deck

XTAL
UNIT
ATOM
ATOM
.
.
XTAL
UNIT
ATOM
.
.

B. Description of Cards

<table>
<thead>
<tr>
<th>Field</th>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>nmxtal</td>
<td>Name of Crystal (Up to 8 characters)</td>
</tr>
</tbody>
</table>

>>>UNIT Card<<<

<table>
<thead>
<tr>
<th>Field</th>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a</td>
<td>length of first primitive vector</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>Length of second primitive vector</td>
</tr>
<tr>
<td>3</td>
<td>c</td>
<td>Length of third primitive vector</td>
</tr>
<tr>
<td>4</td>
<td>alpha</td>
<td>Angle between b-c (in Degrees)</td>
</tr>
<tr>
<td>5</td>
<td>beta</td>
<td>Angle between a-c (in Degrees)</td>
</tr>
<tr>
<td>6</td>
<td>gamma</td>
<td>Angle between a-b (in Degrees)</td>
</tr>
</tbody>
</table>

>>>ATOM Card<<<  (200 allowed per crystal)

<table>
<thead>
<tr>
<th>Field</th>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>z</td>
<td>Number of protons in atom</td>
</tr>
<tr>
<td>2</td>
<td>xatom</td>
<td>a coordinate of atom</td>
</tr>
<tr>
<td>3</td>
<td>yatom</td>
<td>b coordinate of atom</td>
</tr>
<tr>
<td>4</td>
<td>zatom</td>
<td>c coordinate of atom</td>
</tr>
</tbody>
</table>
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. Instructions on how to do this can be obtained from Ed Lent.
References


Figure 1a.

Type of diffraction = BRAGG = reflection

crystal plane

Figure 1b.

Type of diffraction = LAUE = transmission
Figure 2a.

Figure 2b.
Figure 3.
Sample Run of ROCKIT
Input file = BERMIC

XTAL 1 BERYL BRAGG 1.00 3.0
PLANE 1 1
XTAL 2 MICA SRAGG 1.00 3.0
PLANE 2 2
INPUT .01.999 MINUS
OUTPUT -99.9949 50.0068 982843
COGWRT 0.3 20.3 1 1
PROGRAM ROCKIT (VERSION 1)

CONTROL FILE = BERMIC
ENERGY INCIDENT OF PHOTON = 1.0000E+08 KEV
CALCULATE FROM -4.0000E-03 TO 6.0000E-03 RADIANS
2048 TIMES

ROTATE THE CRYSTAL
MINUS POSITION
OUTPUT COG DECK

WITH VIEW Theta = D. (DEG) INCREMENTED 1 TIMES
PHI = 20.000 (DEG) INCREMENTED 1 TIMES

CRYSTAL NUMBER 1 IS BERYL
REFLECTION
THICKNESS IS 1.0000E+00 MM +/- D.
PLANE IS 1 0 0
ANGLE BETWEEN PLANE/SURFACE D. (DEG)

CRYSTAL NUMBER 2 IS MICA
REFLECTION
THICKNESS IS 1.0000E+00 MM +/- D.
PLANE IS 0 0 2
ANGLE BETWEEN PLANE/SURFACE D. (DEG)

STRUCTURE FOR CRYSTAL 1 (BERYL)

UNIT CELL IS ( 9.2060, 9.2060, 9.2060 ) A
( 90.0000, 90.0000, 120.0000 ) DEG

<table>
<thead>
<tr>
<th>PROTONS</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>0.3333</td>
<td>0.6667</td>
<td>0.2500</td>
</tr>
<tr>
<td>13</td>
<td>0.6667</td>
<td>0.3333</td>
<td>0.7500</td>
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<td>0.6667</td>
<td>0.3333</td>
<td>0.7500</td>
</tr>
<tr>
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<td>0.6667</td>
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<td>0.7500</td>
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<td>0.5000</td>
<td>0.7500</td>
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<tr>
<td>4</td>
<td>0.5000</td>
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<td>0.7500</td>
</tr>
<tr>
<td>4</td>
<td>0.5000</td>
<td>0.5000</td>
<td>0.7500</td>
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<tr>
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<td>0.5000</td>
<td>0.5000</td>
<td>0.7500</td>
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<tr>
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<td>0.5000</td>
<td>0.5000</td>
<td>0.7500</td>
</tr>
<tr>
<td>14</td>
<td>0.3820</td>
<td>0.1180</td>
<td>0.</td>
</tr>
<tr>
<td>14</td>
<td>0.6180</td>
<td>0.8820</td>
<td>0.</td>
</tr>
<tr>
<td>14</td>
<td>0.2640</td>
<td>0.3820</td>
<td>0.</td>
</tr>
<tr>
<td>14</td>
<td>0.7360</td>
<td>0.6160</td>
<td>0.</td>
</tr>
<tr>
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<td>0.1180</td>
<td>0.7360</td>
<td>0.</td>
</tr>
<tr>
<td>14</td>
<td>0.0820</td>
<td>0.2640</td>
<td>0.</td>
</tr>
<tr>
<td>14</td>
<td>0.1180</td>
<td>0.3820</td>
<td>0.5000</td>
</tr>
<tr>
<td>14</td>
<td>0.3820</td>
<td>0.6180</td>
<td>0.5000</td>
</tr>
<tr>
<td>14</td>
<td>0.3820</td>
<td>0.2640</td>
<td>0.5000</td>
</tr>
<tr>
<td>14</td>
<td>0.6180</td>
<td>0.7360</td>
<td>0.5000</td>
</tr>
<tr>
<td>14</td>
<td>0.7360</td>
<td>0.1180</td>
<td>0.5000</td>
</tr>
<tr>
<td>14</td>
<td>0.2640</td>
<td>0.8820</td>
<td>0.5000</td>
</tr>
<tr>
<td>8</td>
<td>0.2940</td>
<td>0.2420</td>
<td>0.</td>
</tr>
<tr>
<td>8</td>
<td>0.7960</td>
<td>0.7500</td>
<td>0.</td>
</tr>
<tr>
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<td>0.8520</td>
<td>0.2940</td>
<td>0.</td>
</tr>
<tr>
<td>8</td>
<td>0.9480</td>
<td>0.7500</td>
<td>0.</td>
</tr>
<tr>
<td>8</td>
<td>0.2420</td>
<td>0.9480</td>
<td>0.</td>
</tr>
</tbody>
</table>

File = LROCKIT
Z = 13  \text{FF} = 1.0775E+01 + 7.6291E-01 \text{I}
Z = 4  \text{FF} = 3.7344E+00 + 1.2827E-01 \text{I}
Z = 8  \text{FF} = 4.8660E+00 + 1.7558E+00 \text{I}
\text{NORMAL FF} = -7.3060E+00 + -1.1037E+01 \text{I}
\text{DIRECT FF} = 5.3200E+02 + 7.9572E+01 \text{I}
\text{BRAGG ANGLE} = 51.0297 \text{ (DEG)}
\text{TWO D SPACING} = 15.9453 \text{ (ANGSTROMS)}
\text{MASS ATTENUATION} = 0.2259E+03 \text{ (1/CM)}

\text{STRUCTURE FOR CRYSTAL 2 (MICA)}

\text{UNIT CELL IS (5.1650, 0.9950, 19.9210) A}
\text{(90.0000, 95.1833, 90.0000) DEG}

\text{PROTONS}  \quad X  \quad Y  \quad Z
19  \text{q.}  \quad 0.1016  \quad 0.2560
19  \text{q.}  \quad 0.0964  \quad 0.7530
19  \text{q.}  \quad 0.6016  \quad 0.7530
19  \text{q.}  \quad 0.5960  \quad 0.3940
19  \text{q.}  \quad 0.2434  \quad 0.0971  \quad 0.3216
13  \text{q.}  \quad 0.7516  \quad 0.9129  \quad 0.9964
13  \text{q.}  \quad 0.7516  \quad 0.9129  \quad 0.5016
13  \text{q.}  \quad 0.7516  \quad 0.9129  \quad 0.9964
13  \text{q.}  \quad 0.7516  \quad 0.9129  \quad 0.5016
13  \text{q.}  \quad 0.7516  \quad 0.9129  \quad 0.9964
13  \text{q.}  \quad 0.7516  \quad 0.9129  \quad 0.5016
13  \text{q.}  \quad 0.7516  \quad 0.9129  \quad 0.9964
Z = 19 FF = 1.7902E+01 + 3.9271E+00 i
Z = 13 FF = 1.1052E+01 + 7.6291E+00 i
Z = 14 FF = 1.2389E+01 + 1.0428E+00 i
Z = 20 FF = 8.8166E+00 + 1.7558E+00 i
Z = 1 FF = 9.4621E-01 + 1.6667E-02 i
NORMAL FF = 5.1036E+01 + -1.9356E+00 i
DIRECT FF = 7.9209E+02 + 1.2158E+02 i
BRAGG ANGLE = 38.6722 (DEG)
TWO D SPACING = 19.8395 (ANGSTROMS)
MASS ATTENUATION = 9.1725E+03 (1/CM)

INTEGRATED REFLECTIVITY (XTAL #1) = 5.2832E-05

INTEGRATED REFLECTIVITY (XTAL #2) = 1.3312E-05

DOUBLE INTEGRATED REFLECTIVITY = 2.4286E-05
DISPERSION = -4.3565E-01 (RAD/LAMDA)
BERYL SINGLE CRYSTAL ROCKING CURVE AT 1 KEV

FILES . . SCURVIN P . . SCURV1P A . . SCURV1T
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

- REFLECTIVITY
  - E-03

- THETA-THETAB (RAD)
  - -5  -4  -3  -2  -1  0  1  2  3  4  5
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: 1.866e+01
dist. to viewer: 1.866e+03