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Chapter 1

Introduction

The utilities to SHADOW are a collection of programs written to perform a specific task on either the input or output. They are designed to give the user more information about the results in either tabular or graphic form. Currently the graphics package used is TopDrawer. SHADOW utilities are run through a shell program. Once inside the shell, the utilities are divided into six categories. They are:

- Preprocessors

- Postprocessors

- Macros

- Optical properties

- Graphics

- General

When the shell is invoked, a menu comes up with the first level of options. The up and down arrow keys ($\uparrow$, $\downarrow$)move the cursor to the desired option within a list, <RETURN> moves to the list. Selecting an option moves one level down to the list of utilities that fall in that category. Some utilities may fall in more than one category, in which case they will be found in both. Each category will list the utility followed by a one line description of what the program does. At this point the user can either run the utility (R), get help on the utility (H), quit (Q), or return to the main menu (<RETURN>).

Chapter 2

Preprocessors

This section of the Utilities Manual will cover those utilities that need to be run before SHADOW. The programs generate files, some of them unformatted, that are used as input to SHADOW in various places such as source optimization, crystal diffraction, reflectivities of coatings and/or multilayers, and surface distortions. In this way SHADOW can trace more specific systems with more realistic results.

BRAGG

Purpose:	Create a file which can be used by SHADOW in the computation of the reflectivity of a single crystal.
Input:	Interactive from terminal.
Output:	Formatted files (user specified).

Description:

In order to ray trace an optical system containing a crystal, SHADOW needs some preliminary data. These data are prepared by BRAGG. SHADOW can handle the so called symmetric Bragg case where the crystal planes are parallel to the surface, as well as the asymmetric case. Within the context of the symmetric case, the local reflectivity calculated by the Darwin-Prins formalism is :

$$R = \left| \sqrt{F_H/F_{\bar{H}}} \left[\eta \pm \sqrt{\eta^2 - 1} \right] \right|^2 \tag{2.1}$$

where,

$$\eta = \frac{-\Delta\theta \sin(2\theta_B) + \Gamma \, F_0}{|P| \, \Gamma \, (F_H F_{\bar{H}})} \tag{2.2}$$

θ is the glancing angle, θ_B the Bragg angle, Γ a constant, P a polarization factor, and F_H the structure factor relative to the scattering vector H ($F_{\bar{H}}$ is in the $\bar{H}$ direction).
The structure factor F_H needs more explanation.

$$F_H = \sum_{j=1}^{H} f_j e^{i\vec{r}_j \cdot \vec{H}} \tag{2.3}$$

It is the cell structure factor, and as such depends on:

1. $\vec{H}$, the scattering vector

2. $\vec{r}_j$, the location of atoms within a unit cell in units of a (lattice count).

3. f, the atomic scattering factors of the individual atom.

H is simply the vector defined by (H,K,L), where H, K, and L are the indices of the crystal plane.
Four types of crystal structure are supported. Let say there are atom A and atom B making up the basis within each cubic unit cell, then the locations of each atom for the crystal

structures are :

	A	B	lattice
ZincBlende	(0,0,0)	(1/4,1/4,1/4)	fcc
Rocksalt	(0,0,0)	(1/2,1/2,1/2)	fcc
Simple fcc	(0,0,0)		fcc
CsCl	(0,0,0)	(1/2,1/2,1/2)	cubic

Of course atom A can be the same as atom B. In that case, the ZincBlende reduces to the diamond structure; rocksalt to simple cubic; and CsCl to simple bcc. All together they cover the geometry of most commonly found crystals.

The scattering factor f depends on the atomic propreties. This quantity is complex, and is written as :

$$f = f_0 + f' + i * f"$$ (2.4)

f_0 is the non-dispersive portion of the real part, while f' and $f"$ are the dispersive part. f' and $f"$ are functions of photon energy for each element, and they are readily obtained from our optical constant library (see PREREFL about the library). On the other hand, we don't have a database for f_0 and it must be supplied by the user. f_0 is a function of the perpendicular component of the photon momentum, i.e., $\left(\frac{2\pi}{\lambda}\right)\sin\theta$. At the Bragg peak, $k_\perp$ is exactly $\frac{\pi}{d}$. Since we are working near the Bragg peak, BRAGG asks the user to enter the values of $f_0\left(\frac{\sin\theta}{\lambda}\right)$ at the neighborhood where $\frac{\sin\theta}{\lambda}$ is approximately $\frac{1}{2d}$. Three points at that neighborhood are required in order to do a quadratic fitting.

A good listing of all f_0 values is found in the International Tables of X-Ray Crystallography, Vol. III, sect.2.2, table 2.2A, p.72. A shorter version, adapted from *X-ray Diffraction*, by B.E.Warren, Addison-Wesley, is listed in the SHADOW PRIMER, sect.6.4, p.84.

The example we use here is GaAs(111) crystal. It is the same one as in SHADOW PRIMER. Here we concentrate on the BRAGG part of the modelling, while the user can refer to PRIMER for the SHADOW part. A description on how to run a two crystals case is given there. GaAs has ZincBlende structure with a = 5.65 Å. Note two capitalized letters must be used for each element (Gallium as GA, Tungsten as WW). Then the user is asked to input (3) values of f_0 for each atom. Since the program now knows the 2d spacing, it will type out the value of $\frac{\sin\theta}{\lambda}$ near the Bragg peak in order to assist the user in selecting the correct $f_0\left(\frac{\sin\theta}{\lambda}\right)$. After that, f' and $f"$ are simply defined by the photon energy range. A Debye-Waller factor $\exp^{-M}$ (between 0 and 1) is introduced to account for thermal vibrations. To neglect the finite temperature effect, enter the value of 1 for the Debye-Waller factor. At this point, all the parameters are defined for SHADOW and they are stored in

a formatted file (GAAS.PAR). Rocking curves can also be generated by BRAGG for the user's convenience.

As an example, we pick 11160 eV. BRAGG outputs some useful data. Note θ(graz) is almost the same as Bragg angle, the difference being that the latter is corrected for refraction of the radiation at the crystal surface. The last two items printed are Real(Ss) and Real(Sp), they are the widths of the rocking curves in the two polarizations (s-perpendicular, p-parallel to the plane of incidence). Thus the user can choose the angular range of the rocking curves he wants to generate (60 microradian cover more than twice the width). These data are stored in ROCK_CURVE.PAR, while the rocking curves themselves are stored in ROCK_CURVE.S and ROCK_CURVE.P. Graphs of both files are shown below.

The file GAAS.SHA is the input to SHADOW. It is formatted so that the user may edit the data for f' and f''. The data format is explained in the example. However, we strongly advise not to edit the file unless the data have been determined to be inaccurate e.g. for the description near an absorption edge.

Examples:

The first example will be for a symmetrical case, after which we will run the asymmetrical case.

```
$
$ BRAGG
All crystal structures are refered to a cubic unit cell.
Bravais lattice type :
0 for  ZincBlende
1 for  Rocksalt
2 for simple FCC
3      for     CsCl structure
Then ?
0                              \* select ZincBlende *\
Lattice constant (Angs) ?
5.65                           \* lattice constant *\
Index of crystal plane of reflection H,K,L :
1,1,1                          \* indices *\
*********************************************************
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                                    \* Gallium *\
Enter 2-letters (capitalized) atomic symbol for atom B :
AS                                    \* Arsenic *\
************************************************************
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 ,
For atom A, first set :         \* Ga *\
0.14,27.162                              ! The International Tables for X-ray
         , second set :                 ! Crystallography lists fo as a
0.15,26.783                              ! function of SIN(theta)/Lambda for
         , third set :                  ! each element and some ions.
0.16,26.406                             !
For atom B, first set :         \* As! Here the user needs to supply fo
0.14,28.742                              ! centered around 0.15327..., and
         , second set :                 ! within some limits that SHADOW can
0.15,28.307                              ! interpolate for fo.
         , third set :          !
0.16,27.877
************************************************************
f', f" is furnished from optical constant library within ...
minimum photon energy (eV) :
11100                              \* lower range boundary *\
maximum photon energy (eV) :
11200                              \* upper range boundary *\
energy step (eV) :
10
Do you want to include crystal absorption [1/0] ?
1                                 \* always *\
Temperature (Debye-Waller) factor :
0.979
Output file name (for SHADOW) :
GAAS.SHA                          \* try to use a meaningful name *\
Do you want to generate a rocking curve [1/0] ?
```

```
1                                     \* for examination *\
... at what energy (eV) ?     \* following only for rocking curve *\
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 an asymmetrical cut [1/0] ?
0                                     \* symmetrical this time *\
1/2 width of Rock Curve  s-pol  = :    25.54182356671078     microradians
1/2 width of Rock Curve  p-pol  = :    24.06047395262200     microradians

+/- how many microradians :
60                                    \* width of calculation *\
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] ?
0
$ DIR/SINCE

Directory CXRL$DUA0:[SHADOW.XRAYOP.DOCUMENT.UTIL.BRAGG]

GAAS.SHA;1                    4  19-SEP-1989 13:13:12.77  (RWED,RWED,RE,)
ROCK_CURVE.P;1              20  19-SEP-1989 13:13:25.78  (RWED,RWED,RE,)
ROCK_CURVE.PAR;1             3  19-SEP-1989 13:14:57.71  (RWED,RWED,RE,)
ROCK_CURVE.S;1             20  19-SEP-1989 13:13:25.64  (RWED,RWED,RE,)

Total of 4 files, 47 blocks.
$
```

At the end of the file GAAS.SHA is a table of :
eV   f'(Ga)   f"(Ga)   f'(As)   f"(As)
from the optical constant library. The users can edit this part if they have more accurate
values, especially near an absorption edge.

```
$ TY GAAS.SHA
          0   1562378464.990918        3.2620290209213856E-08
         31              33  0.9790000000000000
 (4.000000000000000,-6.8654264713317982E-17)
 (4.000000000000000,6.8654264713317982E-17)
 (8.4736075498395345E-17,-4.000000000000000)
 (8.4736075498395345E-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 11600 eV.
$ !
$
$ TY 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
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)
The width of the Rock Curve is
1/2 width for s-pol  = :    25.54182356671078     microradians
1/2 width for p-pol  = :    24.06047395262200     microradians
Theta (graz)      =    9.804650841199757     degrees
Bragg angle(corr)  =    9.807153296220226     degrees
$
$ TY ROCK_CURVE.S
-6.0000000000000001E-05  4.4734048523468558E-02
-5.9396984924623116E-05  4.5743273694228373E-02
-5.8793969849246232E-05  4.6788310752051259E-02
          :                      :
          :                      :
 5.8793969849246230E-05  4.6607134825068392E-02
 5.9396984924623114E-05  4.5572622137689755E-02
 5.9999999999999999E-05  4.4573179462104161E-02
$ !
$ ! Plot out the rocking curve for S- and P-polarization.
$ !
 The following example was run for an asymmetrical\index{crystal, asymmetric}
cut silicon crystal\index{crystal} with the
```

cut at seven degrees between the face and Bragg\index{Bragg} planes. We run between 7700
 and 7800 eV, and generate a rocking curve at 7750 eV. Notice for this case you
 get a rocking curve for the incidence and reflection\index{reflection} at the crystal\index{crystal}. The
 parameter file that acts as input to SHADOW does not specify symmetric or
 asymmetric. This information is input to SHADOW when tracing, so once a file
 is set up for a crystal\index{crystal}, one does not have to rerun
BRAGG\index{BRAGG} for the other case of
 the same crystal\index{crystal} unless new rocking curves are desired.
 $
 $ BRAGG
 All crystal structures are refered to a cubic unit cell.
 Bravais lattice type :
 0 for ZincBlende
 1 for Rocksalt
 2 for simple FCC
 3   for   CsCl structure
 Then ?
 0
 Lattice constant (Angs) ?
 5.43
 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 :
 SI
 Enter 2-letters (capitalized) atomic symbol for atom B :
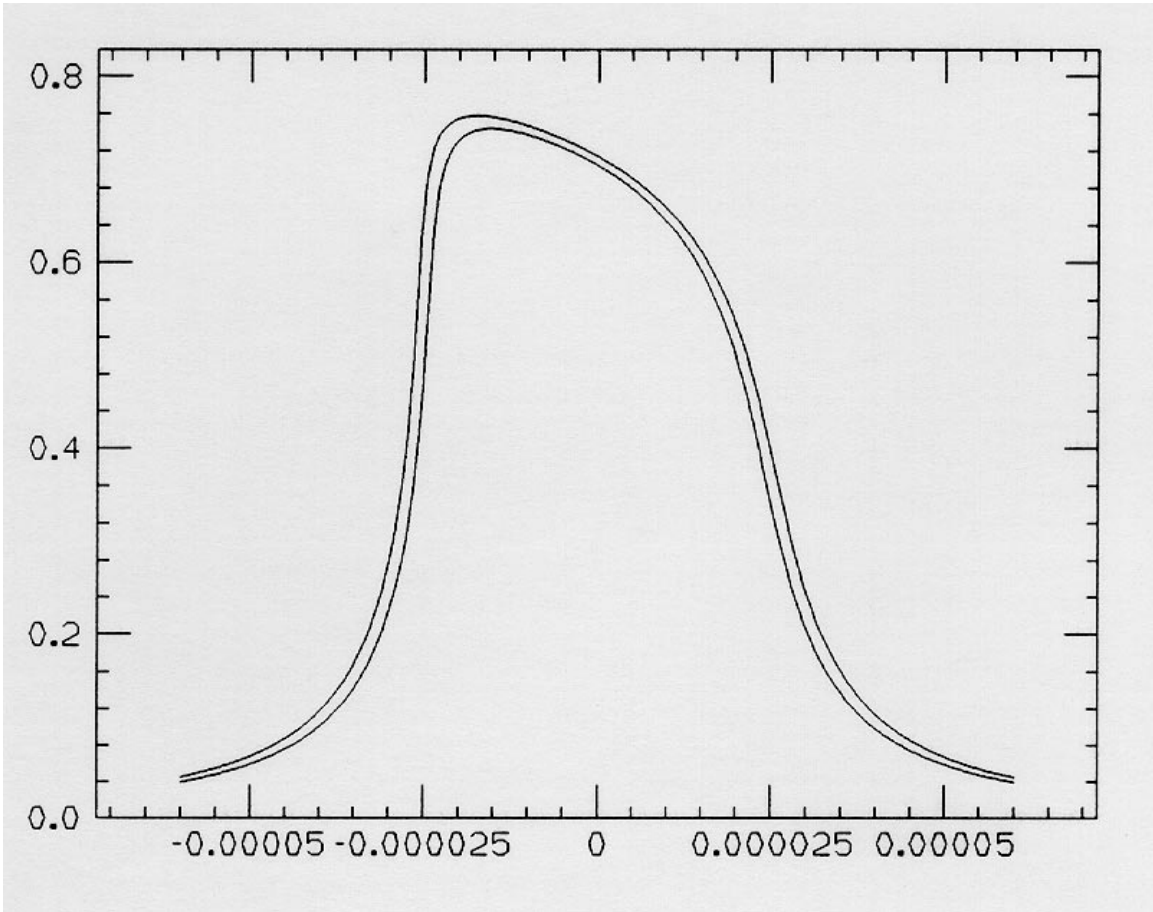
Figure 2.1: BRAGG: Rocking curve for S- and P- polarization

```
 SI
************************************************************
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 =   0.1594890246380182     ratio.
************************************************************
Please enter 1) SIN(theta)/Lambda, 2) fo ,
```

```
For atom A, first set :
0.1,12.16
          , second set :
0.2,9.67
          , third set :
0.3,8.22
For atom B, first set :
0.1,12.16
          , second set :
0.2,9.67
          , third set :
0.3,8.22
***********************************************************
f', f" is furnished from optical constant library within ...
minimum photon energy (eV) :
7700
maximum photon energy (eV) :
7800
energy step (eV) :
10
Do you want to include crystal absorption [1/0] ?
1
Temperature (Debye-Waller) factor :
1.0
Output file name (for SHADOW) :
SI.PAR
Do you want to generate a rocking curve [1/0] ?
1
... at what energy (eV) ?
7750

So far, we are working with:
Lambda    =    1.599809032258065     Angstroms
Theta (graz)   =    14.78259099147192     degrees
Bragg angle    =     14.78449376730854      degrees
Structure factor  = (61.29837293588675,1.976536272774998)
refraction index = 1 - delta - i*beta :
          delta =   8.1919893381993125E-06
           beta =   2.0040488614427989E-07
Absorption coeff =   157.4164179247638     cm-1
```

```
Do you want an asymmetrical cut [1/0] ?
1                                            \* aysmmetrical cut *\
Angle (deg) between face and bragg planes (CW)=
7                                            \* seven degree angle *\
The width of the Rock Curve in function of incident angle is
1/2 width for s-pol  =  :    10.76098572573549    microradians
1/2 width for p-pol  =  :    9.359850847544060    microradians
The width of the Rock Curve in function of reflected angle is
1/2 width for s-pol  =  :    29.48906494122322    microradians
1/2 width for p-pol  =  :    25.64943923522630    microradians
Asymmetric factor b=  :    2.740368372638810


+/- how many microradians :
80
How many points :
150
Do you want to use sec [1/0] ?
1
Do you want the R.C. not centered [1/0] ?
1
Do you want to try another energy [1/0] ?
0
$
$ TY SI.PAR
          0    1760078747.302978      3.1350119616996679E-08
         14            14   1.000000000000000
(4.000000000000000,-6.8654264713317982E-17)
(4.000000000000000,6.8654264713317982E-17)
(8.4736075498395345E-17,-4.000000000000000)
(8.4736075498395345E-17,4.000000000000000)
   15.69000000000000       -40.50000000000000        51.99999999999999
   15.69000000000000       -40.50000000000000        51.99999999999999
          11
   7700.000000000000       0.2846972178807969        0.3536787673872427
  0.2846972178807969       0.3536787673872427
   7710.000000000000       0.2843014434140994        0.3528241239968134
  0.2843014434140994       0.3528241239968134
   7720.000000000000       0.2839056689474015        0.3519694806063841
  0.2839056689474015       0.3519694806063841
```

```
   7730.000000000000        0.2835098944807037        0.3511148372159547
 0.2835098944807037        0.3511148372159547
   7740.000000000000        0.2831141200140062        0.3502601938255254
 0.2831141200140062        0.3502601938255254
   7750.000000000000        0.2827183455473083        0.3494055504350961
 0.2827183455473083        0.3494055504350961
   7760.000000000000        0.2823225710806105        0.3485509070446667
 0.2823225710806105        0.3485509070446667
   7770.000000000000        0.2819267966139127        0.3476962636542374
 0.2819267966139127        0.3476962636542374
   7780.000000000000        0.2815310221472151        0.3468416202638081
 0.2815310221472151        0.3468416202638081
   7790.000000000000        0.2811352476805173        0.3459869768733787
 0.2811352476805173        0.3459869768733787
   7800.000000000000        0.2807394732138195        0.3451323334829494
 0.2807394732138195        0.3451323334829494
$
$ TY ROCK_CURVE.PAR
ZincBlende structure :
For atom A, fo + f' + if" =  (10.83612379466686,0.3494055504350961)
        B,                =  (10.83612379466686,0.3494055504350961)
Lattice constant =    5.430000000000000       Angstroms
d-spacing        =    3.135011961699668       Angstroms
Photon energy  =    7750.000000000000       eV
Lambda    =    1.599809032258065       Angstroms
SIN(theta)/Lambda =   0.1594890246380182      ratio.
Refraction index = 1 - delta - i*beta :
          delta =   8.1919893381993125E-06
           beta =   2.0040488614427989E-07
Absorption coeff =    157.4164179247638       cm-1
Temperature factor =    1.000000000000000
Structure factor F(000) = (114.2617467643785,2.795244403480769)
Structure factor F(hkl) = (61.29837293588675,1.976536272774998)
Width of Rock Curve in function of incident angle:
1/2 width for s-pol = :    10.76098572573549       microrad
1/2 width for p-pol = :    9.359850847544060       microrad
Incident Bragg angle  =    21.78259099147192       degrees
Incident corrected angle   =    21.78388955458310       degrees
Width of Rock Curve in function of reflected angle:
1/2 width for s-pol = :    29.48906494122322       microrad
```
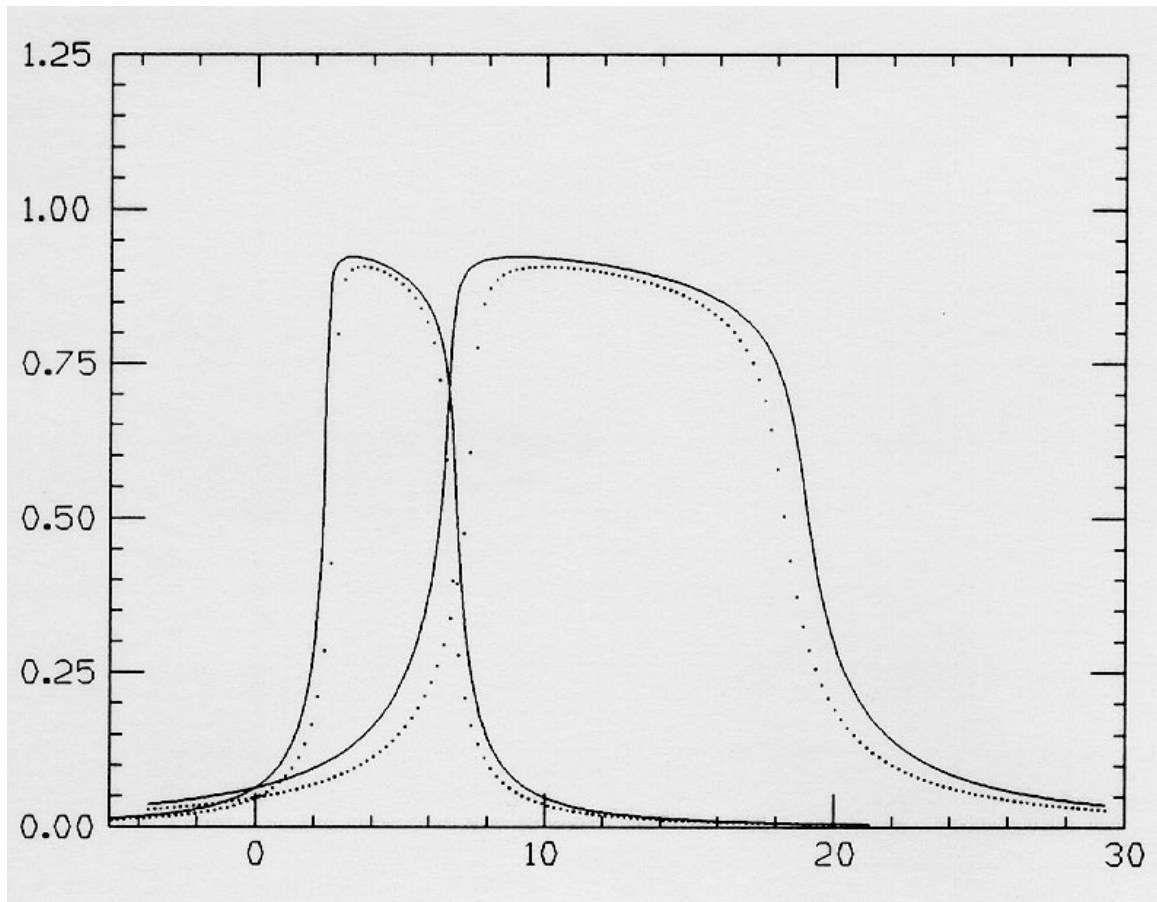
Figure 2.2: BRAGG: Asymmetric Crystal cut

```
1/2 width for p-pol = :      25.64943923522630       microrad
Reflected Bragg angle =    7.782590991471924       degrees
Reflected corrected angle  =    7.786149532751679       degrees
Asymmetric factor b=  :    2.740368372638810
Angle between face and bragg planes (CW)=   7.000000000000000       degrees
```

The following plot shows the rocking curves for incident and reflected light. The S-polarization is denoted by a solid line, while the P-polarization is simply plotted points. We show the pertinent information when running TRACE.

```
$ go trace

Ray Tracing Selected. Begin procedure.

  :
  :
  :

Are we dealing with a crystal [ Y/N ] ?
1
File containing crystal parameters ?
si.par
Is the crystal asymmetric [ Y/N ] ?
1
Enter the angle formed by the crystal planes with the crystal surface. Use a
positive value if the plane normal lies along the +Y direction (focusing),
negative otherwise.
Planes angle [ deg ] ?
7
Automatic Tuning of Crystal [ Y/N ] ?
1
You must then supply the wavelength (or photon energy) at
which you want the crystal tuned.
Energy, in eV, [ 0 ] or wavelength, in Angs., [ 1 ] ?
0
Photon Energy ?
7750

  :
  :
  :
```

ERGSET

Purpose:	To set up an ERG /Grasshopper type monochromator at a user specified photon energy, given an existing system.
Input:	A set of STARTxx files describing the optical system at zero order. The user will also need to input the following parameters: M_0–exit slit distance M_1–codling slit distance codling slit incidence angle grating radius grating incidence angle lines per cm photon energy or wavelength the calculations are desired at the maximum slit-to-slit distance.
Output:	A set of STARTxx files describing the optical system at a user specified photon energy. The user may give them different names from the original system. Also writes the system parameters to a text file or terminal (TT:) if the user chooses.

Description:

The ERG /Grasshopper monochromators are fairly complex to setup because of the correlated rotations of grating, codling slit, and condensing mirror. The user typically knows the beamline parameters at zero order. To avoid annoying calculations, this utility will set up the parameters for an ERG /Grasshopper type monochromator at a given photon energy, given the system at zero order. It will compute zero order slit distance, carriage movement, and codling slit tilt. It will then modify the system to include these parameters, "tuning" the monochromator to the specified wavelength or energy. Notice that no other parameters are modified (e.g reflectivity switches, sizes, errors, etc.) so that the operation is indeed exactly equivalent to retuning the monochromator.

Examples:

Below is the output from SYSINFO on a 2m Grasshopper monochromator at zero order. The output from SYSPLOT for two and three dimensional plots follows.

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S Y S T E M     D E S C R I P T I O N **************
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
System at zero order
2m Grasshopper -- ERGSET Example
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 #    Optical Element:                                  Creation Time:
   1    CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.ERGSET]END.01;5     8-JAN-1990 15:38
   2    CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.ERGSET]END.02;5     8-JAN-1990 15:38
   3    CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.ERGSET]END.03;5     8-JAN-1990 15:39
   4    CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.ERGSET]END.04;5     8-JAN-1990 15:39
   5    CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.ERGSET]END.05;5     8-JAN-1990 15:39
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


Optical Element #              1      System Number:

MIRROR     SPHERICAL              DIM CHECK       COMPUTED        REFLEC. OFF

  Orientation          270.0000000000000     deg.
  Source Plane         230.0000000000000
  Incidence Ang.       88.0000000000000      deg.
  Reflection Ang.      88.0000000000000      deg.
  Image Plane          108.4500000000000
     ----------------

Optical Element #              2      System Number:

MIRROR     ELLIPTICAL             DIM CHECK       COMPUTED        REFLEC. OFF

  Orientation          90.00000000000002     deg.
  Source Plane         108.4500000000000
  Incidence Ang.       88.5000000000002      deg.
  Reflection Ang.      88.5000000000002      deg.
  Image Plane          22.50000000000000
     ----------------

Optical Element #              3      System Number:

MIRROR     CODLING SLIT           DIM CHECK       COMPUTED        REFLEC. OFF
```

```
   Orientation          180.0000000000000      deg.
   Source Plane          22.50000000000000
   Incidence Ang.        88.00000000000000      deg.
   Reflection Ang.       88.00000000000000      deg.
   Image Plane           3.489500000000000
      ----------------

Optical Element #              4       System Number:

GRATING   SPHERICAL            DIM CHECK      EXTERNAL      REFLEC. OFF

   Orientation          180.0000000000000      deg.
   Source Plane          3.489500000000000
   Incidence Ang.        88.00000000000000      deg.
   Reflection Ang.       88.00000000000000      deg.
   Image Plane           6.979899340500188
      ----------------

Optical Element #              5       System Number:

MIRROR    ELLIPTICAL           DIM CHECK      COMPUTED      REFLEC. OFF

   Orientation          180.0000000000000      deg.
   Source Plane          100.0000000000000
   Incidence Ang.        88.00000000000000      deg.
   Reflection Ang.       88.00000000000000      deg.
   Image Plane           100.0000000000000
      ----------------


                    OPTICAL SYSTEM CONFIGURATION
                     Laboratory Reference Frame.

OPT. Elem #        X =                  Y =                  Z =

      0         0.00000000000E+00   0.00000000000E+00   0.00000000000E+00
      1         0.00000000000E+00   230.00000000        0.00000000000E+00
         1'        7.5650895776        338.18582125        0.29010291601E-1

      2         15.130179155        446.37164250        0.58020583202E-15
         2'       16.697548841        468.78607328        1.1775590155
```

3	18.264918527	491.20050405	2.3551180309
3'	18.508296668	494.68097363	2.2942178587
4	18.751674810	498.16144321	2.2333176864
4'	19.237900705	505.11479746	2.5986173929
5	26.203988197	604.73448980	7.8322130172
5'	33.178573147	704.47570145	6.0869723734

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
* * * * * * * * * * * * * * *          E N D          * * * * * * * * * * * * * *
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Three dimensional and two dimensional plots of system at zero order.   Now run ERGSET
on the zero order START files.

```
$
$ ERGSET
Definition of ERG at ZERO Order Position.
Distance M0-exit slit ? 238.9
M1-Codling slit distance ? 45
Codling Slit Incidence Angle ? 88
Grating Radius ? 200
Grating Incidence Angle ? 87.8
Lines per CM ? 12000
Enter [ 0 ] to use eV, [ 1 ] Angs. 0
Then ? 40
Order to be used ? -1
Maximum slit-to-slit distance : 611.5
Do you want to save the inputs [ Y/N ] ? y
File describing M1 ?          START.02
              Codling Slit ? START.03
              Grating ?      START.04
START.04

 read OK.
Enter new file name for grating. To use the same, just type <ret>
```
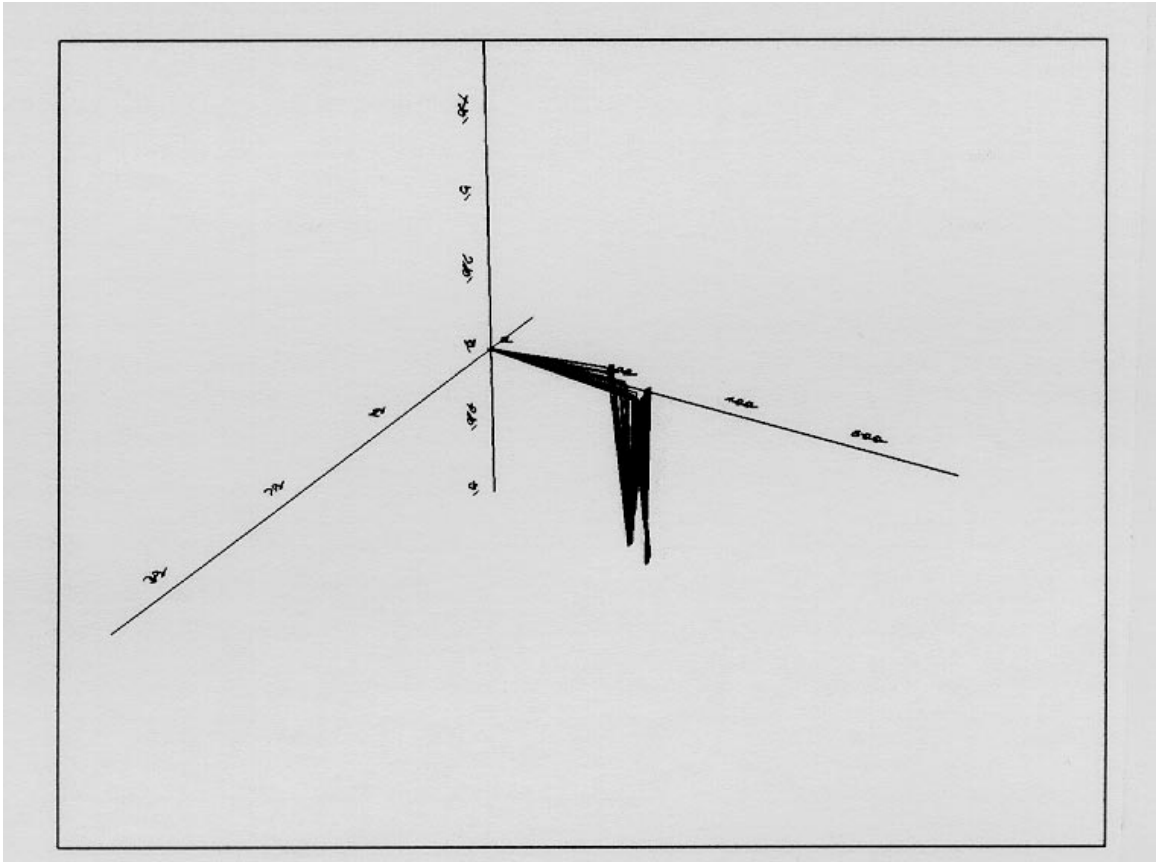
Figure 2.3: Three dimensional before ERGSET
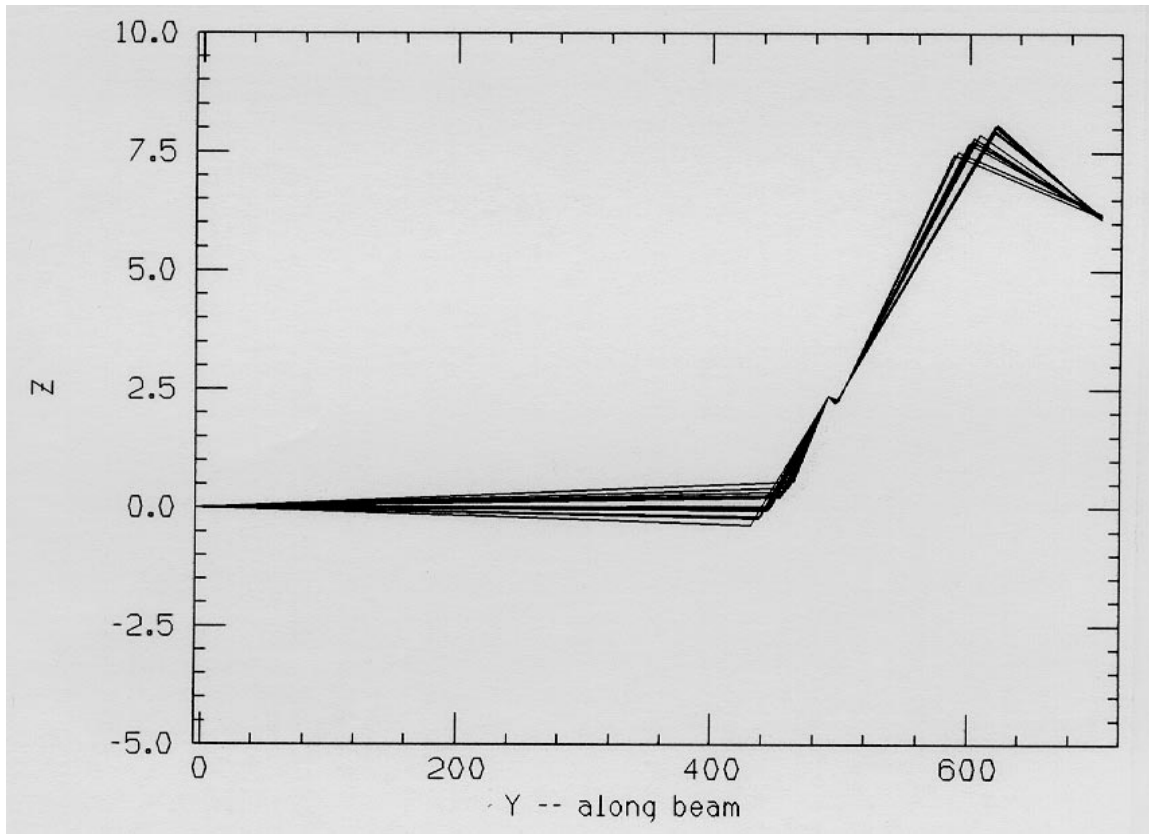
Figure 2.4: Two Dimensional before ERGSET– Side view
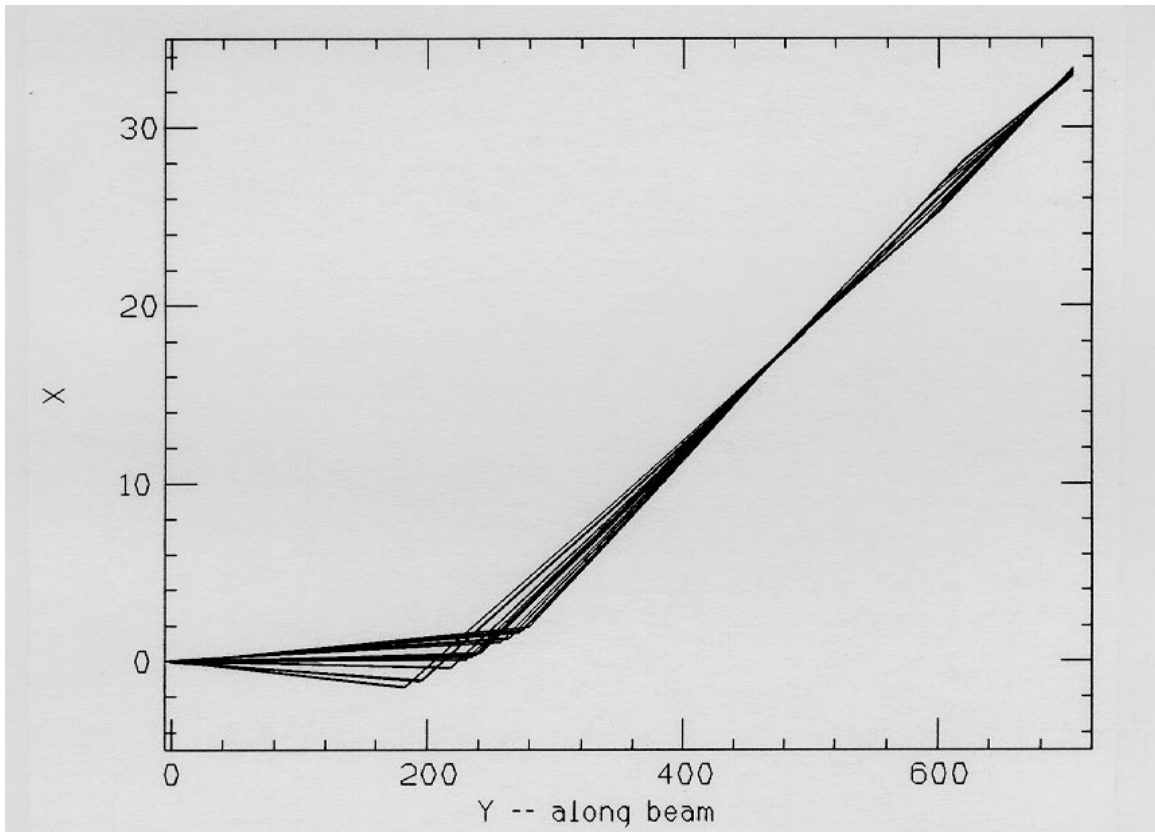
Figure 2.5: Two Dimensional before ERGSET – Top view

```
Then ? 40EV.04
START.03

 read OK.
Enter new file name for Codling Slit. To use the same, just type <ret>
Then ? 40EV.03
Enter new file name for M1. To use the same, just type <ret>
Then ? 40EV.02
File name ? 40EV.PAR
$
$ type 40EV.PAR
   238.9630000000000      ! Distance M0-exit slit
   45.00000000000000      ! Codling slit distance
   88.00000000000000      ! Codling Slit Incidence Angle
   200.0000000000000      ! Grating Radius
   88.00000000000000      ! Grating Incidence Angle
   13.95979868100039      ! Zero order slit distance
   47.19515409835923      ! Carriage movement
   6.902390810838892      ! Codling slit tilt
start.02
 ! M1 file
start.03
 ! Codling Slit file
start.04
 ! Grating file
```

40EV.PAR contains the fixed parameters of the system that we entered when we ran ERGSET. It also contains the parameters it computed for our Grasshopper at 40 eV – the zero order slit distance, carriage movement, and codling slit tilt.
The output from SYSINFO for the new system is shown below.

```
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 ************** S Y S T E M    D E S C R I P T I O N **************
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Grasshopper at 40 eV
ERGSET Example
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
Input file specified:
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 #    Optical Element:                                      Creation Time:
   1   CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.ERGSET.40EV]END.01;1 29-DEC-1989 15:
   2   CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.ERGSET.40EV]END.02;1 29-DEC-1989 15:
   3   CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.ERGSET.40EV]END.03;1 29-DEC-1989 15:
   4   CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.ERGSET.40EV]END.04;1 29-DEC-1989 15:
   5   CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.ERGSET.40EV]END.05;1 29-DEC-1989 15:
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


Optical Element #              1      System Number:

MIRROR     SPHERICAL             DIM CHECK      COMPUTED      REFLEC. OFF

  Orientation          270.0000000000000      deg.
  Source Plane         230.0000000000000
  Incidence Ang.       88.00000000000000      deg.
  Reflection Ang.      88.00000000000000      deg.
  Image Plane          108.4500000000000
     ----------------

Optical Element #              2      System Number:

MIRROR     ELLIPTICAL            DIM CHECK      COMPUTED      REFLEC. OFF

  Orientation          90.00000000000002      deg.
  Source Plane         61.25484590164077
  Incidence Ang.       88.50000000000002      deg.
  Reflection Ang.      88.50000000000002      deg.
  Image Plane          25.00000000000000
     ----------------

Optical Element #              3      System Number:

MIRROR     CODLING SLIT          DIM CHECK      COMPUTED      REFLEC. OFF

  Orientation          180.0000000000000      deg.
  Source Plane         20.00000000000000
  Incidence Ang.       81.09760918916109      deg.
  Reflection Ang.      81.09760918916109      deg.
```

```
   Image Plane              3.489949670250097
     ----------------

Optical Element #              4      System Number:

GRATING   SPHERICAL              DIM CHECK      EXTERNAL      REFLEC. OFF

   Orientation              180.0000000000000      deg.
   Source Plane             3.489949670250097
   Incidence Ang.           88.00000000000000      deg.
   Reflection Ang.          74.19521837832219      deg.
   Image Plane              54.47210960704609
     ----------------

Optical Element #              5      System Number:

MIRROR    ELLIPTICAL             DIM CHECK      COMPUTED      REFLEC. OFF

   Orientation              180.0000000000000      deg.
   Source Plane             100.0000000000000
   Incidence Ang.           88.00000000000000      deg.
   Reflection Ang.          88.00000000000000      deg.
   Image Plane              100.0000000000000
     ----------------


                      OPTICAL SYSTEM CONFIGURATION
                       Laboratory Reference Frame.

OPT. Elem #        X =                  Y =                  Z =

     0          0.00000000000E+00   0.00000000000E+00   0.00000000000E+00
     1          0.00000000000E+00   230.00000000        0.00000000000E+00
         1'        7.5650895776        338.18582125        0.29010291601E-15

     2          11.838011627        399.29145343        0.45395915774E-15
         2'       13.579533500        424.19637651        1.3083989061

     3          14.972750999        444.12031498        2.3551180309
         3'       15.208115658        447.48618642        1.4633436043
```

```
        4              15.443480317        450.85205786        0.57156917764
            4'              19.238055131        505.11700586        3.4224191225

        5              26.204142623        604.73669820        8.6560147468
            5'              33.178727573        704.47790984        6.9107741031


++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
* * * * * * * * * * * * * *              E  N  D              * * * * * * * * * * * * * *
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

The new system is plotted below in two and three dimensions.
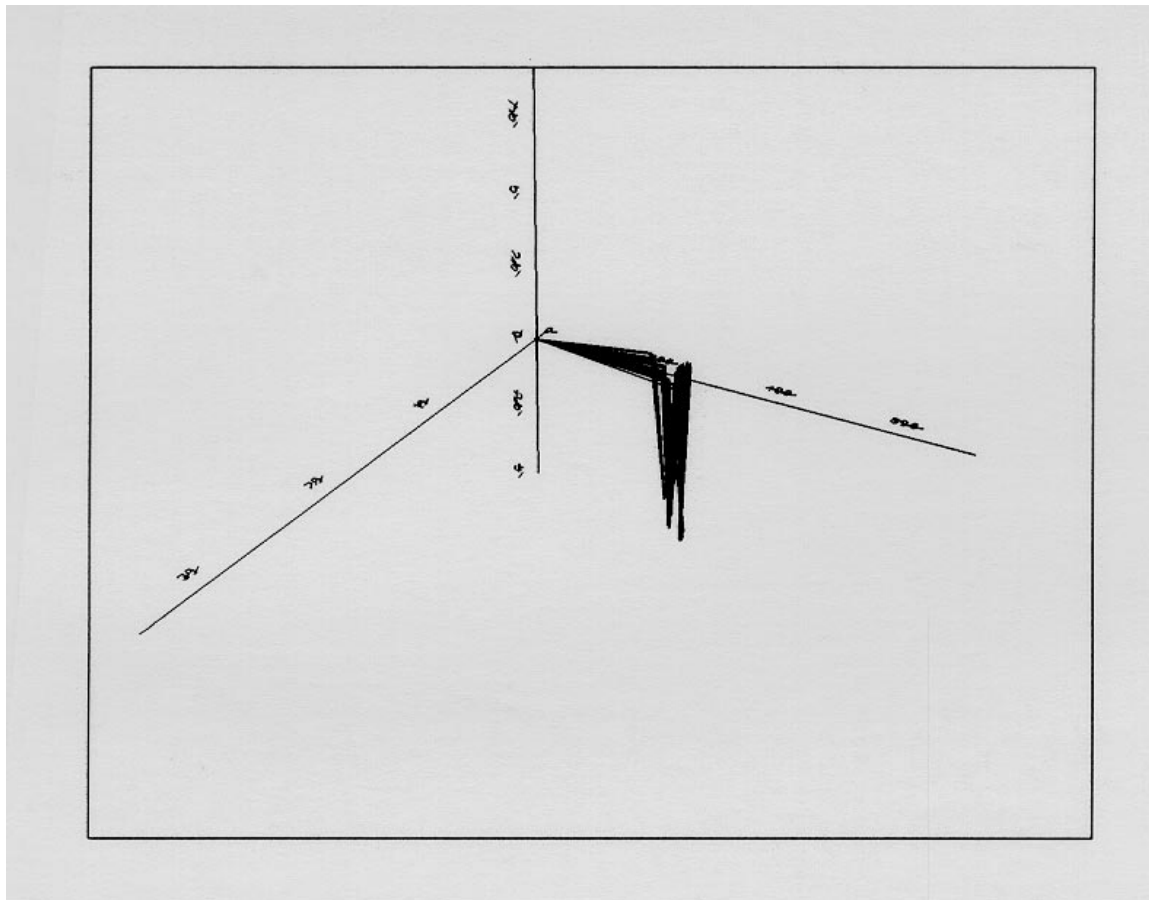
Figure 2.6: Three dimensional after tuning with ERGSET
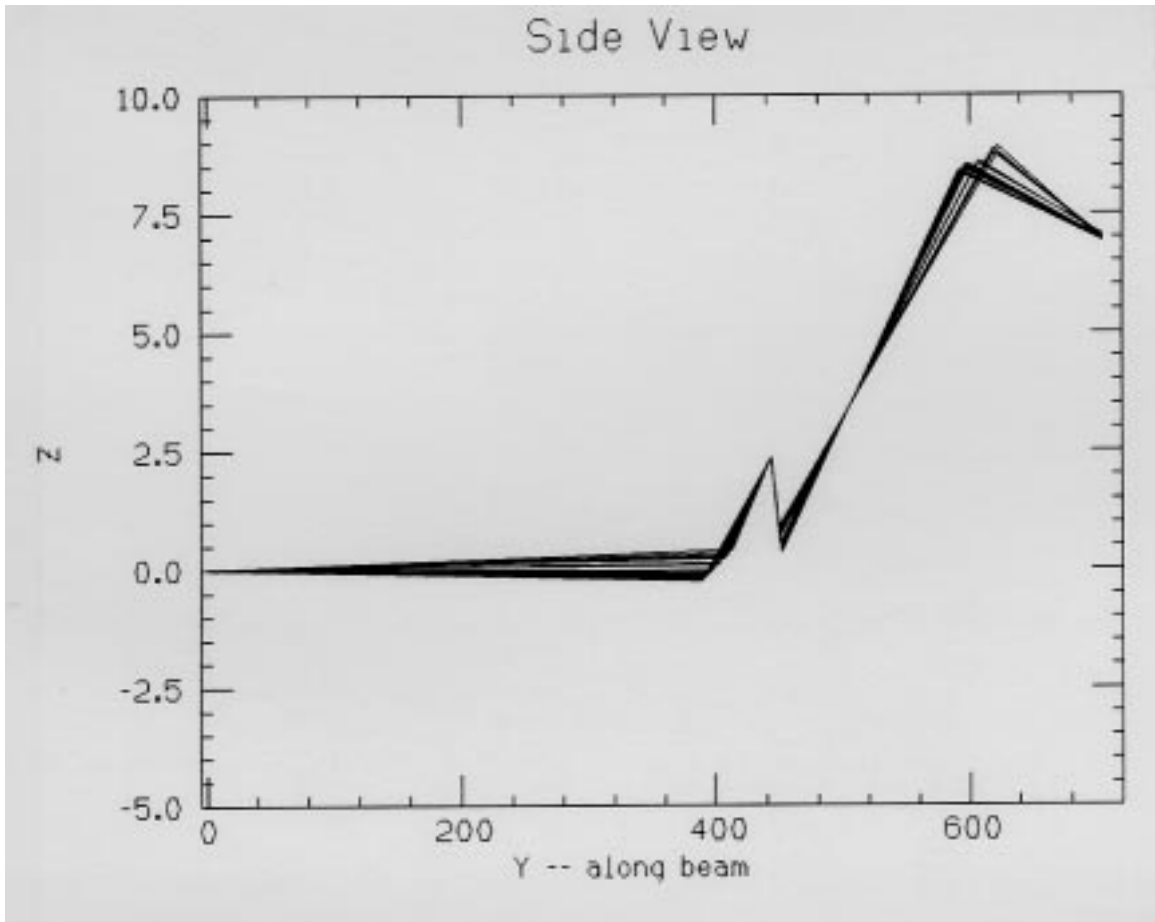
Figure 2.7: Two dimensional side view after tuning with ERGSET
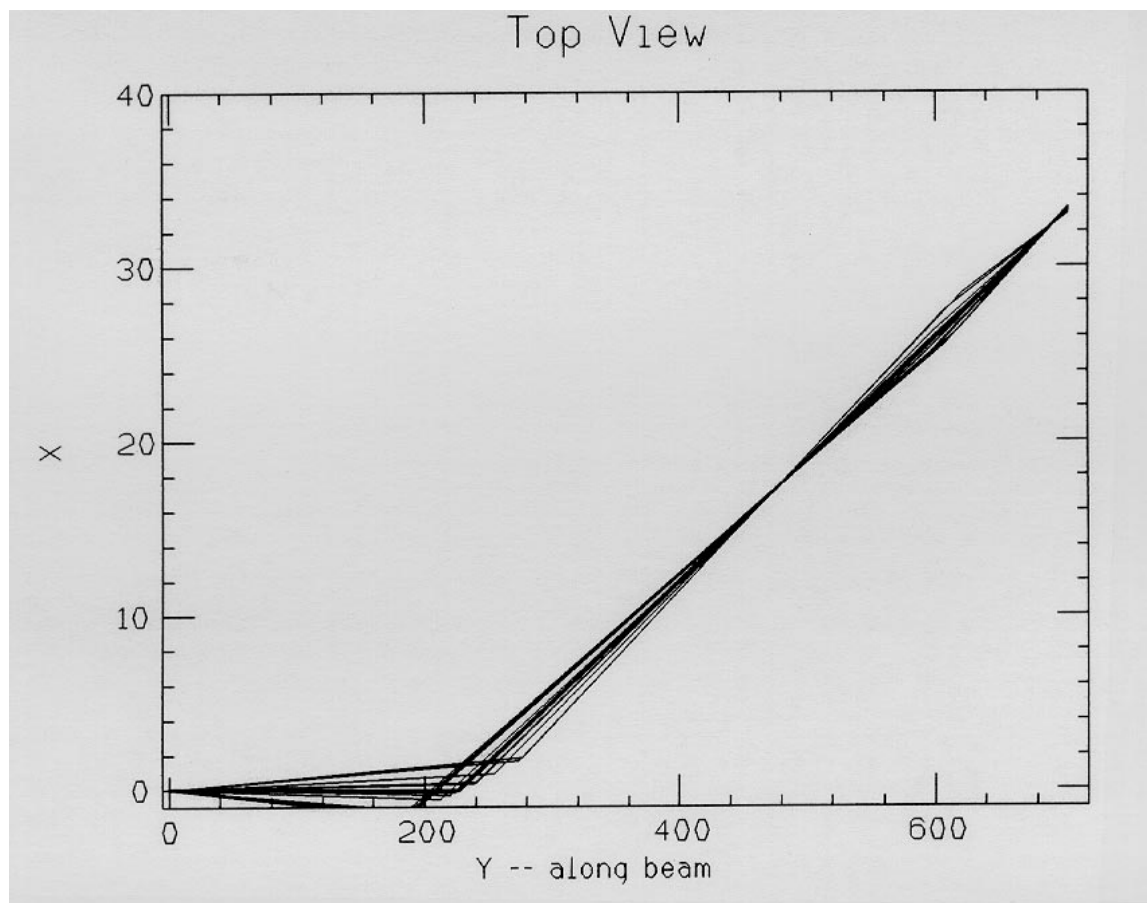
Figure 2.8: Two dimensional top view after tuning with ERGSET

HISTO3

Purpose:	To create a file needed by SHADOW for optimized sources.
Input:	A file generated by REFLAG or SHADOWIT that has modified the source by flagging the rays that will be lost in the system.
Output:	A file that has partitioned the useful volume of phase space into bins. This file will serve as input to the SOURCE option of SHADOW and will be a guide to the 'optimization' of the source.

Description:

HISTO3 defines the volume of phase space in which the rays from the source will not be lost. The steps involved in this matching of the source and system are as follows:

1. Setup source, system and trace as usual.

2. If the number of rays lost in the system is significant, it may be advisable to "optimize" the source. Since SHADOW keeps track of all rays, it is in principle possible to work back toward the source and tag all the rays that are lost somewhere along the line. This can be accomplished with REFLAG (for a single file) or SHADOWIT (for multiple files).

3. The modified source ray file from the previous step is used as input to HISTO3 and is used to define the discrete chunks of phase space which are good or bad. The histograms are given the value 1 if one or more rays that were generated at the source have 'good' flags at the check point in the system. The histograms are created in the phase spaces of (X,X'), (Y,Y'), (Z,Z'). Thus the three coordinates are treated independently (which is not always their true behavior) since the phase space is six-dimensional.

4. The output from HISTO3 is then used as input to the source generation program by selecting the optimization. After the filename has been given to SOURCE, one can exit and let the matching begin. SOURCE will reject any rays that have been generated in the zero space of the histogram. The number of rays accepted and the total number are displayed at regular intervals.

Since HISTO3 seperates good and bad phase space into discrete intervals, it is not guaranteed that all of the rays will be good after one run of the optimization procedure. The above routine may be repeated on the "optimized source" to increase the efficiency further,

but with diminishing returns. By increasing the number of bins, one achieves a finer resolution in phase space at the cost of additional memory and computing time.

Examples:

Here we will consider a typical synchrotron radiation source incident upon a toroidal mirror with an exit slit at the continuation plane, where the image will be formed. The slit has been defined such that it will block a substantial number of rays. Below are the descriptions of the source and system.

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************  S O U R C E      D E S C R I P T I O N  **************
Optimized source
Optimized for exit slit (Star.01)
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
end.00
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.HISTO3]END.00;2
Creation Date            :10-APR-1989 16:05
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Random Source.
Generated total        1000 rays.
Source assumed TRIDIMENSIONAL.
Source Spatial Characteristics: GAUSSIAN
Sigma X     :   0.100000000    Sigma Z   :   0.100000000E-01
Depth:  SYNCHROTRON SOURCE.
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: SYNCHROTRON
Distribution Limits. +X :   0.100000000E-01 -X:   0.100000000E-01 rad
                     +Z :   0.500000000E-02 -Z:   0.500000000E-02 rad
Magnetic Radius =     4.81000000     m.  Beam Energy =   1.5000      GeV.
Beam Emittancies. EPSI_X:   0.000000000E+00 EPSI_Z:   0.000000000E+00
Distance from Waist.  X:   0.000000000E+00     Z:   0.000000000E+00
Polarization Used: SR TOTAL
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: SINGLE LINE
Photon Energy:   1000.0    eV, or   12.399     Angs.
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************              E N D              **************
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*******************   MIRROR  DESCRIPTION   *******************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Torroidal Mirror With Exit Slit.

++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.HISTO3]END.01;2
Creation Date           :10-APR-1989 16:07
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:       TOROIDAL
Cylindrical figure                   NO
Element type                         REFLECTOR
Reflectivity                         OFF
Mirror dimensions                    UNLIMITED
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                    10000.00000000000
Image  Plane                             5000.000000000000
Incidence Angle                          88.99999999999998
Reflection/Diffraction Angle             88.99999999999998

Mirror parameters                    COMPUTED
Same configuration as Central Axis   YES
Objective focus at                       10000.00000000000
Image focus at                           5000.000000000000
Incidence angle                          88.99999999999998
Parameters used follow:
   Major Radius        381874.9072807532
   Minor Radius        116.3493762485566
Source of this O.E. moved            NO
Mirror at pole position ( no mov. )   YES
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

+++

The first plot shows how a large portion of the beam is blocked by the exit slit.
We will now use the lost rays from the exit slit (STAR.01) to modify the good/lost flag in the
source using REFLAG.

```
$ reflag
File to be modified [ e.g. BEGIN.DAT ] ?   begin.dat
File to use as modifier [ e.g. SCREEN.0503 ] ?   star.01
Output file ?   opt.dat
```

Now HISTO3 will divide the phase space up into good and lost bins.

```
$ histo3
Input  file ?   opt.dat
Output      ?   opt.hist
Found        527 good points out of        1000
Here we are.
X max is  0.2972638002614275
X min is -0.3260431318536972
Y max is   24.30820832467235
Y min is  -24.00455259924489
Z max is  2.6589882743400154E-02
Z min is -3.3074220129884787E-02
X prime max is  5.0536091497003565E-03
X prime min is -4.9907608257961093E-03
Y prime max is  0.9999999987862705
Y prime min is  0.9999871499645169
Z prime max is  5.8449901106416506E-04
Z prime min is -5.4485118546760329E-04
How many bins in X  [ default 25 ] ?
How many bins in X`  ?
How many bins in Y   ?
How many bins in Y`  ?
How many bins in Z   ?
How many bins in Z`  ?
```

Now the file genarated by HISTO3 is used as the optimization file in SOURCE. The easiest way to perform this is to enter the menu mode of SOURCE and go into the 'Number of random rays' submenu by using the right arrow. The optimization of source should be changed to 'YES', and the file name is that of the output from HISTO3. Upon exit of SOURCE the number of rays generated vs the number accepted is displayed:

```
Phase space boundaries file read succesfully.
       500    rays have been rejected so far.
       208                    accepted.
Generated          250 rays out of          1000
      1000    rays have been rejected so far.
       393                    accepted.
                500
      1500    rays have been rejected so far.
       595                    accepted.
                750
      2000    rays have been rejected so far.
       778                    accepted.
      2500    rays have been rejected so far.
       963                    accepted.
                1000
Exit from SOURCE
SOURCE => Source has been succesfully generated.

SOURCE procedure completed.
```

Now the system can be retraced in the BATCH mode since the parameters have not changed. We can then examine the exit slit of the optimized system using PLOTXY. Note that 995 out of the 1000 rays have been accepted instead of 527 for the first run. Let's optimize the TGM system with respect to the first mirror. Most of the rays lost are at the edge of the mirror. HISTO3 cannot optimize at the exit slit of a monochromator, because the lost rays are a function of energy, not phase space. In the previous example we plotted the progress against a limiting aperture. In this case we will look at a MINMAX file of the mirror in question to see how the limits change:

```
$ minmax
Input file ?
mirr.01
```
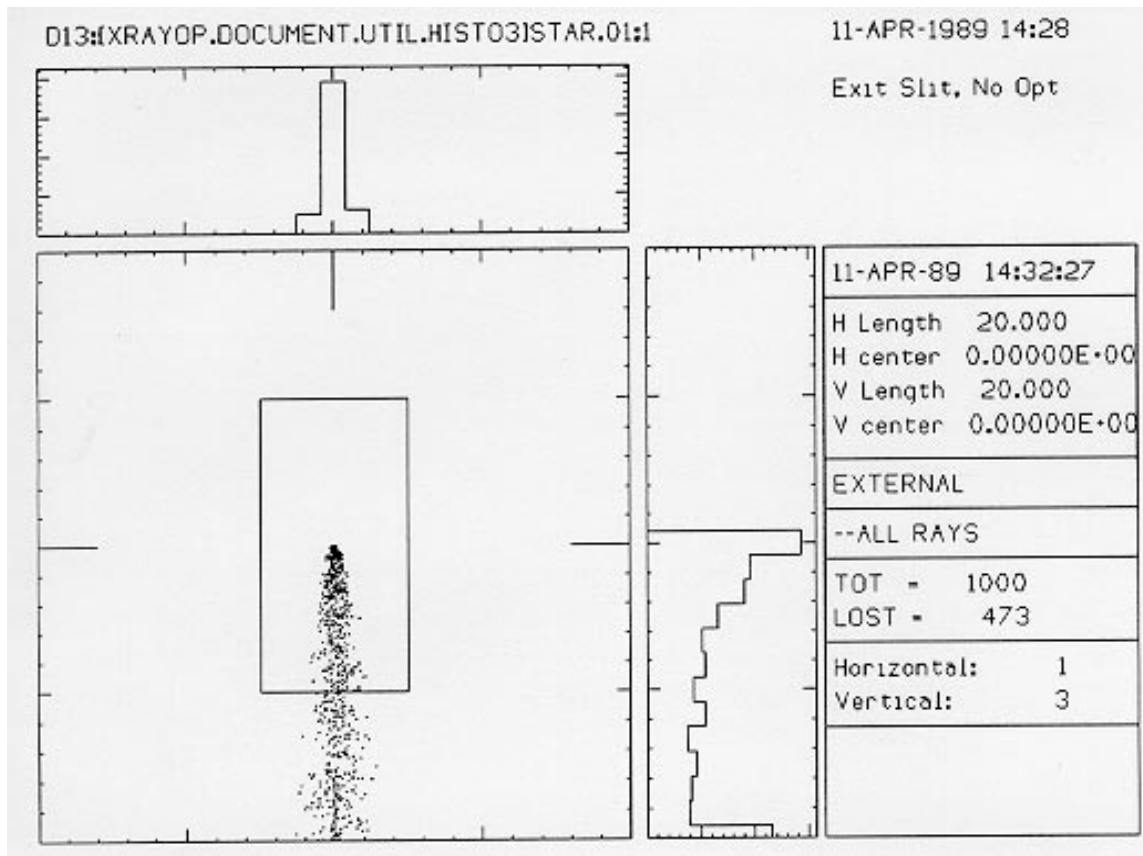
Figure 2.9: HISTO3: Before source optimization
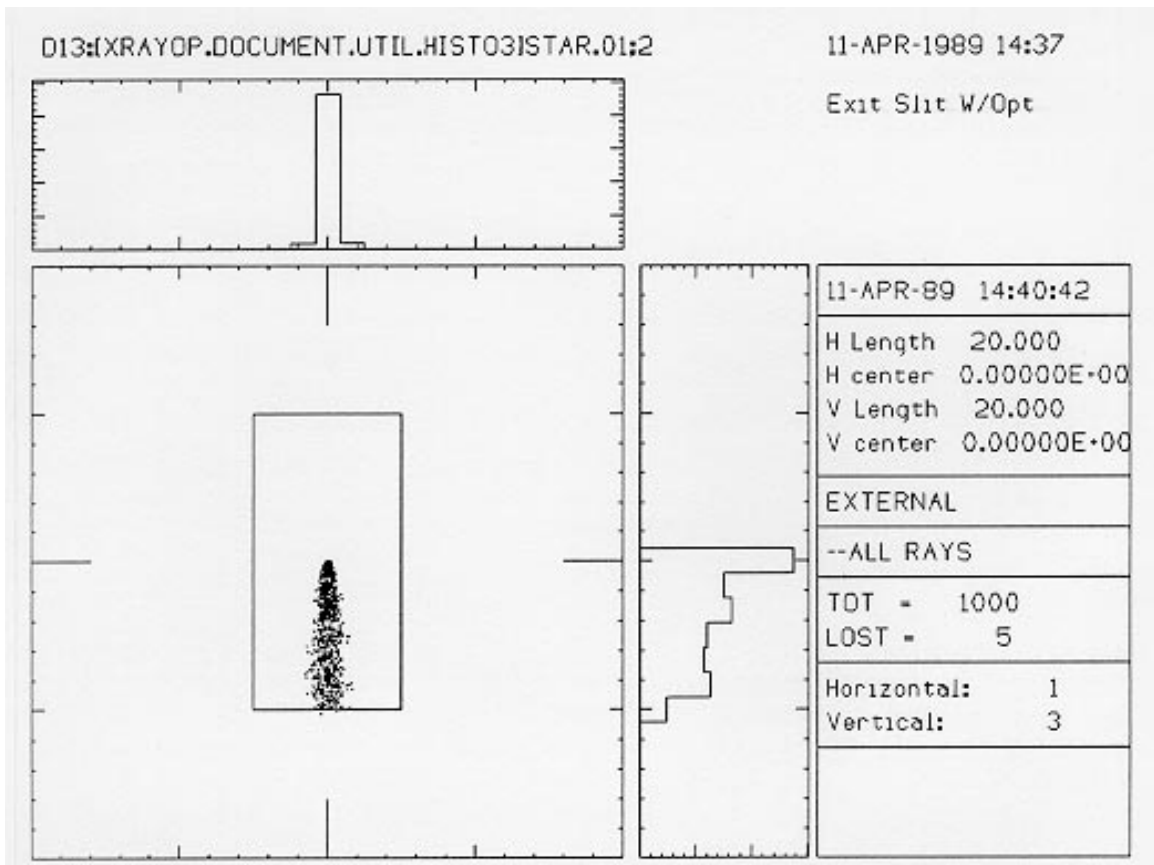
Figure 2.10: HISTO3: After source optimization

```
   Options --- Enter
   0 for excluding the losses
   1 for including losses at a particular O.E.
   2 for including all the losses.
   Then ?
   2
   Comment ?
   First Mirror of TGM without optimization
   ***********
   File examined is :
   D13:[XRAYOP.DOCUMENT.TGM]MIRR.01;29
   Was created :
    9-MAY-1989 11:16
   ***********
   Found           927 good points out of        1000
   Here we are.
   X max is   2.233099
   X min is  -2.203895
   Y max is   4.030588
   Y min is  -5.178271
   Z max is  0.1620322
   Z min is  5.9245693E-05
   X prime max is  1.2591288E-02
   X prime min is -1.3506259E-02
   Y prime max is  0.9964082
   Y prime min is  0.9960193
   Z prime max is  8.9137740E-02
   Z prime min is  8.3950877E-02
```

We pay most attention to the X, Y limits since these define the mirror's edge.

```
 $ reflag
   File to be modified [ e.g. BEGIN.DAT ] ?
   begin.dat
   File to use as modifier [ e.g. SCREEN.0503 ] ?
   mirr.01
   Output file ?
```

```
reflag.opt


$ histo3
Input  file ?
reflag.opt
Output      ?
histo.opt
Found          927 good points out of        1000
Here we are.
X max is  0.2020543762143582
X min is -0.1922062231865444
Y max is   2.489119530789779
Y min is  -2.421645912872256
Z max is  3.3317030366455779E-02
Z min is -3.4645052849801248E-02
X prime max is  1.1941889145443042E-02
X prime min is -1.1634579482826180E-02
Y prime max is  0.9999999788492193
Y prime min is  0.9999280937975692
Z prime max is  1.9853600893657853E-03
Z prime min is -1.9938319051862862E-03
How many bins in X  [ default 25 ] ?
How many bins in X`  ?
How many bins in Y   ?
How many bins in Y`  ?
How many bins in Z   ?
How many bins in Z`  ?
```

The user must change the source parameters to include the optimization file as explained in the SOURCE manual. The following run is made with the file histo.opt as the optimization file.

```
$ go source
```

```
SOURCE selected. Begin procedure.


This procedure generates a SOURCE for SHADOW.
Mode selected [ ? <ret> for HELP ] ? : batch
File containing source description [ START.00 ] ?: synch.00
Phase space boundaries file read succesfully.
Generated           250 rays out of          1000
                    500
                    750
                   1000
Exit from SOURCE
SOURCE => Source has been succesfully generated.
```

Now we'll run MINMAX on the mirror file again to see how the limits have changed. Note that the improvement was slight, but this is where the phase space dependent rays were being lost.

```
$ minmax
Input file ?
mirr.01
Options --- Enter
0 for excluding the losses
1 for including losses at a particular O.E.
2 for including all the losses.
Then ?
2
Comment ?
First mirror of TGM after optimization
***********
File examined is :
D13:[XRAYOP.DOCUMENT.TGM]MIRR.01;30
Was created :
10-MAY-1989 12:47
***********
```

```
Found           973 good points out of           1000
Here we are.
X max is   2.083563
X min is  -2.086486
Y max is   4.180661
Y min is  -4.992939
Z max is  0.1412461
Z min is  5.4842703E-06
X prime max is  1.1868485E-02
X prime min is -1.1789099E-02
Y prime max is  0.9964100
Y prime min is  0.9960120
Z prime max is  8.9194998E-02
Z prime min is  8.3885789E-02
```

PREREFL

Purpose:	To create a file which can be used by SHADOW to calculate reflectivity of mirrors.
Input:	Interactive from terminal.
Output:	Unformatted file.

Description:

PREREFL is a program to compute the complex dielectric function of a given material as a function of photon energy. The results are stored in an unformatted file ready to be read by SHADOW for calculating reflectivity of mirrors (multilayers coatings are handled differently by PRE_MLAYER and crystals by BRAGG). The user must run PREREFL first if he is going to include reflectivity when calling SHADOW later on. (Another case would be absorbing screens along the optical system. The user will still run PREREFL first, specifying the absorbing material, then pass the output file to SHADOW.)

PREREFL looks up an optical constant library which contains all the elements and covers the range 100 eV to 100,000 eV. The lower energy range (100-10,000 eV) is from B. Henke's compilation, while the higher range (10,000-100,000 eV) is calculated by Cromer and Liberman's method. Anything outside the range will create fatal errors. Naturally, the photon energy range should cover the range used in generating the source rays. Some consideration should be given to whether the range includes absorption edges, when choosing the number of points.

In the example, we define an elemental (gold) and a compound (SiC) coatings, from 100 to 500 eV in step of 2 eV. Note silicon must be typed in as SI, and carbon as CC.

Examples:

```
\\ First let us define a gold mirror.

$
$ PREREFL
Element [0] or compound [1] ?
0
Density [ g/cm3 ] ?
19.3
Enter 2-letters (capitalized) atomic symbol ?
AU                                                \\ Must be CAPITALIZED \\
```

```
Enter starting photon energy,end and step
100
500
2
Output file ?
AU.REFL
$
$ DIR AU.REFL

Directory D13:[XRAYOP.DOCUMENT.PREREFL]

AU.REFL;1                    7  22-FEB-1989 21:58  (RWED,RWED,RE,RE)

Total of 1 file, 7 blocks.
$

\\ Now we define another mirror made of SiC.

$ PREREFL
Element [0] or compound [1] ?
1
Density [ g/cm3 ] ?
3.21
The program is setup to compute optical constants of
compounds with up to 5 elements.
How many atomic species ?
2
H2O would be: HH,2 and OO,1. Then ?
Enter 2-letters (capitalized) atomic symbol and formula index for :       1
SI
1
Enter 2-letters (capitalized) atomic symbol and formula index for :       2
CC                                             \\ Must be 2-letters \\
1
Molecular weight is :    40.10000    Number of molecules/cm3:   4.8206819E+22
Enter starting photon energy,end and step
100
500
2
Output file ?
```

```
SIC.REFL
$ DIR *.REFL

Directory D13:[XRAYOP.DOCUMENT.PREREFL]

AU.REFL;1                    7  22-FEB-1989 21:58  (RWED,RWED,RE,RE)
SIC.REFL;1                   7  22-FEB-1989 22:03  (RWED,RWED,RE,RE)

Total of 2 files, 14 blocks.

\\ Either of these files can now be specified to SHADOW for reflectivity
\\ calculation.

-----------------------------------------------------------------------
\\    The followings are typical responses to SHADOW :

Reflectivity of Surface. SHADOW may solve the Fresnel equations locally.
Available options:'No reflectivity              .......... 0
Full polarization dependence .......... 1
No          "           "        .......... 2
Reflectivity mode [ 0,1,2 ] ?
1                              \\ Either 1 or 2 selects reflectivity mode \\

Optical constants from file  ( for multi-line source ) ..... 0
Optical constants from keyboard  (single-line source ) ..... 1
Define multilayer from file                           ..... 2
Optical Constant Source: [file=0,tt:=1], multilayer [2] ?
0
File with optical constants ?
AU.REFL
```

PRESURFACE

Purpose:	To generate a spline file used by SHADOW to simulate distortions in the surface of an optical element.
Input:	A file containing the array size for the distortion and the surface mesh.
Output:	A file readable by SHADOW containing the spline for the distortion.

Description:

This utility takes a file with a surface mesh array and computes the bi-cubic spline for the surface. Normally this is interpreted as an "error surface", although one could use weird shapes by combining suitable error surfaces and plane or other mirrors. It creates a file that can be read by SHADOW under "Distorted Surface?". The system will then be traced as if this defect was present on the mirror. This utility is particularily useful in conjunction with MAKE_PWR and PWR_DENS in modelling the effects of heating on a mirror surface. PRESURFACE takes a file in the format of:

$$N_x, N_y$$
$$Y(1), \ldots, Y(N_y)$$
$$X(1), Z(1,1), \ldots, Z(1,N_y)$$
$$\vdots$$
$$X(N_x), Z(N_x,1), \ldots, Z(N_x, N_y)$$

where N_x and N_y are the size of the surface mesh.

Examples:

To start, we will use a program generated error of the form $\delta z = re^{-r^2/\sigma^2}$ and run that through PRESURFACE. PRESURFACE will then create a binary file for SHADOW. The second example is more complex, but a better demonstration of the usefulness of the program. We look at the distortions to the image of the TGM caused by heat loading on the mirror. This is done by taking the output from PWR_DENS/MAKE_PWR and submitting it to the finite element program ANSYS for analysis. ANSYS then returns a file in the form needed by PRESURFACE so we can give the information to SHADOW.

In the first example, the test program creates a gaussian error file in the form given above for an error with a height of 500 Å. This is run through PRESURFACE and traced through SHADOW as shown below.

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************   S O U R C E        D E S C R I P T I O N  **************
Source used in PRESURFACE Example

+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified: end.00
Full file Specification :CXRL$DUA0:[XRAYOP.DOCUMENT.UTIL.PRESURFACE]END.00;1
Creation Date          : 7-SEP-1989 16:12
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Grid Source.
Generated total       3721 rays.
Source assumed BIDIMENSIONAL (flat).
Source Spatial Characteristics: RECTANGULAR
Source Width:    40.0000000     and Height:    5.00000000
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: UNIFORM
Distribution Limits. +X :    0.000000000E+00 -X:    0.000000000E+00 rad
                     +Z :    0.000000000E+00 -Z:    0.000000000E+00 rad
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************                    E N D                   **************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

$
$ presurface
File containing the surface mesh ? t_error.dat
Setting up          25 by            25 array.
Array read correctly. Compute spline.
Spline succesfully completed.
Please enter file-name for storage: error.dat
Task completed. Spline stored in
error.dat

$

+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
******************   MIRROR  DESCRIPTION   ******************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
PRESURFACE Example
Distorted surface using test program
```

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :CXRL$DUA0:[XRAYOP.DOCUMENT.UTIL.PRESURFACE]END.01;1
Creation Date           : 8-SEP-1989 13:46
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:          PLANE
Cylindrical figure                      NO
Element type                            REFLECTOR
Reflectivity                            OFF
Mirror dimensions                       UNLIMITED
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                       100.0000000000000
Image  Plane                                100.0000000000000
Incidence Angle                             0.0000000000000000E+00
Reflection/Diffraction Angle                0.0000000000000000E+00

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
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

The plots shown below are the cross-sections at the image plane after the mirror. The first is without distortion, the second, after the 500 Å gaussian error was applied. We also show the output from running SURPLOT on the mirror surface to show the distortions in a clearer manner.

CXRL#DUA0:[SHADOW.XRAYOP.DOCUMENT.UTIL.PRESURFACE]STARSUP:1989 14:53

Image before distort

ion

8-SEP-89 14:58:27

H Length   100.00
H center   0.00000E·00
V Length   6.0000
V center   0.00000E·00

EXTERNAL

--GOOD ONLY

TOT =   3721
LOST =   0

Horizontal: 1
Vertical: 3
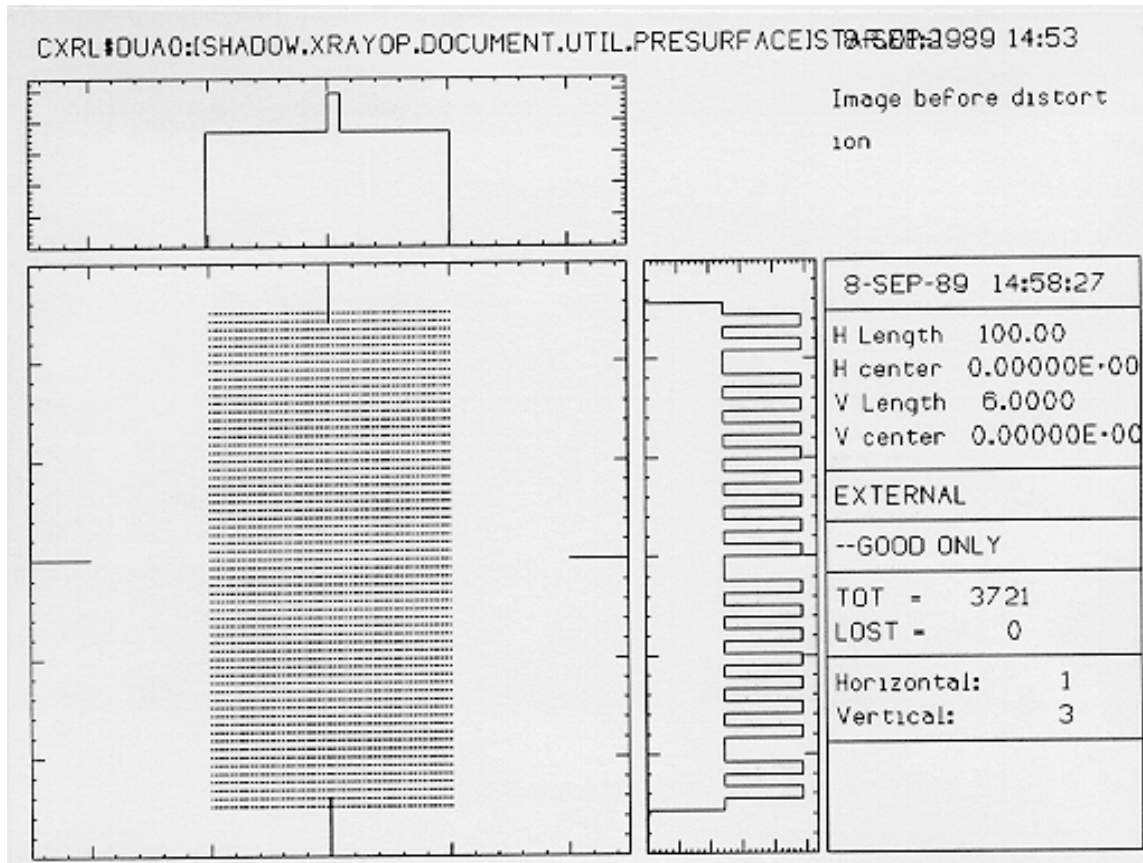
Figure 2.11: PRESURFACE: No distortion

D13:[XRAYOP.DOCUMENT.UTIL.PRESURFACE]STAR.01;25   31-JUL-1989 14:25

Image after 500 A di

stortion

31-JUL-89 14:29:55

H Length   100.00
H center   0.00000E+00
V Length   6.0000
V center   0.00000E+00

AUTOSCALING

--GOOD ONLY

TOT =   3721
LOST -   0

Horizontal: 1
Vertical: 3
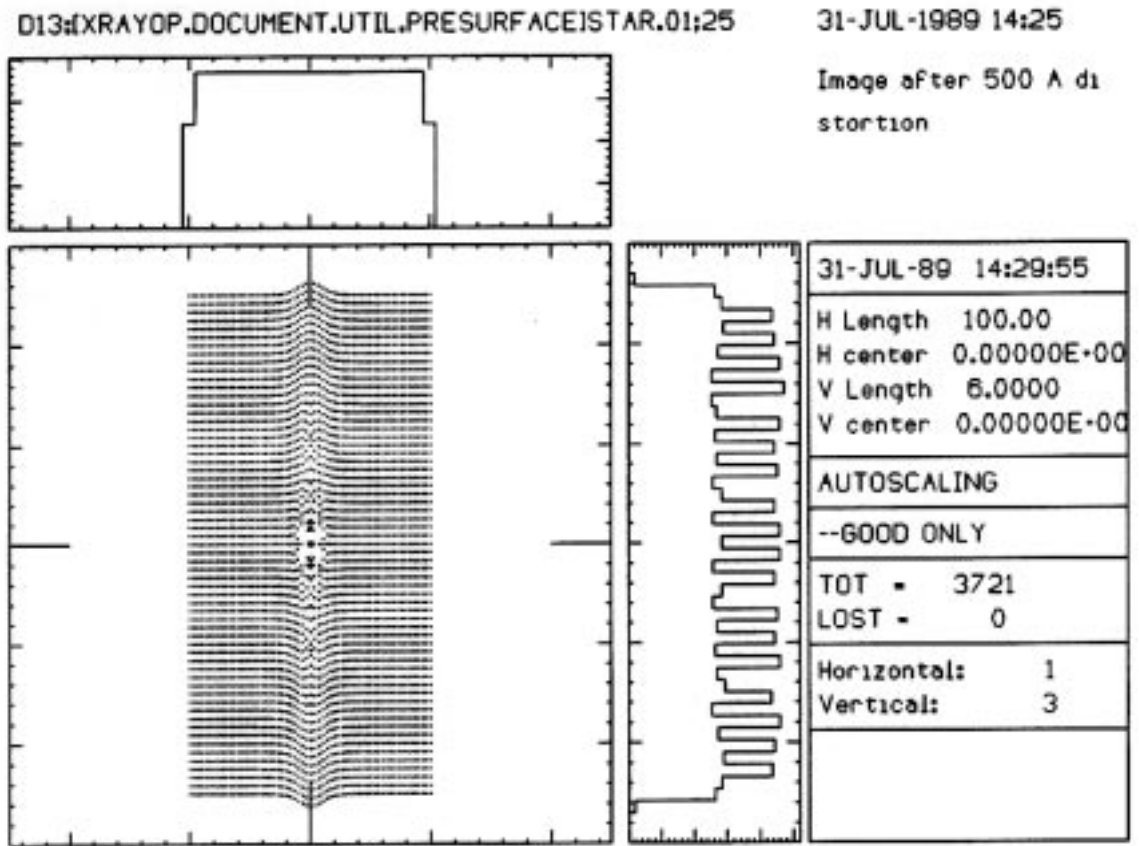
Figure 2.12: PRESURFACE: With gaussian error
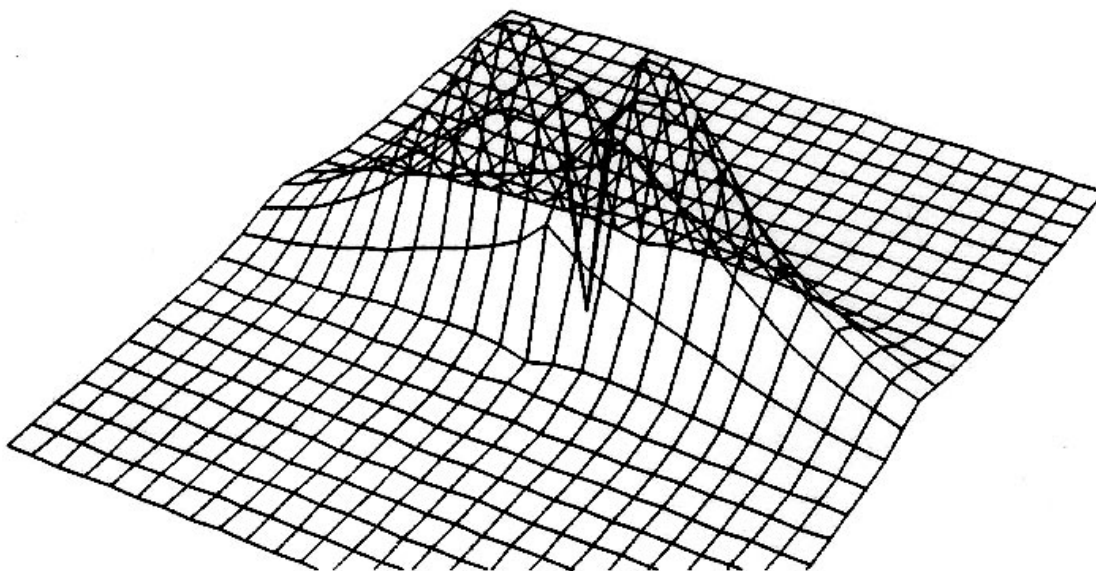
Figure 2.13: PRESURFACE: Surface generated with SURPLOT

PRE_MLAYER

Purpose:	To create a file which has the parameters that SHADOW needs to calculate reflectivity of multilayers.
Input:	Interactive from terminal.
Output:	Unformatted file.

Description:

PRE_MLAYER operates along the same lines as PREREFL. It lets the user specify the multilayer parameters prior to running SHADOW. The necessary complex refractive indices are obtained from an optical constant library (see PREREFL), within the user specified photon energy range. These are stored together with other parameters in a format understandable by SHADOW[1], where both the incident angle and photon energy might vary from ray to ray. Naturally, the photon energy range used here should contain that of the source rays. Valid energies are from 100 to 100,000 eV. Each layer material could be a compound or simply an element. For simplicity, elemental materials are implemented as the case of compounds with only one constituent.

In the example, we defined a 20 layer tungsten-carbon (W-C) multilayers deposited on silicon substrate. The geometrical structure is as follows:

C	14.59 Å	
		20th layer
W	7.74 Å	
C	14.59 Å	
		19th layer
W	7.74 Å	
⋮	⋮	⋮

---

[1]SHADOW uses a multilayer reflectivity code developed by J. H. Underwood.

⋮	⋮	⋮
C	14.59 Å	
		3rd layer
W	7.74 Å	
C	14.57 Å	
		2nd layer
W	7.72 Å	
C	14.56 Å	
		1st layer
W	7.71 Å	
Si		Substrate

Note TWO capitalized letters must be used to specify each element (silicon as SI, tungsten as WW, and so on). Also note the thicknesses are entered upward starting from the substrate as:

        7.71,14.56
        7.72,14.57
        7.74,14.59
        -1,-1

The (-1,-1) means the 4th to 20th layers have the same thicknesses as the last entered layer (3rd layer). Of course, if the thicknesses are different from layer to layer, all twenty pairs must be entered individually in ascending order. If they all have the same thicknesses, then just enter:

        7.71,14.56
        -1,-1

For the reflectivity of these multilayers as a function of angle, at a fixed incident wavelength of 18 Å, refer to the example under MLAYER.

Examples:

```
$ PRE_MLAYER
Name of output file :
CW.REFL
Photon energy (eV) from :
500
                to :
```

```
2000
******************************************************* \\ Si substrate \\
Specify the substrate material :
Density [ g/cm3 ] ?
2.32
How many atomic species (up to 5) ?
1
H2O would be: HH,2 and OO,1. Then ?
Enter 2-letters (capitalized) atomic symbol and formula index for :
SI
1
Formula:
SI( 1)


Molecular weight is :     28.10000     Number of molecules/cm3:   4.9719812E
Atoms/Cm3 of each species:
    SI
 0.49720E+23
 Density    2.320000     g/cm3
******************************************************* \\ W layers \\
Right above the substrate is the even layer material.
Specify the even layer material :
Density [ g/cm3 ] ?
19.3
How many atomic species (up to 5) ?
1
H2O would be: HH,2 and OO,1. Then ?
Enter 2-letters (capitalized) atomic symbol and formula index for :
WW
1
Formula:
WW( 1)


Molecular weight is :     184.0000     Number of molecules/cm3:   6.3166570E
Atoms/Cm3 of each species:
    WW
 0.63167E+23
 Density    19.30000     g/cm3
******************************************************* \\ C layers \\
Odd layer material is on top of the even layer.
```

```
Specify the odd layer material :
Density [ g/cm3 ] ?
2.26
How many atomic species (up to 5) ?
1
H2O would be: HH,2 and OO,1. Then ?
Enter 2-letters (capitalized) atomic symbol and formula index for :          1
CC
1
Formula:
CC( 1)

Molecular weight is :     12.00000     Number of molecules/cm3:   1.1341619E+23
Atoms/Cm3 of each species:
    CC
 0.11342E+24
 Density    2.260000     g/cm3
***************************************************** \\ Thicknesses \\
No. of layer pairs :
20
Now specify the thickness (angstroms) of each pair starting from the substrate
surface.  Type two -1 whenever you want the remaining layers to assume the
thicknesses of the previous one.
Even and odd thicknesses of layer          1
7.71,14.56
Even and odd thicknesses of layer          2
7.72,14.57
Even and odd thicknesses of layer          3
7.74,14.59
Even and odd thicknesses of layer          4
-1,-1

$
$ DIR CW.REFL

Directory D13:[XRAYOP.DOCUMENT.PRE_MLAYER]

CW.REFL;1                   7  23-FEB-1989 20:37  (RWED,RWED,RE,RE)

Total of 1 file, 7 blocks.
```

```
\\ Now CW.REFL can be used by SHADOW to compute the multilayers reflectivit


---------------------------------------------------------------------

\\ The followings are typical responses to SHADOW :


Reflectivity of Surface. SHADOW may solve the Fresnel equations locally.
Available options:'No reflectivity              .......... 0
Full polarization dependence .......... 1
No         "          "       .......... 2
Reflectivity mode [ 0,1,2 ] ?
1                             \\ Either 1 or 2 selects reflectivity mode \\

Optical constants from file  ( for multi-line source ) ..... 0
Optical constants from keyboard  (single-line source ) ..... 1
Define multilayer from file                            ..... 2
Optical Constant Source: [file=0,tt:=1], multilayer [2] ?
2
File with optical constants ?
CW.REFL
```

READCDF

Purpose:	To examine the output from MAKE_ID in a formatted fashion.
Input:	CDF100.DAT type unformatted file created by MAKE_ID.
Output:	A listing to the terminal of the following information contained in CDF100.DAT:
	ENERGY
	THETA
	PHI
	ENERGY CDF
	THETA CDF
	PHI CDF
	POLARIZATION

Description:

This utility may be used after having run MAKE_ID to create an undulator source. MAKE_ID writes two unformatted files called CDF100.DAT and RN100.DAT. The first contains the integrated probability distribution function for the undulator specified. The second contains the unintegrated version (i.e., the probability density function). READCDF will translate these files and display them on the screen, listing them in the following order: $\hbar\omega$, θ, ϕ, $\hbar\omega$ CDF, θ CDF, ϕ CDF, and polarization.

Examples:

Shown here is an abbreviated log run of READCDF. Since we have chosen an array of size (7,31,31), the number of ϕ values is quite high, 6727. Therefore we have indicated where part of the numbers have been taken out for brevity.

```
$
$ run util:readcdf
CDF file name : CDF100.DAT
          7               31              31
ENERGY
  166.6000000000000       166.6514536735605       166.7083895768990
  166.7634291358226       166.8087044526493       166.8511310282644
  166.9000000000000
THETA
```

```
 0.0000000000000000E+00    1.4791657137678076E-05    2.2251941231713891E-05
 2.7687702415863914E-05    3.2313066897178147E-05    3.6571308379987740E-05
          :                         :                         :
          :                         :                         :
 9.2080738694522949E-04    9.2133827633709131E-04    9.2182721517975547E-04
 9.2269959425070353E-04    9.2705937660297172E-04    9.3300299596312150E-04
 9.9999999999999999E-04
PHI
 0.0000000000000000E+00    5.2365113547351804E-02    0.1047198074795338
 0.1570796332030884        0.2094395102445555        0.2617993877992018
          :                         :                         :
          :                         :                         :
          :                         :                         :
 0.9931394837863106        1.052217027334260         1.121618703090235
 1.204075328010145         1.303866401257959         1.426290706607965
 1.570796326794897
ENERGY CDF
 0.0000000000000000E+00    1597452437754297.         3352259513027127.
 5052544494091979.         6617314861817053.         7933820056896882.
 9483864799698803.
THETA CDF
 0.0000000000000000E+00    1137879769018200.         2302194120683513.
 3445473695689648.         4583600464381745.         5719824268258108.
          :                         :                         :
          :                         :                         :
          :                         :                         :
 3.2037618174895696E+16    3.3120834622079286E+16    3.4135948814895818E+16
 3.5239699259666078E+16    3.6636833680816223E+16    3.6745528750518148E+16
 3.6769491832312990E+16
PHI CDF
 0.0000000000000000E+00    2.6945087860844903E+23    5.3884814185598183E+23
 8.0827181134233465E+23    1.0776957448910698E+24    1.3471196810804287E+24
          :                         :                         :
          :                         :                         :
          :                         :                         :
 4.1471861771090057E+19    4.3182396273454665E+19    4.4909831649742257E+19
 4.6637392633570821E+19    4.8364869209620913E+19    5.0091263816753908E+19
 5.1815261815261810E+19
POLARIZATION
 1.000000000000000         1.000000000000000         1.000000000000000
```

```
    1.000000000000000          1.000000000000000          1.000000000000000
            :                          :                          :
            :                          :                          :
            :                          :                          :
    0.8033972364454941         0.6736431273463106         0.5214799388366159
    0.3277322390815726         6.2298305467587064E-02     0.4331000594855148
    0.7127183578208387
$
```

REFLAG

Purpose:	Modifies the good/lost ray flag (column 10) in one BOF (object) according to that of another BOF (control). This utility is typically used to study which rays will be lost from a given source and to define masks for scattered light.
Input:	Two Binary Output Files (Usually BEGIN.DAT and another ray file like STAR.xx).
Output:	A modified version of the first input file.

Description:

The program reads in both files and copies the status flag of the control file to the object file, ray by ray. A typical application is for example, in answering the question "what fraction of the source is the system accepting?" or "how much of a condenser mirror are we really using?". In the first case the object file would be BEGIN.DAT, in the second MIRR.XX, while the control file could be for example the final image STAR.YY.

Another application is that of reducing scattered light. Let's suppose that a beam overfills a mirror thus creating stray rays that may have harmful effects. One can then use REFLAG to see which part of the incoming beam (e.g. at a suitable screen) will miss the mirror and thus design a suitable absorbing mesh that will effectively eliminate stray radiation.

Examples:

First the output from the source and single element system that we'll use for our example.

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S O U R C E      D E S C R I P T I O N **************
REFLAG Example
Source used in REFLAG before optimization
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
end.00
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.REFLAG]END.00;1
Creation Date           :17-MAY-1989 16:26
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Random Source.
Generated total        2000 rays.
Source assumed TRIDIMENSIONAL.
Source Spatial Characteristics: GAUSSIAN
```

```
Sigma X     :    0.100000000     Sigma Z   :    0.100000000E-01
Depth:  SYNCHROTRON SOURCE.
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: SYNCHROTRON
Distribution Limits. +X :   0.100000000E-01 -X:   0.100000000E-01 rad
                     +Z :   0.500000000E-02 -Z:   0.500000000E-02 rad
Magnetic Radius =    4.81000000     m.  Beam Energy =   1.5000     GeV.
Beam Emittancies. EPSI_X:   0.000000000E+00 EPSI_Z:   0.000000000E+00
Distance from Waist.  X:   0.000000000E+00     Z:   0.000000000E+00
Polarization Used: SR TOTAL
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: SINGLE LINE
Photon Energy:   1000.0    eV, or   12.399     Angs.
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************              E N D                 **************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*******************   MIRROR  DESCRIPTION   *******************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
REFLAG Example
Mirror used in REFLAG example
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.REFLAG]END.01;1
Creation Date           :17-MAY-1989 16:26
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


Surface figure was defined as:        TOROIDAL
Cylindrical figure                     NO
Element type                           REFLECTOR
Reflectivity                           OFF
Mirror dimensions                      UNLIMITED
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                      10000.00000000000
Image  Plane                               5000.000000000000
Incidence Angle                            88.99999999999998
Reflection/Diffraction Angle               88.99999999999998
```

```
Mirror parameters                        COMPUTED
Same configuration as Central Axis    YES
Objective focus at                        10000.00000000000
Image focus at                            5000.000000000000
Incidence angle                           88.99999999999998
Parameters used follow:
    Major Radius        381874.9072807532
    Minor Radius        116.3493762485566
Source of this O.E. moved             NO
Mirror at pole position ( no mov. )   YES
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

$
$ reflag
File to be modified [ e.g. BEGIN.DAT ] ? begin.dat
File to use as modifier [ e.g. SCREEN.0503 ] ? star.01
Output file ? refl.dat

$ histo3
Input  file ? refl.dat
Output      ? new.dat
Found          550 good points out of        1000
Here we are.
X max is  0.2730171936559060
X min is -0.2595255943453094
Y max is   24.25826988410192
Y min is  -24.24719610097799
Z max is  3.1774282219930756E-02
Z min is -4.2464660404542004E-02
X prime max is  5.0432633039571831E-03
X prime min is -5.0411845079583304E-03
Y prime max is  0.9999999990291811
Y prime min is  0.9999872410237632
Z prime max is  6.1683691834940080E-04
Z prime min is -5.8033590292263016E-04
How many bins in X  [ default 25 ] ?
How many bins in X`    ?
How many bins in Y     ?
How many bins in Y`    ?
```

```
How many bins in Z    ?
How many bins in Z'   ?
```

The output file from HISTO3 is used to optimize the source.
To perform this optimization, the user should enter the source generation program by typ-
ing: $ GO SOURCE and selecting MENU mode.

1. LOAD SOURCE

2. SEL SOURCE

3. enter the submenu for "Number of Random Rays" by placing the cursor next to the
   '1000' in the rightmost column and pressing the right arrow key.

4. Change 'optimization of source' from NO to YES

5. Enter the name of the file that was generated by HISTO3

6. Exit the menus by pressing the left arrow twice

7. SAVE SOURCE

8. EXIT

The source will now generate only those rays that fit into the bounds defined by HISTO3:
Shown below is the exit from SOURCE after optimization.

```
Phase space boundaries file read succesfully.
        500    rays have been rejected so far.
         46                    accepted.
       1000    rays have been rejected so far.
         82                    accepted.
       1500    rays have been rejected so far.
        115                    accepted.
       2000    rays have been rejected so far.
        157                    accepted.
       2500    rays have been rejected so far.
        197                    accepted.
       3000    rays have been rejected so far.
        233                    accepted.
 Generated          250 rays out of           1000
       3500    rays have been rejected so far.
```

```
   280                    accepted.
  4000   rays have been rejected so far.
   321                    accepted.
  4500   rays have been rejected so far.
   364                    accepted.
  5000   rays have been rejected so far.
   403                    accepted.
  5500   rays have been rejected so far.
   446                    accepted.
  6000   rays have been rejected so far.
   489                    accepted.
               500
  6500   rays have been rejected so far.
   529                    accepted.
  7000   rays have been rejected so far.
   574                    accepted.
  7500   rays have been rejected so far.
   620                    accepted.
  8000   rays have been rejected so far.
   667                    accepted.
  8500   rays have been rejected so far.
   714                    accepted.
               750
  9000   rays have been rejected so far.
   750                    accepted.
  9500   rays have been rejected so far.
   793                    accepted.
 10000   rays have been rejected so far.
   847                    accepted.
 10500   rays have been rejected so far.
   898                    accepted.
 11000   rays have been rejected so far.
   946                    accepted.
 11500   rays have been rejected so far.
   982                    accepted.
              1000
Exit from SOURCE
SOURCE => Source has been succesfully generated.

SOURCE procedure completed.
```

```
Shadow:: exit
```

Exit to DCL

Chapter 3

Postprocessors

After running SHADOW, it is neccesary to have programs to analyze the results and put them in a more understandable form. The Utilities in this section do summarization and ray analysis. They are broken down into four sections: reporting utilities, graphical analysis, non-graphical analysis, and specialized post-processors.

MIRINFO

Purpose: Reads an ERF (exit record file - e.g. END.xx) associated with an op-
                      tical element and displays information (including parameters computed
                      during a trace) about that OE in an intelligible format.
Input: An ERF associated with an optical element.
Output: TT: or a user named and labeled text file.

Description:

Takes the information from an exit record file an puts it into a readable format. The follow-
ing data is included in the output file:

- Exit Record File Data: Name, Creation Date

- Surface Type

- Element Type

- Reflectivity Mode

- Mirror Dimensions

- Source/Image plane Distances

- Incidence/Reflection Angles

- Mirror Parameters

- Focal positions in Object and Image Space

Examples:

Shown below is the output from three runs through MIRINFO. The first run is the first mirror
in the two mirror example from the primer.

```
$ mirinfo


MINFO> Input file MUST be an ERF (Exit Record File) type from SHADOW
```

```
MINFO> Please input filename:
end.01
MINFO> File read correctly.
MINFO> Title ?
Two Mirror Example:  First Mirror
MINFO> Comment ?
Original position from primer example
MINFO> Output file ?
mirr1.inf
MINFO> Prepare output to file : mirr1.inf



+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
******************  MIRROR  DESCRIPTION   *******************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Two Mirror Example:  First Mirror
Original position from primer example
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.MIRINFO]END.01;1
Creation Date           :10-APR-1989 15:03
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


Surface figure was defined as:         ELLIPTICAL
Cylindrical figure                     NO
Element type                           REFLECTOR
Reflectivity                           OFF
Mirror dimensions                      UNLIMITED
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                  2000.000000000000
Image  Plane                           500.0000000000000
Incidence Angle                        88.00000000000000
Reflection/Diffraction Angle           88.00000000000000

Mirror parameters                      COMPUTED
Same configuration as Central Axis     YES
Objective focus at                     2000.000000000000
Image focus at                         500.0000000000000
Incidence angle                        88.00000000000000
```

```
Parameters used follow:
   Semi-major axis      1250.000000000000
   Semi-minor axis      34.89949670250097
   Semi-focal-length  0.0000000000000000E+00
   Eccentricity       0.0000000000000000E+00
Source of this O.E. moved            NO
Mirror at pole position ( no mov. )    YES
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Using the same two mirror example, we move the first mirror in the mirror reference frame. Notice the new information MIRINFO gives:

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*******************  MIRROR  DESCRIPTION  *******************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Two Mirror:  First Mirror moved
Mirror moved 100 units in Z direction (mirror ref frame)
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.MIRINFO]END.01;2
Creation Date           :10-APR-1989 15:09
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:        ELLIPTICAL
Cylindrical figure                    NO
Element type                          REFLECTOR
Reflectivity                          OFF
Mirror dimensions                     UNLIMITED
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                     2000.000000000000
Image  Plane                              500.0000000000000
Incidence Angle                           88.00000000000000
Reflection/Diffraction Angle              88.00000000000000

Mirror parameters                     COMPUTED
Same configuration as Central Axis    YES
```

```
Objective focus at                          2000.000000000000
Image focus at                              500.0000000000000
Incidence angle                             88.00000000000000
Parameters used follow:
   Semi-major axis     1250.000000000000
   Semi-minor axis     34.89949670250097
   Semi-focal-length  0.0000000000000000E+00
   Eccentricity       0.0000000000000000E+00
Source of this O.E. moved                NO
Mirror moved from pole. Parameters :
Displacement along X:     0.0000000000000000E+00
                 Y:     0.0000000000000000E+00
                 Z:      100.0000000000000
 Rotation around X:     0.0000000000000000E+00
                 Y:     0.0000000000000000E+00
                 Z:     0.0000000000000000E+00
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

The final example we show is the first crystal example from the primer. Compare the information in this example with that of earlier examples.

```
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 *******************   MIRROR  DESCRIPTION   *******************
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Crystal Example
Crystal example 1 from Primer
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.MIRINFO]END.01;1
Creation Date           :10-APR-1989 15:20
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

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      ON      coefficients from:  GAAS.PAR
Polarization dependence                      YES
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
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

SOURCINFO

Purpose:	Reads a source ERF and creates a file with all relevant source information in an intelligible format.
Input:	Any source Exit Record File: e.g END.00
Output:	A user defined and labeled file (or TT:) with a description of source.

Description:

Given the source Exit Record File, SOURCINFO will tell the user all of the information regarding creation of the source:

- Type (Random or Grid)

- Number of rays generated

- Source Depth Type

- Spacial Characteristics

- Emission Characteristics (angle distribution)

- Photon Energy Distribution

The user can put a title along with a comment at the top of the file to help identify the source information.

Examples:

We'll run two examples. The first will be the source used in the first crystal example in section 6.4 of the primer.

```
$ sourcinfo


------------------ S O U R C I N F O --------------------
                 vs. 2.01    Feb 1989

INPUT> File containing source specs ?
end.00
```

```
INPUT> Title ?
Primer Crystal 1 Example
INPUT> Comment ?
Source used in sec. 6.4 of primer, crystal example
INPUT> Output file-name ?
xtal.inf
SYSINF> Prepare output to file : xtal.inf
SOURCE_INFO> File
end.00
 read correctly.
$
$ type xtal.inf

  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  **************  S O U R C E      D E S C R I P T I O N  **************
  Primer Crystal 1 Example
  Source used in sec. 6.4 of primer, crystal example
  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  Input file specified:
  end.00
  Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.SOURCINFO]END.00;1
  Creation Date           :26-MAR-1987 14:22
  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  Random Source.
  Generated total        1000 rays.
  Source assumed BIDIMENSIONAL (flat).
  Source Spatial Characteristics: POINT
  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  Source Emission Characteristics
  Distribution Type: LAMBERTIAN
  Distribution Limits. +X :   0.000000000E+00 -X:   0.000000000E+00 rad
                       +Z :   0.600000000E-04 -Z:   0.600000000E-04 rad
  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  Source Photon Energy Distribution: SINGLE LINE
  Photon Energy:   11160.    eV, or   1.1110    Angs.
  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  **************                 E N D                 **************
  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Second example: We'll just show the output of the file synch.inf, a model of the synchrotron source Aladdin.

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************  S O U R C E      D E S C R I P T I O N  **************
Synchrotron Source
Sourcinfo Example 2
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
end.00
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.SOURCINFO]END.00;1

Creation Date           :10-APR-1989 16:38
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Random Source.
Generated total          1000 rays.
Source assumed TRIDIMENSIONAL.
Source Spatial Characteristics: GAUSSIAN
Sigma X    :    0.675000000    Sigma Z   :    0.350000000
Depth:  SYNCHROTRON SOURCE.
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: SYNCHROTRON
Distribution Limits. +X :   0.100000000E-01 -X:   0.100000000E-01 rad
                     +Z :   0.500000000E-02 -Z:   0.500000000E-02 rad
Magnetic Radius =    2.08330000     m.  Beam Energy =   1.0000     GeV.
Beam Emittancies. EPSI_X:   0.000000000E+00 EPSI_Z:   0.000000000E+00
Distance from Waist.  X:   0.000000000E+00     Z:   0.000000000E+00
Polarization Used: SR TOTAL
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: BOX DISTR.
From Photon Energy:    400.000000     or    30.9963000     Angs.
 to  Photon Energy:    5000.00000     or    2.47970400     Angs.
Angular difference in phase is   90.000
Degree of polarization is  0.99462
Source points have INCOHERENT phase.
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************              E N D              **************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

SYSINFO

Purpose: Creates a user friendly simplified description of an optical system from the exit record files after a trace has been completed.

Input: A file containing a listing of the ERF's for all the optical elements in the system. Also the optical axis file is requested as input. A description on how to create the ERF list is given below.

Output: A user defined text file that describes the optical system.

Description:

Gives a description of the optical system from the exit record files. Each optical element is labeled in the following format:

```
          TYPE        (e.g. GRATING)
       SURFACE        (e.g. TOROIDAL)
          SIZE        ( (UN) LIMITED)
    PARAMETERS        ( (not) COMPUTED)
  REFLECTIVITY        (OFF/FULL/NO POL)

  Orientation Ang.    (Degrees)
    Source Plane      (Distance from OE to source: arbitrary units)
   Incidence Ang.     (Degrees)
   Reflection Ang.    (Degrees)
     Image Plane      (Distance from OE to continuation plane)
```

Following the description of each OE, The Optical System Configuration is given in the Laboratory Reference Frame. This involves giving the position in X, Y, Z space of each of the optical elements and of their continuation planes:

```
OPT ELEM #   X=   Y=   Z=
0                        Source Position
1                        OE # 1 Position
        1'       Continuation Plane #1 Position
2                        OE # 2 Position
        2'       Continuation Plane #2 Position
                        ETC …
```

Examples:

Below we show two runs through SYSINFO and the respective files generated. The first
example is the two mirror example from the primer. The second example is the first crystal
example from the primer.


```
 $ sysinfo


 ------------------- S Y S I N F O ----------------------
                 vs. 2.02  June 1989

 Default filenames [ Y/N ] ?y
 How many OE's ? 2
 INPUT> Title ? SYSINFO Example
 INPUT> Comment ? Two Mirror System from Primer Chapter 6
 INPUT> Output file-name ? sysi.twom
 SYSINF> Prepare output to file : sysi.twom
          0
 SYSINF> File
 END.01

  read correctly.
          0
 SYSINF> File
 END.02

  read correctly.
 $ ty sysi.twom


 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
************** S Y S T E M    D E S C R I P T I O N **************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
SYSINFO Example
Two Mirror System from Primer Chapter 6
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 #   Optical Element:                                   Creation Time:
   1   D13:[XRAYOP.PRIMER.CHAPTER6.TWOMIRR]END.01;2        5-MAY-1987 14:
   2   D13:[XRAYOP.PRIMER.CHAPTER6.TWOMIRR]END.02;2        5-MAY-1987 14:
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


Optical Element #               1      System Number:


MIRROR    ELLIPTICAL            UNLIMITED     COMPUTED      REFLEC. OFF

   Orientation             0.0000000000000000E+00 deg.
   Source Plane              2000.000000000000
   Incidence Ang.             88.00000000000000      deg.
   Reflection Ang.            88.00000000000000      deg.
   Image Plane               500.0000000000000
      ----------------


Optical Element #               2      System Number:


MIRROR    ELLIPTICAL            UNLIMITED     COMPUTED      REFLEC. OFF

   Orientation              180.0000000000000      deg.
   Source Plane             1000.000000000000
   Incidence Ang.            88.00000000000000      deg.
   Reflection Ang.           88.00000000000000      deg.
   Image Plane               500.0000000000000
      ----------------


                        OPTICAL SYSTEM CONFIGURATION
                         Laboratory Reference Frame.


OPT. Elem #       X =                Y =                Z =

       0         0.00000000000E+00   0.00000000000E+00   0.00000000000E+00
```

```
     1              0.00000000000E+00     2000.0000000         0.00000000000E+00
          1'           0.00000000000E+00     2498.7820251         34.878236872

     2              0.00000000000E+00     3496.3460754         104.63471062
          2'           0.15370411305E-14     3996.3460754         104.63471062
```

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************              E N D                  **************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


$ sysinfo


-------------------- S Y S I N F O ----------------------
                vs. 2.02   June 1989


Default filenames [ Y/N ] ?y
How many OE's ? 2
INPUT> Title ? SYSINFO Example
INPUT> Comment ? Crystal Example 1 from Primer Chapter 6
INPUT> Output file-name ? sysi.xtal
SYSINF> Prepare output to file : sysi.xtal
          0
SYSINF> File
END.01

 read correctly.
          0
SYSINF> File
END.02

 read correctly.
$ ty sysi.xtal


+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************  S Y S T E M    D E S C R I P T I O N  **************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
SYSINFO Example
Crystal Example 1 from Primer Chapter 6
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
Input file specified:
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 #    Optical Element:                                    Creation Time:
   1   D13:[XRAYOP.PRIMER.CHAPTER6.XTAL1]END.01;1          26-MAR-1987 14:
   2   D13:[XRAYOP.PRIMER.CHAPTER6.XTAL1]END.02;1          26-MAR-1987 14:
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


Optical Element #              1      System Number:

BRAGG     PLANE                 UNLIMITED     COMPUTED      REFLEC. OFF

  Orientation          0.0000000000000000E+00 deg.
  Source Plane         5000.000000000000
  Incidence Ang.       80.19284670377978      deg.
  Reflection Ang.      80.19284670377978      deg.
  Image Plane          149.8956000000000
     ----------------

Optical Element #              2      System Number:

BRAGG     PLANE                 UNLIMITED     COMPUTED      REFLEC. OFF

  Orientation          180.0000000000000      deg.
  Source Plane         149.8956000000000
  Incidence Ang.       80.19284670377978      deg.
  Reflection Ang.      80.19284670377978      deg.
  Image Plane          5000.000000000000
     ----------------


                      OPTICAL SYSTEM CONFIGURATION
                       Laboratory Reference Frame.

OPT. Elem #        X =                 Y =                 Z =

      0         0.00000000000E+00   0.00000000000E+00   0.00000000000E+00
      1         0.00000000000E+00     5000.0000000       0.00000000000E+00
         1'        0.00000000000E+00     5141.1977073        50.317972551

      2         0.00000000000E+00     5282.3954145        100.63594510
         2'        0.73966525681E-13    10282.395415        100.63594510
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
* * * * * * * * * * * * * *           E  N  D           * * * * * * * * * * * * * *
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

TRANSLATE

Purpose:	Tranlates a BOF (e.g. BEGIN.DAT, STAR.xx) into a formatted file. Each of the twelve to eighteen rows (depending on source definition) for each ray is included in the output file.
Input:	Any binary output file.
Output:	A user-named formatted file or the terminal (TT).

Description:

This utility translates a binary output file into a formatted file. The total number of rays in the BOF is given to the user who then chooses how many to translate. The output is in double precision and is displayed in the following format.

X	Y	Z	Spatial coordinates
X'	Y'	Z'	Direction
As_x	As_y	As_z	EM vector (s-)
FF	q	kk	Flag, Wavenumber, ray index
opd	F_s	F_p	Optical path length, phases
Ap_x	Ap_y	Ap_z	EM Vector (p-)

As usual, the number of rows depends on the source definition (i.e. if opd is selected in source but polarization was not, then the number of rows is 13). TRANSLATE tells the user how many rows for each ray will be translated.

Examples:

Here we will use the synchrotron source set up in SOURCINFO, shown below:

```
  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  ************** S O U R C E     D E S C R I P T I O N **************
  Synchrotron Source
  Translate Example
  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  Input file specified:
```

```
end.00
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.SOURCINFO]END.00;1
Creation Date          :10-APR-1989 16:38
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Random Source.
Generated total         1000 rays.
Source assumed TRIDIMENSIONAL.
Source Spatial Characteristics: GAUSSIAN
Sigma X     :   0.675000000     Sigma Z   :   0.350000000
Depth:  SYNCHROTRON SOURCE.
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: SYNCHROTRON
Distribution Limits. +X :   0.100000000E-01 -X:   0.100000000E-01 rad
                     +Z :   0.500000000E-02 -Z:   0.500000000E-02 rad
Magnetic Radius =    2.08330000     m.  Beam Energy =   1.0000     GeV.
Beam Emittancies. EPSI_X:   0.000000000E+00 EPSI_Z:   0.000000000E+00
Distance from Waist.  X:   0.000000000E+00     Z:   0.000000000E+00
Polarization Used: SR TOTAL
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: BOX DISTR.
From Photon Energy:    400.000000     or    30.9963000     Angs.
 to  Photon Energy:    5000.00000     or    2.47970400     Angs.
Angular difference in phase is   90.000
Degree of polarization is  0.99462
Source points have INCOHERENT phase.
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
* * * * * * * * * * * * * *              E N D              * * * * * * * * * * * * * *
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Now let's run BEGIN.DAT through TRANSLATE. Notice the non-zero values for depth and electric field, and compare them to the output from SOURCINFO above.

```
$
$ translate
File for input ?
BEGIN.DAT
```

```
and for output ?
trans.out
Read                    1000 rays.
Each ray has              18 entries.
how many rays to translate ?
5
All done.
$ dir/since


Directory D13:[XRAYOP.DOCUMENT.UTIL.TRANSLATE]


TRANS.OUT;1                   5  13-APR-1989 12:10  (RWED,RWED,RE,RE)


Total of 1 files, 5 blocks.
$
$ type trans.out

  -1.390714334133603        -9.879931896167709        5.0067780073250970E-02
 -4.7392262218636672E-03  0.9999887652748167        9.5178598615866550E-05
  0.9996444645105199        4.7375944414025118E-03    4.5092266573523865E-07
   1.000000000000000        95734809.56938891          1.000000000000000
  0.0000000000000000E+00    3.074243931170887         4.645040257965784
  0.0000000000000000E+00  -2.4974458683843627E-06    2.6239279066775882E-02

  2.7511145072241483E-02   -14.98043983256070         6.6027240850530335E-02
 -7.1906338941880916E-03  0.9999739618211993         6.0865738670193557E-04
  0.8954684439287048        6.4391510223206930E-03    3.9193388862715111E-06
   1.000000000000000        46186641.30730766          2.000000000000000
  0.0000000000000000E+00    2.071735804317716         3.642532131112613
 -4.7124511123640432E-23  -2.7090727399903424E-04    0.4450783412567988

  0.1530800437340783       -14.92438730181352        -0.3691629931304233
 -7.1641626783434953E-03  0.9999742780491507        -3.4353049060675017E-04
  0.9788676621087926        7.0129467309467256E-03  -2.4092230009967500E-06
   1.000000000000000        30557276.28737217          3.000000000000000
  0.0000000000000000E+00    5.645537282077025         4.074740955282128
  1.0819493662900201E-23    7.0210659272627415E-05    0.2043744448811408

  0.7045787542230621       -13.36189239266564        -0.5665608491177220
 -6.4158488038517787E-03  0.9999794153140405         7.6369599785068862E-05
```

```
   0.9997970251734600        6.4146785547840900E-03   4.8989651834470764E-07
    1.000000000000000         186852493.9196818        4.000000000000000
   0.0000000000000000E+00    1.763037151036863        3.333833477831759
   0.0000000000000000E+00   -1.4585901185907957E-06   1.9098700242978440E-02


  -0.6917105883993459       -14.81614060873230        0.1114545705002670
  -7.1093210068994241E-03   0.9999747192975676       -1.3535350638976451E-04
   0.9993560424606797        7.1049223932968824E-03  -9.6170047102332756E-07
    1.000000000000000         21913642.01124334        5.000000000000000
   0.0000000000000000E+00    2.059520134068875        0.4887238072739785
   0.0000000000000000E+00    4.7606793400995139E-06   3.5171301532988853E-02
```

H2KOL

Purpose: To create a histogram of the frequency distribution of ray coordinates, from a selected column in an ASCII file (e.g output from PREPLOT or after processing with FILEX).
Input: Any column formatted file.
Output: TT: or a user defined file.

Description:

This is a specialized version of HISTO1 and uses the same algorithm. H2KOL will create the histogram from a chosen column in a formatted two column file.

Examples:

To demonstrate H2KOL, we'll use a synchrotron source with an energy from 50 - 5000 eV. The output from SOURCINFO is shown. We run BEGIN.DAT through PREPLOT and extract columns 6 (angle distribution in Z) and 11 (photon energy).
Before we create the histogram, we should use FMAX to find the extrema in the data so we can make a reasonable estimate of the center and width of the histogram.

```
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 ************** S O U R C E     D E S C R I P T I O N **************
 H2KOL Example
 Synchrotron Source
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Input file specified:
 end.00
 Full file Specification :CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.H2KOL]END.00;2
 Creation Date          :28-DEC-1989 11:05
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Random Source.
 Generated total        5000 rays.
 Source assumed TRIDIMENSIONAL.
 Source Spatial Characteristics: GAUSSIAN
 Sigma X    :   0.600000000E-01 Sigma Z   :   0.100000000E-01
 Depth:  SYNCHROTRON SOURCE.
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
 Source Emission Characteristics
 Distribution Type: SYNCHROTRON
 Distribution Limits. +X :   0.120000000E-01 -X:   0.120000000E-01 rad
                      +Z :   0.200000000E-02 -Z:   0.200000000E-02 rad
 Magnetic Radius =    2.08330000     m.  Beam Energy = 0.80000     GeV.
 Beam Emittancies. EPSI_X:   0.000000000E+00 EPSI_Z:   0.000000000E+00
 Distance from Waist.  X:   0.000000000E+00     Z:   0.000000000E+00
 Polarization Used: SR TOTAL
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Source Photon Energy Distribution: BOX DISTR.
 From Photon Energy:    50.0000000     or    247.970400     Angs.
  to  Photon Energy:    5000.00000     or    2.47970400     Angs.
 Angular difference in phase is   90.000
 Degree of polarization is  0.62859
 Source points have INCOHERENT phase.
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 ***************              E N D              ***************
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
$
$ dir

Directory CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.H2KOL]

BEGIN.DAT;1              1410  21-DEC-1989 13:19:30.57  (RWED,RWED,RE,)
END.00;1                   7  21-DEC-1989 13:19:35.16  (RWED,RWED,RE,)
H2KOL.ABS;3                1  11-JUL-1989 16:22:53.90  (RWED,RWED,RWED,RE)
H2KOL.DSC;5                1   2-JUN-1989 10:19:00.35  (RWED,RWED,RWED,RE)
H2KOL.EXA;9                9   2-JUN-1989 10:20:01.53  (RWED,RWED,RWED,RE)
H2KOL.INP;1                1  24-JUN-1988 12:17:52.00  (RWED,RWED,RWED,RE)
H2KOL.LOG;1                0  21-DEC-1989 13:21:26.40  (RWED,RWED,RE,)
H2KOL.OUT;2                1  21-FEB-1989 14:25:32.78  (RWED,RWED,RWED,RE)
PHOTONS.DAT;1             313  21-DEC-1989 13:20:46.28  (RWED,RWED,RE,)
SOU.INF;1                  5  21-DEC-1989 13:20:05.54  (RWED,RWED,RE,)
START.00;3                 7  21-DEC-1989 13:17:55.70  (RWED,RWED,RE,)

Total of 11 files, 1755 blocks.
$ fmax
File-name ?
photons.dat
Read        5000 points.
```

```
Found :
XMIN  -1.9855129E-03  . Set at : -2.4330688E-03
XMAX   1.9927619E-03              2.4403178E-03
YMIN    50.12449                 -357.5591
YMAX    3673.979                  4081.663
Good luck !
$
$ h2kol
Input file ? photons.dat
Column to analyze        [ 1 or 2 ] ? 1
Center  ? 0
Width ? 5e-03
Number of bins           [ max=100 ] ? 31
Normalization kind. Enter :
0 for no normalization
1 to normalize to 1          [ at the peak ]
2 to the total counts        [ divide by N ]
3 use the other col. to fill in the bins
<?> 0
Read          5000
Output options :
  [ 0 ] store histogram in a file
  [ 1 ] plot histogram on screen
  [ 2 ] both
Then ? 0
$ dir/since=-00:02

Directory CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.H2KOL]

H2KOL.DAT;1                 4  21-DEC-1989 13:25:17.00  (RWED,RWED,RE,)

Total of 1 file, 4 blocks.
```

The histogram can be normalized or scaled in four ways. The first is not to normalize the plot. The value of each bin is the actual number of points that fall in that bin. The second normalization, to normalize to 1, divides the actual counts by the greatest number of counts to fall in a bin. Thus the maximum value is 1. To normalize to the total counts divides each actual number of points by the total number of points plotted (N). The last type of normalization is most useful when trying to show intensity or amplitude. The phrase "use

the other col. to fill in the bins" means to weight each count by the value of the other column. For our example, this means we are plotting power distribution in angle.

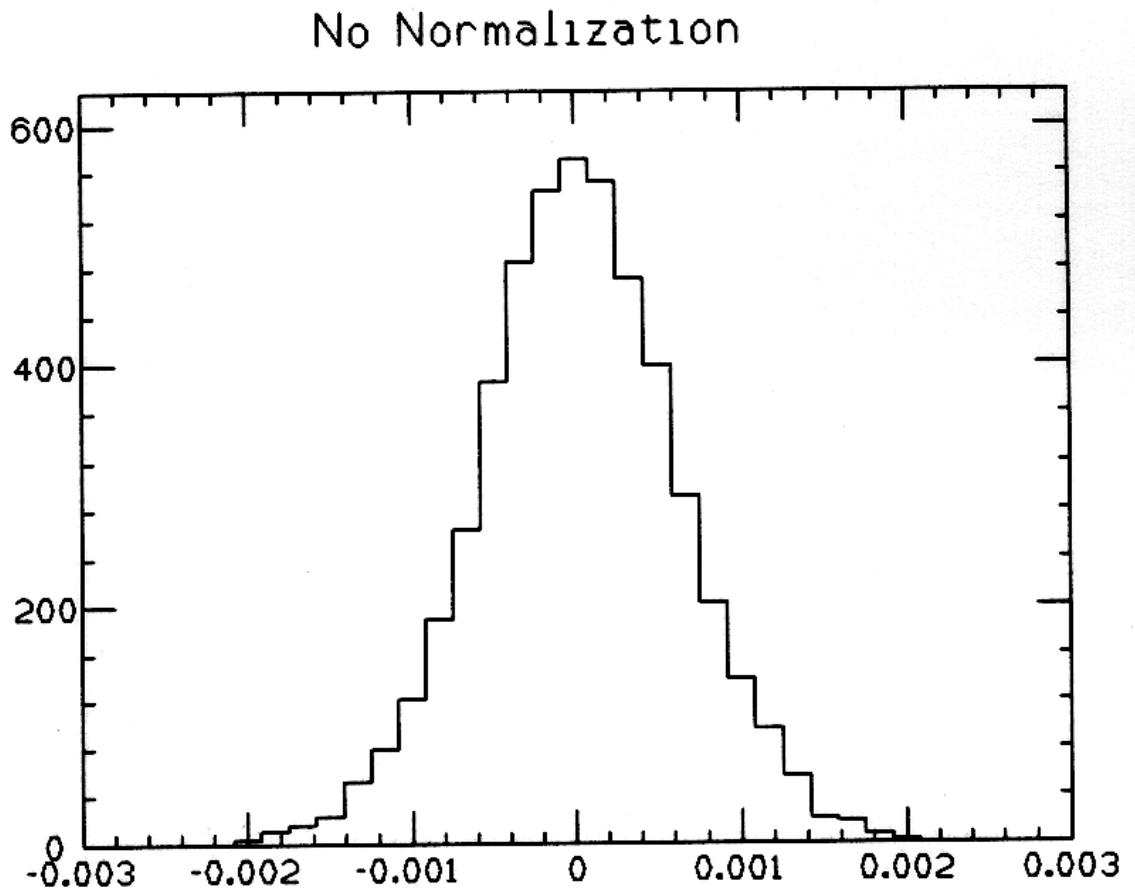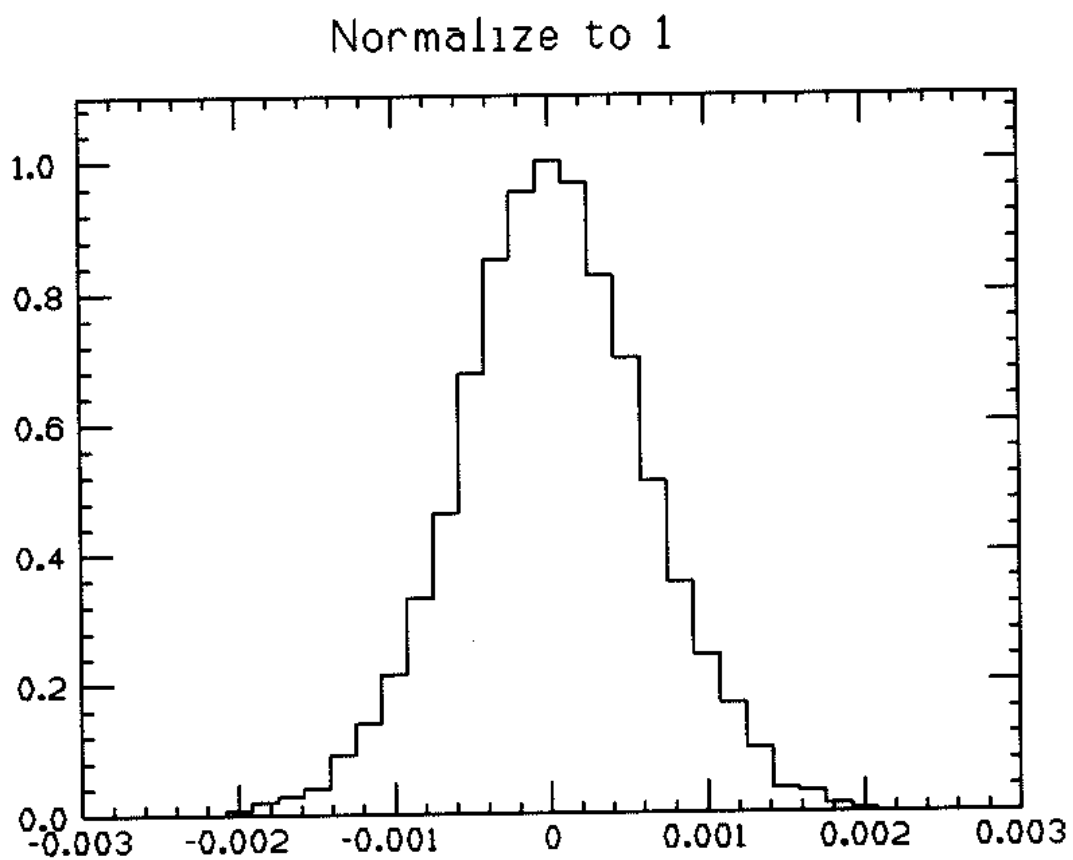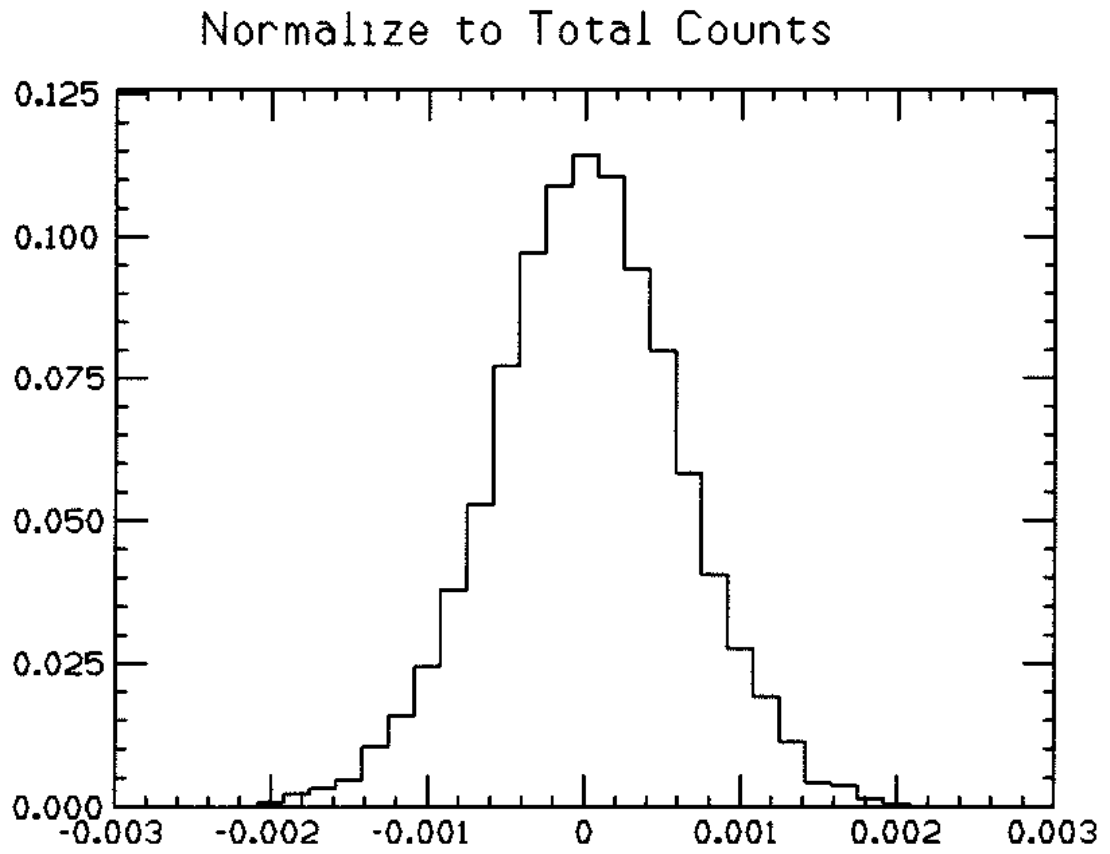Figure 3.1: H2KOL: No Normalization – ray distribution in angle

Normalize to 1

Figure 3.2: H2KOL: Normalize to 1
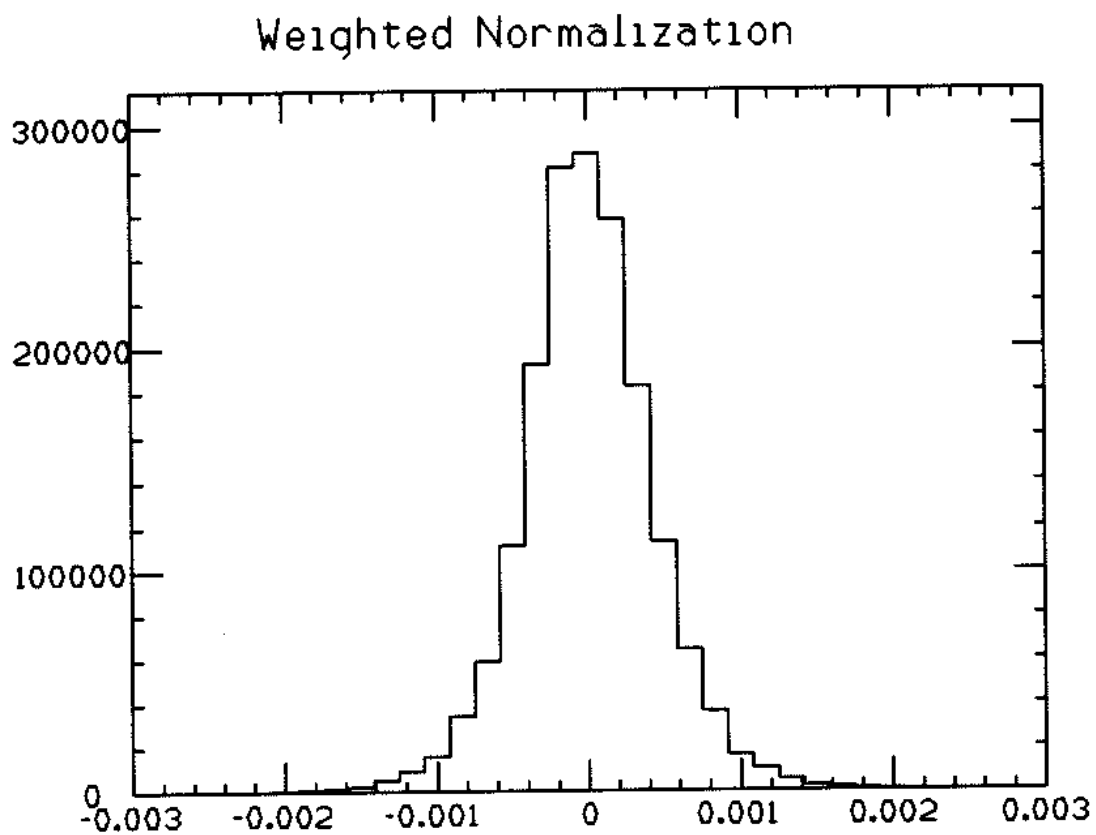
Figure 3.3: H2KOL: Normalize to total counts

Weighted Normalization

Figure 3.4: H2KOL: Weighted Normalization – power distribution in angle

PLOTFOC

Purpose:	To plot a two or three dimensional diagram of the rays near the position of a component of an optical system corresponding to a binary output file. Extends the use of FOCNEW.
Input:	Any Binary Output File.
Output:	A plottable file in two or three dimensions that can be used as input to a graphics routine such as TopDrawer.

Description:

Creates a file suitable for plotting the rays near a continuation plane. The utility asks the user how far in front of and how far beyond the plane the rays should be plotted. The distances are not absolute so the quantity before the plane should be negative. The paths are found by extrapolating:

$$X(d + \Delta) = X(d) + \Delta * X'(d)$$

where d is the location of the continuation plane and Δ is the distance away from the plane along the optical axis.

Examples:

Here we will make a three dimensional plot in the vicinity of the focus in the tangential plane for the example run in FOCNEW. The source has been modified to a conical grid source angle distribution with only twenty rays for the purpose of clarity. From the information we obtained in FOCNEW, we can set the limits to five units on either side of the tangential and sagittal focii.

```
$ plotfoc
Input  file ?  star.01
Output file ?  pf.dat
Read          20 points.
Distance before plane [ <0 ] :  -5
        after        [ >0 ] :  15
Two dimension [ 0 ] or three [ 1 ] ? 1
Only good rays [ 0 ] or all [ 1 ] ?  1
OK. Here we go.
```

$

The following TopDrawer command file was used with the data from PLOTFOC to generate the plot shown below. The outlines of the tangential and sagittal planes were drawn for the sake of clarity.
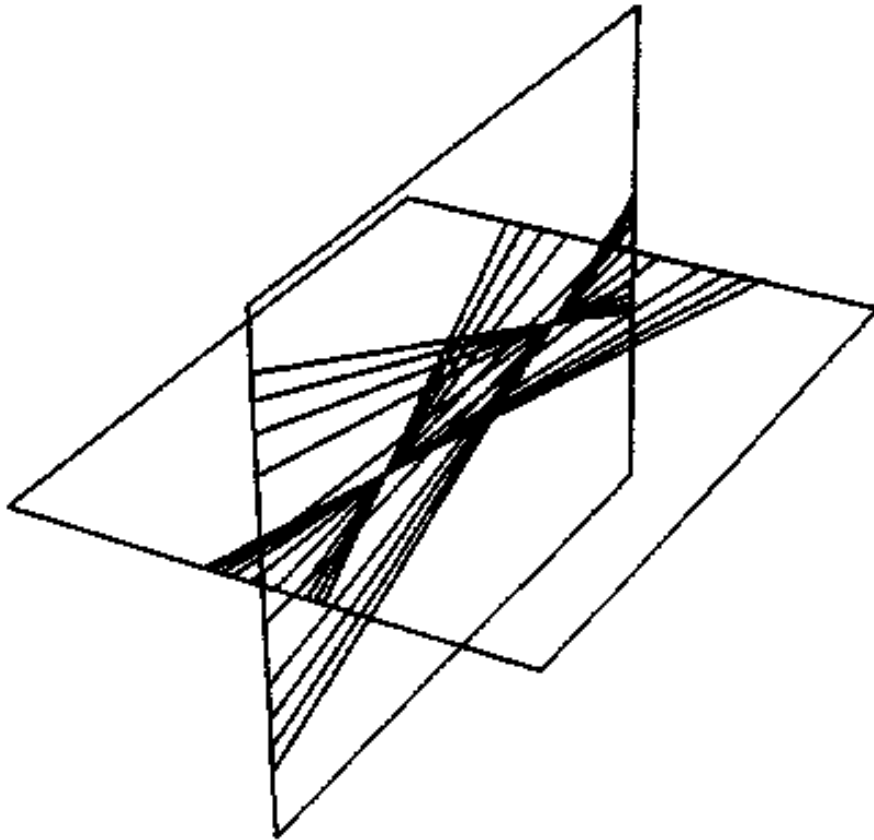
Figure 3.5: PLOTFOC: Tangential and Sagittal focii
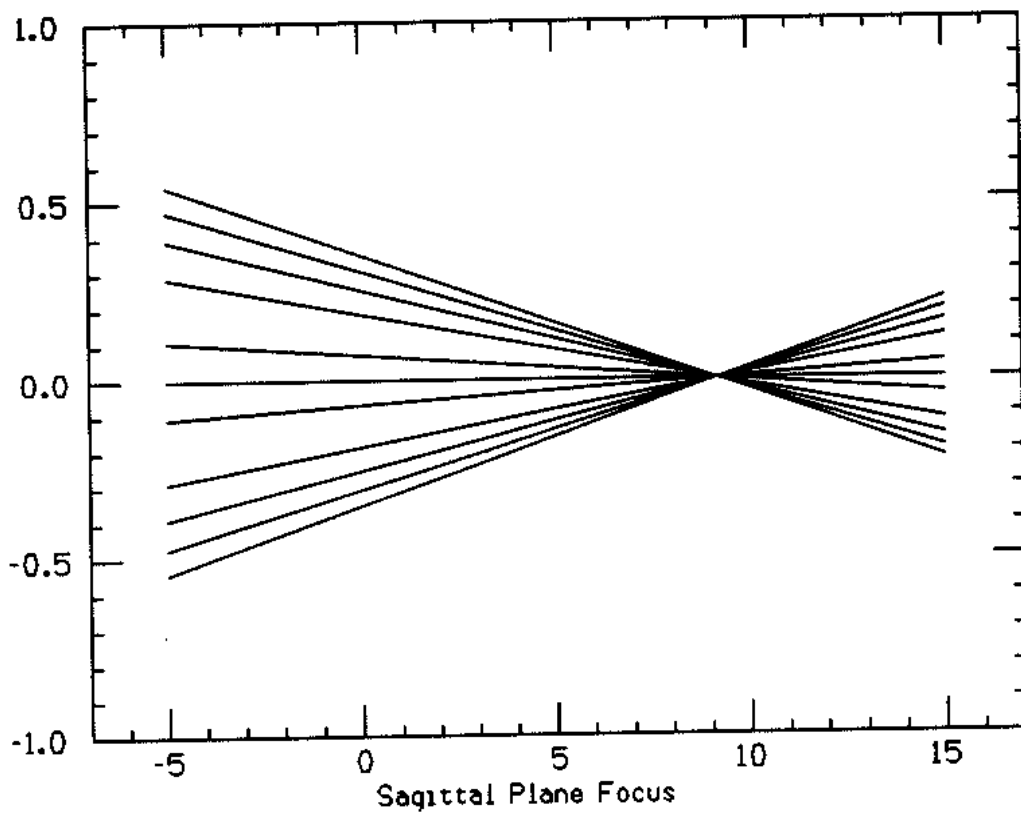
Figure 3.6: PLOTFOC: Sagittal plane focus
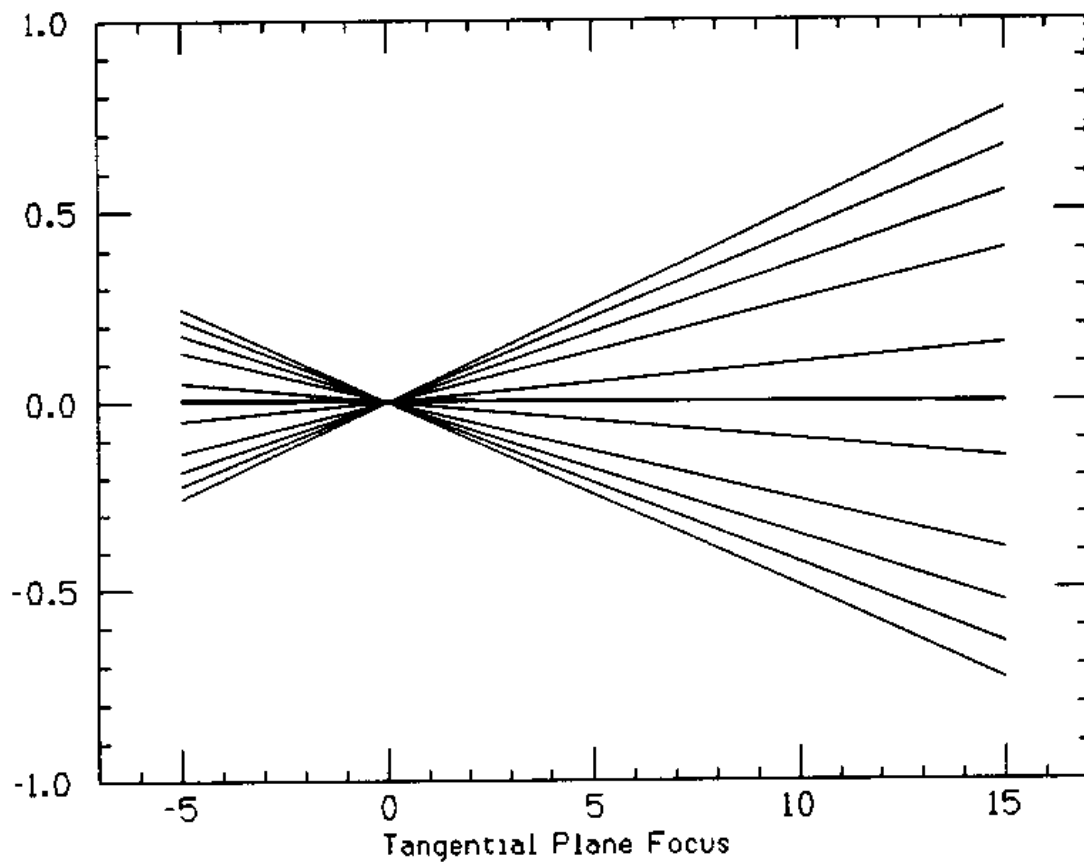
Figure 3.7: PLOTFOC: Tangential plane focus

PLOTSPACE

Purpose: To generate four plots on the same screen of (X,X'), (Z,Z'), (X,Z), (X',Z') of a ray file, thus providing a single view of the phase space.

Input: A BOF file. (such as STAR.xx or MIRR.xx)

Output: Four plots of specified file to terminal.

Description:

This utility will generate four plots on the terminal of a single ray file. The plots, clockwise from the top left, are of X–phase space (X,X'), Z'-X' space, Z–phase space (Z',Z), and the X-Z plane. A TopDrawer command file is not written. If plotting only losses at a given OE, the flag value of those rays must be entered. This is simply the number of the optical element multiplied by 11000.

This program is very useful to have a general overview of the beam properties at any point along the optical axis and to verify, for example, the existence of astigmatism.

Examples:

We'll run this example on the STAR.01 file of the system used in FOCNEW.

```
$ run util:plotspace
PREPLOT> Input file ? star.01
Read               1000 rays.
Each ray has         12 entries.
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
***********
Found         1000 good points out of        1000
Read          1000 good rays. Plot all ?
> 1
PREPLOT> Terminal type: [ 0 ] VT240, [ 1 ] TEK 40xx, [ 2 ] HIREZ, [ 3 ] TEK
7
```

0

We see that the sagittal direction (X) is not at focus while Z is. The meaning of the plots is the following:

3.	4.
X Phase space (X,X')	Far field image (Z',X')
1. Physical image (X,Z)	2. Z Phase space (Z',Z)

where 1. is the beam cross section, 2. and 3. are the phase spaces, 4. is the image detected at large distances (far field). Notice also that the shared boundaries between the plots correspond to the same variables.

Next, we'll run PLOTSPACE on the STAR.03 file from the TGM example. This will show us X phase space, Z phase space, the X-Z plane, and the far field plot of X' vs. Z'.

```
$
$ run util:plotspace
PREPLOT> Input file ? STAR.03
Read                1000 rays.
Each ray has          12 entries.
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
***********
Found         865 good points out of       1000
```
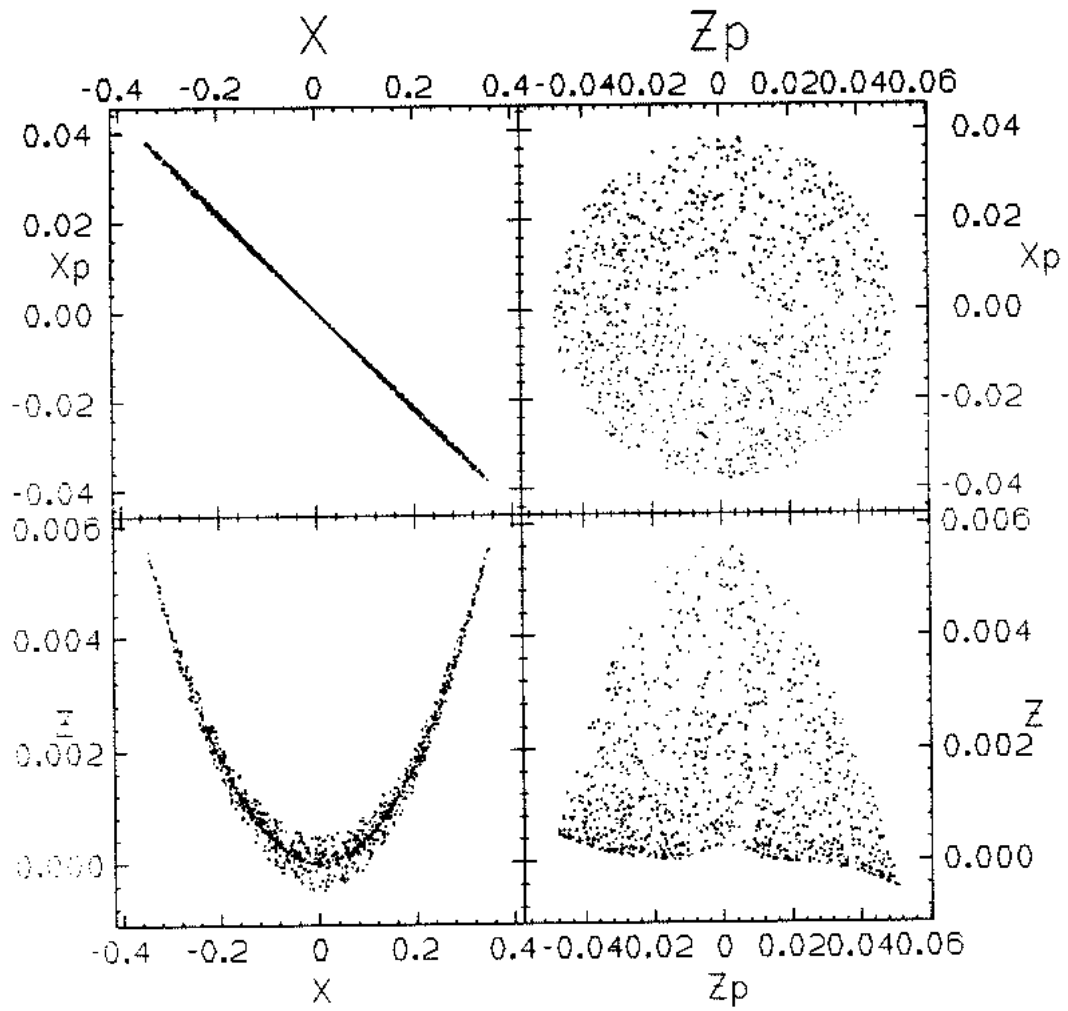
Figure 3.8: PLOTSPACE example one

```
Read           865 good rays. Plot all ?
> y
PREPLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107
0
$
```
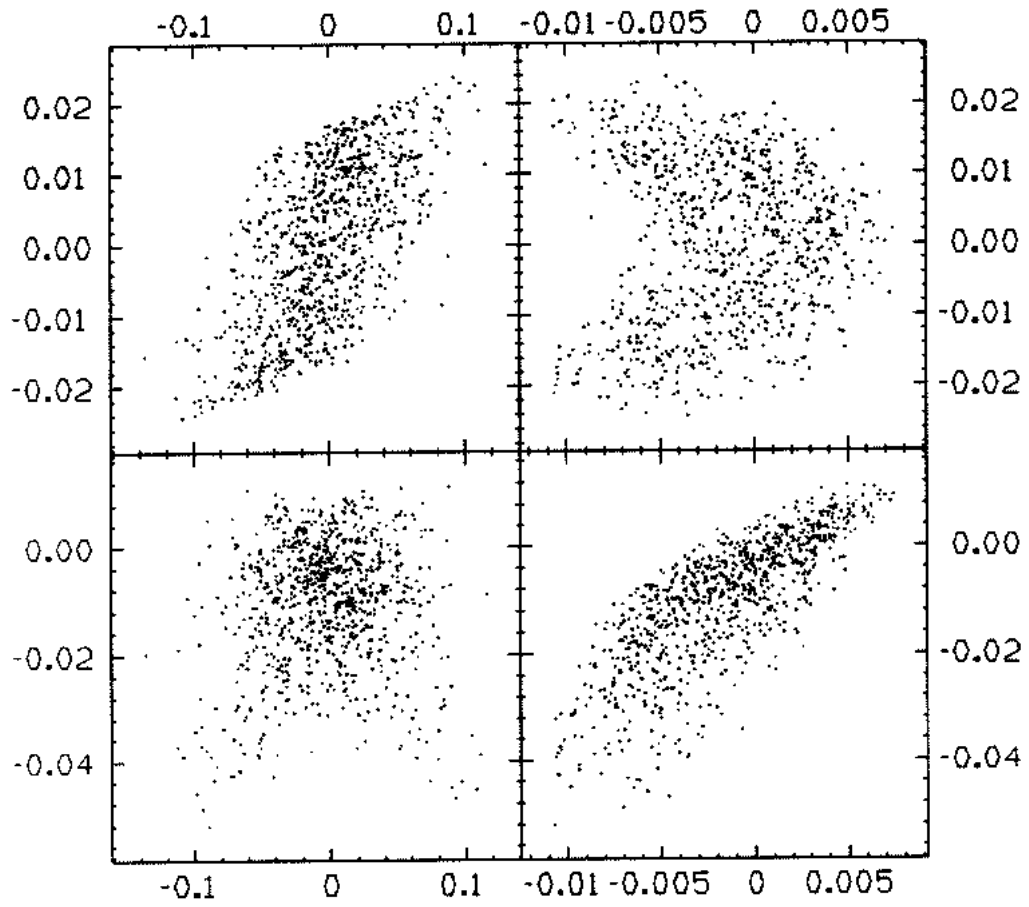
Figure 3.9: PLOTSPACE of TGM final image

PLOTXY

Purpose:	General plotting utility used with SHADOW.
Input:	Unformatted file generated by SHADOW (BEGIN.DAT, STAR.xx, MIRR.xx, SCREEN.xxyy etc.)
Output:	Plot to screen and to file if desired.

Description:

PLOTXY is the basic graphics utility for SHADOW. It will plot any combination of "columns" from the BOF that SHADOW writes, i.e., BEGIN.DAT, MIRR.xx, STAR.xx, SCREEN.xxyy etc. The figure below shows all possible options and, where applicable, the additional information required.

```
                    ┌──────────────┐
                    │    PLOTXY    │
                    └──────────────┘
                            │
                            ▼
                    ┌──────────────┐
                    │  Input file  │
                    └──────────────┘
                            │
                            ▼
                    Display stats
                            │
                            ▼
                    ┌──────────────┐
          ┌─────────│Set ray options│─────────┐
          │         └──────────────┘          │
          ▼                 ▼                  ▼
  ╭──────────────╮  ╭──────────────╮  ╭──────────────╮
  │0:Excluding losses│ │1:Including losses│ │2:Including all rays│
  ╰──────────────╯  ╰──────────────╯  ╰──────────────╯
          │                 │                  │
          └────────►┌──────────────┐◄──────────┘
                    │Read comment  │
                    └──────────────┘
                            │
                            ▼
                Row to plot Horizontal
                            │
                            ▼
            ╭──────────────────────────╮
            │  1 X    2 Y    3 Z       │
            │  4 X'   5 Y'   6 Z'      │
            │  7 Asx 8 Asy 9 Asz       │
            │  10 FF 11 q 12 KK        │
            │  ─ ─ ─ ─ ─ ─ ─ ─ ─ ─     │
            │  13 OPD 14 Fs 15 Fp      │
            │  16 Apx 17 Apy 18 Apz    │
            ╰──────────────────────────╯
```

Row to plot Vertical

```
1 X    2 Y    3 Z
4 X'   5 Y'   6 Z'
7 Asx  8 Asy  9 Asz
10 FF  11 q   12 KK
------------------------
13 OPD 14 Fs  15 Fp
16 Apx 17 Apy 18 Apz
```

Scaling

| 0:Automatic | 1:Cartesian | 2:External Limits
Xmin, Xmax
Ymin, Ymax |

Plotting

| 0:Scattered plot | 1:Connected plot
grid size
Nx by Ny | 2:Contour plot
bins [Nx,Ny]
contours
polynomial |

Hairline

```
                              ┌─────────────────┐
                              │  Contour plot:  │
                              └─────────────────┘
                  ┌───────────────────┐         ┌────────────────────┐
                  │  No reflectivity  │         │ Include reflectivity│
                  └───────────────────┘         └────────────────────┘

                        ┌──────────────────────┐
                        │  0:No normalization  │
                        └──────────────────────┘

        ┌──────────────────┐         ┌────────────────────────┐
        │ 1:Normalize to 1 │         │ 2:Normalize to total   │
        └──────────────────┘         │        counts          │
                                     └────────────────────────┘


   ┌────────────────────────┐  ┌────────────────────────┐  ┌────────────────────────┐
   │ Power density [J/area] │  │ Power density [J/area] │  │ Local reflectivity/    │
   │ absorbed               │  │ reflected/transmitted  │  │ transmission           │
   │     file for Io        │  │                        │  │                        │
   └────────────────────────┘  └────────────────────────┘  └────────────────────────┘

                              ┌──────────────────┐
                              │ Scaling Options  │
                              └──────────────────┘

   ┌────────────────┐  ┌────────────────────┐  ┌────────────────────────────┐
   │  No scaling    │  │ Scaling with user  │  │ Auto scaling for SR        │
   │                │  │ supplied number    │  │ source:                    │
   │                │  │ scaling factor:    │  │    machine radius [m]      │
   │                │  │                    │  │    machine energy [GeV]    │
   │                │  │                    │  │    machine current [A]     │
   │                │  │                    │  │    milliradians of orbit   │
   │                │  │                    │  │    conversion from cm      │
   │                │  │                    │  │     to user units          │
   └────────────────┘  └────────────────────┘  └────────────────────────────┘

                              ┌──────────────┐
                              │  Smoothing   │
                              └──────────────┘
```

Smoothing

Smoothing   No smoothing

Save Option

Save grid file   Don't save file

Hairline

hairline at 0,0   no hairline

Overlay mirror or slit

No mirror/slit   Mirror/slit

Rectangle
  Xmin, Xmax
  Ymin, Ymax

Ellipse
  semi axis along X
  semi axis along Y
  center [X]
  center [Y]

Histograms

−1: to skip histograms

0: same limits as plot

1: 3*standard deviation

2: external limits

(contour plot)

Number of bins in X

Number of bins in Y

Save TD command file?

Don't save command file

Write TD.FIL command file

Terminal type

0: VT240

1: TEK40XX

2: HIREZ

3: TEK4107

Plotting Begins

Examples:

We'll show the contour plot of the footprint on the first mirror of the two mirror example from the primer.

```
$ dir

Directory D13:[XRAYOP.DOCUMENT.UTIL.PLOTXY]

MIRR.01;2                 282   5-MAY-1987 14:55:09.61  (RWED,RWED,RE,RE)

Total of 1 file, 282 blocks.
$
$ plotxy


PLOT> Input file? mirr.01                    \* Use mirror BOF file *\
PLOT> Options --- Enter
PLOT>   0   for excluding the losses
PLOT>   1   for including only the losses
PLOT>   2   for including all the rays.
PLOT> Then ? 0                               \* no losses  *\
PLOT> Comment for plot [ 80 char ] ?    \* a title, if you will  *\
First Mirror footprint

PLOT> File read OK. Full specifications:
      D13:[XRAYOP.DOCUMENT.UTIL.PLOTXY]MIRR.01;2
      Was created :  5-MAY-1987 14:55

PLOT>  Found        1000 good points out of        1000
PLOT>  The following columns are defined for each ray :
       1)   the regular columns [1-12]
       2)   optical path [13]
       3)   phase angle of As [14], Ap [15], and the Ap vector [16-18]



 Col Par Minimum:        Maximum:        Center:        St. Dev.:

  1  X    -12.123        12.010         0.65111E-01       5.7198
```

```
 2  Y     -96.780          66.459         -17.829          29.971
 3  Z      0.42575E-04      2.7165         0.60979         0.55687
 4  X'    -0.22904E-01      0.22887E-01   -0.13710E-03     0.10877E-01
 5  Y'     0.99918          0.99953        0.99941         0.00000E+00
 6  Z'     0.24788E-01      0.39796E-01    0.32624E-01     0.26776E-02
11    Photon Energy  (eV)       500.00            500.00
20    Numerical Aperture       0.30578E-01    0.40520E-01


PLOT> Options. You may plot any two rows from the above
      list versus each other. You may also plot any of
      them versus the ray numerical aperture.
      N.A. -- enter 20.


PLOT> Rows to use for plot :
PLOT>   for horizontal axis ? 1           \* X *\
PLOT>   for vertical axis   ? 2           \* Y *\


PLOT> Scaling options. Enter

      0    For automatic scaling
      1    For cartesian scaling
      2    For external limits
PLOT> Then ? 2                            \* choose external limits *\
PLOT> Enter limits.
PLOT> Horizontal min.: -50
PLOT> Horizontal max.: 50
PLOT> Vertical min.  : -150
PLOT> Vertical max.  : 100
PLOT> Plotting options :
      0    For scattered plot
      1    For connected plot
      2    For contour plot
PLOT> Then ? 2                            \* contour plot *\
PLOT> Number of bins [Nx by Ny] to prepare the contours.   \* odd number *\
PLOT> Nx : 21
PLOT> Ny : 21
PLOT> Number of contours : 11         \* number of lines or levels *\
PLOT> Degree of polynomial used for joining [0=default] : 0
PLOT> Included reflectivity ? 0       \* don't include reflectivity here *\
PLOT> Data normalization :
```

```
        0    For no normalization
        1    For normalized to 1
        2    For normalized to total counts
PLOT> Then ? 2                               \* normalize to total counts *\
Smoothing [ Y/N ] ? 1                        \* choose smoothing  *\
Save grid file [ Y/N ] ? 0
PLOT> Hairline at [ 0,0 ] ? 0
PLOT> Overlay a mirror/slit ? 0
PLOT> Ready for histograms. Enter:
     -1          to skip
      0       for same limits as plot
      1                   3*stdev
      2                   external
PLOT> ? 0
PLOT> Do you want to save the TD command file ? 1    \* save the command file *\
PLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107:0


$ dir/since                                  \* show the command file *\

Directory D13:[XRAYOP.DOCUMENT.UTIL.PLOTXY]

TD.FIL;1                37    2-AUG-1989 10:09:14.99  (RWED,RWED,RE,RE)

Total of 1 file, 37 blocks.
$
```

The command file TD.FIL is plottable using TDTEK and UGTEK.

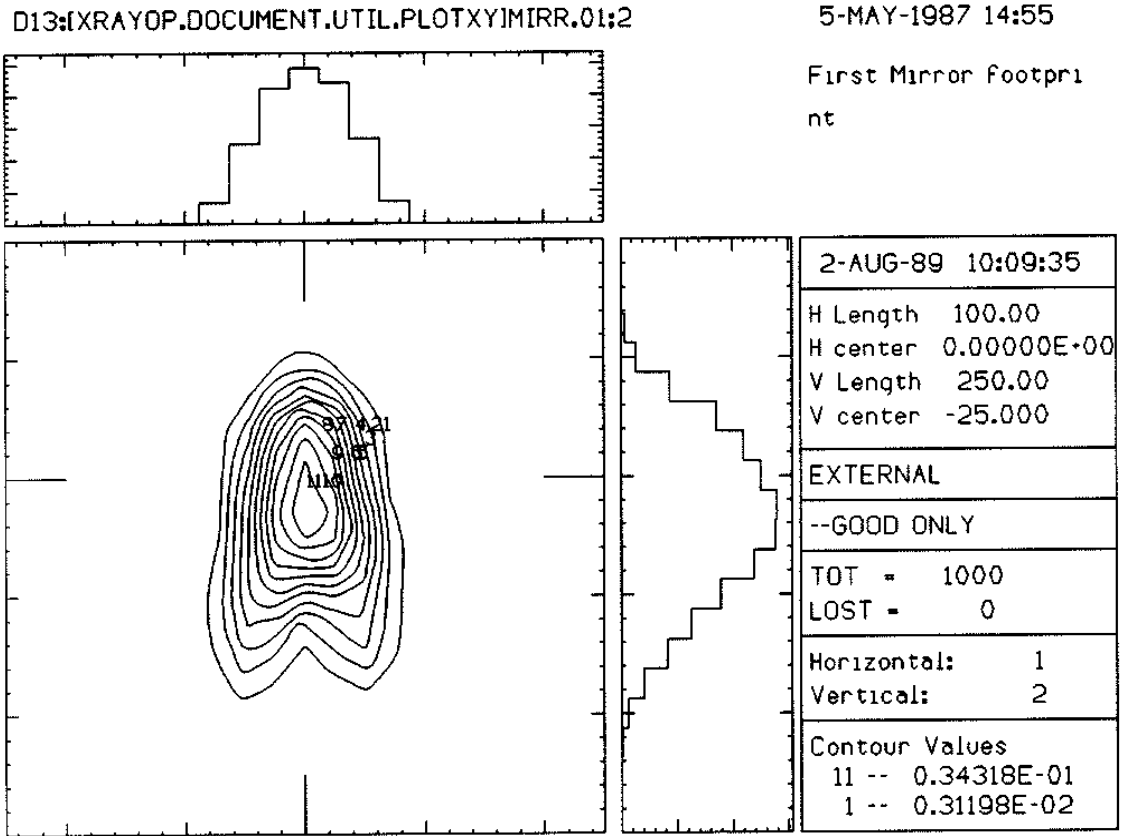D13:[XRAYOP.DOCUMENT.UTIL.PLOTXY]MIRR.01;2

5-MAY-1987 14:55

First Mirror footpri

nt

2-AUG-89 10:09:35	
H Length 100.00	
H center 0.00000E+00	
V Length 250.00	
V center -25.000	
EXTERNAL	
--GOOD ONLY	
TOT = 1000	
LOST = 0	
Horizontal:	1
Vertical:	2
Contour Values	
11 -- 0.34318E-01	
1 -- 0.31198E-02	

Figure 3.10: PLOTXY output

PREPLOT

Purpose:	Creates a two or three column formatted file from a binary output file. The user specifies which two or three columns of the BOF to use for output. The generated file is in a form suitable for input to a graphics routine like TopDrawer or an analysis program that requires formatted input like FMAX or FILEX. Also, a quick alternative to PLOTXY.
Input:	Any Binary output file.
Output:	A user specified file (use TT to direct output to terminal). The file is formatted and in *single precision*.

Description:

PREPLOT generates a two or three column formatted file from a BOF input file. Any of the standard 12 rows (13 or 18 if optical path or polarization is selected when source is defined) may be selected in addition to "rows" 20-23 which are defined during PREPLOT execution (see example). The output can then be used as input to a graphics, histogram, or analysis program that requires formatted input. For example, if one wanted to create a table of optical path length vs. angle from the optical axis at the 2nd image plane, then rows 21 and 13 would be selected from the file STAR.02. **Note:** output is in *single precision*.

Examples:

Let's use the STAR.01 file from sec 2.4 of the primer (spherical mirror).

```
$ 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 :
1
PREPLOT>       2 :
4
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
***********
Found          1000 good points out of        1000
Output options :
  [ 0 ] store rays in a file
  [ 1 ] plot directly on screen
  [ 2 ] both
Then ?
0
PREPLOT> Output file ?
pre.dat
```

Let's look at the first 15 lines of pre.dat

```
$ ty pre.dat
 -0.2780961      1.8455550E-02
 -0.2831062      1.8694960E-02
  0.3307338     -2.2033621E-02
 -0.3311352      2.2213560E-02
 -9.4173871E-02  6.2023830E-03
  0.2767766     -1.8385222E-02
  0.3686378     -2.4258027E-02
  0.1166269     -7.7635958E-03
 -0.3735043      2.5044683E-02
 -0.3660054      2.4130033E-02
```
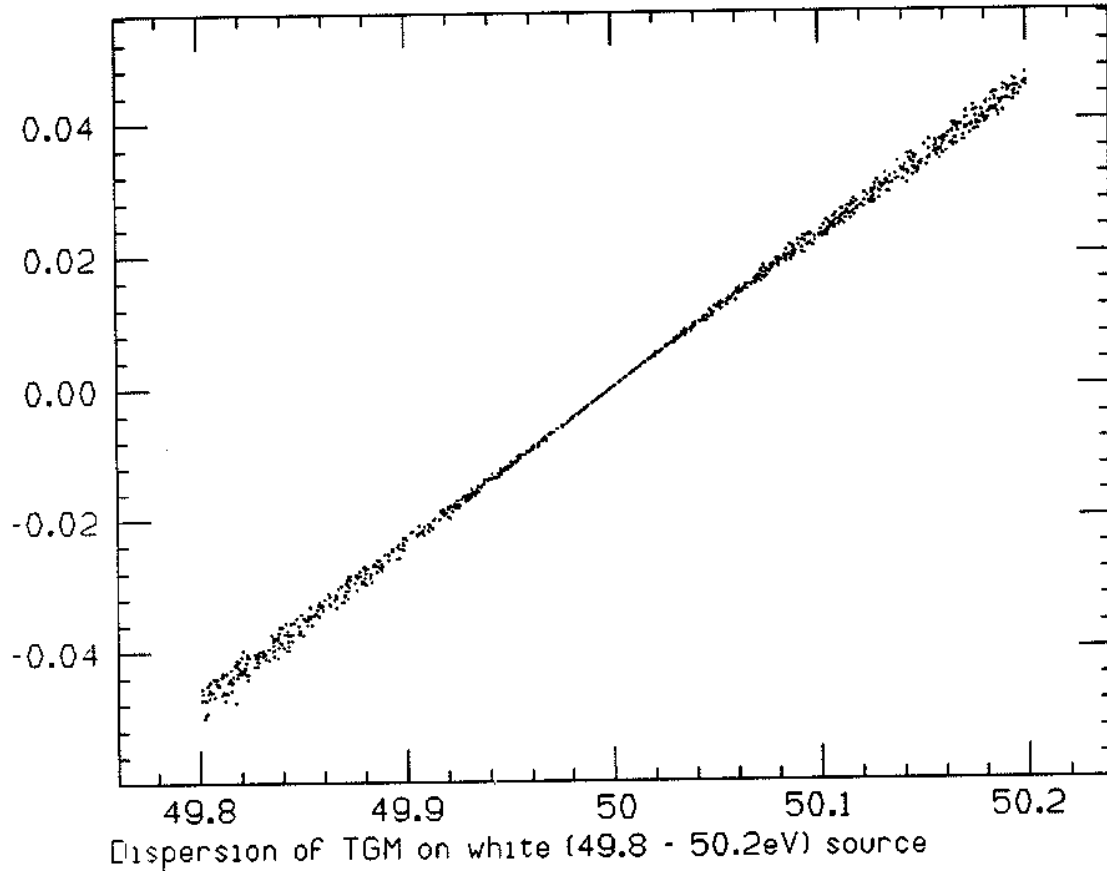
Figure 3.11: PREPLOT: Energy vs. Z for TGM exit slit

```
-9.1828540E-02   6.0481941E-03
 0.3607364      -2.4109263E-02
 0.3719847      -2.5014305E-02
-3.2931246E-02   2.2053795E-03
 0.1509321      -1.0015748E-02
```

PREPLOT2

Purpose:	Creates a two column formatted file from *two* binary output files. The user specifies which row of each ray file to use for output. With this utility it is possible to study the correlation between different optical systems, or between different sections of the same OS.
Input:	Any two binary output files.
Output:	A user-specified formatted two column file or TT.

Description:

This utility allows the user to create a two column file from two different ray files. Any one of the standard twelve to eighteen columns from the first ray file may be tabulated against any column from the second file. The user may then use this data to plot the correlation between various optical systems or between different elements of the same system. For example, the distance off axis in the x-direction at a mirror may be correlated with the optical path length at, say, a image plane further along in the system.

Examples:

One example of PREPLOT2 would be to use it to study the correlation between footprint width on the grating of a TGM and the dispersion at the exit slit. Using out TGM setup at an energy of 59 eV, we run PREPLOT2 using column 1 at the grating (X) and column 3 at the exit slit (Z).

```
$ dir

Directory CXRL$DUA0:[SHADOW.ZDOCUMENT.UTIL.PREPLOT2]

MIRR.02;3              282  28-DEC-1989 10:23:10.19  (RWED,RWED,RE,) <<<
STAR.02;3              282  28-DEC-1989 10:23:13.49  (RWED,RWED,RE,) <<<
SYNCH.00;126             7  28-DEC-1989 10:19:23.61  (RWED,RWED,RE,)
SYSTEMFILE.DAT;2         1  28-DEC-1989 10:22:48.04  (RWED,RWED,RE,)
TGMEG.01;47             12  28-DEC-1989 10:22:46.61  (RWED,RWED,RE,)
TGMEG.02;47             12  28-DEC-1989 10:22:47.11  (RWED,RWED,RE,)
TGMEG.03;48             12  28-DEC-1989 10:22:47.67  (RWED,RWED,RE,)

Total of 7 files, 608 blocks.
$ preplot2
All the losses will be determined by the SECOND file.
```

```
First file to be prepared ?
mirr.02                          \* grating footprint file *\
Second file to be prepared ?
star.02                          \* exit slit (image) file *\
Columns to write out from file
mirr.02
1                                \* X -- width of footprint *\
Columns to write out from file
star.02
3                                \* Z -- height of image at slit *\
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.
? 2                              \* plot all rays to show full dispersion *\
***********
Found           876 good points out of         1000
Output options :
  [ 0 ] store rays in a file
  [ 1 ] plot directly on screen
  [ 2 ] both
Then ? 0
Output file ? aberr
$
```
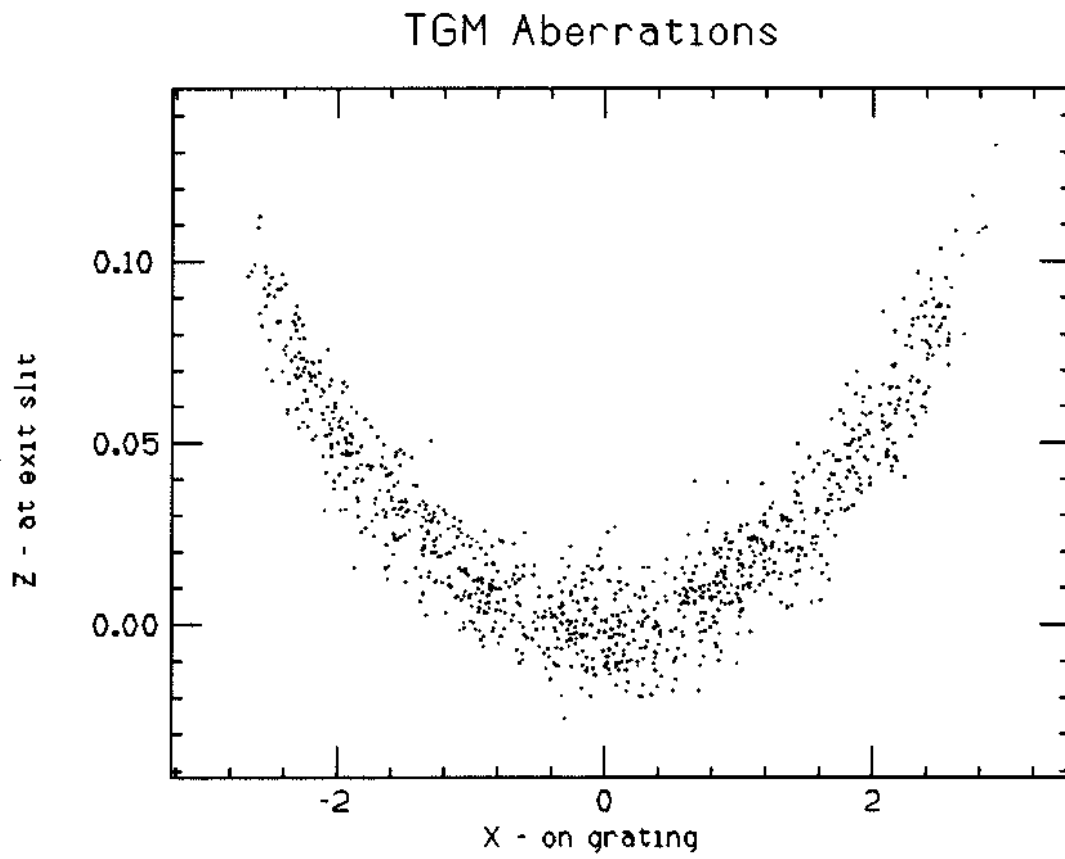
The output is shown in figure 3.12.

Figure 3.12: PREPLOT2 output

SURPLOT

Purpose:	Creates a plottable three dimensional file of a mirror surface. It can be used to plot out the "real" shape of a mirror.
Input:	A Binary Output File (for example MIRR.xx).
Output:	A three dimensional plottable file to be used as input to TDFILE.

Description:

SURPLOT takes a binary output file (BOF) and creates a plottable file that can be put into TopDrawer to create a "real" picture of the mirror surface. It must be used with a rectangular, GRID/GRID source, with the grid in X and Z, and only a 1 x 1 grid in phase space. The source should be about the size of the surface you wish to plot, and should have no depth and zero divergence. This assures that the rays are parallel when they hit the mirror's surface. The system must consist of only the optical element you wish to plot because after the first element the rays will no longer be parallel.

Examples:

We'll show two examples of mirror surfaces, one elliptical and one toroidal. Below is the output from SOURCINFO on the source used, as well as the MIRINFO for each example.

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S O U R C E     D E S C R I P T I O N **************
GRID/GRID Source
Example of source used for SURPLOT
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
end.00
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.SURPLOT]END.00;2
Creation Date           :13-APR-1989 13:48
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Grid Source.
Generated total          225 rays.
Source assumed BIDIMENSIONAL (flat).
Source Spatial Characteristics: RECTANGULAR
Source Width:   8.00000000    and Height:   18.0000000
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: UNIFORM
Distribution Limits. +X :   0.000000000E+00 -X:   0.000000000E+00 rad
                     +Z :   0.000000000E+00 -Z:   0.000000000E+00 rad
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************               E N D                  **************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++



++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*******************   MIRROR  DESCRIPTION   *******************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Elliptical Mirror SURPLOT Example
Elliptical mirror with shape exaggerated.
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.SURPLOT]END.01;6
Creation Date          :14-APR-1989 15:40
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


Surface figure was defined as:        ELLIPTICAL
Cylindrical figure                    NO
Element type                          REFLECTOR
Reflectivity                          OFF
Mirror dimensions ( elliptical ) :
        Major Axis          Minor axis
         -9.0000              -6.0000
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                     100.0000000000000
Image  Plane                              100.0000000000000
Incidence Angle                           0.0000000000000000E+00
Reflection/Diffraction Angle              0.0000000000000000E+00

Mirror parameters                     EXTERNAL
Parameters used follow:
    Semi-major axis     50.00000000000000
    Semi-minor axis     20.00000000000000
    Semi-focal-length  0.0000000000000000E+00
```

```
   Eccentricity        0.0000000000000000E+00
 Source of this O.E. moved               NO
 Mirror at pole position ( no mov. )     YES
  +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Now we'll show a log of the run through SURPLOT and the output after running it through TopDrawer.

```
$ surplot
SURPLOT> File ?
mirr.01
Mesh size must be Nx by Ny.
>> Nx ?
15
>> Ny ?
15
READ          225 POINTS.
$ dir/since

Directory D13:[XRAYOP.DOCUMENT.UTIL.SURPLOT]

SURPLOT.DAT;7            66  11-APR-1989 14:44  (RWED,RWED,RE,RE)

Total of 1 files, 66 blocks.

$ type sur.com
SET THREE

SET ORDER X Y Z
SET LIMITS X -7 7  y -7 7 Z -7 7
SET AXIS OFF
@SURPLOT.DAT
END
```

The plot can be generated using TDTEK and UGTEK with the use of a simple command file in TDTEK, shown above. For best results, the size of the source should not exceed the size of the mirror. The limits in the command file may have to be adjusted slightly to fit the entire mirror.

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*******************   MIRROR  DESCRIPTION   *******************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Toroidal Mirror
Second example of SURPLOT
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.SURPLOT]END.01;3
Creation Date            :13-APR-1989 13:48
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:        TOROIDAL
Cylindrical figure                    NO
Element type                          REFLECTOR
Reflectivity                          OFF
Mirror dimensions ( elliptical ) :
        Major Axis          Minor axis
         -9.0000              -6.0000
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                 100.0000000000000
Image  Plane                          100.0000000000000
Incidence Angle                       0.0000000000000000E+00
Reflection/Diffraction Angle          0.0000000000000000E+00

Mirror parameters                     EXTERNAL
Parameters used follow:
   Major Radius       15.00000000000000
   Minor Radius       5.000000000000000
Source of this O.E. moved             NO
Mirror at pole position ( no mov. )   YES
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```
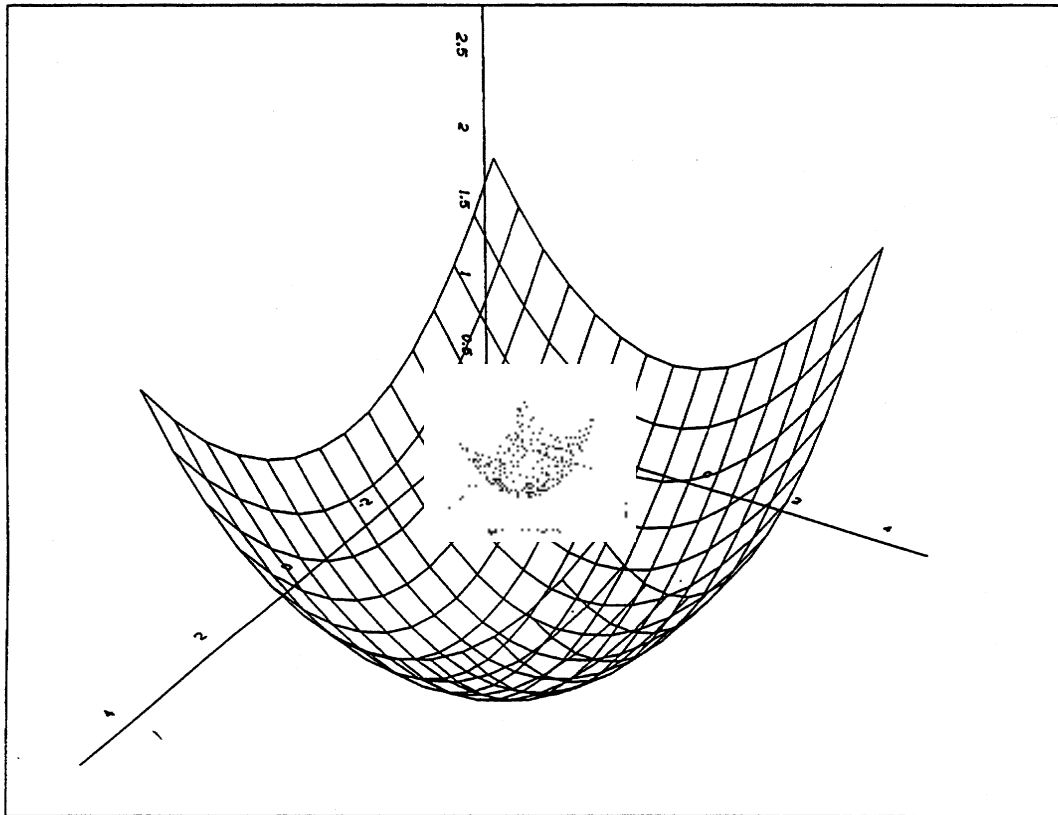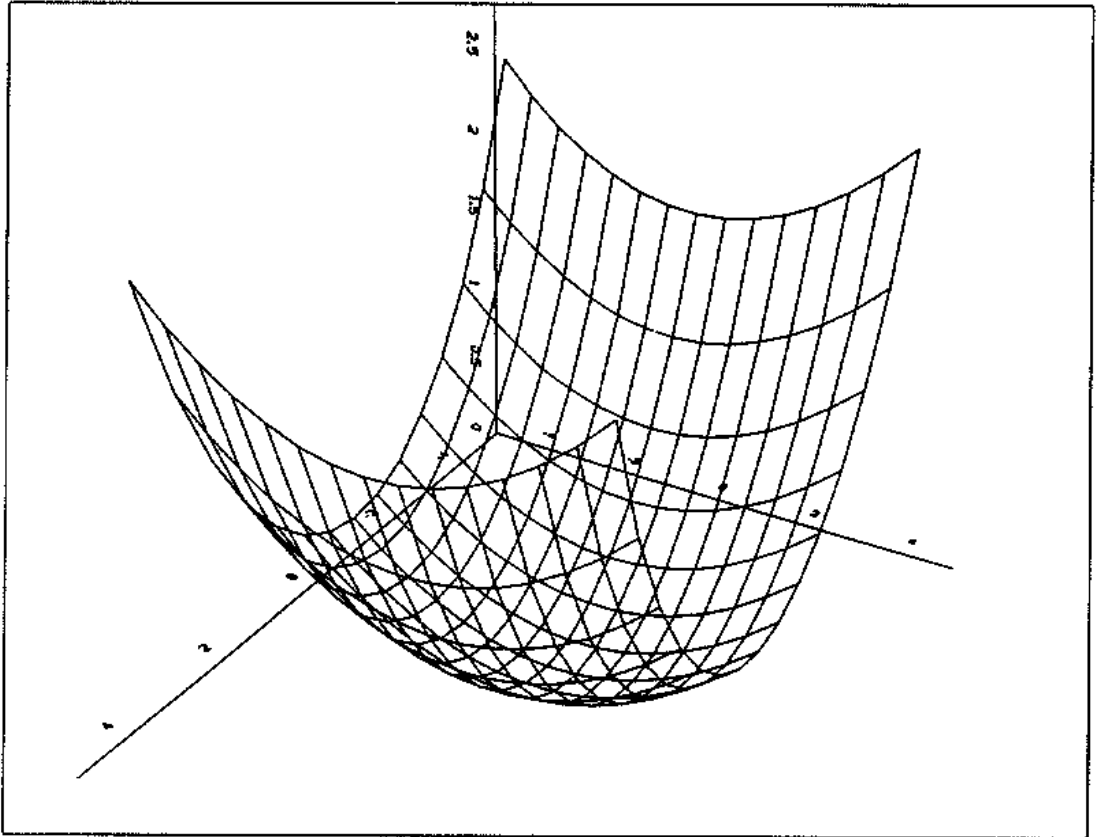
Elliptical Mirror Surface

Figure 3.13: SURPLOT: Elliptical Mirror

A better illustration may be the toroidal grating from the TGM. It is shown below, having been traced with a grid source and run through SURPLOT. The shape is exagerated due to the scaling, X -3 to 3, Y -50 to 50 and Z 0 to 1. The user can also add extra lines to the plot, to better define the mirror shape.

Toroidal Mirror Surface

Figure 3.14: SURPLOT: Toroidal Mirror
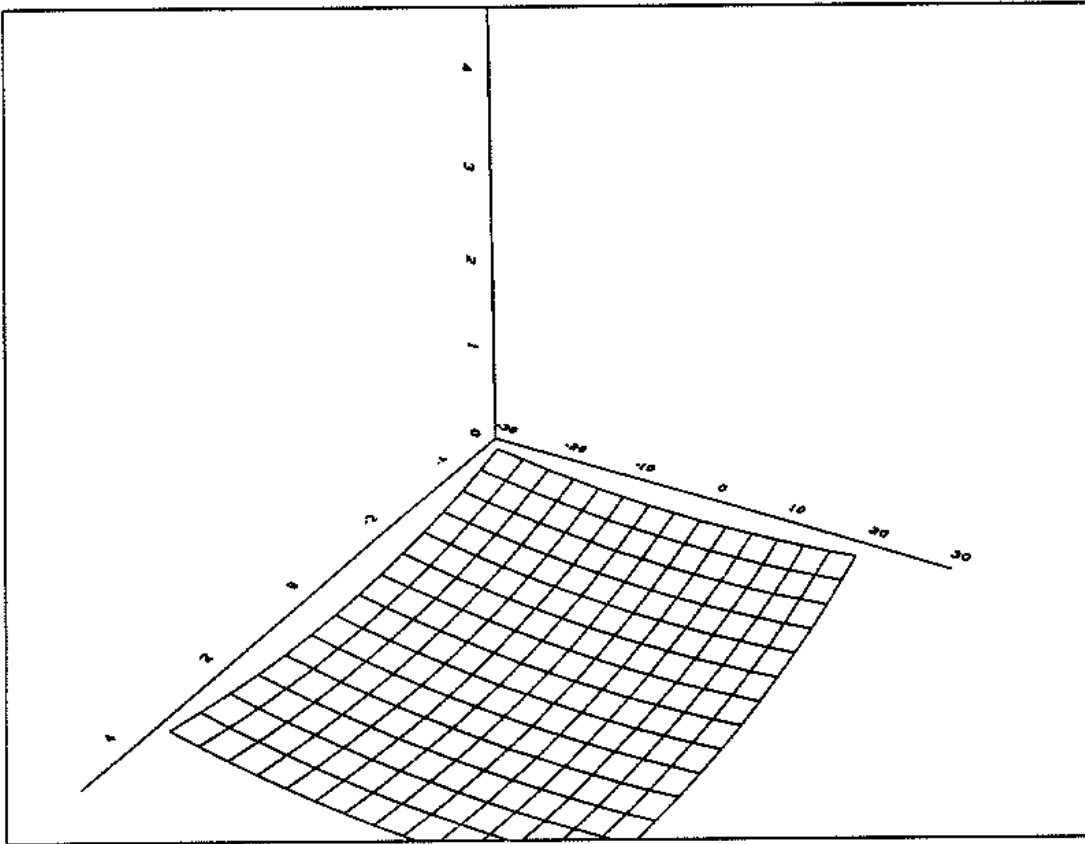
Grating Surface of 6m TGM

Figure 3.15: SURPLOT: TGM Grating

SYSPLOT

Purpose:	Creates a plottable file of all the rays in an optical system in the laboratory reference frame. Either a two or three dimensional plot can be made.
Input:	All of the following are required for input to SYSPLOT:

File	Example
Optical Axis File	OPTAX.nn
Source Binary Output File	BEGIN.DAT
Final Image Binary Output File	STAR.nn
	(There are nn OEs in the OS)
All OE Binary Output Files	MIRR.01-MIRR.nn

Output:	A plottable file SYSPLOT.DAT that can be used as input to TopDrawer.

Description:

SYSPLOT will create a plottable file that shows the path of each ray with respect to the physical optical system. Two dimensional projections of X vs. Y or Z vs. Y can be implemented by selecting columns 2,1 or 2,3 respectively when prompted for horizontal and vertical columns. The output file SYSPLOT.DAT should be examined manually for extrema which will be used to set limits on the plot (see examples below). The output from TDTEK is then used as input to the routine UGTEK to generate the plot.

Examples:

We'll run SYSPLOT on the two mirror example from section 6.1 of the primer. The output from SYSINFO is shown first so one can compare the system to the plot. Ideally one would use a grid/grid source to generate the info for SYSPLOT since the rays would be regularly spaced. We won't do that here to be consistent with data in the Primer.

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S Y S T E M     D E S C R I P T I O N **************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
System shown by SYSPLOT


+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:TT:
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 #    Optical Element:                                    Creation Time:
   1    D13:[XRAYOP.DOCUMENT.UTIL.SYSPLOT]END.01;1          16-MAR-1989 21:55
   2    D13:[XRAYOP.DOCUMENT.UTIL.SYSPLOT]END.02;1          16-MAR-1989 21:56
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Optical Element #              1      System Number:

MIRROR    ELLIPTICAL              UNLIMITED       COMPUTED        REFLEC. OFF

   Orientation            0.0000000000000000E+00 deg.
   Source Plane           2000.000000000000
   Incidence Ang.         88.00000000000000       deg.
   Reflection Ang.        88.00000000000000       deg.
   Image Plane            500.0000000000000
      ----------------

Optical Element #              2      System Number:

MIRROR    ELLIPTICAL              UNLIMITED       COMPUTED        REFLEC. OFF

   Orientation            180.0000000000000       deg.
   Source Plane           1000.000000000000
   Incidence Ang.         88.00000000000000       deg.
   Reflection Ang.        88.00000000000000       deg.
   Image Plane            500.0000000000000
      ----------------


                        OPTICAL SYSTEM CONFIGURATION
                         Laboratory Reference Frame.


 OPT. Elem #        X =                 Y =                 Z =


      0          0.00000000000E+00   0.00000000000E+00   0.00000000000E+00
      1          0.00000000000E+00    2000.0000000       0.00000000000E+00
        1'          0.00000000000E+00    2498.7820251        34.878236872


++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************              E N D                 **************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
$ sysplot
File [ 0 ]  or tt [ 1 ] ?
1
Bidimensional [ 0 ] or 3d plot [ 1 ] ?
1
How many mirrors ?
2
How many rays [ suggest no more than 200 (500 max) ] ?
20
Optaxis file ?
optax.02
Source file and (final) image file ?
begin.dat
star.02
Mirror N.             1 ?
mirr.01
Mirror N.             2 ?
mirr.02
Plot all the losses too [ Y/N ] ?
Y
$ dir/since

Directory D13:[XRAYOP.DOCUMENT.UTIL.SYSPLOT]

SYSPLOT.DAT;5              8  11-APR-1989 13:29  (RWED,RWED,RE,)
SYSPLOT.STR;2             1  11-APR-1989 13:29  (RWED,RWED,RE,)

Total of 2 files, 9 blocks.
```

SYSPLOT creates the two files SYSPLOT.DAT and SYSPLOT.STR. SYSPLOT.DAT can now be plotted using TopDrawer. The limits were chosen by typing the file SYSPLOT.DAT and looking for the extrema. The simplest way to plot the system is to create a command file like the following:

```
set three
set order x y z
```

```
set limits x -50 50 y -100 4100  z -20 120
set ticks off
plot axes at 0 0 0
@sysplot.dat
end
```

To generate a plot on your terminal, use the utilities TDTEK and UGTEK. This is done by first running TDTEK as follows:

```
$ TDTEK
TOP DRAWER (10/10/80) NOW EXECUTING

@SYSPLOT.COM

<ctrl>O  (suppresses output)

$
```
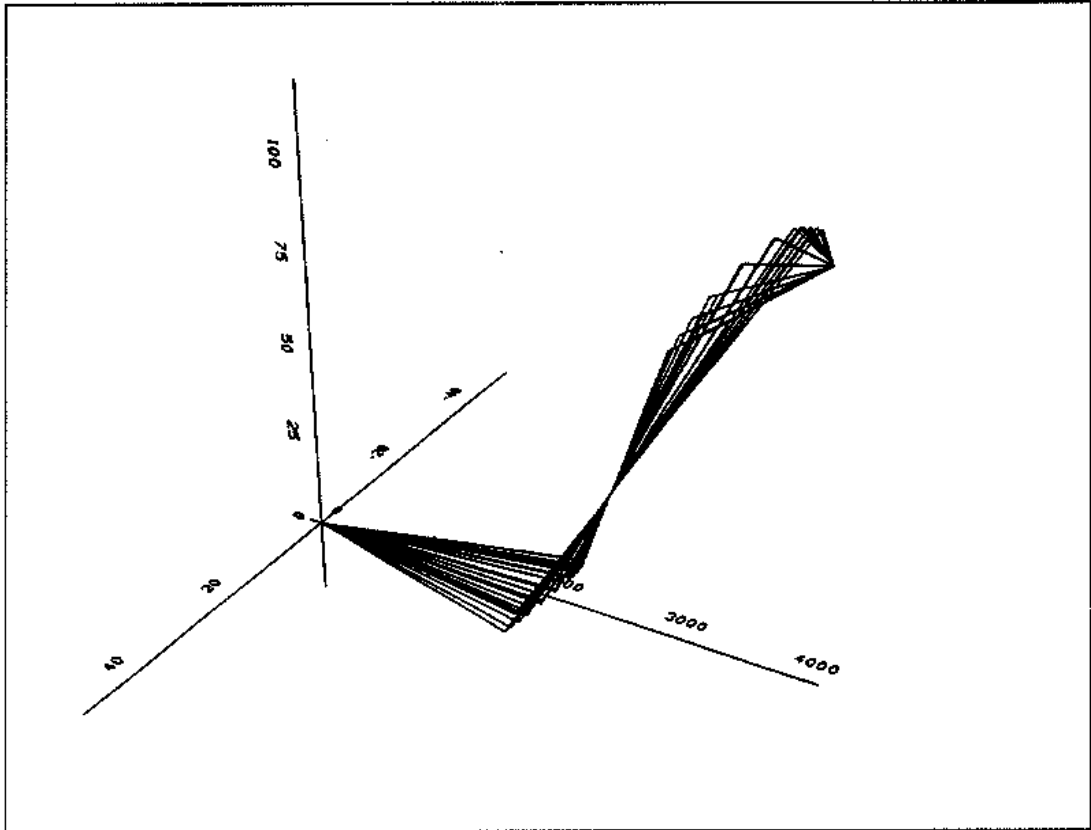
where SYSPLOT.COM is the command file shown above. Then you must put your terminal in graphics mode to run UGTEK on the file created by TDTEK called SAVE.DAT. This is shown in the following:

```
$UGTEK
UG element file: SAVE.DAT
Plot Which Pictures (default=all): <RET>
Enter Picture Scale Factor (default=1.0): <RET>
```

Two Mirror System in 3-D

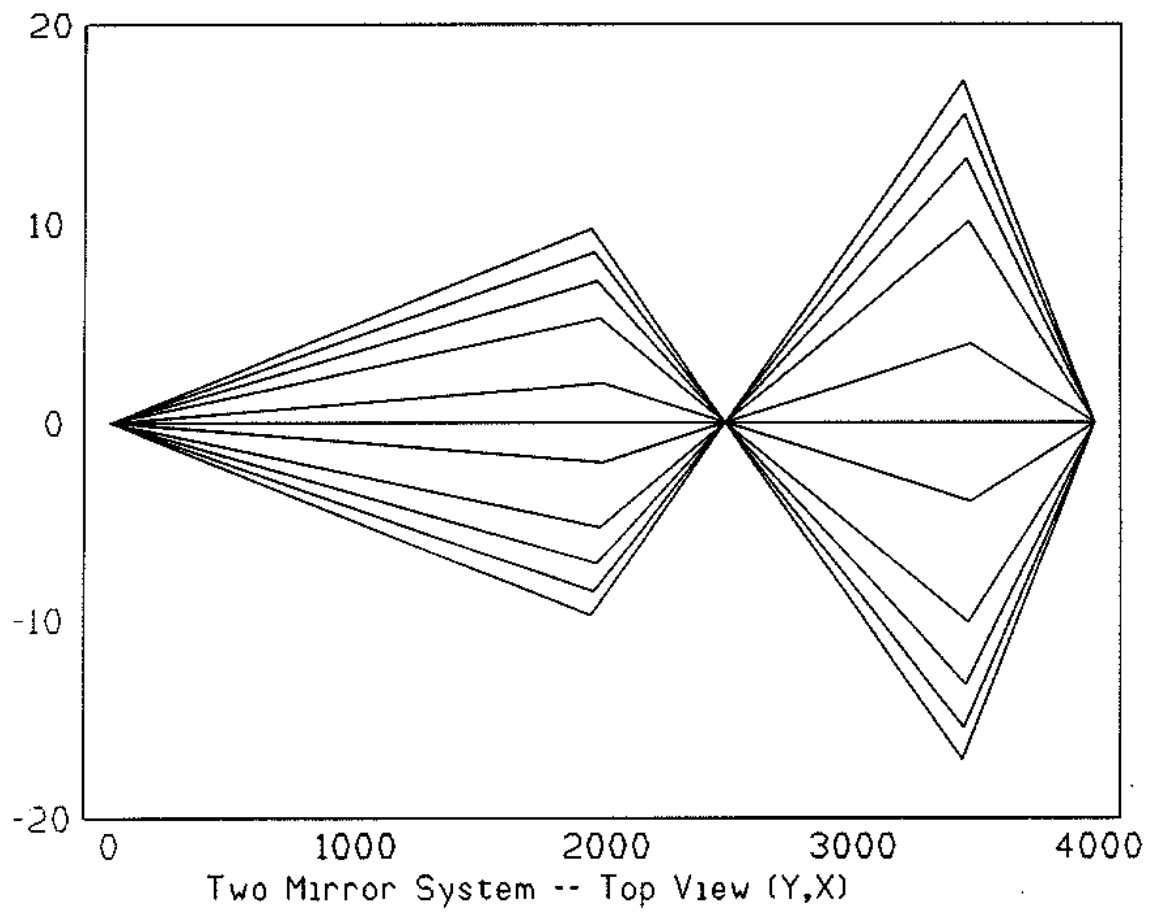Figure 3.16: SYSPLOT: 3-D system
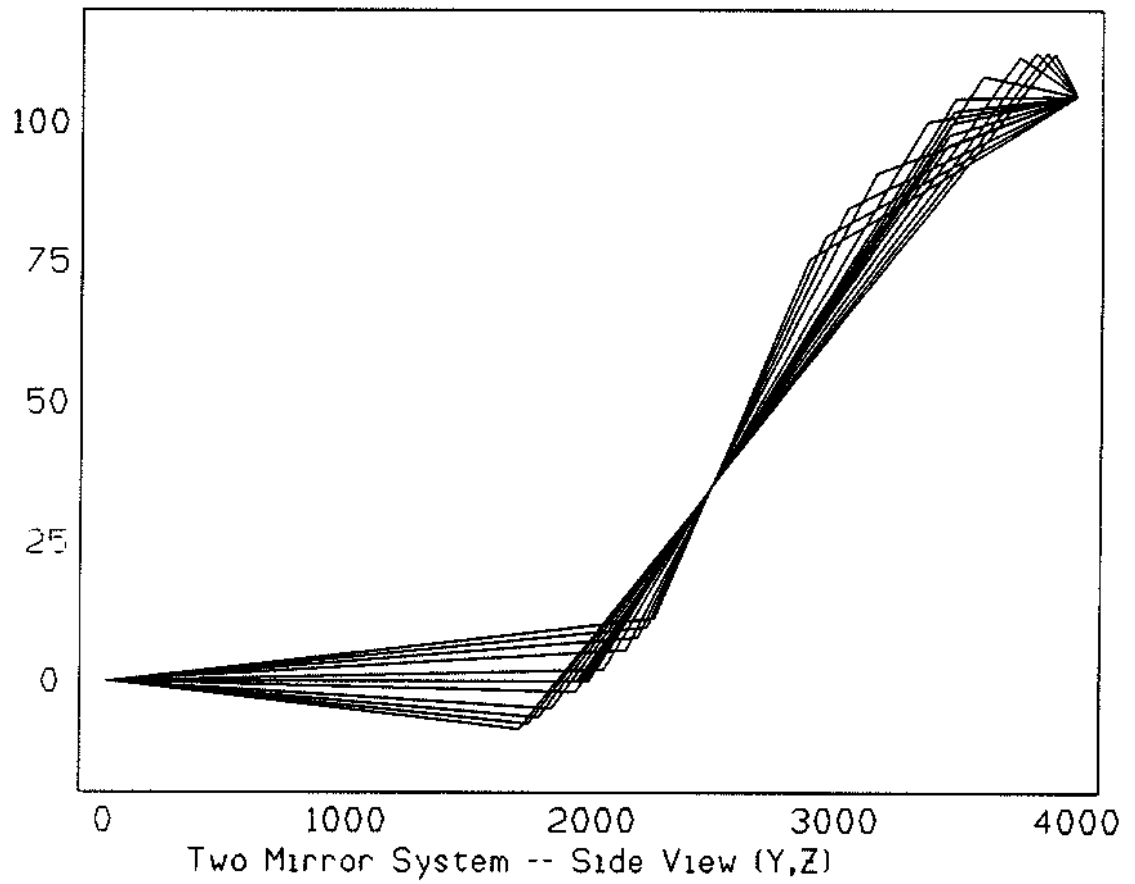
Figure 3.17: SYSPLOT: Top view

Figure 3.18: SYSPLOT: Side view

TDCONN

Purpose:	To generate a connected X-Y plot from a grid RAY file.
Input:	A grid RAY file that has been processed by TRANSLATE and COL_2, or any other two column file.
Output:	A plottable file suitable for TopDrawer output.

Description:

This utility will create a TopDrawer file, that when plotted will be a connected plot. It requires as input a two column formatted file. If one wishes to plot a ray file from SHADOW, it must be a grid file and it must be run through PREPLOT before being suitable for TD-CONN. The maximum number of data points it can handle is 5000. The program assumes that the M{x,y} records describes a grid, $\{N_x, N_y\}$. Thus a first pass is made by joining on {x}, then a second by joining on the other variable. In this way a connected plot is created. Very useful to show for example image distortions.

Examples:

To illustrate this utility, we will use a grid source with conical angle distribution traced through a toroidal mirror. This is the same system used in the SOURCE section of the User's Guide under Conical Angle Distribution. Here we show how to obtain the plot using PREPLOT and TDCONN instead of PLOTXY. The source and mirror are described, then we will show a log of how to get the results, and finally the plot.

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S O U R C E      D E S C R I P T I O N **************
TDCONN Example
Conical Source Angle Distribution-Grid source
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
end.00
Full file Specification :D13:[XRAYOP.DOCUMENT.SOURCE.CONICSAD]END.00;2
Creation Date          :27-MAR-1989 16:35
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Grid Source.
Generated total         160 rays.
Source assumed BIDIMENSIONAL (flat).
Source Spatial Characteristics: POINT
```

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: CONICAL
Cone Outer Aperture :   0.500000000E-02 Inner Aperture :   0.000000000E+00
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************               E N D              **************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*******************  MIRROR  DESCRIPTION   *******************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
TDCONN Example
Conical source traced through mirror
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :CXRL$DUA0:[XRAYOP.DOCUMENT.SOURCE.CONICSAD]END.01;2
Creation Date          :27-MAR-1989 16:36
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


Surface figure was defined as:        TOROIDAL
Cylindrical figure                    NO
Element type                          REFLECTOR
Reflectivity                          OFF
Mirror dimensions                     UNLIMITED
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                 1000.000000000000
Image  Plane                          1000.000000000000
Incidence Angle                       85.99999999999998
Reflection/Diffraction Angle          85.99999999999998

Mirror parameters                     COMPUTED
Same configuration as Central Axis    YES
Objective focus at                    1000.000000000000
Image focus at                        1000.000000000000
Incidence angle                       85.99999999999998
Parameters used follow:
   Major Radius        14265.83055245955
   Minor Radius        69.75647374412529
Source of this O.E. moved             NO
```

```
  Mirror at pole position ( no mov. )      YES
   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


$ preplot
PREPLOT> Input file ? star.01          \* Takes BOF and writes text file *\
Read               160 rays.           \* Maximum number of points allowed
Each ray has        12 entries.     \* by TDCONN is 5000.
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 : 1                    \* Here we show the x phase space *\
PREPLOT>      2 : 4
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
***********
Found          160 good points out of          160
Output options :
  [ 0 ] store rays in a file
  [ 1 ] plot directly on screen
  [ 2 ] both
Then ? 0
PREPLOT> Output file ? conic14.dat
$ r nutil:tdconn
TDCONN> Input file : conic14.dat               \* Read text file to create
Read          160 from                         \* plottable file. *\
conic14.dat

TDCONN> Grid size [ Nx by Ny ].                \* Nx times Ny must equal
TDCONN> Nx : 10                                \* the total number of points
TDCONN> Ny : 16
```
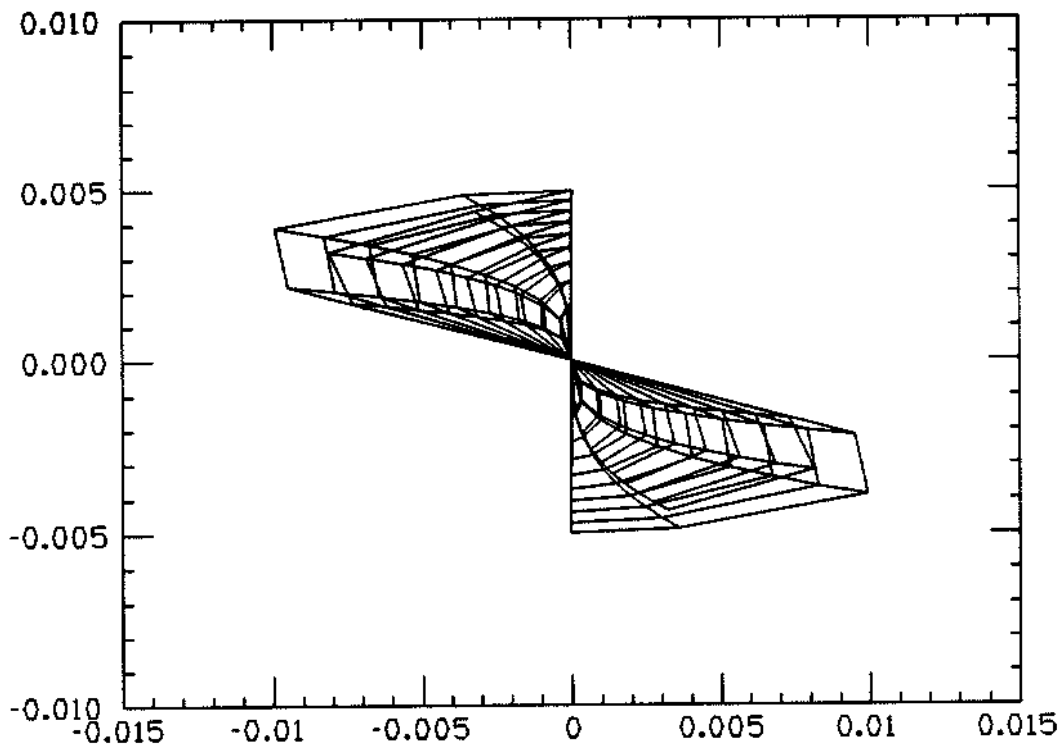
Figure 3.19: TDCONN Example – *X* phase space plot

```
Xmax =    9.9340184E-03 Xmin =   -9.9340184E-03
Ymax =    4.9745785E-03 Ymin =   -4.9745785E-03
TDCONN> Limits to use on the plot :
TDCONN> Xmin : -1.5e-02
TDCONN> Xmax : 1.5e-02
TDCONN> Ymin : -1e-02
TDCONN> Ymax : 1e-02
TDCONN> Output file : conic14.td                    \* Plottable directly using
$                                                   \* TD_NEW
```

HISTO1

Purpose: To determine the distribution of the values in a given column of a ray file. The data are binned in a histogram with conditions specified by the user.

Input: Any BOF (e.g. BEGIN.DAT, STAR.xx).

Output: A plottable file named histo1.dat or TT: or both.

Description:

This utility will create a one dimensional histogram from any column of a BOF. The extrema are given to the user, who must decide what the mean (center) and width of the histogram should be. Options are included to ignore the lost rays, to include reflectivity, and to direct output to the terminal or a file. If the output is in a file, the histogram may be plotted using the graphics routine TopDrawer as in the following example:

```
TDTEK
@ histo1.dat    // <CTRL> O may be toggled to supress output
histo           // The histogram is now plotted
end
```

Examples:

Here we will examine the system set up in the primer section 6.2. We have a rectangular source that models an entrance slit with very narrow vertical divergence. The optical element is a spherical diffraction grating with the slits placed on the Rowland circle. We have an energy range from 198 to 202eV, and will examine how the exit slit determines the output spectrum. For this, we will need to know the photon energy distribution, i.e., the histogram of the number of rays in function of the photon energy. The source and system descriptions follow.

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Incident upon Rowland Circle Mount Grating
HISTO1 Example
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
```

```
end.00
Full file Specification :DISK4:[RUNKLE.UG.UTIL.HISTO1]END.00;3
Creation Date          :25-APR-1989 17:44
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Random Source.
Generated total          5000 rays.
Source assumed BIDIMENSIONAL (flat).
Source Spatial Characteristics: RECTANGULAR
Source Width:    2.00000000     and Height:   0.200000000E-01
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: UNIFORM
Distribution Limits. +X :   0.500000000E-02 -X:   0.500000000E-02 rad
                     +Z :   0.100000000E-01 -Z:   0.100000000E-01 rad
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: BOX DISTR
From Photon Energy   198.000000     or   62.6187879    Angs.
To   Photon Energy   202.000000     or   61.3788119    Angs.
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++




+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
******************** MIRROR  DESCRIPTION   ********************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Rowland Circle Mount Diffraction Grating
HISTO1 Example
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :DISK4:[RUNKLE.UG.UTIL.HISTO1]END.01;7
Creation Date          :25-APR-1989 17:55
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:        SPHERICAL
Cylindrical figure                    NO
Element type                          REFLECTOR
Element type                          GRATING
Order choosen ( inside are < 0 )       -1.000000000000000
Automatic Tuning                      NO
Constant ruling [ lines/cm ]           12000.00000000000
```

```
Reflectivity                            OFF
Mirror dimensions                       UNLIMITED
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                        69.79800000000000
Image  Plane                                253.2330000000000
Incidence Angle                              88.00000000000000
Reflection/Diffraction Angle                 82.72600000000000

Mirror parameters                       EXTERNAL
Parameters used follow:
Spherical Radius                        2000.00000
Source of this O.E. moved               NO
Mirror at pole position ( no mov. )     YES
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

We have added an exit slit with dimensions 10 mm X 3.5 mm at the continuation plane.
We will create a histogram of the photon energy of the rays passing through the slit. The
spectrum is dependent on the slit width, the divergence in the vertical, and on aberrations
in the spherical mirror.

```
$Histo1
 File for analysis ? star.01
 Column to analyze ?  11
 Options : [0] Angstroms
         : [1] eV
         : [2] cm-1
 <?>  1
 Read    :         5000 rays
 Maximum :    201.9990
 Minimum :    198.0021
 Distribution center ?  200
             width ?  1
 Number of bins (odd, please) ?
 25
 Flag checks. Enter :
 0 to exclude lost rays
 1 to include lost rays too
```

```
 2 to use only lost rays
 <?> 0
 Normalization kind. Enter :
 0 for no normalization
 1 to normalize to 1
 2 area normalized to 1
 <?>
 0
 Include reflectivity ?  0
 Output options
   [ 0 ] store histogram in a file
   [ 1 ] plot histogram on screen
   [ 2 ] both
 Then ?  0
 Another run  [ Y/N ] ? 0
 Return to DCL
$
```

The output file can be used as input to TopDrawer by using the folowing commands in TDTEK:


```
@Histo1.dat
Histo
End
```

```
 The results are shown below.
```


Often the histogram assumes a shape close to that of a gaussian curve. This could be the case with the energy profile of a monochromator, or the distribution of rays across an image plane. We will plot the distribution in the vertical direction of rays in the final image plane for the TGM system. The procedure will be to obtain the mean and variance of the vertical distribution using VARIANCE on a PREPLOT file that has been generated from the final image ray file (STAR.03). The same data can be obtained from PLOTXY. These statistics will be used to generate a gaussian curve with the utility TGAUSS. Then HISTO1 will be run on the STAR.03 file using the mean and interval that the gaussian curve was generated with. Finally, both the histogram and superimposed gaussian will be plotted with TopDrawer.
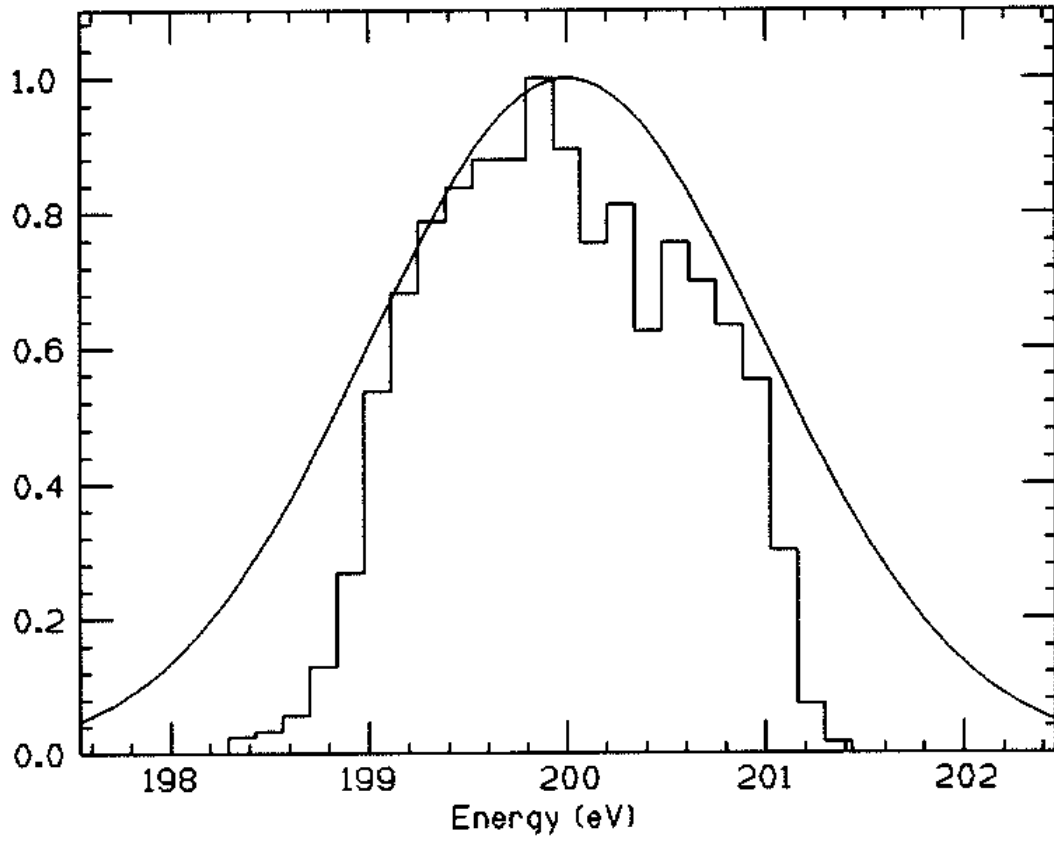
Figure 3.20: HISTO1 example

```
$ preplot
PREPLOT> Input file ?
TGM:star.03
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 :
1
PREPLOT>      2 :
3
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
***********
Found          927 good points out of        1000
Output options :
  [ 0 ] store rays in a file
  [ 1 ] plot directly on screen
  [ 2 ] both
Then ?
0
PREPLOT> Output file ?
pre.dat


$ variance
Log file ?
var.dat
```

```
File for analysis ?
pre.dat
Read           927 from
pre.dat
Column to analyze ?  2

Results from column          2
Mean value:  -1.0513511961653615E-02
Variance  :   1.4434200420233979E-04
Standard deviation :   1.2014241723984905E-02

Enter:
0    to exit
1    new file
2    new column (same file)
3    best fit (plottable)
?
0
```

FILEX must be used on the TGAUSS data file to add the mean value to the data, otherwise the curve would be centered on zero. It is the spherical aberration (notice tail) that gives an apparent shift.

```
$ filex
FILEX >
TG = TG "
FILEX > read           50 records.
FILEX > Succesful completion
FILEX >
TG = TG - %1.037e-2
FILEX > read           50 records.
FILEX > Succesful completion
FILEX >
TG = TG "
FILEX > read           50 records.
FILEX > Succesful completion
FILEX >
FILEX >
```

```
$ histo1
File for analysis ?
TGM:star.03
Column to analyze ?
3
Read     :          1000 rays
Maximum :    1.0586338E-02
Minimum :   -7.2909199E-02
Distribution center ?
-1.037e-2
             width ?
.08
Number of bins (odd, please) ?
25
Flag checks. Enter :
0to exclude lost rays
1to include lost rays too
2to use only lost rays
<?>
0
Normalization kind. Enter :
0for no normalization
1to normalize to 1
2area normalized to 1
<?>
1
Include reflectivity ?
0
Output options :
  [ 0 ] store histogram in a file
  [ 1 ] plot histogram on screen
  [ 2 ] both
Then ?
0
Another run  [ Y/N ] ?
0
Return to DCL
```
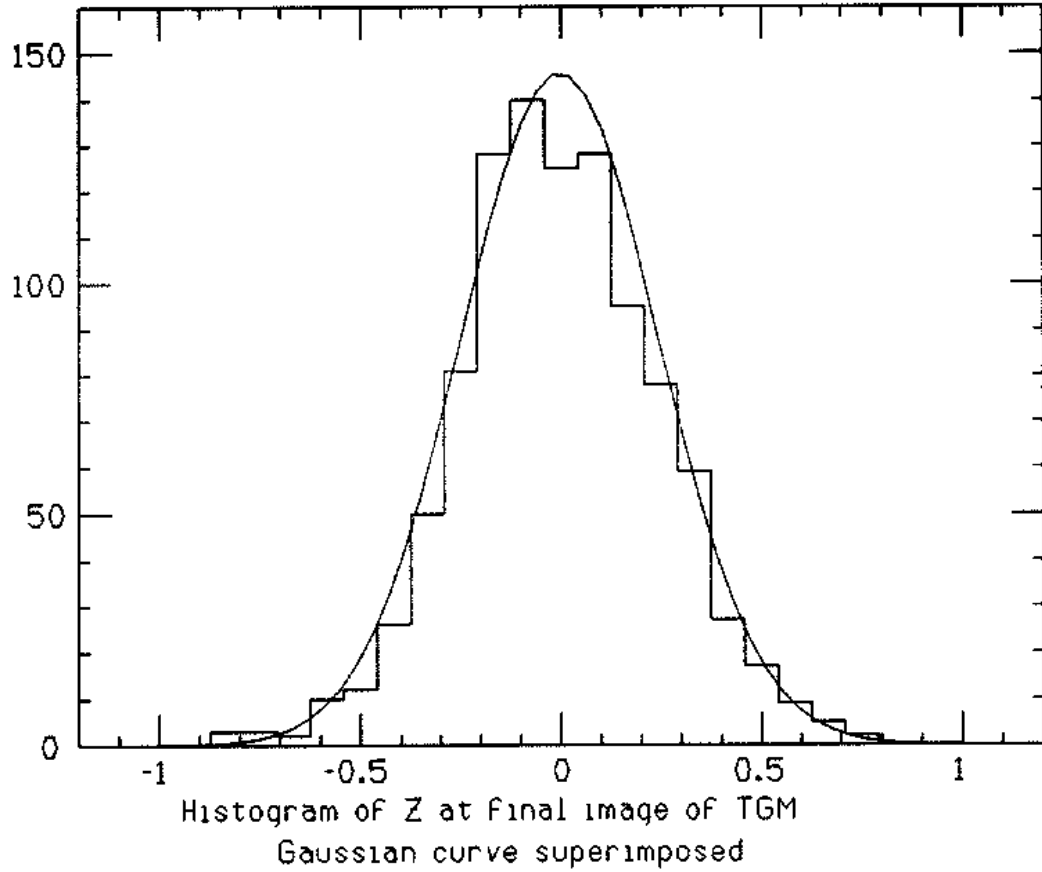
Figure 3.21: HISTO1: Histogram with superimposed gaussian curve

The following TopDrawer commands will superimpose the TGAUSS curve onto the histogram:

```
@histo1.dat
histo
@TG.dat
join 1
end
```

HISTO2

Purpose:	To create a two dimensional histogram from any two of the twelve to eighteen columns of a ray file.
Input:	Any BOF.
Output:	A formatted plottable file named MESH.DAT which can be used as input to a graphics routine like TopDrawer.

Description:

This utility enables the user to create a two dimensional histogram from any two columns of a ray file. The input file should first be run through the utility MINMAX to find the extrema (only for the first 6 columns) since HISTO2 asks for minimum and maximum values for each dimension. Like HISTO1, options for treating lost rays, reflectivity, and normalization are included. The output file MESH.PLT can be plotted using TopDrawer:

```
TDTEK
MESH.PLT    // <CTRL> O may be used to supress output
histo       // histogram is plotted here
end         // Exits TopDrawer
```

We do not have yet a good 3-d plotting utility, so the user will have to use the (limited) resources of TopDrawer or find another package. The NCAR package has powerful contouring capabilities and requires a different file format.

Examples:

Here will make two histograms using the TGM system. We will look at the ray distributions on the first mirror, and at the final image plane. Since HISTO2 asks for the limits, we will run MINMAX on each ray file to determine the appropriate intervals. The output is then used in TopDrawer. Note how the first histogram fills up the space of the mirror, which has a rectangular shape (4 X 9.5). The Final image also has a shape similar to that of the exit slit.

```
$ minmax
Input file ?
tgm:mirr.01
Options --- Enter
```

```
0 for excluding the losses
1 for including losses at a particular O.E.
2 for including all the losses.
Then ?
0
Comment ?
TGM example - first mirror footprint
***********
File examined is :
D13:[XRAYOP.DOCUMENT.TGM]MIRR.01;36
Was created :
15-MAY-1989 07:32
***********
Found            973 good points out of         1000
Here we are.
X max is   1.993178
X min is  -1.999294
Y max is   4.180661
Y min is  -4.735539
Z max is  0.1313010
Z min is  5.4842703E-06
X prime max is  1.1284630E-02
X prime min is -1.1375175E-02
Y prime max is  0.9963850
Y prime min is  0.9960120
Z prime max is  8.9194998E-02
Z prime min is  8.4335230E-02



$ histo2
File for analysis ?
tgm:mirr.01
Data ready. Read        1000 points.
Columns for x-axis and y-axis?
1
2
X min, X max and number of bins :
-5
5
```

```
25
Y min, Y max and number of bins :
-5
5
25
Do you want reflectivity too (Y=1,N=0) ?
0
Data normalization. Enter:
0for no normalization
1to normalize to 1
2to normalize to total counts
1
There were           27lost out of        1000 rays.
Computations done.
File for TOP DRAWER [ 0 ] or NCAR [ 1 ] ?
0
All done.




$ minmax
 Input file ?
 tgm:star.03
 Options --- Enter
 0 for excluding the losses
 1 for including losses at a particular O.E.
 2 for including all the losses.
 Then ?
 0
 Comment ?
 TGM example - Final image
 **********
 File examined is :
 D13:[XRAYOP.DOCUMENT.TGM]STAR.03;36
 Was created :
 15-MAY-1989 07:32
 **********
 Found        927 good points out of        1000
 Here we are.
 X max is  9.4501123E-02
```

```
X min is -0.1043031
Y max is  2.9244185E-15
Y min is -3.3843032E-15
Z max is  1.0586338E-02
Z min is -5.0542224E-02
X prime max is  2.2949979E-02
X prime min is -2.3045009E-02
Y prime max is  0.9999999
Y prime min is  0.9996982
Z prime max is  7.5086863E-03
Z prime min is -1.1798148E-02




$ histo2
File for analysis ?
tgm:star.03
Data ready. Read        1000 points.
Columns for x-axis and y-axis?
1
3
X min, X max and number of bins :
-.15
.15
25
Y min, Y max and number of bins :
-.15
.15
25
Do you want reflectivity too (Y=1,N=0) ?
0
Data normalization. Enter:
0for no normalization
1to normalize to 1
2to normalize to total counts
1
There were        73lost out of        1000 rays.
Computations done.
File for TOP DRAWER [ 0 ] or NCAR [ 1 ] ?
```

```
 0
 All done.
```

The output files from HISTO2 are named MESH.PLT. These files can be plotted by issuing the following commands to TopDrawer:

```
@MESH.PLT    (or a renamed file)
HISTO
END
```
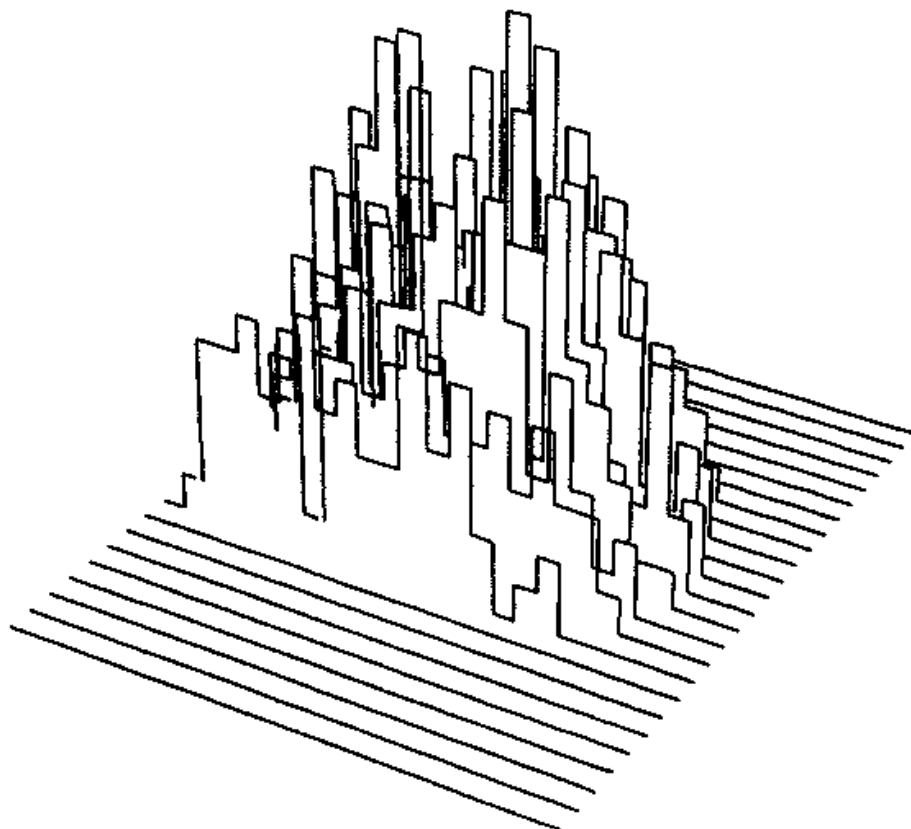
Photon counts on first mirror of TGM

Figure 3.22: HISTO2: First mirror

Histogram of final image plane of TGM

Figure 3.23: HISTO2: Final image

INTENS

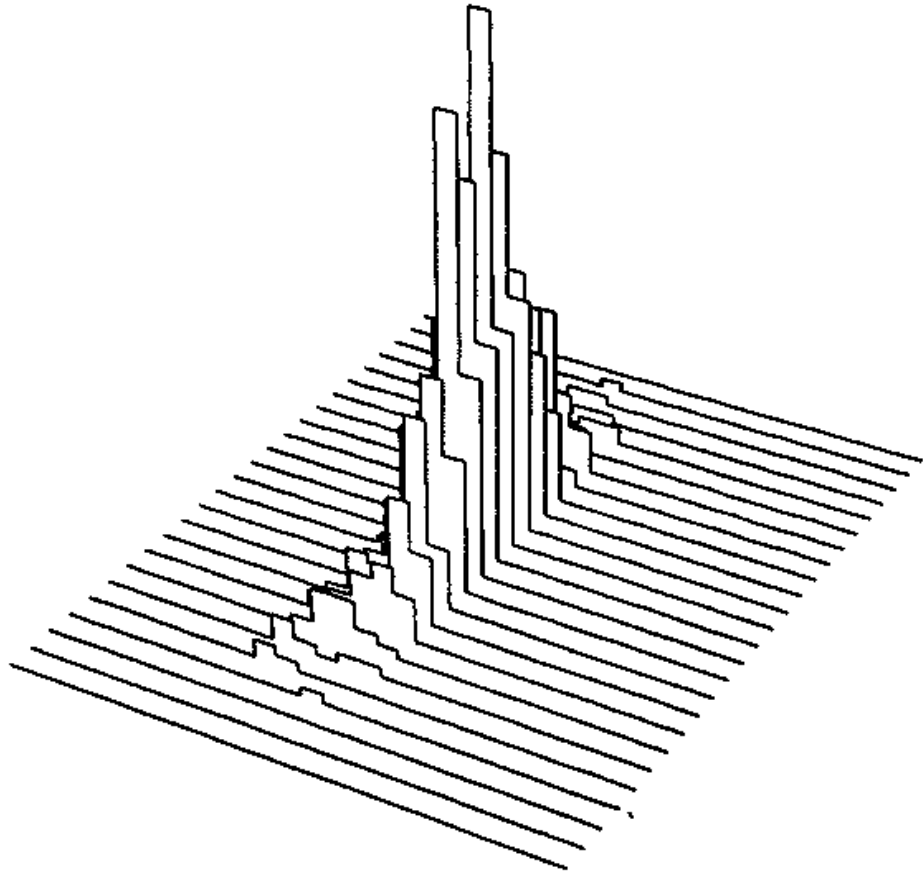|	
Purpose:	Computes the power reflected, absorbed or transmitted ray by ray.
Input:	One or two RAY files such as STAR.xx, MIRR.xx, SCREEN.xxyy
Output:	To a user-specified file of $\{x, y(x)\}$ or $\{x, y, z(x, y)\}$ format.

Description:

The program works by computing the total energy carried by a RAY file after a reflection by a mirror or transmission by a screen. This can be compared with that of the incoming beam and the local reflectivity or absorbed power can then be computed. The program creates a 2 or 3 columns file of the type $\{x, y, z(x, y)\}$ where (x, y) can be any two columns and z is the power. If the rescaling option is selected, then the beam is considered to be a sample of the source (user-specified) power. The output can be plotted out using TopDrawer or further analyzed.

Examples:

For the purpose of demonstration, we use a elliptical mirror to focus a point source. Since the source covers an energy range of 500-2000 eV, the reflectivity of the mirror (Au-coated) will be a function of both the photon energy and the angle. For the narrow divergence (20 mrad) we used, the reflected power shows up mainly depending on the energy. The way the total power is subdivided among rays depends on how the source was generated. In general, SHADOW assumes that the photons are generated by sampling $N(\hbar,\omega)$, unless otherwise specified (as in the SR source).

$$W = \Sigma_{i=1}^{N} n_i \hbar \omega_i$$

In the second case, the photons are generated by sampling $P(\hbar,\omega)$ so that each ray carries the same amount of power:

$$W = \Sigma_{i=1}^{N} W_i$$

To make it more realistic, we assign 100 Watt to the 5000 rays in BEGIN.DAT; that translates into 0.02 Watt per ray, and it is easy to see that the reflected and absorbed power of each ray do add up to 0.02 Watt. Has this not been done, then INTENS simply assumes the intensity of each ray is 1 at the source. The user has the option of writing out the intensity of each ray versus one or two other columns, thus making a bi- or tri-dimensional plot. This is very similar to PREPLOT.

```
$type source.fil
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************  S O U R C E       D E S C R I P T I O N  **************
Example file
Source
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
start.00
Full file Specification :D13:[XRAYOP.DOCUMENT.INTENS]START.00;1
Creation Date           :25-FEB-1989 17:09
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Random Source.
Generated total        5000 rays.
Source assumed BIDIMENSIONAL (flat).
Source Spatial Characteristics: POINT
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: UNIFORM
Distribution Limits. +X :   0.100000000E-02 -X:   0.100000000E-02 rad
                     +Z :   0.100000000E-01 -Z:   0.100000000E-01 rad
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: BOX DISTR.
From Photon Energy:    500.000000    or    24.7970400     Angs.
 to  Photon Energy:    2000.00000    or    6.19926000     Angs.
Angular difference in phase is  0.00000E+00
Degree of polarization is  0.00000E+00
Source points have COHERENT phase.
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************                 E N D                  ***************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
$
$
$
$ type mirror.fil
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*******************   MIRROR  DESCRIPTION   *******************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.INTENS]END.01;2
Creation Date          :25-FEB-1989 17:21
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:        ELLIPTICAL
Cylindrical figure                    NO
Element type                          REFLECTOR
Reflectivity      ON     coefficients from:
AUF1F2
Polarization dependence               YES
Mirror dimensions                     UNLIMITED
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                      1000.000000000000
Image  Plane                               1000.000000000000
Incidence Angle                            84.00000000000001
Reflection/Diffraction Angle               84.00000000000001

Mirror parameters                     COMPUTED
Same configuration as Central Axis    YES
Objective focus at                         1000.000000000000
Image focus at                             1000.000000000000
Incidence angle                            84.00000000000001
Parameters used follow:
   Semi-major axis     1000.000000000000
   Semi-minor axis     104.5284632676535
   Semi-focal-length  0.0000000000000000E+00
   Eccentricity       0.0000000000000000E+00
Source of this O.E. moved             NO
Mirror at pole position ( no mov. )   YES
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
$
$
$ type system.fil


++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S Y S T E M    D E S C R I P T I O N **************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 #    Optical Element:                                   Creation Time:
   1   D13:[XRAYOP.DOCUMENT.UTIL.INTENS]END.01;2         25-FEB-1989 17:21
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Optical Element #           1      System Number:

MIRROR    ELLIPTICAL            UNLIMITED      COMPUTED        REFLEC. ON

  Orientation             0.0000000000000000E+00 deg.
  Source Plane             1000.000000000000
  Incidence Ang.          84.00000000000001      deg.
  Reflection Ang.         84.00000000000001      deg.
  Image Plane             1000.000000000000
     ----------------


                     OPTICAL SYSTEM CONFIGURATION
                      Laboratory Reference Frame.

OPT. Elem #        X =                  Y =                  Z =

     0         0.00000000000E+00   0.00000000000E+00   0.00000000000E+00
     1         0.00000000000E+00    1000.0000000       0.00000000000E+00
       1'        0.00000000000E+00    1978.1476007       207.91169082


+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************               E N D                  ***************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
$
$
$ dir

Directory D13:[XRAYOP.DOCUMENT.INTENS]

AUF1F2.DAT;1                 4  25-FEB-1989 17:05  (RE,RWED,RWED,RE)
BEGIN.DAT;1               1410  25-FEB-1989 17:10  (RE,RWED,RWED,RE)
```

```
EFFIC.01;2                    1   25-FEB-1989 17:21   (RE,RWED,RWED,RE)
END.00;1                      7   25-FEB-1989 17:10   (RE,RWED,RWED,RE)
END.01;2                     11   25-FEB-1989 17:21   (RE,RWED,RWED,RE)
MIRR.01;2                  1410   25-FEB-1989 17:21   (RE,RWED,RWED,RE)
MIRR.FIL;1                    5   25-FEB-1989 17:22   (RE,RWED,RWED,RE)
OPTAX.01;2                    2   25-FEB-1989 17:21   (RE,RWED,RWED,RE)
SOURCE.FIL;1                  4   25-FEB-1989 17:16   (RE,RWED,RWED,RE)
STAR.01;2                  1410   25-FEB-1989 17:21   (RE,RWED,RWED,RE)
START.00;1                    7   25-FEB-1989 17:09   (RE,RWED,RWED,RE)
START.01;3                   11   25-FEB-1989 17:21   (RE,RWED,RWED,RE)
SYSTEM.FIL;3                  4   25-FEB-1989 17:23   (RE,RWED,RWED,RE)
SYSTEMFILE.DAT;2              1   25-FEB-1989 17:21   (RE,RWED,RWED,RE)

Total of 17 files, 4293 blocks.
$
\* We perform now several runs of INTENS to demonstrate
   all the features. *\

$ INTENS
File for Intensity calculations ?  MIRR.01
Read          5000rays.
Each ray has           18 entries.
Total intensity is :    118.2835503036797    \* This is simply the intensit
                                                summed over all the rays.
Normalized intensity is :  2.3656710060735936E-02

                                                \* Total intensity divided b
                                                   the no. of rays.
Options:
Intensity transmitted/reflected ....... 0       \* First compute the power
Intensity absorbed .................. 1            reflected off the mirror.
Local reflectivity/transmission ....... 2
 Then ?   0
Spectrum type :
  [0]    # photons/sec.                          \* The power (Watt) of each
  [1]    Watt                                       will be written out, whic
Then ?   1                                          is from a source of 100 W
Normalize to source power [ Y/N ] ?  1
Total source power emitted ?  100
File-name  for [x,y] file ?  FIRST
Bi [ 0 ] or Tri-dimensional plot [ 1 ] ?  0
```

```
Row for plot x-axis ?  11                          \* Reflected power vs. hv     *\
Enter :
0   cm-1
1   eV
2   angst
Then ?  1
Another run [1/0] ?   1                            \* End of first plot *\
File for Intensity calculations ?  MIRR.01
Read         5000rays.
Each ray has          18 entries.
Total intensity is :   118.2835503036797
Normalized intensity is :  2.3656710060735936E-02
Options:
Intensity transmitted/reflected ....... 0        \* Same as above, except the
Intensity absorbed ................... 1            absorbed power is used.   *\
Local reflectivity/transmission ....... 2
 Then ?  1
Spectrum type :
  [0]    # photons/sec.
  [1]    Watt
Then ?  1
Normalize to source power [ Y/N ] ?  1
Total source power emitted ?  100
Input I0 file :  BEGIN.DAT
File-name  for [x,y] file ?  SECOND
Bi [ 0 ] or Tri-dimensional plot [ 1 ] ?  0
Row for plot x-axis ?  11
Enter :
0   cm-1
1   eV
2   angst
Then ?  1
Another run [1/0] ?   1                            \* End of second run *\
File for Intensity calculations ? MIRR.01    \* this time we use a different
Read          1000rays.                       \* example.  Here we have a
Each ray has          18 entries.            \* single energy source at
Total intensity is :   707.5300660592716    \* 2000 eV incident on a
Normalized intensity is :  0.7075300660592716 \* spherical mirror at 89 deg.
Options:
Intensity transmitted/reflected ....... 0
```

```
Intensity absorbed .................... 1
Local reflectivity/transmission ....... 2
 Then ? 1
Spectrum type :
  [0]    # photons/sec.
  [1]    Watt
Then ? 1
Normalize to source power [ Y/N ] ? 1
Total source power emitted ? 100
Input I0 file : BEGIN.DAT
File-name  for [x,y] file ? ABSORB
Bi [ 0 ] or Tri-dimensional plot [ 1 ] ? 0
Row for plot x-axis ? 2
Another run [1/0] ? 0
$
$
$ dir/since=-00:05

Directory D13:[XRAYOP.DOCUMENT.INTENS]

FIRST.DAT;1                  313  25-FEB-1989 17:28  (RE,RWED,RWED,RE)
SECOND.DAT;1                 313  25-FEB-1989 17:29  (RE,RWED,RWED,RE)

Total of 2 files, 616 blocks.
```

These files are plotted in Figures 3.24 and 3.25

```
$
$ type first.dat \* Units are eV and Watt. *\
  916.4160       4.8564727E-04
  941.6163       4.3134825E-04
  1500.448       5.0780447E-05
  1441.797       6.1421124E-05
  1961.732       1.2236715E-05
  1883.999       1.5970762E-05
    ^Y

$ type second.dat
  916.4160       1.9514352E-02
  941.6163       1.9568652E-02
```
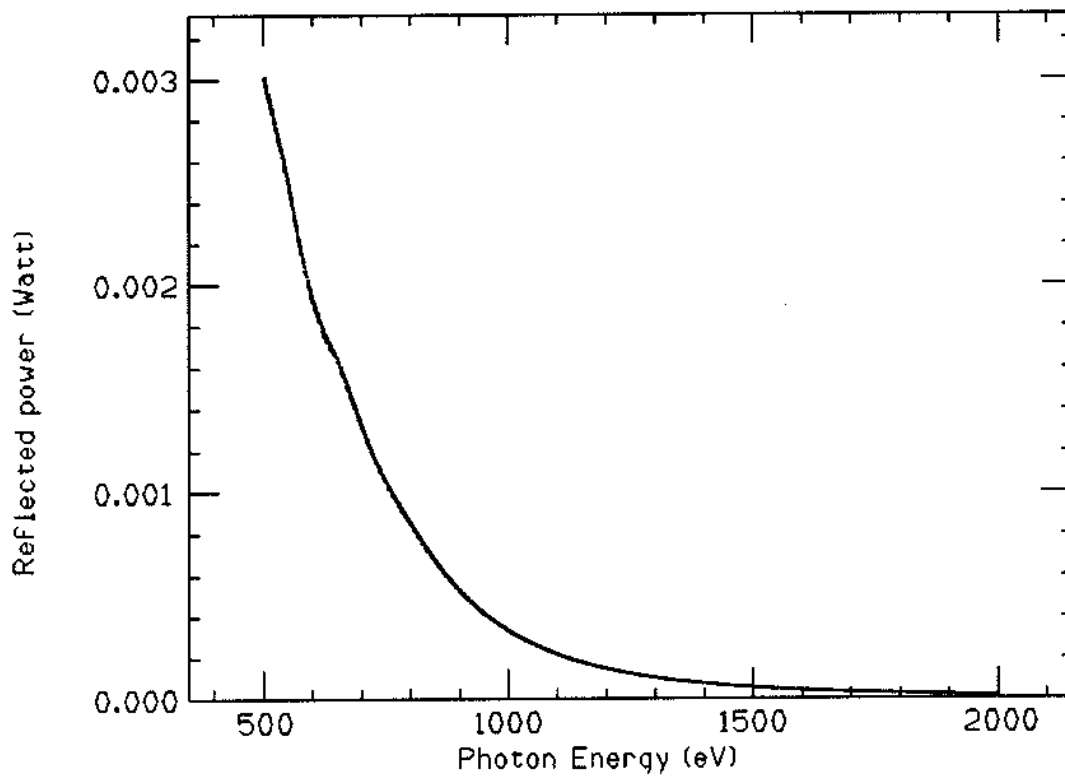
Figure 3.24: INTENS: Reflected Power vs. energy (first.dat)

```
1500.448        1.9949218E-02
1441.797        1.9938579E-02
1961.732        1.9987762E-02
1883.999        1.9984029E-02
   ^Y

$
$
$
```

The last data file (ABSORB.DAT) is plotted in figure 3.26. Following that we ran H2KOL on the data file to generate a histogram. Note that the total power is divided among the bins, so the vertical scale is Watts/bin.
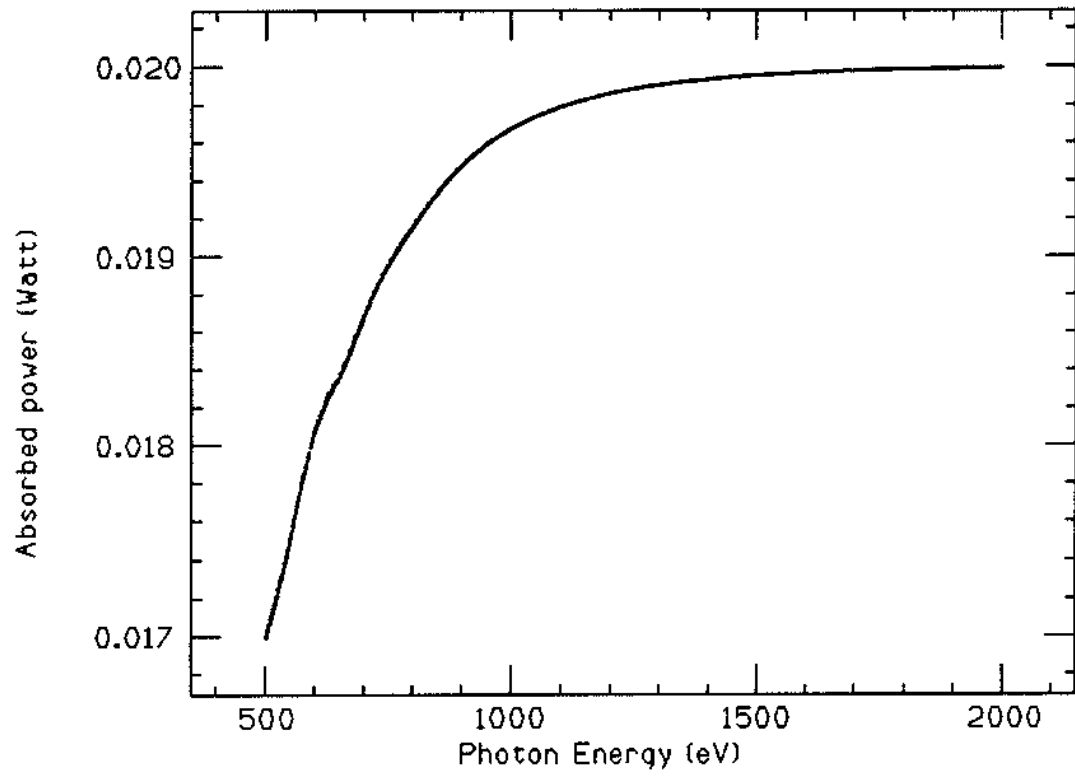
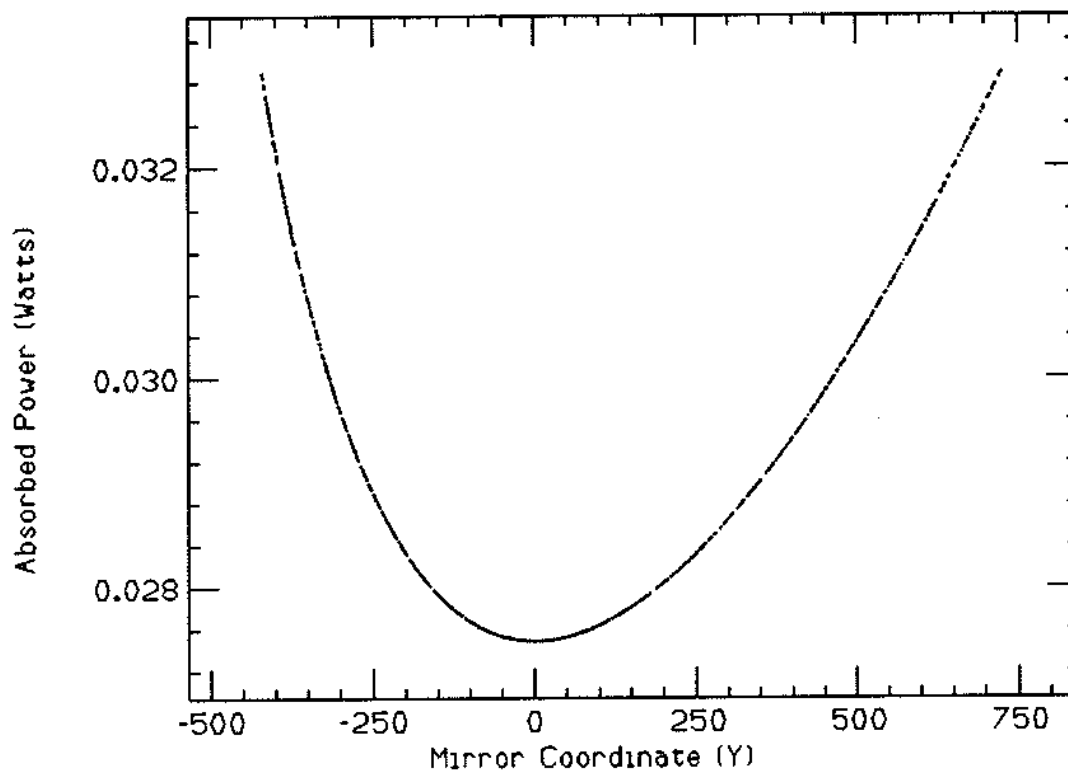Figure 3.25: INTENS: Absorbed power vs. energy (second.dat)

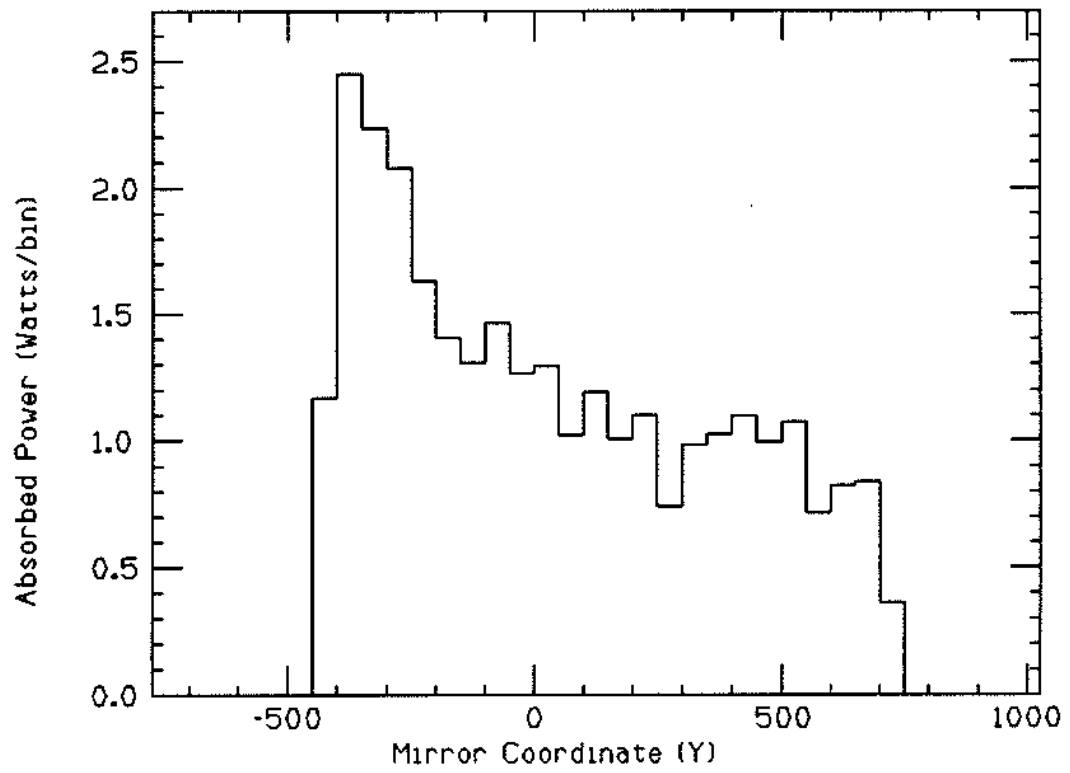Figure 3.26: INTENS: Absorbed power vs. mirror coordinate (Z) (absorb.dat)

Figure 3.27: INTENS: H2KOL output from ABSORB.DAT

MINMAX

Purpose:	To find the extrema of the phase space occupied by a beam described by a RAY file. In other words, finds the extrema of each coordinate (X,Y,Z) and direction cosines (X',Y',Z').
Input:	Binary output file (e.g. STAR.xx)
Output:	TT and formatted file MINMAX.DAT

Description:

Given a ray file it will find the absolute minima and maxima for the three coordinates in position and momentum space. Options to include the lost rays in the analysis are provided. A comment is requested so the output file will have a title. The user may wish to rename this file since all output files will be named MINMAX.DAT. Very useful for quick verification of results.

Examples:

The first example will be using the spherical mirror example from the primer. After that we'll run MINMAX on the STAR.03 and the MIRR.01 files from the TGM example.

```
$ minmax
Input file ?
star.01
Options --- Enter
0 for excluding the losses
1 for including losses at a particular O.E.
2 for including all the losses.
Then ?
0
Comment ?
Simple Spherical Mirror (Primer sec 2.4)
***********
File examined is :
D13:[XRAYOP.PRIMER.CHAPTER2]STAR.01;1
Was created :
 4-MAY-1987 16:37
***********
```

```
 Found           1000 good points out of           1000
 Here we are.
 X max is  0.4081510
 X min is -0.4102450
 Y max is  1.8064706E-15
 Y min is -1.6632746E-15
 Z max is  9.7605148E-03
 Z min is  8.7015678E-07
 X prime max is  2.7311902E-02
 X prime min is -2.7292412E-02
 Y prime max is  0.9999999
 Y prime min is  0.9996073
 Z prime max is  7.4768672E-03
 Z prime min is -7.6602534E-03
```

First we'll show the log of the run, then we'll type the output file to show it's contents.

```
$
$ minmax
Input file ? star.03
Options --- Enter
0 for excluding the losses
1 for including losses at a particular O.E.
2 for including all the losses.
Then ? 0
Comment ?
Image plane after tgm refocus mirror
***********
File examined is :
D13:[XRAYOP.DOCUMENT.UTIL.MINMAX]STAR.03;25
Was created :
 4-MAY-1989 10:40
***********
Found           865 good points out of           1000
Here we are.
X max is  0.1150454
X min is -0.1366614
Y max is  2.7868333E-15
```

```
Y min is -4.3796347E-15
Z max is  1.1263924E-02
Z min is -5.2220654E-02
X prime max is  2.3804422E-02
X prime min is -2.4356563E-02
Y prime max is  0.9999999
Y prime min is  0.9996949
Z prime max is  7.3660947E-03
Z prime min is -1.0705367E-02
$
$ type minmax.star
 Searching file:
 D13:[XRAYOP.DOCUMENT.UTIL.MINMAX]STAR.03;25
  4-MAY-1989 10:40

  Image plane after tgm refocus mirror

 Total rays :          1000
 Lost rays  :           135
 EXCLUDING LOSSES
 X max is          0.115045405924
 X min is         -0.136661350727
 Y max is          0.278683326416E-14
 Y min is         -0.437963467576E-14
 Z max is          0.112639237195E-01
 Z min is         -0.522206537426E-01
 X prime max is    0.238044224679E-01
 X prime min is   -0.243565626442E-01
 Y prime max is    0.999999880791
 Y prime min is    0.999694883823
 Z prime max is    0.736609473825E-02
 Z prime min is   -0.107053667307E-01

$
$ minmax
Input file ? mirr.01
Options --- Enter
0 for excluding the losses
1 for including losses at a particular O.E.
2 for including all the losses.
```

```
Then ? 0
Comment ?
First mirror of tgm
***********
File examined is :
D13:[XRAYOP.DOCUMENT.UTIL.MINMAX]MIRR.01;25
Was created :
 4-MAY-1989 10:40
***********
Found          927 good points out of          1000
Here we are.
X max is   1.998689
X min is  -1.995066
Y max is   4.030588
Y min is  -4.720492
Z max is  0.1304751
Z min is  5.9245693E-05
X prime max is  1.1206643E-02
X prime min is -1.1470584E-02
Y prime max is  0.9963953
Y prime min is  0.9960193
Z prime max is  8.9137740E-02
Z prime min is  8.4174052E-02
$
$ type minmax.mirr
 Searching file:
 D13:[XRAYOP.DOCUMENT.UTIL.MINMAX]MIRR.01;25
  4-MAY-1989 10:40


 First mirror of tgm


 Total rays :          1000
 Lost rays  :           73
 EXCLUDING LOSSES
 X max is          1.99868941307
 X min is         -1.99506604671
 Y max is          4.03058767319
 Y min is         -4.72049236298
 Z max is          0.130475103855
 Z min is          0.592456926825E-04
```

```
 X prime max is     0.112066427246E-01
 X prime min is    -0.114705841988E-01
 Y prime max is     0.996395349503
 Y prime min is     0.996019303799
 Z prime max is     0.891377404332E-01
 Z prime min is     0.841740518808E-01

 $
```

PSPREAD

Purpose:	Creates a histogram of the point spread function at an image plane.
Input:	A ray file corresponding to the location of the desired point spread analysis, along with an interval and variable with respect to which the point spread is computed.
Output:	A file (PSPREAD.DAT) containing data for the point spread histogram and/or a direct screen histogram.

Description:

The point spread function for an optical system is the two dimensional analog of the impulse response function for a linear system. PSPREAD computes a point spread histogram for any plane in the system in which a ray file exists. In order to get a true point spread the system must be traced with a point source in the XZ plane having no depth and a conical angle distribution. The histogram bins are created with respect to one of three variables: constant radius, where each bin represents an equal step outward form the user defined center; constand area, where each bin represents an equal area from the user defined center; or constant volume. The histogram counts may be made with respect to the number of photons or, in the case where reflectivity is used, the number of photons weighted by the electric field intensity. PSPREAD may be used to determine the spread for extended sources, which would be the convolution of the source shape with the point spread if the system was shift invariant.

Examples:

The first example we show is the point spread of a uniform source before it has been traced through an optical system. This shows the ideal point spread when calculated with respect to constant area.

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S O U R C E     D E S C R I P T I O N **************
Uniform Source
PSPREAD Example
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.00
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.PSPREAD]END.00;1
Creation Date           : 7-JUL-1989 09:31
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
 Random Source.
 Generated total          1000 rays.
 Source assumed BIDIMENSIONAL (flat).
 Source Spatial Characteristics: ELLIPTICAL
 Source Width:   0.100000000    and Height:   0.100000000
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Source Emission Characteristics
 Distribution Type: LAMBERTIAN
 Distribution Limits. +X :   0.200000000E-01 -X:   0.200000000E-01 rad
                      +Z :   0.200000000E-01 -Z:   0.200000000E-01 rad
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 ***************                 E N D                  ***************
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Below is a plot of the cross section of the source. We'll now run PSPREAD and show the histogram it produces.

```
$
$ pspread
File for analysis ? begin.dat           \* source file *\
Read    :         1000 rays
Maximum radius :   9.9927226050813235E-02
Minimum radius :   3.9308915161286589E-03
Histogram is done for absolute radius      \* negative values are meaningless
 ...from : 0                               \* here.  Work from zero.  *\
 ...to   : 0.15
Number of bins (odd, please) ? 31       \* must be odd.  31 or 25 work well *\
Generate the histogram at :
0       constant radius
1       constant area
2       constant volume
Then ? 1                                \* choose constant area *\
Flag checks. Enter :
0 to exclude lost rays
1 to include lost rays too
2 to use only lost rays
<?> 0                                   \* no lost rays *\
Include reflectivity ? 0                \* no reflectivity yet *\
```

D13:[XRAYOP.DOCUMENT.UTIL.PSPREAD]BEGIN.DAT;1   7-JUL-1989 09:31

Cross section of uni

form source

7-JUL-89 09:37:01

H Length 0.30000
H center 0.00000E+00
V Length 0.30000
V center 0.00000E+00

CARTESIAN

--GOOD ONLY

TOT = 1000
LOST -   0

Horizontal: 1
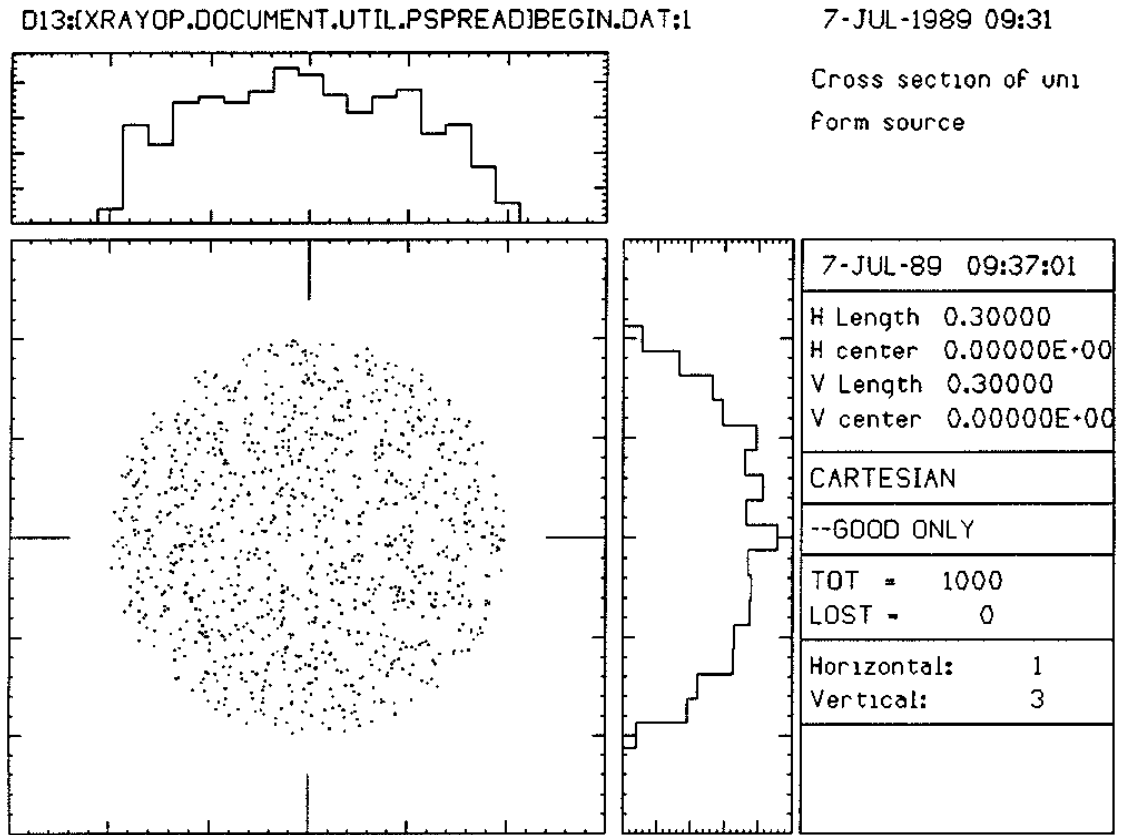Vertical: 3

Figure 3.28: PSPREAD: Source cross section

```
Output options :
  [ 0 ] store histogram in a file
  [ 1 ] plot histogram on screen
  [ 2 ] both
Then ? 0
Another run  [ Y/N ] ?n
Return to DCL
$ dir/since=-00:01                    \* information is output to PSPREAD.DAT *\

Directory D13:[XRAYOP.DOCUMENT.UTIL.PSPREAD]

PSPREAD.DAT;2              5   10-JUL-1989 10:32:43.39   (RWED,RWED,RE,RE)

Total of 1 file, 5 blocks.
$
```

The histogram is shown below.

The next example will run PSPREAD on the STAR.02 file created with the Schwarzchild
source and system. The source and system files are shown below.

```
  +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  **************  S O U R C E      D E S C R I P T I O N  **************
  Schwarzchild Source
  PSPREAD Example
  +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  Input file specified:
  end.00
  Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.PSPREAD.MODEL]END.00;4
  Creation Date           : 7-JUL-1989 10:00
  +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  Random Source.
  Generated total        5000 rays.
  Source assumed BIDIMENSIONAL (flat).
  Source Spatial Characteristics: POINT
  +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  Source Emission Characteristics
  Distribution Type: CONICAL
```
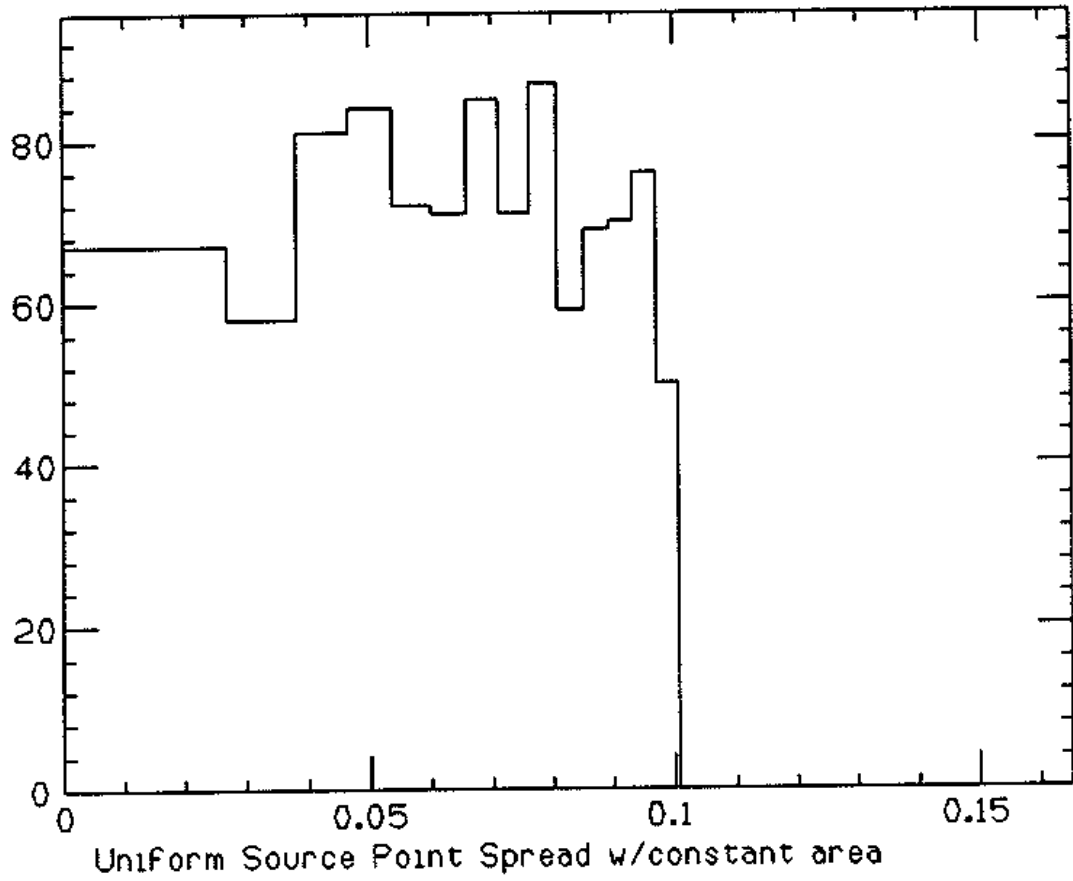
Figure 3.29: PSPREAD output

```
Cone Outer Aperture :   0.100000000E-01 Inner Aperture :   0.500000000E-02
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: SINGLE LINE
Photon Energy:   281.78     eV, or   44.000     Angs.
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************              E N D              **************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++



+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************  S Y S T E M     D E S C R I P T I O N  **************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Schwarchild system
PSPREAD Example
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 #   Optical Element:                                  Creation Time:
   1   D13:[XRAYOP.DOCUMENT.UTIL.PSPREAD.MODEL]END.01;4     7-JUL-1989 10:01
   2   D13:[XRAYOP.DOCUMENT.UTIL.PSPREAD.MODEL]END.02;4     7-JUL-1989 10:01
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Optical Element #           1     System Number:

MIRROR    SPHERICAL           UNLIMITED     EXTERNAL      REFLEC. OFF

  Orientation        0.0000000000000000E+00 deg.
  Source Plane       51.21000000000000
  Incidence Ang.     0.0000000000000000E+00 deg.
  Reflection Ang.    0.0000000000000000E+00 deg.
  Image Plane        2.500000000000000
    ---------------

Optical Element #           2     System Number:

MIRROR    SPHERICAL           UNLIMITED     EXTERNAL      REFLEC. OFF

  Orientation        0.0000000000000000E+00 deg.
  Source Plane       2.701370000000000
  Incidence Ang.     0.0000000000000000E+00 deg.
```

```
    Reflection Ang.       0.0000000000000000E+00 deg.
    Image Plane           11.02186800000000
     ----------------


                         OPTICAL SYSTEM CONFIGURATION
                          Laboratory Reference Frame.


  OPT. Elem #          X =                  Y =                  Z =


        0            0.00000000000E+00    0.00000000000E+00    0.00000000000E+00
        1            0.00000000000E+00     51.210000000        0.00000000000E+00
           1'           0.00000000000E+00     48.710000000         0.28605943631E-

        2            0.00000000000E+00     46.008630000         0.59516038809E-16
           2'           0.00000000000E+00     57.030498000        -0.19271670896E-


  +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  * * * * * * * * * * * * * *             E N D             * * * * * * * * * * * * * *
    +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Shown below is the PLOTXY output of the second image file.
The STAR.02 file was run through PSPREAD. The run is shown below, followed by the
histogram created with PSPREAD.DAT.

```
$
$ pspread
File for analysis ? star.02                \* image file *\
Read     :         5000 rays
Maximum radius :   2.7598328716075391E-06
Minimum radius :   2.1388662054996055E-10
Histogram is done for absolute radius
 ...from : 0
 ...to   : 4.0E-06
Number of bins (odd, please) ? 31
Generate the histogram at :
0       constant radius
1       constant area
2       constant volume
```

D13:[XRAYOP.DOCUMENT.UTIL.PSPREAD.MODEL]STAR.02:4   7-JUL-1989 10:01

Image plane cross se
ction

7-JUL-89 10:08:46

H Length 0.10000E-04
H center 0.00000E+00
V Length 0.10000E-04
V center 0.00000E+00

CARTESIAN

--GOOD ONLY

TOT =   5000
LOST =   0

Horizontal: 1
Vertical: 3
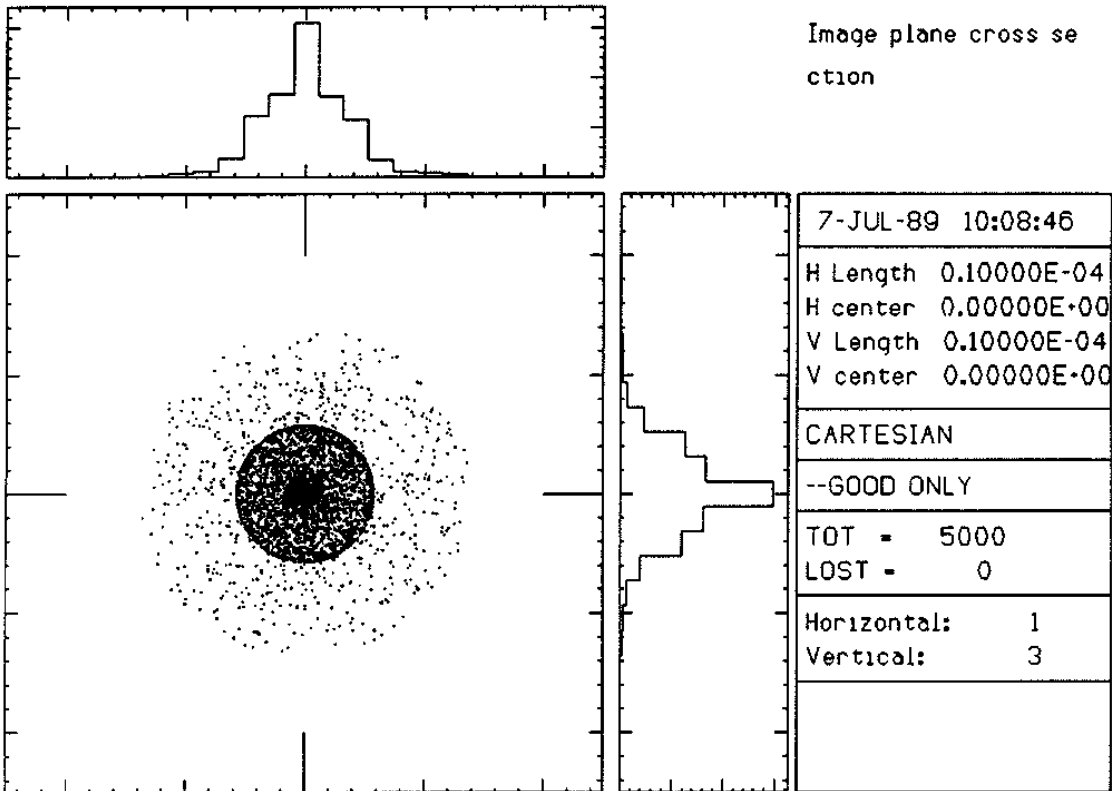
Figure 3.30: PSPREAD: Second Image

```
Then ? 1                                    \* use constant area *\
Flag checks. Enter :
0 to exclude lost rays
1 to include lost rays too
2 to use only lost rays
<?> 0
Include reflectivity ? 0                    \* no reflectivity included *\
Output options :                            \* in this example *\
  [ 0 ] store histogram in a file
  [ 1 ] plot histogram on screen
  [ 2 ] both
Then ? 0
Another run  [ Y/N ] ?n
Return to DCL
$
```

Notice how the PSPREAD graph shows a constant density in the radius, while the histograms from PLOTXY show a peaked structure (because of the binning procedure).
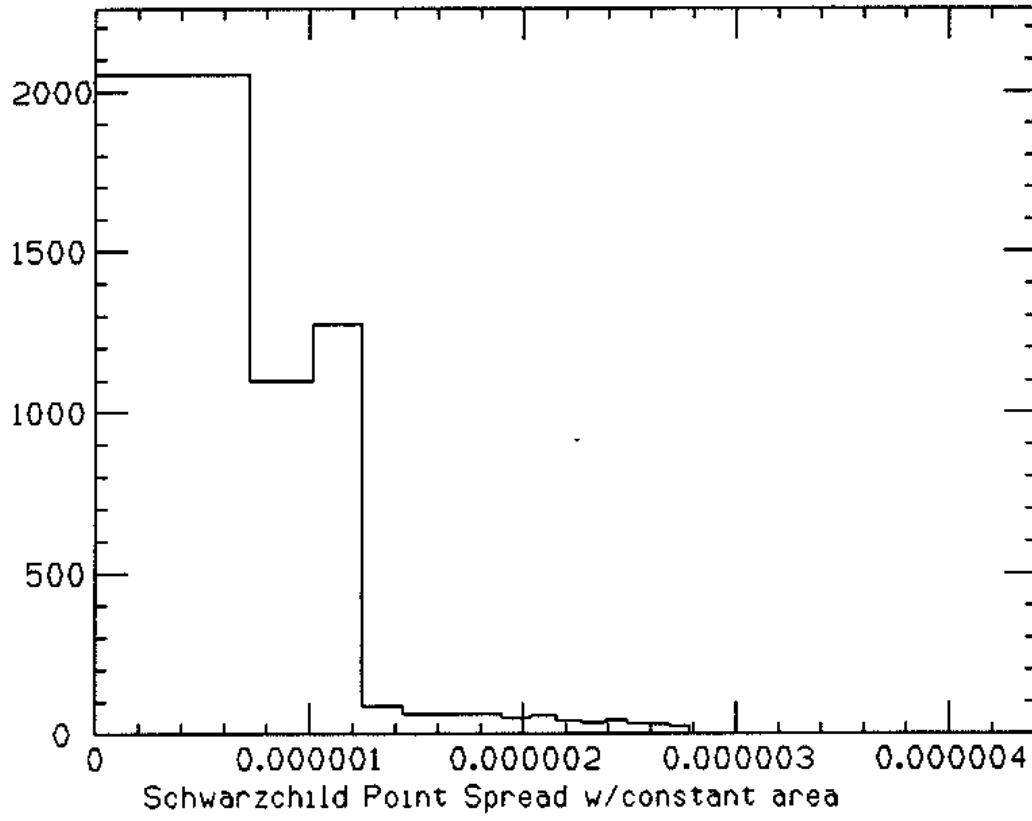
Figure 3.31: PSPREAD output of STAR.02

PWR_DENS

Purpose:	To generate a two-dimensional histogram containing the power density using an output file from SHADOW.
Input:	Source file (i.e., BEGIN.DAT) and file for analysis (i.e., MIRR.xx etc).
Output:	A file containing the power density grid in one of the following formats: TopDrawer, NCAR, generic format, or ANSYS, suitable for further processing.

Description:

PWR_DENS calculates the power at a given point in an optical system. It can be power transmitted/reflected, power absorbed, local reflectivity/transmission, or incoming power. The program reads a source file (BEGIN.DAT) and for all options except the power transmitted/reflected, the binary output file of the previous element. (For the first element in a system this would also be BEGIN.DAT.)

SHADOW stores the amplitudes of all the rays as they are traced through the system. The MIRR.xx file for an element stores the amplitude of the i-th ray "after" reflection. The incoming intensity is calculated from the source file for the element in question, the previous STAR file or BEGIN.DAT for the first element. If the amplitude, $\vec{A}_s$ and $\vec{A}_p$, is represented by "columns" 7, 8, 9 and 13, 14, 15 respectively, the intensity "after" reflection can be written as:

$$A_s^2 + A_p^2 = I_{after}\{x, y\} \tag{3.1}$$

A binning operation is done so that the reflected intensity is:

$$I_{after}(x, y) = \sum_{j=1}^{M} \left[A_{js}^2 + A_{jp}^2 \right] \tag{3.2}$$

Along the same lines, we can write the absorbed intensity as:

$$I_{absorbed} = \sum_{j=1}^{M} \left[I_{j,reflected} - (I_{j,incoming}) \right] \tag{3.3}$$

The local reflectivity is then:

$$r_s(x, y) = \frac{I_{after}}{I_{before}} \tag{3.4}$$

For this utility to give meaningful results, the source must have full polarization and reflectivities must be turned on for the elements in question.

For cleaner statistics, the utility MAKE_PWR will take the user through PWR_DENS and create a file that can be submitted as a batch job to run SHADOW iteratively as many times as desired.

Examples:

```
$
$ pwr_dens
Interactive [0] or namelist mode [1] : 0
This program needs a file containing the source spectrum computed within the
limits used. Or you can  specify the total power.
Source file [0] or total power [1] : 1
Total power in Watt : 100

Please specify now the file containing the SOURCE array (e.g., BEGIN.DAT)
Then ? BEGIN.DAT
Read          5000 rays. The file has           18 columns.
Computing renormalizing factor.

All preliminaries completed.
Ready to proceed with density analysis.

File for analysis ? MIRR.01
Data ready. Read          5000 points.
Options --- Enter
0 for excluding the losses
1 for including losses at a particular O.E.
2 for including all the losses.
Then ? 0
***********
File examined is :

Was created :

***********
Found          4717 good points out of          5000
Found:
Column 1: X max is   1.999296941008725
```

```
        1: X min is  -1.999883817471559
        2: Y max is   3.568274926989652
        2: Y min is  -4.166031351586952
        3: Z max is  0.1300002931936204
        3: Z min is  3.5289946631600344E-07
 for a photon energy range:
  101.1613479791329      to    2959.045637676470
I need to define the two-dimensional histogram for the power density. Please
specify:
Columns for x-axis and y-axis?
1
2
Limits to use for the histogram.
To use           scaling, enter:
      automatic                0
      external                 1
Then? 0
Number of bins in X [ max 51 ] ? 31
                 Y [ max 51 ] ? 31
Optical Properties options.


To select                           enter

Power transmitted/reflected ........ 0
Power absorbed .................... 1
Local reflectivity/transmission .... 2
Incoming Power .................... 3


Then ?
1
File to use for Io ? BEGIN.DAT
The program need to know how many iterations have been already performed. En
[ 0 ] if this is the first time.
No. of time this power density case has run : 0
How many times will you be looping through ? 1
There were        283 lost out of         5000 rays.
Begin verification.
Total power in file:    72.12355434039542
Compare with:           100.0000000000000
Computations done. Ready to store output data.
```

```
The files contain the power density at the nodes but
for the case of ANSYS, that stores total power.
File for:
 TOP DRAWER           [ 0 ]
 NCAR                 [ 1 ]
 Generic              [ 2 ] ** to be used for loop
 For ANSYS            [ 3 ]
2
Output file ? MIRR1
All done.
$ DIR/SINCE


Directory D1:[SHADOW.XRAYOP.DOCUMENT.TGM]


MIRR1.DAT;1                 102   7-AUG-1989 10:38:55.61  (RWED,RWED,RE,RE)
PWR_DENS_PAR.DAT;1            3   7-AUG-1989 10:38:58.14  (RWED,RWED,RE,RE)


Total of 2 files, 105 blocks.
$ TY MIRR1.DAT
 -1.9354      -4.0413      0.00000000E+00         0
 -1.9354      -3.7918      0.35433976E-01         1
 -1.9354      -3.5423      0.00000000E+00         0
 -1.9354      -3.2928      0.35721396            4
 -1.9354      -3.0433      0.55205592E-01         2
 -1.9354      -2.7938       2.8768778            15
 -1.9354      -2.5443       4.1098812            12
 -1.9354      -2.2948       4.6196552            12
 -1.9354      -2.0453       5.7607246            14
 -1.9354      -1.7958       3.5439385            11
 $
```

COMB_RAY

Purpose:	To combine two RAY files in a single one in order to merge two sources or two images.
Input:	Two Binary RAY files, e.g., STAR.01;0, STAR.01;2
Output:	A binary Ray file.

Description:

The program reads two ray files and combines them by appending the second to the first in anew file. The counter flag is reset to take in account the addition of rays. If the total number of rays exceeds 5000 an error message is typed and no output file produced. This program is designed to create "special" sources.

Examples:

As an example, let's create two source files with a circular and rectangular shape. They are illustrated in Fig. 3.32 and fig. 3.33. After running COMB_RAY we obtain the source shown in Fig. 3.34. This program can be used to generate quite complicated sources; one could also combine STAR files with other STAR or BEGIN files for interesting systems.

D13:[XRAYOP.DOCUMENT.UTIL.COMB_RAY]BEGIN.DAT;4   24-FEB-1989 23:01

First source

19-JUL-89 15:08:15

H Length   17.000
H center   0.00000E+00
V Length   17.000
V center   0.00000E+00

CARTESIAN

--GOOD ONLY

TOT =   2000
LOST -   0

Horizontal: 1
Vertical: 3

Figure 3.32: COMB_RAY: Source one

D13:[XRAYOP.DOCUMENT.UTIL.COMB_RAY]BEGIN.DAT;5   24-FEB-1989 23:16

Second source

19-JUL-89 15:11:16

H Length	11.000
H center	0.00000E+00
V Length	11.000
V center	0.00000E+00

CARTESIAN

--GOOD ONLY

TOT = 2000
LOST = 0

Horizontal: 1
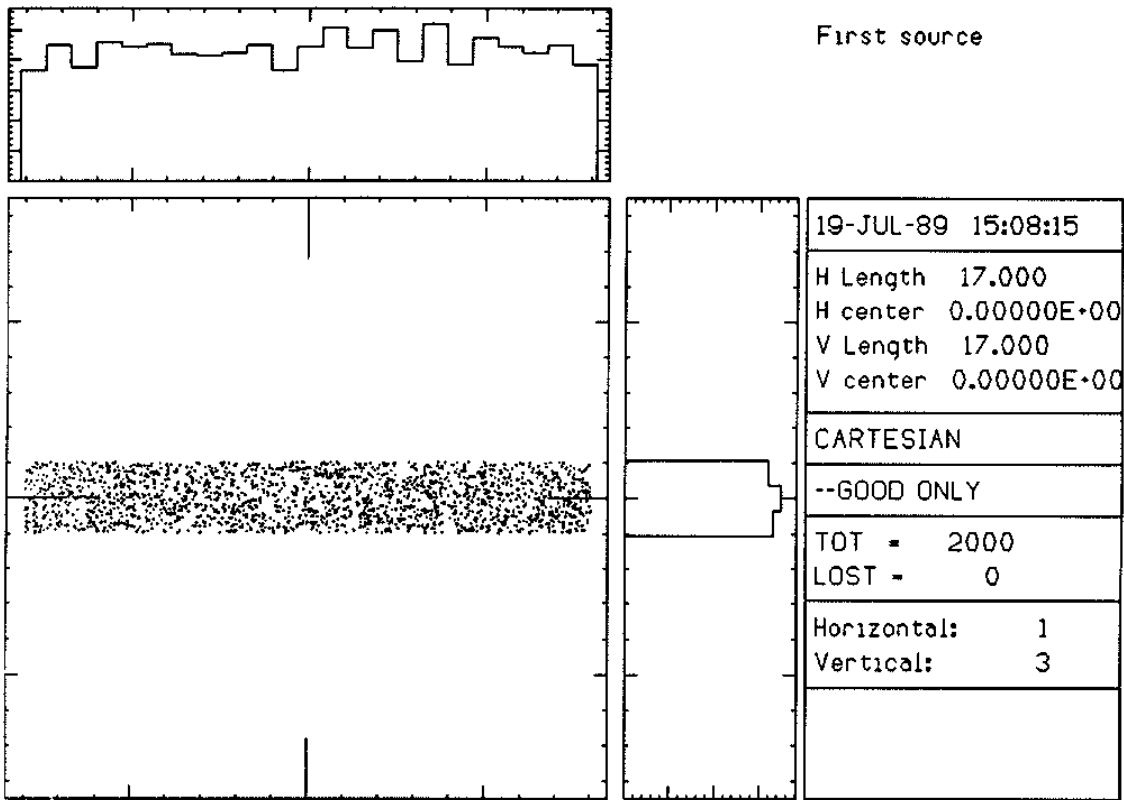Vertical: 3
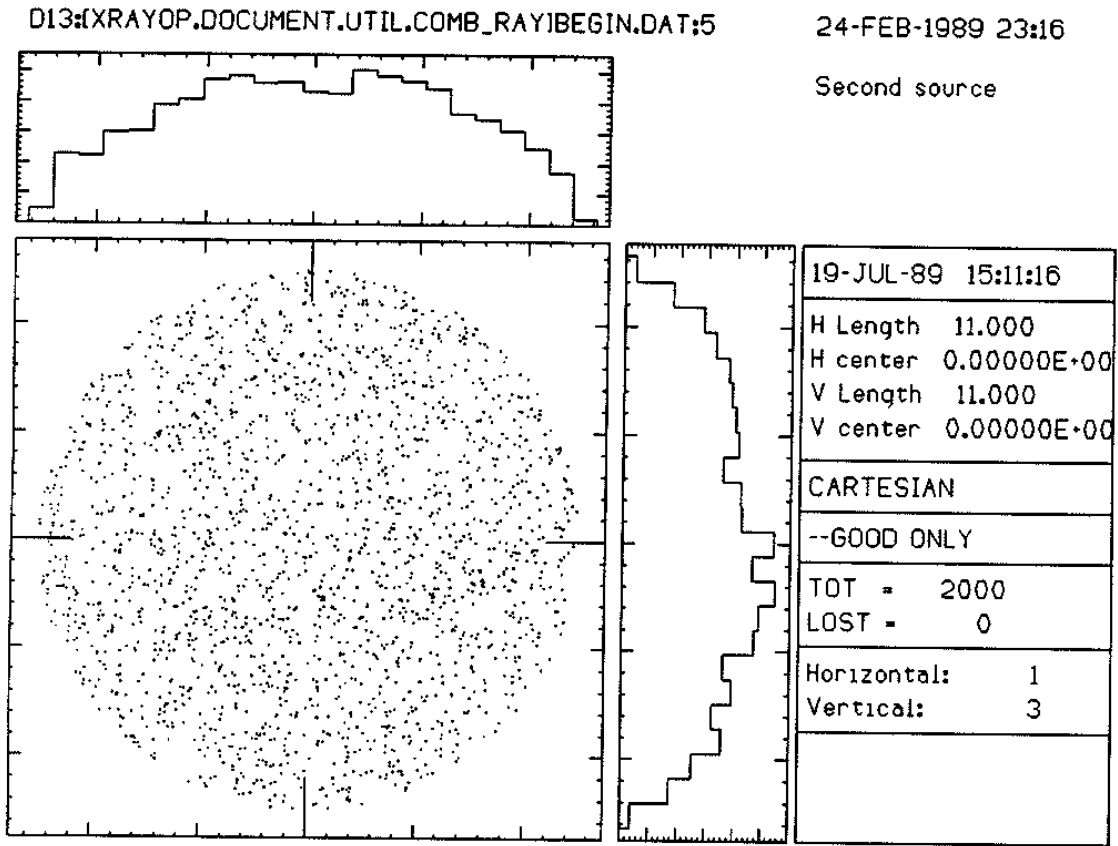
Figure 3.33: COMB_RAY: Source two

D13:[XRAYOP.DOCUMENT.UTIL.COMB_RAY]COMBINED.DAT;2   24-FEB-1989 23:17

After COMB_RAY

19-JUL-89 15:16:08
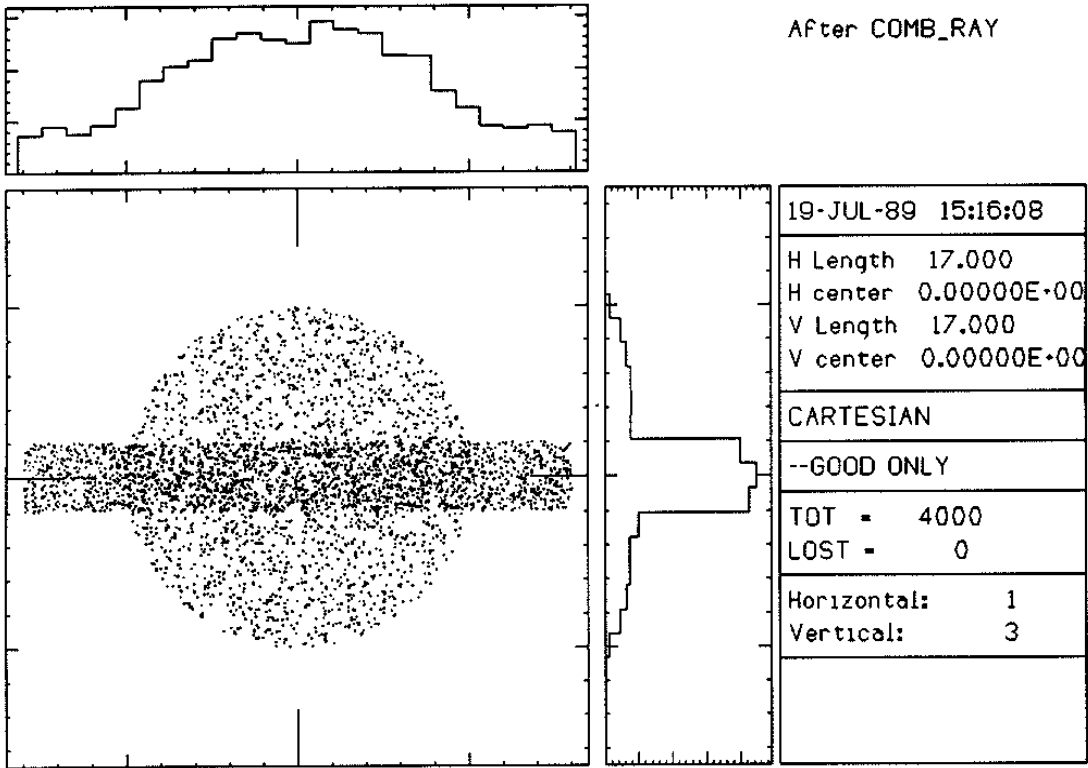
H Length   17.000
H center   0.00000E+00
V Length   17.000
V center   0.00000E+00

CARTESIAN

--GOOD ONLY

TOT =   4000
LOST =   0

Horizontal: 1
Vertical: 3

Figure 3.34: COMB_RAY: Combined source

FFRESNEL

Purpose:	To calculate the diffraction image from an aperture using the Fresnel-Kirchoff integral.
Input:	Interactive from terminal and a SCREENxxxx.DAT file.
Output:	Formatted 2-columns file.

Description:

Ordinarily, SHADOW is a ray-tracing program using *geometrical* optics. But it also has the capability of working in the *physical* optics regime. This is accomplished by properly defining the source and using FFRESNEL. It can be shown that the diffracted ("real") image can be computed by applying the Fresnel-Kirchoff Integral at the exit pupil of an optical system where the information on the illumination function has been obtained by geometrical optics. The placement of the pupil is arbitrary (as long as proper scaling is applied) since a shift leads to a phase change only. It is particularly useful for well corrected systems where most of the geometrical aberrations have been cancelled out and the image is diffraction limited. Such a case can be found in the Schwarzschild objective which we will be using as example here.

FFRESNEL is basically a numerical implementation of the *full* Fresnel-Kirchoff integral. It integrates over all the rays across a suitably located aperture. The priciple is discussed in B. Lai, K. Chapman and F. Cerrina, *SHADOW: New Developments*, Nucl. Instr. and Meth. **A266**, 544-549 (1988). Briefly, the FK integral can be written as:

$$A'(\vec{r'}) = \frac{i\bar{u}}{\lambda} \int_S A(\vec{r}) \frac{e^{ikR}}{R} d\vec{r} \tag{3.5}$$

where $R = |\vec{r} - \vec{r'}|$ and $r(r')$ is the position vector at the image (exit pupil) plane. $A(A')$ is the electric field at the same positions. SHADOW knows exactly $A(\vec{r})$ at the exit pupil while the mapping performed by the ray tracing operation has transformed the integral from a Riemann to a Stieltjes type. In order to do that, it must know for each ray the amplitude and phase of the electric field vector $\vec{A}$. In general, we separate $\vec{A}$ into two components :

$$\vec{A} = \vec{A_s}e^{i\theta_s} + \vec{A_p}e^{i\theta_p} \tag{3.6}$$

where s and p are the perpendicular and parallel component (respect to the plane of incidence). At the source, they are along the X and Z direction. Thus the $\vec{A}$ vector is defined

initially at SOURCE by :

$$degree\ of\ polarization \quad = \quad \frac{\vec{A}_x}{\vec{A}_x + \vec{A}_z} \tag{3.7}$$

$$phase\ difference \quad = \quad \theta_z - \theta_x \tag{3.8}$$

From then on, both the phase and amplitude may be modified upon reflecting off a surface (be it a grating, crystal, multilayers or reflective coatings), and these are all tracked by SHADOW ray by ray. In addition, the user also has the option of storing the optical path distance (OPD) of each ray from the source. This fully specifies (with 18 columns) all the rays anywhere along the optical system. With this information, FFRESNEL can easily evaluate the integral.

A very important point is that, since we are dealing with interference pattern, good cancellation *cannot* be achieved if we just use a random source due to finite sampling. Thus a *grid* source with coherent phase should be used if FFRESNEL is to give meaningful results. The type of source to use requires careful analysis. For example, a SR source is essentially fully incoherent so that the final image will be a <u>convolution</u> of the diffracted image (computed from a point source) with the geometrical optics image (computed from the extended source).

The first example shows the diffraction of a very simple system, a spherical mirror with the point source located at the center of curvature. The geometrical image is clearly a point while the diffracted image is given by an Airy pattern of width depending on the radiation numerical aperture. The first minimum is indeed located at

$$\Delta = \frac{\lambda}{2N.A.} \tag{3.9}$$

In the second example, a conical source is used to match the acceptance of the Schwarzschild objective. We place 30 points along the radius and only 20 points around the circle since the system is spherically symmetric. This system then images the point source to 11.02 cm after the second mirror. MINMAX tells us that the geometrical spot is about 276 Å which demonstrates the quality of the image. So we define an aperture, using the screen option in SHADOW, 1 cm after the second mirror and use FFRESNEL to calculate the diffraction image 10.02 cm from the screen. At 44 Åwavelength, the diffraction image size is certainly comparable to that of the geometric image. Note that we do not specify the photon energy in SOURCE and input it as parameter in FFRESNEL for flexibility. The user can do it the other way if he wants to use a chromatic source.

Examples:

The first example we will is show is a simple case of a point source at the focal point of
a spherical mirror. We run the example with three different numerical apertures, 0.1, 0.2,
and 0.4. The diffraction patterns are plotted together following the example.

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S O U R C E     D E S C R I P T I O N **************
Spherical mirror source example
FFRESNEL Example
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
end.00
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.FFRESNEL.EXAMPLE]END.00;
Creation Date          :25-JUL-1989 16:12
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Grid Source.
Generated total        2601 rays.
Source assumed BIDIMENSIONAL (flat).
Source Spatial Characteristics: POINT
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: CONICAL
Cone Outer Aperture :  0.200000000    Inner Aperture :   0.000000000E+00
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: SINGLE LINE
Photon Energy:  2.4797    eV, or   5000.0    Angs.
Angular difference in phase is  0.00000E+00  \* full specification of rays
Degree of polarization is  0.50000          \* neccesary.  *\
Source points have COHERENT phase.
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************              E N D                **************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*******************  MIRROR  DESCRIPTION   *******************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Spherical mirror
FFRESNEL example
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
```

```
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.FFRESNEL.EXAMPLE]END.01;17
Creation Date           :11-JUL-1989 11:14
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:        SPHERICAL
Cylindrical figure                    NO
Element type                          REFLECTOR
Reflectivity                          OFF
Mirror dimensions                     UNLIMITED
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                           100.0000000000000
Image  Plane                                    100.0000000000000
Incidence Angle                                 0.0000000000000000E+00
Reflection/Diffraction Angle                    0.0000000000000000E+00

Mirror parameters                     EXTERNAL
Parameters used follow:
Spherical Radius                      100.000000    \* source at focus *\
Source of this O.E. moved             NO
Mirror at pole position ( no mov. )   YES
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

A screen was defined 10 cm after the mirror for the purposes of running FFRESNEL.

```
$
$ ffresnel

Define integration limits [ cm ].
From               -5E-04
 to                5E-04
No. of points      201                      \* odd number works best. *\
Integration direction [ 0 = x, 90 = z ] ? 0
Distance from plane [ cm ] ? 90              \* distance of screen from image *\
Ray input file ? screen.0101                \* input SCREEN.xxyy file *\
[ 0 ] to discard losses, [ 1 ] to keep them. 0
Do you want to override the wavelength in the file ? 0
Files read OK.
```

```
Conversion to [ cm ] factor (*) ? 1.0
Include the S- and P- phase shifts in the computations ?1
$ dir/since=-00:02

Directory D13:[XRAYOP.DOCUMENT.UTIL.FFRESNEL.EXAMPLE]

FFPAR.DAT;23                    1  11-JUL-1989 11:20:03.11  (RWED,RWED,RE,RE)
FFRESNEL.DAT;16                20  11-JUL-1989 11:20:03.81  (RWED,RWED,RE,RE)

Total of 2 files, 21 blocks.
$
```

The plot follows.

Next the source was offset by 0.5 units to test its affect on the diffraction pattern. This offsets the image the same distance in the opposite direction, so our integration will no longer be around zero. The output from SOURCINFO is the same as the previous example. The numerical aperture is 0.2. The mirror description follows.

```
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 ******************   MIRROR   DESCRIPTION   ******************
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Spherical Mirror--Offset
 FFRESNEL Example
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Input file specified:end.01
 Full file Specification :D1:[XRAYOP.DOCUMENT.UTIL.FFRESNEL.EXAMPLE]END.01
 Creation Date          : 2-AUG-1989 16:32
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 Surface figure was defined as:        SPHERICAL
 Cylindrical figure                    NO
 Element type                          REFLECTOR
 Reflectivity                          OFF
 Mirror dimensions                     UNLIMITED
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Central Axis parameters :
 Source Plane Distance                         100.0000000000000
 Image  Plane                                  100.0000000000000
```
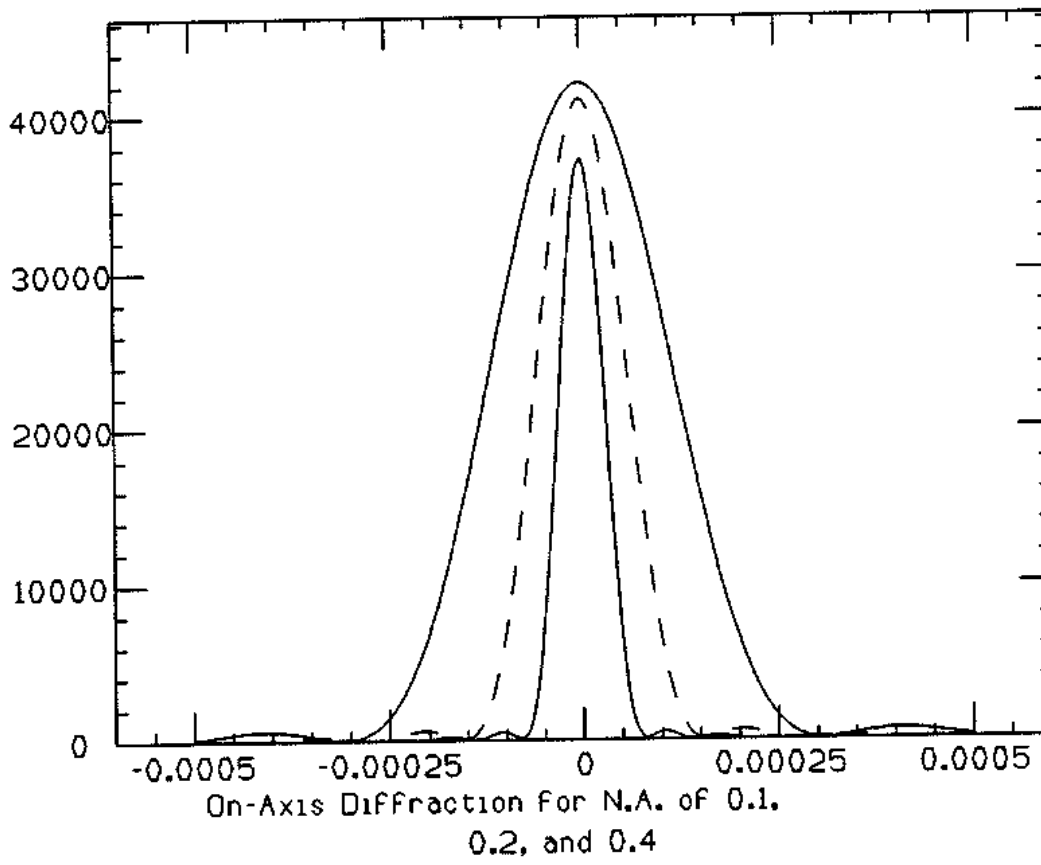
Figure 3.35: FFRESNEL output with N.A. 0.1, 0.2, 0.4

```
 Incidence Angle                             0.0000000000000000E+00
 Reflection/Diffraction Angle                0.0000000000000000E+00

 Mirror parameters                      EXTERNAL
 Parameters used follow:
 Spherical Radius                       100.000000
 Source of this O.E. moved              YES
 In SOURCE reference frame:
 Source Movement X:   0.0000000000000000E+00
                 Y:   0.0000000000000000E+00
                 Z:   0.5000000000000000    <<< offset source 0.5 cm *\
 Source rotat  X:   0.0000000000000000E+00
               Y:   0.0000000000000000E+00
               Z:   0.0000000000000000E+00
 In MIRROR reference frame:
 Source distance       100.0000000000000
       rotation       0.0000000000000000E+00
 Incidence angle       0.0000000000000000E+00
 Source offset X:   0.0000000000000000E+00
                Y:   0.0000000000000000E+00
                Z:   0.0000000000000000E+00
 Mirror at pole position ( no mov. )     YES
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 $ ffresnel


Define integration limits [ cm ].
From               0.495         \* offset integration as well *\
 to                0.505
No. of points      201
Integration direction [ 0 = x, 90 = z ] ? 90  \* integrate in Z since
                                    \* offset in Z         *\
Distance from plane [ cm ] ? 90
Ray input file ? SCREEN.0101
[ 0 ] to discard losses, [ 1 ] to keep them. 0
Do you want to override the wavelength in the file ? 0
Files read OK.
Conversion to [ cm ] factor (*) ? 1.0
```

```
Include the S- and P- phase shifts in the computations ?1
$ DIR/SINCE

Directory D1:[SHADOW.XRAYOP.DOCUMENT.UTIL.FFRESNEL.EXAMPLE]

FFPAR.DAT;1                        1   2-AUG-1989 16:44:52.84  (RWED,RWED,RE,RE)
FFRESNEL.DAT;1                    20   2-AUG-1989 16:44:53.24  (RWED,RWED,RE,RE)

Total of 2 files, 21 blocks.
$ TY FFPAR.DAT
From   0.4950000000000000      to   0.5050000000000000
     Step   5.0000000000000010E-05
Wavelength   0.0000000000000000E+00 angs.
 Image located at     90.00000000000000
 Integration direction    90.00000000000000
 Scale factor [ units ] *    1.000000000000000     = [ cm ]
Losses: NOT INCLUDED
S- and P- phase shifts :      INCLUDED
Files used:
SCREEN.0101

$
```

The offset plot superimposed on the first example with N.A.=0.2 follows.
The next example is more complex. It involves the Schwarzchild source and system. First
SHADOW was run to define the source and the Schwarzschild objective. The output from
SOURCINFO and SYSINFO follows.

```
  +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  ************** S O U R C E     D E S C R I P T I O N **************
  Source for FFRESNEL

  +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  Input file specified:
  end.00
  Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.FFRESNEL]END.00;2
```
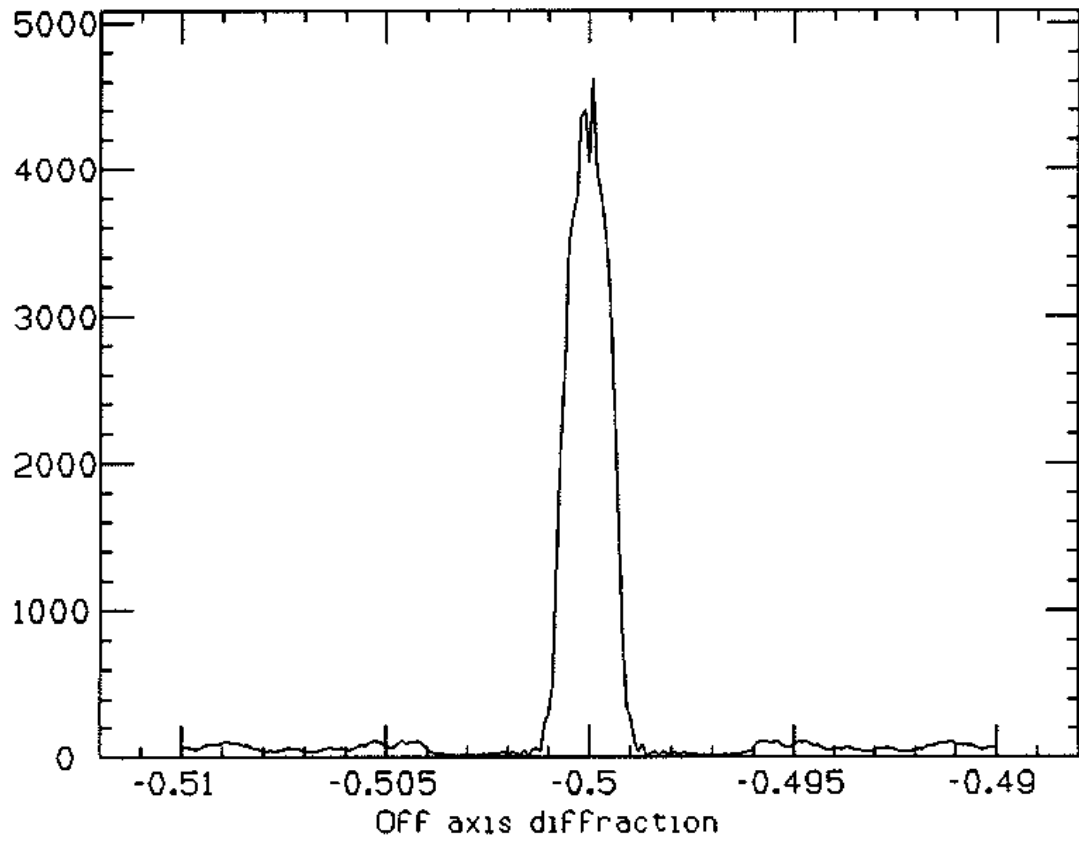
Figure 3.36: FFRESNEL: Offset example

```
Creation Date            : 3-JUL-1989 13:45
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Grid Source.                                   \* grid source a must \*
Generated total          600 rays.
Source assumed BIDIMENSIONAL (flat).
Source Spatial Characteristics: POINT
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: CONICAL
Cone Outer Aperture :   0.100000000E-01 Inner Aperture :   0.500000000E-02
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: SINGLE LINE
Photon Energy:   281.78     eV, or   44.000     Angs.
Angular difference in phase is  0.00000E+00     \* full specification of rays
Degree of polarization is  0.50000               \* needed OPD + A vector
Source points have COHERENT phase.               \* No random phase
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************              E N D               ***************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


\\ Now define the first mirror (convex). \\
\\ Then define the second mirror (concave). \\
\\ Following the log from the screen defintion is the system output from
SYSINFO. \\
\\ Define a screen as our aperture. \\
        :
        :
Any screens in this OE [ Y/N ] ?  1
How many in this OE [ total ] ?  1
Screen N.             1
Is this screen before mirror [ Y/N ] ?  0
Distance from mirror [ absolute ] ?  1.0
Is Screen Carrying an Aperture Stop [ Y/N ] ?  0
Include absorption [ Y/N ] ?  0
        :
        :


+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************  S Y S T E M    D E S C R I P T I O N **************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

FFRESNEL Example

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 #    Optical Element:                                        Creation Time:
   1   D13:[XRAYOP.DOCUMENT.UTIL.FFRESNEL]END.01;2            3-JUL-1989 14
   2   D13:[XRAYOP.DOCUMENT.UTIL.FFRESNEL]END.02;2            3-JUL-1989 14
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Optical Element #              1     System Number:

MIRROR    SPHERICAL              UNLIMITED       EXTERNAL       REFLEC. ON

  Orientation          0.0000000000000000E+00 deg.
  Source Plane          51.21000000000000
  Incidence Ang.       0.0000000000000000E+00 deg.
  Reflection Ang.      0.0000000000000000E+00 deg.
  Image Plane           2.500000000000000
    ----------------

Optical Element #              2     System Number:

MIRROR    SPHERICAL              UNLIMITED       EXTERNAL       REFLEC. ON

  Orientation          0.0000000000000000E+00 deg.
  Source Plane          2.701370000000000
  Incidence Ang.       0.0000000000000000E+00 deg.
  Reflection Ang.      0.0000000000000000E+00 deg.
  Image Plane           11.02186800000000
    ----------------
   SCREENS:           1 defined.
BEFORE Mirror         at    1.000000000000000
    ----------------

                      OPTICAL SYSTEM CONFIGURATION
                       Laboratory Reference Frame.

 OPT. Elem #        X =                 Y =                Z =
```

```
   0                0.00000000000E+00    0.00000000000E+00    0.00000000000E+00
   1                0.00000000000E+00      51.210000000       0.00000000000E+00
        1'             0.00000000000E+00      48.710000000       0.28605943631E-16

   2                0.00000000000E+00      46.008630000       0.59516038809E-16
        2'             0.00000000000E+00      57.030498000      -0.19271670896E-15


   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
   ***************                    E N D                   ***************
   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


   \\ First check the geometric image size. \\


   $
   $ MINMAX
   Input file ? STAR.02
   Options --- Enter
   0 for excluding the losses
   1 for including losses at a particular O.E.
   2 for including all the losses.
   Then ? 0
   Comment ?Geometrical Image
   ***********
   File examined is :
   D13:[XRAYOP.DOCUMENT.UTIL.FFRESNEL]STAR.02;2
   Was created :
    3-JUL-1989 14:32
   ***********
   Found          600 good points out of          600
   Here we are.
   X max is  2.7609133E-06
   X min is -2.7609133E-06
   Y max is  2.2204460E-16
   Y min is  0.0000000E+00
   Z max is  2.7609133E-06
   Z min is -2.7609133E-06
   X prime max is  0.2000885
   X prime min is -0.2000885
   Y prime max is  0.9949863
```

```
Y prime min is  0.9797778
Z prime max is  0.2000885
Z prime min is -0.2000885
$
$ DIR SCREEN*                        \* The aperture file \*

Directory D13:[XRAYOP.DOCUMENT.UTIL.FFRESNEL]

SCREEN.0201;2              170    3-JUL-1989 14:32:26.41  (RWED,RWED,RE,RE)

Total of 1 file, 170 blocks.
$
$ FFRESNEL                           \* calculate the diffraction image \*


Define integration limits [ cm ].
From                -500E-8         \* -500 to 500 Angstroms \*
 to                  500E-8
No. of points        101
Integration direction [ 0 = x, 90 = z ] ? 0    \* along the horizontal \*
Distance from plane [ cm ] ? 10.021868
Ray input file ? SCREEN.0201
[ 0 ] to discard losses, [ 1 ] to keep them. 0
Do you want to override the wavelength in the file ? 0

Files read OK.
Conversion to [ cm ] factor (*) ? 1.0
Include the S- and P- phase shifts in the computations ?1
$
$ DIR FF*

Directory D13:[XRAYOP.DOCUMENT.UTIL.FFRESNEL]

FFPAR.DAT;2                  1    3-JUL-1989 15:00:20.70  (RWED,RWED,RE,RE)
FFRESNEL.DAT;2              10    3-JUL-1989 15:00:21.49  (RWED,RE,RE,RE)

Total of 2 files, 11 blocks.
$
$ TY FFPAR.DAT                \* stores parameters for FFRESNEL \*
From  -5.0000000000000000E-06 to   5.0000000000000000E-06
```

```
      Step    1.0000000000000000E-07
 Wavelength    0.0000000000000000E+00 angs.
 Image located at     10.02186800000000
 Integration direction    0.0000000000000000E+00
 Scale factor [ units ] *     1.000000000000000      = [ cm ]
 Losses: NOT INCLUDED
 S- and P- phase shifts :     INCLUDED
 Files used:
 SCREEN.0201
 $
 $ TY FFRESNEL.DAT                        \* the diffraction image \*
 -5.0000000000000000E-06   1973087.868071882
 -4.9000000000000000E-06   1695296.044110004
 -4.8000000000000000E-06   1316561.473098089
            :                       :
            :                       :
  4.8000000000000000E-06   1316561.466332203
  4.9000000000000001E-06   1695296.058811655
  5.0000000000000000E-06   1973087.881998670
 $
```
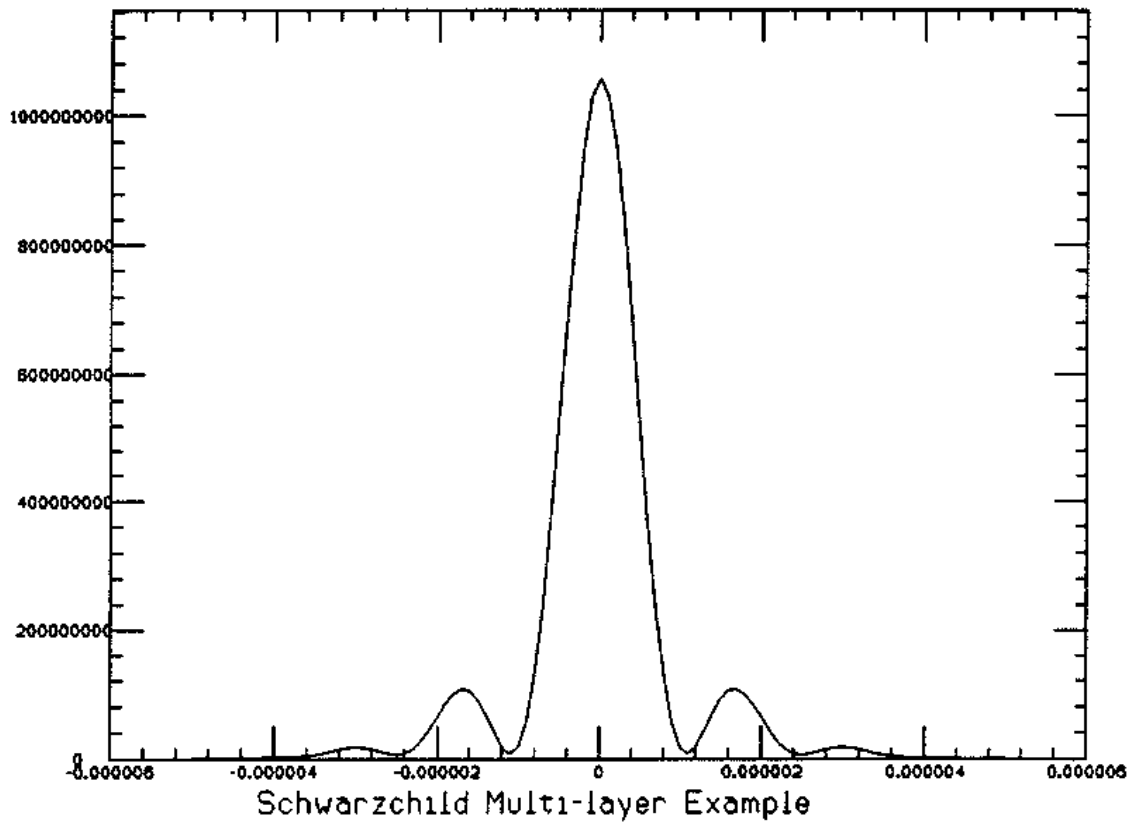
Figure 3.37: FFRESNEL: Schwarzchild example

FOCNEW

Purpose:	To search a BOF for the location of the minimum beam waist (i.e. the best gaussian focus in both the sagittal (x) and tangential (z) directions).
Input:	STAR.xx
Output:	A file FOCUS.DAT containing the analysis results plus an optional user defined plottable file that tabulates waist size vs. distance along optical axis. Analysis results are also displayed on terminal.

Description:

Locates the waist of the beam by minimizing the variance in real space with respect to the optical axis in the sagittal, tangential planes and for the circle of least confusion. If x_i is the coordinate of the ith ray (in the sagittal plane), and v_i is its direction vector then the variance will be:

$$\sigma(t) = \frac{1}{N} \sum_{i=1}^{N} (x_i + v_i t)^2$$

Expanding the sum:

$$\sigma(t) = \frac{1}{N} \sum_{i=1}^{N} (x_i^2 + 2x_i v_i + v_i^2 t^2)$$

For many purposes, the focus can be defined as the position where the beam spread is minimum. Thus we have to find the minimum of the above expression, which is just a parabola, with respect to t. Setting the derivative equal to zero and solving for t we have,

$$t = -\frac{\sum_{i=1}^{N} x_i v_i}{\sum_{i=1}^{N} v_i^2}$$

The expressions for the tangential focus and circle of least confusion are similar. The user may also choose a center of the distribution other than the optical axis.
This utility is very important in the study of monochromators and spectrographs, since it allows the user to verify the real location of the focal position.

Note: One must be careful in using FOCNEW and verify with PLOTXY that the calculations are correct. This is because with strongly asymmetric or multimodel distribution the standard deviation is not a good measure of the image "size".

Examples:

Here we will have a spherical mirror create an astigmatic image by having a point source incident upon it at 20 degrees. SHADOW computes the curvature of the mirror to satisfy the focal condition for the tangential plane. The sagittal focus occurs further away from the mirror, and the circle of least confusion is located between the two. Below are the source and mirror descriptions.

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S O U R C E      D E S C R I P T I O N **************
Point source
Focnew Example
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
end.00
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.FOCNEW]END.00;1
Creation Date          :11-APR-1989 10:56
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Random Source.
Generated total           1000 rays.
Source assumed BIDIMENSIONAL (flat).
Source Spatial Characteristics: POINT
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: CONICAL
Cone Outer Aperture :   0.500000000E-01 Inner Aperture :   0.100000000E-01
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************           E N D            **************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
******************* MIRROR  DESCRIPTION  *******************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Spherical Mirror Illuminated at 20 degrees incidence
Focnew Example to Generate Astigmatic Image
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
```

```
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.FOCNEW]END.01;1
Creation Date           :11-APR-1989 10:56
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:          SPHERICAL
Cylindrical figure                      NO
Element type                            REFLECTOR
Reflectivity                            OFF
Mirror dimensions                       UNLIMITED
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                        30.00000000000000
Image  Plane                                 30.00000000000000
Incidence Angle                              20.00000000000000
Reflection/Diffraction Angle                 20.00000000000000

Mirror parameters                       COMPUTED
Same configuration as Central Axis      YES
Objective focus at                           30.00000000000000
Image focus at                               30.00000000000000
Incidence angle                              20.00000000000000
Parameters used follow:
Spherical Radius                        31.9253332
Source of this O.E. moved               NO
Mirror at pole position ( no mov. )     YES
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

We will have FOCNEW create files for the sagittal and tangential focii as well as the circle of least confusion. These files will then be used as input to TopDrawer to plot the results.

```
$ focnew

Input file ?  star.01
We have            1000 good points out of            1000
```

```
 Row Par Minimum:        Maximum:         Center:          St. Dev.:

  1  X   -0.35104        0.35104          0.36242E-17      0.17898
  2  Y   -0.74221E-15    0.59533E-15     -0.29388E-16      0.37404E-15
  3  Z   -0.50159E-03    0.56424E-02      0.14659E-02      0.20068E-02
  4  X'  -0.38286E-01    0.38286E-01     -0.45285E-18      0.19524E-01
  5  Y'   0.99870        0.99997          0.99948          0.37334E-03
  6  Z'  -0.49071E-01    0.50888E-01      0.76300E-04      0.25491E-01
Options:
center at origin              [ 0 ]
center at center of gravity   [ 1 ]
external                      [ 2 ]
Then ? 0
-------------------------------------------------------------------------
Searching file :
star.01
D13:[XRAYOP.DOCUMENT.UTIL.FOCNEW]STAR.01;5                11-APR-1989 10:56
-------------------------------------------------------------------------
Center at :Origin
X =   0.0000000000000000E+00    Z =   0.0000000000000000E+00
-------------------------------------------------------------------------
.............  S A G I T T A L   ............
X coefficients :   0.3815973746E-03 -0.3496278593E-02  0.3203366904E-01
Center : 0.3624200855E-17   Average versor : 0.2795689524E-18
Sagittal   focus at       :   9.162218680
Waist size at best focus (rms) :  0.0000000000E+00
Waist size at origin              :  0.1789795213
.............  T A N G E N T I A L  .............
Z coefficients :   0.6510081993E-03 -0.5464547342E-05  0.6176084572E-05
Center : 0.1465870279E-02   Average versor : 0.7687155566E-04
Tangential focus at       :   0.8393976217E-02
Waist size at best focus (rms) :  0.2475927158E-02
Waist size at origin              :  0.2485172946E-02
.............  LEAST CONFUSION  ...............
T coefficients :   0.1032605574E-02 -0.3501743141E-02  0.3203984512E-01
Center : 0.1465870279E-02   Average versor : 0.7687155566E-04
Circle of least confusion :   3.391172031
Waist size at best focus (rms) :  0.1420029286
Waist size at origin              :  0.1789967741
All done. File out data.
```

```
Do you want a plottable file ?   1
Enter :
1 for X
2 for Z
3 for T
4 for all
 Then ?   4
Please specify Limits [ YMIN, YMAX, STEP ] ?
Ymin ?   -5
Ymax ?   15
Ystep ? 0.5
 File root [ 7 letters max ] ?  foc.dat
Enter :
0 for another plot
1 to restart
2 to exit
 Then ?   2


$
```

Shown below are the Phase space projections in X and Z showing lack of focus in the sagittal plane and focus in the tangential plane, since the points are uncorrelated.

Notice how the beam is smallest at the slit position.

A more complex case may be that of the toroidal grating monochromator(TGM. This mount is based on the use of a Toroidal grating rotated around its surface with fixed slits located at p and q respectively. A Rowland Circle mount would give the best image when the Rowland circle condition is satisfied, but the quality degrades quickly if the grating is rotated. In the TGM mount the quality of the "best" focus is sacrificed so that a wider range with "acceptable" resolution is maintained.

Typically, the entrance slit is located "inward" relative to the rowland circle position at zero order (asymmetric mount) so that its image moves outward. When scanning the wavelength the change in angle of incidence brings the image back closer to the grating until it is located at the exit slit; this is the first "sweet spot" of the TGM. Then the image moves even closer to a minimum distance and the process reverses, with the image moving away through the second "sweet spot" of the spectrum.

Clearly if one could move the exit slit to follow the "best" focus, the performance of the monochromator would be improved. This has originated many designs based on movable exit slits. FOCNEW is particulary important because it allows one to locate the position
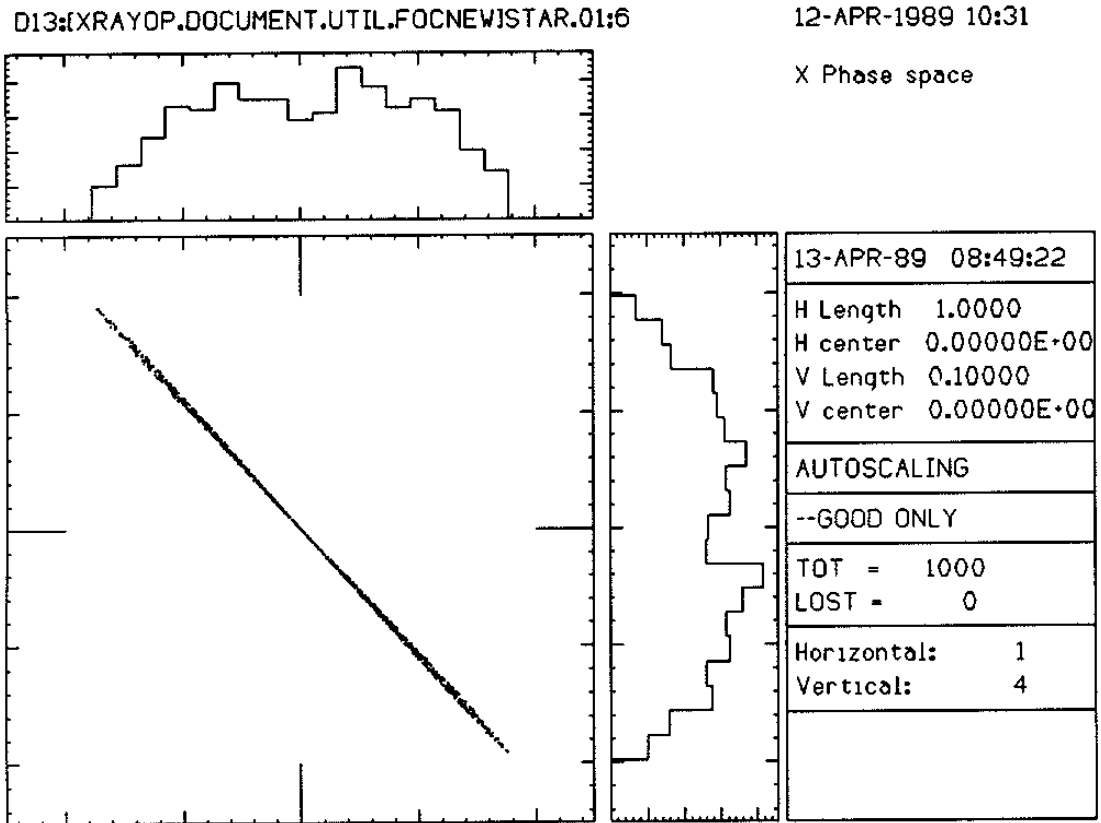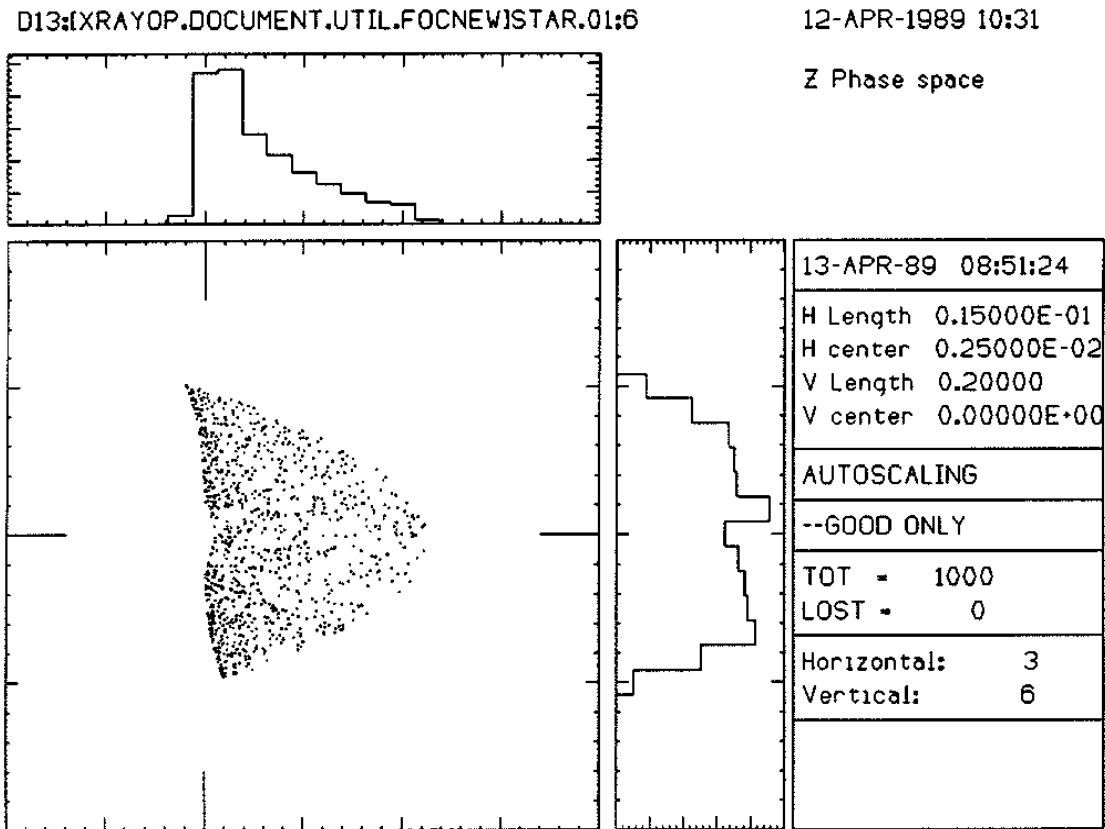
D13:[XRAYOP.DOCUMENT.UTIL.FOCNEW]STAR.01;6   12-APR-1989 10:31

X Phase space

13-APR-89 08:49:22

H Length   1.0000
H center   0.00000E+00
V Length   0.10000
V center   0.00000E+00

AUTOSCALING

--GOOD ONLY

TOT   =   1000
LOST =   0

Horizontal: 1
Vertical: 4

Figure 3.38: FOCNEW: X phase space

D13:[XRAYOP.DOCUMENT.UTIL.FOCNEW]STAR.01:6   12-APR-1989 10:31

Z Phase space

| 13-APR-89 08:51:24 |
| H Length 0.15000E-01 |
| H center 0.25000E-02 |
| V Length 0.20000 |
| V center 0.00000E+00 |
| AUTOSCALING |
| --GOOD ONLY |
| TOT = 1000 |
| LOST =   0 |
| Horizontal: 3 |
| Vertical: 6 |

Figure 3.39: FOCNEW: Z phase space
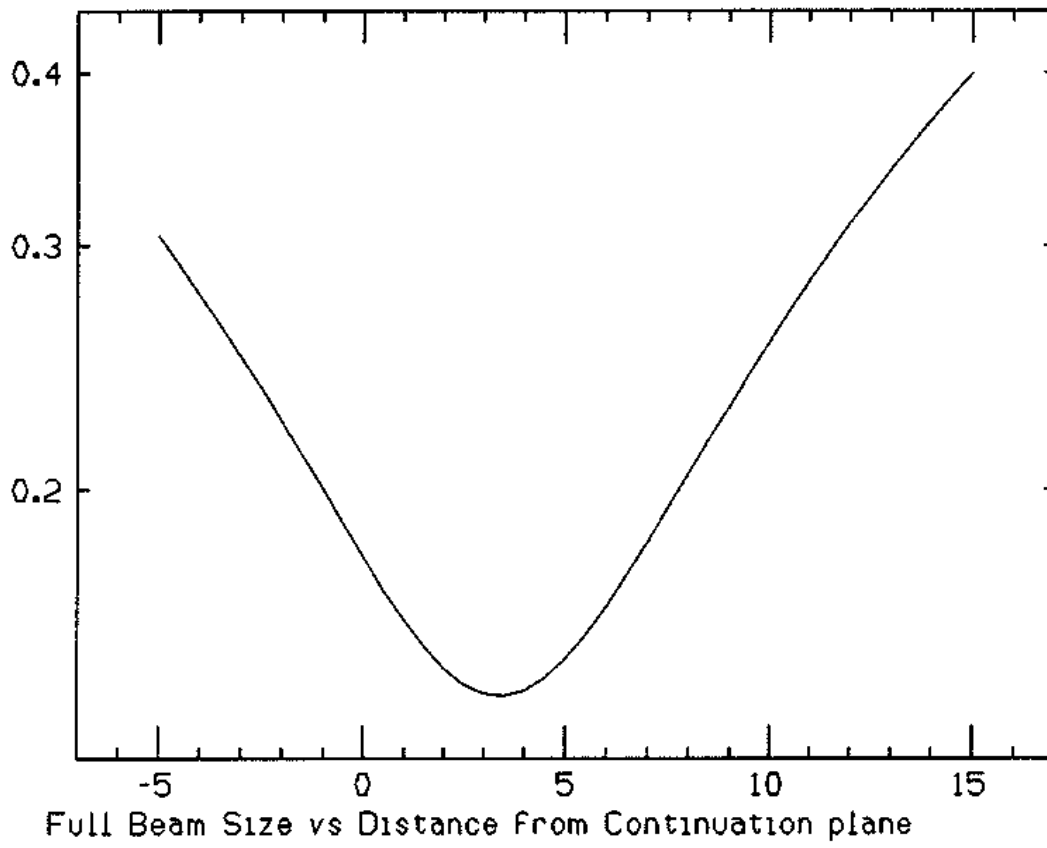
Figure 3.40: FOCNEW: Full beam size
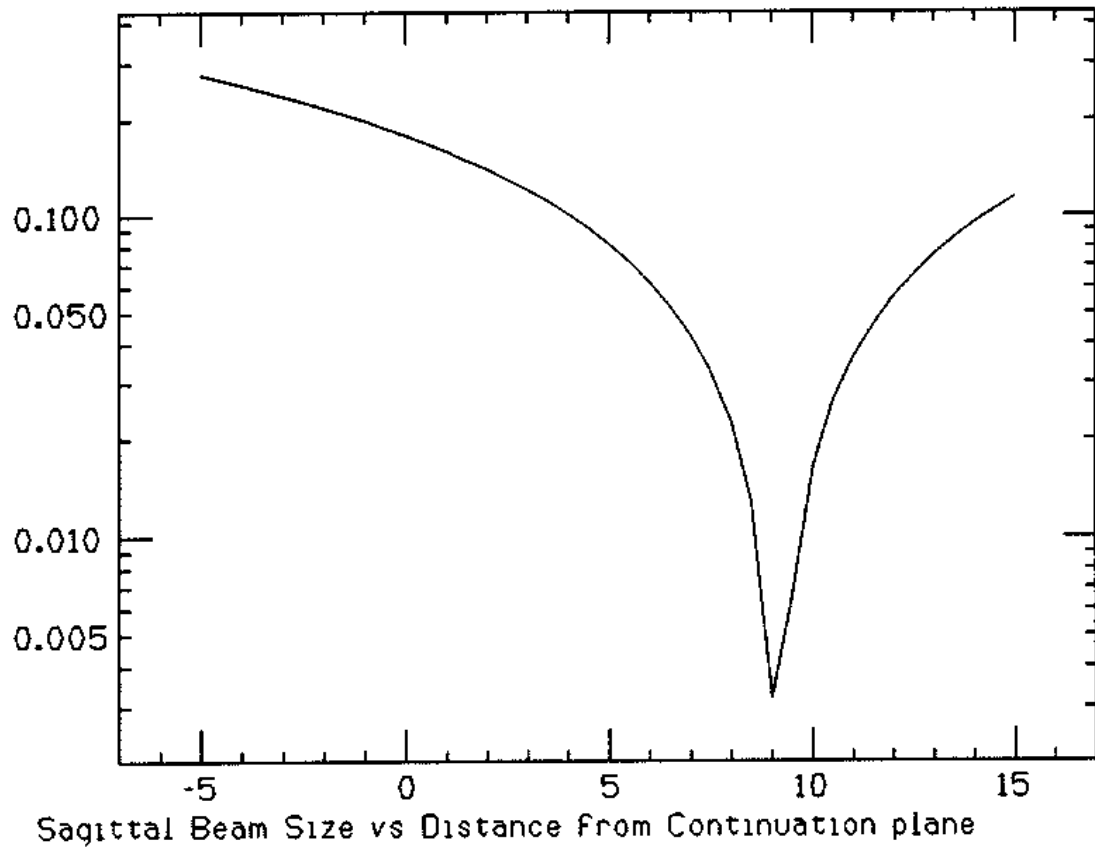
Figure 3.41: FOCNEW: Sagittal beam size
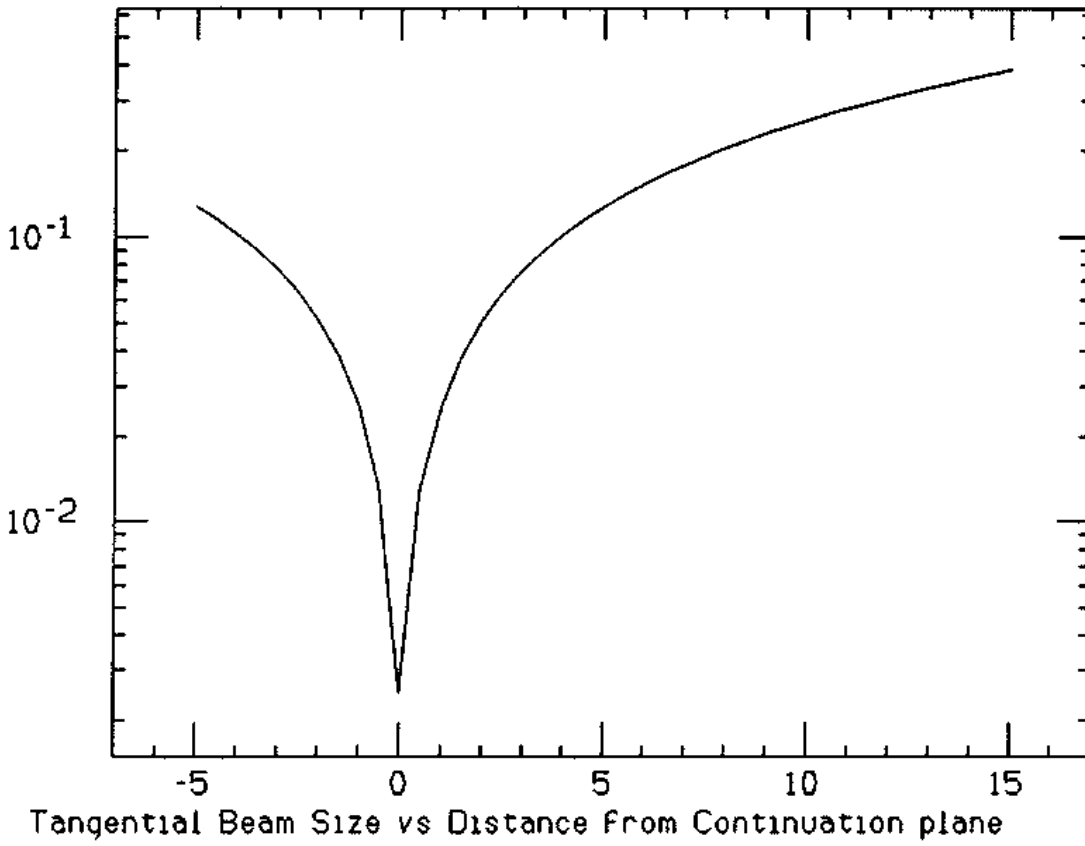
Figure 3.42: FOCNEW: Tangential beam size

of this best focus. It is also useful to verify that the optical system we have just traced is indeed performing as expected.

With the TGM, let's look at how the tangential focus at the final image plane is dependent upon the beam energy. We first examined the focus at 50eV, the energy to which the grating was tuned. Note that the center of gravity was used, because at different energies, the ray bundle will be displaced from the origin. Then the source was recolored to 50.1eV, the system was retraced, and FOCNEW was run in the same manner, again using the center of gravity for the distribution center. The FOCNEW file FOCUS.DAT for each run is displayed below, along with a plot around the tangential focal points.

```
--------------------------------------------------------------------------
Searching file :
tgm:star.03
D13:[XRAYOP.DOCUMENT.TGM]STAR.03;29                          9-MAY-1989 11:1
--------------------------------------------------------------------------
Center at :Baricenter
X =   0.0000000000000000E+00    Z =   0.0000000000000000E+00
--------------------------------------------------------------------------
Working with  865 "good" rays out of 1000
.............. S A G I T T A L  ..............
X coefficients :   0.1279945686E-03  0.2849121654E-03  0.1589516586E-02
Center : 0.3572783631E-02   Average versor : 0.2159759878E-03
Sagittal   focus at        :  -2.232813118
Waist size at best focus (rms) :  0.3064103890E-01
Waist size at origin               :   0.3970833417E-01
.............. T A N G E N T I A L ..............
Z coefficients :   0.1814695449E-04  0.5456865017E-04  0.2534060565E-03
Center : 0.1037995525E-01   Average versor : 0.1706396676E-02
Tangential focus at        :  -2.419161809
Waist size at best focus (rms) :  0.7516725477E-02
Waist size at origin                 :   0.1206907559E-01
..............    LEAST CONFUSION  ..............
T coefficients :   0.1461415231E-03  0.3394808156E-03  0.1842922642E-02
Center : 0.1097762515E-01   Average versor : 0.1720010245E-02
Circle of least confusion :  -2.252641249
Waist size at best focus (rms) :  0.3155704656E-01
Waist size at origin                 :   0.4150198054E-01
```

```
--------------------------------------------------------------------------
Searching file :
tgm:star.03;28
D13:[XRAYOP.DOCUMENT.TGM]STAR.03;28                          9-MAY-1989 11:10
--------------------------------------------------------------------------
Center at :Baricenter
X =   0.0000000000000000E+00    Z =   0.0000000000000000E+00
--------------------------------------------------------------------------
Working with  865 "good" rays out of 1000
.............. S A G I T T A L  ..............
X coefficients :   0.1300886749E-03  0.2994988597E-03  0.1629528588E-02
Center : 0.3521177601E-02   Average versor : 0.2175865878E-03
Sagittal   focus at       :  -2.308996827
Waist size at best focus (rms) :  0.3039438956E-01
Waist size at origin             :   0.4021355364E-01
.............. T A N G E N T I A L .............
Z coefficients :   0.1549933837E-04  0.3405311760E-04  0.2902239386E-03
Center : 0.1251010550E-01   Average versor : 0.4472218222E-04
Tangential focus at       :  -2.233454297
Waist size at best focus (rms) :  0.7511028279E-02
Waist size at origin             :   0.1156378826E-01
..............   LEAST CONFUSION  .............
T coefficients :   0.1455880133E-03  0.3335519773E-03  0.1919752527E-02
Center : 0.1299620835E-01   Average versor : 0.2221350868E-03
Circle of least confusion :  -2.300952861
Waist size at best focus (rms) :  0.3130995822E-01
Waist size at origin             :   0.4184317263E-01
```
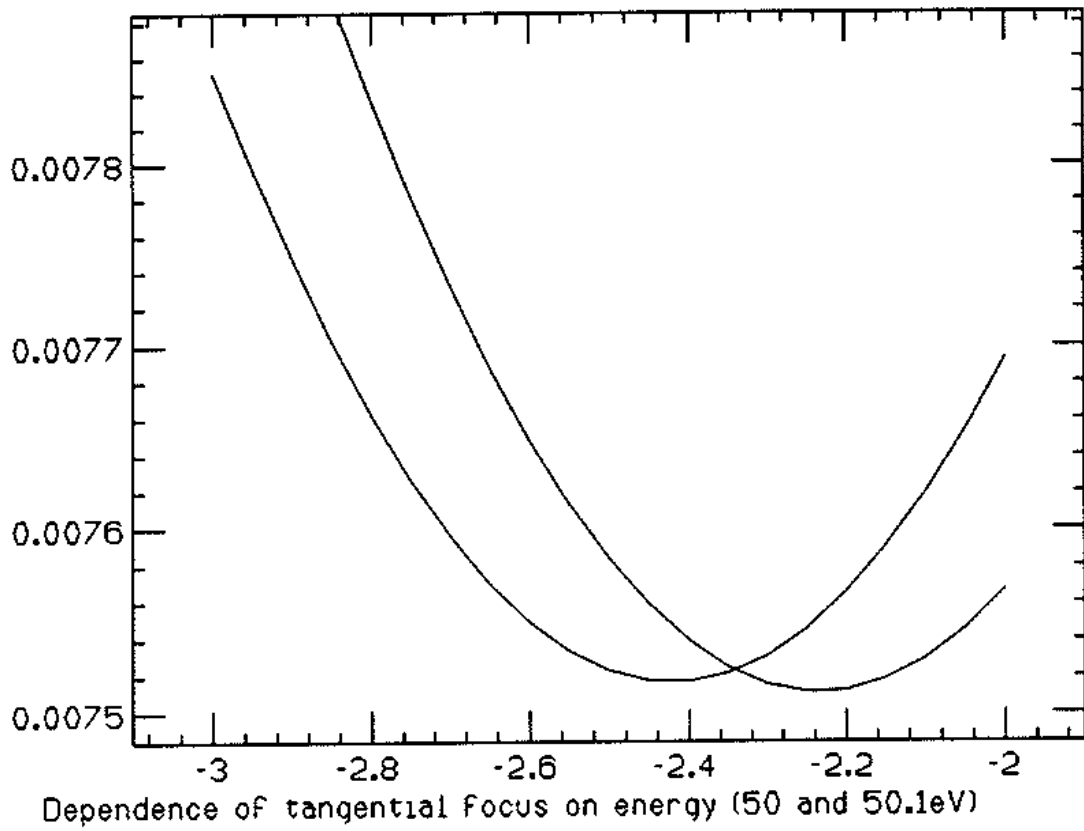
Figure 3.43: TGM example with FOCNEW

RECOLOR

Purpose:	To modify the photon energies of each ray in a source array file according to a user defined distribution. Only random photon energy distributions are allowed.
Input:	A ray Binary Output File.
Output:	A ray Binary Output File.

Description:

This utility will create a ray file with a distribution of energies. Such a modification is useful in studying the effects of a nonmonochromatic source. For example, one may wish to examine how power is absorbed in a mirror as a function of wavelength or one could determine how different energies are diffracted in a given crystal. A typical application can be found when one runs first a monochromatic source through a system dispersing, say, in Z. PREPLOT can be used to extract FIL1 = $\{\hbar\omega_o, z\}$. Then RECOLOR is used to modify $\hbar\omega_o$ to the range $\hbar\omega_o \pm \Delta\hbar\omega$. After running SHADOW, one creates FIL2 = $\{\hbar\omega, z\}$. Then using FILEX:

$$DISP = FIL2 - FIL1$$

and plot DISP. The graph will show directly $\Delta(\hbar\omega)$ around $\hbar\omega_o$. Notice that for extended sources the values of Z in FIL1 will *not* be all the same.

RECOLOR will change the photon energy distribution to one of the following:

1. *Monochromatic:* All rays have the same energy.

2. *Multi Lines:* Discrete energies, each specified by the user (not necessarily equispaced), are assigned to rays at random.

3. *Uniform Distribution:* Any value between user specified limits may be assigned at random to the ray energy.

The energies can be expressed in eV or as a function of wavelength.

Examples:

We will examine an ERG monochromator with a monochromatic point source having a much larger vertical divergence than horizontal. Then we will use RECOLOR to create a white source with the energy distribution centered on that of the tuned grating. The beam will be dispersed in the tangential plane as a function of energy. The dispersion may be

examined by finding the difference between the Z coordinates for the monochromatic and white rays and plotting this vs energy. Below are descriptions of the source and system.

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S O U R C E      D E S C R I P T I O N **************
Point source to be incident upon ERG
Recolor Example
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
end.00
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.RECOLOR]END.00;2
Creation Date           :13-APR-1989 09:26
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Random Source.
Generated total        1000 rays.
Source assumed BIDIMENSIONAL (flat).
Source Spatial Characteristics: POINT
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: LAMBERTIAN
Distribution Limits. +X :   0.100000000E-03 -X:   0.100000000E-03 rad
                     +Z :   0.200000000E-01 -Z:   0.200000000E-01 rad
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: SINGLE LINE
Photon Energy:   400.00     eV, or   30.996     Angs.
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************              E N D              **************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++




++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
******************* MIRROR  DESCRIPTION  *******************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
ERG auto tuned to order -1
RECOLOR EXAMPLE
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.RECOLOR]END.01;2
Creation Date           :13-APR-1989 09:27
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:       SPHERICAL
Cylindrical figure                   NO
Element type                         REFLECTOR
Element type                         GRATING
Order choosen ( inside are < 0 )      -1.000000000000000
Automatic Tuning                     YES
Mount                                ERG
Grating tuned at  [ eV ]              400.0000000000000
Constant ruling [ lines/cm ]          12000.00000000000
Reflectivity                         OFF
Mirror dimensions                    UNLIMITED
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                         174.5000000000000
Image  Plane                                  464.7235755591278
Incidence Angle                               88.00000000000000
Reflection/Diffraction Angle                  84.66696278217028

Mirror parameters                    EXTERNAL
Parameters used follow:
Spherical Radius                      5000.00000
Source of this O.E. moved             NO
Mirror at pole position ( no mov. )   YES
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Now we will create a file with the energy and Z coordinate of each ray in the image plane.

```
PREPLOT> Input file ?
400ev.img
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 :  3
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
***********
Found        1000 good points out of       1000
Output options :
  [ 0 ] store rays in a file
  [ 1 ] plot directly on screen
  [ 2 ] both
Then ?  0
PREPLOT> Output file ?  400ev.dat
```

Now we will create the white light source in the interval 395 to 405eV. The system is then retraced with the new source.

```
$ RECOLOR
File for input ? BEGIN.DAT
and for output ? BEGIN.DAT
Data ready. Read        1000 points.
Are you going to specify energies in eV [ 0 ] or wavelengths in angstroms [1]
? 0
Available options :
```

```
1 single line
2 multi lines
3 box distribution
Then ? 3
Minimum value ? 395
Maximum value ? 405
Enter seed for random number generator : 12312377
All done.
$
```

After rerunning TRACE in the BATCH mode on the system, we create the file of Z coordinate vs energy on the new image file with the aid of PREPLOT.

```
$ preplot
PREPLOT> Input file ?
delev.img
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 :  3
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
***********
Found          1000 good points out of          1000
Output options :
  [ 0 ] store rays in a file
  [ 1 ] plot directly on screen
  [ 2 ] both
Then ?   0
PREPLOT> Output file ?   delev.dat
```

Use FILEX to get the difference between the Z coordinates.

```
$ filex
FILEX >
disper = delev - 400ev
FILEX > read          1000 records.
FILEX > Succesful completion
FILEX >
```

The file disper.dat can now be plotted using TDTEK or TDFILE and UGTEK. Notice the variance in the dispersion away from 400eV. This is a result of the spherical aberration of the grating since the divergence in the tangential plane is significant.

D13:[XRAYOP.DOCUMENT.UTIL.RECOLOR]STAR.01:3   13-APR-1989 09:39

Diffracted Image at
   400eV

13-APR-89 09:45:21

H Length   2.0000
H center   0.00000E+00
V Length   2.0000
V center   0.00000E+00

CARTESIAN

--GOOD ONLY

TOT =   1000
LOST =   0

Horizontal: 1
Vertical: 3
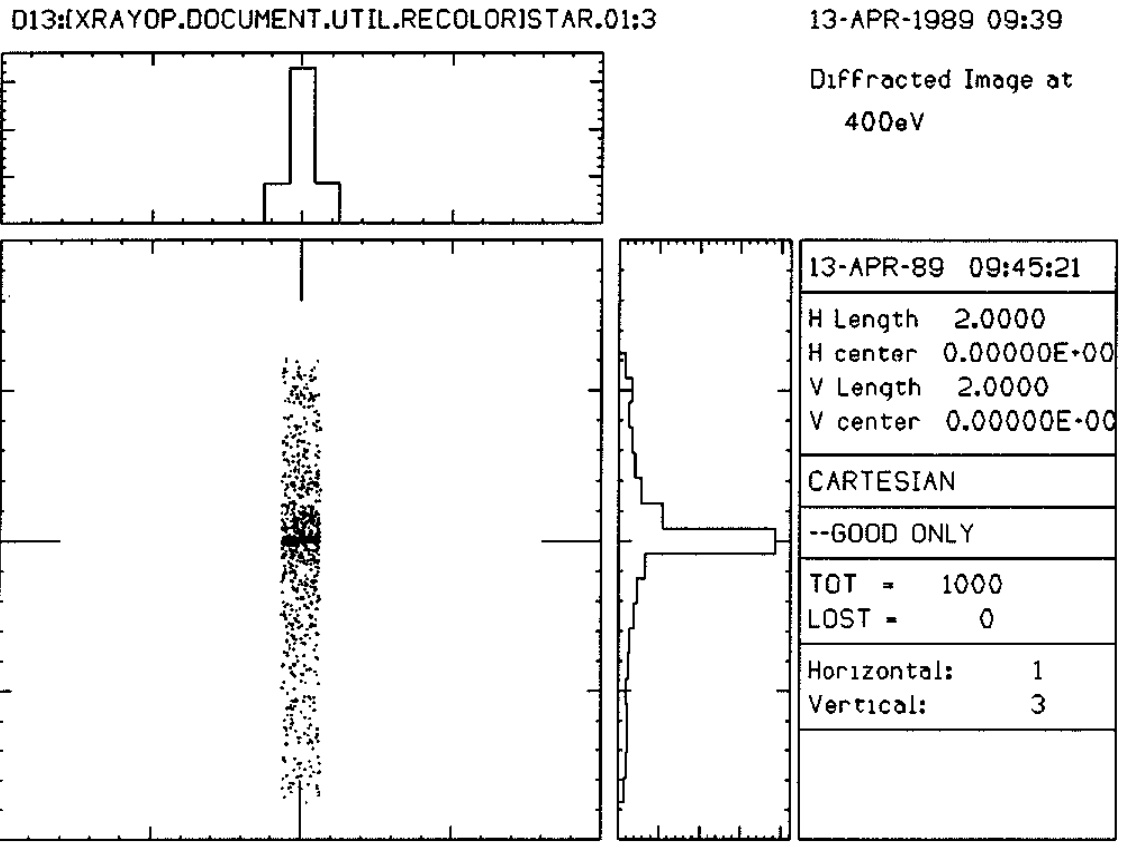
Figure 3.44: RECOLOR: Image at 400 eV

D13:[XRAYOP.DOCUMENT.UTIL.RECOLOR]STAR.01:3   13-APR-1989 10:10

Diffracted Image

395-405eV

13-APR-89 10:20:48

H Length   2.0000
H center   0.00000E+00
V Length   2.5000
V center -0.25000

CARTESIAN

--GOOD ONLY

TOT =   1000
LOST =   0

Horizontal: 1
Vertical: 3
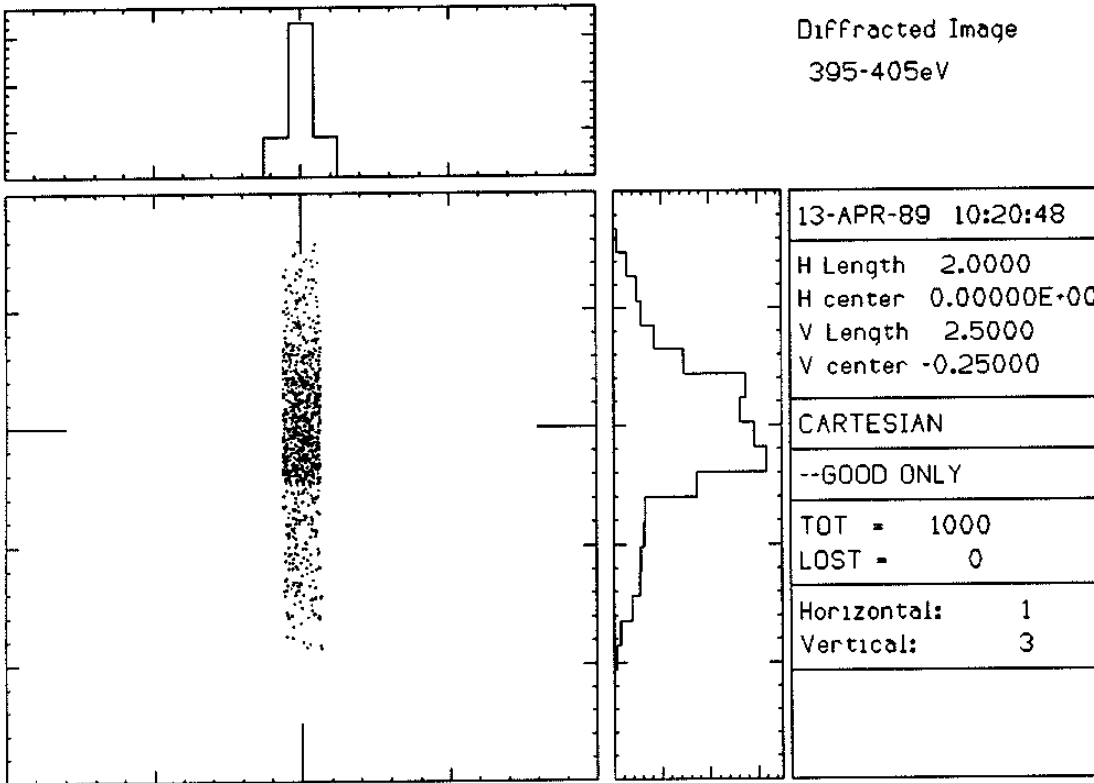
Figure 3.45: RECOLOR: Image from 395-405 eV
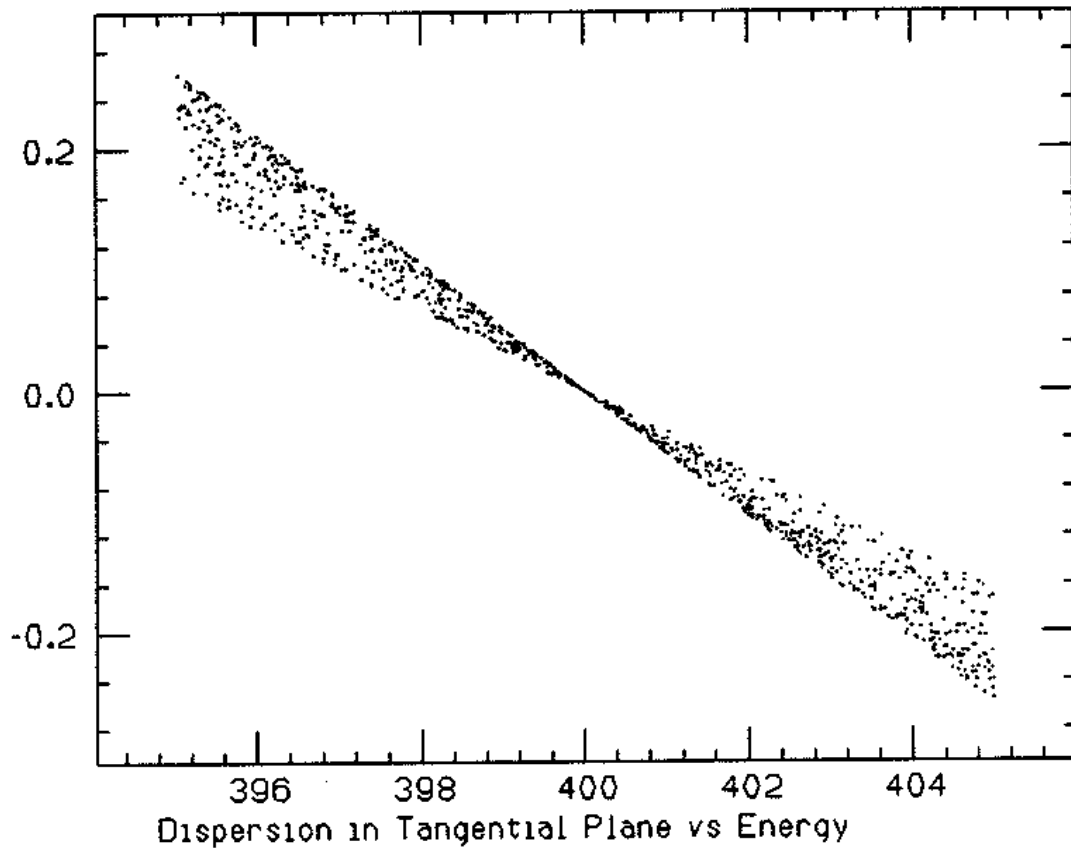
Figure 3.46: RECOLOR: Dispersion in tangential plane from 395-405 eV

RETRACE

Purpose:	To create a new BOF (e.g. STAR.xx) from an existing BOF at a different position along the optical axis by continuing the trajectory of the rays. Notice that the distance is arbitrary so that for example it is possible to study virtual images.
Input:	Any BOF
Output:	A BOF

Description:

This utility enables the user to look at the 'image' formed by the rays at some distance along the optical axis from the location of the continuation plane. The rays are assumed to be undeflected between the continuation plane and the desired location. Thus the new position can be calculated as follows:

$$X(t) = X(0) + X't$$

Here X' is assumed constant, of course.

RETRACE should be used in conjunction with FOCNEW and PLOTFOC, for example, to look at the image at the circle of least confusion without having to go back into SHADOW to modify the image plane and retrace the entire system.

Examples:

In this example we will examine the astigmatic image that was generated in Section 2.4 of the Primer. Recall that FOCNEW told us that the sagittal focus and the circle of least confustion were about 9.151 and 3.281 units away from the tangential focus. We may plot out the cross sections of the beam or use other utilities to analyze the new ray files. In order to create a BOF for the beam at the position of the sagittal focus and circle of least confusion without retracing the system, we can let RETRACE do the work for us:

```
$ retrace
RETRACE> Ray input file ?  star.01
RETRACE> Ray output file ? ret.dat
RETRACE> Distance ?  9.151
Read        1000 rays.
```

D13:[XRAYOP.DOCUMENT.UTIL.RETRACE]RET.DAT;2   12-APR-1989 15:37

Sagittal Focus

12-APR-89 15:39:52

H Length 0.20000E-01
H center 0.00000E+00
V Length   2.0000
V center 0.00000E+00

AUTOSCALING

--GOOD ONLY

TOT =   1000
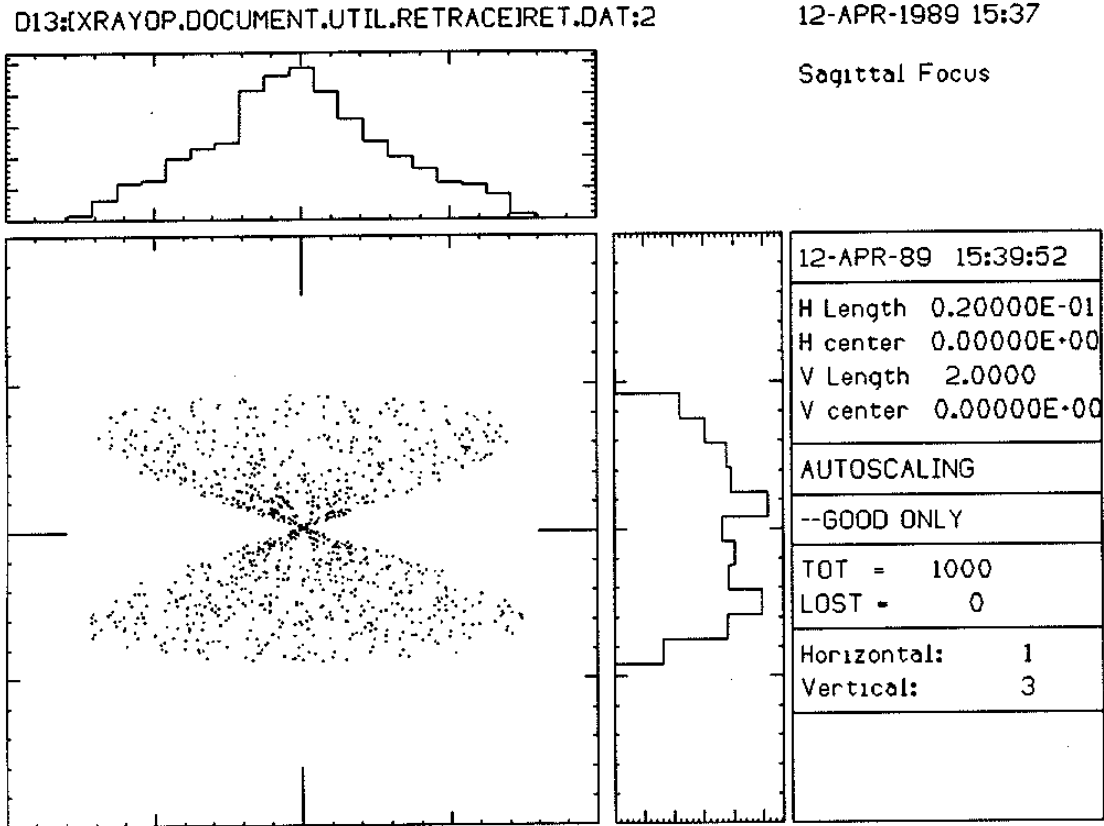LOST =   0

Horizontal: 1
Vertical: 3

Figure 3.47: RETRACE: Sagittal focus

```
Another run [ Y/N ] ? y
RETRACE> Ray input file ? star.01
RETRACE> Ray output file ? ret2.dat
RETRACE> Distance ?  3.281
Read         1000 rays.
Another run [ Y/N ] ? 0
```

Now that we have the ray files for the desired positions, we can plot out the images of the beam. Notice that neither coordinate is in focus, but that the optical size is smaller.

D13:[XRAYOP.DOCUMENT.UTIL.RETRACE]STAR.01;6   12-APR-1989 10:31

Tangential Focus

12-APR-89 15:05:07
H Length   1.0000
H center   0.00000E+00
V Length   0.15000E-01
V center   0.25000E-02
AUTOSCALING
--GOOD ONLY
TOT =   1000
LOST =   0
Horizontal: 1
Vertical: 3
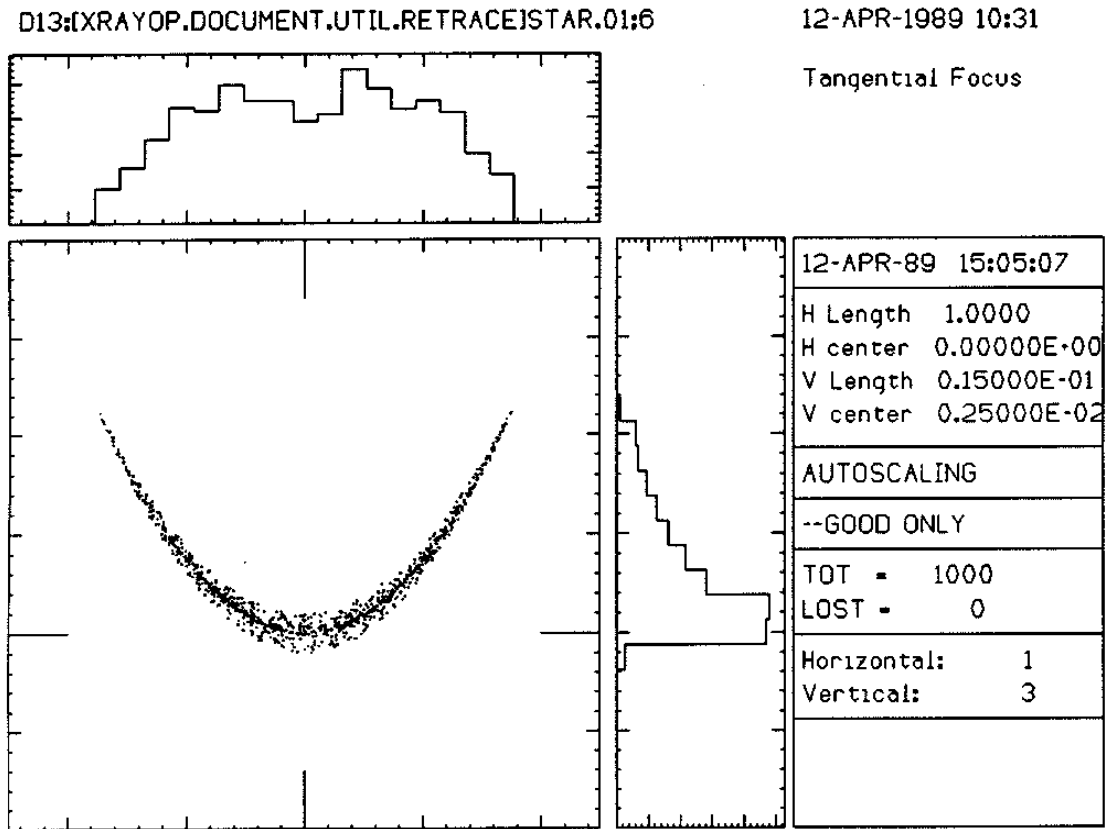
Figure 3.48: RETRACE: Tangential focus

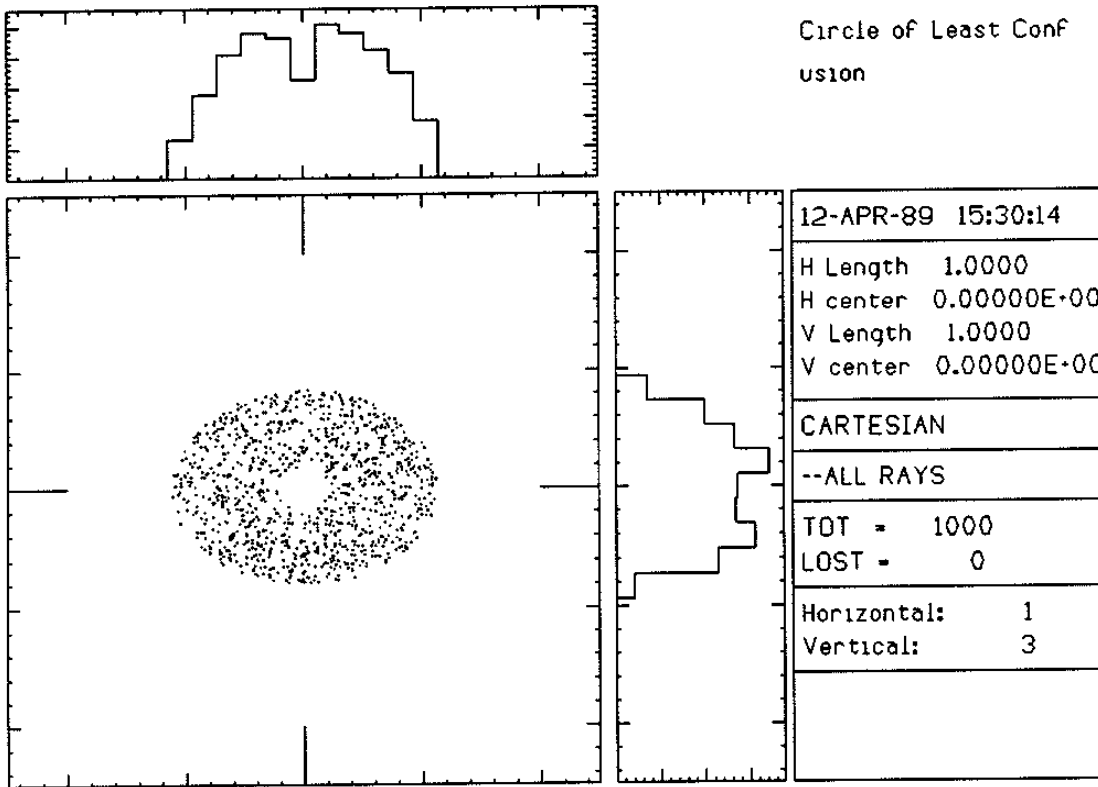D13:[XRAYOP.DOCUMENT.UTIL.RETRACE]RET1.DAT;1   12-APR-1989 15:26

Circle of Least Conf
usion

12-APR-89 15:30:14
H Length   1.0000
H center   0.00000E+00
V Length   1.0000
V center   0.00000E+00
CARTESIAN
--ALL RAYS
TOT =   1000
LOST -   0
Horizontal: 1
Vertical: 3

Figure 3.49: RETRACE: Circle of least confusion

SECTOR

Purpose:	To combine up to four tracings from SHADOW in a single sectored output.
Input:	A BEGIN/STAR file and the corresponding START.xx file, up to four MIRR.xx files, one for each sector.
Output:	A STAR.00 file containing the image from the sectored surface and a MIRRS.00 file containing the combined MIRR file.

Description:

This utility will combine up to four separate tracings from SHADOW to create a "compound" mirror otherwise not possible with SHADOW. Each tracing is done separately by the user, using the same source or previous optical element. Then the utility is run. The utility reads in a source file and its corresponding namelist file (i.e. BEGIN.DAT and START.00 or STAR.02 and START.02, etc.). It then reads in up to four mirror files (MIRR.xx). Using these files, the program computes the optical path to the mirror. The intercepts associated with shorter optical paths are then put into a single continuation file. The program writes two binary files; MIRRS.00 and STAR.00, the mirror file and continuation plane file respectively. These files can be plotted with PLOTXY, like any other mirror or image file.

Examples:

The following example shows how one would trace a flashlight composed of two cylindrical parabolical mirrors with the cylinder axes 90 degrees apart. First we show the output from MIRINFO on each of the mirrors we start with.

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*******************   MIRROR  DESCRIPTION   *******************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
SECTOR Example - First Mirror
0 deg orientation
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.SECTOR.M1]END.01;5
Creation Date           :12-JUN-1989 13:35
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:          PARABOLICAL
```

```
Cylindrical figure                    YES                       << note angle
Cylinder axis angle from X-axis        0.0000000000000000E+00   of cylinder
Element type                          REFLECTOR                 axis
Reflectivity                          OFF
Mirror dimensions                     UNLIMITED
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                       1.000000000000000
Image  Plane                                5.000000000000000
Incidence Angle                             0.0000000000000000E+00
Reflection/Diffraction Angle                0.0000000000000000E+00

Mirror parameters                     COMPUTED
Same configuration as Central Axis    YES
Objective focus at                          1.000000000000000
Image focus at                              5.000000000000000
Incidence angle                             0.0000000000000000E+00
Parameters used follow:
   Parabola Param.    2.000000000000000
Source of this O.E. moved             NO
Mirror at pole position ( no mov. )   YES
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*******************   MIRROR  DESCRIPTION   *******************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
SECTOR Example - Second Mirror
0 deg orientation
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.SECTOR.M2]END.01;5
Creation Date           :12-JUN-1989 13:39
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


Surface figure was defined as:        PARABOLICAL
Cylindrical figure                    YES                     << note angle of
Cylinder axis angle from X-axis        90.00000000000002    cylinder axis
Element type                          REFLECTOR
```

```
Reflectivity                                OFF
Mirror dimensions                           UNLIMITED
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                          1.000000000000000
Image  Plane                                   5.000000000000000
Incidence Angle                                0.0000000000000000E+00
Reflection/Diffraction Angle                   0.0000000000000000E+00

Mirror parameters                           COMPUTED
Same configuration as Central Axis          YES
Objective focus at                             1.000000000000000
Image focus at                                 5.000000000000000
Incidence angle                                0.0000000000000000E+00
Parameters used follow:
   Parabola Param.    2.000000000000000
Source of this O.E. moved                   NO
Mirror at pole position ( no mov. )         YES
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Using the renamed mirror files from the above mirrors, we'll now run SECTOR using the
same source used in tracing of each of the separate mirrors.

```
$
$ run util:sector
Source file ? BEGIN.DAT                      \* or the previous STAR.xx file \*
Parameter file [ START.xx ] ? START.00 \* or START.xx file corresponding
How many sectors [ max 4 ] ? 2          \* to previous optical element \*
Call to SETSOUR
Exit from SETSOUR
Call to IMREF
Exit from IMREF
Call to OPTAXIS
Exit from OPTAXIS
Read          1000 from
BEGIN.DAT

Sector #              1
```

```
File name ? MIRR1.01                      \* MIRR.xx file of first sector \*
Sector #          2
File name ? MIRR2.01                      \* MIRR.xx file of second sector \*
Call to RESTART
Exit from RESTART
Call to IMAGE
Exit from IMAGE
$ DIR/SINCE=-00:05


Directory D13:[XRAYOP.DOCUMENT.UTIL.SECTOR]

MIRRS.00;3                188    8-JUN-1989 16:18:59.20  (RWED,RWED,RE,RE)
OPTAX.00;3                  0    8-JUN-1989 16:18:37.54  (RWED,RWED,RE,RE)
STAR.00;3                 188    8-JUN-1989 16:19:02.36  (RWED,RWED,RE,RE)

Total of 3 files, 376 blocks.
$ \* Both MIRRS.00 and STAR.00 are binary files plottable using PLOTXY \*
  \* giving the results of the combined mirror \*
```

The image and footprint plots are shown below as well as plots of the resulting system
generates by SYSPLOT.
For comparison, we also show the results of tracing a full parabolical mirror.

```
   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
   *******************  MIRROR  DESCRIPTION   *******************
   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
   Sector Example - Full Parabolical Mirror w/o SECTOR
   0 deg orientation
   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
   Input file specified:end.01
   Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.SECTOR.PARAB]END.01;1
   Creation Date            :12-JUN-1989 14:16
   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

   Surface figure was defined as:       PARABOLICAL
   Cylindrical figure                   NO
   Element type                         REFLECTOR
   Reflectivity                         OFF
   Mirror dimensions                    UNLIMITED
   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```
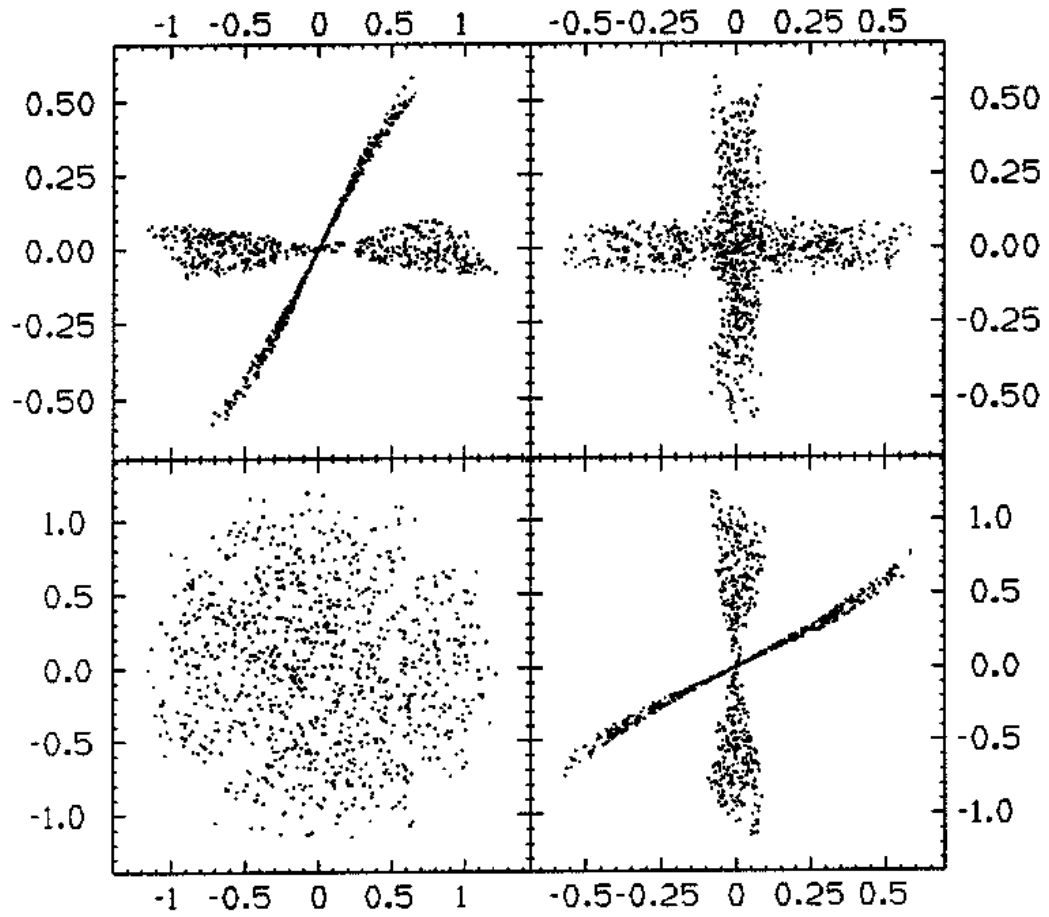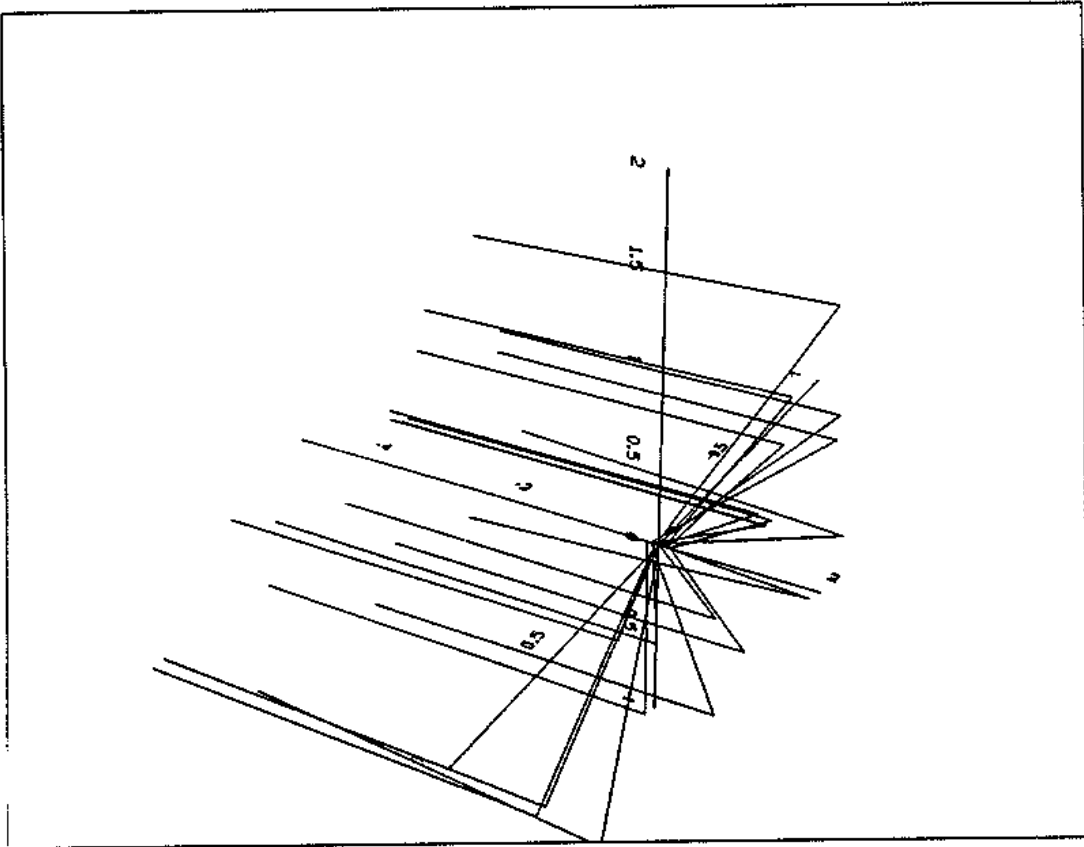
Figure 3.50: SECTOR: PLOTSPACE output of SECTORed mirror

Sectored Mirror

Figure 3.51: SECTOR: System in 3-D
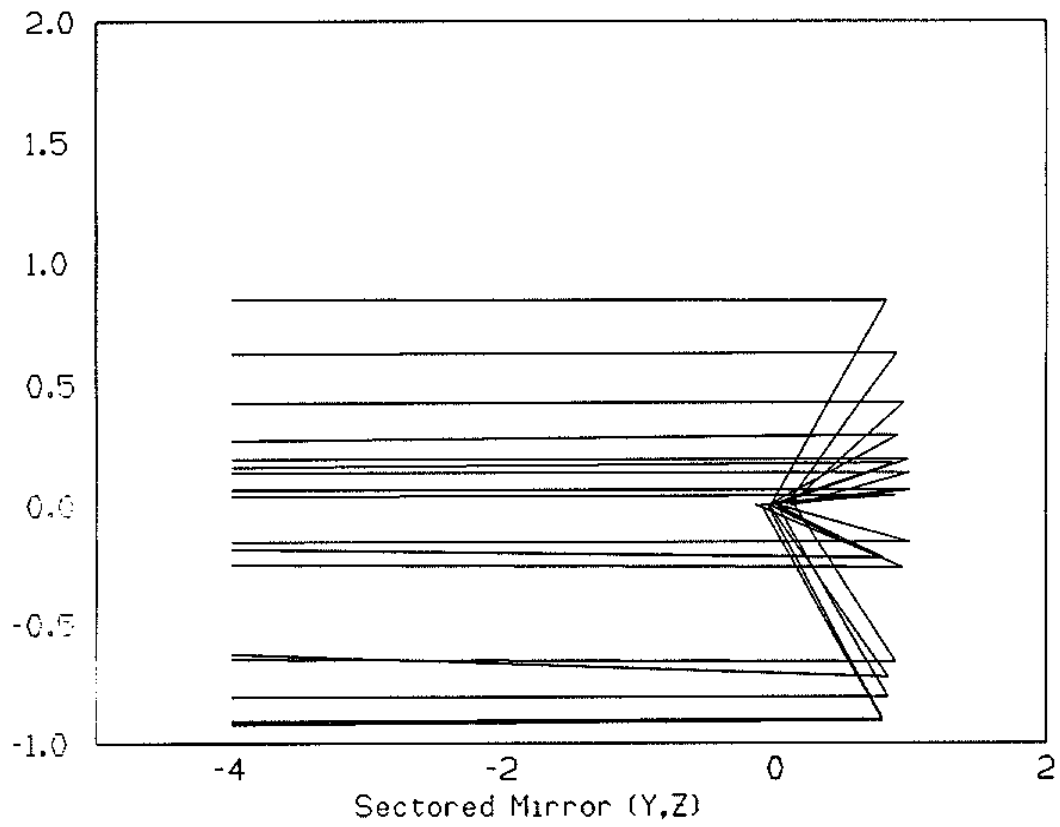
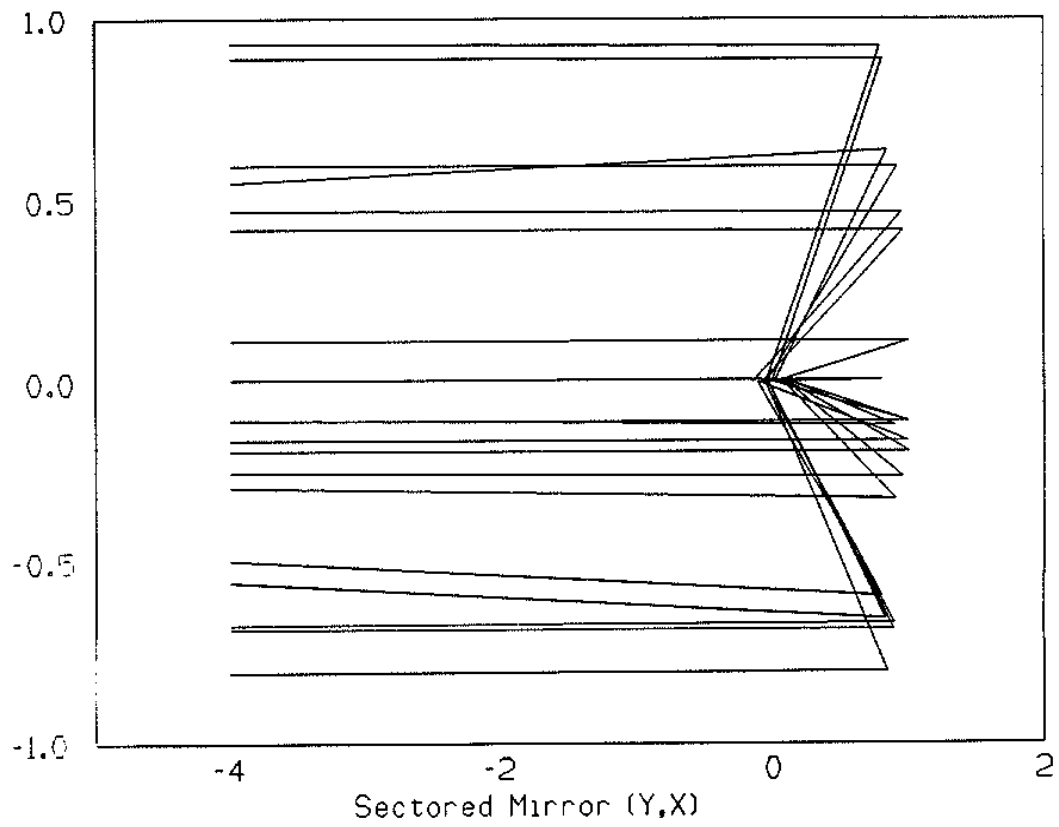Figure 3.52: SECTOR: Side view of resulting system

Figure 3.53: SECTOR: Top view

```
Central Axis parameters :
Source Plane Distance                    1.000000000000000
Image  Plane                             5.000000000000000
Incidence Angle                          0.0000000000000000E+00
Reflection/Diffraction Angle             0.0000000000000000E+00


Mirror parameters                  COMPUTED
Same configuration as Central Axis   YES
Objective focus at                       1.000000000000000
Image focus at                           5.000000000000000
Incidence angle                          0.0000000000000000E+00
Parameters used follow:
   Parabola Param.    2.000000000000000
Source of this O.E. moved            NO
Mirror at pole position ( no mov. )  YES
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```
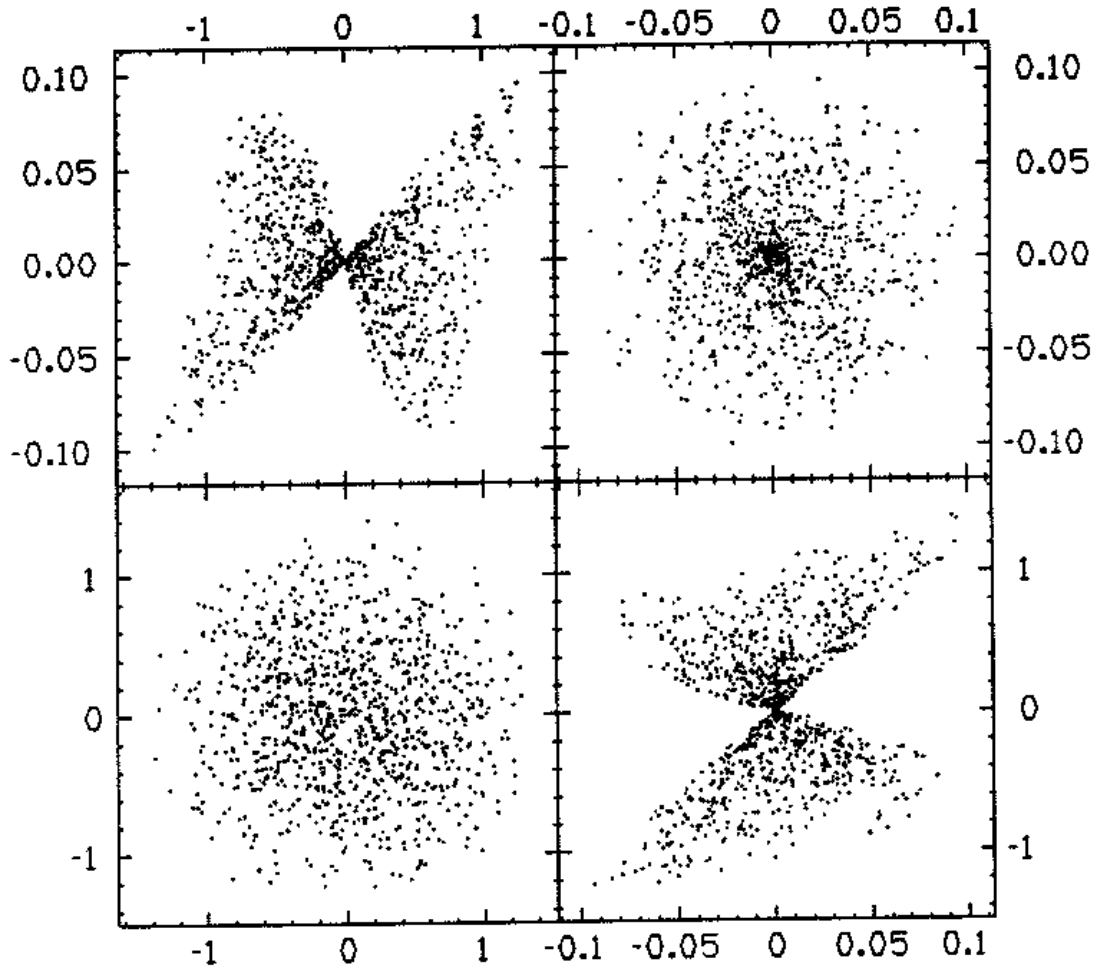
Figure 3.54: SECTOR: PLOTSPACE of full parabolical mirror
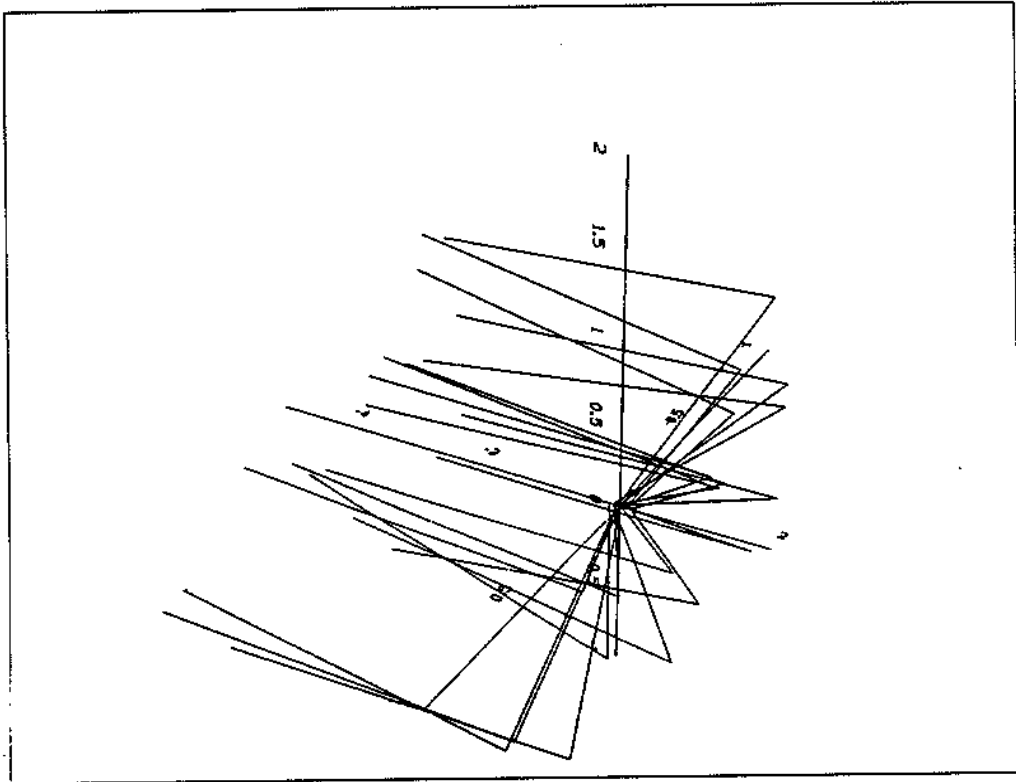
Parabolical Mirror

Figure 3.55: SECTOR: System in 3-D

Figure 3.56: SECTOR: Top view
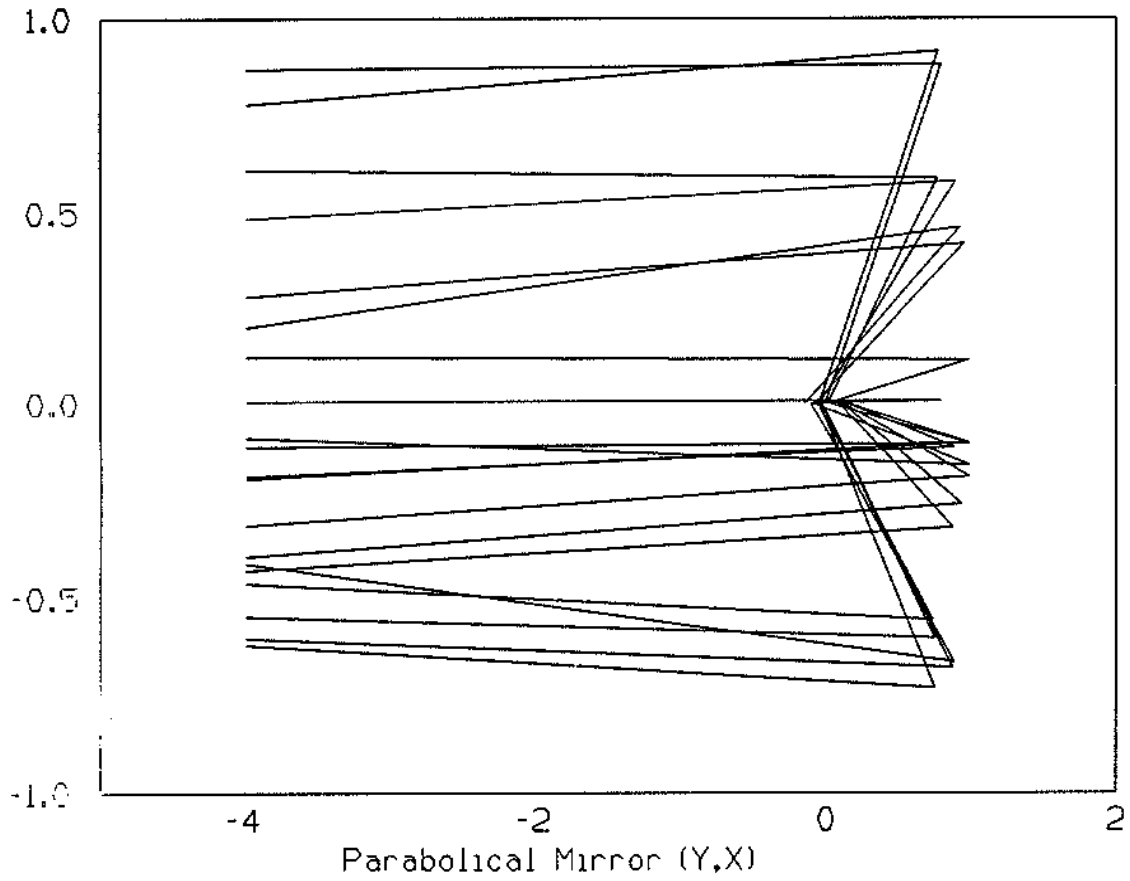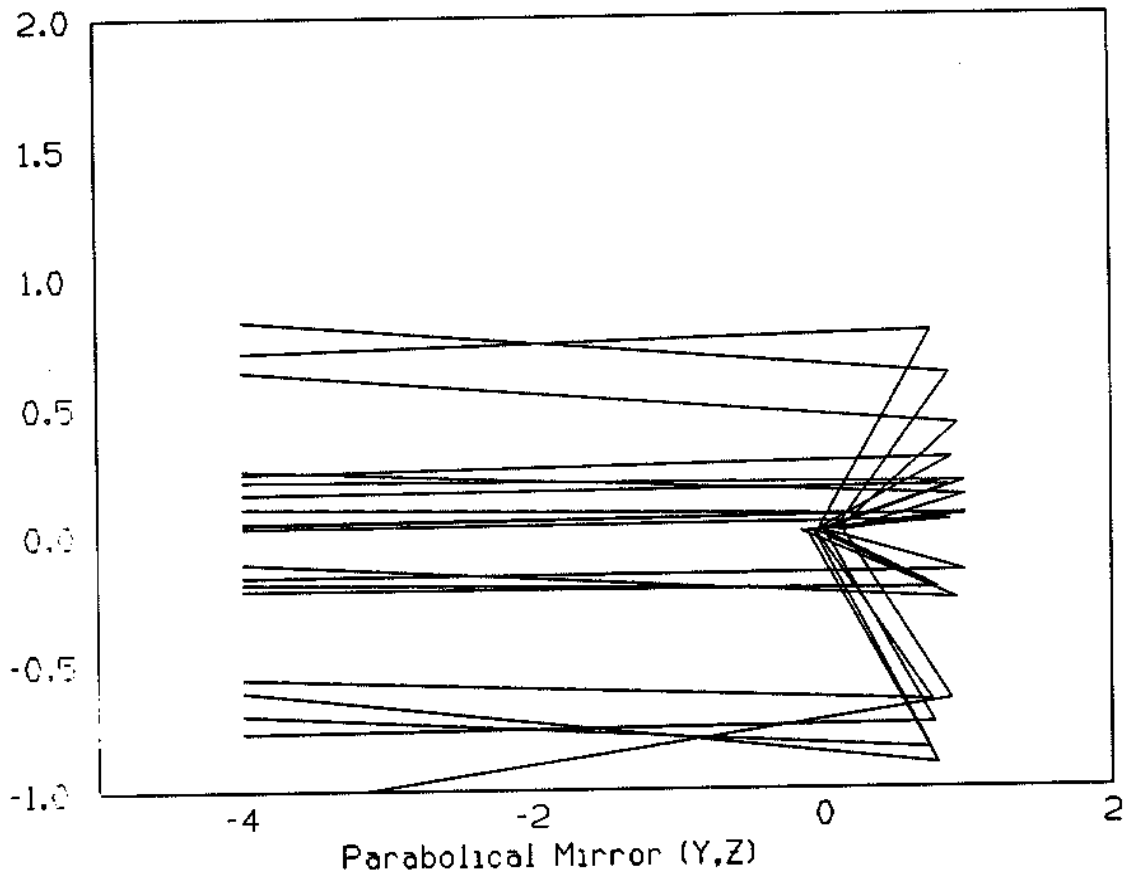
Figure 3.57: SECTOR: Side view

SLITS

Purpose:	To study the resolving power (resolution) of monochromators.
Input:	The ray files where the entrance and exit slits will be positioned, along with the maximum and minimum slit sizes, and number of steps for each slit.
Output:	A file containing energy and lost ray statistics for each combination of entrance and exit slit width.

Description:

SLITS will aid the user in determining the performance of a monochromator i.e., its resolution. The program answers the basic question of "what is the <u>resolution</u> of the real system for given slit settings?".

The program is based on the following algorithm: Given two ray files located at the entrance and exit slit positions (e.g. STAR.xx or SCREEN.xxyy),the program sets the width of the entrance slit and then computes the number of rays that are transmitted for a given exit slit setting. From that, the transmitted photon energy distribution (i.e., bandwidth or resolution) is easily computed. The setting of the exit slit is then modified, and the process is repeated to show the trends in the resolution. After the computations have been performed for all exit slit settings, the entrance slit is modified, and the entire process is repeated.

The entrance slit should be set to an opening that brackets the source image. Ideally, the optical system must be designed to relay an image of the source consistent with the required resolution. For example, let us consider a grating in a Rowland geometry. A line source will have a resolution limited by the spherical aberration of the grating. This means that the overall resolution will not be affected too much by the entrance slit size. The image will be (figuratively speaking):

$$\Delta_{image} = \Delta_{source} + \Delta_{aberr}$$

SLITS allows one to easily assess these terms by changing Δ_{source} and studying the effects on Δ_{image}.

The following steps must be taken by the user before running SLITS:

1. All limiting apertures between the desired entrance and exit slit should be turned off in the system. This includes slits at continuation planes and screens.

2. The source should have a continuous energy range. The extent of the range may be varied according to the number of rays lost at the exit slit: if more than 70 percent of rays are lost for the widest slit use a narrower distribution. The energy range may be easily changed with the utility RECOLOR.

3. The system must be retraced after the slits are removed and for each redefinition of the source energy

The output from SLITS is arranged in rows. Each row presents the statistics for each combination of slit openings. The entries are in the order: Entrance slit width, Exit slit width, Minimum energy passing through exit slit, Maximum transmitted energy, Mean transmitted energy, standard deviation of transmitted energy, number of transmitted rays, and average intensity of the electric field (maximum intensity = 1).

Perhaps the most useful information is the standard deviation and the number of good rays, for these provide luminosity and resolution of the monochromator. The slit widths are varied in increments specified by the user. One of the slits may be held at a constant width to determine the effect of the other slit on the beam as demonstrated in the TGM example below.

After running SLITS, make sure to restore the slits and screens in the system.

Examples:

To start let's run SLITS on a Rowland circle grating found in a 2m Grasshopper.
The system is described below. We run SLITS for six different entrance slit widths through the same range of exit slit widths. We then plot exit slit vs. the standard deviation on energy to show the resolution of the system.

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S O U R C E      D E S C R I P T I O N **************
Source used in SLITS

++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified: end.00
Full file Specification :CXRL$DUA0:[XRAYOP.DOCUMENT.UTIL.SLITS.ROWLAND]END.00;
Creation Date          :25-AUG-1989 16:30
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Random Source.
Generated total        5000 rays.
Source assumed TRIDIMENSIONAL.
Source Spatial Characteristics: GAUSSIAN
Sigma X    :   0.600000000E-01 Sigma Z   :   0.100000000E-01
Depth:  SYNCHROTRON SOURCE.
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: SYNCHROTRON
```

```
Distribution Limits. +X :    0.120000000E-01 -X:   0.120000000E-01 rad
                      +Z :    0.200000000E-02 -Z:   0.200000000E-02 rad
Magnetic Radius =     2.08330000       m.  Beam Energy =  0.80000      GeV.
Beam Emittancies. EPSI_X:   0.000000000E+00 EPSI_Z:   0.000000000E+00
Distance from Waist.   X:   0.000000000E+00      Z:   0.000000000E+00
Polarization Used: SR TOTAL
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: BOX DISTR.
From Photon Energy:    450.000000     or    27.5522667     Angs.
 to  Photon Energy:    550.000000     or    22.5427636     Angs.
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************              E N D                 ***************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
********************   MIRROR  DESCRIPTION   ********************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Rowland mount grating used in SLITS Example


++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :CXRL$DUA0:[XRAYOP.DOCUMENT.SLITS.ROWLAND]END.01;
Creation Date          :25-AUG-1989 15:14
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


Surface figure was defined as:        SPHERICAL
Cylindrical figure                    NO
Element type                          REFLECTOR
Element type                          GRATING
Order choosen ( inside are < 0 )       -1.000000000000000
Automatic Tuning                      YES
Mount                                 Const. INCIDENCE
Grating tuned at  [ eV ]               500.0000000000000
Constant ruling [ lines/cm ]           12000.00000000000
Reflectivity                          OFF
Mirror dimensions                     UNLIMITED
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                         6.978000000000000
Image  Plane                                  25.32000000000000
```

```
 Incidence Angle                              88.00000000000000
 Reflection/Diffraction Angle                 85.14710385779864

 Mirror parameters                    EXTERNAL
 Parameters used follow:
 Spherical Radius                     200.000000
 Source of this O.E. moved            NO
 Mirror at pole position ( no mov. )  YES
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

$ slits
Entrance slit file : begin.dat
Exit slit file     : star.01
Units : [ 0 ]  eV
        [ 1 ]  Angstroms
        [ 2 ]  cm-1
Then ? 0
So far we are working with :
  Total number of rays          =          5000
  Number of rays transmitted    =          5000
  Intensity of transmitted rays =    5000.000000000000
Maximum entrance slit width : 0.4
Minimum entrance slit width : 0.4
No. of points : 1
Maximum exit slit width : 0.3
Minimum exit slit width : 0.001
No. of points : 101
Output file : slits.dat
$ type slits.dat

   \* EnS          ExS         Min NRG       Max NRG       Mean NRG      std. dev

 0.40000E+00  0.30000E+00  0.45001E+03  0.54997E+03  0.49729E+03  0.28377E+02
#good rays  Avg reflectivity *\
 4994        0.10000E+01


 0.40000E+00  0.29701E+00  0.45001E+03  0.54997E+03  0.49729E+03  0.28377E+02
 4994   0.10000E+01
```

```
 0.40000E+00  0.29402E+00  0.45001E+03  0.54997E+03  0.49730E+03  0.28373E+0
 4993  0.10000E+01


    ...           ...          ...          ...          ...          ...
 $
```

Let's now look at the TGM to determine appropriate values for the entrance and exit slits. The slits are located at the image continuation planes of the first and second OE. We will run SLITS two times: first to determine the width of the entrance slit that begins to limit the divergence of the incoming rays; then with the threshold value of the entrance slit we will look at the resolution (standard deviation of the energy) as the exit slit width varies.

```
$ slits
Entrance slit file :
tgm:star.01
Exit slit file    :
tgm:star.02
Units : [ 0 ]  eV
        [ 1 ]  Angstroms
        [ 2 ]  cm-1
Then ?
0
So far we are working with :
  Total number of rays        =         1000
  Number of rays transmitted    =          927
  Intensity of transmitted rays =    450.9344767072463
Maximum entrance slit width :
.5
Minimum entrance slit width :
.025
No. of points :
20
Maximum exit slit width :
1
Minimum exit slit width :
1
No. of points :
1
```
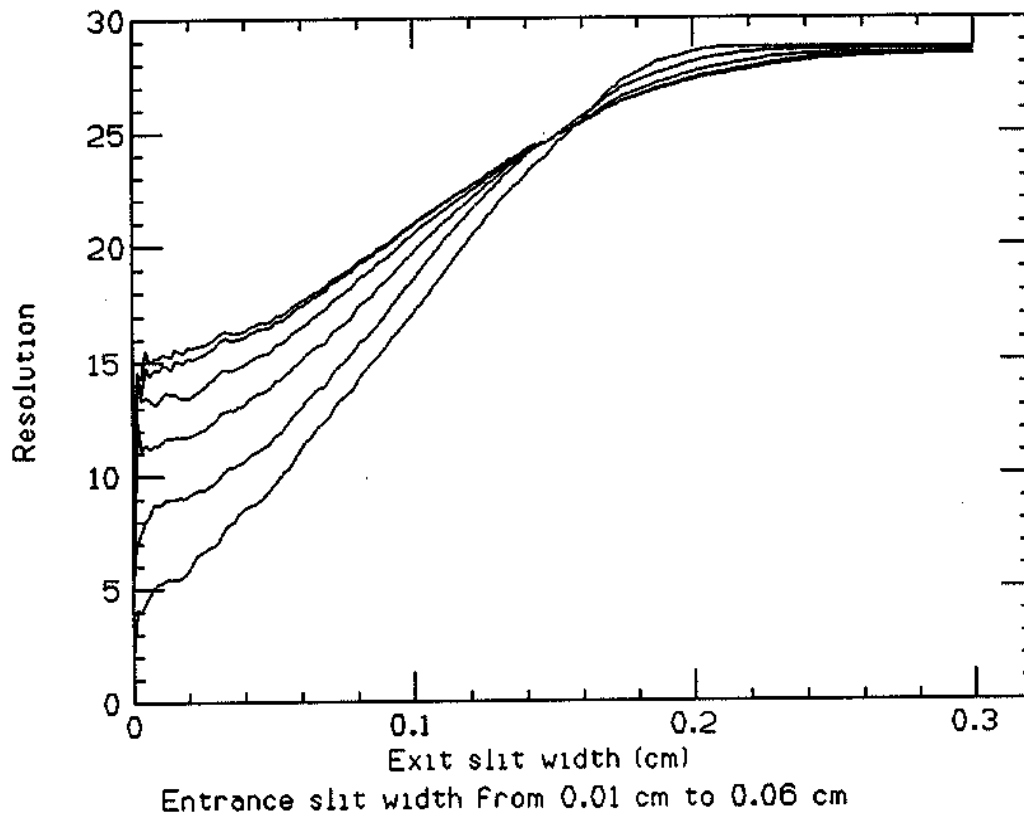
Figure 3.58: SLITS: Resolution of Rowland circle grating
Notice the saturation of the resolution
for large entrance slit sizes.

```
Output file :
entrance.dat
$
$ ty entrance.dat
 0.5000000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.4750000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.4500000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.4250000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.4000000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.3750000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.3500000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.3250000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.3000000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.2750000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.2500000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.2250000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.2000000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.1750000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.1500000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.1250000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 0.1000000        1.000000        49.60062        50.39836        50.00345
 0.2290445             927  0.4864450
 7.5000003E-02    1.000000        49.60062        50.39836        50.00284
 0.2289153             925  0.4864450
```

```
  5.0000001E-02    1.000000          49.60062          50.39836          50.00109
  0.2284425                   905  0.4864449
  2.5000000E-02    1.000000          49.60107          50.39836          50.00358
  0.2327612                   679  0.4864448
```

Notice that the rays start to be limited by the slit at a width of 0.075cm. We will then use 0.1 cm as our entrance slit width. Any source that has a larger divergence will then be limited to that of the current source (4 mrad in the z direction).

```
$ slits
Entrance slit file :
tgm:star.01
Exit slit file     :
tgm:star.02
Units : [ 0 ]  eV
        [ 1 ]  Angstroms
        [ 2 ]  cm-1
Then ?
0
So far we are working with :
  Total number of rays          =          1000
  Number of rays transmitted    =           927
  Intensity of transmitted rays =    450.9344767072463
Maximum entrance slit width :
.1
Minimum entrance slit width :
.1
No. of points :
1
Maximum exit slit width :
1
Minimum exit slit width :
.05
No. of points :
20
Output file :
exit.dat
```

Now we can look at the energy range for the various exit slit widths:
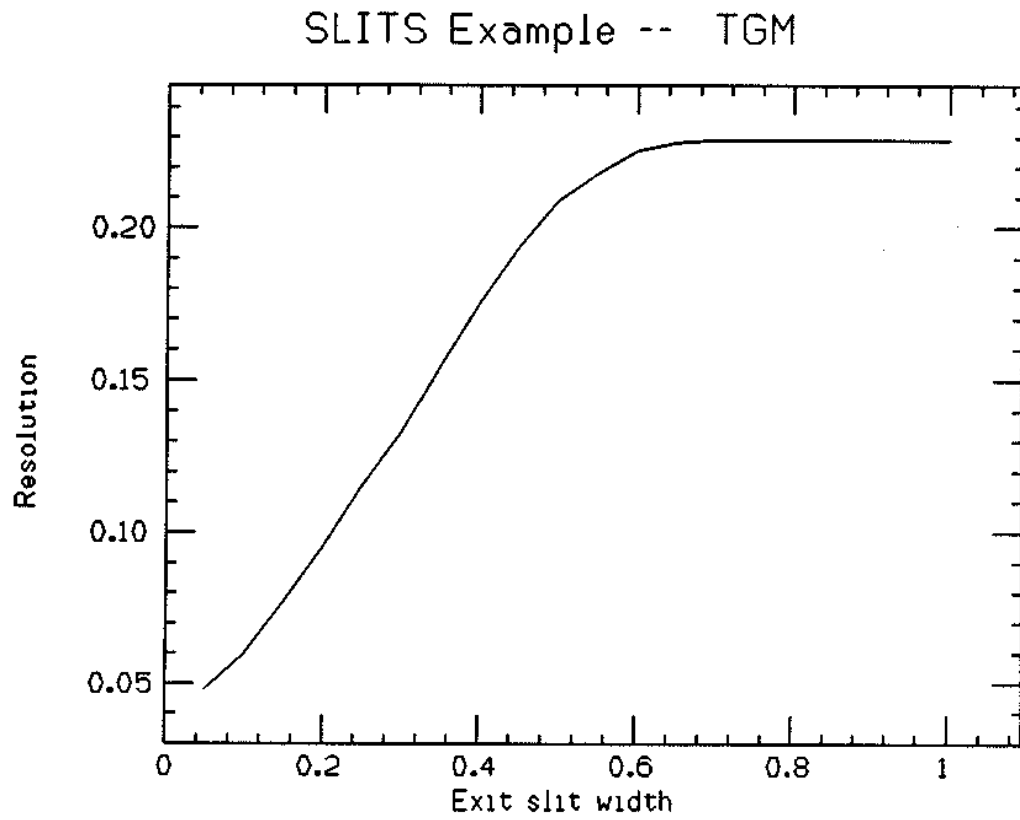
Figure 3.59: TGM SLITS example

Chapter 4

Macros

The programs are defined as macros because they are command files rather than straight executables. They generally call other programs. The functions of the programs in this category are not neccesarily similar; MAKE_ID is basically a preprocessor, MAKE_PWR is a postprocessor.

MAKE_ID

Purpose:	To prepare the files describing an insertion device for use by SHADOW. Includes wigglers and transverse undulators.
Input:	From terminal.
Output:	Files for SHADOW to use to define the source.

Description:

MAKE_ID generates the insertion device parameters for both the wiggler source and the undulator source. For both sources, the *single electron* trajectory is generated. The program then splits to compute the photon radiation depending on the insertion device desired.

Undulator:
Since no simple scaling relations exist for an undulator, the photon distribution is function of $(\hbar\omega, \theta, \phi)$ where θ and ϕ are the polar and azimuthal angles respectively referred to the SOURCE Y-axis (foreward direction). Thus the distribution must be recomputed every time the photon energy range or the polar angle range is changed (ϕ is always taken from 0 to 2π), even though the physical parameters of the undulator are the same.

This process makes the undulator calculation very computer time-consuming, so we limit the $(\hbar\omega, \theta, \phi)$ array to a maximum size of (51,31,31). If the user is only looking at the peak of a harmonic, $\approx$ 5 array points in ω is sufficient (at least 2 points are needed for the interpolation scheme to work). For a good description of an entire harmonic, $\approx$ 10 to 20 points should be used to cover the wider energy range. Finally to cover more than one harmonic, the full 51 points should be used. For the angular part, we recommend using the (31,31) points whenever possible. This is especially true for the θ array because it has more structures, while the features are usually not as sharp in the azmuthal ϕ direction.

For the Undulator Radiation part, the user can choose between entering the parameters from terminal (TT:) or a namelist file. At the end of each run a namelist file called UP-HOT.PAR is always created; this can be used (ITER must be reset to 0 though, see Appendix in User's Guide on User's Program) by the user if he needs to run the program again. For the first pass, one must use the interactive process. We provide a general purpose program to compute the undulator radiation distribution, which is sufficient for most cases; but the user can use his own program if he finds our program insufficient for his needs (see Appendix in User's Guide on User's Program).

To make better use of the array $(\hbar\omega, \theta, \phi)$, the variables are not equally spaced; rather they are put where there are more photons. This involves computing the angular "rings" at each energy for the first pass, and what we call the optimization for the latter passes. At

the end of the first pass, we know the approximate photon distribution. The optimization process then comes in: it finds out where there are higher emission of photons according to the existing distribution, relocates the array points in ($\hbar\omega$, θ, ϕ), and then recomputes the entire photon distribution for the new array using either the radiation program we provided or the User's Program. The upper and lower limits on the three variables are of course unchanged. This procedure can be repeated as many time as needed, we do it four times for the example. The angular patterns as a result of each optimization are shown here as X'-Z' plots. We note that the overall features are fairly evident even before optimization, while the plot after the last optimization looks more realistic. So the last distribution (stored in CDF100.DAT;5) should be used in subsequent ray tracing. A warning here about artifact: a higher amount of rays may be generated between the rings due to the linear interpolation scheme used[1].

The essential output of MAKE_ID is in CDF100.DAT (CDF100.DAT;1 is before optimization, CDF100.DAT;5 after fourth optimization). It contains the integrated probability distribution function (CDF) ready as input to SOURCE. An unintegrated version is found in RN100.DAT:*. They are both unformatted files and use exactly the same format. For SOURCE, we select a zero emittance source. Since the photon energy and the angle range are already pre-determined by MAKE_ID, there is no need to specify them in SOURCE.

Wiggler:

For insertion devices with large K, SHADOW uses the wiggler source. It basically assumes incoherent emission processes, thus the wiggler can be approximated by bending magnets of changing magnetic radius. Then the task is divided into computing: a) electron trajectory, b) photon radiation. They are both computed by MAKE_ID which must be called before running SOURCE.

The correction field factor is used to adjust the end magnetic fields so there is smooth transition in and out of the wiggler. Typically, 101 points is sufficient to describe the trajectory of *each period*. The output of this first part is in WIGGLER.PAR and WIGGLER.TRAJ. The first file simply stores the parameters for the trajectory, while the second file stores the actual trajectory in the following format:

$$
\begin{array}{ccc}
X & Y & Z \\
\beta_x & \beta_y & 1/R
\end{array}
$$

where (X,Y,Z) is the usual SOURCE reference frame, β=v/c, R the instanteous radius of curvature. They are both formatted files and metric units (meter) are used.

The second part uses the trajectory file (WIGGLER.TRAJ) from the first part and computes the radiation at each point, within the photon energy range specified by the user. The out-

---

[1]This part of the code is under intensive development and interested users should contact us for the latest version.

put file (RADIAT.DAT) then stores the CDF of photon emission along the wiggler in binary form ready for input to SOURCE. Note that the highest critical energy λ_c is determined by the smallest radius of curvature.

Examples:

In the example below, we take an undulator of λ = 3.5cm, K=1.87, E=1.3GeV (as suitable for an undulator on SSRL). The correction field factor modifies the magnetic fields at the two ends so that the electron trajectory transits smoothly in and out of the undulator. 101 points are used for each period. That fully defines the trajectory, whose parameters are stored in the file SSRL.PAR and the trajectory itself in SSRL.TRAJ. An optional plottable file SSRL.PLOT is also created for demonstration, which is a formatted 5 columns file in $(X,\beta_x,Y,1-\beta_y,t)$ where (X,Y,Z) is the usual SOURCE coordinates, β is v/c, and t the time. The computation uses metric units and are equally spaced in the Y-axis.

In this example we are centered at the peak of the first harmonic, so 7 points in energy are enough. From the parameters of the trajectory file we note that the first harmonic is at 166.81 eV, and so we take the range from 166.6 to 166.9 eV which is still narrower then the width for a 100 periods undulator. For θ we go from 0 to 1.0 mrad. Now the calculation is fully defined which involves 6727 (7x31x31) points, and the user can tell our program to update on the screen whenever it finishes every 20 or 50 points.

```
 $
 $ MAKE_ID

 ----------------------------------------------------------------------

 Type of Insertion Device.
 Enter:
 for wiggler    (large K)       [ 1 ]
 for undulator (small K)        [ 2 ]
 Then ?   2

 ----------------------------------------------------------------------


 Define Insertion Device parameters:

       wavelength of insertion device (m) :   0.035
       deflection parameter K :   1.87
       correction field factor (=1) :   1.0
```

```
        electron energy (GeV) :   1.3
        Enter the number of points to be used in the  trajectory calculation.
        ( max = 1001, suggested 101 ) :   101


    -----------------------------------------------------------------------


    Two files will be created. One will contain a  record of the parameters used
    in the calculation, the other the trajectory itself. The names of the files
    can be specified by the user, e.g., MYFILE.PAR and MYFILE.TRJ.

    Output files specification:

        Name for parameter file:  SSRL.PAR
        Name for UNDULATOR trajectory file:  SSRL.TRAJ
        Do you want a plottable file [ Y/N ] ?  Y
        Name for plottable file:  SSRL.PLOT

    -----------------------------------------------------------------------



    Calculation Completed. File out results.



    -----------------------------------------------------------------------



    Files:

    SSRL.TRAJ
    SSRL.PAR
    SSRL.PLOT

    Written to disk.

    -----------------------------------------------------------------------

    All Done. Trajectory computed and stored on Disk.
```

```
********************** UNDULATOR RADIATION **********************


Parameters from :
User interactive process   (0)
NAMELIST file   (1)
Choice :  0
Computation done by :
      supplied program       (0)
      user's program         (1)
Choice :  0


----------------------------------------------------------------



Define Radiation Computational parameters:

Polar coordinate is used here.
Number of points in energy (51 max) :  7
                   theta (31 max) :  31
                     phi (31 max) :  31


----------------------------------------------------------------

----------------------------------------------------------------


    Enter name of trajectory file from EPATH  (input ) : SSRL.TRAJ


----------------------------------------------------------------


Undulator case.
Trajectory computed by EPATH with following parameters:

Number of points        :        101
Undulator wavelength    :  3.5000000000000000E-02meters
Deflection parameter    :  1.870000000000000
Peak magnetic field     : 0.5722597698020819    tesla
Electron energy         :  1.300000000000000    GeV
Gamma       :   2543.735230444036
******
Fundamental energy      :  166.8162940850640    eV
```

```
Fundamental wavelength :    74.33307164977071     Angstrom
******


-------------------------------------------------------------------------
 Parameters for Radiation Computation.
Please note value of first harmonic from above table.

  Enter number of periods:  100
        spectrum starting energy [ eV ] :  166.6
                final          [ eV ] :  166.9
        electron current       [ A ] :  1.0
Maximum angle between radiation and undulator axis [ mrad ]:  1.0


All undulator parameters defined.
How many times of optimization ?   4
How often do you want a report on calculations ?
E.G., 20, 50,... ?   4500


-------------------------------------------------------------------------

\\ First pass (before optimization):  \\

-------------------------------------------------------------------------



Begin calculations.



Phi / Horz:  Theta / Vert : Energy:        CPU Time:       % Completed:

 0.209E-03    0.917E-03      167.          290.            66.89


-------------------------------------------------------------------------

Spectra Computations completed.

Total CPU time used so far:    435.5199794769287
CPU time per point:   6.4742081087695661E-02
```

```
------------------------------------------------------------------------

Calculation completed.
------------------------------------------------------------------------


------------------------------------------------------------------------

Begin computation of total power.
Total Power emitted in the specified angles is:
0.1967898468476837
Watts.

Preliminary calculations completed.

Number of optimization finished :             0

Do you want to write out spectra ?  1
Name of file for storing spectra:  RN100.DAT
Do you want to create a SHADOW file ?  1
Name of (binary) file for SHADOW:  CDF100.DAT
File name for parameter info :  UNDULATOR.PAR
------------------------------------------------------------------------

Files:
UNDULATOR.PAR
RN100.DAT
CDF100.DAT
written to disk.
------------------------------------------------------------------------


------------------------------------------------------------------------

\\ First optimization :  \\

------------------------------------------------------------------------


Begin calculations.
```

```
Phi / Horz:   Theta / Vert : Energy:        CPU Time:      % Completed:

 0.209E-03   0.921E-03       167.           280.             66.89

---------------------------------------------------------------------


---------------------------------------------------------------------


Begin calculations.


Phi / Horz:   Theta / Vert : Energy:        CPU Time:      % Completed:

 0.209E-03   0.804E-03       167.           283.             66.89

---------------------------------------------------------------------


---------------------------------------------------------------------


Begin calculations.


Phi / Horz:   Theta / Vert : Energy:        CPU Time:      % Completed:

 0.209E-03   0.804E-03       167.           283.             66.89

---------------------------------------------------------------------

Spectra Computations completed.

Total CPU time used so far:   425.2399902343750
CPU time per point:   6.3213912625891927E-02
```

```
-------------------------------------------------------------------------

Calculation completed.
-------------------------------------------------------------------------


-------------------------------------------------------------------------

Begin computation of total power.
Total Power emitted in the specified angles is:
0.2482396424982191
Watts.

Preliminary calculations completed.

Number of optimization finished :            1

Do you want to write out spectra ?  1
Name of file for storing spectra:  RN100.DAT
Do you want to create a SHADOW file ?  1
Name of (binary) file for SHADOW:  CDF100.DAT
File name for parameter info :   UNDULATOR.PAR
-------------------------------------------------------------------------

Files:
UNDULATOR.PAR
RN100.DAT
CDF100.DAT
written to disk.
-------------------------------------------------------------------------


-------------------------------------------------------------------------

\\ Second optimization :  \\

-------------------------------------------------------------------------


Begin calculations.
```

```
Phi / Horz:   Theta / Vert : Energy:        CPU Time:       % Completed:

 0.209E-03    0.921E-03       167.            292.              66.89

------------------------------------------------------------------------


------------------------------------------------------------------------


Begin calculations.


Phi / Horz:   Theta / Vert : Energy:        CPU Time:       % Completed:

 0.209E-03    0.661E-03       167.            285.              66.89

------------------------------------------------------------------------


------------------------------------------------------------------------


Begin calculations.


Phi / Horz:   Theta / Vert : Energy:        CPU Time:       % Completed:

 0.209E-03    0.661E-03       167.            284.              66.89

------------------------------------------------------------------------

Spectra Computations completed.

Total CPU time used so far:    428.3701171875000
```

```
CPU time per point:    6.3679220631410733E-02

-------------------------------------------------------------------

Calculation completed.
-------------------------------------------------------------------


-------------------------------------------------------------------

Begin computation of total power.
Total Power emitted in the specified angles is:
0.2960115135632488
Watts.

Preliminary calculations completed.

Number of optimization finished :              2

Do you want to write out spectra ?  1
Name of file for storing spectra:  RN100.DAT
Do you want to create a SHADOW file ?  1
Name of (binary) file for SHADOW:  CDF100.DAT
File name for parameter info :  UNDULATOR.PAR
-------------------------------------------------------------------

Files:
UNDULATOR.PAR
RN100.DAT
CDF100.DAT
written to disk.
-------------------------------------------------------------------


-------------------------------------------------------------------

\\ Third optimization :  \\

-------------------------------------------------------------------
```

```
Begin calculations.


Phi / Horz:   Theta / Vert : Energy:        CPU Time:      % Completed:

 0.209E-03    0.690E-03       167.            286.            66.89

-----------------------------------------------------------------------


-----------------------------------------------------------------------


Begin calculations.


Phi / Horz:   Theta / Vert : Energy:        CPU Time:      % Completed:

 0.209E-03    0.653E-03       167.            285.            66.89

-----------------------------------------------------------------------


-----------------------------------------------------------------------


Begin calculations.


Phi / Horz:   Theta / Vert : Energy:        CPU Time:      % Completed:

 0.209E-03    0.653E-03       167.            286.            66.89

-----------------------------------------------------------------------

Spectra Computations completed.
```

```
Total CPU time used so far:    430.8698730468750
CPU time per point:   6.4050821026739259E-02


-----------------------------------------------------------------------


Calculation completed.
-----------------------------------------------------------------------


-----------------------------------------------------------------------


Begin computation of total power.
Total Power emitted in the specified angles is:
0.2668414494602727
Watts.


Preliminary calculations completed.


Number of optimization finished :             3


Do you want to write out spectra ?  1
Name of file for storing spectra:  RN100.DAT
Do you want to create a SHADOW file ?  1
Name of (binary) file for SHADOW:  CDF100.DAT
File name for parameter info :  UNDULATOR.PAR
-----------------------------------------------------------------------


Files:
UNDULATOR.PAR
RN100.DAT
CDF100.DAT
written to disk.
-----------------------------------------------------------------------


-----------------------------------------------------------------------


\\ Fourth optimization :  \\


-----------------------------------------------------------------------
```

Begin calculations.

```
Phi / Horz:   Theta / Vert : Energy:        CPU Time:        % Completed:

 0.209E-03   0.921E-03       167.           283.             66.89
```

Begin calculations.

```
Phi / Horz:   Theta / Vert : Energy:        CPU Time:        % Completed:

 0.209E-03   0.851E-03       167.           287.             66.89
```

Begin calculations.

```
Phi / Horz:   Theta / Vert : Energy:        CPU Time:        % Completed:

 0.209E-03   0.851E-03       167.           287.             66.89
```

Spectra Computations completed.

```
Total CPU time used so far:    430.2602539062500
CPU time per point:   6.3960198291400327E-02


--------------------------------------------------------------------

Calculation completed.
--------------------------------------------------------------------


--------------------------------------------------------------------

Begin computation of total power.
Total Power emitted in the specified angles is:
0.2533485171223082
Watts.

Preliminary calculations completed.

Number of optimization finished :              4

Do you want to write out spectra ?  1
Name of file for storing spectra:  RN100.DAT
Do you want to create a SHADOW file ?  1
Name of (binary) file for SHADOW:  CDF100.DAT
File name for parameter info :  UNDULATOR.PAR
--------------------------------------------------------------------

Files:
UNDULATOR.PAR
RN100.DAT
CDF100.DAT
written to disk.
--------------------------------------------------------------------

FORTRAN STOP
$
$ DIR

Directory DEVEL:[MAXIMUM.FRANCO.FRINGE.DEMO]
```

```
CDF100.DAT;5              324  13-MAR-1989 23:31  (RE,RWED,RE,RE)
CDF100.DAT;4              324  13-MAR-1989 23:03  (RE,RWED,RE,RE)
CDF100.DAT;3              324  13-MAR-1989 22:33  (RE,RWED,RE,RE)
CDF100.DAT;2              324  13-MAR-1989 21:59  (RE,RWED,RE,RE)
CDF100.DAT;1              324  13-MAR-1989 21:33  (RE,RWED,RE,RE)
RN100.DAT;5              324  13-MAR-1989 23:31  (RE,RWED,RE,RE)
RN100.DAT;4              324  13-MAR-1989 23:03  (RE,RWED,RE,RE)
RN100.DAT;3              324  13-MAR-1989 22:33  (RE,RWED,RE,RE)
RN100.DAT;2              324  13-MAR-1989 21:59  (RE,RWED,RE,RE)
RN100.DAT;1              324  13-MAR-1989 21:32  (RE,RWED,RE,RE)
SSRL.PAR;1                2  13-MAR-1989 21:20  (RE,RWED,RE,RE)
SSRL.PLOT;1               21  13-MAR-1989 21:21  (RE,RWED,RE,RE)
SSRL.TRAJ;1               16  13-MAR-1989 21:21  (RE,RWED,RE,RE)
UNDULATOR.PAR;5            4  13-MAR-1989 23:31  (RE,RWED,RE,RE)
UNDULATOR.PAR;4            4  13-MAR-1989 23:03  (RE,RWED,RE,RE)
UNDULATOR.PAR;3            4  13-MAR-1989 22:33  (RE,RWED,RE,RE)
UNDULATOR.PAR;2            4  13-MAR-1989 21:59  (RE,RWED,RE,RE)
UNDULATOR.PAR;1            4  13-MAR-1989 21:33  (RE,RWED,RE,RE)
UPHOT.DAT;13            320  13-MAR-1989 23:20  (RE,RWED,RE,RE)
UPHOT.PAR;13             2  13-MAR-1989 23:20  (RE,RWED,RE,RE)


Total of 20 files, 3621 blocks.
$
\\ SSRL.PAR is the parameters file from trajectory calculation. \\

$
$ TY SSRL.PAR
Parameters used for run creating
UNDULATOR case. Trajectory stored in:
SSRL.TRAJ
and in (formatted file):
SSRL.PLOT
The UNDULATOR case uses 1 period only.
------   INPUT    ---------
Insertion device  Wavel. [ m ] =   3.5000000000000000E-02
Beam Energy          [ GeV ] =   1.300000000000000
K                            =   1.870000000000000
Field correction factor      =   1.000000000000000
------   OUTPUT   ---------
Gamma                        =   2543.735230444036
```

```
Peak Magnetic field   [ Tesla ] =    0.5722597698020819
Fundamental               [ Ev ] =    166.8162940850640
Fundamental      [ Angstroms ] =    74.33307164977071
Equivalent SR C.W.     [ Angs ] =    19.23237966486749
            C.E.       [ eV ] =    644.6690537546344
$
\\ SSRL.PLOT is the plottable file of the trajectory.  The first 3 points
\\ are shown.  \\


$
$ TY SSRL.PLOT
0.000000000000E+00  0.677626357803E-20 -0.211243686708E-01  0.772727220405E
0.297898968623E-09  0.211239131844E-05 -0.207018812973E-01  0.772749531308E
0.237647068755E-08  0.842528581107E-05 -0.202793939239E-01  0.773082147604E
       :                    :                   :                      :
$
\\UNDULATOR.PAR is the parameter file from the radiation part.  \\


$
$ TY UNDULATOR.PAR

-------------------------------------------

Trajectory computed by EPATH with following     parameters:
Number of points :           101
Wavelen. (und)   :    3.5000000000000000E-02 meters
Fundamental wvl  :    74.33307164977071     angstroms
Fund.    energy  :    166.8162940850640     eV
K is             :    1.870000000000000
Gamma            :    2543.735230444036
Beta0            :    0.9999999227272780    C units
Field B0         :    0.5722597698020819    tesla
Electron energy  :    1.300000000000000     GeV

-------------------------------------------

Read          101 trajectory records from SSRL.TRAJ
Number periods used in ERAD:          100
Total power radiated in the limits [ W ]:   1.8898209057174996E-04
```

```
-------------------------------------------

Working with constant dE (units eV) .
Energy interval =   0.0000000000000000E+00
Limits:    166.6000000000000         166.9000000000000
Step  :   0.0000000000000000E+00 Number of points:           7

-------------------------------------------

POLAR ANGLES CHOSEN
Azimutal angle (units rad) .
Limits:   0.0000000000000000E+00  1.5707963267948966E-03
Step  :   0.0000000000000000E+00 Number of points:          31

-------------------------------------------

Polar angle (units mrad) .
Limits:   0.0000000000000000E+00   1.000000000000000
Step  :   0.0000000000000000E+00 Number of points:          31
Spectra written into (binary) file:
RN100.DAT
in units: PHOTONS/SEC/eV/RAD**2

-------------------------------------------


-------------------------------------------
$
\\ UPHOT.PAR is a namelist file generated at the end of each optimization.\\

$
$ TY UPHOT.PAR
$PARAIN
NCOMP   =          100,
RCURR   =   1.000000000000000    ,
ICOMP   =            1,
BPASS   =   0.0000000000000000E+00,
IANGLE  =            1,
IAPERTURE       =           2,
IEXTERNAL       =           0,
```

```
FOUT    = '
',
FIN     = '
',
FTRAJ   = 'SSRL.TRAJ
          ',
EMIN    =    166.6000000000000      ,
EMAX    =    166.9000000000000      ,
THEMIN  =  0.0000000000000000E+00,
THEMAX  =  9.9999999999999999E-04,
PHIMIN  =  0.0000000000000000E+00,
PHIMAX  =  1.5707963267948966E+00,
NE      =             7,
NT      =            31,
NP      =            31,
NCHECK  =          4500,
IOPT    =             4,
ITER    =             4,
IPASS   =             0
$END
```

Shown below are the plots from the first pass and the subsequent optimizations.

D13:[XRAYOP.DOCUMENT.SOURCE.UNDULATOR]BEGIN.DAT:2   15-MAR-1989 18:10

Zero optimization

15-MAR-89 18:31:24

H Length	0.24000E-02
H center	0.00000E+00
V Length	0.24000E-02
V center	0.00000E+00

EXTERNAL

--GOOD ONLY

TOT	=	2500
LOST	=	0

Horizontal:	4
Vertical:	6
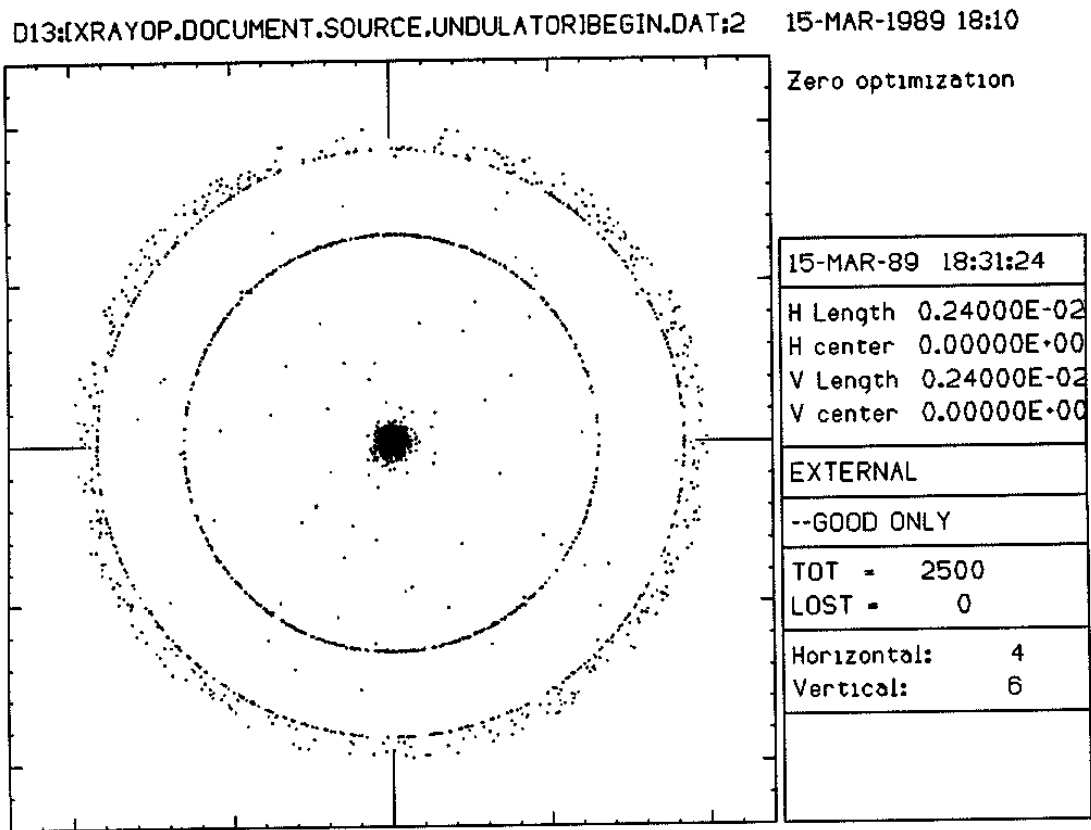
Figure 4.1: MAKE_ID: Before optimization

D13:[XRAYOP.DOCUMENT.SOURCE.UNDULATOR]BEGIN.DAT;3   15-MAR-1989 18:35

First optimization

15-MAR-89 18:36:08

H Length 0.24000E-02
H center 0.00000E+00
V Length 0.24000E-02
V center 0.00000E+00

EXTERNAL

--GOOD ONLY

TOT =   2500
LOST =   0

Horizontal: 4
Vertical: 6
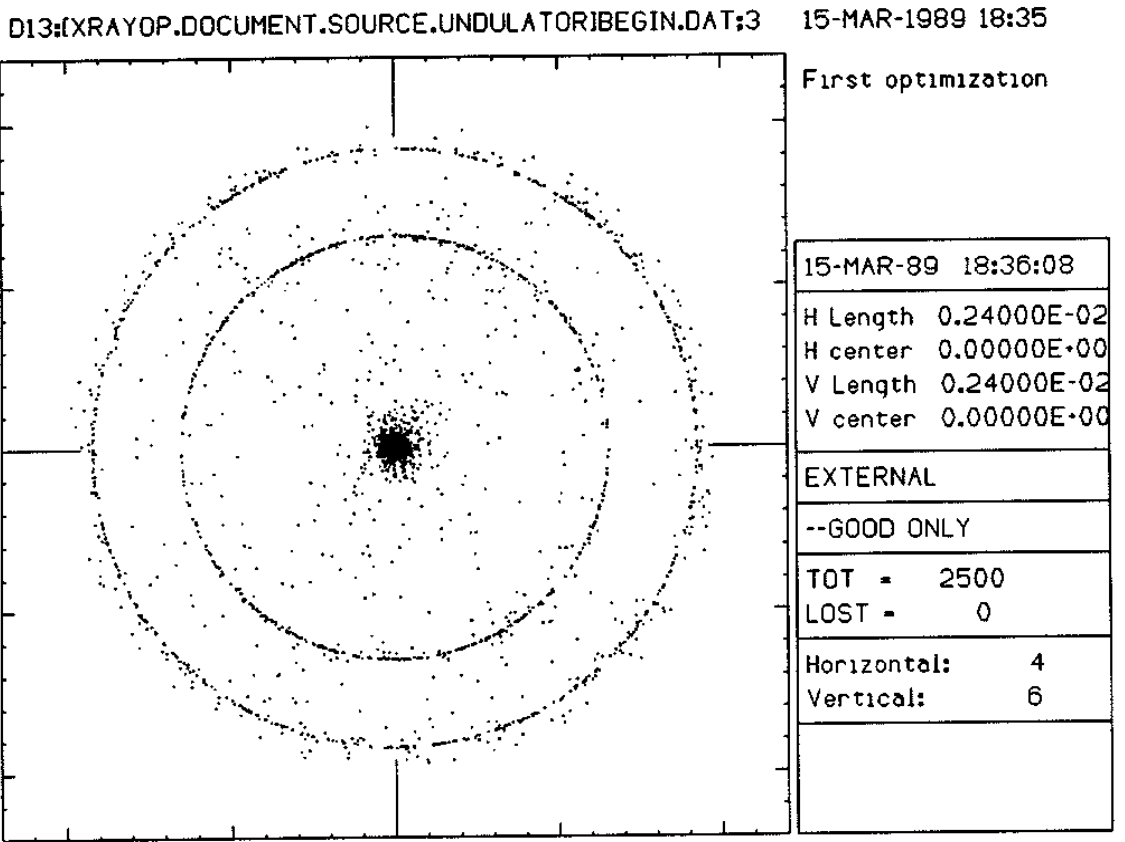
Figure 4.2: MAKE_ID: After first pass

D13:[XRAYOP.DOCUMENT.SOURCE.UNDULATOR]BEGIN.DAT:4   15-MAR-1989 18:36

Second optimization

| 15-MAR-89 18:37:26 |
| H Length   0.24000E-02 |
| H center   0.00000E+00 |
| V Length   0.24000E-02 |
| V center   0.00000E+00 |
| EXTERNAL |
| --GOOD ONLY |
| TOT =   2500 |
| LOST =   0 |
| Horizontal: 4 |
| Vertical: 6 |
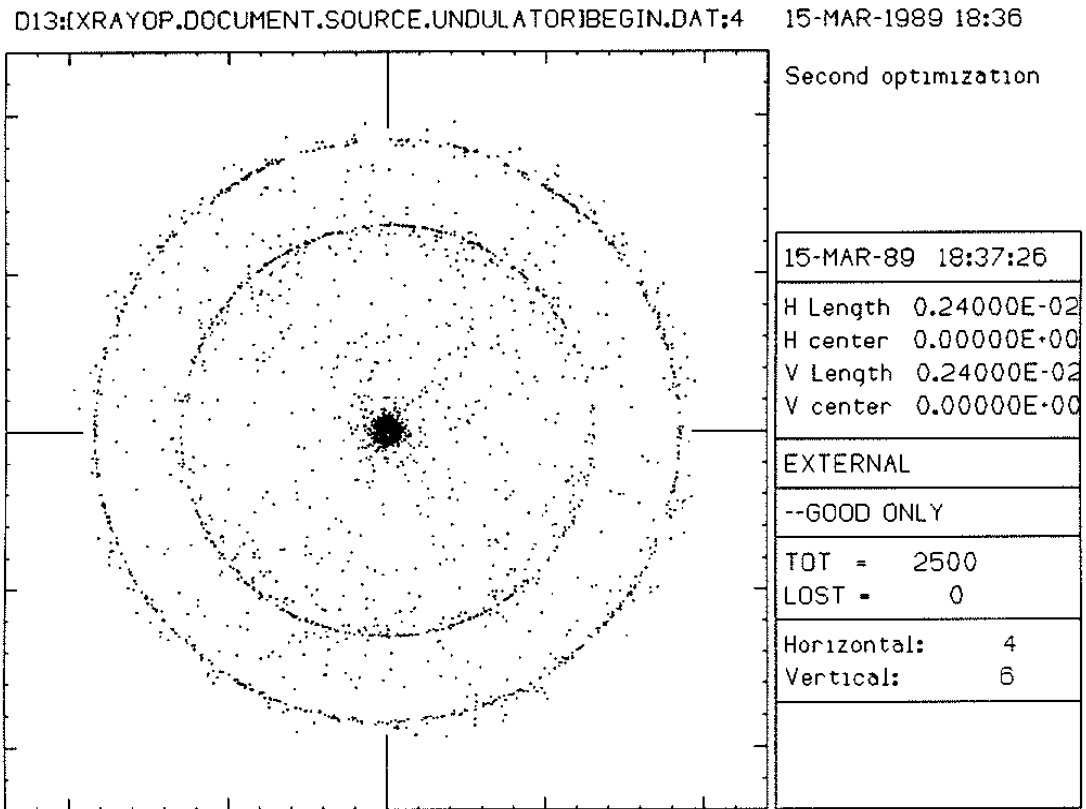
Figure 4.3: MAKE_ID: After second pass

D13:[XRAYOP.DOCUMENT.SOURCE.UNDULATOR]BEGIN.DAT;5   15-MAR-1989 18:37

Third optimization

15-MAR-89 18:38:38

H Length	0.24000E-02
H center	0.00000E+00
V Length	0.24000E-02
V center	0.00000E+00

EXTERNAL

--GOOD ONLY

TOT =	2500
LOST =	0

Horizontal:	4
Vertical:	6
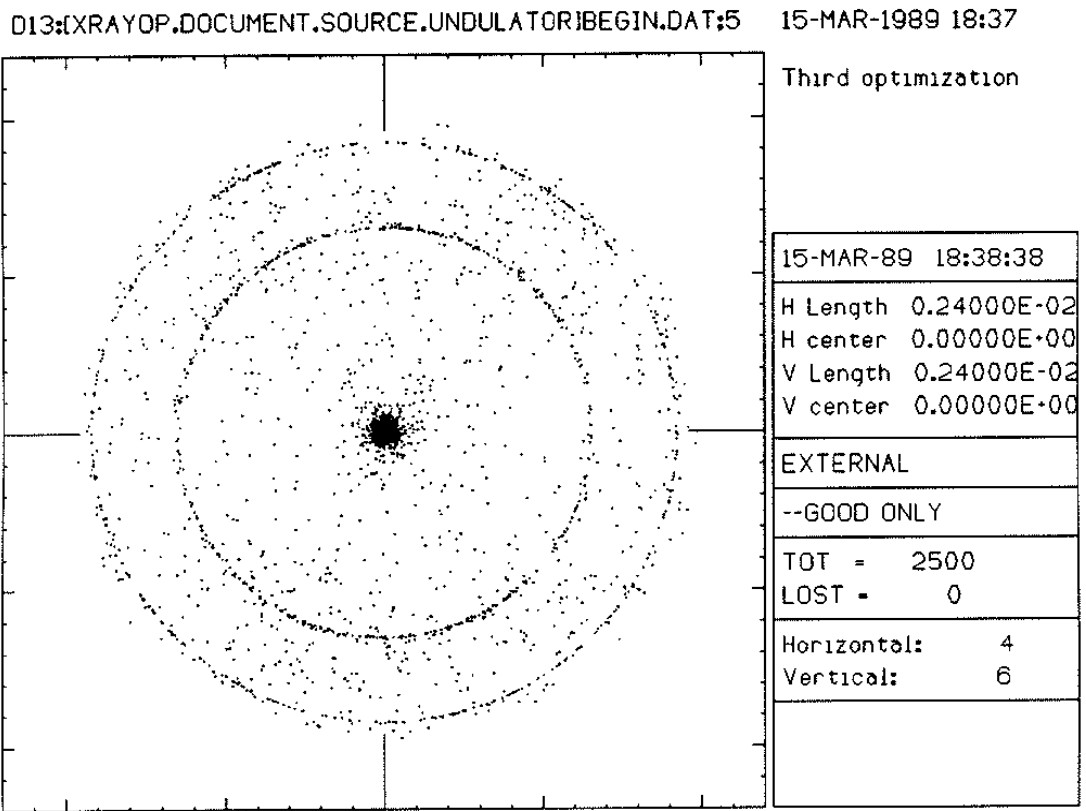
Figure 4.4: MAKE_ID: After third pass
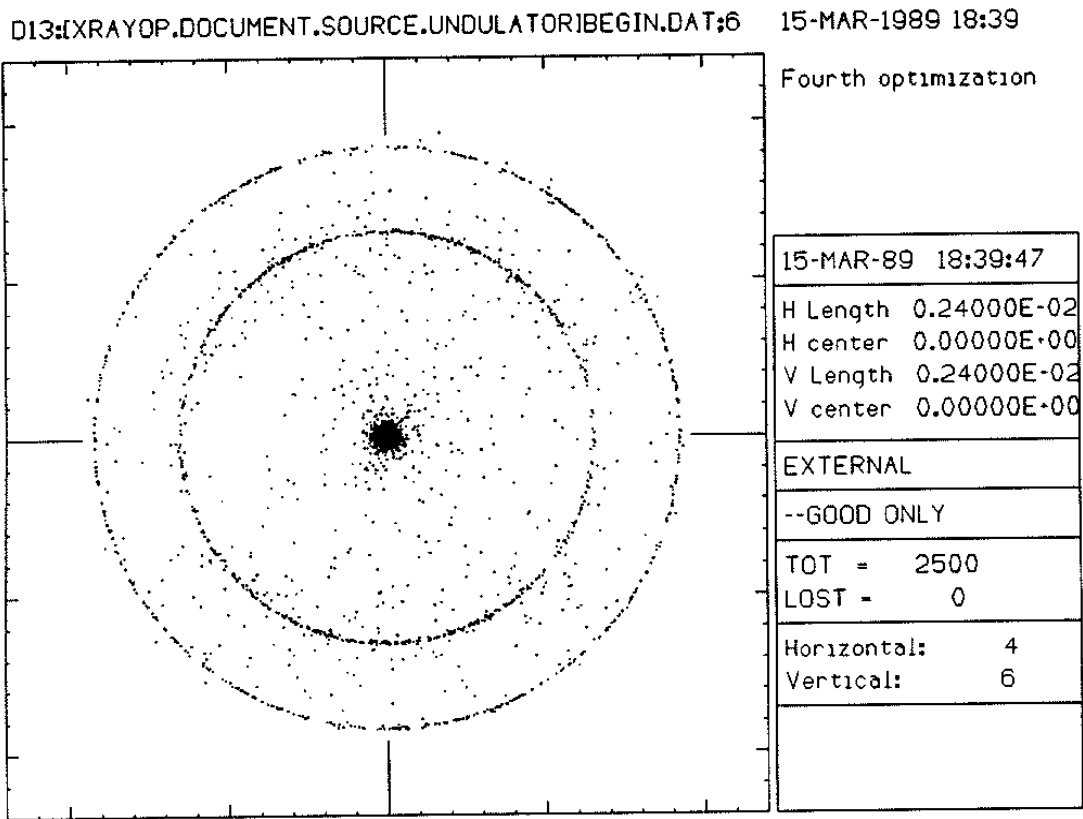
Figure 4.5: MAKE_ID: After fourth pass

Wiggler Example:
This example illustrates how to generate a wiggler source with the following parameters:
N=10 periods, λ=10 cm, K=14.94, E=1 GeV. For the SOURCE part, we use finite emittance
to demonstrate its effects which can be seen at both the top view and cross view. The
electrons come to a waist at the middle of the wiggler, as we have specified in SOURCE.
Most photons are clearly generated near turning points, thus giving rise to the two loops
seen when viewing the wiggler head on. Note the entire wiggler is offset to the positive
x-axis. The photon energy range, on the other hand, is taken from MAKE_ID (1-100 eV).

```
$
$ MAKE_ID


-----------------------------------------------------------------------


Type of Insertion Device.
Enter:
for wiggler   (large K)      [ 1 ]
for undulator (small K)      [ 2 ]
Then ?  1


-----------------------------------------------------------------------



Define Insertion Device parameters:

Enter number of periods :  10
      wavelength of insertion device (m) :  0.1
      deflection parameter K :  14.94
      correction field factor (=1) :  1.0
      electron energy (GeV) :  1.0
      Enter the number of points to be used in the  trajectory calculation.
      ( max = 1001, suggested 101 ) :  101


----------------------------------------------------------------------

 Two files will be created. One will contain a  record of the parameters use
 in the calculation, the other the trajectory itself. The names of the files
 can be specified by the user, e.g., MYFILE.PAR and MYFILE.TRJ.

 Output files specification:
```

```
        Name for parameter file:  WIGGLER.PAR
        Name for WIGGLER trajectory file:  WIGGLER.TRAJ


----------------------------------------------------------------------


Trajectory Calculations begins.


Calculation Completed. File out results.


----------------------------------------------------------------------


Files:

WIGGLER.TRAJ


*********************** WIGGLER RADIATION ***********************

Name of input file :
WIGGLER.TRAJ
Read           1001 points from input file.
Beam energy (GeV) =    1.000000000174087
Radius of curvature (max.) =   6.2266522507136881E+16 m
                   (min.) =     2.084481700350993     m
Critical Energy (max.) =    1063.821612058376     eV
               (min.) =   3.5613305408526866E-14 eV
Initial photon energy [ eV ] :  1
Final photon energy [ eV ]   :  100
Name of output file :  RADIAT.DAT
Total no.of photons =   1.7399069816581998E+16
$
$ DIR

Directory DEVEL:[MAXIMUM.FRANCO.FRINGE.WIGGLER]
```

```
RADIAT.DAT;1                  87  13-MAR-1989 22:19  (RE,RWED,RE,RE)
WIGGLER.PAR;1                   2  13-MAR-1989 22:15  (RE,RWED,RE,RE)
WIGGLER.TRAJ;1                290  13-MAR-1989 22:15  (RE,RWED,RE,RE)

Total of 3 files, 379 blocks.
$
$ TY WIGGLER.PAR \\ Parameter file. \\
Parameters used for run creating
WIGGLER case. Trajectory stored in:
WIGGLER.TRAJ
Number of periods                =          10
------   INPUT     ---------
Insertion device  Wavel. [ m ] =   0.1000000000000000
Beam Energy            [ GeV ] =   1.000000000000000
K                               =   14.94000000000000
Field correction factor         =   1.000000000000000
------   OUTPUT    ---------
Gamma                           =   1956.719408033874
Peak Magnetic field   [ Tesla ] =   1.600185121255940
Fundamental             [ Ev ] =   0.8432615847877075
Fundamental      [ Angstroms ] =   14704.76986532713
Equivalent SR C.W.    [ Angs ] =   11.62365513397686
            C.E.       [ eV ] =   1066.662754279258

$
\\ WIGGLER.TRAJ is the actual trajectory.  The first three points are liste
$
$ TY WIGGLER.TRAJ
 0.0000000000000000E+00 -0.5000000000000000        0.0000000000000000E+00
 0.0000000000000000E+00  0.9999998694090963        0.4797355620016315
 2.3978852546284019E-07 -0.4990000000000000        0.0000000000000000E+00
 4.7941990834775524E-04  0.9999997544873504        0.4787889134551865
 9.5820947756009422E-07 -0.4980000000000000        0.0000000000000000E+00
 9.5694776534338392E-04  0.999994115344188         0.4759527038051818
```
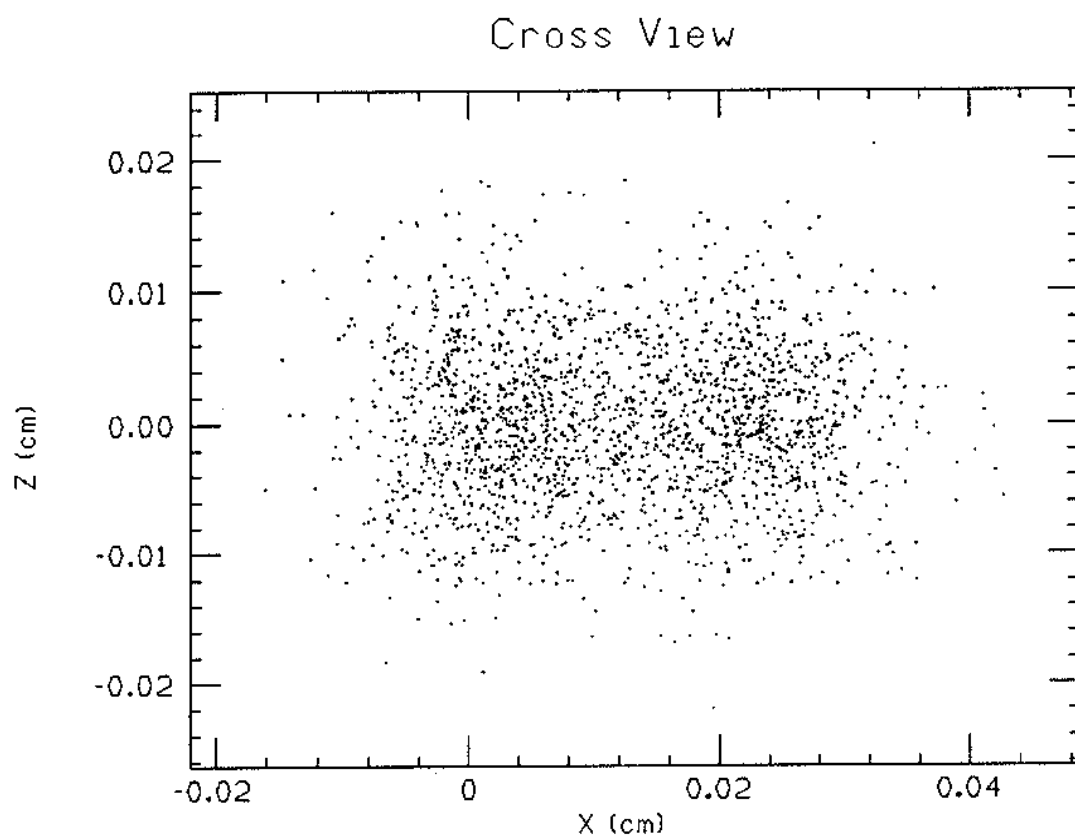
Cross View

Figure 4.6: MAKE_ID: Cross view
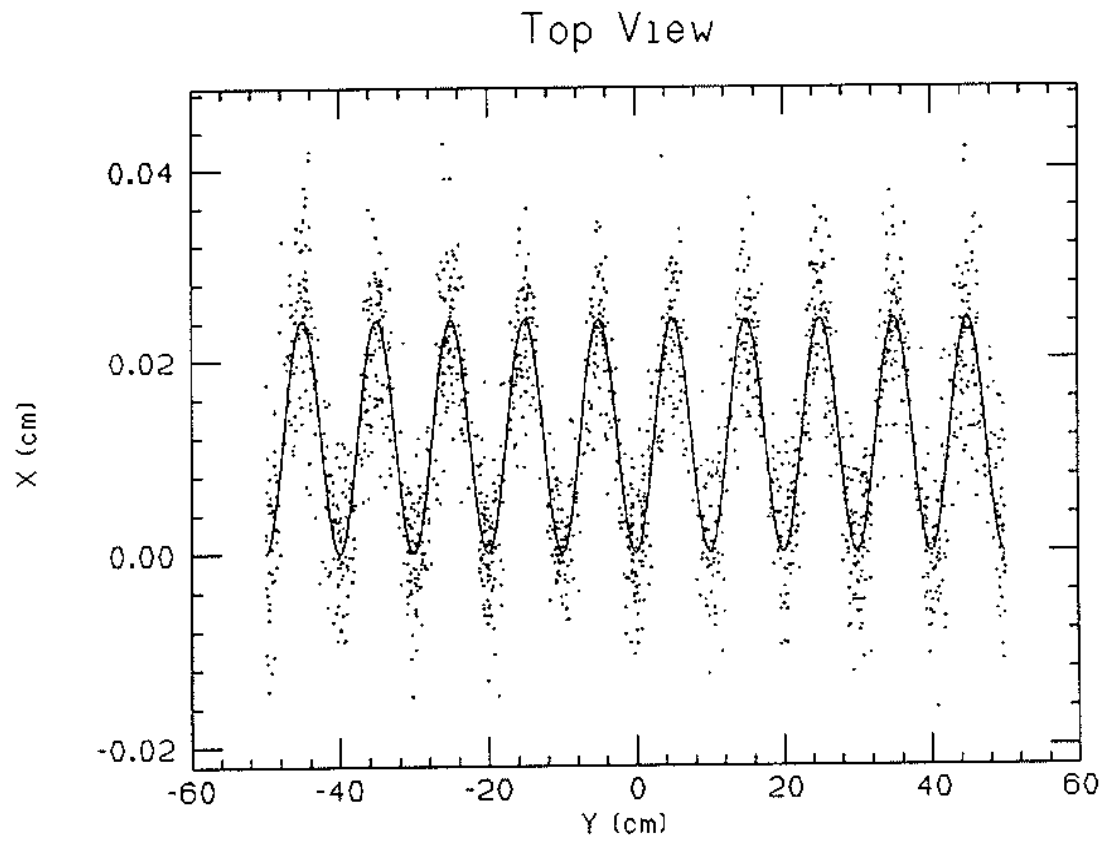
Figure 4.7: MAKE_ID: Top view

MAKE_PWR

Purpose:	To generate a batch command file for power density calculations on a given optical element or elements.
Input:	Mirror file and BEGIN file for element interested in.
Output:	A batch file that when submitted generates two data files and two namelist files for each iteration.

Description:

When computing a two-dimensional power distribution it is essential to accumulate a good statistics in order to have a clean result. This program creates a batch file that, when submitted, runs SHADOW iteratively for a specified number of times; at the same time, the power absorbed is accumulated in a file. At the last iteration a file suitable for input to ANSYS is generated. The batch file purges after every run, leaving the two latest versions. The file before the ANSYS file can be used as input to TopDrawer as well.

Examples:

We have turned on the reflectivities and put a gold coating on the first mirror and the grating of the 6m TGM. We run MAKE_PWR to generate a command file that can be submitted in batch mode. When submitted, the intermediate files are in a generic form of X, Y, power, and counts per bin. The data file generated after the last loop is in a form that can be input to ANSYS for further power analysis. It may be useful to use the LOG option when submitting the batch file so if the job does not terminate correctly, you have some indication of the reason.

```
$ sd [.xrayop.document.tgm]
$ MAKE_PWR
--------------------------------------------------

Name for the batch job [ myjob.com ] ? : MYJOB1.COM  \*command file  *\

How many elements do you want to analyze ? : 2  \* analyze the mirror
                                             \* and grating *\
Defining element: 2                          \* grating *\

Interactive [0] or namelist mode [1] : 0   \* first time must be interactive
```

This program needs a file containing the source spectrum computed within the
limits used. Or you can specify the total power.
Source file [0] or total power [1] : 1   * choose total power *\
Total power in Watt : 100

Please specify now the file containing the SOURCE array (e.g., BEGIN.DAT)
Then ? BEGIN.DAT
Read   5000 rays. The file has   18 columns.
Computing renormalizing factor.

All preliminaries completed.
Ready to proceed with density analysis.

File for analysis ?
MIRR.02   * grating file *\
Data ready. Read   5000 points.
Options --- Enter
0 for excluding the losses
1 for including losses at a particular O.E.
2 for including all the losses.
Then ? 0
****
File examined is :

Was created :

****
Found   4483 good points out of   5000
Found:
Column 1: X max is   2.247921404888549
       1: X min is -2.248152741557152
       2: Y max is   3.733963121236766
       2: Y min is -3.241366038463902
       3: Z max is 5.5920629967978197E-02
       3: Z min is 9.8741963938664412E-07
 for a photon energy range:
  101.074845359784   to   2971.487995770237
I need to define the two-dimensional histogram for the power density. Please
specify:
Columns for x-axis and y-axis?

```
1                                         \* calculate the power on the surface
2                                         \* of the mirror ($X,Y$)            *\
Limits to use for the histogram.
To use          scaling, enter:
      automatic                  0
      external                   1
Then? 0
Number of bins in X [ max 51 ] ? 31     \* odd number of bins works best *\
                Y [ max 51 ] ? 31
Optical Properties options.


To select                           enter

Power transmitted/reflected ........ 0
Power absorbed .................... 1  <<<<
Local reflectivity/transmission .... 2
Incoming Power .................... 3

Then ?
1                                         \* choose power absorbed  *\
File to use for Io ?                      \* source file, i.e. BEGIN.DAT *\
BEGIN.DAT
The program need to know how many iterations have been already performed. En
[ 0 ] if this is the first time.
No. of time this power density case has run : 0
How many times will you be looping through ? 50  \* this number will be ente
                                          \* again, remember it! *\
There were          517 lost out of          5000 rays.
Begin verification.
Total power in file:    83.98999144696705
Compare with:          100.0000000000000
Computations done. Ready to store output data.
The files contain the power density at the nodes but
for the case of ANSYS, that stores total power.
File for:
 TOP DRAWER          [ 0 ]
 NCAR                [ 1 ]
 Generic             [ 2 ] ** to be used for loop
 For ANSYS           [ 3 ]
2                        \* for running more than once, choose generic *\
```

```
Output file ? GRATING        \* file name, no extension *\
All done.


Output file name for this element [ ele1.pwr, ele2.pwr, ... ] ? : ELE2G


Defining element: 1         \* first mirror *\


Interactive [0] or namelist mode [1] : 0
This program needs a file containing the source spectrum computed within the
limits used. Or you can  specify the total power.
Source file [0] or total power [1] : 1
Total power in Watt : 100


Please specify now the file containing the SOURCE array (e.g., BEGIN.DAT)
Then ? BEGIN.DAT
Read          5000 rays. The file has            18 columns.
Computing renormalizing factor.


All preliminaries completed.
Ready to proceed with density analysis.


File for analysis ?
MIRR.01                                          \* mirror file *\
Data ready. Read          5000 points.
Options --- Enter
0 for excluding the losses
1 for including losses at a particular O.E.
2 for including all the losses.
Then ? 0
***********
File examined is :

Was created :

***********
Found          4696 good points out of          5000
Found:
Column 1: X max is   1.999925668739772
       1: X min is  -1.998543900746248
       2: Y max is   3.943993346718717
```

```
      2: Y min is  -4.268345358794168
      3: Z max is  0.1313206504810491
      3: Z min is  6.9529741764107200E-07
 for a photon energy range:
  101.0305579596815      to     2971.487995770237
I need to define the two-dimensional histogram for the power density. Please
specify:
Columns for x-axis and y-axis?
1
2
Limits to use for the histogram.
To use          scaling, enter:
      automatic              0
      external               1
Then? 0
Number of bins in X [ max 51 ] ? 31
               Y [ max 51 ] ? 31
Optical Properties options.


To select                         enter

Power transmitted/reflected ....... 0
Power absorbed .................... 1   <<<
Local reflectivity/transmission .... 2
Incoming Power .................... 3

Then ?
1
File to use for Io ? BEGIN.DAT
The program need to know how many iterations have been already performed. En
[ 0 ] if this is the first time.
No. of time this power density case has run : 0  \* still 0, hasn't finished
How many times will you be looping through ? 50  \* same as before *\
There were          304 lost out of         5000 rays.
Begin verification.
Total power in file:    72.89175060410695
Compare with:          100.0000000000000
Computations done. Ready to store output data.
The files contain the power density at the nodes but
for the case of ANSYS, that stores total power.
```

```
File for:
 TOP DRAWER          [ 0 ]
 NCAR                [ 1 ]
 Generic             [ 2 ] ** to be used for loop
 For ANSYS           [ 3 ]
2
Output file ? MIRROR
All done.


Output file name for this element [ ele1.pwr, ele2.pwr, ... ] ? : ELE1M


----------------------------------------------------


Input completed. Prepare batch file.
Job File name ? MYJOB1.COM            \* same job name as above *\
Command used to define SHADOW environment [ setsha, setup, ... , no $ sign] ?
@[SHADOW]SETUP
Default directory for calculations ? [SHADOW.XRAYOP.DOCUMENT.TGM]
How many OE's in this system ? 2   \* # of OE's for calculations *\
How many loops ? 50               \* same loop number again *\
Read          2 files.


----------------------------------------------------


Batch file ready. Check for the file:
%SHOW-S-NOTRAN, no translation for logical name JOBFILE
in your default directory.
You may use the command:

 $submit/notify/noprinter myjob.com

----------------------------------------------------


$
$ DIR/SINCE

Directory D1:[SHADOW.XRAYOP.DOCUMENT.TGM]

ELE1M.DAT;1               3  31-JUL-1989 10:38:58.42  (RWED,RWED,RE,RE)
ELE2G.DAT;1               3  31-JUL-1989 10:37:28.48  (RWED,RWED,RE,RE)
```

```
GRATING.DAT;1              102  31-JUL-1989 10:37:26.25  (RWED,RWED,RE,RE)
MIRROR.DAT;1              102  31-JUL-1989 10:38:56.16  (RWED,RWED,RE,RE)
MYJOB1.COM;2               2  31-JUL-1989 10:39:35.40  (RWED,RWED,RE,RE)
MYJOB1.COM;1               1  31-JUL-1989 10:36:24.63  (RWED,RWED,RE,RE)

Total of 6 files, 213 blocks.
$
$ TY MYJOB1.COM                    \* job file to be submitted *\
$SET DEFAULT [SHADOW.XRAYOP.DOCUMENT.TGM]
$ASSIGN SYS$COMMAND TT:
$@[SHADOW]SETUP
$YES_TYPE == "SECOND"
$ASSIGN SYS$COMMAND TT:
$PWR_DENS :== RUN UTIL:PWR_DENS
$ASSIGN SYS$COMMAND TT:
$SEED :== RUN UTIL:SEED
$I = 0
$AGAIN:
$GO
SOURCE
BATCH
START.00                          \* if you have renamed the namelist
TRACE                             \* files for your source and system
BATCH                             \* you must edit the command file
0                                 \* and replace the defaults with
START.01                          \* the correct names or rename your
0                                 \* namelist files to START.xx   *\
START.02
0
%EXIT
EXIT
$ASSIGN/USER_MODE ELE2G PWR_DENS_PAR
$PWR_DENS
1
$ASSIGN/USER_MODE ELE1M PWR_DENS_PAR
$PWR_DENS
1
$PURGE/KEEP=2                     \* only two latest versions kept *\
$SEED
START.00                          \* make sure to change name of namelist
```

```
$I = I + 1                                \* file here as well or job will abort. *\
$IF I .EQ.  50 THEN $EXIT
$SHOW SYMBOL I
$GOTO AGAIN
$EXIT
$
$ TY MIRROR.DAT   \* in form of generic file after running MAKE_PWR *\
\*  X              Y              power              # per bin    *\
 -1.9341        -4.1359        0.00000000E+00           0
 -1.9341        -3.8710        0.93015110E-01           2
 -1.9341        -3.6061        0.56923885E-01           2
 -1.9341        -3.3411        0.33663763               1
 -1.9341        -3.0762        0.37450902               4
 -1.9341        -2.8113        0.78836927               5
 -1.9341        -2.5464         1.9283763               10
 -1.9341        -2.2815         4.3062616               12
 -1.9341        -2.0166         3.4735672               11
 -1.9341        -1.7517         6.3110739               8
^Y
$
$ TY GRATING.DAT
\*   X             Y              power              # per bin    *\
 -2.1756        -3.1289        0.00000000E+00           0
 -2.1756        -2.9039        0.00000000E+00           0
 -2.1756        -2.6788        0.00000000E+00           0
 -2.1756        -2.4538        0.00000000E+00           0
 -2.1756        -2.2288        0.00000000E+00           0
 -2.1756        -2.0038        0.00000000E+00           0
 -2.1756        -1.7788        0.00000000E+00           0
 -2.1756        -1.5538        0.00000000E+00           0
 -2.1756        -1.3288        0.00000000E+00           0
 -2.1756        -1.1038        0.00000000E+00           0
^Y
```

After the batch job was completed, the latest generic data files were run through a contouring program. The results were plotted with TopDrawer. The plots show the outline of the mirror and grating and how the power is absorbed on each.
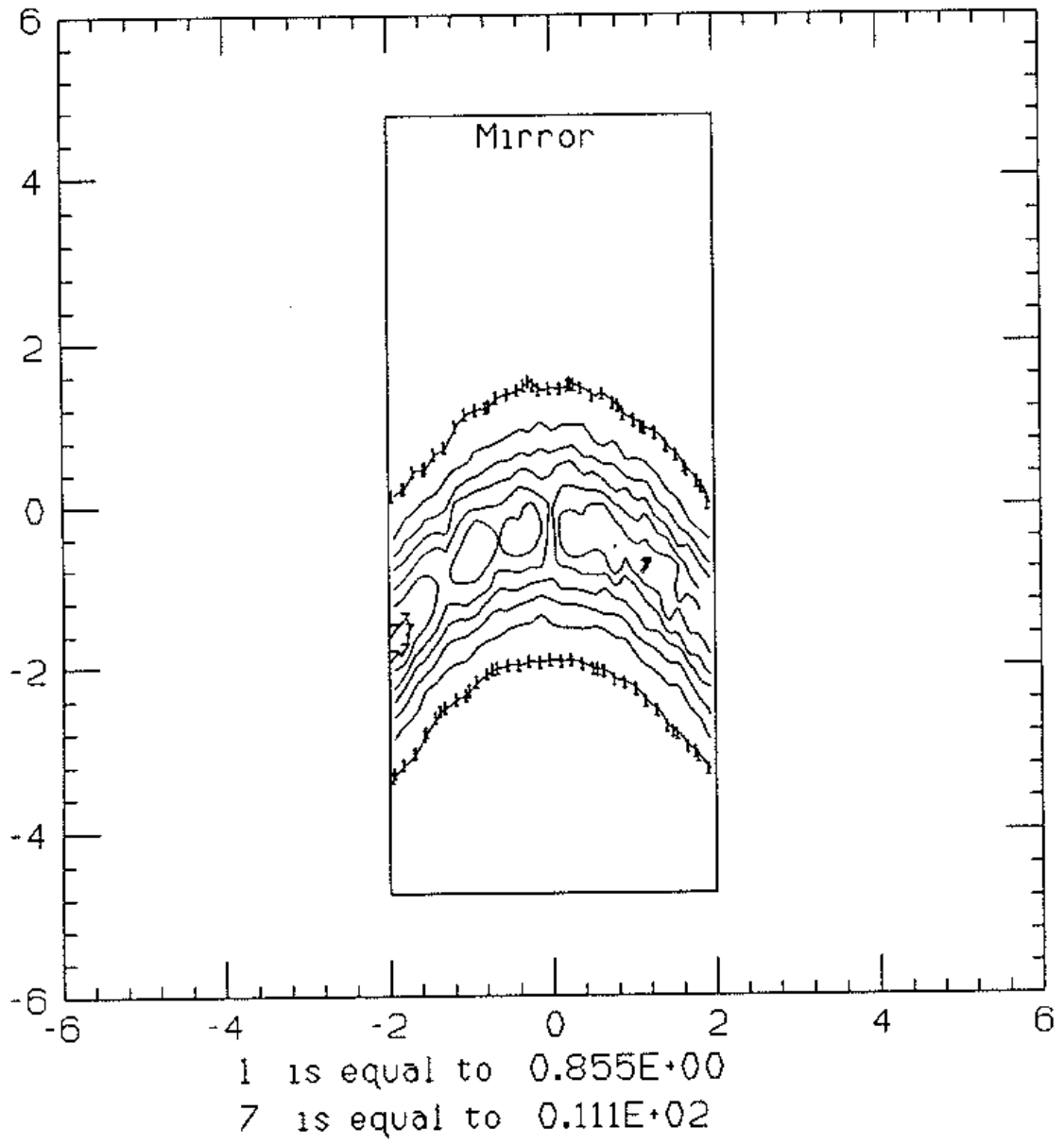
Figure 4.8: MAKE_PWR: Mirror

1 is equal to 0.935E+00
7 is equal to 0.122E+02
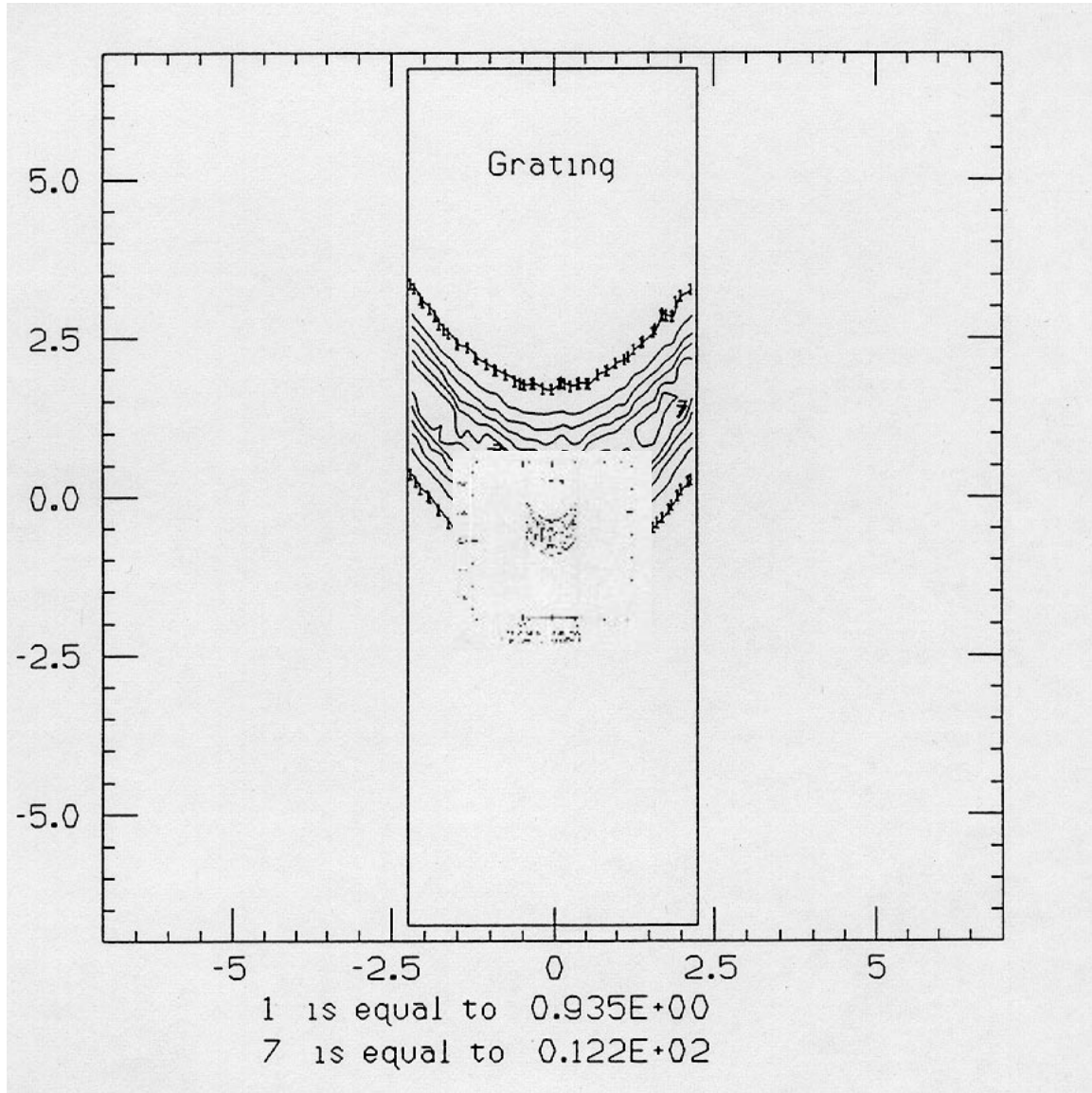
Figure 4.9: MAKE_PWR: Grating

Chapter 5

Optics Utilities

The optical utilities are mainly standalone programs that perform optical calculations that may be of use when running SHADOW. They provide information about element/compound characteristics, grating information, multilayer calculations, synchrotron spectra and the resulting transmission through a system. They do not generate any files that can be input to SHADOW itself, however similar utilities for some exist in Preprocessors. Again we have broken them down into several sections for convienience: Optical properties, sources, and geometrical optics.

ABREFC

Purpose:	Computes several properties of a given material (over a specified photon energy range) that are important for physical optics calculations.
Input:	From terminal:

1. Material Density

2. Material formula

3. Photon range

Output:	ABSOR_COEFF.DAT
	CROSS_SECTION.DAT
	DIELEC_FUNC.DAT
	ELECTRON_YIELD.DAT
	ENERGY_LOSS.DAT
	REFLECTIVITY.DAT
	REFRAC_INDEX.DAT
	TRANSMISSION.DAT

Description:

The program is based on the compilation of atomic scattering factor by B.Henke, with extension to 10,000 by G.Tirsell. We have extended it to 100,000 eV by using the tables from Cromer and Liberman. The division is then:

1. 100-2000 eV, B. L. Henke, P. Lee, T. J. Tanaka, R. Shimabukuro and B. K. Fujikawa, Atom. Data Nucl. Data Tables 27 (1982).

2. 2000-10000 eV, J. M. Auerbach and G. Tirsell, "Software for Reflectivity calculations of X-ray Mirrors", Lawrence Livermore National Labs Report UCRL91230, (1984).

3. 10000-100000 eV, CXrL (S. Sasaki, "Anomolous Scattering Factors for Synchrotron Radiation Users, Calculated using Cromer and Liberman's Method", KEK 83-22, 1984.
   D. T. Cromer and D. Liberman: J. Chem. Physics, **53**, 1891-1898 (1970).
   D. T. Cromer and D. A. Liberman: Acta Crystallog., **A37**, 267-268 (1981).

The program requires no user input beside the knowledge of the material atomic composition and its density. The formulae used are described in detail in B.Henke's article in *Low Energy X-ray Diagnostics* and are valid for the x-ray region.

The program can compute the optical properties of materials containing up to five atomic species. Notice that when specifying the formula the atomic symbols must be capitalized and two-letters long (e.g. SI for silicon and WW for tungsten). Another input parameter needed by the program is the density, ρ, in g/cm^3 of the material.

Finally the program prompts for "Full printout at terminal". If the user answers yes, then all the results are printed to the terminal beside being saved in a file. This is useful only if one is interested in the value at one or two photon energies.

The files are saved with fixed file names. It is a good idea to rename them immediately (e.g REFLECTIVITY.DAT → REFLEC.AU_89) to keep things orderly.

The following properties are computed over the specified photon energy range:

- **Dielectric Function:** The complex dielectric function is computed and stored in a file called DIELEC_FUNC.DAT. The units are in $farad/cm$ and the program stores α, β where:

$$\tilde{\epsilon} = 1 - \alpha + i\beta \qquad (5.1)$$

- **Absorption Coefficient:** Units are in cm^{-1} and the result is stored in the file ABSOR_COEFF.DAT.

- **Transmission:** The transmission through a film of thickness d (as specified by the user):

$$T(\hbar\omega) = e^{-d\,\mu(\hbar\omega)} \qquad (5.2)$$

and is stored in the file TRANSMISSION.DAT.

- **Reflectivity:** The $s-$ and $p-$components of the reflectivity R are computed from the Fresnel equations and the dielectric function as obtained above. The file includes average, $s-$ and $p-$ reflectivities.

- **Refraction Index:** This value is again obtained from the dielectric function above ($n^2 = \epsilon$); only the real part is stored. The complex refractive index is of the form: $1 - \delta - i\beta$. The output is formatted (ANSI).

- **Cross Section:** for photoelectric effect. Obtained directly from f_1, f_2 in cm^2. It is the basic "ingredient" of the absorption coefficient μ.

- **Electron Yield:** as defined by B.Henke. In essence, the primary electron yield is proportional to the square of the electric field at the surface of the material.

- **Energy Loss:** The rate at which energetic electrons lose energy when travelling through a medium is proportional to the imaginary part of the dielectric function.

This is obtained directly from the linear medium response theory in the limit of small q (Raether, 1960),

$$R(\Delta E) = -Im\frac{1}{\epsilon}$$ (5.3)

The files are all in a two or three columns tabular format and can be plotted out using Top-Drawer. It may be a good idea to run CLIP on the files if an error is obtained when running TopDrawer because of possible underflows.

$\boxed{\textbf{Examples:}}$

```
$ abrefc
Full printout at Terminal ?
n                               \* suppresses extra output *\
Thickness (microns) ?
1.0                             \* needed for transmission *\
The program is setup to compute optical constants of
compounds with up to 5 elements.
How many atomic species ?
2                               \* choose a compound *\
H2O would be: HH,2 and OO,1. Then ?
Enter 2-letters (capitalized) atomic symbol and formula index for :     1
SI                              \* silicon *\
1
Enter 2-letters (capitalized) atomic symbol and formula index for :     2
CC                              \* carbon *\
1
Density ?
3.44                            \* g/cm^3 *\
Enter starting photon energy,end and step
200,5000,20                     \* computation range *\
Incidence angle ?
88                              \* for reflectivity *\
Molecular weight is :    40.10000
Atoms/Cm3
 5.1660890E+22  5.1660890E+22  0.0000000E+00  0.0000000E+00  0.0000000E+00
$ dir

Directory D13:[XRAYOP.DOCUMENT.UG.ABREFC]
```

```
ABSOR_COEFF.DAT;1          16  17-JUN-1988 00:06  (RWED,RWED,RE,RE)
CROSS_SECTION.DAT;1
                           16  17-JUN-1988 00:06  (RWED,RWED,RE,RE)
DIELEC_FUNC.DAT;1          23  17-JUN-1988 00:06  (RWED,RWED,RE,RE)
ELECTRON_YIELD.DAT;1
                           16  17-JUN-1988 00:06  (RWED,RWED,RE,RE)
ENERGY_LOSS.DAT;1          16  17-JUN-1988 00:06  (RWED,RWED,RE,RE)
REFLECTIVITY.DAT;1         30  17-JUN-1988 00:06  (RWED,RWED,RE,RE)
REFRAC_INDEX.DAT;1         16  17-JUN-1988 00:06  (RWED,RWED,RE,RE)
TRANSMISSION.DAT;1         16  17-JUN-1988 00:06  (RWED,RWED,RE,RE)

Total of 9 files, 149 blocks.
$
$
$ type absor_coeff.dat               \\ units  are in cm-1
  200.0000        179319.5
  220.0000        148879.4
  240.0000        124486.7
  260.0000        104718.1
  280.0000        88981.34
  300.0000        125351.2
  320.0000        107683.3
  340.0000        93240.84
  360.0000        81363.08
  380.0000        71451.71
  400.0000        63132.95
  420.0000        56095.28
  440.0000        50092.01
  460.0000        44927.46
  480.0000        40454.81
  500.0000        36563.99
  520.0000        33177.92
  540.0000        30197.32
  560.0000        27553.70
     .....          ....
$
$
$ t cross_section.dat                \\ cm^2
  200.0000     3.4710877E-18
  220.0000     2.8818582E-18
```

```
    240.0000        2.4096892E-18
    260.0000        2.0270288E-18
    280.0000        1.7224119E-18
    300.0000        2.4264235E-18
    320.0000        2.0844250E-18
    340.0000        1.8048632E-18
    360.0000        1.5749454E-18
    380.0000        1.3830910E-18
    400.0000        1.2220647E-18
    420.0000        1.0858365E-18
    440.0000        9.6963125E-19
    460.0000        8.6966089E-19
      .....           ......
$
$ type dielec_func.dat

    photon            real           imaginary
    energy            part             part

   200.0000      2.3322932E-02  1.7692428E-02
   220.0000      2.0575328E-02  1.3353705E-02
   240.0000      1.7792486E-02  1.0235325E-02
   260.0000      1.5051441E-02  7.9476433E-03
   280.0000      1.0406492E-02  6.2709148E-03
   300.0000      1.1901873E-02  8.2451245E-03
   320.0000      1.1594478E-02  6.6403067E-03
   340.0000      1.0792673E-02  5.4114950E-03
   360.0000      9.9309748E-03  4.4597946E-03
   380.0000      9.1089029E-03  3.7103852E-03
   400.0000      8.3512999E-03  3.1144836E-03
   420.0000      7.6613128E-03  2.6355239E-03
   440.0000      7.0428853E-03  2.2464965E-03
   460.0000      6.4875023E-03  1.9272763E-03
   480.0000      5.9888614E-03  1.6631020E-03
   500.0000      5.5409130E-03  1.4430239E-03
     ......          .......        .......
$
$ type refrac_index.dat

    photon             real
```

```
   energy              part

 200.0000        1.1661466E-02
 220.0000        1.0287664E-02
 240.0000        8.8962428E-03
 260.0000        7.5257206E-03
 280.0000        5.2032461E-03
 300.0000        5.9509366E-03
 320.0000        5.7972390E-03
 340.0000        5.3963363E-03
 360.0000        4.9654874E-03
 380.0000        4.5544514E-03
 400.0000        4.1756500E-03
 420.0000        3.8306564E-03
 440.0000        3.5214426E-03
 460.0000        3.2437511E-03
 480.0000        2.9944307E-03
 500.0000        2.7704565E-03
   ......          .......
$
$ type reflectivity.dat

   photon           r              r_s             r_p
   energy
 200.0000        0.7642972       0.7672730       0.7613214
 220.0000        0.7695174       0.7719697       0.7670650
 240.0000        0.7701561       0.7722075       0.7681047
 260.0000        0.7644928       0.7662324       0.7627532
 280.0000        0.6992385       0.7007588       0.6977182
 300.0000        0.6961607       0.6979848       0.6943366
 320.0000        0.7215253       0.7230968       0.7199538
 340.0000        0.7340940       0.7354625       0.7327254
 360.0000        0.7424233       0.7436262       0.7412204
 380.0000        0.7487475       0.7498126       0.7476823
 400.0000        0.7537164       0.7546662       0.7527666
 420.0000        0.7576135       0.7584658       0.7567613
 440.0000        0.7609170       0.7616860       0.7601480
 460.0000        0.7636897       0.7643870       0.7629924
 480.0000        0.7660290       0.7666641       0.7653939
   .....           ......          .....           ......
```

```
$
$ type transmission.dat

  photon         transmission
  energy

 200.0000       1.6302495E-08
 220.0000       3.4217771E-07
 240.0000       3.9229426E-06
 260.0000       2.8323737E-05
 280.0000       1.3664376E-04
 300.0000       3.5980481E-06
 320.0000       2.1055983E-05
 340.0000       8.9248650E-05
 360.0000       2.9271599E-04
 380.0000       7.8866363E-04
 400.0000       1.8120520E-03
 420.0000       3.6627993E-03
 440.0000       6.6762352E-03
 460.0000       1.1189881E-02
  ......         ........

$
$ type energy_loss.dat

 photon
 energy        Im (1/epsilon)

 200.0000       1.8541420E-02
 220.0000       1.3918069E-02
 240.0000       1.0608352E-02
 260.0000       8.1918687E-03
 280.0000       6.4032399E-03
 300.0000       8.4443605E-03
 320.0000       6.7967018E-03
 340.0000       5.5300575E-03
 360.0000       4.5496193E-03
 380.0000       3.7788621E-03
 400.0000       3.1671315E-03
 420.0000       2.6763568E-03
```
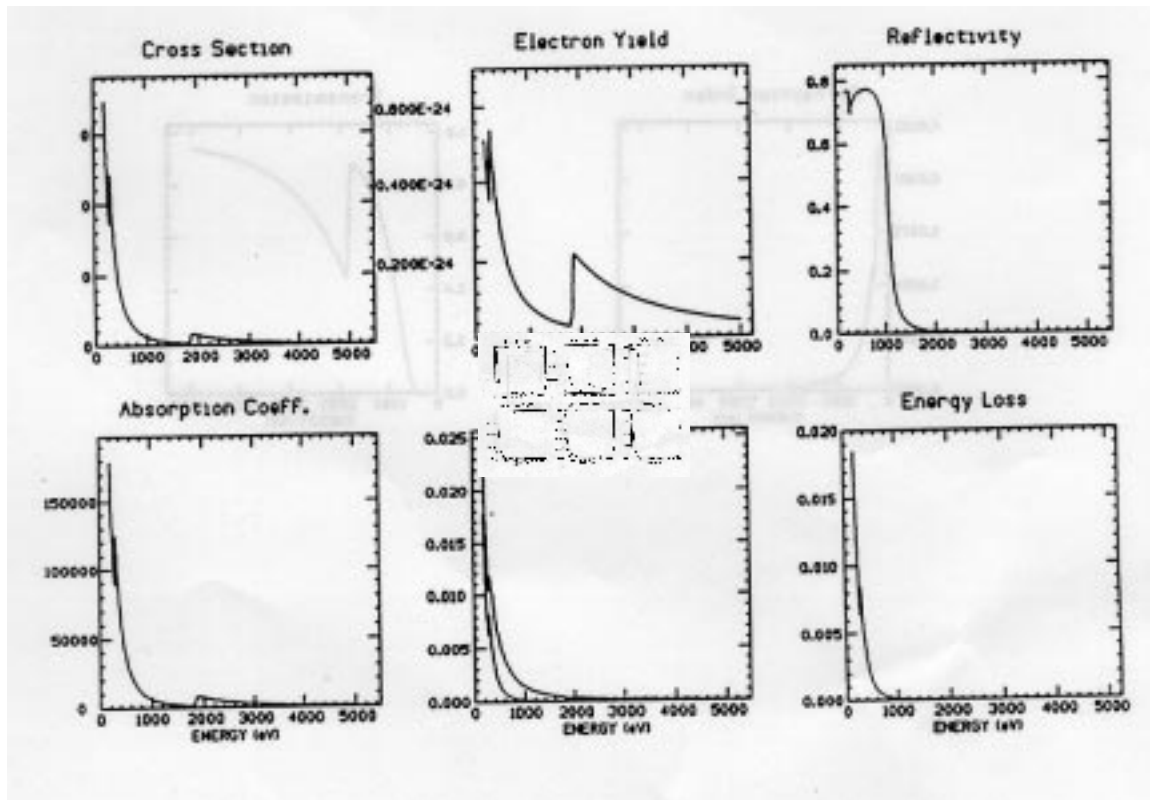
Figure 5.1: ABREFC output

```
440.0000        2.2784660E-03
460.0000        1.9525208E-03
480.0000        1.6831977E-03
 ......          .......
```

The files are plotted in the following two figures.
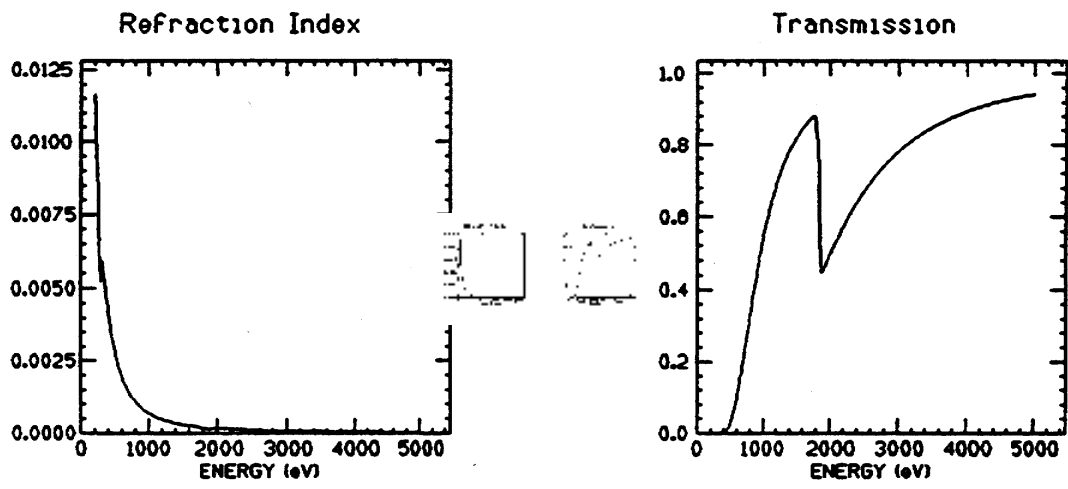
Figure 5.2: ABREFC output continued

CUTOFF

Purpose:	Computes the reflectivity cutoff angle for a given element.
Input:	From the Keyboard.
Output:	To two {x,y} files, CUTOFFDEG.DAT (degrees, reflectivity) and CUT-OFF.DAT (radians, reflectivity).

Description:

The program is based on the optical constants described in ABREFC. At each photon the cutoff wavelength, i.e., the extrapolation to zero is computed. The formula is defined by B. Henke in *Low Energy X-ray Diagnostics*. Notice that for an absorbing system this wavelength is not well defined as it is for a dielectric.

Examples:

We will consider the case of a gold mirror.

```
$CUTOFF
Enter 2-letters (capitalized) atomic symbol ?
AU
Density ?
19.7
Enter starting photon energy,end and step
200,5000,25
$
$ dir *.dat

Directory D13:[XRAYOP.DOCUMENT.CUTOFF]

CUTOFF.DAT;2            13  25-FEB-1989 13:02  (RE,RWED,RWED,RE)
CUTOFFDEG.DAT;2         13  25-FEB-1989 13:02  (RE,RWED,RWED,RE)

Total of 2 files, 26 blocks.
$
$
```

Au Reflectivity Cutoff Angle
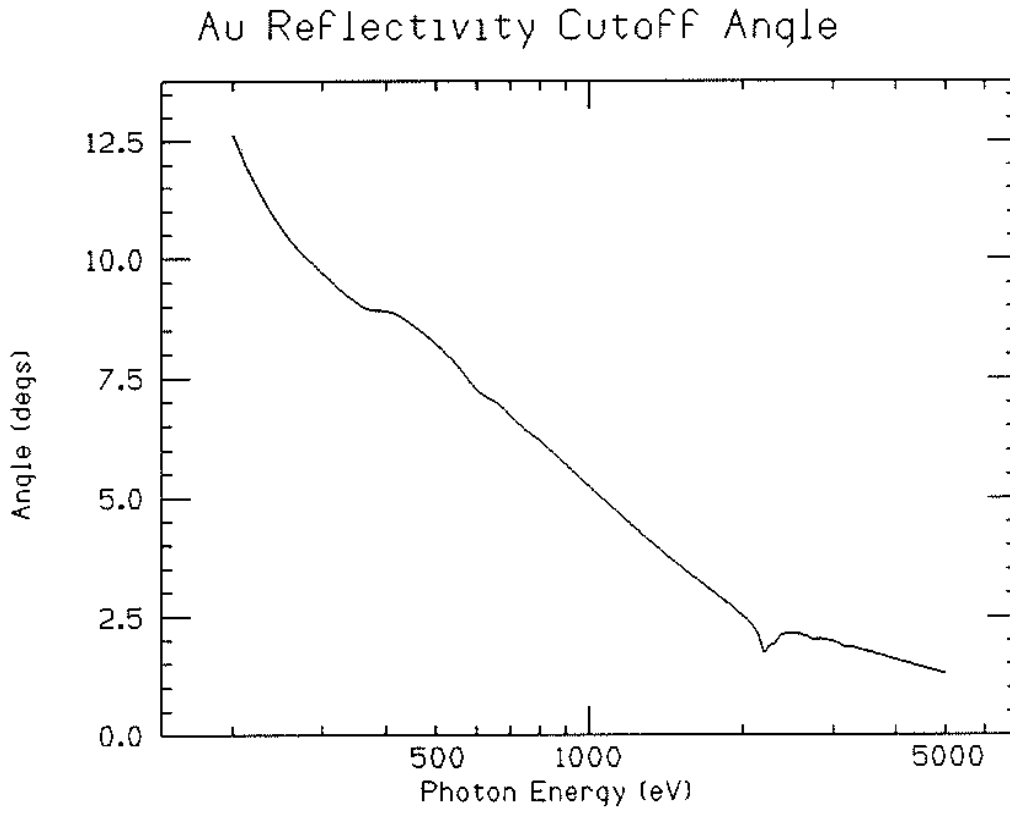
Figure 5.3: CUTOFF example using gold

TopDrawer was then used to generate the plot displayed here.

DOSE

Purpose:	Computes the absorbed X-ray dose in a given material vs. depth.
Input:	Incoming power data file (as generated by TRANSMIT)
	Absorption coefficient file (as generated by ABREFC)
Output:	A file z,dose with the value of the absorbed dose within the material.

Description:

The program relies on two preprocessors, TRANSMIT and ABREFC to generate respectively the incoming power density file and the absorption coefficient. Beer's law is used to compute the local absorbed power. Particularly useful for radiation damage studies. No geometrical information is used so that the implicit geometry is that of the x-rays incoming normally onto the sample.

Examples:

In order to demonstrate the program, we will prepare a system consisting of a thin Be window followed by an X-ray mask; an organic material (a resist) is located behind the mask and absorbs the radiation. We will compute the power density absorbed in function of the depth in this material. The absorbed dose is given by:

$$D(z) = \int_{E_1}^{E_2} I(z, \hbar\omega)\mu(\hbar\omega) \, d\,\hbar\omega \tag{5.4}$$

$$I(z, \hbar\omega) = I_o e^{-\mu(\hbar\omega)z} \tag{5.5}$$

where μ is the absorption coefficient. It is necessary to compute the incoming power density file and the absorption coefficient of the material under study. TRANSMIT generates a file that represents the <u>Watts</u> of radiation incident on a given area, hence the units are W/cm^2. Since μ is in [cm^{-1}], the dose is obtained in W/cm^3. If one is interested in a monochromatic or narrow band source, then create with EDT or another program, a file of the same format as TRANSMIT, i.e., {photon energy, power}.

Note: care must be taken that the different files be coherent for the photon energy range and energy steps.

```
$TRANSMIT
Do you want to generate a source file ?: y
```

```
Machine name ?
Aladdin                                              \* obviously *\
Title ?
Demo for Dose        Session
Machine Radius [ m ] and Beam Energy [ GeV ] ?
2.0833
1.0
Current [ A ] and milliradians of orbit (horizontal) ?
.100
5
Minimum photon energy, maximum, step :
200,2500,25                             \* calculation range *\
Spectrum type:
dE = constant            0          [ Photons/sec/eV ]
dL = constant            1          [ Photons/sec/Angs ]
dL/L = constant          2          [ Photons/sec/%bandwidth ]
dE/E = constant          3          [ Photons/sec/%bandwidth ]
Power dL=const           4          [ Watt/Angs ]
Power dE=const           5          [ Watt/eV ]          \* use this *\
Then ? 5
Do you want to specify the vertical acceptance ? 0
Read         1001 records.
+++++++++++++++++++++++++++++++++++++++++++
 Spectrum completed
+++++++++++++++++++++++++++++++++++++++++++
: DATA file roots for local properties ?
> loc
: CUMULATIVE DATA file roots ?
> tot
Do you want a conversion to Watts/cm^2 ? [Y/N] ? > y  \* not neccessary *\
Please enter the vertically scanned height (including overshoot) in CM.
> 10
The program will assume that you have used 1 mrad of orbit. If you have
specified 1 mrad when creating the source, simply enter 1. If not, enter the
number of milliradians you used.
Number of milliradians used: 5
Please enter the horizontal dimension of the exposed field [cm].
> 2.0                                \* we willuse an area of 20 cm^2 *\
Distance from the tangent point [m] ?
> 5                                  \* located at 5 m from the source *\
```

```
Total area is:    20.00000
All set.
Is the source spectrum in function of : [1] eV  [2] Angs ? 1
Read          93 records.
Initial power is:   0.1030330


Currently at Element N.      0

: Enter a negative number to exit, zero to cancel; OE ?
> 1
: Enter [ 0 ] for pure element, [ 1 ] for compound
> 0
Enter 2-letters (capitalized) atomic symbol ?
BE
Density ?
1.98
Mirror [ 1 ] or filter [ 0 ] ?
0
Thickness (microns) ?
15
OUT > Power density [W/cm^2] is   3.0929089E-02
Comment for this OE > Op  First filter


Currently at Element N.       1

: Enter a negative number to exit, zero to cancel; OE ?
> 2
: Enter [ 0 ] for pure element, [ 1 ] for compound
> 1
Density [ g/cm3 ] ?
4.6
Mirror [ 1 ] or filter [ 0 ] ?
0
Thickness (microns) ?
2
The program is setup to compute optical constants of
compounds with up to 5 elements.
How many atomic species ?
3
H2O would be: HH,2 and OO,1. Then ?
```

```
Enter 2-letters (capitalized) atomic symbol and formula index for :    1
BB
4
Enter 2-letters (capitalized) atomic symbol and formula index for :    2
NN
1
Enter 2-letters (capitalized) atomic symbol and formula index for :    3
HH
1
OUT > Power density [W/cm^2] is   2.0523597E-02
Comment for this OE > This could be an X-ray mask membrane

Currently at Element N.       2

: Enter a negative number to exit, zero to cancel; OE ?
> -2
$
$
$ dir *.dat

Directory D13:[XRAYOP.DOCUMENT.DOSE]

LOC1.DAT;1                     6  25-FEB-1989 13:25  (RE,RWED,RWED,RE)
LOC2.DAT;1                     6  25-FEB-1989 13:26  (RE,RWED,RWED,RE)
MACHINE.DAT;1                  3  25-FEB-1989 13:24  (RE,RWED,RWED,RE)
SRCOMP.DAT;1                   6  25-FEB-1989 13:24  (RE,RWED,RWED,RE)
TOT1.DAT;1                     6  25-FEB-1989 13:26  (RE,RWED,RWED,RE)
TOT2.DAT;1                     6  25-FEB-1989 13:26  (RE,RWED,RWED,RE)
TRANSMIT.DAT;1                 4  25-FEB-1989 13:24  (RE,RWED,RWED,RE)
TRANSMIT.LOG;1                 6  25-FEB-1989 13:26  (RE,RWED,RWED,RE)

Total of 8 files, 43 blocks.
$
$  \* verify that the limits are OK *\
$ fmax
File-name ?
tot1.dat
Read          93 points.
Found :
XMIN       200.0000      . Set at :  -58.75000
```

```
XMAX        2500.000                    2758.750
YMIN      0.0000000E+00               -2.6425714E-06
YMAX      2.3489521E-05                2.6132093E-05
Good luck !
$
$                              \* compute absorption coefficient *\
$ ABREFC
Full printout at Terminal ? 0
Thickness (microns) ?
2
The program is setup to compute optical constants of
compounds with up to 5 elements.
How many atomic species ?
3
H2O would be: HH,2 and OO,1. Then ?
Enter 2-letters (capitalized) atomic symbol and formula index for :     1
CC
7
Enter 2-letters (capitalized) atomic symbol and formula index for :     2
OO
6
Enter 2-letters (capitalized) atomic symbol and formula index for :     3
HH
11
Density ?
2.03
Enter starting photon energy,end and step
200,2500,25
Incidence angle ?
0
Molecular weight is :    191.1100
Atoms/Cm3
 4.4777364E+22  3.8380595E+22  7.0364425E+22  0.0000000E+00  0.0000000E+00
$
$
$ dir abs* \* this file contains the abs. coeff. in cm-1 *\

Directory D13:[XRAYOP.DOCUMENT.DOSE]

ABSOR_COEFF.DAT;1          6  25-FEB-1989 13:29  (RE,RWED,RWED,RE)
```

```
Total of 1 file, 6 blocks.
$
$ dose
Power density file ? tot2.dat
Absorption Coefficient File ? absor_coeff.dat
Output file ? dose    abs_dose
Files read OK.
Thickness (MICRONS) ? 2         \* film thickness *\
Step size (MICRONS) ? 0.05 2    \* calculation step -- 41 points *\
Area over which power is spread [ cm2 ] ? 20
All calculations completed
$
$
$ type abs_dose.dat
 0.0000000E+00   1.639008
 2.0000000E-02   1.630774
 3.9999999E-02   1.622603
 5.9999999E-02   1.614495
 7.9999998E-02   1.606449
 9.9999994E-02   1.598465
 0.1200000       1.590542
 0.1400000       1.582678
 0.1600000       1.574874
 0.1800000       1.5671\
    Interrupt

$
$ dir .dat;0

Directory D13:[XRAYOP.DOCUMENT.DOSE]

ABSOR_COEFF.DAT;1          6  25-FEB-1989 13:29  (RE,RWED,RWED,RE)
ABS_DOSE.DAT;1            7  25-FEB-1989 13:30  (RE,RWED,RWED,RE) <<<<<<
CROSS_SECTION.DAT;1
                         6  25-FEB-1989 13:29  (RE,RWED,RWED,RE)
DIELEC_FUNC.DAT;1        9  25-FEB-1989 13:29  (RE,RWED,RWED,RE)
ELECTRON_YIELD.DAT;1
                         6  25-FEB-1989 13:29  (RE,RWED,RWED,RE)
ENERGY_LOSS.DAT;1        6  25-FEB-1989 13:29  (RE,RWED,RWED,RE)
```

```
LOC1.DAT;1                 6  25-FEB-1989 13:25   (RE,RWED,RWED,RE)
LOC2.DAT;1                 6  25-FEB-1989 13:26   (RE,RWED,RWED,RE)
MACHINE.DAT;1              3  25-FEB-1989 13:24   (RE,RWED,RWED,RE)
REFLECTIVITY.DAT;1        12  25-FEB-1989 13:29   (RE,RWED,RWED,RE)
REFRAC_INDEX.DAT;1         6  25-FEB-1989 13:29   (RE,RWED,RWED,RE)
SRCOMP.DAT;1               6  25-FEB-1989 13:24   (RE,RWED,RWED,RE)
TOT1.DAT;1                 6  25-FEB-1989 13:26   (RE,RWED,RWED,RE)
TOT2.DAT;1                 6  25-FEB-1989 13:26   (RE,RWED,RWED,RE)
TRANSMISSION.DAT;1         6  25-FEB-1989 13:29   (RE,RWED,RWED,RE)
TRANSMIT.DAT;1             4  25-FEB-1989 13:24   (RE,RWED,RWED,RE)

Total of 16 files, 101 blocks.
$
$                \* The session of Transmit is recorded in TRANSMIT.LOG *\
$
$ type transmit.log
---------------------------------------------------------------------------
Demo Session
Parameters of Aladdin
---------------------------------------------------------------------------
Magnetic Radius     :    2.083300      meters
Beam energy         :    1.000000      GeV
Gamma               :    1957.000
Magnetic Field      :    1.600695      tesla
---------------------------------------------------------------------------
Critical ENERGY     :    1064.883      eV
          WAVELENGTH:    11.64308      Angstroms
Power/Amp           :    42.48068      kilowatts/amp
Total Power         :    4.248068      kilowatts
     at current of  :    0.1000000     Amperes.
Total Power/mrad    :    0.6761010     watts/mrad
For unlimited vertical acceptance,
  power accepted    :    3.380505      watts
  hori. acceptance  :    5.000000      mrads
---------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
         PROGRAM   TRANSMIT V1.0 -- SEPTEMBER 1984
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
Photon energy range used:
      start             :     200.0000
      end               :     2500.000
      step              :     25.00000


Results are in Watts/cm^2.


Power in source file [W] =    2.575826
Full power in W/cm^2 =   0.1030330


Exposure field is defined by:


Horizontal [cm] =     2.000000
Vertical   [cm] =     10.00000
Area       [cm] =     20.00000
Milliradians   =     4.000000
Distance   [m ] =     5.000000


================================================
================================================
Optical Element :          1
Defined FILTER   15.000      microns thick
Working with   Z =   4       Symbol: BE
Atomic Weight:    9.010000    and density   1.980000    g/cm3

--------------------------
OE #             1
First filter
OUT > Power density [W/cm^2] is   3.0929089E-02


================================================
================================================
Optical Element :          2
```

```
Defined FILTER    2.0000      microns thick
Formula:  BB( 4) NN( 1) HH( 1)

Molecular weight is :     58.21000      Number of molecules/cm3:    4.7589159E
Atoms/Cm3 of each species:
     BB              NN               HH
 0.19036E+24  0.47589E+23    0.47589E+23
 Density    4.600000      g/cm3


--------------------------
OE #               2
This could be an X-ray mask membrane
OUT > Power density [W/cm^2] is    2.0523597E-02



$
$
$
$
```
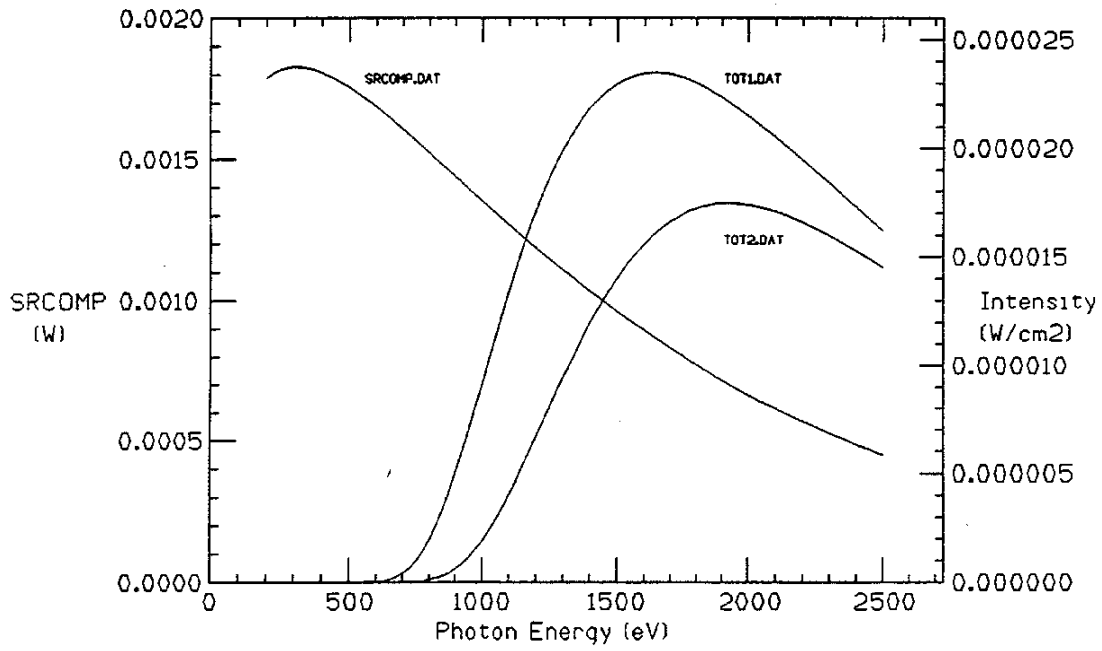
Figure 5.4: DOSE: Graphical output from TRANSMIT
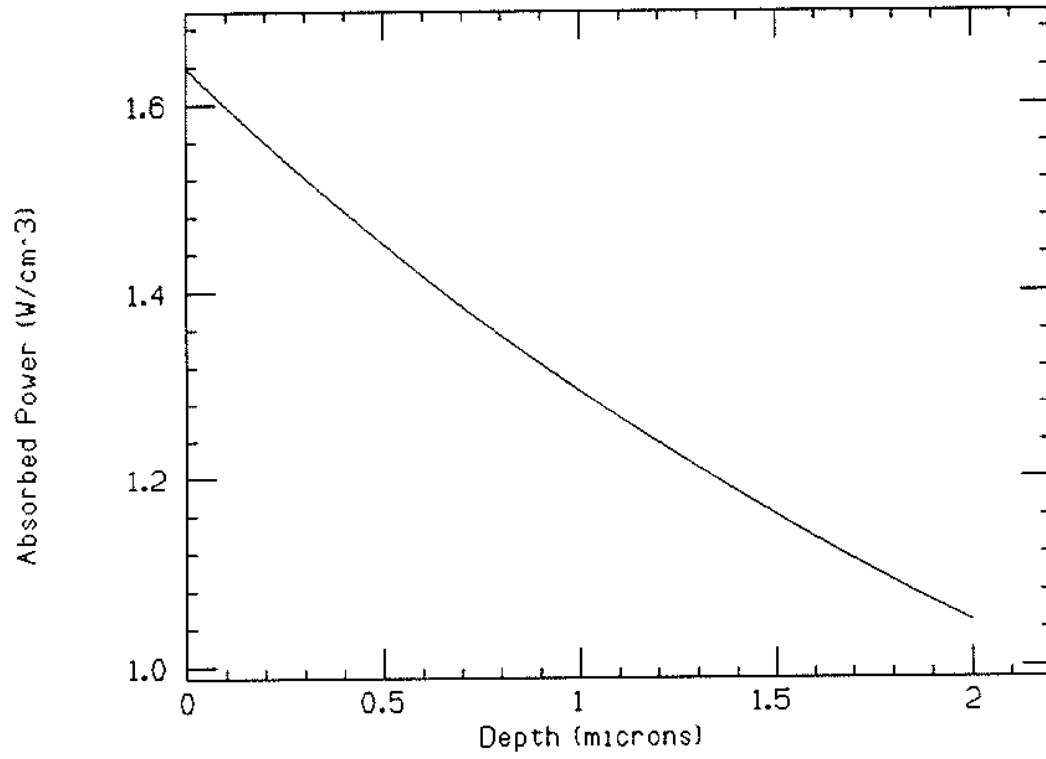
Figure 5.5: DOSE: Dose seen by photo-resist

MLAYER

Purpose:	A standalone program to compute the reflectivity of multilayers. (J.H. Underwood)
Input:	Multilayers defined either from terminal or by a formatted file.
Output:	Formatted (8 columns) file.

Description:

MLAYER is not really a utility to SHADOW but rather, a standalone program written by J. H. Underwood of the Center for X-ray Optics. It can calculate the reflectivity of multilayer as a function of a) incident angle or b) incident wavelength, leaving the other one fixed. MLAYER also assumes that a narrow wavelength range will be used, so that a set of constant refractive indices (supplied by the user) is sufficient. Thus a possible sequence of events may be:

1. Run MLAYER to get an idea of how the multilayers perform

2. Run PRE_MLAYER to set up the multilayers

3. Run SHADOW for a complete simulation.

MLAYER has the following options :
 OPTIONS
1	=	fixed wavelength, scan angle, periodic layers
2	=	fixed angle, scan wavelength, periodic layers
3	=	fixed wavelength, scan angle, individual layers defined
4	=	fixed angle, scan wavelength, individual layers defined
5	=	fixed angle, scan wavevector, individual layers defined

Whether the multilayers are periodic or not depends on whether the absorbing and non-absorbing materials all have the same thicknesses for all layers. Of course, the user can always define the thicknesses one by one.

For the example here we use the same W-C multilayers as in PRE_MLAYER (see PRE_MLAYER). We use option 3 to scan the *glancing* angle from 0 to 90 degrees, at a fixed wavelength of 18 Å. Then the user can direct the program to read all the input parameters from a file or type them in from the terminal. For the first pass, we use the latter mode. We proceed to define the complex refractive indices of the substrate and the multilayers by δ and β:

$$n = (1 - \delta) - i * (\beta)$$

The δ's and β's can in turn be obtained at the energy you are interested in from ABREFC. We put the wavelength at 18 Åand the initial angle 0 degrees. Using a step size of 0.5 and 181 points, this will take us up to 90 degrees. Had we chosen to scan the wavelength instead (option 4), the same step size and number of points will scan from 18 to 108 Å(but then the refractive indices are not nearly constant). After that, we type in the individual thickness of the layers. This process fully specifies the multilayers, and the parameters can be saved in a file (CW.PAR). In future run, the user can direct MLAYER to read from the file, saving the labor of re-defining the multilayers.

The output of this calculation is saved in a formatted file (CW.OUT). There are eight columns and they have the following meanings :

COLUMN

1	λ (or θ, whichever is varied)
2	S reflectivity
3	P reflectivity
4	Average reflectivity
5	S phase shift
6	P phase shift
7	S (electric field)^2
8	P (electric field)^2

where S is the perpendicular component and P the parallel component (to the plane of incidence). Phase shift is in units of π.

Examples:

```
\\ For the geometry, refer to the example in PRE_MLAYER. \\


$
$ MLAYER
option 1, 2, 3, 4, or 5?  (0 = help, 6 = exit)
0                                                          \\ Help menu \\
1 = fixed wavelength, scan angle, peroidic layers
2 = fixed angle, scan wavelength, periodic layers
3 = fixed wavelength, scan angle, individual layers defined
4 = fixed angle, scan wavelength, individual layers defined
5 = fixed angle, sacn wavevector, individual layers defined
option 1, 2, 3, 4, or 5?  (0 = help, 6 = exit)
3
use existing input file?  (cr = yes)
```

```
N
input multilayer parameters
substrate material is      .  (cr = no change)         \\ Substrate \\
SI
delta =    0.00000,       beta =    0.00000(, = no change)
1.0E-3,1.0E-4
odd layer material is      .  (cr = no change)          \\ Odd layer \\
W
delta =    0.00000,       beta =    0.00000(, = no change)
1.1E-2,1.25E-2
even layer material is       .  (cr = no change)          \\ Even layer \\
C
delta =    0.00000,       beta =    0.00000(, = no change)
1.3E-3,1.86E-4
lambda(begin) =   0.00000   theta(begin) =   0.00000(, = no change)
18.0,0.0                                         \\ wavelength, angle \
step size =    0.00000   number of steps =    0(, = no change)
0.5,181
number of layer pairs =    0  (, = no change)
20
for layer pair    1,
  odd thickness =    0.00000   even thickness =    0.00000 (, = no change)
7.71,14.56
for layer pair    2,
  odd thickness =    0.00000   even thickness =    0.00000 (, = no change)
7.72,14.57
for layer pair    3,
  odd thickness =    0.00000   even thickness =    0.00000 (, = no change)
7.74,14.59
for layer pair    4,
  odd thickness =    0.00000   even thickness =    0.00000 (, = no change)
7.74,14.59
for layer pair    5,
  odd thickness =    0.00000   even thickness =    0.00000 (, = no change)
7.74,14.59


      :                              :                              :
      :                              :                              :
      :                              :                              :
```

```
for layer pair   19,
  odd thickness =    0.00000   even thickness =    0.00000  (, = no change)
7.74,14.59
for layer pair   20,
  odd thickness =    0.00000   even thickness =    0.00000  (, = no change)
7.74,14.59
save layer parms in which file? (cr = don't save)
CW.PAR
name of output file:
CW.OUT
option 1, 2, 3, 4, or 5?  (0 = help, 6 = exit)
6
FORTRAN STOP
$
$ DIR CW

Directory D13:[XRAYOP.DOCUMENT.MLAYER]

CW.OUT;1                   36  23-FEB-1989 23:13  (RWED,RWED,RE,RE)
CW.PARCN;1                  2  23-FEB-1989 23:13  (RWED,RWED,RE,RE)

Total of 2 files, 38 blocks.

\\ CW.PARCN can be edited or simply reused for input to MLAYER. \\


$
$ TY CW.PARCN
SI                                        \\ Substrate
   0.00100    0.00010                     \\ delta, beta
W                                         \\ Odd layer
   0.01100    0.01250                     \\ delta, beta
C                                         \\ Even layer
   0.00130    0.00019                     \\ delta, beta
  18.00000    0.00000                     \\ wavelength, angle
   0.50000 181                            \\ step size, no. of points
  20                                      \\ no. of layers
   7.71000  14.56000                      \\ thickness (odd, even)
   7.72000  14.57000
   7.74000  14.59000
   7.74000  14.59000
```

```
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
      7.74000   14.59000
```

\\ CW.OUT is the output we are interested in. \\

```
$
$ TY CW.OUT               \* the file CW.OUT contains the eight values on a
                          \* single line, however to display the values, we
                          \* have continued them on the next line. *\
  90.000000    0.000025   0.000025    0.000025    1.988236    0.988236
   1.009956    1.009956

  89.500000    0.000025   0.000025    0.000025    1.988777    0.988776
   1.009947    1.009945

  89.000000    0.000024   0.000024    0.000024    1.990377    0.990375
   1.009917    1.009911

  88.500000    0.000024   0.000024    0.000024    1.992974    0.992969
   1.009863    1.009849

      :            :          :           :           :           :
      :            :          :           :           :           :

   1.500000    0.703394   0.696951    0.700172    0.892246    0.895151
   0.121218    3.276859
```

```
1.000000    0.793120    0.788295    0.790707    0.928310    0.930251
0.056958    3.521553

0.500000    0.891299    0.888593    0.889946    0.964200    0.965171
0.015056    3.762622

0.000000    1.000000    1.000000    1.000000    1.000000    1.000000
0.000000    4.000000
```

\\ Now let us graph the average reflectivity (col. 4) vs the angle (col. 1)
\\ using TOPDRAWER.

```
$
$ TDTEK
TOP DRAWER (10/10/80) NOW EXECUTING

MOD NOECHO
         1  MOD NOECHO

SET ORDER X DUMMY DUMMY Y DUMMY DUMMY DUMMY DUMMY
         2  SET ORDER X DUMMY DUMMY Y DUMMY DUMMY DUMMY DUMMY

@CW.OUT
READING FROM INDIRECT COMMAND FILE: CW.OUT
         3      90.000000    0.000025    0.000025    0.000025    1.988236
                             0.988236    1.009956    1.009956
END OF INDIRECT COMMAND FILE
JOIN 1
       184  JOIN 1

END
       185  END
```
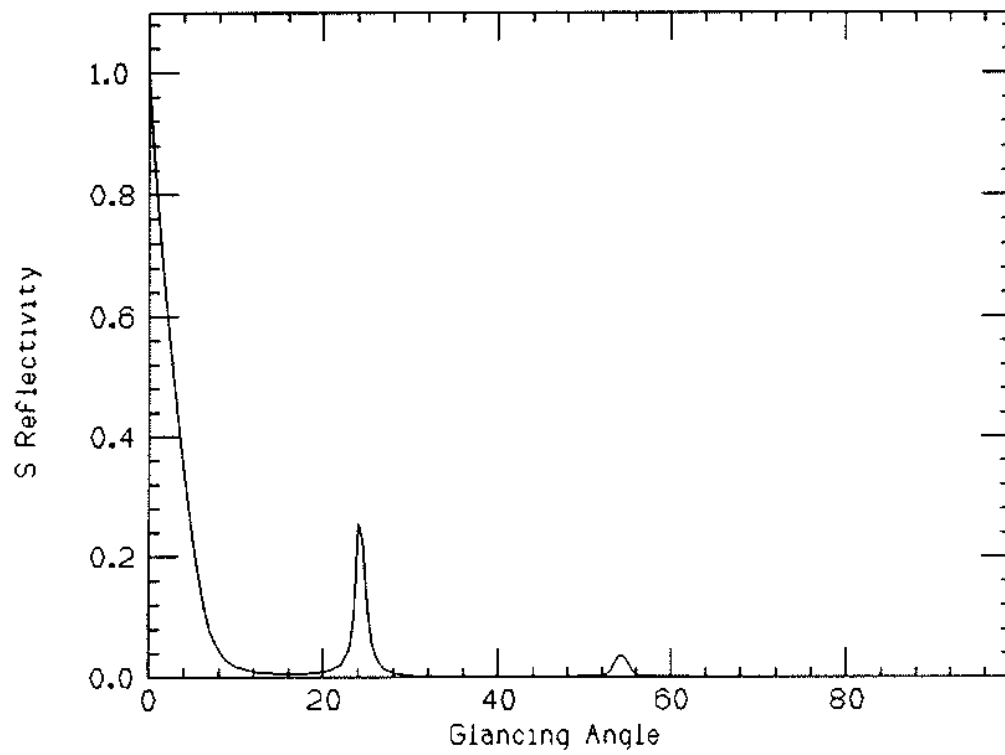
Figure 5.6: MLAYER: S-reflectivity vs. angle
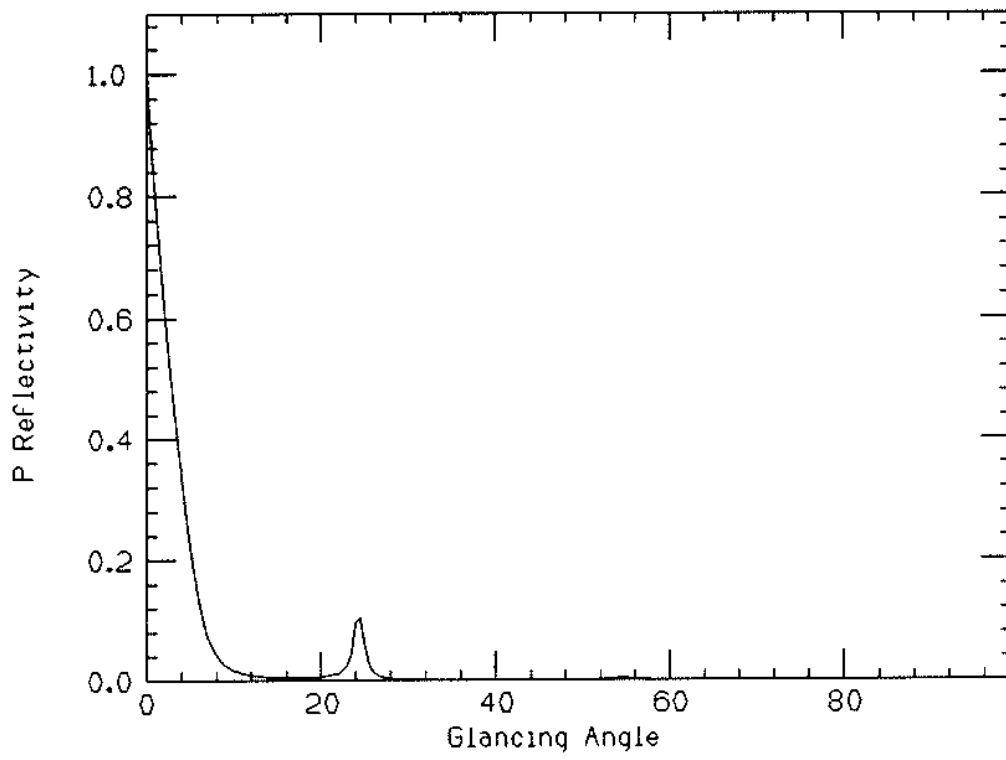
Figure 5.7: MLAYER: P-reflectivity vs. angle
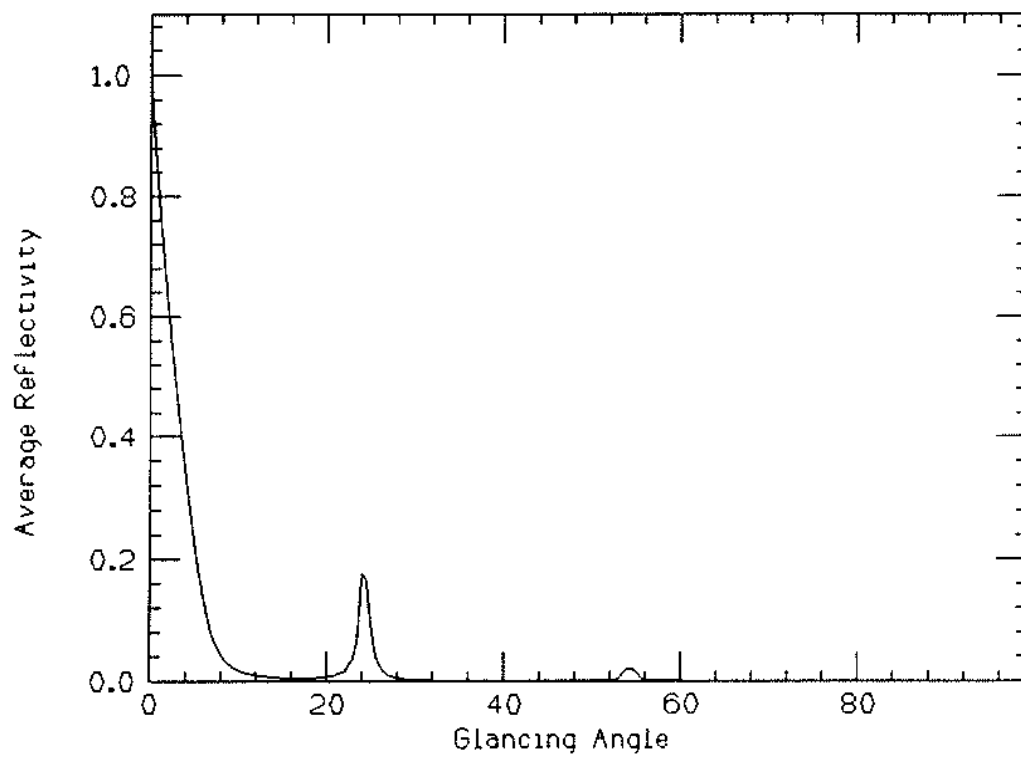
Figure 5.8: MLAYER: Average reflectivity

TRANSMIT

Purpose:	To compute the transmission in terms of energy vs. power of an x-ray beamline from the universal SR curves (C. K. Green. *BNL Internal Report*. Upton, 1976.) with reflectivities and transmission coefficents as obtained from the Fresnel equations and a comprehensive optical constants database.
Input:	Machine parameters, photon energy, and system information.
Output:	Formatted ASCII files containing the source spectra {photon energy, power}, and for each element a file with local properties and cummulative properties, and a log file of the session.

Description:

The TRANSMIT code was developed for the modelling of x-ray lithography systems – hence the terminology. It is however of wide application and the program performs calulations for mirrors, filters, masks and photo resists consisting of single elements or compounds of up to five atomic species.

The program is file oriented. A user interface creates a set of files describing the calculations to be performed and then invokes a computational engine to compute the actual physical properties. The program requires a set of startup files with a generic machine description for the source, a generic x-ray beamline, and a resist. These files can then be created and modified in a menu driven interface to represent specific machines and beamlines. New startup files are then saved for future use. They can be named by the user. The program outputs several files. The first is a data file containing the source spectra in the form {photon energy, power}. For each optical element, two files are written when the LOGGING option is on. One contains the local properties for that element, the other contains the cumulative properties. The final file that can be written is a log file of the session. Whether or not this file is written is dependent on the value given to the LOGGING flag in the main menu. The log file contains all the information found in a summary to the screen, plus a simple ASCII graph of the flux after each element. It is recommended that the user make all the changes and additions to his system, then turn the logging flag on and run TRANSMIT. This way only the latest version of the system is written to the log file. Otherwise, if the flag is turned on when starting, every time a change is made and saved and TRANSMIT is run, a log of the entire system is written. This can lead to a very large file containing duplicate information; from another point of view, it will contain a log of the entire session.

TRANSMIT is run by a menu driven shell program. The shell allows the user to enter a source and system, generate the flux characteristics, and then modify any parameter without having to reenter the entire source and system. The same source or system can also be used with other runs, providing the startup files have been saved. TRANSMIT provides information on the spectral power distribution generated by a source and modified by an optical system. The program provides information on the total power along the beamline, making it quite useful for the estimation of power loadings. The units of the files created by TRANSMIT (e.g. Watts) may also be scaled to a given surface, thus giving W/cm^2.

The program can model a specific storage ring when the parameters of the machine are input. The characteristics of the user's machine are scaled to the universal SR curve based on formulas calculated by C. K. Green. The source spectra is then calculated and stored. The user can then specify optical elements in a beamline or system. An optical element can consist of mirrors, filters, a mask or a photo resist. The user must input the materials used (element or compound), their densities, and other variables depending on the type of optical element (i.e. thickness for a filter). The reflectivity/transmission characteristics for various polarizations are calculated using an optical constants library shared with SHADOW. Meaningful energies are from 100 eV to 100,000 eV. If energies below 100 eV are entered, the program will assume an energy of 100 eV. If both the minimum and maximum energy are chosen to be below 100 eV, the program will abort. The information is output in the form of energy or wavelength vs. power.

Examples:

The following example uses the SR source Aladdin at 800 MeV to generate the power profiles. The x-ray beamline contains three mirrors at 88, 89, 89 degrees angle of incidence with a beryllium window and silicon carrier/gold absorber mask. The photoresist is modelled by 1 μm of PMMA.

Moving around in the shell is accomplished with the up/down arrows and the return key. The arrow keys move you vertically within a menu. The return key selects an item for modification and moves from the main menu down to the sub-menus, and returns to the main menu. Each screen shown below will have a description below it of what is being done and how to move to the next screen.
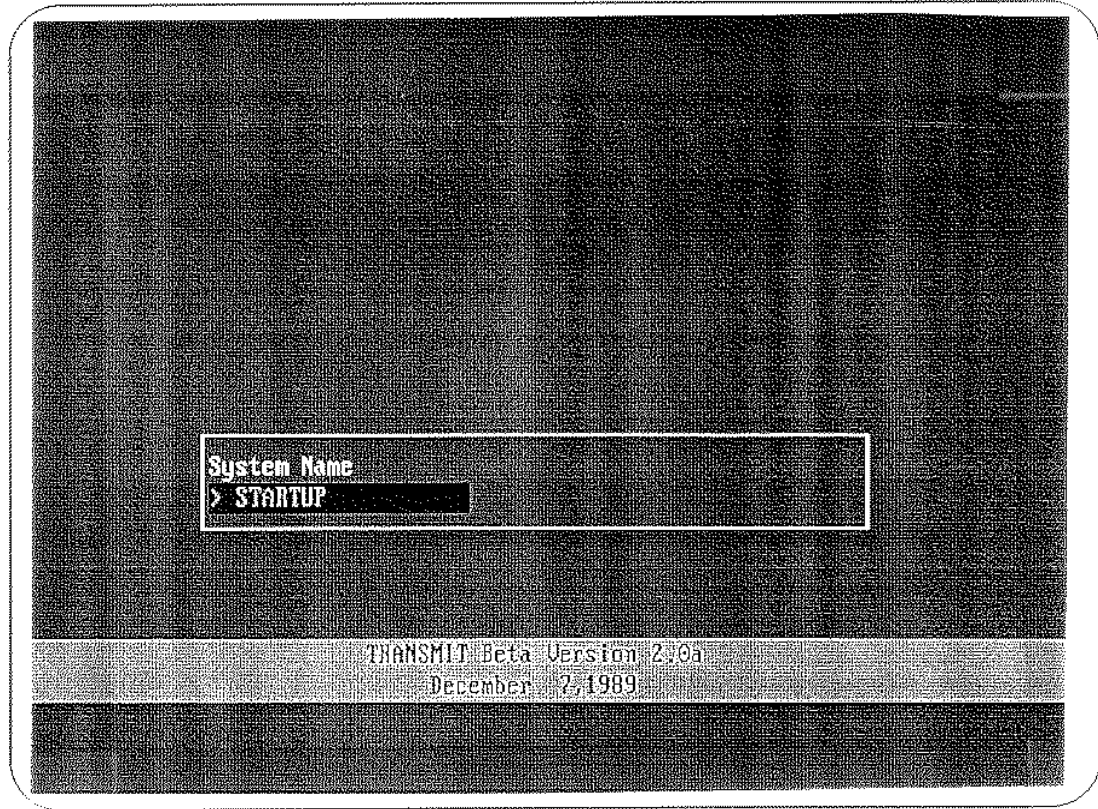
The program is started by typing TRANSMIT at the DCL level. The screen displays a prompt for system name. For first time users, this will be a generic system. The system name is input in the main menu at the EXIT & SAVE option. At this point, hitting <RETURN> will take you to the main menu.
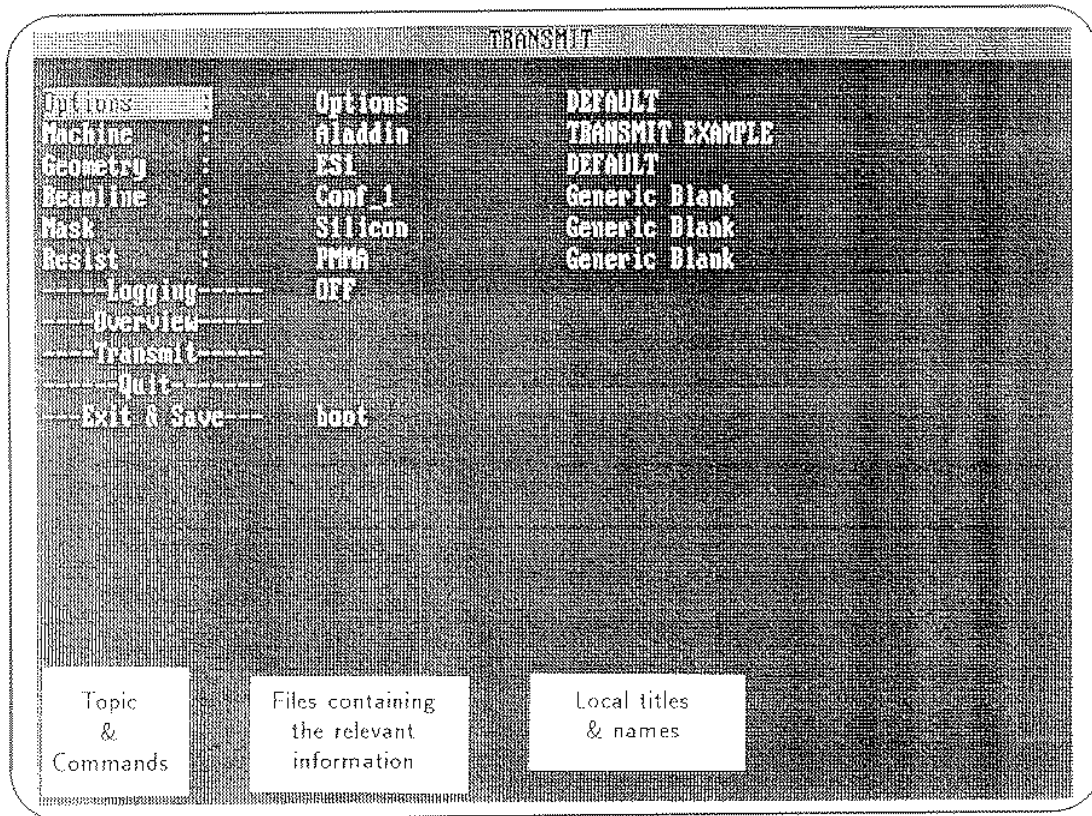
This is the generic startup menu. It contains basic machine parameters for a source, but does not have any kind of beamline set up. Options, Machine, Geometry, Beamline, Mask and Resist are all sub-menus where parameters can be entered. These will be shown. The Logging flag should be OFF for now, turn it on after the system is completely set up, then move the highlight bar to Transmit and hit <RETURN> to generate a log file of the final system. Overview will give a summary of the system to the terminal. Quit will exit without saving any parameters. The last option, EXIT & SAVE, is where the user's system name should be entered after setting up the rest of the parameters. Using the arrow keys, position the highlighted bar so it is on Options@, then hit <RETURN>.
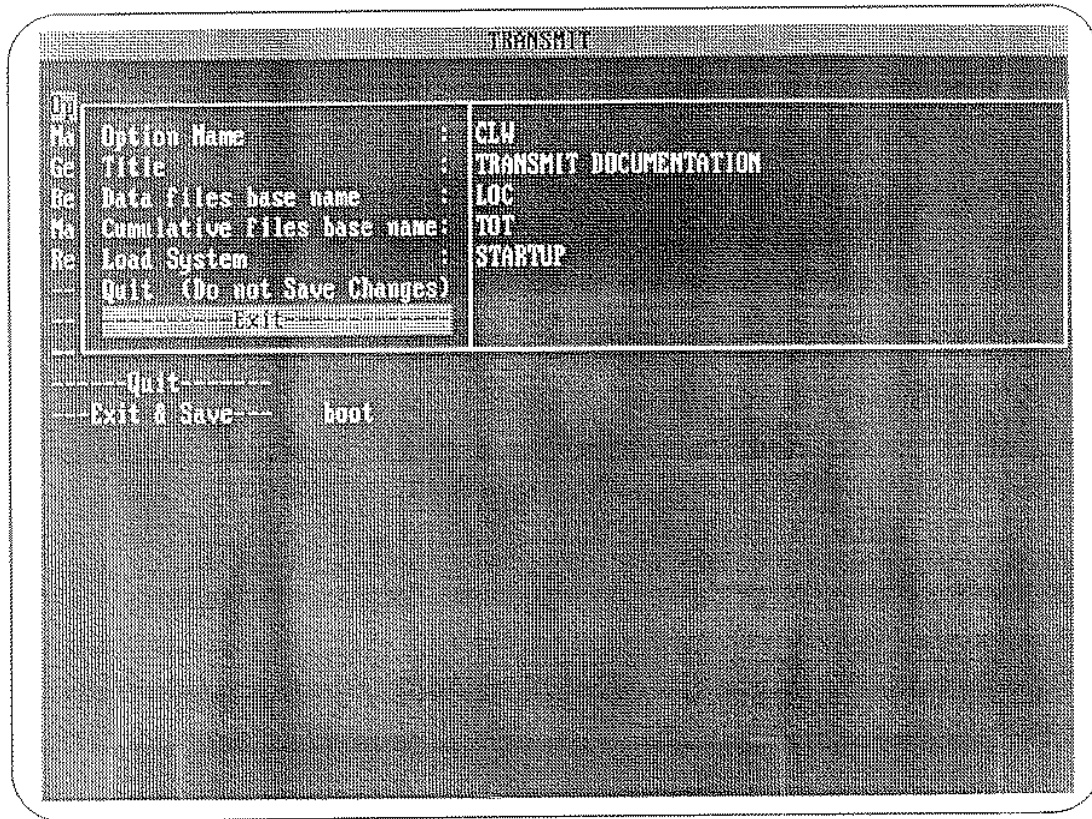
This is the `Options` menu. It allows the user to give meaningful names to the data files that TRANSMIT writes and to give a default system or set of files to read. The title is just a comment to the user, it has no bearing on the program. This is where the first time user should name the Option file. That way the parameters displayed in this menu will be saved in a file as specified in the `Option Name` field. If changes have been made, choose the `Exit@` option, otherwise choose `Quit@` by moving the arrow keys and hitting `<RETURN>` to return to the main menu. Enter the `Machine@` sub-menu by highlighting the option and again hitting `<RETURN>`.

The machine menu sets up the basic x-ray source. Here we model the synchrotron called Aladdin. To enter the specific parameters interested in, move the arrow to highlight the parameter and hit return, then enter the correct data. Under Spectrum type, there are five options. Highlighting and hitting return will list the available spectra. Create Source will generate the source with the given parameters, and among other things, calculate the critical energy, wavelength, and total power/mrad. Exit will also save the parameters and generate the source. Return to the main menu. At this point we notice that next to Machine name is the name of the machine we have generated. This name can be used in future runs if the parameters are desired. Next move down to Geometry@ and enter that menu.
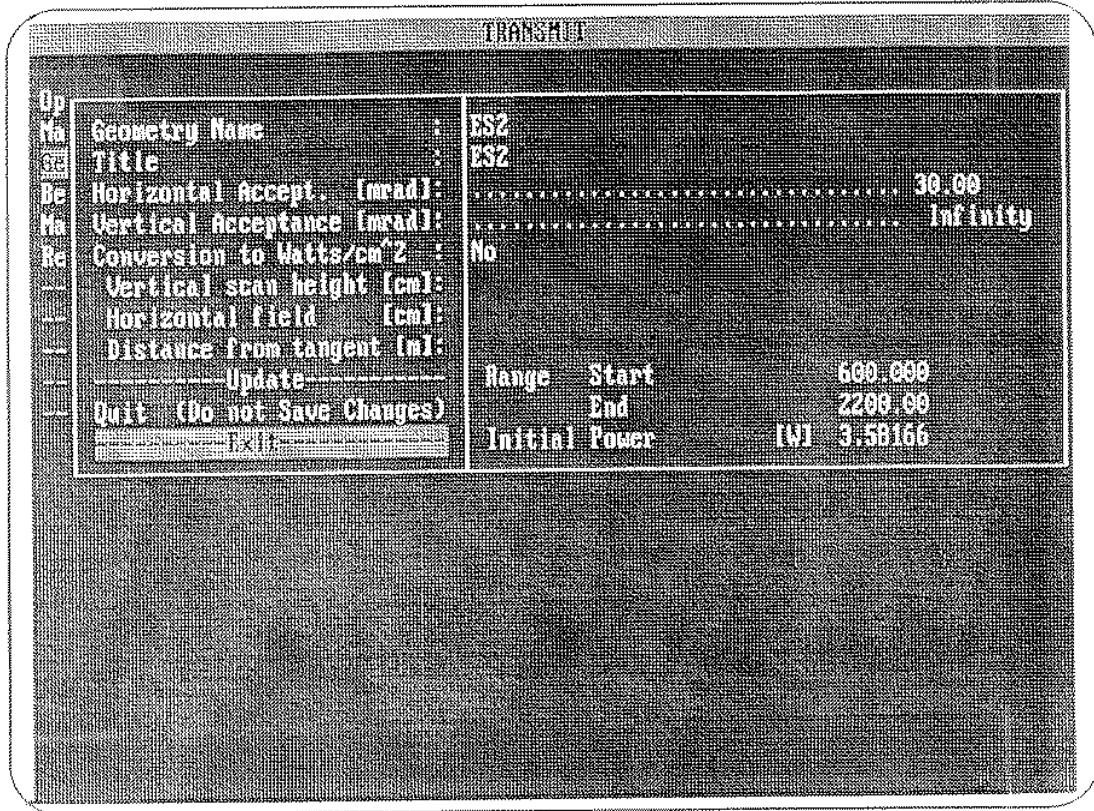
The geometry menu refers to the acceptance of the system in terms of mrads. This is usually specific to location in relation to the source. The vertical acceptance can either be specified or assumed infinite. If the user desires a conversion to Watts/cm^2, he will need also to enter the scan height, horizontal field, and distance from tangent. `Update` will perform the calculations and remain in this menu so that the user can see the results immediately, if desired, `Exit` will also run the calculations, but will return you to the main menu when complete.

The next menu is the `Beamline` menu. At this point the user can set up any combination of mirrors and filters knowing the element or compound they are made of, the material density, the formula, and either the incidence angle of the light or the thickness of the filter. `Add optical element` adds a new element on the end of the beamline. `Delete optical element` asks which element you wish to delete. `Run Transmit` recalculates the power. `Quit` returns to the main menu without saving any changes or updating any numbers. `Exit` saves, updates, and returns to the main menu.

The `Mask` menu appears much like the beamline menu. The elements of the mask are entered in the same fashion; the only difference being the user must distinguish between a carrier and an absorber.
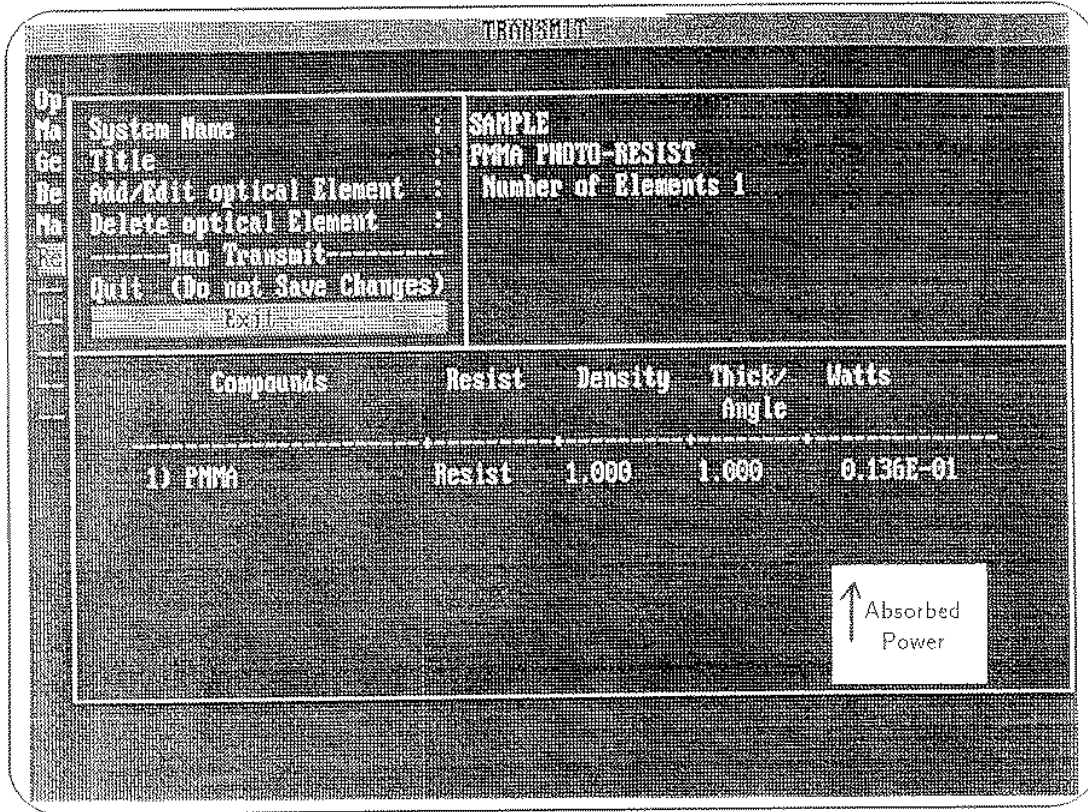
The final step in an x-ray beamline is the photo resist. The `Resist` menu is similar in setup to the beamline and mask menus. Here we demonstrate a compound, PMMA, with molecular formula $C_5H_8O_2$.
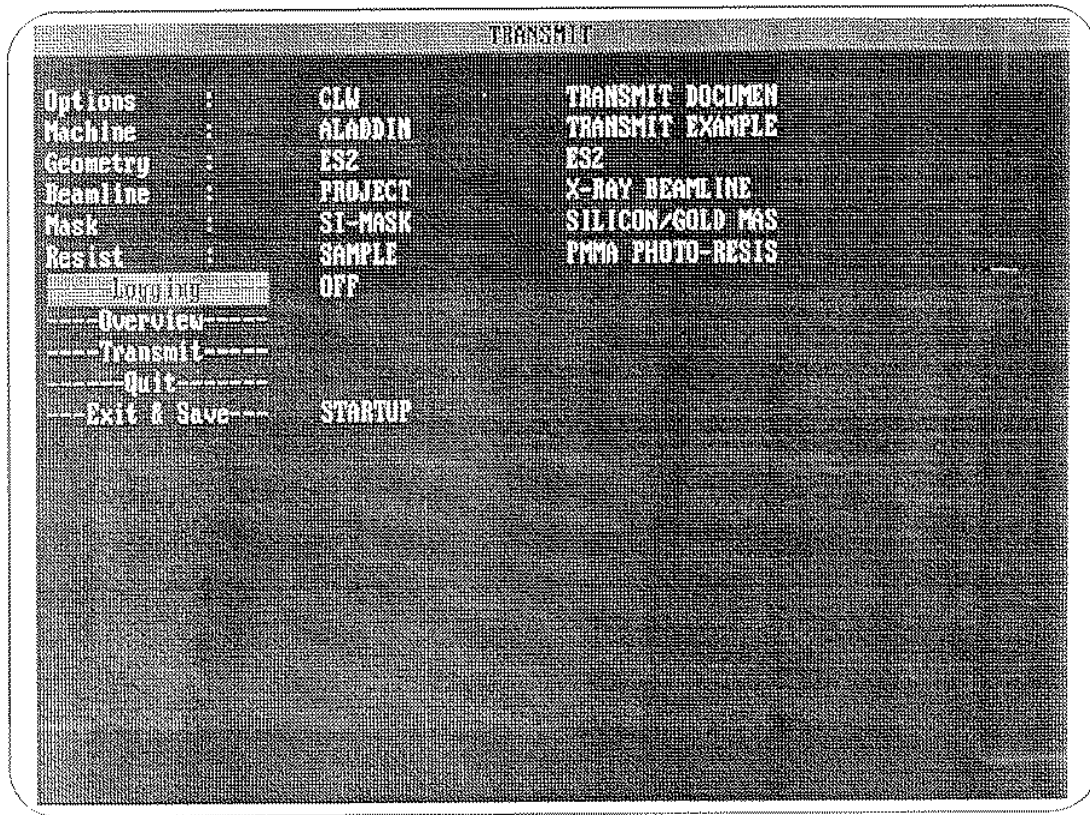
We return to the main menu and notice all the system names and titles appear here. This is where if the user had existing beamlines or masks etc., and wished to use them, he could load the specific system by name. If the user wishes to get a hardcopy of the entire system, this is the time to turn `Logging` on, run TRANSMIT, and turn it back off. The `Overview` option will give the same information as is in the log file, only to the screen. A sample run through the `Overview` option is shown in figures 5.9 – **??**. To save the source, beamline, mask, and resist so that they can all be loaded together at another time, move down to the `Exit & Save` option and name the startup file.

When we exit the program we get an assortment of files similar to the following:

```
Directory D1:[CWELNAK.TEMP]

101LOC.DAT;1            11  \* local properties at first mirror *\
101TOT.DAT;1            11  \* cummulative properties at first  *\
```

Figure 5.9: TRANSMIT: Overview screen

Compounds	Filter/ Mirror	Density	Thick/ Angle	Watts
1) M1	Mirror	19.30	88.00	1.92
2) M2	Mirror	19.30	89.00	1.51
3) M3	Mirror	19.30	89.00	1.19
4) BE	Filter	1.850	15.00	0.274
5) HE	Filter	.1786E-03	.2000E+06	0.245

Page 2
Press a key to continue

Figure 5.10: TRANSMIT: Overview screen

Figure 5.11: TRANSMIT: Overview screen

Figure 5.12: TRANSMIT: Overview screen

	T	Power	Ave E	3 %	50 %	97 %	Sigma	Std
Source		S 3.582	1098	610	1010	2010	350	31
Beam	1	M 1.924	950	610	1016	1740	282	25
Beam	2	M 1.513	950	610	1014	1740	282	25
Beam	3	M 1.190	950	610	1013	1730	280	25
Beam	4	P .2739	1330	840	1342	1890	262	22
Beam	5	P .2451	1350	860	1364	1900	260	22
Mask	1	C .1600	1390	930	1392	1810	220	19
Mask	2	A .1486E-01	1590	1160	1575	1940	195	16
Res CtA	1	A .1361E-01	1600	1170	1582	1950	195	15
Res C	1	C .1401	1410	950	1410	1810	215	19

POWER

Page 6
Press a key to continue

Figure 5.13: TRANSMIT: Overview screen
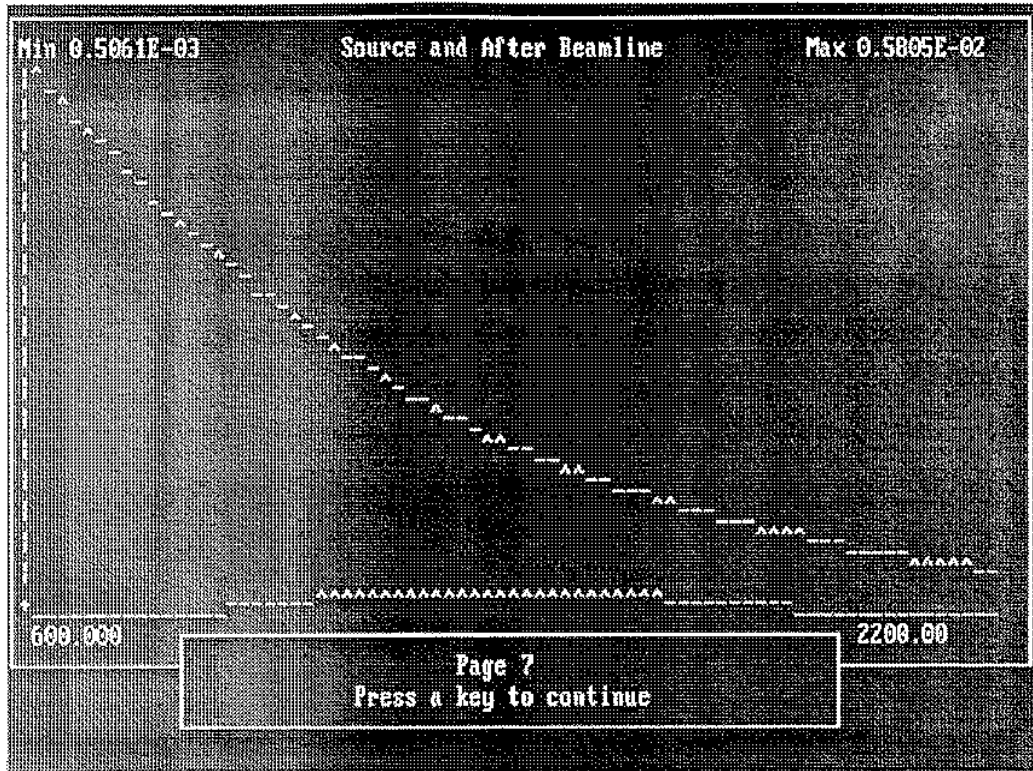
Figure 5.14: TRANSMIT: Overview screen
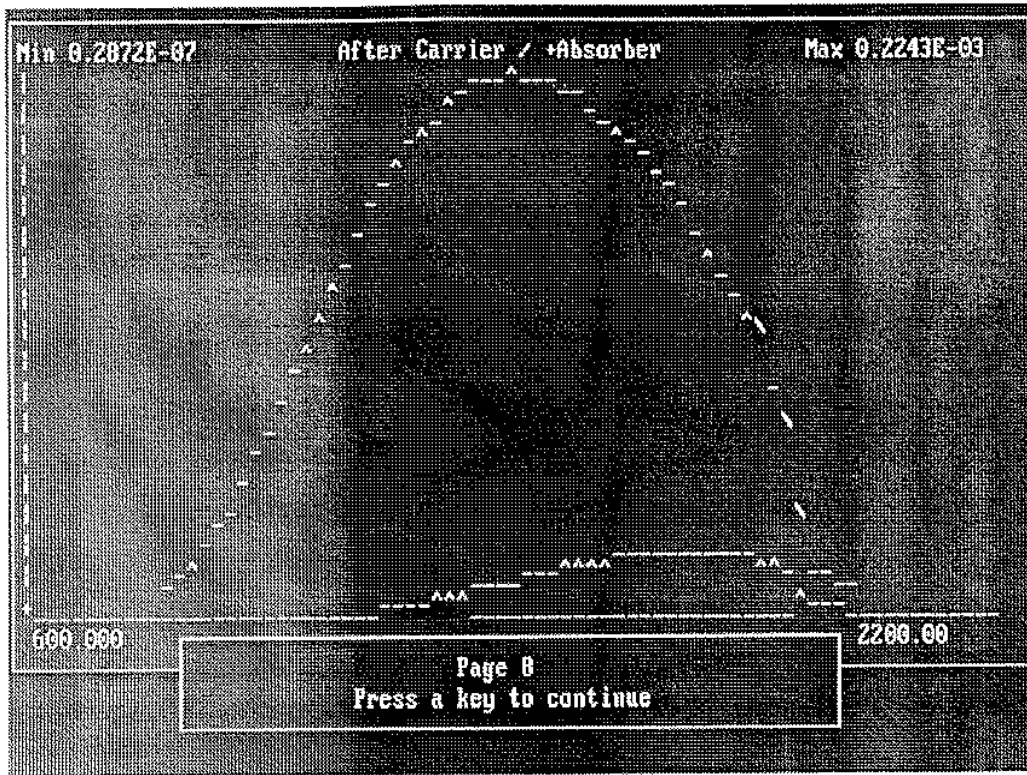
Figure 5.15: TRANSMIT: Overview screen

```
102LOC.DAT;1              11  \* second mirror                      *\
102TOT.DAT;1              11  \*                                    *\
103LOC.DAT;1              11  \* third mirror                       *\
103TOT.DAT;1              11  \*                                    *\
104LOC.DAT;1              11  \* beryllium filter                   *\
104TOT.DAT;1              11  \*                                    *\
105LOC.DAT;1              11  \* helium pathway                     *\
105TOT.DAT;1              11  \*                                    *\
201LOC.DAT;1              11  \* silicon carrier                    *\
201TOT.DAT;1              11  \*                                    *\
202LOC.DAT;1              11  \* gold absorber                      *\
202TOT.DAT;1              11  \*                                    *\
301LOC.DAT;1              11  \* photo-resist-carrier+absorber      *\
301TOT.DAT;1              11  \*                                    *\
401LOC.DAT;1              11  \* photo-resist after carrier only  *\
401TOT.DAT;1              11  \* above files generated w/logging on *\
BOOTSTRAP.DAT;19           1  \* system start-up files             *\
G-ES2.DAT;41               1  \*                                    *\
M-ALADDIN.DAT;42           1  \*                                    *\
MACHINE.DAT;4              3  \*                                    *\
O-CLW.DAT;14               1  \*                                    *\
S-EXAMPLE.DAT;22           5  \*                                    *\
S-PMMA.DAT;32              5  \*                                    *\
S-SIMASK.DAT;31            5  \*                                    *\
SRCOMP.DAT;4              11  \* source spectra                     *\
STARTUP.DAT;19             2  \* start-up file                      *\
TRANS.DAT;1                1  \*                                    *\
TRANSMIT.LOG;4            57  \* contains log of session            *\

Total of 30 files, 291 blocks.
```

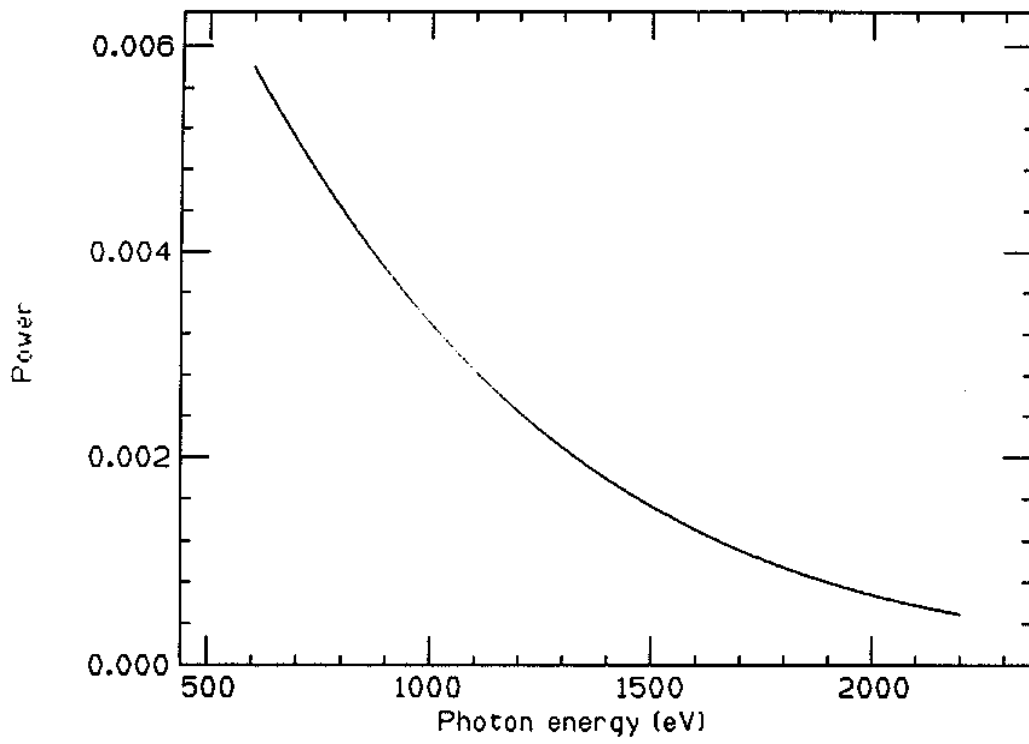Next we'll show plots generated by TopDrawer of some of the various data files generated.

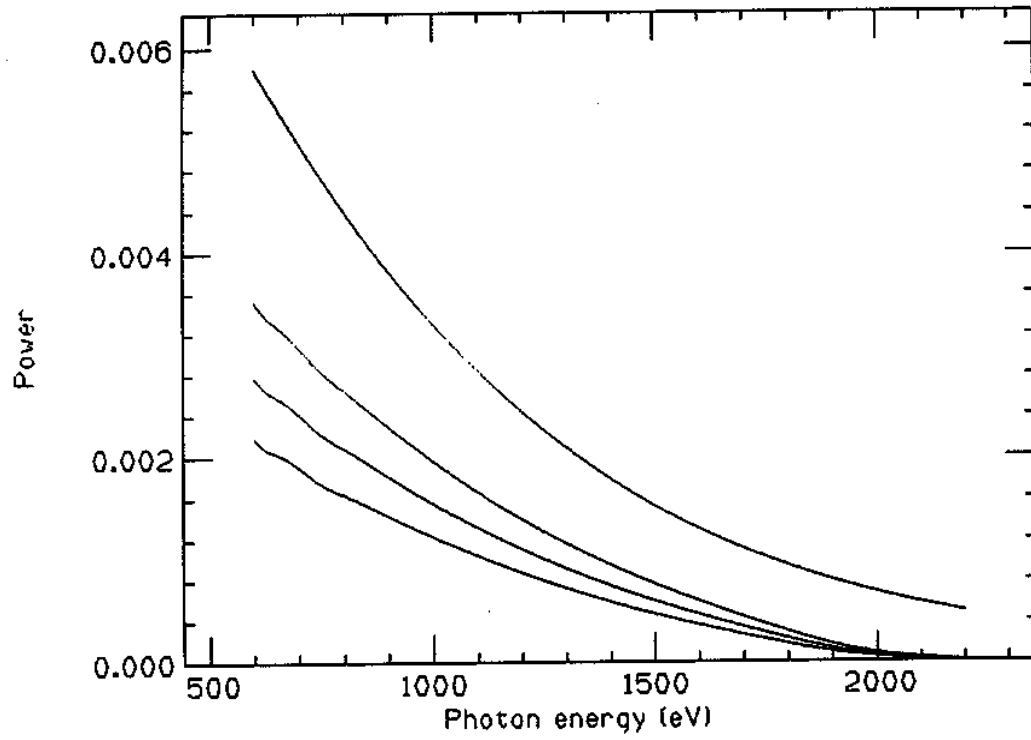Figure 5.16: TRANSMIT: Source spectra – SRCOMP.DAT

Figure 5.17: TRANSMIT: Source spectra and after each of the three mirrors
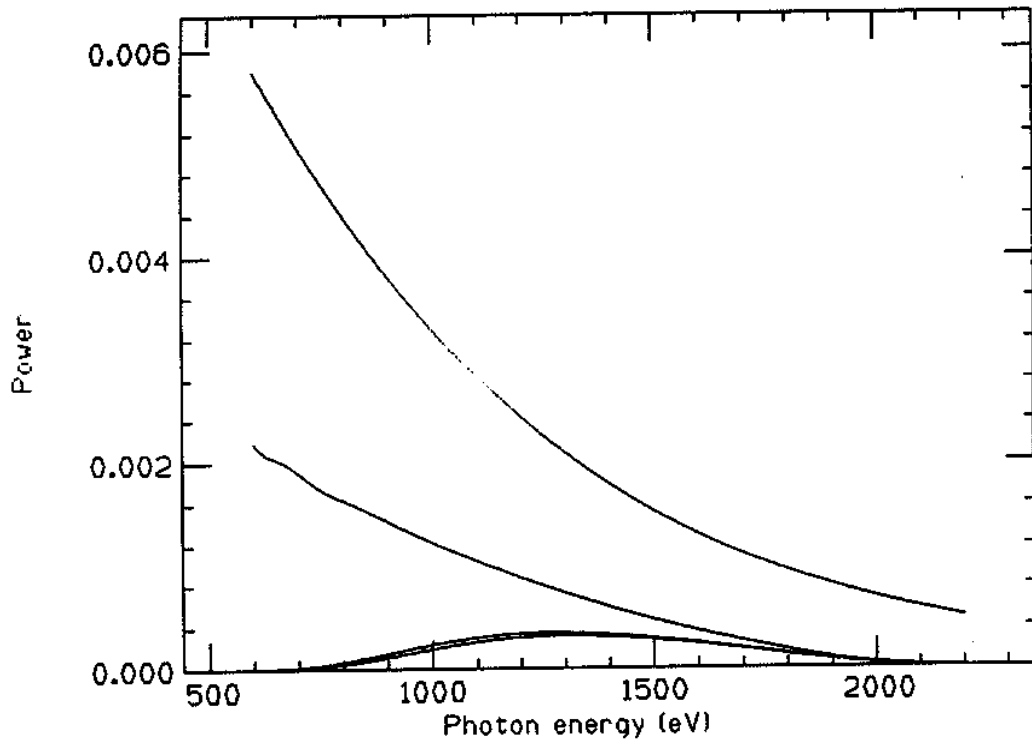
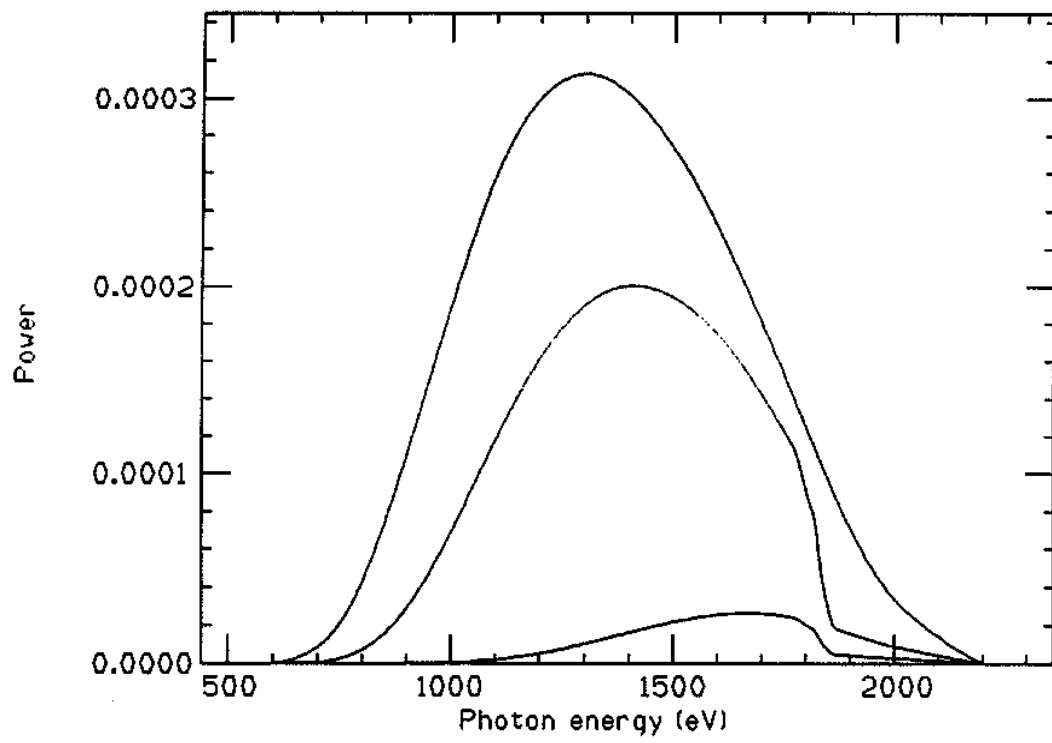Figure 5.18: TRANSMIT: Source, third mirror, beryllium window, and helium pathway

Figure 5.19: TRANSMIT: After complete beamline, after Si carrier, after Au absorber

SYNC_SPECTRA

Purpose: To generate the synchrotron spectra for a given machine.
Input: Machine parameters and energy range interested in.
Output: File containing photon energy, θ, power in TopDrawer format if desired.

Description:

SYNC_SPECTRA takes the parameters of the user's machine and scales them to the universal curves using the formula from C. K. Green. From this information, it generates a spectra in the desired form at the desired photon energy. The results can be scaled by several factors including to the critical energy, to the beam energy, logarithmically, and changing θ by a factor of γ.

Examples:

The following example uses the SR machine Aladdin for its parameters. The output file is plotted using TopDrawer for θ vs. power.

```
$
$ r sync_spectra
Machine radius  [ m ] : 2.083       \* Machine parameters *\
        energy  [ GeV ] : 0.8        \*
        current [ A ] : 0.1          \*
Subtended angle [ mrads ] : 30       \* geometry at port *\
Critical energy =    545.2986288035259    \* calculated by SYNC_SPECTRA *\
Options:
dE = const  0 [ phot/sec/mrad(V)/ eV ]
dL = const  1 [ phot/sec/mrad(V)/ Angs ]
dL/L = const  2 [ phot/sec/mrad(V)/%bandwidth ]
dE/E = const  3 [ phot/sec/mrad(V)/%bandwidth ]
Power dL = const  4 [ watts/mrad(V)/angs ]
Power dE = const  5 [ watts/mrad(V)/eV ]
Then ? 5                             \* here choose power in watts/mrad *\
Maximum Photon energy [wavelength]: 2200   \* "white" source *\
Minimum                 : 600
Number of points in energy [wavelength]: 17
Log Scale [ Y/N ] ? 0
```

```
Maximum vertical angle [ mrad ] : 1.25
Minimum                         : -1.25
No. of points in THETA : 250              \* vertical angle of above *\
Polarization [1,2,3] : 3                  \* parallel, perpindicular, total *\
Scale energy to critical energy [ Y/N ] ? 0
Scale flux to beam energy [ Y/N ] ? 0
Multiply theta by gamma [ Y/N ] ? 0
File for 3d Top Drawer ? 0
File for Top Drawer (with embedded JOIN)? 1  \* 2d plot *\
Output file name: spectd.dat
$ dir/since=-00:02

Directory CXRL$DUA0:[SHADOW.XRAYOP.DOCUMENT.UTIL.SYNC_SPECTRA]

SPECTD.DAT;1              399  27-SEP-1989 15:27:29.91  (RWED,RWED,RE,)

Total of 1 file, 399 blocks.
$ ty spectd.dat
  photon          theta           power
  energy

      :               :               :
      :               :               :
  600.0000      -1.019076       0.0000000E+00
  600.0000      -1.009036       0.0000000E+00
  600.0000      -0.9989960      0.0000000E+00
  600.0000      -0.9889558      0.0000000E+00
  600.0000      -0.9789157      0.0000000E+00
  600.0000      -0.9688755      0.0000000E+00
  600.0000      -0.9588354      0.0000000E+00
  600.0000      -0.9487952      0.0000000E+00
  600.0000      -0.9387550      0.0000000E+00
  600.0000      -0.9287149      9.8043092E-05
  600.0000      -0.9186747      1.1077573E-04
  600.0000      -0.9086345      1.3059203E-04
  600.0000      -0.8985944      1.4686001E-04
  600.0000      -0.8885542      1.6397580E-04
  600.0000      -0.8785141      1.8351113E-04
  600.0000      -0.8684739      2.0489228E-04
  600.0000      -0.8584337      2.2823217E-04
```
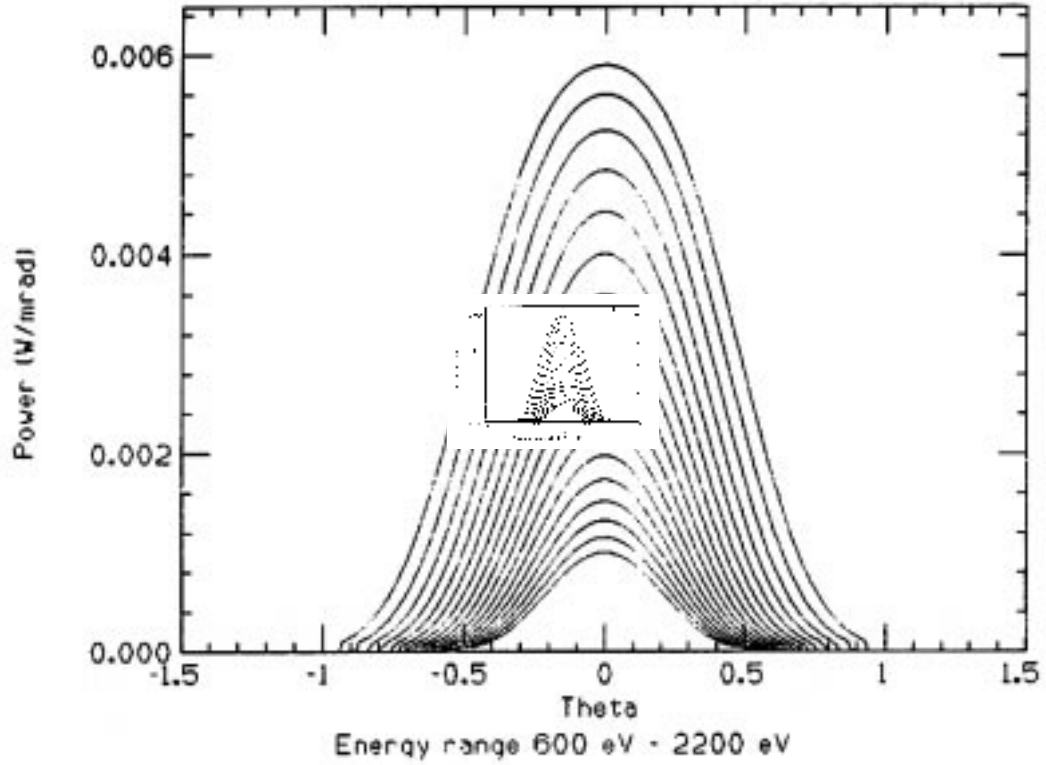
Figure 5.20: SYNC SPECTRA output

```
600.0000        -0.8483936        2.5364381E-04
600.0000        -0.8383534        2.8124033E-04
600.0000        -0.8283132        3.1113272E-04
600.0000        -0.8182731        3.4342680E-04
    :                 :                 :
    :                 :                 :
```

A plot of θ vs. power follows. Notice the decrease of the FWHM with the photon energy.

GRATING_SET

Purpose:	To compute some useful angles for diffraction gratings studies.
Input:	From keyboard.
Output:	To the terminal and a file DIFFRAC.DAT

Description:

The program recognizes the following cases:

1. Blazed grating. The grating is set at an angle relative to the incoming radiation that satisfies the grating equation for that wavelength and the specular reflection from the groove facet. Double grating systems can be configured efficiently in this mount.

2. Constant Incidence Angle. The user specify the incidence angle and the program computes the diffraction angles that satisfies the grating equation. Rowland Circle monochromators belong to this class.

3. Constant Included Angle. The deflection angle of the radiation (included angle) is kept constant and the incidence angle is computed to satisfy the diffraction condition. Typical examples of this case several varieties of Toroidal Grating Monochromators.

Examples:

We will consider each of the three cases that the program can handle. The data will also be stored in the file DIFFRAC.DAT. All the cases are based on the grating equation:

$$\sin(\alpha) - \sin(\beta) = m\frac{\lambda}{d} \tag{5.6}$$

where d is the grating spacing. The difference between the three cases is explained in the following figure. If the wavelength is too long to satisfy the grating equation, an error message will be issued.
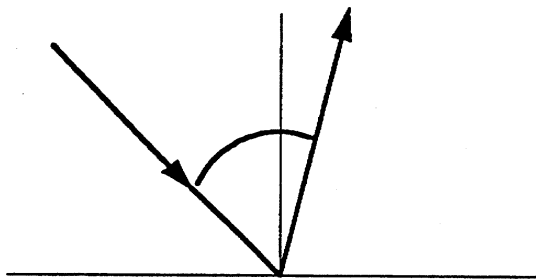
```
$RUN UTIL:GRATING_SET
File out the results ? 1 yes
Options:
Diffraction angles for given blaze..... [ 0 ]
              fixed incidence angle..... [ 1 ]
                fixed included angle..... [ 2 ]
```
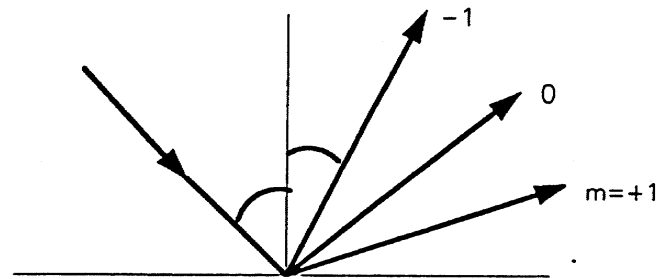
Constant Incidence Angle
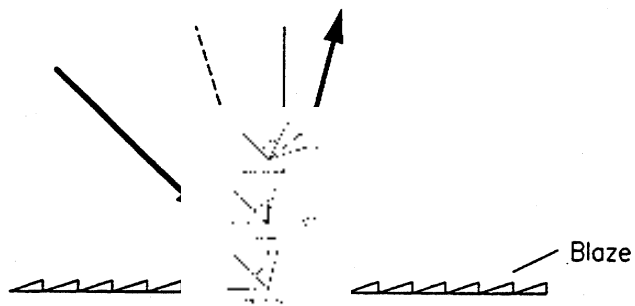
Blazed Grating

Constant Included Angle

Figure 5.21: GRATING_SET: Three diffraction cases available

```
Choice ? 1
Do you want to use eV [ 0 ] or Angstroms [ 1 ] ?
Choice ? 0
Photon Energy ? 500
Grating Line Density [ Lines / mm ] ? 1200
Order [ negatives are inside ] ? -1
Incidence Angle [ degrees ]? 88
Diffraction angle BETA:    85.14710385779866
Options:
Diffraction angles for given blaze..... [ 0 ]
             fixed incidence angle..... [ 1 ]
               fixed included angle..... [ 2 ]

Choice ? 0
Do you want to use eV [ 0 ] or Angstroms [ 1 ] ?
Choice ? 0
Photon Energy ? 800
Grating Line Density [ Lines / mm ] ? 1200
Order [ negatives are inside ] ? -1
Blaze angle [ degrees ]: 1
Incidence angle   ALPHA:    87.94575321306993
Diffraction angle BETA:    85.94575321306993
Options:
Diffraction angles for given blaze..... [ 0 ]
             fixed incidence angle..... [ 1 ]
               fixed included angle..... [ 2 ]

Choice ? 2
Do you want to use eV [ 0 ] or Angstroms [ 1 ] ?
Choice ? 0
Photon Energy ? 250
Grating Line Density [ Lines / mm ] ? 1200
Order [ negatives are inside ] ? -1
Included Angle [ degs ]? 170
Incidence   Angle [ degs ]:    86.95655527500508
Diffraction Angle [ degs ]:    83.04344472499492
Rotation    Angle [ degs ]:    1.956555275005078
Options:
Diffraction angles for given blaze..... [ 0 ]
```

```
                 fixed incidence angle..... [ 1 ]
                  fixed included angle..... [ 2 ]

 Choice ?
 ^Y
 $
 $
```

The following example was run using the TGM example. The six meter TGM has a fixed included angle of 160 degrees.

```
$
$ run util:grating_set
File out the results ? 1
Options:
Diffraction angles for given blaze..... [ 0 ]
              fixed incidence angle..... [ 1 ]
               fixed included angle..... [ 2 ]

Choice ? 2
Do you want to use eV [ 0 ] or Angstroms [ 1 ] ?
Choice ? 0
Photon Energy ? 50
Grating Line Density [ Lines / mm ] ? 1200
Order [ negatives are inside ] ? -1
Included Angle [ degs ]? 160
Incidence   Angle [ degs ]:    84.91514459719740
Diffraction Angle [ degs ]:    75.08485540280260
Rotation    Angle [ degs ]:    4.915144597197396
Options:
Diffraction angles for given blaze..... [ 0 ]
              fixed incidence angle..... [ 1 ]
               fixed included angle..... [ 2 ]

Choice ? 2
Do you want to use eV [ 0 ] or Angstroms [ 1 ] ?
Choice ? 0
Photon Energy ? 60
```

```
Grating Line Density [ Lines / mm ] ? 1200
Order [ negatives are inside ] ? -1
Included Angle [ degs ]? 160
Incidence   Angle [ degs ]:    84.09441581524222
Diffraction Angle [ degs ]:    75.90558418475778
Rotation    Angle [ degs ]:    4.094415815242220
Options:
Diffraction angles for given blaze..... [ 0 ]
             fixed incidence angle..... [ 1 ]
              fixed included angle..... [ 2 ]

Choice ?
<CTRL>Y
$ dir/since


Directory D13:[XRAYOP.DOCUMENT.UTIL.GRATING]

DIFFRAC.DAT;3              3  10-MAY-1989 14:56:22.01  (RWED,RWED,RE,RE)

Total of 1 file, 3 blocks.
$
$ type diffrac.dat
 --------------------------------------------
 --------------------------------------------
          Fixed Included Angle.
 --------------------------------------------
 Photon Energy      [ eV ]:   50.00000000000000
       Wavelength [ Angs ]:   247.9704000000000
 Line density      [ mm-1 ]:   1200.000000000000
 Order                 :   -1.000000000000000
 Included Angle    [ degs ]:   1.396263401595464

 Incidence   Angle [ degs ]:   84.91514459719740
 Diffraction Angle [ degs ]:   75.08485540280260
 Rotation angle    [ degs ]:   4.915144597197396
 --------------------------------------------
                end
 --------------------------------------------
 --------------------------------------------
 --------------------------------------------
```

```
        Fixed Included Angle.
---------------------------------------------
Photon Energy       [ eV ]:    60.00000000000000
      Wavelength [ Angs ]:    206.6420000000000
Line density      [ mm-1 ]:    1200.000000000000
Order                   :    -1.000000000000000
Included Angle    [ degs ]:    1.396263401595464

Incidence   Angle [ degs ]:    84.09441581524222
Diffraction Angle [ degs ]:    75.90558418475778
Rotation angle    [ degs ]:    4.094415815242220
---------------------------------------------
                end
---------------------------------------------
```

TORUS

Purpose:	Computes the major and minor radii for a toroidal mirror given the setup parameters.
Input:	The distances to the tangential and sagittal object and image planes, and the angle of incidence with respect to the mirror normal.
Output:	A log file containing the input parameters and the computed focal lengths and radii of curvature for the tangential and sagittal planes.

Description:

If a toroidal mirror is to be used in a system where the object and image distances for the tangential and sagittal planes as well as the angle of incidence are known, TORUS may be used to compute the parameters of the mirror surface without setting up and tracing the system. The object and image distances need not be coincident for the tangential and sagittal planes. If they are coincident, TORUS computes the parameters that minimize astigmatism for the optical element. The focal length is computed in the conventional method:

$$\frac{1}{p} + \frac{1}{q} = \frac{1}{f}$$

where p and q are the object and image distances and f is the focal length. The radii of curvature for the tangental and sagittal planes may be computed from the relations

$$\frac{1}{p} + \frac{1}{q} = \frac{2}{R\cos\theta}$$

and

$$\frac{1}{p} + \frac{1}{q} = \frac{2\cos\theta}{r}$$

where R and r are the radii for the tangential and sagittal planes respectively, and θ is the angle of incidence. Notice that {R,r} are the "optical" radii of the mirrors (R is, for example, the maximum radius). Sometimes other definitions are used in the equations defining the surface so that there may be an apparent difference of r or 2r with the values of R used by different authors.

Examples:

In this example we will have TORUS compute the radii for a toroidal mirror that has object and image distances both 100 cm from the mirror, and is illuminated at 85 degrees incidence. The results will be compared to a SHADOW run where a similar system is traced

with a point source having a conical angle distribution of 10 mrad. Note that we wish to
have the tangential and sagittal focal planes coincide. Let's run TORUS first:

```
$ run util:torus
 Name to use for log file ?  tor.par
 Tangential Object:  100
            Image:  100
 Sagittal   Object:  100
            Image:  100
 Incidence   Angle:  85

 Tangential.
 Focal length          =     50.00000000000000
 Optical Radius        =     1147.371324566986      \* R_0
 Sagittal.
 Focal length          =     50.00000000000000
 Radius                =     8.715574274765817
 Continue ?  0
```

After tracing the system described above, we check out the computed
mirror parameters using MIRINFO\index{MIRINFO}:

```
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 ******************** MIRROR  DESCRIPTION  ********************
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Toroidal Mirror
 TORUS example
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Input file specified:end.01
 Full file Specification :DISK4:[RUNKLE.UG.UTIL.TORUS]END.01;1
 Creation Date           : 1-MAY-1989 14:31
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Surface figure was defined as:          TOROIDAL
 Cylindrical figure                      NO
 Element type                            REFLECTOR
 Reflectivity                            OFF
 Mirror dimensions                       UNLIMITED
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Central Axis parameters :
```

```
   Source Plane Distance                    100.0000000000000
   Image  Plane                             100.0000000000000
   Incidence Angle                          84.99999999999999
   Reflection/Diffraction Angle             84.99999999999999

   Mirror parameters                   COMPUTED
   Same configuration as Central Axis  YES
   Objective focus at                       100.0000000000000
   Image focus at                           100.0000000000000
   Incidence angle                          84.99999999999999
   Parameters used follow:
      Major Radius      1138.655750292220    \* R_1    *\
      Minor Radius      8.715574274765816    \* rho    *\
   Source of this O.E. moved           NO
   Mirror at pole position ( no mov. )  YES
   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Notice that the radii computed by TORUS and SHADOW are in agreement. Indeed:

$$R_1 = R_0 - \rho$$

We can also look at the positions of the sagittal and tangential focii with respect to the final continuation plane by using FOCNEW:

```
   -----------------------------------------------------------------------
   Searching file :
   star.01
   DISK4:[RUNKLE.UG.UTIL.TORUS]STAR.01;1                      1-MAY-1989 14:3
   -----------------------------------------------------------------------
   Center at :Origin
   X =   0.0000000000000000E+00    Z =   0.0000000000000000E+00
   -----------------------------------------------------------------------
   Working with  500 "good" rays out of  500
   .............. S A G I T T A L  ..............
   X coefficients :   0.2539159622E-04 -0.5607838486E-05  0.2861789653E-05
   Center : 0.8078084052E-04   Average versor : 0.1794262007E-03
   Sagittal   focus at      :  0.2208541140
   Waist size at best focus (rms) :  0.1274078276E-02
```

```
Waist size at origin                    :   0.1691682492E-02
.............. T A N G E N T I A L ..............
Z coefficients :   0.2398763062E-04 -0.2063942800E-04  0.2015928704E-04
Center : 0.1149163952E-03   Average versor : 0.5822703881E-04
Tangential focus at        :   0.8604196190
Waist size at best focus (rms) :  0.1549425142E-02
Waist size at origin                    :   0.4489909469E-02
..............   LEAST CONFUSION  ..............
T coefficients :   0.4937922683E-04 -0.2624726648E-04  0.2302107669E-04
Center : 0.1404682245E-03   Average versor : 0.1886376144E-03
Circle of least confusion :  0.5315447034
Waist size at best focus (rms) :  0.3011557938E-02
Waist size at origin                    :   0.4798028417E-02
```

In practice it is quite difficult to eliminate astigmatism, but the toroidal mirror performed reasonably well here, considering the grazing angle of incidence.

Chapter 6

Graphics

This chapter covers the core level graphical utilities used with SHADOW and its utilities. They are a subset of TopDrawer a graphics program written at Stanford University.

TDTEK

Purpose:	General graphics program used in plotting much of the output from SHADOW and it's utilities.
Input:	TopDrawer commands or a command file containing TopDrawer commands and reference to a data file.
Output:	Terminal (TT:) and TD metafile with default name SAVE.DAT.

Description:

TDTEK is a graphics program that is part of TopDrawer. The output to the terminal can be suppressed by hitting <CTRL>O, as shown in specific examples. For the purpose of SHADOW and its utilities, example command files are given in the example for that utility. For more information on commands and other functions of TopDrawer, see the TopDrawer manual.

Notice that TDTEK writes to the virtual device UGDEVICE, which is often assigned to the terminal ($ASSIGN TT: UGDEVICE) but can be assigned to another terminal if the system implementation allows it ($ASSIGN RRE7: UGDEVICE). In this way text I/O will be directed to the standard terminal while the graphics will go to RRE7:. This is the best way to run TDTEK, otherwise text and graphics get hopelessly mingled.[1] TDTEK is quite useful for a "quick and dirty" examination of data files.

Examples:

Here we will use the example shown in SYSPLOT. We will wait to hit <CTRL>O, to demonstrate the output to the terminal.

```
$
$ type sysplot.com
set three
set order x y z
set limits x -50 50 y -100 4100  z -20 120
set ticks off
plot axes at 0 0 0
@sysplot.dat
end
```

---

[1]New graphics packages are being developed.

```
$
$ TDTEK
TOP DRAWER (10/10/80) NOW EXECUTING

@SYSPLOT.COM
READING FROM INDIRECT COMMAND FILE: SYSPLOT.COM
          1  set three

          2  set order x y z

          3  set limits x -50 50 y -100 4100  z -20 120

          4  set ticks off

          5  plot axes at 0 0 0

<CTRL>O                                  \\ suppresses output to screen
$                                        \\ It's probably a good idea to
$                                        \\ hit <CTRL>O sooner than shown
$ dir/since                              \\ if not running in graphics mode.

Directory D13:[XRAYOP.DOCUMENT.UTIL.TDTEK]

SAVE.DAT;1              11   5-MAY-1989 09:16:29.40  (RWED,RWED,RE,RE)
TD.FIL;1                1   5-MAY-1989 09:16:20.09  (RWED,RWED,RE,RE)

Total of 2 files, 12 blocks.
$
$ type td.fil
@SYSPLOT.COM
$
```

TDFILE

Purpose:	Non interactive version of TopDrawer.
Input:	A set of TopDrawer commands or a TopDrawer command file.
Output:	A TopDrawer log file (TD.FIL) that contains the commands for the non-interactive session, and a file (SAVE.DAT) to be input to the Unified Graphics utilities for graphics output.

Description:

TDFILE controls a non-interactive session of TopDrawer. The procedures for runing Top-Drawer through TDFILE are the same as those in TDTEK except that there is no direct graphics output. Advantages of running in this mode include an absence of clutter from a mixture of text and graphics and creating graphics files on terminals without graphics capability to be plotted elsewhere, as it may happen in a batch run. The graphics file SAVE.DAT may be used as input to UGTEK or a similar Unified Graphics utility for video display or hard copy.

TD_NEW

Purpose:	General purpose graphics program.
Input:	TopDrawer command file or commands and data file.
Output:	Plot to terminal.

Description:

This utility calls a general graphics program that processes a TopDrawer command file and plots the information to the screen. The terminal must be in graphics mode before calling TD_NEW. The command file input would be the same as for TDTEK. Instead of writing the information to a TD metafile, it is plotted to the screen directly.

Examples:

As with UGTEK, the transition between text and graphics mode cannot be shown well. We will again use the files SYSPLOT.COM and SYSPLOT.DAT to illustrate this utility.

To get output to an LN03 laser printer is fairly simple with TD_NEW. One need not put the terminal graphics mode. Simply make the first line typed or in the command file SET DEVICE LASER. This generates a file with the default name LN03.PLOT that can be printed using a standard print command with no set format.

```
$
$ TYPE SYSPLOT.COM
set three
set order x y z
set limits x -50 50 y -100 4100  z -20 120
set ticks off
plot axes at 0 0 0
@sysplot.dat
end
$
$ DTEKON            \\ terminal in graphics mode

$ TD_NEW
Top Drawer 08/11/82
@SYSPLOT.COM
```

```
                        \\ at this point the plot is being drawn to the screen.
                        \\ hitting <return> will get you back to the DCL prompt
                        \\ when finished plotting.
FORTRAN STOP
$
$ DTEKOFF           \\ terminal returns to text mode.
$
```

UGTEK

Purpose:	Plots a TopDrawer metafile to the screen.
Input:	A TopDrawer metafile (i.e. SAVE.DAT from TDTEK or TDFILE).
Output:	A plot on the screen.

Description:

The command UGTEK will plot a TopDrawer metafile to the screen. The terminal must be in graphics mode for the plot to be drawn to the screen. A TD metafile is created by running either TDTEK or TDFILE on a TopDrawer command file. It's default name is SAVE.DAT. If there is more than one picture in a SAVE.DAT file, UGTEK gives you the opportunity to specify which pictures to plot, defaulting to plotting all (sequentially), and also gives you the chance to reduce the size of the picture.

Examples:

The page does not show well the transition from text to graphics mode, and consequently the output of UGTEK. However, we will show how to run through UGTEK, the result being a plot on the screen.

```
$
$ DTEKON                  \\ puts the terminal in graphics mode.  Clears scree
                          \\ for plot.
$ UGTEK

  UG element file: SAVE.DAT
  Plot which pictures (default=all)?
  Enter picture scale factor (default=1.0):
```

At this point the screen clears again to make space for the plot. Hitting <RETURN> will return you to the DCL command level when the plot has finished.

```
$ DTEKOFF                 \\ Returns the terminal to text mode.
```

UGHP7470

Purpose: To plot a TopDrawer metafile on an HP 7470 plotter in high quality.

Input: TopDrawer metafile such as SAVE.DAT output from TDTEK or TDFILE.

Output: High quality plot of TopDrawer metafile on HP plotter.

Description:

The command UGHP7470 will plot a TopDrawer metafile to an HP plotter in high quality, suitable for publication. A TD metafile is created by running either TDTEK or TDFILE on a TopDrawer command file. Its default name is SAVE.DAT. If there is more than one picture in a SAVE.DAT file, UGHP7470 gives you the opportunity to specify which pictures to plot, defaulting to plotting all, and also gives you the chance to reduce the size of the picture. Notice that the program expects the plotter to be connected between the computer and the terminal with the "Y" cable. Alternatively, the file can be captured in a log session or (if using a PC emulator) on a local media for later plotting.
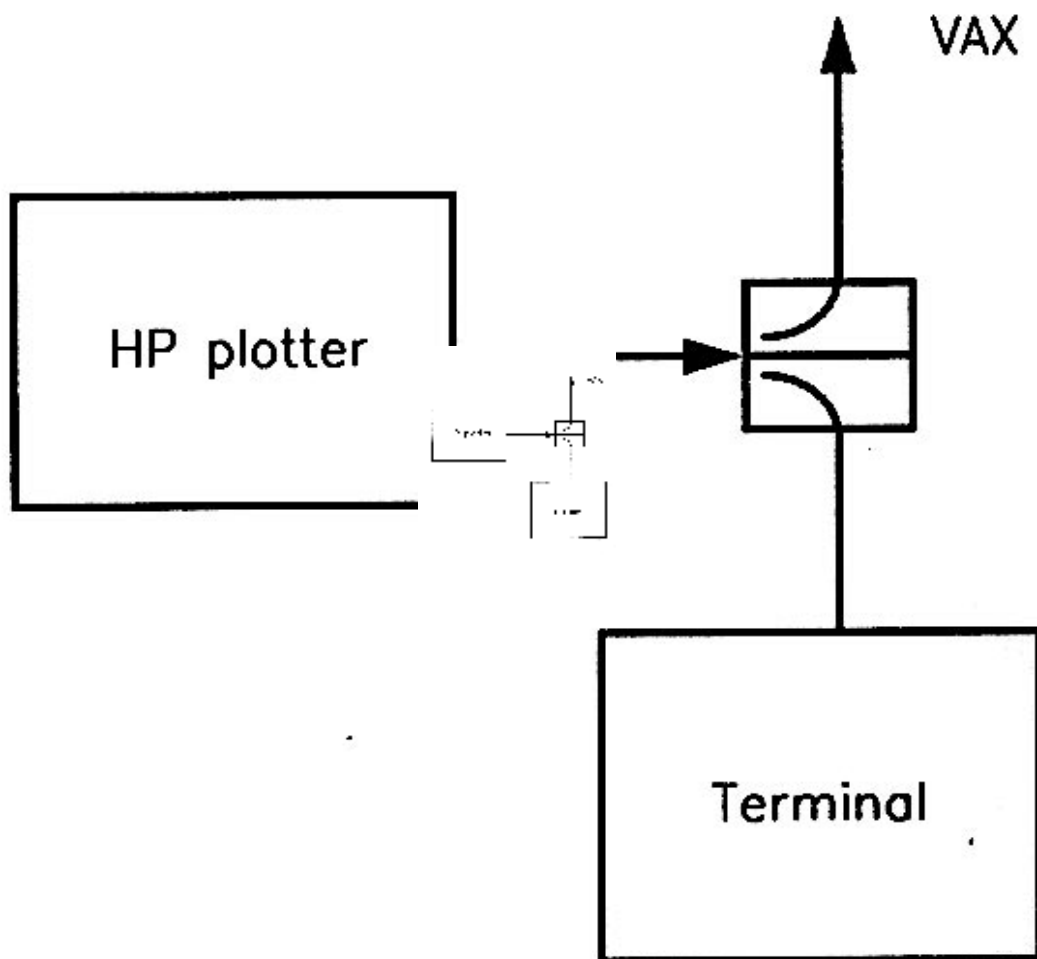
Figure 6.1: UGHP7470: Plotter/terminal setup

UGHP7470S

Purpose: To plot a TopDrawer metafile on an HP 7470 plotter in draft quality.
Input: TopDrawer metafile such as SAVE.DAT output from TDTEK or TDFILE.
Output: Draft quality plot of TopDrawer metafile on HP plotter.

Description:

The command UGHP7470S will plot a TopDrawer metafile to an HP 7470 plotter in draft quality. A TD metafile is created by running either TDTEK or TDFILE on a TopDrawer command file. Its default name is SAVE.DAT. If there is more than one picture in a SAVE.DAT file, UGHP7470S gives you the opportunity to specify which pictures to plot, defaulting to plotting all, and also gives you the chance to reduce the size of the picture.
The same setup as in UGHP7470 applies here as well.

Chapter 7

General Utilities

The utilities in this chapter are more convenience utilities than SHADOW utilities. They perform tasks that, though rather simple, take multiple steps and are easier used in program form.

CLIP

Purpose: Clips the second column in a two column formatted file. CLIP gives the user the extrema for the second column, and asks for upper and lower clipping values. If any data is outside the specified range it is set equal to the clippping bound.
Input: Any two column formatted file (e.g. output from PREPLOT).
Output: A two column formatted file (similar to input file).

Description:

This utility clips the second column of a two column formatted file using the following rules:

> IF Y $>$ MAX THEN Y:=MAX
> IF Y $<$ MIN THEN Y:=MIN

The input file is scanned and the extrema are displayed. Then the user can enter the desired values for MAX and MIN. This program is useful for cleaning up files that have some rays that fall far from the mean. Then the clipped file can be plotted without overscaling to accomodate the stray rays. Also, the graphics program TopDrawer crashes if the range is too wide. TD converts first to integers then checks for limits; in this step a very small number (10^{-30}) will cause an overflow while zero values are handled correctly. This may happen when computing absorption or transmission data near an edge. In this case, CLIP to zero.

Examples:

We'll run CLIP on the first 15 rows in the file PRE.DAT (See PREPLOT document for details on how PRE.DAT was generated).

```
$ clip
Input file ?  pre.dat
Output file ?  clip.dat
CLIP> Read   15 records.
Enter 0  to clip at zero only, 1 to other limits
 1
Found:
Ymax =    2.5044683E-02
```

```
Ymin =  -2.5014305E-02
CLIP> Enter Ymin,Ymax
CLIP> Ymax =  2.0e-2
CLIP> Ymin =  -2.0e-2
CLIP> Do you want IF (y,lt.1.0e-10) y = 0  [ y=1,n=0 ] ? 1
```

Here's a before and after look at the data.

Before:

```
-0.2780961        1.8455550E-02
-0.2831062        1.8694960E-02
 0.3307338       -2.2033621E-02
-0.3311352        2.2213560E-02
-9.4173871E-02  6.2023830E-03
 0.2767766       -1.8385222E-02
 0.3686378       -2.4258027E-02
 0.1166269       -7.7635958E-03
-0.3735043        2.5044683E-02
-0.3660054        2.4130033E-02
-9.1828540E-02  6.0481941E-03
 0.3607364       -2.4109263E-02
 0.3719847       -2.5014305E-02
-3.2931246E-02  2.2053795E-03
 0.1509321       -1.0015748E-02
```

After:

```
-0.2780961        1.8455550E-02
-0.2831062        1.8694960E-02
 0.3307338       -2.0000000E-02
-0.3311352        2.0000000E-02
-9.4173871E-02  6.2023830E-03
 0.2767766       -1.8385222E-02
```

```
  0.3686378      -2.0000000E-02
  0.1166269      -7.7635958E-03
 -0.3735043       2.0000000E-02
 -0.3660054       2.0000000E-02
 -9.1828540E-02  6.0481941E-03
  0.3607364      -2.0000000E-02
  0.3719847      -2.0000000E-02
 -3.2931246E-02  2.2053795E-03
  0.1509321      -1.0015748E-02
```

Another example is the transmission of a 25 μm beryllium window in the energy range 100-1000 eV. We run ABREFC to get the TRANSMISSION.DAT file, then run that through CLIP.

```
$
$
$ abrefc
Full printout at Terminal ?
0
Thickness (microns) ?
25
The program is setup to compute optical constants of
compounds with up to 5 elements.
How many atomic species ?
1
H2O would be: HH,2 and OO,1. Then ?
Enter 2-letters (capitalized) atomic symbol and formula index for :
1
BE                                              \* beryllium *\
1
Density ?
1.96                                            \* g/cm^3 *\
Enter starting photon energy,end and step
100
1000
50
Incidence angle ?
0
Molecular weight is :    9.010000
```

```
Atoms/Cm3
 1.3100236E+23  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00
$ dir/since

Directory D13:[XRAYOP.DOCUMENT.UTIL.CLIP]

ABSOR_COEFF.DAT;1            2  13-JUL-1989 15:06:36.28  (RWED,RWED,RE,RE)
CROSS_SECTION.DAT;1
                            2  13-JUL-1989 15:06:38.09  (RWED,RWED,RE,RE)
DIELEC_FUNC.DAT;1           2  13-JUL-1989 15:06:36.91  (RWED,RWED,RE,RE)
ELECTRON_YIELD.DAT;1
                            2  13-JUL-1989 15:06:37.48  (RWED,RWED,RE,RE)
ENERGY_LOSS.DAT;1          2  13-JUL-1989 15:06:37.20  (RWED,RWED,RE,RE)
REFLECTIVITY.DAT;1         3  13-JUL-1989 15:06:35.97  (RWED,RWED,RE,RE)
REFRAC_INDEX.DAT;1         2  13-JUL-1989 15:06:37.75  (RWED,RWED,RE,RE)
TRANSMISSION.DAT;1         2  13-JUL-1989 15:06:36.53  (RWED,RWED,RE,RE) <<<

Total of 9 files, 17 blocks.
$ ty transmission.dat              \* original file.  Notice the very small
  100.0000     2.7356200E-17       \* values that would trip up a program
  150.0000     0.0000000E+00       \* like TopDrawer.
  200.0000     0.0000000E+00
  250.0000     0.0000000E+00
  300.0000     8.6374230E-39   <<< crash site
  350.0000     3.3791325E-26
  400.0000     1.2199397E-18
  450.0000     1.2972137E-13
  500.0000     2.6327970E-10
  550.0000     4.6298648E-08
  600.0000     1.9180404E-06
  650.0000     2.9635275E-05
  700.0000     2.2219188E-04
  750.0000     1.0262434E-03
  800.0000     3.3866602E-03
  850.0000     8.6356746E-03
  900.0000     1.7964149E-02
  950.0000     3.2535858E-02
  1000.000     5.3043921E-02
$ clip
Input file ? transmission.dat
```

```
Output file ? trans_clip.dat
CLIP> Read   19 records.
Enter 0  to clip at zero only, 1 to other limits
1
Found:
Ymax =   5.3043921E-02
Ymin =   0.0000000E+00
CLIP> Enter Ymin,Ymax
CLIP> Ymax = 6e-02
CLIP> Ymin = 0
CLIP> Do you want IF (y,lt.1.0e-10) y = 0  [ y=1,n=0 ] ?1  \* get rid of 1E-
$                                                   \* values.  *\
$ type trans_clip.dat                        \* after *\
   100.0000      0.0000000E+00
   150.0000      0.0000000E+00
   200.0000      0.0000000E+00
   250.0000      0.0000000E+00
   300.0000      0.0000000E+00
   350.0000      0.0000000E+00
   400.0000      0.0000000E+00
   450.0000      0.0000000E+00
   500.0000      2.6327970E-10
   550.0000      4.6298648E-08
   600.0000      1.9180404E-06
   650.0000      2.9635275E-05
   700.0000      2.2219188E-04
   750.0000      1.0262434E-03
   800.0000      3.3866602E-03
   850.0000      8.6356746E-03
   900.0000      1.7964149E-02
   950.0000      3.2535858E-02
   1000.000      5.3043921E-02
$
```

COL_2

Purpose: Extract any two columns from an ASCII, N column file.
Input: A file with N columns.
Output: A file with any two columns extracted from the input file.

Description:

This utility reads in a formatted ASCII file with a known number of columns, and allows the user to choose any two columns to be written to another file in the order specified by the user. This utility will not work on binary output files such as MIRR.xx or STAR.xx without first running them through TRANSLATE.

Examples:

Two examples follow. The first example demonstrates the most common type of file this utility works on, a simple file with multiple columns, where each line is a column. The second example demonstrates how the utility works on a translated ray file.

```
$
$ type example.lis
   1  101  102  103  104
   2  201  202  203  204
   3  301  302  303  304
   4  401  402  403  404
   :    :    :    :    :
   :    :    :    :    :
 101  111  222  333  444
$
$ col_2
input file : example.lis
How many columns in the input file : 5
output file : col2.out
Column 1 : 2
Column 2 : 4
$
$ type col2.out
    \* column 2                 column 4 \*
```

```
   101.0000000000000        103.0000000000000
   201.0000000000000        203.0000000000000
   301.0000000000000        303.0000000000000
   401.0000000000000        403.0000000000000
            :                        :
            :                        :
   111.0000000000000        333.0000000000000
 $
```

For this example we'll use the synchrotron source file BEGIN.DAT created for use with the
TGM examples. First we'll run TRANSLATE to format the file. Then we'll run COL_2 to
extract columns 4 and 6, the angle distribution. For this example we'll only use 20 rays.

```
 $
 $ translate
 File for input ? begin.dat
 and for output ? tbegin.dat
 Read                 1000 rays.
 Each ray has           12 entries.
 how many rays to translate ?
 20
 All done.
 $

 $ col_2
 input file : tbegin.dat
 How many columns in the input file : 12
 output file : col.out
 Column 1 : 4
 Column 2 : 6
 $
 $ dir/since

 Directory D13:[XRAYOP.DOCUMENT.UTIL.COL_2]

 COL.OUT;1                    2   5-MAY-1989 14:24:28.07  (RWED,RWED,RE,RE)
 TBEGIN.DAT;1                12   5-MAY-1989 14:14:02.81  (RWED,RWED,RE,RE)
```

```
Total of 2 files, 14 blocks.
$
$ type col.out
 7.1207349033216965E-03  4.2598658113385647E-04
-2.6712548929609998E-03 -5.3321707887277658E-04
-4.2450409837258438E-04  8.9222914618205597E-04
-1.5401936936191181E-03  1.4590310682053907E-03
 1.0545386278912323E-02  5.3498849279228146E-04
 1.5371153788922542E-03 -2.9422052535095319E-04
-9.0826729006043025E-04 -4.2770848179471979E-04
 6.4885397124077561E-03  2.6606883484927588E-04
-9.0210832491599969E-03  1.1547317216979092E-03
 4.5896466841608658E-03  1.1607701177610969E-03
 6.0678659520798649E-03  7.6186301014691257E-04
-7.8908855034182015E-04  4.8762170237351560E-04
-2.0309429492565774E-03 -4.3717432212851493E-05
 1.4943430919349669E-03 -3.8288106268715352E-04
-7.6212021143264583E-03 -4.8180567614367067E-05
-8.3078372735220177E-03  5.8870256818982272E-04
 9.5664992971012362E-03 -2.8970588545932720E-04
-1.7791916484991329E-03  6.1577849756395542E-04
 3.7020178414177026E-03 -1.9409225197437758E-04
-2.5605721601357427E-04 -5.8362582323245487E-04
$

\* now compare the above list with the entries in columns 4 and 6 from *\
\* the first two records of tbegin.dat *\

$ type tbegin.dat
  5.0982915276736750E-04   1.483496817385351      -1.3608385926677304E-02
  7.1207349033216965E-03  0.9999745565112491       4.2598658113385647E-04
  0.9999746472458372      -7.1207342572083670E-03 -3.0334144220366471E-06
    1.000000000000000      2533844.889220482       1.000000000000000

 -1.8923075843487773E-02 -0.5565551450115362      -5.9508659084241021E-03
 -2.6712548929609998E-03  0.9999962900315399      -5.3321707887277658E-04
  0.9999964321922838       2.6712545132120622E-03 -1.4243638128054778E-06
    1.000000000000000      2533844.889220482       2.000000000000000
            :                       :                       :
            :                       :                       :
```

DIRTIME

Purpose: Prepares a file with a listing of the default directory sorted by date.
Input: None.
Output: A file DIRTIME.LIS containing the sorted directory.

Description:

The utility writes a file of the default directory to disk and then sorts it according to the date, using VMS $DIRECTORY and $SORT commands. Strangely enough, VMS does not have a switch to change the sorting of the directory listing. It is sometimes important to see when files were created relative to others. This simple utility fills the gap.

Examples:

```
$ show def
  BEAMROOT:[XRAYOP.DOCUMENT]
$ DIRTIME
Sorted listing ready in DIRTIME.LIS.
$
$
$ type dirtime.lis


  Directory          D13:[XRAYOP.DOCUMENT]

\* name                                        size       date  *\

  UG.DIR;1                                        2      16-JUN-1988 23:
  PAGE.TEX;2                                      2       8-JUL-1988 22:
  DIRTEX.DAT;2                                    2      10-JUL-1988 11:
  DIRTEMP.DAT;9                                   1      11-JUL-1988 15:
  DIRTRY.DAT;1                                    1      11-JUL-1988 15:
  DOC_PREP.FOR;28                                11      11-JUL-1988 16:
  DOC_PREP.EXE;19                                14      11-JUL-1988 17:
  DOCPROG.DAT;6                                   4       2-AUG-1988 11:
  INTRODUCTION.DIR;1                              1       6-DEC-1988 10:
```

SOURCE.DIR;1	4	12-DEC-1988 15:57
CLIP.DIR;1	1	30-JAN-1989 12:46
HISTO2.DIR;1	1	30-JAN-1989 12:48
MIRINFO.DIR;1	1	30-JAN-1989 12:48
FMAX.DIR;1	1	30-JAN-1989 12:48
FILEX.DIR;1	1	30-JAN-1989 12:48
MINMAX.DIR;1	1	30-JAN-1989 12:48
H2KOL.DIR;1	1	30-JAN-1989 12:48
HISTO1.DIR;1	1	30-JAN-1989 12:48
FOCNEW.DIR;1	1	30-JAN-1989 12:48
MERGEROW.DIR;1	1	30-JAN-1989 12:48
HISTO3.DIR;1	1	30-JAN-1989 12:48
DOSE.DIR;1	1	30-JAN-1989 12:48
PLOTXY.DIR;1	1	30-JAN-1989 12:53
PLOTFOC.DIR;1	1	30-JAN-1989 12:53
PREPLOT.DIR;1	1	30-JAN-1989 12:54
REFLAG.DIR;1	1	30-JAN-1989 12:54
RECOLOR.DIR;1	1	30-JAN-1989 12:54
PREPLOT2.DIR;1	1	30-JAN-1989 12:54
RETRACE.DIR;1	1	30-JAN-1989 12:57
SURPLOT.DIR;1	1	30-JAN-1989 12:58
REVPRINT.DIR;1	1	30-JAN-1989 12:58
SCAN.DIR;1	1	30-JAN-1989 12:58
SOURCINFO.DIR;1	1	30-JAN-1989 12:58
SYSINFO.DIR;1	1	30-JAN-1989 13:00
COP.COM;7	1	30-JAN-1989 13:00
TRANSLATE.DIR;1	1	30-JAN-1989 13:01
VARIANCE.DIR;1	1	30-JAN-1989 13:01
SYSPLOT.DIR;1	1	30-JAN-1989 13:01
DIR.LST;4	2	30-JAN-1989 13:07
TRACE.DIR;1	1	17-FEB-1989 15:56
PREREFL.DIR;1	1	22-FEB-1989 21:52
PRE_MLAYER.DIR;1	1	23-FEB-1989 20:33
MLAYER.DIR;1	1	23-FEB-1989 21:56
ABREFC.DIR;1	1	24-FEB-1989 21:02
COMB_RAY.DIR;1	1	24-FEB-1989 22:42
CUTOFF.DIR;1	1	25-FEB-1989 12:53
DIRTIME.DIR;1	1	25-FEB-1989 13:08

```
Total of   48 files.


$
$
```

FILEX

Purpose:	To perform simple algebraic operations on the second column of a two column formatted fileand to plot out the results. A list of legal operations is given to the user upon request.
Input:	Any two column ASCII files such as those generated by PREPLOT. One or two files may be used as input.
Output:	A two column ASCII file.

Description:

It is often desirable to perform simple algebraic operations among files, such as division or multiplication without having to write every time a program ex-novo. The operation may be performed between two files or a file and a scalar. FILEX implements a logic as described below. This guide to FILEX can be displayed by typing ? after the prompt FILEX>.

```
                  PROGRAM        FILEX


  This program is a file manipulation utility. Operations are performed on
two files having the format of an (x,y) table and the same number of elem
Command format is:

                  file-out = file1 /oper/ file2

where /oper/ is an operation symbol, like *, +, -, /.

 If file2 is written as %123, then 123 will be used as a factor for the
Y (second) column.

 The following symbols operates only on one file. They are

     &       Sum of X, Y                           #       Computes 1/Y
     ^       Derivative of Y                        ~       SQRT (Y)
     @       Integral of second column             "       Interchange X and Y
     \       Inverts the sequential order ( 1 --> N, N --> 1 )
     |       Replace Y with X*Y
     [       Mean and st. dev. of X weighed by Y
```

```
     To plot out a file, type:    %Plot = file-name
```

If the extension of the files in the command line is *.dat, then the extension may be omitted. Also, the file-out may have the same name as one of the files on which the operation is being performed. This helps keep the directory clean when several operations are to be applied to a file.

Examples:
Add X, Y :   file.out = file1 + file2
Multiply Y by 200:   file.out = file1 * %200
Subtract Y2 from Y1:   file.out = file1 - file2

Note: Because of the simple parser used, correct spacing of the '=' and operations between filenames is critical for proper generation of output file.

Examples:

Here we will examine the reflectivity of a gold coated mirror as a function of grazing angle. The mirror will be illuminated by a 100 points between 0 and 12 degrees. PREPLOT will be used to create a two column file with the intensity vs divergence in radians in the image plane. We will use FILEX to convert the radians to degrees and to add the grazing angle of the central ray to the angle of all the rays. FILEX will also be used to plot out the results. The source and system descriptions follow:

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
************** S O U R C E      D E S C R I P T I O N **************
Point source with Grid angle distribution
Filex Example
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
end.00
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.FILEX]END.00;4
Creation Date           :14-APR-1989 14:44
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Mixed Type Source. Spatial: RANDOM, directions: GRID
Generated total          100 rays.
Source assumed BIDIMENSIONAL (flat).
Source Spatial Characteristics: POINT
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Emission Characteristics
Distribution Type: LAMBERTIAN
Distribution Limits. +X :   0.000000000E+00 -X:   0.000000000E+00 rad
                    +Z :   0.100000000    -Z:   0.100000000    rad
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Source Photon Energy Distribution: SINGLE LINE
Photon Energy:   1000.0     eV, or   12.399     Angs.
Angular difference in phase is  0.00000E+00
Degree of polarization is  0.50000
Source points have INCOHERENT phase.
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************                 E N D               **************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++




++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
********************  MIRROR  DESCRIPTION   *******************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Gold coated spherical mirror
Filex example
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.01
Full file Specification :D13:[XRAYOP.DOCUMENT.UTIL.FILEX]END.01;3
Creation Date            :14-APR-1989 14:46
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:        PLANE
Cylindrical figure                    NO
Element type                          REFLECTOR
Reflectivity       ON    coefficients from:
auf1.opt
Polarization dependence               YES
Mirror dimensions                     UNLIMITED
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                    10.00000000000000
```

```
Image  Plane                                   10.00000000000000
Incidence Angle                                84.00000000000001
Reflection/Diffraction Angle                   84.00000000000001

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
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

$ preplot
PREPLOT> Input file ?  star.01
Read                100 rays.
Each ray has         18 entries.
PREPLOT> How many columns to write out ?  2
Row [1-18]  : 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 :   23       \* intensity vs. *\
PREPLOT>        2 :  6        \* Z'          *\
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
**********
Found          100 good points out of          100
Output options :
  [ 0 ] store rays in a file
  [ 1 ] plot directly on screen
```

```
   [ 2 ] both
 Then ?  0
 PREPLOT> Output file ?  reflec2.dat


 $ filex
 FILEX >  reflec = reflec * %57.30   \* converts radians to degrees *\
 FILEX > read          100 records.
 FILEX > Succesful completion
 FILEX >  reflec = reflec + %6       \* Adds grazing angle of central *\
                                     \* ray to all rays *\
 FILEX > read          100 records.
 FILEX > Succesful completion
 FILEX >  reflec = reflec "          \* Switches columns for plotting *\
 FILEX > read          100 records.
 FILEX > Succesful completion
 FILEX > %plot = reflec2             \* Writes to plottable file *\
```
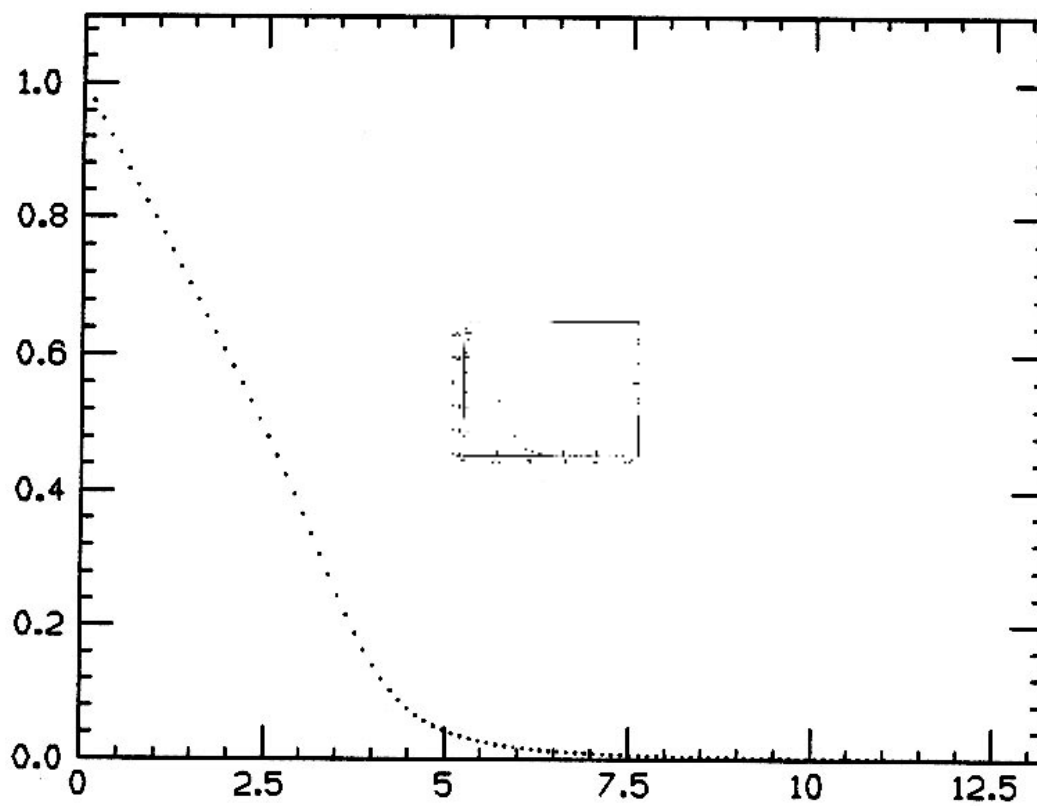
Figure 7.1: FILEX example – grazing angle vs. reflectivity

FMAX

Purpose:	Scans an ASCII two column file and returns the extrema.
Input:	Any formatted two column file (e.g. output from the utility PREPLOT is suitable for input to FMAX).
Output:	TT:

Description:

FMAX accepts as input a formatted two column file (e.g. output from PREPLOT) and returns the extrema found in the two columns. The first column lists the absolute extrema. The second column lists extrema with a slightly larger variance than the absolute extrema so that these values can be used to set, e.g., limits of a plot. The program is similar to MINMAX and useful to verify if data are reasonable, and to figure out plotting limits.

Examples:

We'll use the formatted file generated from PREPLOT using the STAR.01 file from the primer sec 2.4 (Refer to PREPLOT example).

```
$ fmax
File-name ?
pre.dat
Read         1000 points.
Found :
XMIN  -0.4102450      . Set at : -0.5023146
XMAX   0.4081510                  0.5002205
YMIN  -2.7292412E-02             -3.3435397E-02
YMAX   2.7311902E-02              3.3454888E-02
Good luck !
```

LOCPRI

Purpose:	To insert a Form Feed every 60 lines and prepare a nicely formatted file. Can directly drive a local printer connected to the printer port of a terminal.
Input:	A formatted/text file.
Output:	A nicely printable formatted file or printout.

Description:

This utility will take a file and format it to print "nice" pages. The output can be written to a file or sent directly to a printer if one is connected to the terminal on the "printer" port.

Examples:

For an example we'll run LOCPRI on the file REFLEC2.DAT used in H2KOL. Here we write the formatted output to a file.

```
$
$
$ run util:locpri
Input file ? reflec2.dat
Output file ? lreflec.dat
End of file found.
$
$ ty lreflec.dat

 --------------------------------------------------------------------------
 reflec2.dat                                                        Page  1
 --------------------------------------------------------------------------
     11.98835424000000      7.0040433999999999E-04
     11.86866027000000      7.3150668000000001E-04
     11.74888608000000      7.6436024000000000E-04
     11.62903906170000      7.9908548000000000E-04
     11.50911554790000      8.3581248000000001E-04
     11.38911909120000      8.7468227000000000E-04
     11.26905089490000      9.1584772000000000E-04
     11.14891267800000      9.5947435999999999E-04
     11.02870615950000      1.0057425000000000E-03
```

```
10.90843260000000        1.0548475000000000E-03
10.78809371850000        1.1070025000000000E-03
10.66769083290000        1.1624395000000000E-03
10.54722560490000        1.2214115000000000E-03
10.42669975350000        1.2841950000000000E-03
10.30611494040000        1.3510921000000000E-03
10.18547254080000        1.4224338000000000E-03
10.06477421640000        1.4985824000000000E-03
9.944021227800000        1.5799359000000000E-03
9.823215294000000        1.6669319000000000E-03
9.702358592400000        1.7600515000000000E-03
9.581451925200000        1.8598255000000000E-03
9.460497240600000        1.9668394000000000E-03
9.339496200300000        2.0817409000000000E-03
9.218450351400000        2.2052468000000000E-03
9.097361183700000        2.3381521000000000E-03
8.976230416200000        2.4813407000000000E-03
8.855059653300000        2.6357956000000000E-03
8.733850556700000        2.8026134000000000E-03
8.612604444300000        2.9830188000000000E-03
8.491323207000000        3.1783830000000000E-03
8.370008563800000        3.3902437000000000E-03
8.248661775300000        3.6203295000000000E-03
8.127284847000000        3.8705876000000000E-03
8.005879096800000        4.1432166000000000E-03
7.884464729000000        4.4407044000000000E-03
7.762988350500000        4.7658742000000000E-03
7.641506391300000        5.1219380000000000E-03
7.520002371600000        5.5125575000000000E-03
7.398477723900000        5.9419232000000000E-03
7.276934224500000        6.4148409000000000E-03
7.155373477800000        6.9368407000000000E-03
7.033797088200000        7.5143059000000000E-03
6.912206832000000        8.1546307000000000E-03
6.790604199000000        8.8664079000000001E-03
6.668990850900000        9.6596609999999999E-03
6.547368506700000        1.0546126000000000E-02
6.425738719230000        1.1539599000000000E-02
6.304103196030000        1.2656363000000000E-02
6.182463558690000        1.3915719000000000E-02
```

```
     6.060821463180000        1.5340646000000000E-02
     5.939178536820000        1.6958624000000000E-02
     5.817536441310000        1.8802667000000000E-02
     5.695896803970000        2.0912619000000000E-02
     5.574261280770000        2.3336785000000000E-02
     5.452634933000000        2.6133977000000000E-02
     5.331009149100000        2.9376088000000000E-02
     5.209395801000000        3.3151280000000000E-02
     5.087793168000000        3.7567887000000000E-02
     4.966202911800000        4.2759053000000000E-02
```

```
----------------------------------------------------------------------
reflec2.dat                                                    Page   2
----------------------------------------------------------------------
     4.844626522200000        4.8888013000000000E-02
     4.723065775500000        5.6153461000000000E-02
     4.601522276100000        6.4793922000000000E-02
     4.479997628400000        7.5088702000000000E-02
     4.358493608700000        8.7351263000000000E-02
     4.237011649500000        0.1019087000000000
     4.115553527100000        0.1190601000000000
     3.994120903200000        0.1390117000000000
     3.872715153000000        0.1617977000000000
     3.751338224700000        0.1872196000000000
     3.629991436200000        0.2148423000000000
     3.508676793000000        0.2440649000000000
     3.387395555700000        0.2742399000000000
     3.266149443300000        0.3047836000000000
     3.144940346700000        0.3352407000000000
     3.023769583800000        0.3652977000000000
     2.902638816300000        0.3947659000000000
     2.781549648600000        0.4235510000000000
     2.660503799700000        0.4516253000000000
     2.539502759400000        0.4790034000000000
     2.418548074800000        0.5057266000000000
     2.297641407600000        0.5318510000000000
     2.176784706000000        0.5574403000000000
     2.055978772200000        0.5825618000000000
     1.935225783600000        0.6072831000000000
     1.814527459200000        0.6316712000000000
```

```
 1.693885059600000       0.6557913000000000
 1.573300246500000       0.6797072000000000
 1.452774395100000       0.7034808000000000
 1.332309167100000       0.7271726000000000
 1.211906281500000       0.7508422000000000
 1.091567400000000       0.7745487000000000
0.9712938405000000       0.7983509000000000
0.8510873220000000       0.8223084000000000
0.7309491051000000       0.8464814000000000
0.6108809088000000       0.8709326000000000
0.4908844521000000       0.8957261000000000
0.3709609383000000       0.9209299000000000
0.2511139200000000       0.9466155000000000
0.1313397300000000       0.9728594000000000
1.1645759999999949E-02   0.9997437000000000
```

$

MERGEROW

Purpose: Takes two files of similar format and combines them into one file by taking alternate rows from each input file.

Input: Any two text files of similar format, especially column files (e.g. output from TRANSLATE or PREPLOT).

Output: A single file with alternating rows from the two input files.

Description:

This utility makes it easy to compare the rows of two files like those that are output from TRANSLATE or PREPLOT or similar column formatted files. Two input files are requested and are combined row by row with the labels 1: and 2: at the left of each row to designate which file it belongs to.

Examples:

Let's translate a couple of BOFs and then merge them.

```
$ translate star.01
File for input ?
star.01
and for output ?
star.dat
Read                  1000 rays.
Each ray has            12 entries.
how many rays to translate ?
2
All done.


$ translate
File for input ?
mirr.01
and for output ?
mirr.dat
Read                  1000 rays.
```

```
Each ray has               12 entries.
how many rays to translate ?
2
All done.



$ run util:merge
First file ?
star.dat
Second file ?
mirr.dat
Output file ?
mrg.dat
End of file found.
```

We'll type the input files and the merged file:

```
$ ty star.dat
-0.2780960640374226       1.0318894176630788E-16  4.3164806578071226E-03
 1.8455549611618461E-02  0.9998271538721697      -2.2483479289981678E-03
 0.9989241080626123      -1.8534474303775961E-02 -4.2509994043719599E-02
  1.000000000000000        0.0000000000000000E+00  1.000000000000000

-0.2831061672594486       1.7334495384241366E-15  4.6566385577880755E-03
 1.8694959705118020E-02  0.9998115448711023      -5.2319426682332429E-03
 0.9988783014611897      -1.8904690404164647E-02 -4.3413725372642238E-02
  1.000000000000000        0.0000000000000000E+00  2.000000000000000



$ ty mirr.dat
 -1.016798475029074      -9.5158502246510235E-02  1.4295016022463081E-02
 1.8455549611618461E-02  0.3440737824260938       0.9387612182741329
 0.9989241080626123       3.3607164154692846E-02 -3.1955982989010609E-02
  1.000000000000000        0.0000000000000000E+00  1.000000000000000
```

```
    -1.032199854951956      -0.2224876977694570      1.5282134990743490E-02
    1.8694959705118020E-02  0.3468721057931864       0.9377261011106732
    0.9988783014611897      3.4329772451938084E-02 -3.2612966645288010E-02
     1.000000000000000      0.0000000000000000E+00   2.000000000000000
```

Notice how much easier it is to compare ray values.

```
$ty mrg.dat
1:  -0.2780960640374226      1.0318894176630788E-16  4.3164806578071226E-03
2:   -1.016798475029074     -9.5158502246510235E-02  1.4295016022463081E-02
1:   1.8455549611618461E-02  0.9998271538721697      -2.2483479289981678E-03
2:   1.8455549611618461E-02  0.3440737824260938       0.9387612182741329
1:   0.9989241080626123    -1.8534474303775961E-02 -4.2509994043719599E-02
2:   0.9989241080626123      3.3607164154692846E-02 -3.1955982989010609E-02
1:    1.000000000000000      0.0000000000000000E+00   1.000000000000000
2:    1.000000000000000      0.0000000000000000E+00   1.000000000000000
1:
2:
1:  -0.2831061672594486      1.7334495384241366E-15  4.6566385577880755E-03
2:   -1.032199854951956     -0.2224876977694570      1.5282134990743490E-02
1:   1.8694959705118020E-02  0.9998115448711023      -5.2319426682332429E-03
2:   1.8694959705118020E-02  0.3468721057931864       0.9377261011106732
1:   0.9988783014611897    -1.8904690404164647E-02 -4.3413725372642238E-02
2:   0.9988783014611897      3.4329772451938084E-02 -3.2612966645288010E-02
1:    1.000000000000000      0.0000000000000000E+00   2.000000000000000
2:    1.000000000000000      0.0000000000000000E+00   2.000000000000000
1:
2:
```

PP

Purpose:	Arithmetic double-precision calculator.
Input:	Numbers and functions suitable for calculator input.
Output:	The results of the calculations.

Description:

Simulates a double-precision calculator, like an HP. Old and crude, but useful at 3:00 AM when you have lost your HP. Functions are chosen by entering the appropriate number. The inverse of a function may be used by entering a negative of the number. For example, to take the square root, one enters 7, to square a number, one enters -7.

Examples:

A simple example using this utility follows.

```
$ run util:pp
This program simulates an RPN calculator, like an HP.
It works in double precision. For the moment, the stack
is 10 registers.The trig functions work in radians,but
there is an easy conversion key.
The "display" is the lowest register in the stack.
Enter the number correspondent to the function. Use the
negative code for the inverse function.
Press RETURN when ready to go



- 10    clear all
0  enter X
1   SIN ,2   COS  ,3   TAN
4   LN  ,5   LOG  ,6  - not used yet-
7   SQRT
8   to degrees
9  +9 CHS, -9 1/x
10 EXIT
11 (*) , 12 (+) , 13 (-) ,14 (/)
```

```
15 write x to register
16 read in x from register
17 exchange the two lowest stack regs.
18 step up (down) the stack
19 E (G) Format
20 print the registers and stack
Register 11 contains conversion eV-angstroms,12 PI.

----------------------------------------------------
  Display =          0.0000000000000000E+00
----------------------------------------------------
0
?
25

- 10    clear all
0  enter X
1   SIN ,2   COS  ,3   TAN
4   LN  ,5   LOG  ,6  - not used yet-
7   SQRT
8   to degrees
9  +9 CHS, -9 1/x
10 EXIT
11 (*) , 12 (+) , 13 (-) ,14 (/)
15 write x to register
16 read in x from register
17 exchange the two lowest stack regs.
18 step up (down) the stack
19 E (G) Format
20 print the registers and stack
Register 11 contains conversion eV-angstroms,12 PI.

----------------------------------------------------
  Display =          25.00000000000000
----------------------------------------------------
7

- 10    clear all
0  enter X
1   SIN ,2   COS  ,3   TAN
```

```
4   LN  ,5   LOG  ,6  - not used yet-
7   SQRT
8   to degrees
9  +9 CHS, -9 1/x
10 EXIT
11 (*) , 12 (+) , 13 (-) ,14 (/)
15 write x to register
16 read in x from register
17 exchange the two lowest stack regs.
18 step up (down) the stack
19 E (G) Format
20 print the registers and stack
Register 11 contains conversion eV-angstroms,12 PI.

--------------------------------------------------
  Display =         5.000000000000000
--------------------------------------------------
-10

- 10    clear all
0  enter X
1   SIN ,2   COS  ,3   TAN
4   LN  ,5   LOG  ,6  - not used yet-
7   SQRT
8   to degrees
9  +9 CHS, -9 1/x
10 EXIT
11 (*) , 12 (+) , 13 (-) ,14 (/)
15 write x to register
16 read in x from register
17 exchange the two lowest stack regs.
18 step up (down) the stack
19 E (G) Format
20 print the registers and stack
Register 11 contains conversion eV-angstroms,12 PI.

--------------------------------------------------
  Display =        0.0000000000000000E+00
--------------------------------------------------
```

$

REVPRINT

Purpose:	Displays a formatted file in reverse order line by line.
Input:	A formatted file of 10,000 lines or less.
Output:	TT:

Description:

Displays a file in reverse order line by line. REVPRINT can be useful when the data are in a large file and the last entries are to be examined. A typical case could be to examine a long .LOG file to find the reason for a crash.

Examples:

We'll run REVPRINT on a short PREPLOT output file Here's the file before REVPRINT:

```
$ ty pre.dat
-0.2780961       1.8455550E-02
-0.2831062       1.8694960E-02
 0.3307338      -2.2033621E-02
-0.3311352       2.2213560E-02
-9.4173871E-02  6.2023830E-03
 0.2767766      -1.8385222E-02
 0.3686378      -2.4258027E-02
 0.1166269      -7.7635958E-03
-0.3735043       2.5044683E-02
-0.3660054       2.4130033E-02
-9.1828540E-02  6.0481941E-03
 0.3607364      -2.4109263E-02
 0.3719847      -2.5014305E-02
-3.2931246E-02  2.2053795E-03
 0.1509321      -1.0015748E-02
```

After:

```
$ revprint
Input file ?
pre.dat
  0.1509321      -1.0015748E-02
 -3.2931246E-02  2.2053795E-03
  0.3719847      -2.5014305E-02
  0.3607364      -2.4109263E-02
 -9.1828540E-02  6.0481941E-03
 -0.3660054       2.4130033E-02
 -0.3735043       2.5044683E-02
  0.1166269      -7.7635958E-03
  0.3686378      -2.4258027E-02
  0.2767766      -1.8385222E-02
 -9.4173871E-02  6.2023830E-03
 -0.3311352       2.2213560E-02
  0.3307338      -2.2033621E-02
 -0.2831062       1.8694960E-02
 -0.2780961       1.8455550E-02
```

TGAUSS

Purpose:	Creates a two column formatted file of a discrete gaussian function.
Input:	The standard deviation and interval for the gaussian function, and the number of points on the interval for which the function is to be computed.
Output:	A user named two column file that contains the value of the gaussian function for each point on the interval.

Description:

TGAUSS may be used to compare a randomly generated distribution to an actual gaussian with the same parameters. It could also be useful for comparing with the spectrum from the output of a narrow band device such as a monochromator. For demonstrations, see the example in HISTO1. If the normalization is to be to the area, then the integral over the interval is equal to one. If normalization is to one, the value of the gaussian at the mean (zero) is one and the other values are weighted accordingly.

Examples:

To start out, let's make a plot of a gaussian function with a four s standard deviation width on either side of the mean. We'll normalize to area and use TopDrawer to plot out the results.

```
$ run util:tgauss
 Output file ?
 Gauss.dat
 Enter Mean, Stnd. Dev., Interval Width, Number of Points
 0
 1
 8
 100
 Normalize to area [ 1 ] or to 1 [ 0 ]?
 1
$
```

Figure 7.2: TGAUSS Example

TYPEOUT

Purpose:	Prints a file, one page at a time, forward or backwards.
Input:	A file to be displayed on the terminal.
Output:	The contents of the file printed one page at a time.

Description:

TYPEOUT allows scrolling through a file one page at a time in either direction. Maximum file size is 1000 lines.

Examples:

The following run was done using the file reflec2.dat used in H2KOL.

```
$
$ typeout
Input file ? reflec2.dat


    11.98835424000000        7.0040433999999999E-04
    11.86866027000000        7.3150668000000001E-04
    11.74888608000000        7.6436024000000000E-04
    11.62903906170000        7.9908548000000000E-04
    11.50911554790000        8.3581248000000001E-04
    11.38911909120000        8.7468227000000000E-04
    11.26905089490000        9.1584772000000000E-04
    11.14891267800000        9.5947435999999999E-04
    11.02870615950000        1.0057425000000000E-03
    10.90843260000000        1.0548475000000000E-03
    10.78809371850000        1.1070025000000000E-03
    10.66769083290000        1.1624395000000000E-03
    10.54722560490000        1.2214115000000000E-03
    10.42669975350000        1.2841950000000000E-03
    10.30611494040000        1.3510921000000000E-03
    10.18547254080000        1.4224338000000000E-03
    10.06477421640000        1.4985824000000000E-03
    9.944021227800000        1.5799359000000000E-03
    9.823215294000000        1.6669319000000000E-03
```

```
   9.702358592400000       1.7600515000000000E-03

Cursor at page:    1; Page printed:    1
<ret>, +n, -n
<ret>

   9.581451925200000       1.8598255000000000E-03
   9.460497240600000       1.9668394000000000E-03
   9.339496200300000       2.0817409000000000E-03
   9.218450351400000       2.2052468000000000E-03
   9.097361183700000       2.3381521000000000E-03
   8.976230416200000       2.4813407000000000E-03
   8.855059653300000       2.6357956000000000E-03
   8.733850556700000       2.8026134000000000E-03
   8.612604444300000       2.9830188000000000E-03
   8.491323207000000       3.1783830000000000E-03
   8.370008563800000       3.3902437000000000E-03
   8.248661775300000       3.6203295000000000E-03
   8.127284847000000       3.8705876000000000E-03
   8.005879096800000       4.1432166000000000E-03
   7.884464729000000       4.4407044000000000E-03
   7.762988350500000       4.7658742000000000E-03
   7.641506391300000       5.1219380000000000E-03
   7.520002371600000       5.5125575000000000E-03
   7.398477723900000       5.9419232000000000E-03
   7.276934224500000       6.4148409000000000E-03

Cursor at page:    2; Page printed:    2
<ret>, +n, -n
-1

   11.98835424000000       7.0040433999999999E-04
   11.86866027000000       7.3150668000000001E-04
   11.74888608000000       7.6436024000000000E-04
   11.62903906170000       7.9908548000000000E-04
   11.50911554790000       8.3581248000000001E-04
   11.38911909120000       8.7468227000000000E-04
   11.26905089490000       9.1584772000000000E-04
   11.14891267800000       9.5947435999999999E-04
   11.02870615950000       1.0057425000000000E-03
```

```
    10.90843260000000          1.0548475000000000E-03
    10.78809371850000          1.1070025000000000E-03
    10.66769083290000          1.1624395000000000E-03
    10.54722560490000          1.2214115000000000E-03
    10.42669975350000          1.2841950000000000E-03
    10.30611494040000          1.3510921000000000E-03
    10.18547254080000          1.4224338000000000E-03
    10.06477421640000          1.4985824000000000E-03
    9.944021227800000          1.5799359000000000E-03
    9.823215294000000          1.6669319000000000E-03
    9.702358592400000          1.7600515000000000E-03

Cursor at page:   2; Page printed:   1
<ret>, +n, -n
+2



    2.297641407600000          0.5318510000000000
    2.176784706000000          0.5574403000000000
    2.055978772200000          0.5825618000000000
    1.935225783600000          0.6072831000000000
    1.814527459200000          0.6316712000000000
    1.693885059600000          0.6557913000000000
    1.573300246500000          0.6797072000000000
    1.452774395100000          0.7034808000000000
    1.332309167100000          0.7271726000000000
    1.211906281500000          0.7508422000000000
    1.091567400000000          0.7745487000000000
   0.9712938405000000          0.7983509000000000
   0.8510873220000000          0.8223084000000000
   0.7309491051000000          0.8464814000000000
   0.6108809088000000          0.8709326000000000
   0.4908844521000000          0.8957261000000000
   0.3709609383000000          0.9209299000000000
   0.2511139200000000          0.9466155000000000
   0.1313397300000000          0.9728594000000000
    1.1645759999999949E-02     0.9997437000000000

 Cursor at page:   5; Page printed:   5
```

```
<ret>, +n, -n
```

```
$
```

VARIANCE

Purpose: Analyzes a formatted two column file (such as output from PREPLOT) and returns the mean, variance and standard deviation for the selected column. A plottable file of the distribution function is optional.
Input: Any formatted two column file.
Output: TT and a user-named log file. A plottable file is optional.

Description:

Gives parameters for the statistical distribution of a column from a formatted file: mean, variance, standard deviation. The results are saved in a log file named by the user. A best fit plottable file is also optional: the user specifies the interval, mean and number of points to plot in the interval. It is useful to define the interval as the difference between the extrema of the data, which can be found using FMAX before running VARIANCE as in the example below.

Examples:

```
                              //If we want a plottable file, we should find th
                              // extrema using FMAX.

                              // We're using the spherical mirror example (pri
                              // sec 2.4).

$ fmax
File-name ?
pre.dat
Read        1000 points.
Found :
XMIN  -0.4102450      . Set at : -0.5023146
XMAX   0.4081510                  0.5002205
YMIN  -2.7292412E-02             -3.3435397E-02
YMAX   2.7311902E-02              3.3454888E-02
Good luck !
```

```
                        //Now let's run VARIANCE on the data.

$ variance
Log file ?
var.dat
File for analysis ?
[.ug.variance]pre.dat
Read        1000 from
[.ug.variance]pre.dat
Column to analyze ?
1


Results from column             1
Mean value:  -8.8223701815000001E-03
Variance   :   5.5424558469452820E-02
Standard deviation :   0.235424209607790 4


Enter:
0    to exit
1    new file
2    new column (same file)
3    best fit (plottable)
?
3
Output file name ?
var.plt
Enter interval width,number of points
Interval width ?
1
Interval center ?
0
Number of points ?
30
Area = 1 ?
1
Enter:
0    to exit
1    new file
2    new column (same file)
3    best fit (plottable)
```
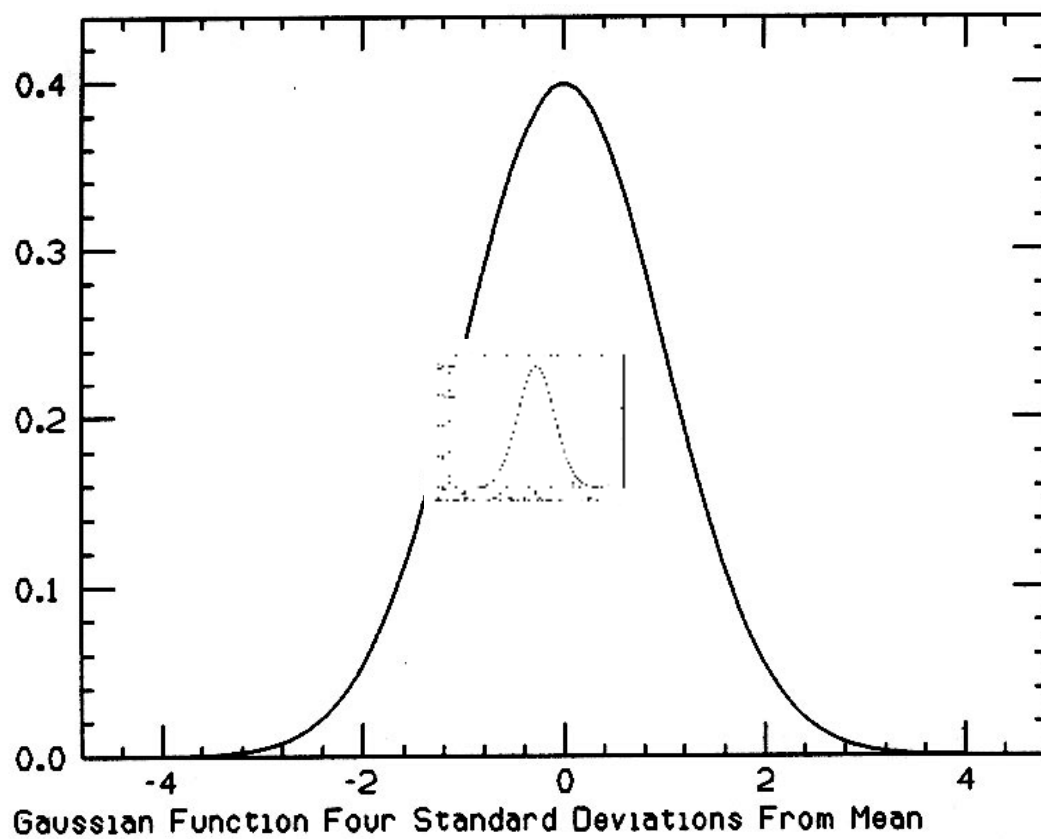
?
0

Figure 7.3: VARIANCE best fit example

Appendix A

Toroidal Grating Monochromator

Throughout the examples in this manual we have referred to a 6 meter toroidal grating monochromator (TGM). The monochromator modelled is a six-meter installed at the Synchrotron Radiation Center on the ring Aladdin. The system consists of an elliptical entrance mirror, an entrance slit, a toroidal grating, an exit slit and an elliptical refocus mirror. The two mirrors and the grating are gold coated. It has three holographic gratings, low, medium and high energy. The grating we have used for all our examples is the medium energy grating.

We follow with the output from SYSINFO and MIRINFO for each element. The screens defined are there to show the location of valves or future filters.

```
     +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
     *************  S Y S T E M     D E S C R I P T I O N  *************
     +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
     6-m TGM


     +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
     Input file specified:
     +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
      #    Optical Element:                                    Creation Time:
        1   CXRL$DUA0:[SHADOW.XRAYOP.DOCUMENT.TGM]END.01;56        1-NOV-1989 10:
        2   CXRL$DUA0:[SHADOW.XRAYOP.DOCUMENT.TGM]END.02;55        1-NOV-1989 10:
        3   CXRL$DUA0:[SHADOW.XRAYOP.DOCUMENT.TGM]END.03;5         1-NOV-1989 10:
     +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Optical Element #            1      System Number:
```

```
MIRROR    ELLIPTICAL            DIM CHECK      COMPUTED       REFLEC. OFF

   Orientation            180.0000000000000      deg.
   Source Plane           180.0000000000000
   Incidence Ang.         84.99999999999999      deg.
   Reflection Ang.        84.99999999999999      deg.
   Image Plane            180.0000000000000
     ----------------

Optical Element #             2      System Number:

GRATING   TOROIDAL            DIM CHECK      EXTERNAL       REFLEC. OFF

   Orientation            180.0000000000000      deg.
   Source Plane           211.1000000000000
   Incidence Ang.         80.0000000000002       deg.
   Reflection Ang.        80.0000000000002       deg.
   Image Plane            388.8000000000000
     ----------------
   SCREENS:            4 defined.
AFTER  Mirror          at    190.0000000000000
   Type :SLIT        ELLIPTICAL
AFTER  Mirror          at    76.00000000000000
BEFORE Mirror          at    329.0000000000000
   Type :SLIT        ELLIPTICAL
BEFORE Mirror          at    388.7900000000000
     ----------------

Optical Element #             3      System Number:

MIRROR    ELLIPTICAL            UNLIMITED      COMPUTED       REFLEC. OFF

   Orientation            180.0000000000000      deg.
   Source Plane           240.0000000000000
   Incidence Ang.         80.0000000000002       deg.
   Reflection Ang.        80.0000000000002       deg.
   Image Plane            80.00000000000000
     ----------------


              OPTICAL SYSTEM CONFIGURATION
```

```
                    Laboratory Reference Frame.

 OPT. Elem #        X =                Y =                Z =


     0              0.00000000000E+00   0.00000000000E+00   0.00000000000E+00
     1              0.00000000000E+00    180.00000000       0.00000000000E+00
        1'            0.13774432066E-14    357.26539554      -31.256671980

     2              0.29928779894E-14    565.15831220      -67.913802286
        2'           -0.58425516932E-14    948.05156657      -0.39939080863

     3             -0.11296520633E-13   1184.4054273        41.276171831
        3'           -0.94785309865E-14   1263.1900475       27.384317618


 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 **************          E N D            **************
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

To show the system layout, we ran the beamline through SYSPLOT.

```
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 ******************   MIRROR  DESCRIPTION   ******************
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Condensing mirror
 Orientation 180 deg.
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Input file specified:end.01
 Full file Specification :D1:[SHADOW.XRAYOP.DOCUMENT.TGM]END.01;55
 Creation Date           :28-JUL-1989 22:58
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 Surface figure was defined as:        ELLIPTICAL
 Cylindrical figure                    NO
 Element type                          REFLECTOR
 Reflectivity      ON     coefficients from:
 AU.REF
 Polarization dependence               YES
 Mirror dimensions ( rectangular ):
      X plus            X minus            Y plus            Y minus
      2.0000           -2.0000             4.7500            -4.7500
```
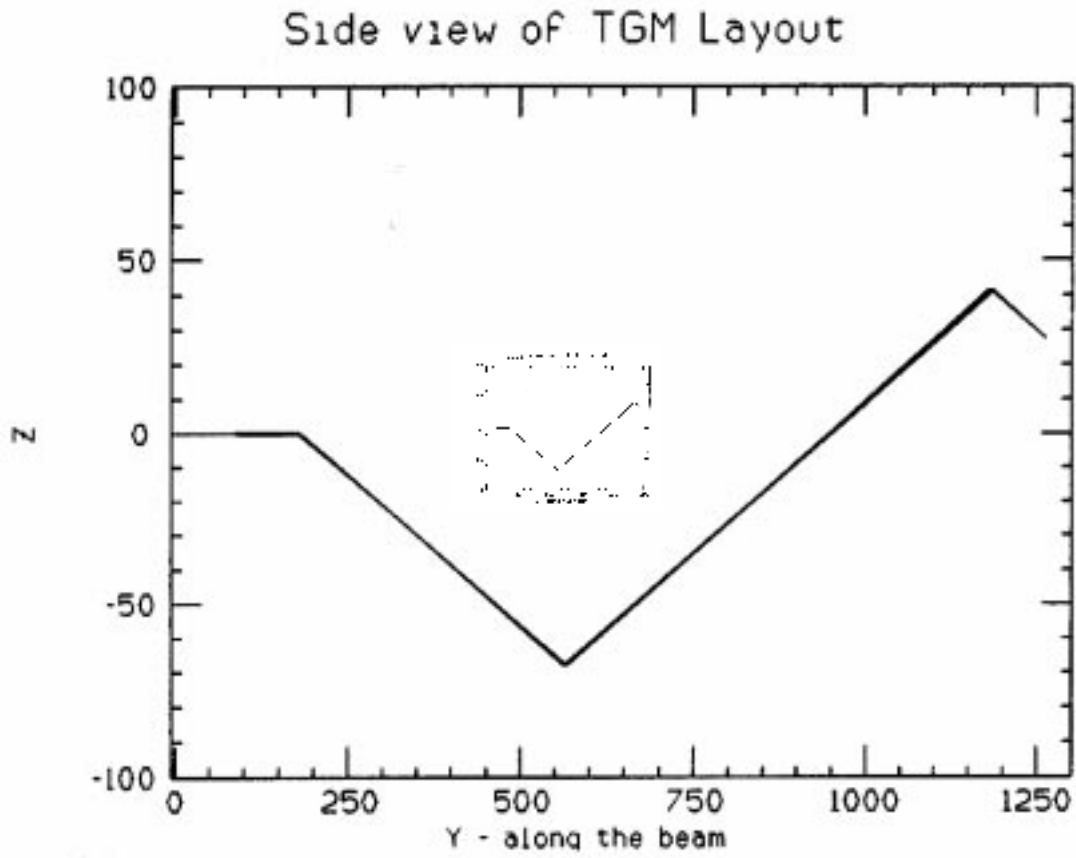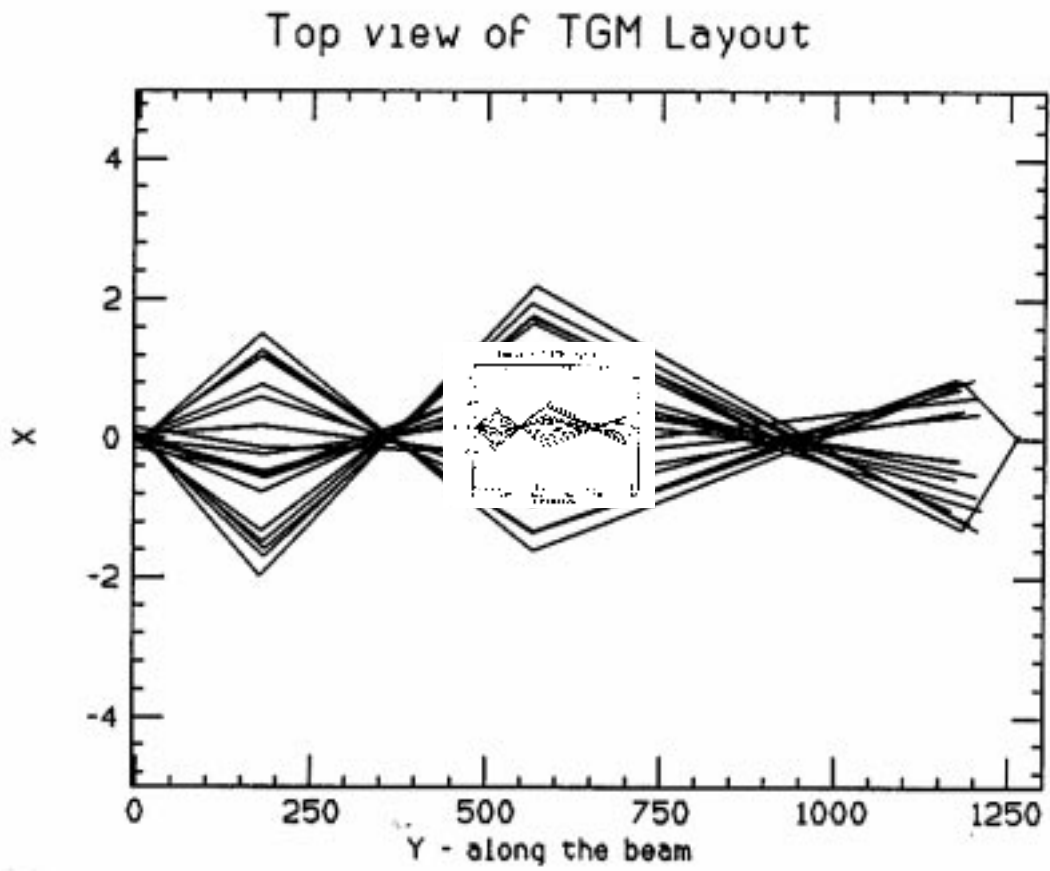
Figure A.1: TGM Layout – side view

Figure A.2: TGM Layout – top view

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                      180.0000000000000
Image  Plane                               180.0000000000000
Incidence Angle                            84.99999999999999
Reflection/Diffraction Angle               84.99999999999999

Mirror parameters                      COMPUTED
Same configuration as Central Axis     YES
Objective focus at                         180.0000000000000
Image focus at                             180.0000000000000
Incidence angle                            84.99999999999999
Parameters used follow:
   Semi-major axis     180.0000000000000
   Semi-minor axis     15.68803369457847
   Semi-focal-length  0.0000000000000000E+00
   Eccentricity       0.0000000000000000E+00
Source of this O.E. moved                  NO
Mirror at pole position ( no mov. )    YES
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*******************  MIRROR  DESCRIPTION   *******************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Grating
Orientation 180 deg
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.02
Full file Specification :D1:[SHADOW.XRAYOP.DOCUMENT.TGM]END.02;55
Creation Date            :28-JUL-1989 23:00
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:        TOROIDAL
Cylindrical figure                     NO
Element type                           REFLECTOR
Element type                           GRATING
Order choosen ( inside are < 0 )        -1.000000000000000
Automatic Tuning                       YES
Mount                                  SEYA / TGM
```

```
Grating tuned at  [ eV ]                        59.00000000000000
Holographic grating. Recording Wavelength:    4879.860000000000
Input Slit Dist.  Exit Slit Dist.    Input Slit Angle    Exit Slit Angle
  919.300000       619.000000          10.3600000         -12.8100000
Input  Slit rotation angle   0.0000000000000000E+00
Output Slit rotation angle   0.0000000000000000E+00
Spherical / Spherical
Spherical  / Spherical
Real      / Real
Reflectivity      ON     coefficients from:
AU.REF
Polarization dependence              YES
Mirror dimensions ( rectangular ):
      X plus            X minus            Y plus            Y minus
       2.2500           -2.2500            6.7500            -6.7500
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                   211.1000000000000
Image  Plane                            388.8000000000000
Incidence Angle                         80.00000000000002
Reflection/Diffraction Angle            80.00000000000002

Mirror parameters                    EXTERNAL
Parameters used follow:
   Major Radius       1877.550000000000
   Minor Radius       47.05000000000000
Source of this O.E. moved             NO
Mirror moved from pole. Parameters :
Displacement along X:     0.0000000000000000E+00
                Y:     0.0000000000000000E+00
                Z:     0.0000000000000000E+00
Rotation around X:     2.853995871245999
             Y:     0.0000000000000000E+00
             Z:     0.0000000000000000E+00
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
******************   MIRROR  DESCRIPTION   ******************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
Refocus Mirror
Orientation 180 deg.
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:end.03
Full file Specification :CXRL$DUA0:[SHADOW.XRAYOP.DOCUMENT.TGM]END.03;3
Creation Date          :24-OCT-1989 15:15
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Surface figure was defined as:        ELLIPTICAL
Cylindrical figure                    NO
Element type                          REFLECTOR
Reflectivity                          OFF
Mirror dimensions                     UNLIMITED
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Central Axis parameters :
Source Plane Distance                       240.0000000000000
Image  Plane                                80.00000000000000
Incidence Angle                             80.00000000000002
Reflection/Diffraction Angle                80.00000000000002

Mirror parameters                     COMPUTED
Same configuration as Central Axis    YES
Objective focus at                          240.0000000000000
Image focus at                              80.00000000000000
Incidence angle                             80.00000000000002
Parameters used follow:
   Semi-major axis     160.0000000000000
   Semi-minor axis     24.06139730886965
   Semi-focal-length   0.0000000000000000E+00
   Eccentricity        0.0000000000000000E+00
Source of this O.E. moved             NO
Mirror at pole position ( no mov. )   YES
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Appendix B

Glossary

Active Surface	A surface where the rays are reflected/refracted.
Aligned System	An optical system where nothing has been "moved" when running SHADOW.
Aperture	A slit or hole at a screen that limits the latitude of the beam.
BATCH mode	Input mode that takes parameter files (START.xx, SYSTEM-FILE.DAT) generated by a previous input session and supplies them to SHADOW for a re-run. You will simply be prompted for these parameter file names.
Beam	A collection of rays, pretty much like in flashlight beam. The rays can be random or ordered (grid). The beam is stored in the BOF at different locations.
Beamline	The hardware implementation of an optical system for XUV, used to relay with or without monochromatization the beam from source to sample. Optical System.
Bins	Divisions of a histogram that determine the resolution of ray statistics; A greater number of bins yields higher resolution but less reliable statistics, i.e. a smaller signal/noise ratio.
Blaze	The blaze condition proper applies only to triangular grooves, when the light is incident and diffraction angles, relative to the grating normal, are such that the ray is exactly "reflected" by the facet. In other words, the incoming ray forms with the facet normal the same angle as the diffracted beam. It is the condition of maximum efficiency of the grating. Lamellar and sinusoidal gratings have both high-efficiency angles, but for other reasons (see *Gratings*).

BOF	Binary Output File – the large binary files generated by the run of SHADOW. They contain the full beam description at some location along the optical system. Use TRANSLATE to type/print them.
Central Ray	The ray generated by SOURCE with $x = y = z = 0$, $x' = z' = 0$, and $y' = 1$. It is the ray propagating exactly along the source Y axis. It coincides with the optical axis, in the case of an aligned system.
Collimated	The condition of a beam in which all rays are parallel, i.e., the object/image is at infinity.
Column	Each ray has up to eighteen values defining it in terms of X, Y, Z, X', Y', Z' etc.; they form the columns containing X, Y, etc.
Continuation Plane	An intermediate plane perpendicular to the Y axis that acts as a delimiter between two optical elements, or as the image plane at the end of the optical system. Continuation planes may or may not coincide with the beam focus. The beam information for the XXth continuation plane is located in the BOF STAR.XX.
Cylindrical Figure	A figure originated by the translation of a plane curve perpendicular to the plane. If the plane curve is an ellipse, we speak of elliptical cylinder; if it is a circle, of circular cylinder; etc.
DCL	DIGITAL Command Language - The command language for the VAX/VMS operating system.
DEFINE	(OE, SCREEN) This MENU mode command is used declare existence of OEs and SCREENs in the System. The elements are numbered starting from the source, which is OE 0. Elements can be inserted and deleted from the system, since the pattern for numbering the OEs of the OS follows that of a stack. Similarly, SCREENS are placed within each OE.
DELETE	(OE, SCREEN) Menu mode command used to remove either an OE from the SYSTEM list or a screen from an OE. The system is renumbered down.

Diffraction Grating	An element whose surface produces a strongly peaked auto-correlation power series. The relative height of the first, second, etc. peak represent the relative efficiency of the first, second, ... diffraction order. As the ACF depends on the coherent spacing for the peak position, the diffraction angles are determined solely by the grating pitch. The height of the peaks represents the Fourier components of the surface at each groove, so that the efficiency depends on the shape of the grooves. The condition of blaze is usually the most efficient.
Diffraction Limit	The observed width of a (geometrically) point-like image. It is due to the finite wavelength of the radiation used to reconstruct the image and to the finite convergence angle. Typically: $$\delta = \frac{\lambda}{2N.A.}$$
Diffraction Limited Optics	An optical system where the dimensions of the image are larger than those of the geometrical image and defined by the radiation employed. For a focusing system, the diffraction limited focus is given by $\frac{\lambda/2}{N.A.}$, N.A. being the numerical aperture of the system. Aberrations and figure errors mainly modify the intensity distribution within the limits predicted by the diffraction limit.
Diffraction Order	See Order.
Element	The part of an optical system that encloses an active surface.
ERF	Exit Record File - Contains information about a source or optical element after the rays have been traced through the system. Information such as computed parameters, and positions in the X,Y,Z and Laboratory Reference Frames are given. SHADOW gives the ERFs the default name END.XX.
EXIT	Exit from SHADOW command level to VMS DCL level, restoring the terminal status to the standard one.
External	Pertaining to the definition of an optical element; the parameters are supplied by the user rather than being computed by SHADOW.
Figure	The mathematical function describing the surface of a mirror or of a lens. We speak of elliptical figure, etc.

Figure Limited Optics	Optical systems where the dimensions of the image are dominated by the figure errors. At grazing angle, slope errors are the most serious. Common problems with high brightness sources (small dimensions).
Flag	Tags a ray if it was not transmitted through an OE or screen. The Flag is 1 if the ray passed and < 0 if it was lost. The Flag is the tenth column in the BOFs; it may assume other values as well.
Footprint	The intensity pattern of a beam on the surface of an optical element.
Fresnel Equations	Determine the reflectivity of a medium for the two polarization directions as a function of incident and transmitted angles:

$$R_\perp = \frac{\sin^2(\theta_i - \theta_t)}{\sin^2(\theta_i + \theta_t)}, \qquad R_\parallel = \frac{\tan^2(\theta_i - \theta_t)}{\tan^2(\theta_i + \theta_t)}$$

	where θ_i and θ_t are the angles of incidence and transmission respectively, and $R_\perp$ and $R_\parallel$ correspond to the reflectivities in the perpendicular (s-polarization) and parallel (p-polarization) directions with respect to the plane of incidence.
Geometrical Optics	The study of an optical system purely on the basis of geometrical relations between rays and surfaces.
GOTO	MENU mode command that allows the user to set the pointer to a particular OE. Useful for forgotten screens or if you're in the (good) habit of DEFINing all OEs at once and then using the SELECT command to input parameters.
Grating Horizon	The wavelength such that, for a particular incidence angle, the diffracted first order would be at $-90°$, i.e., diffracted back and tangent to the surface. Longer wavelengths would be diffracted 'inside' the surface, so that the grating behaves like a normal mirror for wavelengths beyond the horizon.

Grating Mount	The particular optical system configuration chosen to implement an instrument. A mount is specified by the geometry of the grating element and by focal conditions. Also used, more loosely, to indicate a type of scanning action, like in "TGM mount": this simply means a mount with Constant Included angle and rotation achieved by simple rotation of the grating.
Grazing Angle	An Incidence or reflection angle in which the rays are nearly parallel to the optical surface.
Groove Shape	Refers to a grating's grooves. They can be generally divided in lamellar, triangular or sinusoidal.
HELP	Evokes the help facility at the SHADOW command level and provides some on-line description of the local commands and their purposes.
HELPSHA	Invokes SHADOW help facility at DCL command level.
Image Distance	The distance along the Y axis from an optical element to the next continuation plane, which may or may not be the location of a real image or focus point.
Incidence Angle	The angle that an incident ray makes with respect to the normal of the optical surface in question.
Input Modes	Means to enter the parameters characterizing source and OE. The three input modes are PROMPT, MENU and BATCH.
LIST	Menu mode command that gives a list of the currently defined OEs and SCREENs in an OS and their relative numbering.
LOAD	(SYSTEM, SOURCE, OE) MENU mode command that invokes the LOAD menu. This command LOADs an already existing SYSTEM, OE or SOURCE by reading existing parameter file(s) into memory. This is useful for major or minor modifications. The parameters requested are the directory and file-name root describing the location of the information you wish the menu to access. Use "[ ]" or nothing to specify the current directory; the default file-root name is START unless you've renamed it. When you have defined the files, hit the ← to return to the "Ready::" prompt.

Marginal Rays	The rays on the periphery (margin) of the beam. They are normally the ones suffering the most aberration.
MENU	This command is used to define, examine and modify parameters defining source and/or optical elements. The order of entry is entirely free. The system displays a list of variables with their current values; each item is accessed using the cursor's arrows. No calculations are performed and only START files are generated.
MENU mode	One of the three input modes. The program for MENU is subdivided into a COMMAND interpreter and a set of screen oriented menus. It is the most powerful method. A list of parameters are presented on the screen and these can be randomly accessed. This method offers the flexibility to make a single change thus bypassing the lengthy process of the PROMPT mode. It allows also the possibility of going back and forth between the parameters specifying an OE or source. On the other hand, one runs the risk of leaving out a single parameter, and spending a sleepless night wondering why a plane mirror magnified the source. MENU has its own command level and the prompt is "Ready::". The possible commands are: DEFINE, DELETE, GOTO, LIST, LOAD, SAVE, SELECT, SPAWN.
Momentum Space	The monemtum $\vec{p}$ is the conjugate variable to the coordinate $\vec{r}$. In general,

$$\vec{p} = \frac{2\pi}{\lambda}\{\alpha_x, \alpha_y, \alpha_z\}$$

where α's are the cartesian cosines

$$\alpha_i = \frac{\vec{p}}{p} \cdot \hat{x}_j$$

Rows 4,5,6 store the α's of the ray, while $|p| = \frac{2\pi}{\lambda}$ is stored in row 11. The coordinates in momentum space for a ray are in columns 4, 5, and 6 in any BOF. Also called reciprocal space.

Monochromator	An optical instrument capable of transmitting a very narrow bandpass of a white spectrum. Normally consisting of one or more gratings/crystals in a particular mount. Notice that the monochromator is an optical device whose function is simply to define the bandpass: it does not necessarily refocus the diffracted beam. It is normally teamed with condensing and refocusing optics.
Namelist	Text file that contains the input parameters for the source or optical system. These files (named by SHADOW as START.XX) are the only files that are needed, besides the files created by the preprocessors, to regenerate the beam data for the entire system.
Normal	A vector which is perpendicular to the surface in question. Usually located at the geometric center of an optical surface.
Numerical Aperture	The sine of the angle formed by a ray with the optical axis.
Optical Axis	The ray connecting the poles of the optical elements. It connects the origin points of the consecutive OE's. Notice that even when the mirror are "moved", the optical axis remains the same. Same as central ray, if the source has not been "moved" in SHADOW.
Optical Efficiency	The ratio of the number of photons departing to the number incident on an optical element (or system).
Optical Element or O.E.	The part of the optical system encompassing an active surface. It is delimited by two planes (source/object and image, respectively) located along the optical axis at some convenient location.
Optical Path	The optical path of a ray is given by:

$$T_{BA} = \int_a^b n(s)ds$$

	where $n(s)$ is the index of refraction as a function of position, and a and b are the initial and terminal points of the ray. The focal condition states that all the optical paths are the same, independent of angle.
Optical system	The collection of optical elements under study.

Orders	The labels tagged to a beam when diffracted from a grating. The European convention defines negative the orders diffracted inside (inside order) the zero-order reflection beam, positive those laying outside. The American convention is the opposite. Most XUV systems work in the first order and the XUV community follows the European convention.
Phase Space	The union of Real and Momentum spaces. Phase space projections may aid in interpreting the character of the beam at a given point in the system by determining the correlation between two of the components such as X and X'. The volume of phase space occupied by a beam is always conserved.
Physical Optics	The study of an optical system that explicitly includes physical aspects, such as reflectivity, diffractions, etc.
Preprocessor	Any utility that generates data that is used for SOURCE generation or defining an element of the optical system, e.g., PREREFL is used to determine the reflection and transmission coefficients for a given Atomic Number.
PROMPT mode	Input mode in SHADOW that asks the user for parameters to cover the full specification of a source or OE. Useful when setting up a new system.
Ray	The path described by a single photon. It is specified by 12-18 double precision real numbers. They are described by a starting point, a direction, an electric field, a phase, a polarization degree, an energy, a status flag.
Ray Index	Index used to number the rays in order of their generation: the first ray is given Ray Index 1, the second 2, etc... The Ray index is the 12th column in the BOFs.
Real Space	The ordinary geometrical space. The real space coordinates for a ray are in columns 1, 2, and 3 in the BOFs.
Reflection Angle	The angle that a reflected or refracted ray that is coincident with the Y axis makes with respect to the normal of the optical surface in question.

Roughness	The incoherent part of a surface height autocorrelation power series. It causes a diffuse scattering of radiation away from the geometrical image. Although it does not affect the image sharpness, it decreases the system MTF. The roughness becomes less important at glancing angles, due to the roll-off in the power spectrum and to the increase in the photon horizontal wavevector at glancing angles.
Sagittal	A direction perpendicular to the incidence plane (s-polarization).
SAVE	(SYSTEM, SOURCE, OE) MENU mode command that invokes the SAVE menu. The parameters requested are the directory and the file-name root, i.e., where and under what name do you want the data stored. This is the command to use to write the definition of OE, SOURCE or entire SYSTEM to disk. SAVE SYSTEM also creates SYSTEM-FILE.DAT; when in doubt, always use SAVE SYSTEM. NOTE: You *MUST* issue the SAVE command on exit from the MENU or else the data is lost. SHADOW will warn you if you have modified a file and not saved it.
Seed	An odd eight-digit number used as input to a pseudo-random number generator for creating source photon distributions.
SELECT	(SOURCE, OE, SCREEN) MENU mode command that SELECTs which OE or SCREEN you wish to characterize. This applies also for the SOURCE. After issuing the SELECT OE (or SCREEN) command, you are prompted for the element number (screen/slit number). This positions the pointer to the chosen location. Note, an OE or screen must be DEFINEd before SELECTed, though SELECT SOURCE automatically verifies its existence. Before issuing the SELECT SCREEN command, you must be in a defined (i.e., existing) OE.
Shape	The shape of the mirror outline or contour: a spherical mirror can be round or rectangular. The same is true for any mirror figure.
Sigma	Usually refers to the standard deviation of the distribution function in question.

SOURCE   Used to define the source parameters and generate the source rays. After entering the command the user will be prompted to choose an input mode during which the physical description is set up.

Source Depth   The distribution of the source points in the Y direction.

Source Distance   The distance along the Y axis from the source or previous continuation plane to the next optical element in the system.

Source Limited optics   An optical system where the dimensions of the image are dominated by the aberrations caused by the large extent of the source, either in plane or in angle. Diffraction and figure errors have a small effect.

SPAWN   MENU mode command that spawns the process, giving full access to DCL without interrupting the menu session, by creating a new VMS session. The program will resume where it left when you log off from the sub-process.

                                Note: Be sure to "log-off" from all sub-processes when done.

Tangential   A direction laying in the incidence plane (p-polarization).

TRACE   Used to define the optical elements and the optical system. On completion of the OS definition, TRACE computes the path of each ray through the OS. A source must exist before issuing the command TRACE.

Virtual Image   Rays emerging from an OE or OS in image space are diverging, so image appears to exist in object space.

Virtual Object   Rays entering an OE or OS from object space are converging, so object appears to exist in image space.

Wavenumber   The wavenumber for a photon is given by $K = \frac{2\pi}{\lambda}$, where λ is the wavelength. (see *Momentum*.)

Zero order   The beam reflected by a grating without scattering, whereby it acts like a simple mirror.