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Ray-Tracing Lab

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Two Crystals I

The main purpose of this section is to demostrate how to ray-trace a crystal monochromator. SHADOW needs a data file to ray trace a crystal. This file is prepared by BRAGG. In addition, BRAGG may allow the user to visualize the diffraction patterns or rocking curves of the crystal in consideration. SHADOW deals with crystals in both reflection (Bragg) and transmission (Laue) mounting. Two crystal models are allowed in SHADOW: perfect crystals (i.e. Silicon, Diamond) and mosaic crystals, where the crystal block is made by an aglutination of small microcrystals (i.e. graphite, berylium). Perfect crystals may be symmetric (the Bragg planes are parallel to the crystal surface in Bragg mounting, and perpendicular in Laue mounting) and asymmetric, when the crystal planes form an arbitrary angle alfa with the crystal surface. Mosaic crystals can only be symmetrical in SHADOW.

Ground-bent crystals (the so-called Johansson geometry) for perfect crystals are also allowed in SHADOW. We remind the reader that a symmetric perfect crystal in Bragg mounting is essentially a mirror with a very narrow bandwidth in energy or angle, determined by its rocking curve or diffraction pattern. An asymmetric crystal does not act as a mirror, but as a grating, where the "grating ruling" is provided by the intersection lines between the Bragg planes and crystal surface. In addition,the rocking curve determines the energy or angular acceptance, as in symmetric crystals.

In all the crystal cases of three-dimensional Bragg scattering, only the rays close to the Bragg condition will be diffracted; the other ones will be *absorbed* by the crystal. For this reason, to only look at the scatter plot of the reflected (outgoing) beam, like we did in the case of the grating, is not enough. This is because of the way SHADOW carries the intensity information; to each ray is associated the vector potential A that contains, in its modulus, the intensity (and polarization) information. For this reason a simple scatter plot does not convey any information on the *intensity* of the rays; it is necessary then to use either the facilities provided by PLOTXY in the CONTOUR mode (two dimensional case), or make use of the INTENSITY flag in PREPLOT (one dimensional case). Since PLOTXY has already been demonstrated, we will concentrate on PREPLOT. In this example we will then show how to:

- To use BRAGG in generating the files needed by SHADOW to perform the calculations.
- To run SHADOW for the CRYSTAL case
- To run SHADOW by restarting from an Optical Element instead than from a source
- To use PREPLOT in order to analyze the results

The case that we will consider is that of a two-crystal monochromator in an antiparallel configuration. After considering the ideal case, we will introduce some rotational misalignment and study its effect on the transmitted spectrum. See figure 1 below.

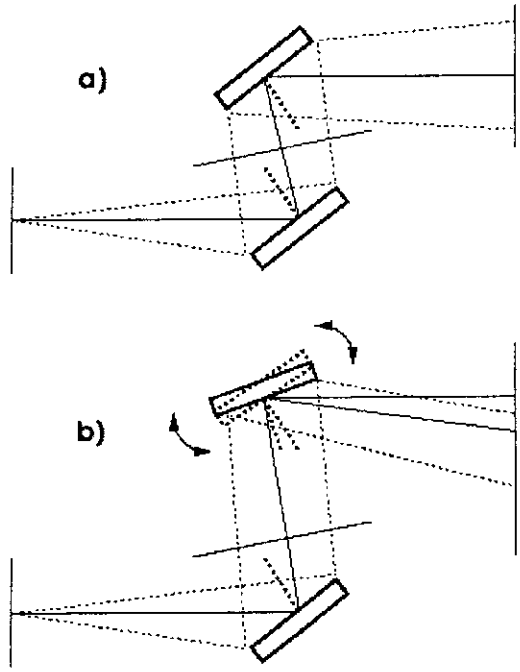

Fig. 1 - Two-crystal monochromator with diverging radiation and antiparallel configuration: a) ideal case, b) misaligned second crystal

In order to do that, we will restart the calculations at the second OE, since the first one will have been left unchanged. The source that we will be using will be a point source of single wavelength. The BRAGG condition

$$n \lambda = 2 d \sin \theta$$

will change along the crystal surface, since θ will be changing and rays hitting at different positions will be attenuated by different amounts.

Another section will describe the complementary case of a collimated broad-band source. Notice that for a real source, i.e., both diverging and with a continuous distribution, the output from Preplot will not be a "nice" curve but instead a *band* of values. To analyze it it will be necessary to resort to HISTO1, as shown in the previous section on the radiation power density study.

In order to prepare BRAGG it is necessary to have a table of the real part of the atomic scattering coefficients in function of $\sin(\theta)/\lambda$. An exhaustive table can be found in the International Tables of X-Ray Crystallography, Vol.III, Sect.2.2, Table 2.2A, p.72. A shorter version can be found in *X-ray Diffraction* , by B.E.Warren, Addison-Wesley. BRAGG will prompt about the coefficients.

BRAGG is the program that generates the crystal parameters in a format suitable for input to SHADOW. Let us use the GaAs (111) plane, with incident energy of 11160 eV.

$ **BRAGG**

```
All crystal structures are referred to a cubic unit cell.
Bravais lattice type :
0       for ZincBlende
1       for Rocksalt
2       forsimple FCC
3       for     CsCl structure
Hexagonal Bravais lattice type:
4       for     Hexagonal Close-Packed structure
5       for     Hexagonal Graphite structure
```

Then ? **0**

Lattice constant (Angs) ? **5.65**

Index of crystal plane of reflection H,K,L : **1,1,1**

```
 ********************************************************
 The ZINCBLENDE structure is defined by atom A located at
 (0,0,0) and atom B at (1/4,1/4,1/4) of the fcc lattice.
 ********************************************************
```

Enter 2-letters (capitalized) atomic symbol for atom A : **GA**

Enter 2-letters (capitalized) atomic symbol for atom B : **AS**

```
 ********************************************************
 Atomic scattering factor is defined by fo + f' + if", where
     fo = fo(SIN(theta)/Lambda) is the non-dispersive part
     f', f" (Lambda) are the dispersive part.
 ********************************************************
 We need fo at 3 different values of SIN(theta)/Lambda, which
 should cover the range of interest and center around :
 SIN(theta)/Lambda =   0.1532788325282192     ratio.
 ********************************************************
 Please enter 1) SIN(theta)/Lambda, 2) fo ,

\ At this point, take the International Tables or the ones from Warren, and
\ find the values tabulated for Ga and As at values of Sin(theta)/lambda
\ bracketing the one quoted above. BRAGG will automatically interpolate.
```

For atom A, first set : **0.14, 27.162**

. , second set : **0.15, 26.783**

. , third set : **0.16,26.406**

For atom B, first set : **0.14, 28.742**

. , second set : **0.15, 26.783**

. , third set : **0.16, 27.877**

```
 ********************************************************
 f', f" is furnished from optical constant library within ...

\ The other part of the atomic scattering factors is read from the library.
\ Enter the photon energy range, keeping it reasonably narrow.
```

minimum photon energy (eV) : **11100**

maximum photon energy (eV) : **11200**

energy step (eV) : **10**

Do you want to include crystal absorption [1/0] ? **1**

Temperature (Debye-Waller) factor : **0.979**

This is the value of the Debye-Waller coefficient, $\exp(-1/2\ G^2u^2)$ where **G** is the scattering vector and **u** the rms atomic displacement. If in doubt, enter 1.0. This will ignore then DW effects.

Output file name (for SHADOW) : **GAAS.PAR**

Do you want to generate a rocking curve [1/0] ? **1**

What do you want to calculate ?:

[1] Diffracted beam in Transmission (Laue) geometry

[2] Diffracted beam in Reflection (Bragg) geometry

[3] like [2] using thick crystal approximation

<?> **3**

... at what energy (eV) ? **11160**

```
 So far, we are working with:
 Lambda  =    1.110978494623656     Angstroms
 Theta (graz)  =    9.804650841199757     degrees
 Bragg angle      =    9.807153296220226     degrees
 Structure factor  =  (142.6426218594671,11.03752285669588)
 Refraction index = 1 - delta - i*beta :
           delta =   7.3270650274570581E-06
            beta =   4.8385681505652676E-07
 Absorption coeff =    547.2944878508624     cm-1
```

Do you want to calculate a mosaic crystal ? **0**

Do you want an asymmetrical cut [1/0] ? **0**

```
 Real(Ss) :  25.541823566710784 microradians
 Real(Sp) :  24.060473952622004 microradians

\ Ss and Sp represent the width of the Bragg peak, and will be used as
\ 'reduced units' in some of the plots, so that the peak will extend
\ from -1 to +1.
```

+/- how many microradians : **60**

How many points : **200**

Do you want to use sec [1/0] ? **0**

Do you want the R.C. not centered [1/0] ? **0**

Do you want to try another energy [1/0] ? **O**

$

VMS
$
$ DIR

```
Directory D13:[XRAYOP.XTAL]

GAAS.PAR;1           4     26-MAR-1987     14:17     (RWED,RWED,RE,RE)
ROCK_CURVE.P;1      20     26-MAR-1987     14:17     (RWED,RWED,RE,RE)
ROCK_CURVE.PAR;1     3     26-MAR-1987     14:17     (RWED,RWED,RE,RE)
ROCK_CURVE.S;1      20     26-MAR-1987     14:17     (RWED,RWED,RE,RE)

Total of 4 files, 47 blocks.
```

UNIX
%ls -al

```
-rw-r--r--  1 shadow      1789 Mar  9 15:23 gaas.par
-rw-r--r--  1 shadow      9800 Mar  9 15:27 rock_curve.p
-rw-r--r--  1 shadow      1051 Mar  9 15:27 rock_curve.par
-rw-r--r--  1 shadow      9800 Mar  9 15:27 rock_curve.s
```

GAAS.PAR will be the input parameter file to SHADOW. At the end of the file GAAS.PAR is a table of: eV f'(Ga) f''(Ga) f'(As) f''(As) which form the optical constant library. The user can edit this file if more accurate values are available, especially near an absorption edge.

$ TYPE GAAS.PAR

```
           0   1562378464.990918      3.2620290209213856E-08
          31          33  0.9790000000000000
(4.000000000000000,-6.8654264713317982E-17)
(4.000000000000000,6.8654264713317982E-17)
(8.473607549839534 5E-17,-4.000000000000000)
(8.473607549839534 5E-17,4.000000000000000)
  32.67800000000011       -40.80000000000018       10.00000000000364
  35.35699999999986       -50.74999999999727       24.99999999999272
          11
  11100.00000000000       -1.895109680624937       3.414937245198015
 -2.436850441775594       0.5607204097485073
  11110.00000000000       -1.880106255382257       3.410127243375178
 -2.449320912049193       0.5598036778163483
  11120.00000000000       -1.865102830139578       3.405317241552341
 -2.461791382322792       0.5588869458841894
  11130.00000000000       -1.850099404896898       3.400507239729505
 -2.474261852596391       0.5579702139520304
  11140.00000000000       -1.835095979654219       3.395697237906668
 -2.486732322869990       0.5570534820198715
  11150.00000000000       -1.820092554411540       3.390887236083831
 -2.499202793143589       0.5561367500877125
  11160.00000000000       -1.805089129168860       3.386077234260994
 -2.511673263417189       0.5552200181555536
  11170.00000000000       -1.790085703926181       3.381267232438158
 -2.524143733690788       0.5543032862233946
  11180.00000000000       -1.775082278683501       3.376457230615321
 -2.536614203964387       0.5533865542912357
  11190.00000000000       -1.760078853440822       3.371647228792484
 -2.549084674237986       0.5524698223590767
  11200.00000000000       -1.745075428198142       3.366837226969648
 -2.561555144511585       0.5515530904269178
```

ROCK_CURVE.PAR lists the parameters used to generate the rocking curve at 11160 eV, which are a function of the real part of Ss and Sp (for the S- and P-polarization). For this case, Ss = 25.541 and Sp = 24.060 microradians.

$ TYPE ROCK_CURVE.PAR

```
ZincBlende structure :
For atom A, fo + f' + if" =  (24.85407850869210,3.386077234260994)
        B,                =  (25.65378599830614,0.5552200181555536)
Lattice constant =     5.650000000000000      Angstroms
d-spacing        =     3.262029020921386      Angstroms
Photon energy  =    11160.00000000000      eV
Lambda  =     1.110978494623656      Angstroms
Theta (graz)  =     9.804650841199757      degrees
Bragg angle      =     9.807153296220226      degrees
SIN(theta)/Lambda =    0.1532788325282192      ratio.
Refraction index = 1 - delta - i*beta :
           delta =    7.3270650274570581E-06
            beta =    4.8385681505652676E-07
Absorption coeff =     547.2944878508624      cm-1
Temperature factor =    0.9790000000000000
Structure factor F(000) =  (238.7329504296558,15.76518900966619)
Structure factor F(hkl) =  (142.6426218594671,11.03752285669588)
Real(Ss) :  25.541823566710784 microradians
Real(Sp) :  24.060473952622004 microradians
```

NOW we can run SHADOW (finally). To check things out, let us use a monochromatic source with only vertical divergence.

$ GO SOURCE

```
SOURCE selected. Begin procedure.
This procedure generates a SOURCE for SHADOW.
```

Mode selected [? <ret> for HELP] ? : **prompt**

```
Call to INPUT

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Defining source :
When prompted for a yes/no answer, you may enter:
```

```
for YES     answer     Y, 1
for NO      answer     anything else
```

Do you want a verbose [1] or terse [0] output ? **0**

```
------------ SOURCE SPECS ------------------
```

Source modelling type [0-5] ? **0**

How many rays [1 - 5 000] ? **1000**

Seed [odd, 1000 - 1 000 000] ? **12345**

Do you want to optimize the source ? **0**

```
Source type : [ 0 ] regular source
              [ 1 ] normal wiggler
              [ 2 ] undulator
              [ 3 ] elliptical wiggler
```

Then ? **0**

X-Z plane source type [0-3] ? **0**

Source Depth [1-4] ? **1**

Source Angle Distribution [1-6] ? **2**

Horizontal half-divergence [(+)x, rads] ? **0**

. [(-)x, rads] ? **0**

Vertical [(+)z, rads] ? **60E-6**

. [(-)z, rads] ? **60E-6**

Do you want a Photon energy [Y/N] ? **1**

Energy distribution [1-3] ? **1**

Photon Energy [0] or Angstroms [1] ? **0**

Energy [eV] ? **11160**

Do you want to store the optical paths (OPD) [Y/N] ? **0**

Do you want to generate the A vectors (electric field) [Y/N] ? **0**

```
Exit from INPUT_SOURCE
Generated          250 rays out of         1000
                   500
                   750
                  1000
Exit from SOURCE
SOURCE => Source has been successfully generated.
SOURCE procedure completed.
```

Shadow:: **trace**

```
Ray Tracing Selected. Begin procedure.
```

Mode selected [? <ret> for HELP] ? : **prompt**

```
PROMPT selected.
Call to RESET
Exit from RESET

Mode selected is:
PROMPT
Options:      to start anew [ 0 ]
              to restart from a given OE [ 1 ]
```

Then ? **0**

```
Call to INPUT_OE

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When prompted for a yes/no answer, you may enter: for YES answer Y, 1 for NO answer anything else

Defining Optical Element: 1
```

Continue ? [^Z or %EXIT to terminate OS] **<ret>**

Do you want a verbose [1] or terse [0] output ? **0**

```
 You may save disk space by not writing out the  intermediate STAR or MIRR
data files. In general you will not need them unless you have specific
needs (footprints, etc.)

Files to write out. Options:
All.............................. [ 0 ]
Mirror only.....................[ 1 ]
Image at CP only................[ 2 ]
None............................[ 3 ]
```

Then ? **0**

```
 Optical Element definition:
```

Incidence Angle ? **10**

Source Distance ? **5000**

Reflection Angle? **10**

Image Distance ? **150**

```
//  The angles here do not matter, as they will be replaced by the exact
//  Bragg angle when you choose autotuning of the crystal and neither do
//  distances.
```

Reflector [0] or refractor [1] ? **0**

A: Is this a Kumakhov system? **0**

A: Is this mirror faceted [Y/N] ? **0**

Mirror surface [1-9] ? **5**

Is the mirror Cylindrical ? **0**

Is this optical element a Fresnel Zone Plate ? **0**

Are we dealing with a Grating ? **0**

Are we dealing with a crystal [Y/N] ? **1**

```
\  After we specify the mirror to be a crystal, SHADOW asks further questions
\  to define the problem. We will tell the program that we want the crystal to
\  be automatically set at the photon energy of 11160 eV.
```

File containing crystal parameters ? **GAAS.PAR**

Is it a mosaic crystal [Y/N] ? **0**

Is the crystal asymmetric [Y/N] ? **0**

Are we working in Johansson geometry [Y/N] ? **0**

Automatic Tuning of Crystal [Y/N] ? **1**

Energy, in eV, [0] or wavelength, in Angs., [1] ? **0**

Photon Energy ? **11160**

Is the mirror convex [Y/N] ? **0**

Reflectivity mode [0,1,2] ? **0**

Orientation Angle [Alpha] ? **0**

Mirror Dimensions finite [Y/N] ? **0**

Do you want to move the Source [Y/N] ? **0**

Do you want to move the mirror itself [Y/N] ? **0**

Distorted surface [Y/N] ? **0**

Do you want to include surface roughness [Y/N] ? **0**

Any screens in this OE [Y/N] ? **0**

Slit at continuation plane [Y/N] ? **0**

Extra Image plates [Y/N] ? **0**

File containing the source array ? **BEGIN.DAT**

```
 Exit from INPUT
 Tracing optical element #            1
 Call to SETSOUR
    ........
 Exit from RESET

Call to INPUT_OE

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Defining Optical Element: 2
```

Continue ? [^Z or %EXIT to terminate OS] **<ret>**

Do you want a verbose [1] or terse [0] output ? **0**

```
 You may save disk space by not writing out the  intermediate STAR or MIRR
data files. In general you will not need them unless you have specific
needs (footprints, etc.)

Files to write out. Options:
All.............................. [ 0 ]
Mirror only.....................[ 1 ]
Image at CP only................[ 2 ]
None............................[ 3 ]
```

Then ? **0**

```
 Optical Element definition:
```

Incidence Angle ? **10**

Source Distance ? **150**

Reflection Angle? **10**

Image Distance ? **5000**

Reflector [0] or refractor [1] ? **0**

A: Is this a Kumakhov system? **0**

A: Is this mirror faceted [Y/N] ? **0**

Mirror surface [1-9] ? **5**

Is the mirror Cylindrical ? **0**

Is this optical element a Fresnel Zone Plate ? **0**

Are we dealing with a Grating ? **0**

Are we dealing with a crystal [Y/N] ? **1**

File containing crystal parameters ? **GAAS.PAR**

Is it a mosaic crystal [Y/N] ? **0**

Is the crystal asymmetric [Y/N] ? **0**

Are we working in Johansson geometry [Y/N] ? **0**

Automatic Tuning of Crystal [Y/N] ? **1**

Energy, in eV, [0] or wavelength, in Angs., [1] ? **0**

Photon Energy ? **11160**

Is the mirror convex [Y/N] ? **0**

Reflectivity mode [0,1,2] ? **0**

Orientation Angle [Alpha] ? **180**

Mirror Dimensions finite [Y/N] ? **0**

Do you want to move the Source [Y/N] ? **0**

Do you want to move the mirror itself [Y/N] ? **0**

Distorted surface [Y/N] ? **0**

Do you want to include surface roughness [Y/N] ? **0**

Any screens in this OE [Y/N] ? **0**

Slit at continuation plane [Y/N] ? **0**

Extra Image plates [Y/N] ? **0**

```
 Exit from INPUT
 Tracing optical element #            2
 Call to SETSOUR
    ........
 Exit from RESET

Call to INPUT_OE

------------------------ S H A D O W ------------------------ May 1993 F.Cerrina CXrL/ECE - UW

Defining Optical Element: 3 Continue ? [ ^Z or %EXIT to terminate OS ] ^Z

 End of session
 Procedure completed. Return to COMMAND level
```

Shadow:: **exit**

The tracing has been completed. Let us look at the files that have been generated by SHADOW. You should have the following ones:

VMS

$ DIR

```
 Directory D13:[XRAYOP.XTAL]

BEGIN.DAT;1          188     26-MAR-1987 14:22     (RWED,RWED,RE,RE)
EFFIC.01;1             1     26-MAR-1987 14:41     (RWED,RWED,RE,RE)
EFFIC.02;1             1     26-MAR-1987 14:48     (RWED,RWED,RE,RE)
END.00;1               6     26-MAR-1987 14:22     (RWED,RWED,RE,RE)
END.01;1              11     26-MAR-1987 14:41     (RWED,RWED,RE,RE)
END.02;1              11     26-MAR-1987 14:48     (RWED,RWED,RE,RE)
GAAS.PAR;1             4     26-MAR-1987 14:17     (RWED,RWED,RE,RE)
MIRR.01;1            188     26-MAR-1987 14:41     (RWED,RWED,RE,RE)
MIRR.02;1            188     26-MAR-1987 14:48     (RWED,RWED,RE,RE)
OPTAX.01;1             2     26-MAR-1987 14:40     (RWED,RWED,RE,RE)
OPTAX.02;1             3     26-MAR-1987 14:48     (RWED,RWED,RE,RE)
ROCK_CURVE.P;1        20     26-MAR-1987 14:17     (RWED,RWED,RE,RE)
ROCK_CURVE.PAR;1       3     26-MAR-1987 14:17     (RWED,RWED,RE,RE)
ROCK_CURVE.S;1        20     26-MAR-1987 14:17     (RWED,RWED,RE,RE)
SAVE.DAT;1             8     26-MAR-1987 14:19     (RWED,RWED,RE,RE)
STAR.01;1            188     26-MAR-1987 14:41     (RWED,RWED,RE,RE)
STAR.02;1            188     26-MAR-1987 14:48     (RWED,RWED,RE,RE)
START.00;1             6     26-MAR-1987 14:22     (RWED,RWED,RE,RE)
START.01;1            11     26-MAR-1987 14:40     (RWED,RWED,RE,RE)
START.02;1            11     26-MAR-1987 14:48     (RWED,RWED,RE,RE)
TD.FIL;1               1     26-MAR-1987 14:19     (RWED,RWED,RE,RE)
```

```
Total of 23 files, 1089 blocks.
```

UNIX

% ls-al

```
total 1248
drwxr-sr-x   2 shadow       512 Jun 10 12:41 .
drwxr-sr-x   4 shadow       512 Mar  9 14:58 ..
-rw-rw-r--   1 shadow    104020 Jun 10 12:10 begin.dat
-rw-rw-r--   1 shadow       371 Jun 10 12:41 effic.01
-rw-rw-r--   1 shadow       371 Jun 10 12:41 effic.02
-rw-rw-r--   1 shadow      1498 Jun 10 12:10 end.00
-rw-rw-r--   1 shadow      4540 Jun 10 12:41 end.01
-rw-rw-r--   1 shadow      4555 Jun 10 12:41 end.02
-rw-r--r--   1 shadow      1485 Jun 10 10:20 gaas.par
-rw-rw-r--   1 shadow    104020 Jun 10 12:41 mirr.01
-rw-rw-r--   1 shadow    104020 Jun 10 12:41 mirr.02
-rw-rw-r--   1 shadow       297 Jun 10 12:41 optax.01
-rw-rw-r--   1 shadow       742 Jun 10 12:41 optax.02
-rw-rw-r--   1 shadow       103 Jun 10 11:31 rc.com
-rw-r--r--   1 shadow      9080 Jun 10 10:21 rock_curve.p
-rw-r--r--   1 shadow      1185 Jun 10 10:21 rock_curve.par
-rw-r--r--   1 shadow      9048 Jun 10 11:40 rock_curve.s
-rw-rw-r--   1 shadow    104020 Jun 10 12:41 star.01
-rw-rw-r--   1 shadow    104020 Jun 10 12:41 star.02
-rw-rw-r--   1 shadow      1493 Jun 10 12:10 start.00
-rw-rw-r--   1 shadow      4451 Jun 10 12:41 start.01
-rw-rw-r--   1 shadow      4466 Jun 10 12:41 start.02
-rw-rw-r--   1 shadow        30 Jun 10 12:41 systemfile.dat
```

Note the P-polarization has smaller average reflectivity, because of narrower width of the rocking curve (smaller value of Sp relative to Ss).

$ ty effic.01

```
 Of a total of   1000 rays, of which   1000 formed the input set
      0 were out of the mirror N.     1
 The mirror collects   1.0000     of the incoming flux.
 The average reflectivities are :
 S-pol                      0.37464
 P-pol                      0.35000
 Total                      0.36232
 The overall efficiency of the mirror is : 0.36232
```

We know that SHADOW must have changed the optical system angles, in order to satisfy Bragg's equation. To check the new values, let us run MIRINFO.

$ mirinfo

```
 ------------------- M I R I N F O ----------------------
                  vs. 3.0 - May 1993

MINFO> Mirror descriptor file. It must be an END.xx type.
```

MINFO> Please input filename: **end.01**

```
 MINFO> File read correctly.
```

MINFO> Title ? **plane crystal reflection**

MINFO> Comment ? **to test SHADOW computation of the rocking curve**

MINFO> Output file ? **mirr.inf**

```
 MINFO> Prepare output to file : mirr.inf

// Notice the incident and reflected angle have been replaced by the
// Bragg angle.
```

$

$

$ type mirr.inf

```
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 ********************   MIRROR  DESCRIPTION   ********************
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 plane crystal reflection
 to test SHADOW computation of the rocking curve.
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Input file specified:end.01
 Full file Specification :D13:[XRAYOP.XTAL]END.01;1
 Creation Date           :26-MAR-1987 14:41
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:          PLANE
Cylindrical figure                       NO
Element type                             REFLECTOR
Element type                             CRYSTAL
Lattice Spacing                           3.2620290209213856E-08
Bragg Reflection from
GAAS.PAR
Reflectivity                             OFF
Mirror dimensions                        UNLIMITED
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                       5000.000000000000
Image Plane                                 150.0000000000000
Incidence Angle                             80.19284670377978
Reflection/Diffraction Angle                80.19284670377978

Mirror parameters                        COMPUTED
Same configuration as Central Axis       NO
Objective focus at                          0.0000000000000000E+00
Image focus at                              0.0000000000000000E+00
Incidence angle                             0.0000000000000000E+00
Parameters used follow:
Plane mirror
```

```
Source of this O.E. moved                NO
Mirror at pole position ( no mov. )      YES
*********************************************************************
```

Now let us verify that SHADOW also computes the same rocking curve. Since the source we used was a point source, the incidence angle changes continuously along the mirror surface, accordingly to the aperture of the ray from the central axis. If we then plot the ray intensity versus z', i.e., the sine of the aperture at the image plane, we should obtain a curve that duplicates exactly the Bragg rocking curve. Let's compare the following plot with that done earlier using ROCK_CURVE.S. We use PREPLOT to display the rocking curve and generate a plottable file.

$

$

$ PREPLOT

PREPLOT> Input file ? **star.01**

```
Read                1000 rays.
Each ray has          12 entries.
```

PREPLOT> How many columns to write out ? **2**

```
Row [1-12]  : the individual column
Row   [20]  : R = SQRT(X**2 + Y**2 + Z**2)
Row   [21]  : angle from the Y-axis
Row   [22]  : the magnitude of A vector
Row   [23]  : A**2
```

PREPLOT> Row # 1 : **6**

PREPLOT> 2 : **23**

```
Options - Enter
0     for excluding the losses
1     for including losses at a particular O.E.
2     for plotting all the rays .
3     for plotting ONLY the losses (all of them)
4     for plotting ONLY the losses at a given O.E.
```

PREPLOT> Then ? **0**

VMS

```
Output options :
  [ 0 ] store rays in a file
  [ 1 ] plot directly on screen
  [ 2 ] both
```

Then ? **2**

PREPLOT> Output file ? **STAR.01.PLT**

PREPLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 : OOOOOOO

```
**********
Found         1000 good points out of        1000
```

UNIX

Found 1000 good points out of 1000

Display type:

[0] Xwindow

[1] Tektronix

[2] Postscript file

Terminal type: **0**

The default filename is preplot.dat -- it is a good idea to change the name to something meaningful.

% mv preplot.dat star.01.dat

We will now create a plottable file of the intensity after the second crystal, but we will be plotting it out later. If you are interested, plot it now just as we did for STAR01.PLT. The Bragg curve should be sharper.

$ PREPLOT

PREPLOT> Input file ? **star.02**

```
Read                1000 rays.
Each ray has          12 entries.
```

PREPLOT> How many columns to write out ? **2**

```
Row [1-12]  : the individual column
Row   [20]  : R = SQRT(X**2 + Y**2 + Z**2)
Row   [21]  : angle from the Y-axis
Row   [22]  : the magnitude of A vector
Row   [23]  : A**2
```

PREPLOT> Row # 1 : **6**

PREPLOT> 2 : **23**

```
Options - Enter
0     for excluding the losses
1     for including losses at a particular O.E.
2     for plotting all the rays .
3     for plotting ONLY the losses (all of them)
4     for plotting ONLY the losses at a given O.E.
```

PREPLOT> Then ? **0**

VMS

```
 Output options :
   [ 0 ] store rays in a file
   [ 1 ] plot directly on screen
   [ 2 ] both
```

Then ? **0**

PREPLOT> Output file ? **STAR.02.PLT**

PREPLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 : **1**

```
 ***********
Found         1000 good points out of        1000
```

UNIX

Found 1000 good points out of 1000

Display type:

[0] Xwindow

[1] Tektronix

[2] Postscript file

Terminal type: **0**

% mv preplot.dat star.02.dat

To illustrate the case of Bragg diffraction, we will now offset slightly the second crystal from its ideal position. At first, we will be setting directly (no autotuning or other features) the second crystal to the ``wrong'' angle, i.e., 2.777E-3 degrees away from the nominal Bragg angle (that we know exactly from the run of MIRINFO). It is a good idea to create a new subdirectory for clarity. We will copy down the image of the first mirror and restart the calculation from the second optical element.

VMS
$
$ CREATE/DIRECTORY [.OFFSET]
$ SET DEF [.OFFSET]
$ COPY [-]STAR.01,GAAS.PAR [ ]
$ COPY [-]OPTAX.01 [ ]

UNIX
%
% mkdir offset
% cd offset
% cp ./../star.01
% cp ./../gaas.par
% cp ./../optax.01

$ GO TRACE

```
 Ray Tracing Selected. Begin procedure.
```

Mode selected [? <ret> for HELP] ? : **PROMPT**

```
 PROMPT selected.
 Call to RESET
 Exit from RESET

Mode selected is:
PROMPT
Options:      to start anew                [ 0 ]
              to restart from a given OE   [ 1 ]
```

Then ? **1**

Previous element number : **1**

Image file of the previous OE ? **STAR.01**

Do you want to change the input mode ? **0**

```
 Call to INPUT_OE

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Defining Optical Element: 2
```

Continue ? [^Z or %EXIT to terminate OS] **<ret>**

Do you want a verbose [1] or terse [0] output ? **1**

```
 You may save disk space by not writing out the  intermediate STAR or MIRR
data files. In general you will not need them unless you have specific
needs (footprints, etc.)

Files to write out.Options:
All.............................. [ 0 ]
Mirror only.....................[ 1 ]
Image at CP only................[ 2 ]
None............................[ 3 ]
```

Then ? **0**

```
 Optical Element definition:
```

Incidence Angle ? **80.1956244**

Source Distance ? **150**

Reflection Angle? **80.1900690**

Image Distance ? **5000**

Reflector [0] or refractor [1] ? **0**

A: Is this a Kumakhov system? **0**

A: Is this mirror faceted [Y/N] ? **0**

Mirror surface [1-9] ? **0**

Is the mirror Cylindrical ? **0**

Is this optical element a Fresnel Zone Plate ? **0**

Are we dealing with a Grating ? **0**

Are we dealing with a crystal [Y/N] ? **1**

File containing crystal parameters ? **GAAS.PAR**

Is it a mosaic crystal [Y/N] ? **0**

Is the crystal asymmetric [Y/N] ? **0**

Are we working in Johansson geometry [Y/N] ? **0**

Automatic Tuning of Crystal [Y/N] ? **0**

Is the mirror convex [Y/N] ? **0**

Reflectivity mode [0,1,2] ? **0**

Orientation Angle [Alpha] ? **180**

Mirror Dimensions finite [Y/N] ? **0**

Do you want to move the Source [Y/N] ? **0**

Do you want to move the mirror itself [Y/N] ? **0**

Distorted surface [Y/N] ? **0**

Do you want to include surface roughness [Y/N] ? **0**

Any screens in this OE [Y/N] ? **0**

Slit at continuation plane [Y/N] ? **0**

Extra Image plates [Y/N] ? **0**

```
 Exit from INPUT
 Tracing optical element #            2
 Call to SETSOUR
   ........
 Exit from RESET
```

Do you want to change input mode ? **0**

```
 Call to INPUT_OE

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Defining Optical Element: 3
```

Continue ? [^Z or %EXIT to terminate OS] **^Z**

```
 End of session
 Procedure completed. Return to COMMAND level
```

Shadow:: **exit**

Exit to DCL

$

$

The tracing has been completed. Notice how easy it is to restart from any given point along the optical system. We now generate another plottable file, similarly to what we did before.

$ PREPLOT

PREPLOT> Input file ? **STAR.02**

```
 Read                1000 rays.
 Each ray has          12 entries.
```

PREPLOT> How many columns to write out ? **2**

```
 Row [1-12]  : the individual column
 Row   [20]  : R = SQRT(X**2 + Y**2 + Z**2)
 Row   [21]  : angle from the Y-axis
 Row   [22]  : the magnitude of A vector
 Row   [23]  : A**2
```

PREPLOT> Row # 1 : **6**

PREPLOT> 2 : **23**

```
Options - Enter
0     for excluding the losses
1     for including losses at a particular O.E.
2     for plotting all the rays .
```

```
3      for plotting ONLY the losses (all of them)
4      for plotting ONLY the losses at a given O.E.
```

PREPLOT> Then ? **0**

VMS

```
Output options :
  [ 0 ] store rays in a file
  [ 1 ] plot directly on screen
  [ 2 ] both
```

Then ? **0**

PREPLOT> Output file ? **STAR.02.PLT**

PREPLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 : **1**

```
**********
Found         1000 good points out of         1000
```

UNIX

Found 1000 good points out of 1000

Display type:

[0] Xwindow

[1] Tektronix

[2] Postscript file

Terminal type: **0**

% mv preplot.dat star.02.dat

We can now plot out the two cases, offset and not, together. This is a typical mode of using SHADOW, in order to appreciate the changes induced by small variations in the OS. Notice that we first read all the files and only at the end we PLOT. This is because TopDrawer determines the plot limits at the first occurrence of the PLOT command (unless they are user-specified). Since we are plotting the intensity versus the *angle* , the offset of the second crystal will cause the third plot to be out of bounds (try it). We created the following command file to plot the three images on the same graph.

Several interesting observations can be drawn from this plot. Notice the three curves. The highest one represents the intensity transmitted at each wavelength by the first crystal; notice that it is essentially identical with the rocking curve and is centered around zero. The second (lower) curve centered around zero represents the intensity transmitted by the *two* crystals; it is, in this case, equal to the square of the original intensity. The sides are thus more sharply defined, while the ``bandpass'' is not changed substantially. However, the fact that the sides are sharper means that the transmitted intensity is a better approximation to a rectangle, i.e., to an ideal monochromator. The third and smallest curve is clearly offset to the side. This is due to the rotation imparted to the second crystal, so that the rays are not anymore coming out centered along the optical axis. This displaces the rocking curves of the two crystals relative to each other, thus giving the typical ``spike''. A careful observation will reveal the onset of the two different rocking curves. This is highlighted by the added traces.

Two Crystals II

In this section of the primer we will reconsider the case of the two crystals, but with a different type of source. We will be using a *collimated* source with a continuous energy distribution. The crystals will be set at the same conditions as for the former case. There the change of angle across the face of the crystal produced the change in reflectivity and thus in intensity. In the present case it will be the change in *wavelength* that will give rise to a different reflectivity. Besides this, the run is exactly like the former one, so we will not repeat the full description.

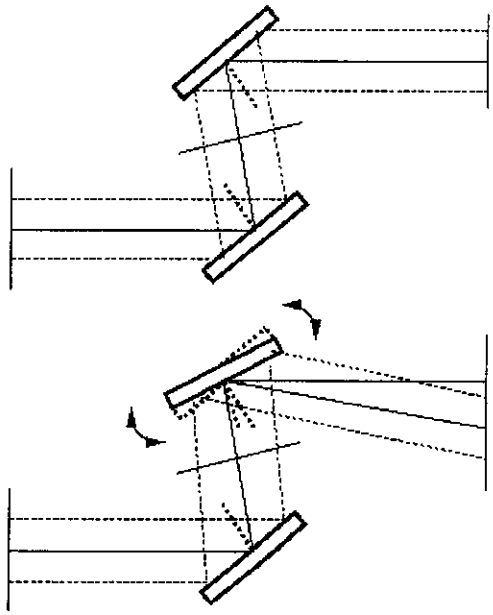

Fig. 1 - Two-crystal monochromator in parallel radiation

VMS

$ CREATE/DIRECTORY [.XTAL2]
$ SD [XRAYOP.XTAL2]
$ COPY [GAAS.PAR] [ ]*.*

UNIX
% mkdir ./xtal2
% cd ./xtal2
% cp ./../gaas.par

GO SOURCE

```
 SOURCE selected. Begin procedure.
 This procedure generates a SOURCE for SHADOW.
```

Mode selected [? <ret> for HELP] ? : **PROMPT**

```
 Call to INPUT

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Defining source : When prompted for a yes/no answer, you may enter: for YES answer Y, 1 for NO answer anything else
```

Do you want a verbose [1] or terse [0] output ? **0**

```
------------- SOURCE SPECS ------------------
```

Source modelling type [0-5] ? **0**

How many rays [1 - 5 000] ? **1000**

Seed [odd, 1000 - 1 000 000] ? **12345**

Do you want to optimize the source ? **0**

```
Source type : [ 0 ] regular source
              [ 1 ] normal wiggler
              [ 2 ] undulator
              [ 3 ] elliptical wiggler
```

Then ? **0**

X-Z plane source type [0-3] ? **1**

Source Width [x] ? **1**

Height [z] ? **1**

Source Depth [1-4] ? **1**

Source Angle Distribution [1-6] ? **1**

Horizontal half-divergence [(+)x, rads] ? **0**

. | (-)x, rads] ? **0**

Vertical [(+)z, rads] ? **0**

. | (-)z, rads] ? **0**

Do you want a Photon energy [Y/N] ? **1**

Energy distribution [1-3] ? **3**

Photon Energy [0] or Angstroms [1] ? **0**

From photon energy or wavelength ... ? **11156**

... to photon energy or wavelength : ? **11164**

Do you want to store the optical paths (OPD) [Y/N] ? **0**

Do you want to generate the A vectors (electric field) [Y/N] ? **0**

```
 Exit from INPUT_SOURCE
 Generated          250 rays out of         1000
                    500
                    750
                   1000
 Exit from SOURCE
 SOURCE => Source has been successfully generated.
 SOURCE procedure completed.
```

Shadow:: **TRACE**

```
 Ray Tracing Selected. Begin procedure.
```

Mode selected [? <ret> for HELP] ? : **PROMPT**

```
 PROMPT selected.
 Call to RESET
 Exit from RESET

Mode selected is: PROMPT Options: to start anew [ 0 ] to restart from a given OE [ 1 ] Then ? 0

 Call to INPUT_OE

------------------------ S H A D O W -------------------------
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When prompted for a yes/no answer, you may enter:
for YES answer Y, 1
for NO answer anything else

Defining Optical Element: 1 Continue ? [ ^Z or %EXIT to terminate OS ] <ret>

Do you want a verbose [ 1 ] or terse [ 0 ] output ? 0

 You may save disk space by not writing out the  intermediate STAR or MIRR
data files. In general you will not need them unless you have specific
needs (footprints, etc.)

Files to write out. Options:
All.............................. [ 0 ]
Mirror only.....................[ 1 ]
Image at CP only................[ 2 ]
None............................[ 3 ]

Then ? 0

 Optical Element definition:
```

Incidence Angle ? **10**

Source Distance ? **5000**

Reflection Angle? **10**

Image Distance ? **149.8956**

Reflector [0] or refractor [1] ? **0**

A: Is this a Kumakhov system? **0**

A: Is this mirror faceted [Y/N] ? **0**

Mirror surface [1-9] ? **5**

Is the mirror Cylindrical ? **0**

Is this optical element a Fresnel Zone Plate ? **0**

Are we dealing with a Grating ? **0**

Are we dealing with a crystal [Y/N] ? **1**

File containing crystal parameters ? **GAAS.PAR**

Is it a mosaic crystal [Y/N] ? **0**

Is the crystal asymmetric [Y/N] ? **0**

Are we working in Johansson geometry [Y/N] ? **0**

Automatic Tuning of Crystal [Y/N] ? **1**

Energy, in eV, [0] or wavelength, in Angs., [1] ? **0**

Photon Energy ? **11160**

Is the mirror convex [Y/N] ? **0**

Reflectivity mode [0,1,2] ? **0**

Orientation Angle [Alpha] ? **0**

Mirror Dimensions finite [Y/N] ? **0**

Do you want to move the Source [Y/N] ? **0**

Do you want to move the mirror itself [Y/N] ? **0**

Distorted surface [Y/N] ? **0**

Do you want to include surface roughness [Y/N] ? **0**

Any screens in this OE [Y/N] ? **0**

Slit at continuation plane [Y/N] ? **0**

Extra Image plates [Y/N] ? **0**

File containing the source array ? **BEGIN.DAT**

```
Exit from INPUT
Tracing optical element #            1
Call to SETSOUR
   ........
Exit from RESET
```

Do you want to change input mode ? **0**

```
Call to INPUT_OE

------------------------ S H A D O W -------------------------
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```

Defining Optical Element: 2 Continue ? [^Z or %EXIT to terminate OS] **<ret>**

Do you want a verbose [1] or terse [0] output ? **0**

```
 You may save disk space by not writing out the  intermediate STAR or MIRR
data files. In general you will not need them unless you have specific
needs (footprints, etc.)

Files to write out. Options:
All............................ [ 0 ]
Mirror only.....................[ 1 ] Image at CP only.............[ 2 ]
None............................[ 3 ]
```

Then ? **0**

```
 Optical Element definition:
```

Incidence Angle ? **10**

Source Distance ? **149.8956**

Reflection Angle? **10**

Image Distance ? **5000**

Reflector [0] or refractor [1] ? **0**

A: Is this a Kumakhov system? **0**

A: Is this mirror faceted [Y/N] ? **0**

Mirror surface [1-9] ? **5**

Is the mirror Cylindrical ? **0**

Is this optical element a Fresnel Zone Plate ? **0**

Are we dealing with a Grating ? **0**

Are we dealing with a crystal [Y/N] ? **1**

File containing crystal parameters ? **GAAS.PAR**

Is it a mosaic crystal [Y/N] ? **0**

Is the crystal asymmetric [Y/N] ? **0**

Are we working in Johansson geometry [Y/N] ? **0**

Automatic Tuning of Crystal [Y/N] ? **1**

Energy, in eV, [0] or wavelength, in Angs., [1] ? **0**

Photon Energy ? **11160**

Is the mirror convex [Y/N] ? **0**

Reflectivity mode [0,1,2] ? **0**

Orientation Angle [Alpha] ? **180**

Mirror Dimensions finite [Y/N] ? **0**

Do you want to move the Source [Y/N] ? **0**

Do you want to move the mirror itself [Y/N] ? **0**

Distorted surface [Y/N] ? **0**

Do you want to include surface roughness [Y/N] ? **0**

Any screens in this OE [Y/N] ? **0**

Slit at continuation plane [Y/N] ? **0**

Extra Image plates [Y/N] ? **0**

```
 Exit from INPUT
 Tracing optical element #            2
 Call to SETSOUR
    ........
 Exit from RESET
```

Do you want to change input mode ? **0**

```
 Call to INPUT_OE

 ---------------------- S H A D O W -------------------------
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Defining Optical Element: 3
```

Continue ? [^Z or %EXIT to terminate OS] **^Z**

```
 End of session
 Procedure completed. Return to COMMAND level
```

Shadow:: **EXIT**

```
 Exit to DCL
```

$ TYPE EFFIC.01

```
 Of a total of   1000 rays, of which   1000 formed the input set
      0 were out of the mirror N.     1
 The mirror collects   1.0000     of the incoming flux.
 The average reflectivities are :
 S-pol                    0.36560
 P-pol                    0.34058
 Total                    0.35309
 The overall efficiency of the mirror is : 0.35309
```

$ MIRINFO

```
 -------------------- M I R I N F O ----------------------
                   vs. 3.0 - May 1993

MINFO> Mirror descriptor file. It must be an END.xx type.
```

MINFO> Please input filename: **END.01**

MINFO> File read correctly.

MINFO> Title ? **PLANE CRYSTAL REFLECTION 2**

MINFO> Comment ? **<ret>**

MINFO> Output file ? **MIRR.INF**

```
 MINFO> Prepare output to file : MIRR.INF
```

$ TYPE MIRR.INF

```
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 ********************   MIRROR  DESCRIPTION   ********************
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 PLANE CRYSTAL REFLECTION 2
 MIRR.INF
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Input file specified:END.01
 Full file Specification :D13:[XRAYOP.XTAL2]END.01;1
 Creation Date           :30-MAR-1987 14:04
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:      PLANE
Cylindrical figure                      NO
Element type                            REFLECTOR
Element type                            CRYSTAL
Lattice Spacing                             3.2620290209213856E-08
Bragg Reflection from
GAAS.PAR
Reflectivity                            OFF
Mirror dimensions                       UNLIMITED
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                       5000.000000000000
Image Plane                                 149.8956000000000
Incidence Angle                             80.19284670377978
```

```
 Reflection/Diffraction Angle              80.19284670377978

 Mirror parameters                         COMPUTED
 Same configuration as Central Axis        NO
 Objective focus at                           0.0000000000000000E+00
 Image focus at                               0.0000000000000000E+00
 Incidence angle                              0.0000000000000000E+00
 Parameters used follow:
    Plane mirror
 Source of this O.E. moved                 NO
 Mirror at pole position ( no mov. )       YES
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

VMS
$ DIR

```
 Directory D13:[XRAYOP.XTAL2]

BEGIN.DAT;1          188 30-MAR-1987 14:01     (RWED,RWED,RE,RE)
EFFIC.01;1             1 30-MAR-1987 14:03     (RWED,RWED,RE,RE)
EFFIC.02;1             1 30-MAR-1987 14:05     (RWED,RWED,RE,RE)
END.00;1               6 30-MAR-1987 14:01     (RWED,RWED,RE,RE)
END.01;1              11 30-MAR-1987 14:04     (RWED,RWED,RE,RE)
END.02;1              11 30-MAR-1987 14:05     (RWED,RWED,RE,RE)
GAAS.PAR;1             4 26-MAR-1987 14:17     (RWED,RWED,RE,RE)
MIRR.01;1            188 30-MAR-1987 14:03     (RWED,RWED,RE,RE)
MIRR.02;1            188 30-MAR-1987 14:05     (RWED,RWED,RE,RE)
MIRR.INF;1             5 30-MAR-1987 14:07     (RWED,RWED,RE,RE)
OPTAX.01;1             2 30-MAR-1987 14:03     (RWED,RWED,RE,RE)
OPTAX.02;1             3 30-MAR-1987 14:05     (RWED,RWED,RE,RE)
STAR.01;1            188 30-MAR-1987 14:03     (RWED,RWED,RE,RE)
STAR.02;1            188 30-MAR-1987 14:05     (RWED,RWED,RE,RE)
START.00;1             6 30-MAR-1987 14:01     (RWED,RWED,RE,RE)
START.01;1            11 30-MAR-1987 14:03     (RWED,RWED,RE,RE)
START.02;1            11 30-MAR-1987 14:05     (RWED,RWED,RE,RE)

Total of 17 files, 1012 blocks.
```

UNIX
% ls -al

```
total 1192
drwxrwsr-x   2 shadow       512 Jun 11 11:22 .
drwxr-sr-x   4 shadow      1024 Jun 11 11:09 ..
-rw-rw-r--   1 shadow    104020 Jun 11 11:12 begin.dat
-rw-rw-r--   1 shadow       371 Jun 11 11:12 effic.01
-rw-rw-r--   1 shadow       371 Jun 11 11:12 effic.02
-rw-rw-r--   1 shadow      1506 Jun 11 11:12 end.00
-rw-rw-r--   1 shadow      4540 Jun 11 11:12 end.01
-rw-rw-r--   1 shadow      4555 Jun 11 11:12 end.02
-rw-r--r--   1 shadow      1485 Jun 11 11:09 gaas.par
-rw-rw-r--   1 shadow    104020 Jun 11 11:12 mirr.01
-rw-rw-r--   1 shadow    104020 Jun 11 11:12 mirr.02
-rw-rw-r--   1 shadow      2262 Jun 11 11:22 mirr.inf
-rw-rw-r--   1 shadow       297 Jun 11 11:12 optax.01
-rw-rw-r--   1 shadow       742 Jun 11 11:12 optax.02
-rw-rw-r--   1 shadow    104020 Jun 11 11:12 star.01
-rw-rw-r--   1 shadow    104020 Jun 11 11:12 star.02
-rw-rw-r--   1 shadow      1500 Jun 11 11:11 start.00
-rw-rw-r--   1 shadow      4451 Jun 11 11:12 start.01
-rw-rw-r--   1 shadow      4466 Jun 11 11:12 start.02
-rw-rw-r--   1 shadow        30 Jun 11 11:12 systemfile.dat
```

$ PREPLOT

PREPLOT> Input file ? **STAR.02**

```
 Read                 1000 rays.
 Each ray has           12 entries.
```

PREPLOT> How many columns to write out ? **2**

```
 Row [1-12]  : the individual column
 Row   [20]  : R = SQRT(X**2 + Y**2 + Z**2)
 Row   [21]  : angle from the Y-axis
 Row   [22]  : the magnitude of A vector
 Row   [23]  : A**2
```

PREPLOT> Row # 1 : **11**

PREPLOT> 2 : **23**

```
// Note, here we are plotting energy vs. amplitude squared.

Option: Angstroms          [ 0 ]
        Electronvolts      [ 1 ]
        Cm-1               [ 2 ]
```

PREPLOT> Then ? **1**

```
 Options - Enter
 0      for excluding the losses
 1      for including losses at a particular O.E.
 2      for plotting all the rays .
 3      for plotting ONLY the losses (all of them)
 4      for plotting ONLY the losses at a given O.E.
```

PREPLOT> Then ? **0**

VMS

```
 Output options :
   [ 0 ] store rays in a file
   [ 1 ] plot directly on screen
   [ 2 ] both
```

Then ? **0**

PREPLOT> Output file ? **STAR02.PLT**

PREPLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 : **2**

```
**********
Found         1000 good points out of         1000
```

UNIX

Found 1000 good points out of 1000

Display type:

[0] Xwindow

[1] Tektronix

[2] Postscript file

Terminal type: **0**

% MV PREPLOT.DAT STAR.02.DAT

Now the second crystal will be offset.

VMS
$
$ CREATE/DIRECTORY [.OFFSET2]
$ SET DEF [.OFFSET2]
$ COPY [-]STAR.01,GAAS.PAR [ ]
$ COPY [-]OPTAX.01 [ ]

UNIX
%
% mkdir offset2
% cd offset2
% cp ./../star.01
% cp ./../gaas.par
% cp ./../optax.01

$ GO TRACE

```
 Ray Tracing Selected. Begin procedure.
```

Mode selected [? <ret> for HELP] ? : **PROMPT**

```
 PROMPT selected.
 Call to RESET
 Exit from RESET
Mode selected is: PROMPT Options: to start anew [ 0 ] to restart from a given OE [ 1 ] Then ? 1
```

Previous element number : **1**

Image file of the previous OE ? **STAR.01**

Do you want to change the input mode ? **0**

```
 Call to INPUT_OE
---------------------- S H A D O W ------------------------ May 1993 F.Cerrina CXrL/ECE - UW
Defining Optical Element: 2 Continue ? [ ^Z or %EXIT to terminate OS ] <ret>
```

Do you want a verbose [1] or terse [0] output ? **0**

```
 You may save disk space by not writing out the  intermediate STAR or MIRR
data files. In general you will not need them unless you have specific
needs (footprints, etc.)

Files to write out. Options:
All.............................. [ 0 ]
Mirror only.....................[ 1 ]
Image at CP only................[ 2 ]
None............................[ 3 ]
```

Then ? **0**

```
 Optical Element definition:
```

Incidence Angle ? **10**

Source Distance ? **149.8956**

Reflection Angle? **10**

Image Distance ? **5000**

Reflector [0] or refractor [1] ? **0**

A: Is this a Kumakhov system? **0**

A: Is this mirror faceted [Y/N] ? **0**

Mirror surface [1-9] ? **5**

Is the mirror Cylindrical ? **0**

Is this optical element a Fresnel Zone Plate ? **0**

Are we dealing with a Grating ? **0**

Are we dealing with a crystal [Y/N] ? **1**

File containing crystal parameters ? **GAAS.PAR**

Is it a mosaic crystal [Y/N] ? **0**

Is the crystal asymmetric [Y/N] ? **0**

Are we working in Johansson geometry [Y/N] ? **0**

Automatic Tuning of Crystal [Y/N] ? **1**

Energy, in eV, [0] or wavelength, in Angs., [1] ? **0**

Photon Energy ? **11160**

Is the mirror convex [Y/N] ? **0**

Reflectivity mode [0,1,2] ? **0**

Orientation Angle [Alpha] ? **180**

Mirror Dimensions finite [Y/N] ? **0**

Do you want to move the Source [Y/N] ? **0**

Do you want to move the mirror itself [Y/N] ? **1**

Rotation around X axis [degrees] ? **2.777E-3**

. Y. ? **<ret>**

. Z. ? **<ret>**

Mirror Offset. In X ? **<ret>**

. Y ? **<ret>**

. Z ? **<ret>**

Distorted surface [Y/N] ? **0**

Do you want to include surface roughness [Y/N] ? **0**

Any screens in this OE [Y/N] ? **0**

Slit at continuation plane [Y/N] ? **0**

Extra Image plates [Y/N] ? **0**

Exit from INPUT

```
Tracing optical element #            2
Call to SETSOUR
  ........
Exit from RESET
```

Do you want to change input mode ? **0**

```
Call to INPUT_OE

------------------------ S H A D O W -------------------------- May 1993 F.Cerrina CXrL/ECE - UW

Defining Optical Element: 3
```

Continue ? [^Z or %EXIT to terminate OS] **^Z**

```
End of session
Procedure completed. Return to COMMAND level
```

Shadow:: **EXIT**

```
Exit to DCL
```

$ PREPLOT

PREPLOT> Input file ? **STAR.01**

```
Read                1000 rays.
Each ray has          12 entries.
```

PREPLOT> How many columns to write out ? **2**

```
Row [1-12]  : the individual column
Row   [20]  : R = SQRT(X**2 + Y**2 + Z**2)
Row   [21]  : angle from the Y-axis
Row   [22]  : the magnitude of A vector
Row   [23]  : A**2
```

PREPLOT> Row # 1 : **11**

PREPLOT> 2 : **23**

```
Option:    Angstroms        [ 0 ]
           Electronvolts    [ 1 ]
           Cm-1             [ 2 ]
```

PREPLOT> Then ? **1**

```
Options - Enter
0      for excluding the losses
1      for including losses at a particular O.E.
2      for plotting all the rays .
3      for plotting ONLY the losses (all of them)
4      for plotting ONLY the losses at a given O.E.
```

PREPLOT> Then ? **0**

VMS

```
Output options :
  [ 0 ] store rays in a file
  [ 1 ] plot directly on screen
  [ 2 ] both
```

Then ? **0**

PREPLOT> Output file ? **STAR01.PLT**

```
**********
Found         1000 good points out of        1000
```

UNIX

Found 1000 good points out of 1000

Display type:

[0] Xwindow

[1] Tektronix

[2] Postscript file

Terminal type: **0**

% mv preplot.dat star.01.dat

$

$

$ PREPLOT

PREPLOT> Input file ? **STAR.02**

```
Read                  1000 rays.
Each ray has            12 entries.
```

PREPLOT> How many columns to write out ? **2**

```
Row [1-12]  : the individual column
Row   [20]  : R = SQRT(X**2 + Y**2 + Z**2)
Row   [21]  : angle from the Y-axis
Row   [22]  : the magnitude of A vector
Row   [23]  : A**2
```

PREPLOT> Row # 1 : **11**

PREPLOT> 2 : **23**

```
Option:    Angstroms          [ 0 ]
           Electronvolts      [ 1 ]
           Cm-1               [ 2 ]
```

PREPLOT> Then ? **1**

```
Options - Enter
0      for excluding the losses
1      for including losses at a particular O.E.
2      for plotting all the rays .
3      for plotting ONLY the losses (all of them)
4      for plotting ONLY the losses at a given O.E.
```

PREPLOT> Then ? **0**

VMS

```
Output options :
  [ 0 ] store rays in a file
  [ 1 ] plot directly on screen
  [ 2 ] both
```

Then ? **0**

PREPLOT> Output file ? **STAR.02.PLT**

```
**********
Found         1000 good points out of        1000
```

UNIX

Found 1000 good points out of 1000

Display type:

[0] Xwindow

[1] Tektronix

[2] Postscript file

Terminal type: 0

% mv preplot.dat star.02.dat