SHADOW

PRIMER 2.0

CXrL

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Foreword

This book contains the Primer to SHADOW. We have tried to explain in detail all the aspects of the code that may be useful to the user in setting up his or her calculations. We have insisted on the description of the physical models rather than on the implementation of the algorithms used in the code in order not to obscure the physical aspects of the problems. SHADOW is a program in continuous evolution and development and thus some of the information contained in the manual may become obsolete rather quickly.

SHADOW is a multifaceted program and has been used to study optical systems ranging from flashlights to x-ray telescopes and microscopes. Many beamlines and monochromators around the world have been designed and studied with the help of SHADOW and the list is constantly growing. It is the interaction with all our users that has helped us in extending and debugging the code; we have always been (and will be) interested in implementing new cases and in incorporating extensions developed by others. As our users know, SHADOW is released in the form of a Fortran and C library of subroutines which are largely undocumented. This is because we want to avoid the uncontrolled proliferation of versions of the code: when that happens it becomes impossible to maintain the code. What we suggest to the user that has a valuable idea or code for the extension of SHADOW is to get in touch with us and we will incorporate the extension/addition in future releases of the code for the benefit of the whole community. It will be impossible to thank here all the users that have helped us with input and criticisms in the past; we look forward to keep this interaction going in the future.

SHADOW is a public domain software and we intend to keep it that way. The only exception would be to companies or individuals using the code for commercial resale or development for others. A code of the size of SHADOW needs however resources beyond part-time student workers, so that we have sought in the past support from Federal agencies (and will continue to in the future). The development of SHADOW has been supported by several sources over the years; significant support was received from the Synchrotron Radiation Center, the Department of Energy via the Center for X-ray Optics at Berkeley,the Department of Defense URI program, the Wisconsin Alumni Research Foundation, Brookhaven National Laboratory, Los Alamos National Laboratory and, more recently, the Naval Research Laboratory.

It is also appropriate to name all the persons that have directly contributed to the development of SHADOW . Barry Lai has written and debugged extensive parts of the code; Karen Chapman has developed an important fraction of the undulator source and written the original Primer. Paul Runkle and Chris Welnak have written most of the User's Guide for the Source and the Utilities and performed the computations described therein. Chris Welnak and Mumit Khan have ported the code to several Unix machines, and Luigi Capodieci has written the graphics interpreter for the Unix versions. Manuel Sanchez del Rio has written several extensions to the crystal model; Guan Jye Chen has written the Kumakhov lens and faceted mirror extensions.

F. Cerrina,
Madison, March, 1994.

Contents

Chapter 1

INTRODUCTION

The PRIMER describes the basic features of the programs and provides the user with the first hands-on experience. It is intended for the newcomer to the programs and provides annotated examples as a 'guided tour'. The reader should refer to the User's Guide for more in-depth coverage of the topics. The Glossary may also be quite helpful. In order to run the examples indicated below, we will assume that SHADOW has been installed and is successfully running.

In this PRIMER we will describe how to access SHADOW and some utility programs. Further examples can be found in the DEMOs included with the program, where some more advanced cases are illustrated, and in the USER's GUIDE (hereafter UsG) where specific examples for each program are given.

Please report any bugs or comments to *shadow@xraylith.wisc.edu*.

1.1 SHADOW structure

SHADOW is a software package that is designed to study the propagation of a photon beam through an optical system. The program is general, but is optimized for the case of X-rays and reflective optics such as those encountered in the XUV and in Synchrotron Radiation. The code is designed to be simple and reliable, with prompt- and menu-driven programs. SHADOW runs on the following computers: VAX running VMS, SUN running SUN OS 4.1+ or Solaris 2.1 (SUN OS 5.x), Decstation running Ultrix 3.+, and IBM RS6000 running AIX 3.1+.
SHADOW is formed by a core of main programs and by a collection of utilities used to process the output from the main programs. As shown in Fig. 1.1, there are three groups of programs falling under the confines of SHADOW. The first group is used in the I/O session to define the characteristics of the source and of the optical system. The second is the one performing the actual calculations, i.e., generating and tracing the photon beam through the optical system. The third includes analysis programs necessary to interpret the results

of the calculations performed earlier. The programs are run sequentially by the user in an interactive I/O session; they can also be run in batch mode.

The communication between different programs is via disk files. The files are normally created in the current directory [see INIT, below] and may be quite large, so that we strongly recommend VMS users to PURGE the disk area often. Some files have default names (like the ones indicated above), other have names that are supplied by the user. Briefly, we will encounter:

1.1.1 Data files:

Data files are normally in binary (unformatted) for accuracy and speed of disk access. NON printable. SHADOW creates these files containing the ray in a given position of the optical system (O.S.). Typical names are BEGIN.DAT for the beam at the source position, MIRR.xx (where xx is a number from 01 to 20) standing for the beam at the optical element (O.E.), STAR.xx for the image of each individual O.E., and SCREEN.xxyy for screens associates with O.E.'s. These files are quite large (in excess of 189 blocks for a 1000 rays file).

1.1.2 Parameter Files:

Parameter files are typically named START.xx, and are NAMELIST format. They list the values of the parameters used by SHADOW in setting up a calculation of a source or of an optical system. They can be EDITED (but we do not recommend it); there are modes to simply change single parameters. The DIFFERENCE (VAX DCL) utility may be useful in checking modifications on VMS. All data files can be regenerated from the START.XX files and, in some cases, preprocessor files.

1.1.3 Analysis Files:

Files created by the analysis programs vary widely in type and internal structure. Refer to the USER's GUIDE – Utilities for a description of the files generated by each program.

Notice that the internal structure of the files used by SHADOW is rigid, in particular for the DATA files, and cannot be modified by the user.

1.2 Definitions and Nomenclature

Here we describe the most commonly used terms in the code which are necessary in order to correctly set-up the calculations, when in doubt, look up the GLOSSARY. SHADOW operates on an OPTICAL SYSTEM, which is in turn formed by a SOURCE and by (one or more) OPTICAL ELEMENTS. Figure 1.2 illustrates an OPTICAL SYSTEM, formed

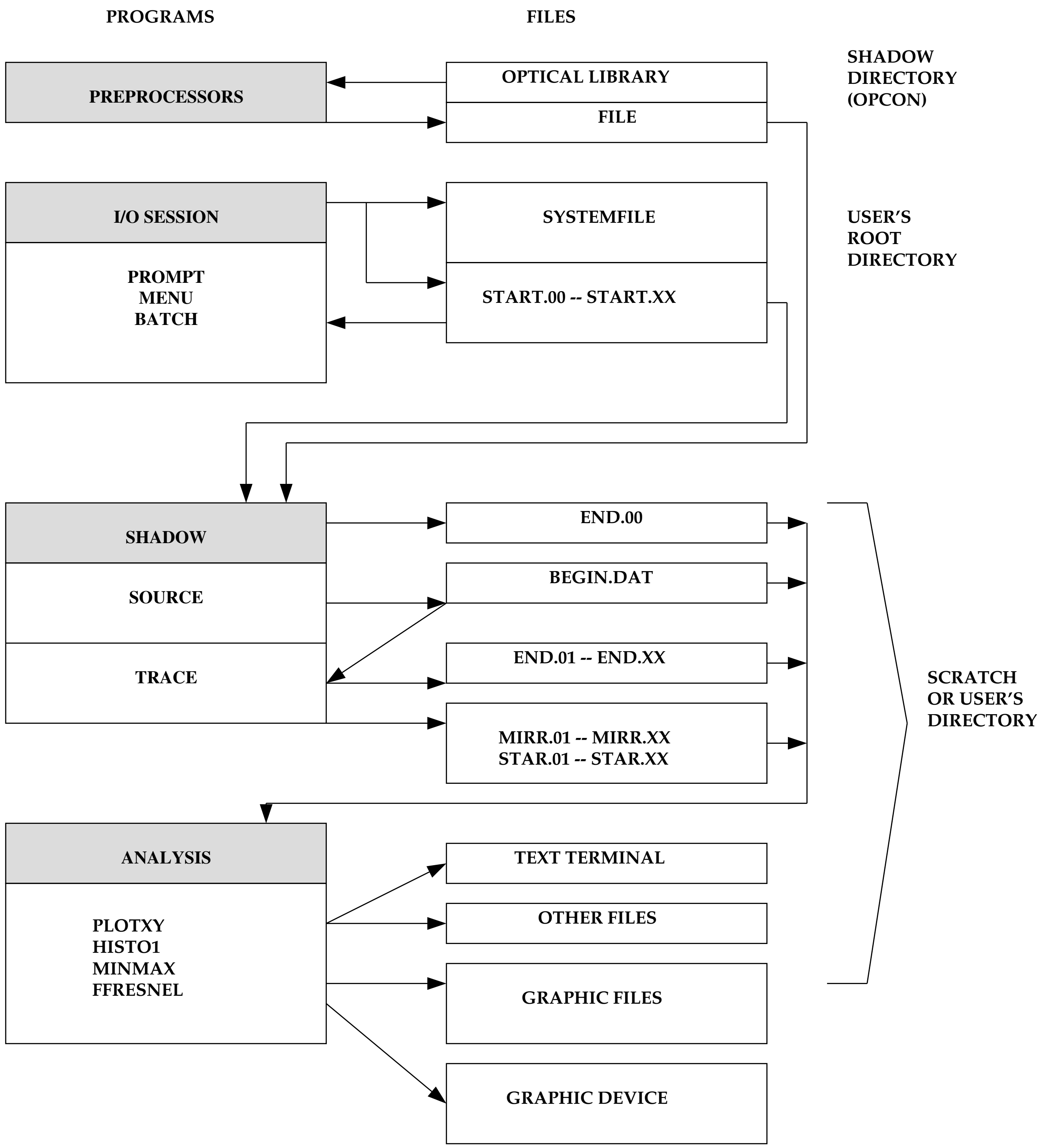

Figure 1.1: SHADOW structure

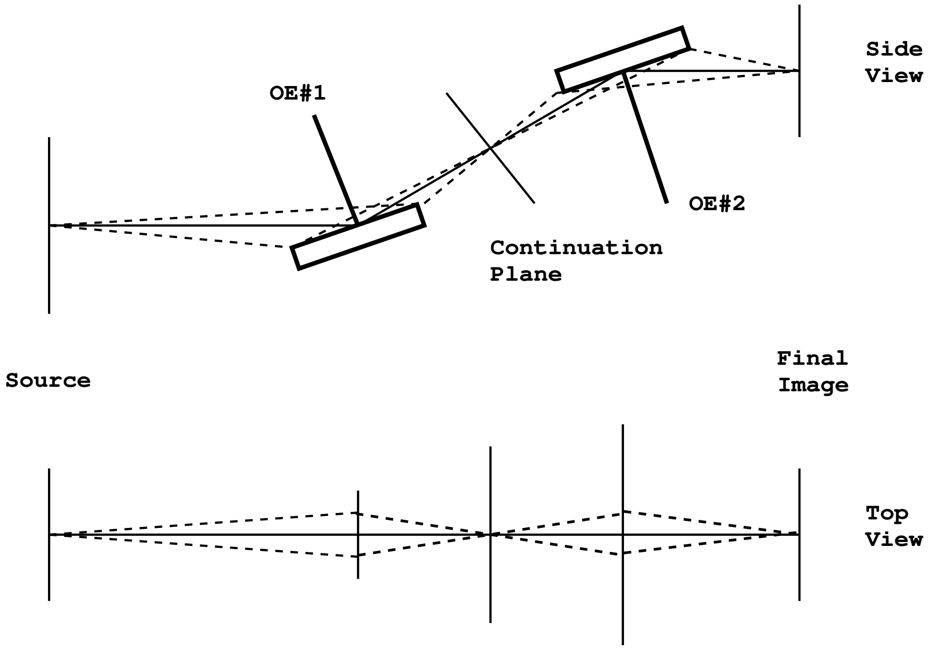

Figure 1.2: Two-mirrors Optical System

by two mirrors.

The solid line represents the 'central axis' or 'optical axis'; it connects the poles of the mirrors and defines the 'backbone' of the system.

The photon beam generated at the source is traced on the first mirror to the 'continuation plane', where an intermediate image is generated. This image becomes the source for the next mirror and is traced through to the final image position. SHADOW allows great flexibility in specifying the position and the type of mirrors used in the calculations. DATA files are generated at each 'critical' position in the optical element, i.e., at the mirror and at the continuation planes; more, if some options are selected.

In this way, many OE's can be concatenated together (up to 20). The files are automatically numbered to keep track of what belongs where.

Before beginning the description of a session, it is necessary to define briefly the geometry used by the programs (more in the *UsG*). SHADOW works in a cartesian reference frame, always using the full specification of the vectors. Most optical ray-tracing programs

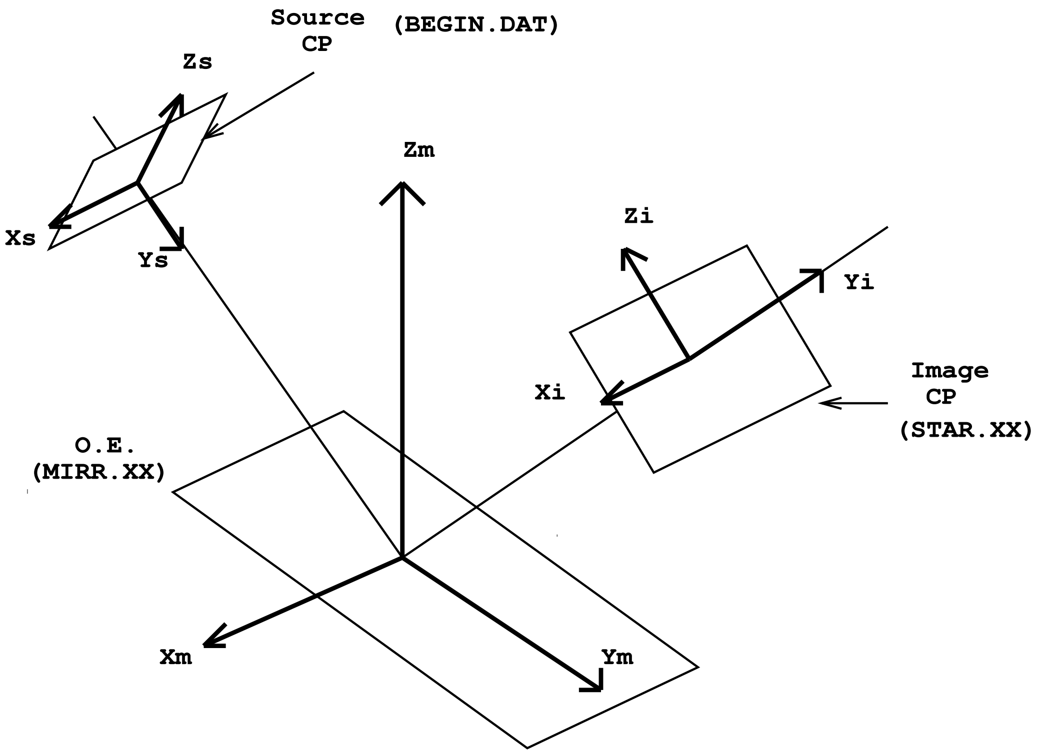

Figure 1.3: Optical Element Geometry and Continuation Planes

refer the rays components to the optical axis but, although cheaper in terms of storage, this solution is rigid and makes exotic geometries impossible to implement. We thus define the geometry shown in figure 1.3. Notice that this geometry is somewhat different from other codes (in particular machine physics conventions). Notice also how for an off-center system the reference frame of the source *flows* in that of the mirror.

This is all that is needed for a first run of SHADOW. We will introduce other terms as needed.

Chapter 2

OVERVIEW

2.1 HOW TO GET STARTED

Part of this manual is intended to take the user through the first steps in using SHADOW. It defines how to access the programs and presents some simple cases. To this purpose we present the literal screen output, as it should appear to the user: this text will be in `typewriter` style. Throughout the text, we will make use of several abbreviations and symbols to indicate I/O operations. Here is a list of some of these symbols. In the program listings that follow, the answer supplied by the user to the system questions are normally enclosed in a box, i.e., $\boxed{\text{BOXED}}$.

```
Symbol    Definition

  $       Represents the prompt from your host computer
          (VAX VMS). The prompt may be followed by a
          question asked by the computer or a command
          which the user is to enter.
  %       Represents the c-shell prompt from your host
          computer (UNIX).
  /       Used in the examples of interactive sessions
          to denote comments.
  OE      Optical Element (a mirror, grating, crystal,
          or lens).
  OS      Optical System (consists of one or more OE).
  TT      TT means the user's terminal in DEC's language.
 (or TT:)
  UsG     User's Guide
```

In cases where a command is different on VMS and UNIX, we will provide both. If it is a relatively short section, the text will be split into two columns and labeled *VMS* and *UNIX*, listing the appropriate commands for each system. If the example is sufficiently long, and will show a different screen on VMS and UNIX systems, the VMS example will be listed first with the UNIX example following. An example of the two column system is:

VMS	*UNIX*
$ DIR/SIZE/DATE/PROT *.DAT	% ls -al *.dat

We assume SHADOW is installed and running on your system. Access the system by logging in.[1] Before running SHADOW, it is necessary to define some logical names and commands. This is done by entering the command:

VMS	*UNIX*
$ @D0:[SHADOW]SETUP.COM	% source /usr/local/shadow/.shadowrc
	or for Bourne shell users:
	% . /usr/local/shadow/.shadowrc.sh

From this point on, Unix commands will be given in c-shell only.
There are several graphics devices supported. For VMS: Tektronix 40xx and 41xx, and Dec VT240 terminals. Hardcopy is available on Digital LN03 printers and HPGL. For Unix: xterminal and tektronix are supported displays, hardcopy is available on any Postscript device. To correctly plot your results, the display must be set, and the host machine must allow the connections.
Since SHADOW may generate a considerable amount of disk files, we recommend that you create a new directory for each project or new variation on the project, in order to keep an orderly data structure.

VMS	*UNIX*
$ CREATE/DIRECTORY [.test]	% mkdir test
$ SET DEF [.test]	% cd test

At this point, all the logical names are defined and you are ready to start SHADOW itself. The directory in which you currently are will be your 'root' directory for the rest of the session.

> A caution to UNIX users: Remember, the UNIX operating system is case sensitive! To make it easier on the user, we have tried to keep all file names in lower case for UNIX. In the examples, most of the file names are shown upper case, for the standard SHADOW files, use lower case to avoid "File not found" errors.

[1]For demonstration purposes, we assume that SHADOW is installed in the D0:[SHADOW] directory for VMS users, and the /usr/local/shadow directory for UNIX. It may be different on your system, hence, please verify where it is installed before starting.

An exception is the startup command GO.

2.2 SHADOW'S COMMAND LEVEL

To access SHADOW programs from the system prompt level, enter $\boxed{\text{GO}}$. This takes you to SHADOW command level where the prompt is "**Shadow::**". The available commands are: HELP, SOURCE, TRACE, MENU, INIT, EXIT. Each of these commands perform a specific function and after completion you are returned to SHADOW's command level. We describe the function of each command below. We notice that only two of these commands, SOURCE and TRACE, perform actual calculations. MENU is used to define new and/or modify already existing parameters. For this reason both SOURCE and TRACE ask the user to supply the path to a set of parameters that will form the basis of the calculations performed. After the user has supplied the data (using one of the input modes described below) the calculations are performed.

2.2.1 HELP

VMS only at this time. Invokes the help facility at the SHADOW command level and provides some on-line description of the local commands and of their purposes.

2.2.2 SOURCE

Used to define the source parameters and then generate the relative model. After entering the command, you will be prompted to choose an input mode (see below) during which the source physical description is "set-up". The source will then be generated automatically after the I/O session is completed. Chapter 5 contains several examples of this process.

2.2.3 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.

2.2.4 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 on VMS, on UNIX you may need to use >, < for the right and left arrows, and *<ctrl>P*, or *<return>* and *<ctrl>N* or *<backspace>* for the up and down arrows. No calculations are performed and only START files are generated.

2.2.5 INIT

(Not implemented on Unix.) The position in the VMS DCL structure when you type the command

VMS

$ @D0:[SHADOW]SETUP

is the location defined as your "root directory". All input and output is sent to the root directory unless you redirect it using the INIT command. This command is useful ONLY for systems with scratch area or scratch disk space (again, check with your system manager). The scratch area is often implemented in systems with limited disk space and defines an area that is regularly purged (e.g., once a day) so that data cannot accumulate. For such systems, INIT is used to define the disk area(s) where the program I/O operations are written. Use of the command is a desirable alternative to the accumulation of lengthy files in your root directory. Calculations, outputs and temporary files are directed to the scratch area while important files defining the OS remain in your root directory.

2.2.6 EXIT

Exit from SHADOW command level to operating system command level, restoring the terminal status to the standard one.

2.3 INPUT MODES

There are three ways to enter parameters characterizing source and OE. They are the three input modes, PROMPT, MENU, BATCH and are described below.

PROMPT mode

The user answers questions from SHADOW designed to cover the full specification of source or OE. The questions branch depending on the answers supplied; we *strongly* recommend to consult the I/O session flowchart in order to get familiar with the capabilities of the program. This is recommended as a starting point until familiarity with the minimum necessary parameters is achieved, since in this mode it is not possible to "forget" a parameter and generate surprising results. The mode is particularly useful (and safe) when setting up a new system. It is somewhat limited by the fact that it is not possible (yet) to back-track during the session to alter a single parameter without going through the process from the beginning.

MENU mode

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 some parameters, key to a particular setup, 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.`

`DEFINE (OE, SCREEN)`

This command tells SHADOW how many optical elements (i.e., surfaces) there are in the system. It is used to declare existence of OEs and SCREENs in the System. The elements are numbered starting from the source, which is always 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. For example, suppose 3 OEs already exist, and you want to define an additional OE between OE #2 and OE #3. You may use the DEFINE OE command and assign it as element number 3. The stack moves up to accommodate the new entry.

```
Ready::          DEFINE OE
Element number?  3
```

will generate a system as:

old OE	1		OE	1
old OE	2		OE	2
new OE	3	$\Longleftarrow$	OE	3
old OE	3		OE	4

The stack operates the same way for SCREENs on a single OE. Note, the maximum number of screens on a single OE is ten.

`DELETE (OE, SCREEN)`

Used to remove either an OE from the SYSTEM list or a screen from an OE. The system is renumbered down.

`GOTO`

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.

`LIST`

Gives a list of the currently defined OEs and SCREENs in an OS and their relative numbering.

`LOAD (SYSTEM, SOURCE, OE)`

Invokes the LOAD menu. This command LOADs an already defined 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 entered the correct file name root, hit the ← to return to the "Ready::" prompt.

`SAVE (SYSTEM, SOURCE, OE)`

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 SYSTEMFILE.DAT; when in doubt, *always use SAVE SYSTEM.*

> NOTE: You **MUST** issue the SAVE command before exiting from the MENU or else the data are lost. SHADOW will warn you if you have modified a file and not saved it.

`SELECT (SOURCE, OE, SCREEN)`

Before entering the screen driven menu you must SELECT which OE or SCREEN you wish to edit (modify). 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.

SPAWN

Spawns the process, giving full access to the operating system command level without interrupting the menu session, by creating a new 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.

MENU Editing Keys

The MENU programs use the arrows of a DEC type terminal to position the cursor in the menu. On VMS, the program works best on a VT100-VT200 type terminal.

$\uparrow, \downarrow$	are used to move between the menu lines
<ctrl>P, <ctrl>N	UNIX command to move between lines
$\rightarrow$, >	are used to enter a submenu or to move between OE's.
$\leftarrow$,<	to go back to next higher menu. If none, the program returns to the command level. It is equivalent to an EXECUTE command.
<ctrl>W	refreshes the screen.
?	VMS only: will give help on the specific line where the cursor is currently located.
<ctrl>C,	as well as EXIT, STOP, RETURN, QUIT will return the menu to the command level.

Unrecognized inputs will result in a brief listing of valid entries: when in doubt, enter some gibberish and the system will prompt you with a list of proper answers.

BATCH mode

This method takes a parameter file (START.xx, SYSTEMFILE.DAT) generated by a previous input session and supplies it to SHADOW for a re-run. You will simply be prompted for this parameter file name.

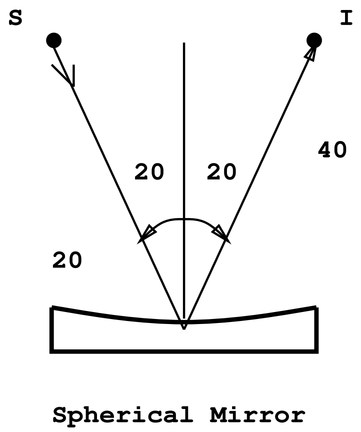

Figure 2.1: Spherical Mirror Geometry

2.4 PROMPT Mode Run

In this section we will give an example of how to run an interactive session with SHADOW. We have included a transcript of an actual session so that you should be able to duplicate the results. For the start, we will choose a very simple case, that is, a point source illuminating a spherical mirror, as illustrated in Fig. 2.1. Let's assume that we want to study an optical system focusing a (point) source located at 30 cm before the mirror to a distance 40 cm after the mirror. The source has an aperture of ± 0.1 rads in horizontal and ± 0.02 in vertical. We need an angle of incidence of 20^o and we do not know the radius of the mirror needed to satisfy the focal condition. We would like SHADOW to compute all the missing parameters for us. After the calculation we will have a look at the results using one of the utilities, PLOTXY. In this example we will then demonstrate how:

- To generate a simple source
- To trace a simple 1-mirror optical system
- To display some of the information

It may be a good idea to create a hard-copy of your session. This is particularly useful since it allows you to cross-check answers supplied earlier during the session. The specific command is terminal-dependent, for example on a VT220 (VT240) you may go in SETUP mode and set the PRINTER menu option to AUTO-PRINT. On an X-Windows system, you can start a new window and then print its contents.
In the following text, any line prefixed with " /* " represents a comment to the I/O record. Let's assume that we have started SHADOW successfully (if not return to beginning of chapt. 2) and let's

VMS

$ GO

UNIX

% GO

```
  ::::::: :::    ::          ::: :::::::     :::::   :::  ::  ::
 :::::::: :::    ::         :::: ::::::::   :::::::  :::  ::  ::
:::       :::    ::        ::: : :::   ::: :::    :: :::  ::  ::
:::       :::    ::       ::: :: :::    :: :::    :: :::  ::  ::
 :::::::  :::::::::      :::  :: :::    :: :::    :: :::  ::  ::
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:::::::   :::    :: :::       :: :::::::     :::::     ::: :::



VMS/Ultrix/Sun/AIX VERSION 2.0                    01 May 1993



 Hit <RETURN> when ready: <ret>
                               SHADOW

 Commands Available at this level:

 HELP       More information on the following commands
 SOURCE     Generates a source file
 TRACE      Starts the tracing of an Optical System from a
            specified source file
 MENU       Begins the process of defining an Optical System
 INIT       Defines scratch directories and set default to
            scratch
 EXIT       Returns to DCL

/* Shadow:: is the prompt at this level.  To begin the SOURCE procedure
/* type 'source'. If uncertain, enter a '?' to get a list of
/* commands. The procedures could be accessed directly by entering, for
/* instance,
```

VMS

$ GO SOURCE

UNIX

% GO SOURCE

```
/* This procedure generates a SOURCE for SHADOW.

   Shadow:: source


 SOURCE selected. Begin procedure.

   Mode selected [ enter ? for HELP ] ? : ?

  Enter :
 MENU       for screen-driven menus
 PROMPT            prompted session
 BATCH        file-oriented session

/* In response to our query SHADOW lists all the possible I/O modes. In
/* the present case we will select PROMPT.


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

 Call to INPUT

/* start of the I/O session

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

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

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


/*  Questions in verbose output are asked in a more descriptive manner.
/*  Terse questions supply very sparse information, if any.
/*  Initiate characterization of source.


 ------------- SOURCE SPECS ------------------
 Options available:
 Random in  BOTH REAL and MOMENTUM space                0
 Grid              BOTH                                 1
 Grid              REAL, random  MOMENTUM               2
 Random            REAL,  grid   MOMENTUM               3
```

```
 Ellipses in PHASE space, random around each ellipse     4
 Ellipses in PHASE space,   grid around each ellipse     5

 Source modeling type [ 0-5 ] ? 0
 How many rays [ 1 - 5 000 ] ? 1000
 Seed [ odd, 1000 - 1 000 000 ] ? 10001
 Do you want to optimize the source ? 0


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

 Then ? 0


  The source is specified in the laboratory reference frame. The program will
then rotate the set of rays in the mirror frame.
 Type of source,now.
          use  ( 0 ) for point source
               ( 1 ) for rectangular s.
               ( 2 ) for elliptical  s.
               ( 3 ) for gaussian    s.

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

 Source depth. The actual source will be centered on the no-depth
position. Use:
          ( 1 ) for no depth,
          ( 2 ) for flat depth distribution,
          ( 3 ) for gaussian depth distribution,
          ( 4 ) for a synchrotron source depth distr.
 Then ?

 Source Depth [ 1-4 ] ? 1

 O.K., got it so far.
          Source distribution now. We may use
              ( 1 ) for a flat source
              ( 2 )       uniform   s.
              ( 3 )       gaussian  s.
              ( 4 )       synchrotron
              ( 5 )       conical
              ( 6 )       exact synchrotron
```

```
Source Angle Distribution   [ 1-6 ] ? [1]
Horizontal half-divergence  [ (+)x, rads ] ? [.05]
.                           [ (-)x, rads ] ? [.05]
Vertical                    [ (+)z, rads ] ? [.01]
.                           [ (-)z, rads ] ? [.01]
Do you want a Photon energy [ Y/N ] ? [0]
Do you want to store the optical paths (OPD) [Y/N] ? [0]
Do you want to generate the A vectors (electric field) [Y/N] ? [0]
Exit from INPUT_SOURCE        /* all defined; calculation begins.
                              /* SHADOW always lets us know that calculations
                              /* are progressing.

Generated          250 rays out of         1000
                   500
                   750
                  1000
Exit from SOURCE

Source has been successfully generated.

SOURCE procedure completed.   /* Returns to shadow command level.


Shadow:: [exit]
Exit to DCL
/* SOURCE has now generated 1000 rays that have the distribution in angle, space
/* and photon energy as specified by the answer to the prompts. We can verify
/* that the following files have been generated:
```

VMS

```
$ [dir]
Directory DO:[SHADOW.TEST]

BEGIN.DAT;1 196  29-DEC-1992 13:35:21 /* file containing the 1000 rays
END.00;1      7  29-DEC-1992 13:35:23 /* parameter file (output) from SOURCE
START.00;1    7  29-DEC-1992 13:35:16 /*                (input) to SOURCE

Total of 3 files, 210 blocks.
```

UNIX

```
% [ls -al]
```

```
total 120
drwxr-xr-x  2 shadow       512 Dec 29 13:57 .
drwxrwxr-x  3 shadow      1536 Dec 29 13:56 ..
-rw-rw-r--  1 shadow    104020 Dec 29 13:57 begin.dat
-rw-rw-r--  1 shadow      3142 Dec 29 13:57 end.00
-rw-rw-r--  1 shadow      3142 Dec 29 13:57 start.00

/* Since we now have a file with a source, we can begin to trace the
/* mirror. Notice how the commands for generating the source and tracing the
/* system are separate.
```

VMS	*UNIX*
$ GO trace	$ GO trace

```
/* This bypasses the shadow command level since a command has been
/* specified following 'GO' and takes us directly to the TRACE option.

 Ray Tracing Selected. Begin procedure.

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

 PROMPT selected.
 Call to RESET                /* SHADOW clears definitions and initializes
 Exit from RESET              /* variables

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

/* SHADOW is inquiring if we are starting a calculation from the
/* beginning of the system or we want to resume a tracing interrupted
/* at an intermediate position.

 Then ? 0

 Call to INPUT_OE

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

```
/* self-explanatory

 Defining Optical Element:  [1]
 Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] [<ret>]


/* SHADOW inquires if it is necessary to continue tracing or if the end of the
/* system has been reached.

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

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

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

 Then ?  [0]

 Let's define the optical or central axis of the system  for this particular
optical element.  By this I mean a ``virtual'' line that runs throughout  the
optical system. Along this line are located the  ``continuation'' planes, where
the OS is subdivided in the  individual OE. This line does not have to coincide
with the  true optical axis, as it is used mainly for bookkeeping the  data,
but it helps greatly in the data analysis if this  identity is preserved as
everything in the program is referred to it.  Once established, you still have
complete freedom of  ``moving'' around the mirrors.  In the case of a grating,
you will have several choices. The  program may override your specifications
for the central axis  and locate the source and image at the ``best'' position.
 You will be prompted later for this option.  It is recommended to use CM as
units. This is not critical for most cases, but it is in the case of
diffraction elements.
\* Most importantly, use the same units throughout the specification of
\* source and system unless otherwise specified.
 Optical Element definition:

 Incidence Angle ?    [20].         //Degrees
 Source Distance ?    [20]
 Reflection Angle?    [20].         //Degrees
```

```
Image Distance  ?   [40]
Reflector [ 0 ] or refractor [ 1 ] ?   [0]

Kumakhov lenses are formed from tube arrays
their packing pattern are Wigner-Seitz type cell

A: Is this a Kumakhov system? [0]

Compound mirrors ( or lenses) are formed
by several smaller mirrors ( facets) combined together.

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

 Lets define the mirror. I may compute its parameters, like the  radius or the
axes. This will not affect the rest of the calculations;  all the geometrical
parameters may be modified later.  Or, you may wish to specify the mirror
parameters yourself.

What kind of surface are we dealing with ?
spherical    = 1
elliptical   = 2
toroidal     = 3
paraboloid   = 4
plane        = 5
Codling slit = 6
hyperbolical = 7
cone         = 8
polynomial   = 9

Mirror surface [ 1-9] ?   [1]
Do you want to specify the mirror parameters ?  [0]
Is the mirror Cylindrical ?   [0]
Is this optical element a Fresnel Zone Plate ? [0]
Are we dealing with a Grating ?   [0]
Are we dealing with a crystal [ Y/N ] ?   [0]
Is the mirror convex [ Y/N ] ?   [0]

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 ] ?   [ 0 ]
```

Mirror orientation angle. Angles are measured CCW, in deg,
referring to the mirror normal. Alpha=0 is the mirror
sitting at the origin, facing up. Alpha = 90 is the
mirror standing at your right and facing left when you
look along the beam STANDING ON THE PREVIOUS MIRROR and so on.

Orientation Angle [Alpha] ? $\boxed{0}$
Mirror Dimensions finite [Y/N] ? $\boxed{0}$

The mirror will be computed from the optical parameters
that you supply. For example, in the case of a spherical mirror
I will compute the radius of the mirror to satisfy the equation
1/p + 1/q = 2/(R*cos(theta)) given p,q and theta.
This will NOT affect in any way the placement of the mirror in
the optical element.

Foci placed at continuation planes [Y/N] ? $\boxed{1}$

The Optical Element and the the relative mirror are now fully
defined. The mirror pole is now located at the ‘‘center’’ of the
optical element. It is possible to override this situation and
‘‘move’’ the mirror without affecting the rest of the system.
It is also possible to move the ‘‘source’’ without affecting the
rest of the system.
The movements are expressed in the DEFAULT Mirror Ref. Frame
so that if you move BOTH source and mirror the relative
movement is the vector sum of the individual ones.
A word of caution: SOURCE movements and MIRROR movements are
NOT equivalent from the point of view of the whole system.

Do you want to move the Source [Y/N] ? $\boxed{0}$

----- Mirror rotations and position. -----

We define three angles, as rotations around the three axis.
These rotation are defined in the program as corrections to
the mirror nominal position; that is, they modify the mirror
position relative to the Default Mirror Reference Frame, where
all the calculations are performed. Remember that rotations
do NOT commute. I apply them in the same order of entry.
CW ROTATIONS are (+) angles. A translation can be also applied
to the mirror.

Do you want to move the mirror itself [Y/N] ? $\boxed{0}$
Distorted surface [Y/N] ? $\boxed{0}$

```
 Do you want to include surface roughness [Y/N] ?  [0]
 Any screens in this OE [ Y/N ] ?   [0]
 Slit at continuation plane [ Y/N ] ?   [0]
 Extra Image plates [ Y/N ] ?   [0]
 File containing the source array ?   [begin.dat]


Exit from INPUT

Tracing optical element #  1        /* SHADOW always lets the user know
 Call to SETSOUR                    /* that calculations are in progress.
 Exit from SETSOUR
 Call to IMREF
 Exit from IMREF
 Call to OPTAXIS
 Exit from OPTAXIS
 Call to MSETUP
 Exit from MSETUP
 Call to RESTART
 Exit from RESTART
 Call to MIRROR
 Exit from MIRROR
 Call to IMAGE
 Exit from IMAGE
 Call to RESET
 Exit from RESET                       /* OE completed; ready for next.


Do you want to change input mode ?   [0]


 Call to INPUT_OE

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 Defining Optical Element: 2

 Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ]    [exit]
 Shadow:: [EXIT]
 Return to DCL
```

We have achieved our goal, so we have returned to DCL. Let us have a look at the results of the calculation.

VMS

```
$
$
$ dir/since
 Directory D0:[SHADOW.TEST]

EFFIC.01;10             1  29-DEC-1992 14:50
END.01;10              13  29-DEC-1992 14:50
MIRR.01;1             196  29-DEC-1992 14:50
OPTAX.01;12             2  29-DEC-1992 14:50
STAR.01;1             196  29-DEC-1992 14:50
START.01;12            13  29-DEC-1992 14:50

Total of 6 files, 421 blocks.
```

UNIX

```
% ls -al
-rw-r--r--  1 shadow      162 Dec 29 14:45 effic.01
-rw-r--r--  1 shadow     6272 Dec 29 14:45 end.01
-rw-r--r--  1 shadow   104020 Dec 29 14:45 mirr.01
-rw-r--r--  1 shadow      597 Dec 29 14:45 optax.01
-rw-r--r--  1 shadow   104020 Dec 29 14:45 star.01
-rw-r--r--  1 shadow     6272 Dec 29 14:45 start.01
```

This is a 'minimal' set of files, since SHADOW may generate more if other options are selected. The large STAR and MIRR are the files containing the arrays with the 1000 rays at the image plane and mirror surface, respectively. SHADOW is a verbose program and likes to generate large amount of data; from this the usefulness of the 'scratch' area. We now may have a first look to the results. For that, we will make use of PLOTXY (see UsG), a graphics utility that quickly plots any projection of the beam at any position where an output file has been generated. We will look first at the STAR.01 file, the image at the continuation plane.

VMS

```
$
$ plotxy
```

UNIX

```
% plotxy
```

```
 PLOT> Input file? star.01

 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]
PLOT> Comment for plot [ 80 char ] ? [Image at continuation plane]


PLOT> File read OK. Full specifications:
      DO:[SHADOW.TEST]STAR.01;1
      Was created : 29-DEC-1992 14:50

PLOT> Found         1000 good points out of        1000

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

 1  X   -0.40999        0.40627        0.14771E-02    0.24263
 2  Y   -0.17154E-14    0.17942E-14    0.10171E-15    0.58061E-15
 3  Z    0.71211E-07    0.96965E-02    0.34127E-02    0.28083E-02
 4  X'  -0.27145E-01    0.27335E-01   -0.97068E-04    0.16155E-01
 5  Y'   0.99960         1.0000        0.99986        0.00000E+00
 6  Z'  -0.76371E-02    0.74764E-02   -0.23875E-03    0.42787E-02
11   Photon Energy  (eV)     0.00000E+00    0.00000E+00

/* The former table gives some statistical information about the rays traced
/* by SHADOW. To understand the meaning, refer to Fig. 1.3, that describes the
/* geometry used by SHADOW. Since we are plotting a STAR file, i.e., the
/* intercepts at the image plane, it is easily understood that Y (row 2) will
/* be zero within the machine precision, while Y' (Y direction of ray) will be
/* always very close to 1.


PLOT> Rows to use for plot :
PLOT>   for horizontal axis ?  [1]
PLOT>   for vertical axis   ?  [3]

PLOT> Scaling options. Enter
      0   For automatic scaling
      1   For cartesian scaling
      2   For external limits

PLOT> Then ?  [0]

PLOT> Plotting options :
      0   For scattered plot
      1   For connected plot
      2   For contour plot
```

```
PLOT> Then ?  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> Number of bins for X axis [default = 25] : <ret>
PLOT> Number of bins for Y axis [default = 25] : <ret>
```

VMS

```
PLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107: 2
PLOT> Do you want to save the TD command file ?  1
```

UNIX

```
Display type:
  [ 0 ] Xwindow
  [ 1 ] Tektronix
  [ 2 ] Postscript file
Terminal type:  0
```

This completes this first simple example. Why not try to plot out other projections of the beam? If you enter MIRR.01 and then specify 1 and 2 you will have a picture of the radiation's footprint on the mirror. Furthermore, if you specify again STAR.01 but rows $\{1,4\}$ or $\{3,6\}$ instead of $\{1,3\}$, you will plot out respectively the x or z phase space. These plots are very important in finding the distance from the focus; you should see that the z phase space is quite symmetric relative to the vertical axis of the plot (z'), indicating that the beam is at a waist at that position, while the x phase space should have a distinctive slant to it. The slope is indeed equal to $1/\Delta$, if Δ is the distance of the *sagittal* focus from the continuation plane: the system is quite astigmatic. Furthermore, an ideal focusing system would give a straight line in phase space: deviations from it directly indicate the existence of aberrations.

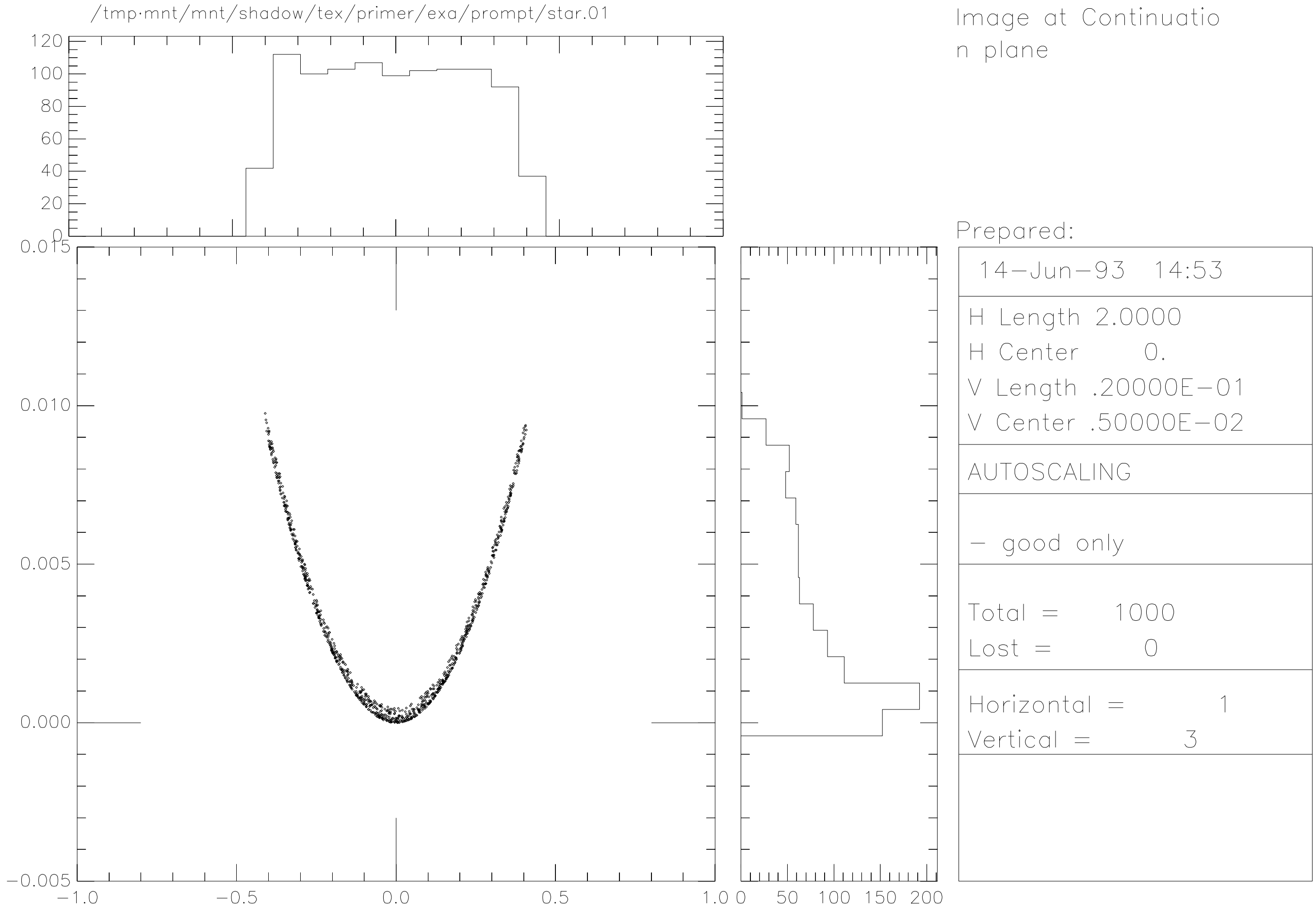

Figure 2.2: Image at continuation plane

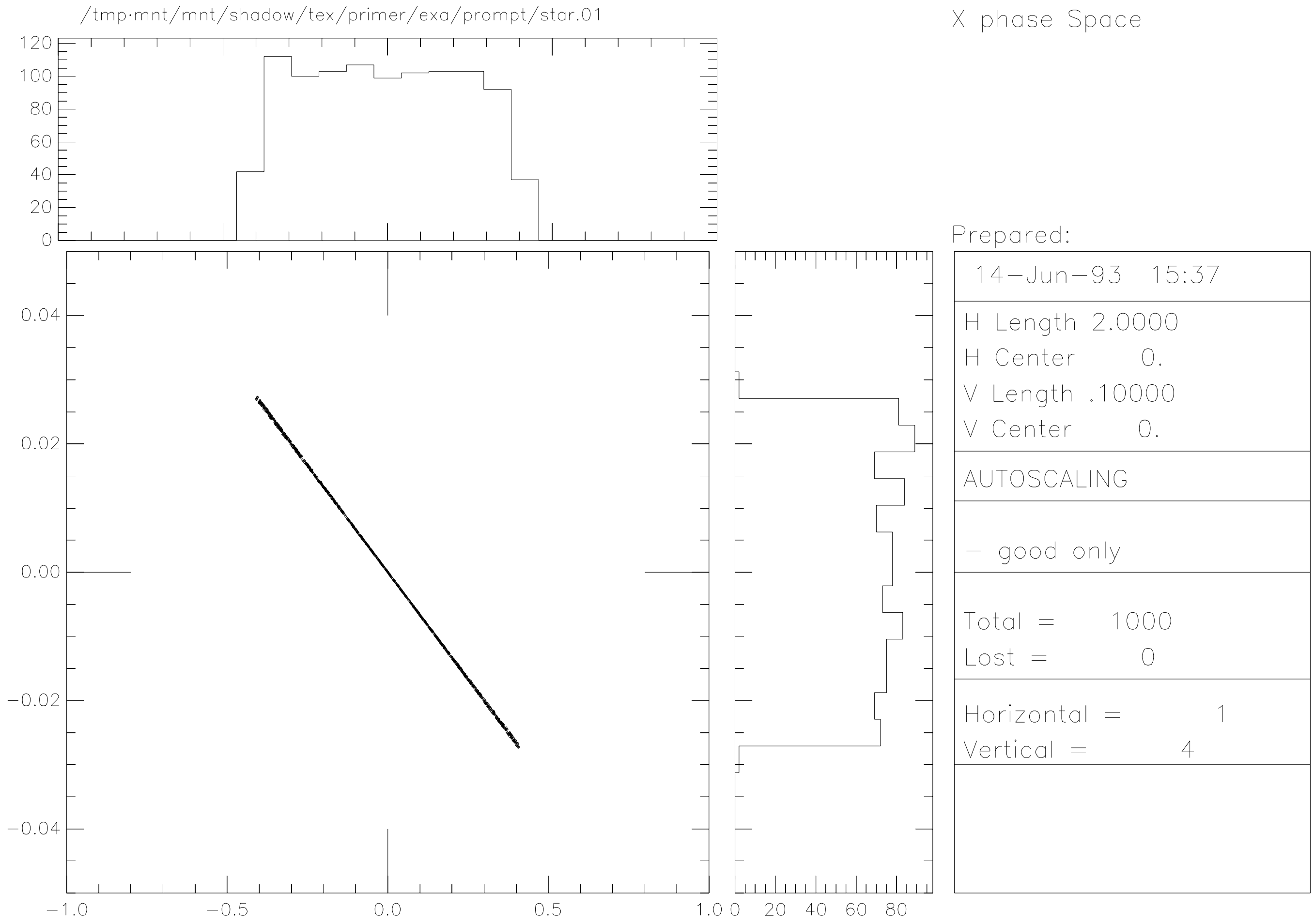

Figure 2.3: X-phase space

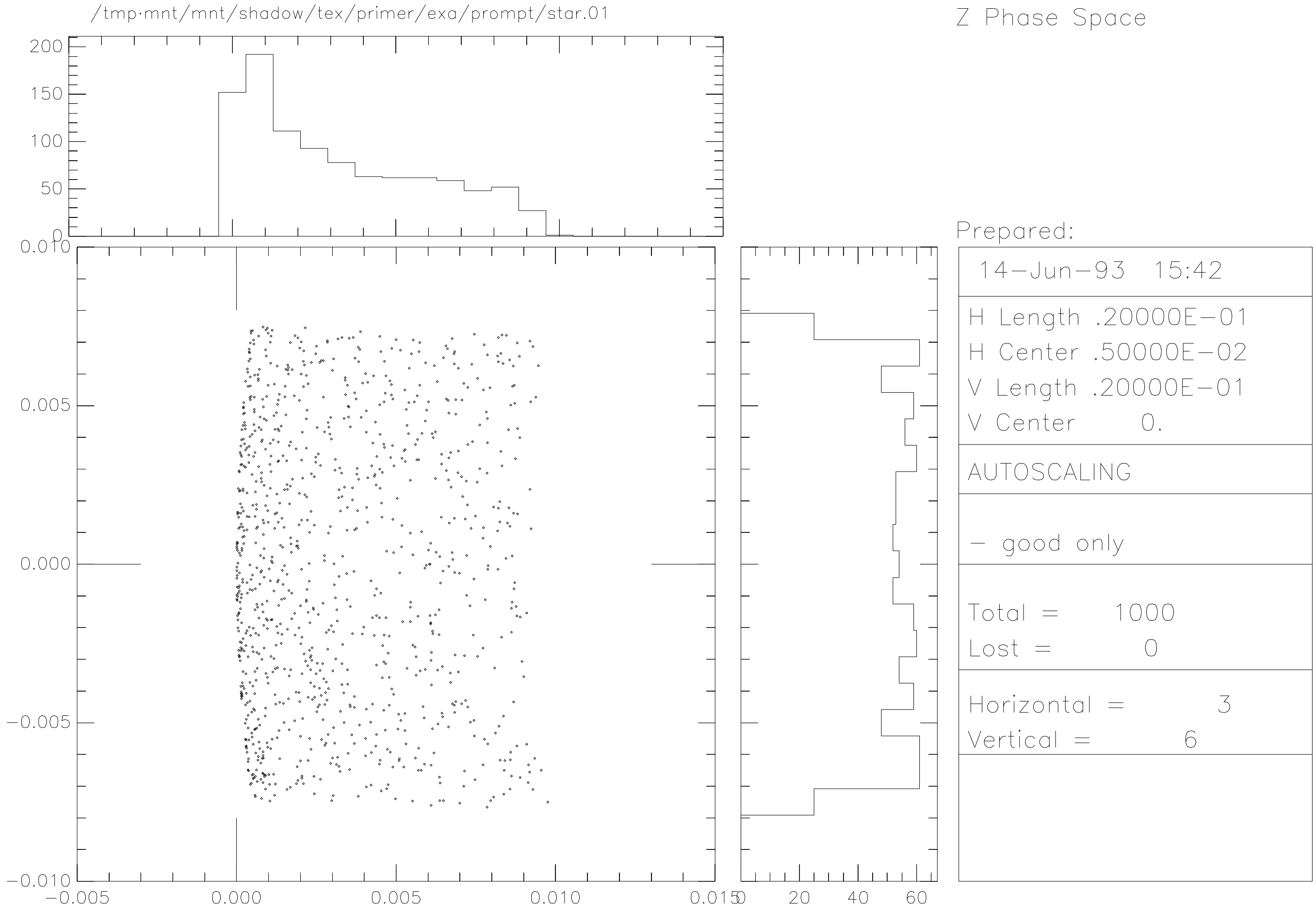

Figure 2.4: Z-phase space

2.5 MENU Mode Run

In this section we will demonstrate the use of the MENU input mode. As usual, we have included a transcript of an actual session, with comments. The example used in the calculations is the same as in the PROMPT mode, i.e., a simple spherical mirror. Due to the extensive screen manipulations performed by MENU, it is difficult to present a hard-copy. We simulate the cursor as ▮, while each part of text limited as

is meant to represent a typical MENU screen. We will also show the use of two programs, MIRINFO and SYSINFO, that can be used to obtain an organized description of the mirror and of the system, respectively. The user will then learn how:

- To use the MENU mode to specify a SOURCE
- To use the MENU mode to trace an Optical Element
- To use the MENU mode to define a SCREEN in the Optical Element
- To use the MIRINFO and SYSINFO programs

This said, let us

```
$ GO

                                SHADOW

 Commands Available at this level:

 HELP                 More information on the following commands
 SOURCE               Generates a source file
 TRACE                Starts the tracing of an Optical System from a specified
                      source file
 MENU                 Begins the process of defining an Optical System
 INIT                 Defines scratch directories and set default to scratch
 EXIT                 Returns to DCL


  Shadow:: SOURCE
  SOURCE selected. Begin procedure.
  This procedure generates a SOURCE for SHADOW.
  Mode selected [ ? <ret> for HELP ] ? : MENU

  Prepare MENU...
```

```
Ready:: SEL SOURCE
```
/* The MENU screens have all the same structure. We have:

```
Definition area                       Value            Dialogue
-------------------------------------------------------------------

Source Definition

File to store the rays                BEGIN
Source Type (+)                       RAN/RAN
Number of random rays                 1000
Spatial Type (+)                      POINT
Depth                                 OFF
Angle Distribution (+)                FLAT             ▌
Photon Energy distribution (+)        OFF
Store optical path                    NO
Polarization (+)                      NO
Coherence                             COHERENT

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

/* For example, we can position the cursor at the line:

```
Angle Distribution (+)                FLAT          ▌
```
/* the (+) indicates that there is more information available in a lower
/* sub-menu. We can access the sub-menu by hitting the → key.
/* The screen now shows:

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

Source Angle Distribution

Angle distribution (+)             FLAT                     ▌

Use RADIANS for angles here.
Use ABSOLUTE values.

Horizontal divergence [(+)X]       0.0000000000000E+00
                      [(-)X]       0.0000000000000E+00
Vertical divergence   [(+)Z]       0.0000000000000E+00
                      [(-)Z]       0.0000000000000E+00
Cone internal half-aperture   n/a  0.0000000000000E+00
     external                 n/a  0.0000000000000E+00
Vertical Sigma         [ Z ]  n/a  0.0000000000000E+00
Horizontal             [ X ]  n/a  0.0000000000000E+00

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

```
/* Let's bring the cursor to the line
.     Horizontal divergence [(+)X]          0.0000000000000E+00
/* and then let's enter 0.05, without hitting <ret> yet.
/* The screen will show:
.     Horizontal divergence [(+)X]          0.0000000000000E+00   0.05
/* and, when we hit <ret> or any of the arrows, the field will be updated to
.     Horizontal divergence [(+)X]          0.5000000000000E-01
/* and we can then enter all the other values. When we are done, the screen
/* may look somewhat like:
```

```
Source Angle Distribution

Angle distribution (+)            FLAT

Use RADIANS for angles here.
Use ABSOLUTE values.

Horizontal divergence [(+)X]       0.5000000000000E-01
                      [(-)X]       0.5000000000000E-01
Vertical divergence   [(+)Z]       0.1000000000000E-01
                      [(-)Z]       0.1000000000000E-01
Cone internal half-aperture   n/a  0.0000000000000E+00
     external                 n/a  0.0000000000000E+00
Vertical Sigma         [ Z ]  n/a  0.0000000000000E+00
Horizontal             [ X ]  n/a  0.0000000000000E+00
```

Notice the "n/a" field. It means *Not Available* for modification by the user. A value may be entered and SHADOW will dutifully store it, but at execution time the program will ignore that variable and consider only those that are *not* prefixed nu 'N/A'. It means that the values defining, for example, the vertical σ of a gaussian source will not be used since the source is FLAT. This said, at this point we can hit the left arrow ← and return to the higher level. As a further example, let's assume we would like to specify a rectangular source. We bring the cursor to the field

```
    Spatial Type (+)                          POINT
/* and enter:
    Spatial Type (+)                          POINT         RECT <ret>
/* to obtain:
    Spatial Type (+)                          RECTANGLE
/* at this point we can access the sub-menu, as we did before, by hitting the
/* right arrow →. The screen will show:
```

```
Source Spatial Characteristics

Source type                           RECTANGLE          ▮
    Depth                             OFF
    width [ X ]                       0.0000000000000E+00
    height [ Z ]                      0.0000000000000E+00
    depth [ Y ]                  n/a  0.0000000000000E+00
sigma X                          n/a  0.0000000000000E+00
sigma Z                          n/a  0.0000000000000E+00
sigma Y                          n/a  0.0000000000000E+00
```

/* once more, we position the cursor to the line

```
.         width  [ X ]                  0.0000000000000E+00    ▮
```

/* and enter

```
.         width  [ X ]                  0.0000000000000E+00   0.2 <ret>
```

/* to obtain

```
.         width  [ X ]                  0.2000000000000E+00
```

/* and we do the same for the height. At this point we have defined all the
/* parameters that we need, and we may try to EXIT in order to generate the
/* source. But after our command we receive a warning:

Ready:: $\boxed{\text{EXIT}}$
Source has not been SAVED.
Confirm EXIT [Y/N] ? $\boxed{\text{N}}$

/* we forgot to store the definition on disk and SHADOW reminds us.
/* We have then to enter:

Ready:: $\boxed{\text{SAVE SOURCE}}$

```
Save Source Description

Directory name                        SYS$START:  ▮
File name                             START
```

/* this menu has the same structure as the ones above. We could rename the
/* file and the directory, but usually it is not worth it and we can leave
/* the default values. We can simply enter ← to execute the
/* command. We get in return the message

Writing to file SYS$START:START.00

/* and we can then exit the MENU level. SHADOW will start immediately to
/* generate the source.

Ready:: $\boxed{\text{EXIT}}$

```
Exit from MENU to SHADOW COMMAND level

Generated          250 rays out of         1000
                   500
                   750
                  1000
Exit from SOURCE

SOURCE => Source has been successfully generated.
SOURCE procedure completed.

Shadow::
```

At this point SHADOW has computed the array describing the source and is waiting for further commands. We are ready to follow the evolution of the rays propagating through the system and for that we start the TRACE session.

```
Shadow:: [TRACE]
Ray Tracing Selected. Begin procedure.
Mode selected [ ? <ret> for HELP ] ? : [MENU]
MENU selected.
Execute existing SYSTEMFILE ? : [N]


...Prepare MENU


Ready:: [DEF OE]

Element: [1]
Ready:: [DEF SCREEN]
Screen/Slit: [1]
Ready:: [SEL OE]
Number of Element: [1]
```

```
MAIN MENU                         Optical Element 1

Files to write out                ALL
Source plane distance             0.0000000000000E+00
Image plane distance              0.0000000000000E+00
Incidence angle                   0.0000000000000E+00
Reflection angle                  0.0000000000000E+00
Mirror Orientation Angle          0.0000000000000E+00
Source file                       BEGIN

Type of element (+)               REFLECTOR
Figure (+)                        PLANE                 ?
Diffraction (+)                   MIRROR
Crystal (+)                       NO
Mirror movement (+)               NO
Exit Slit (+)                     NO
Modified Surface (+)              NO
Source Movement (+)               NO
     Goto OE (+) ?
```

To each field there is an HELP associated. For example, is the user does not know what type of mirrors can be defined, SHADOW will volunteer the information. Position the cursor at Figure (+) and hit ? followed by <ret>. The screen will display a description of the variable name you've inquired about and of the possible inputs, as well as any other pertinent information. In this case the screen will display:

```
FMIRR

        Flag describing the mirror figure. So far, we have:

          Spherical                    Hyperbolical
          Elliptical                   Conical (axicon)
          Parabolic                    Polynomial
          Plane                        External (in prep)
          Codling Slit                 Spline (in prep)

  Topic? <ret>
```

MENU is also error-proof, in the sense that you can always modify your inputs if you realize you have made a mistake. If the input is not one of the acceptable values, MENU will prompt you with a list of choices. Suppose instead that you enter some gibberish followed by <ret>. SHADOW will display a list of valid entries on the lower portion of the screen.

The menu remains intact and the lower portion of the screen will display:

```
Use SPHERICAL ELLIPTICAL TOROIDAL PARABOLICAL PLANE CODLING SLIT ...  (Return)
```

We need to enter the geometry of the system as in the prompt example. Starting on the second line, enter the Source plane distance (30), image plane (40), and the incidence and reflection angles (20). Position the cursor to the ninth line and type SPHERICAL followed by <ret>; this tells SHADOW that we want to use a spherical mirror. Four letters are normally sufficient for the parser to resolve ambiguities. Let us now define the location of the optical screen. The screen menu is invoked as:

`Ready::` SEL SCREEN

```
Screen/Slit:  1

View Screen/Slit Data       Optical Element 1 Screen 1

Position rel.  to mirror         BEFORE
Distance (abs) from mirror       0.0000000000000E+00
Aperturing                       NO
Open slit/ solid stop       n/a  SLIT
Aperture shape              n/a  RECTANGULAR
Slit width/ x-axis          n/a  10.00000000000
Slit height/ z-axis         n/a  10.00000000000
Absorption                       NO
Thickness [ CM ]            n/a  0.0000000000000E+00
Opt.  Const.  File-name     n/a  NONE SPECIFIED
     Goto Screen/Slit (+)
```

Position the cursor to the first line and type AFTER followed by <ret>. Position the cursor to the second line and type 90.00 followed by <ret>. These instructions tell SHADOW to position an observation screen at 90.0 units AFTER the mirror (i.e., downstream).

`Ready::` SAVE SYSTEM

```
Save Optical System Description

Directory name                   SYS$START:
File name                        START
```

after you hit ← , MENU will display:

```
 Writing to file SYS$START:START.01
 Ready:: EXIT

Exit from MENU to SHADOW COMMAND level
Call to RESET
Exit from RESET

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

 Then ? 1

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

Procedure completed. Return to COMMAND level

Procedure completed.

 Shadow:: EXIT
 Exit to DCL
```

VMS

```
$
$ DIREC/SIZE/DATE

Directory DO:[SHADOW.TEST]

BEGIN.DAT;1            196  30-DEC-1992 15:26
EFFIC.01;1               1  30-DEC-1992 15:26
END.00;1                 7  30-DEC-1992 15:26
END.01;1                13  30-DEC-1992 15:26
MIRR.01;1              196  30-DEC-1992 15:26
OPTAX.01;2               2  30-DEC-1992 15:26
SCREEN.0101;1          196  30-DEC-1992 15:26
STAR.01;1              196  30-DEC-1992 15:26
START.00;1               7  29-DEC-1992 13:35
START.01;2              13  30-DEC-1992 15:23
```

```
 SYSTEMFILE.DAT;1         1  30-DEC-1992 15:23

 Total of 11 files, 828 blocks.
```

UNIX

% ls -al

```
total 460
drwxr-xr-x  2 shadow       512 Dec 30 15:28 .
drwxrwxr-x  3 shadow      1536 Dec 30 11:24 ..
-rw-rw-r--  1 shadow    104020 Dec 29 13:57 begin.dat
-rw-r--r--  1 shadow       162 Dec 30 15:28 effic.01
-rw-rw-r--  1 shadow      3142 Dec 29 13:57 end.00
-rw-r--r--  1 shadow      6515 Dec 30 15:28 end.01
-rw-r--r--  1 shadow    104020 Dec 30 15:28 mirr.01
-rw-r--r--  1 shadow       597 Dec 30 15:28 optax.01
-rw-r--r--  1 shadow    104020 Dec 30 15:28 screen.0101
-rw-r--r--  1 shadow    104020 Dec 30 15:28 star.01
-rw-rw-r--  1 shadow      3142 Dec 29 13:57 start.00
-rw-r--r--  1 shadow      6429 Dec 30 15:28 start.01
-rw-r--r--  1 shadow        15 Dec 30 15:28 systemfile.dat
```

The meaning of these files is described later; we already know that BEGIN is the source, MIRR the mirror image and STAR the image file. We can plot them out by using PLOTXY (see previous section). Let us instead inspect in some detail the type of mirror that SHADOW has produced; for this we will need the END files.

```
$
$
$ MIRINFO

  -------------------- M I R I N F O ----------------------
                    vs. 3.0 - May 1993
  MINFO> Mirror descriptor file. It must be an END.xx type.
  MINFO> Please input filename: END.01
  MINFO> File read correctly.
  MINFO> Title ? PRIMER
  MINFO> Comment ? FIRST MIRROR
  MINFO> Output file ? MIRRO1.LIS
  MINFO> Prepare output to file : MIRR01.LIS
$
$
$ TYPE MIRRO1
```

```
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
********************   MIRROR  DESCRIPTION   ********************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
PRIMER
FIRST MIRROR
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:END.01
Full file Specification :D0:[SHADOW.TEST]END.01;1
Creation Date          :30-DEC-1992 15:26
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

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                              40.00000000000000
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                            40.00000000000000
Incidence angle                           20.00000000000000
Parameters used follow:
Spherical Radius                       36.4860951
Source of this O.E. moved              NO
Mirror at pole position ( no mov. )    YES
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
***************                E N D                ***************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Notice how SHADOW supplies us the mirror radius satisfying the requested focal conditions. Let us have a look now at the system geometry.

$
$
$ $\boxed{\text{SYSINFO}}$

```
  -------------------- S Y S I N F O ----------------------
```

```
                   vs. 2.02  June 1989
 Default filenames [ Y/N ] ? Y
 How many OE's ? 1
 INPUT> Title ? PRIMER
 INPUT> Comment ? System Description
 INPUT> Output file-name ? SYSTEM.LIS
 SYSINF> Prepare output to file : system.lis
 SYSINF> File END.01
  read correctly.

 $ TYPE SYSTEM
```

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
**************  S Y S T E M     D E S C R I P T I O N  **************
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
PRIMER
System Description
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Input file specified:
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 #    Optical Element:                                       Creation Time:
   1   D2:[SHADOW.TEST]END.01;1                           30-DEC-1992 15:26

++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Optical Element #            1      System Number:

MIRROR   SPHERICAL           UNLIMITED      COMPUTED       REFLEC. OFF

  Orientation          0.0000000000000000E+00 deg.
  Source Plane          30.00000000000000
  Incidence Ang.        20.00000000000000     deg.
  Reflection Ang.       20.00000000000000     deg.
  Image Plane           40.00000000000000
    ----------------
  SCREENS:            1 defined.
AFTER Mirror         at    90.00000000000000
    ----------------

                        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    30.000000000       0.00000000000E+00
        1'      0.00000000000E+00  -0.64177772476        25.711504387

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

Notice how SYSINFO lists the location of all elements in the laboratory reference frame. We can plot out the beam at the SCREEN location by using PLOTXY, just like we did before for STAR (the reference frame is the same).

2.6 BATCH mode run

This section will demonstrate the use of the BATCH input mode. This mode is particularly useful when used to re-trace an OE or a system defined in an earlier session. It assumes that the following files are existing:

VMS

$ DIR

```
Directory D0:[SHADOW.TEST]

START.00;1            7  29-DEC-1992 13:35  (RWED,RWED,RE,RE)
START.01;2           13  30-DEC-1992 15:23  (RWED,RWED,RE,RE)
SYSTEMFILE.DAT;1      1  30-DEC-1992 15:23  (RWED,RWED,RE,RE)

Total of 3 files, 21 blocks.
```

UNIX

% ls -al

```
-rw-rw-r--  1 shadow      3142 Dec 29 13:57 start.00
-rw-r--r--  1 shadow      6429 Dec 30 15:28 start.01
-rw-r--r--  1 shadow        15 Dec 30 15:28 systemfile.dat
```

The file START.00 contains the parameters describing the source, while START.01 those describing the optical element no. 1. The file SYSTEMFILE.DAT contains the names of the files describing the OS, in this case START.01;1. However, SYSTEMFILE.DAT may contain the names of files located in other directories and not necessarily named START.xx. It is a good practice to get rid of the calculation outputs (like STAR, MIRR, etc.) and to keep only the START files (and the optical constants, if used). SHADOW is a very efficient program and it is often better to just regenerate the output rather than storing large amount of data. In any event, tree-structured directories are very helpful in keeping things straight. Meaningful names are also very helpful. This section will then simply describe how:

- To generate a SOURCE in BATCH
- To trace an Optical Element in BATCH

We can access directly the source by typing:
$ 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 ] ?: START.00


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

 SOURCE procedure completed.

/* The source is now generated, and the array describing it is stored in
/* BEGIN.DAT, as usual.

 Shadow:: TRACE
 Ray Tracing Selected. Begin procedure.
 Mode selected [ enter ? for HELP ] ? : BATCH

 BATCH selected.
 Call to RESET
 Exit from RESET
 Mode selected is:             /* This is simply a declaration from SHADOW
 BATCH
 Options: to start anew                [ 0 ]
             to restart from a given OE [ 1 ]

 Then ? 0
 Input file [ exit(Unix) or %EXIT(VMS) terminates OS ] ? START.01


 Tracing optical element # 1    /* The usual series of notifications from
 Call to SETSOUR                /* SHADOW to let us know something is indeed
 Exit from SETSOUR              /* going on.
    . . .
 Exit from IMAGE
 Call to RESET
 Exit from RESET                /* First OE completed, inquire about more.


 Do you want to change input mode ?  No
 Input file [ exit(Unix) or %EXIT(VMS) terminates OS ] ? exit
```

```
/* We have notified SHADOW that we do not have more OE's to trace.

 Procedure completed. Return to COMMAND level.

 Shadow:: EXIT
 Exit to DCL.
$
```

The calculation is completed. Now we could run PLOTXY as shown earlier to out about the ray's distribution. They should be identical to those obtained in the earlier runs.

Chapter 3

OUTPUT FILES

The disk files used by SHADOW have different purposes depending on their type. We notice that the name structure of the output files is fixed, while the input ones can be named at the user's pleasure (with the exception of SYSTEMFILE.DAT). The only output files that may play any role *on input* are the STARs (and maybe SCREENs). In particular, END files should *never* be used as input files instead of STARTs. After a run of SHADOW through a single OE you will typically find the following files.

```
Directory D9:[XRAYOP.USER]

BEGIN.DAT;1         188   3-FEB-1987 15:49  (RWED,RWED,RE,RE)
EFFIC.01;1            1   3-FEB-1987 16:06  (RWED,RWED,RE,RE)
END.00;1              6   3-FEB-1987 15:49  (RWED,RWED,RE,RE)
END.01;1             11   3-FEB-1987 16:06  (RWED,RWED,RE,RE)
MIRR.01;1           188   3-FEB-1987 16:06  (RWED,RWED,RE,RE)
OPTAX.01;1            2   3-FEB-1987 16:05  (RWED,RWED,RE,RE)
SCREEN.0101         188   3-FEB-1987 16:06  (RWED,RWED,RE,RE)
STAR.01;1           188   3-FEB-1987 16:06  (RWED,RWED,RE,RE)
START.00;1            6   3-FEB-1987 15:46  (RWED,RWED,RE,RE)
START.01;1           11   3-FEB-1987 15:48  (RWED,RWED,RE,RE)
SYSTEMFILE.DAT;1      1   3-FEB-1987 15:48  (RWED,RWED,RE,RE)

Total of 18 files, 1192 blocks.
```

The binary output files (double precision array) describe the collection of rays defining the beam at a particular location in the OS. Binary files generated by SHADOW are:

```
BEGIN.DAT
STAR.xx
MIRR.xx
SCREEN.xxyy
```

Parameter (or namelist) files contain the listing of the variables' values that define a source or an OE. Examples of this type are:

```
START.xx
END.xx
```

A closer look at each file will help you find the information you need.

BEGIN.DAT
Binary file which contains an array describing the source. Generated on exit from SOURCE.

MIRR.xx
Binary file storing the intercepts of the beam on a surface, OE xx, in the mirror reference frame. This file is notable for its use in plotting the illuminated area on the OE. Generated on exit from TRACE.

STAR.xx
Binary file storing the intercepts at an image (or continuation) plane xx. Generated on exit from TRACE.

START.xx
START.00 is a parameter file containing the data entered during SOURCE to describe the source. Similarly, START.xx contains data describing OE xx.

END.xx
END.00 is a parameter file which contains the parameters for the source (state) at the end of the SOURCE run. END.xx contains parameters for OE xx on exit from TRACE. When the actual source generation and tracing processes occur, some variables of START.xx may be modified or recalculated and stored in END.xx. END.xx files are need by:

```
SYSINFO   -->  returns information on the whole OS
MIRINFO   -->                      on a given OE
SOURCinfo  -->                     on the source
```

SCREEN.xxyy
Binary file containing the intercepts of the beam at screen yy in OE xx. Generated on exit from TRACE.

EFFIC.xx
This file contains information on the "optical efficiency" of OE xx. It will tell you the number of rays transmitted through a particular OE, as well as the mirror average reflectivity. Generated on exit from TRACE.

SYSTEMFILE.DAT
File containing the names of the START.xx files to be used in the TRACing process. It is normally generated at the end of a MENU session (PROMPT does not generate it). It is used in batch and menu mode to supply the names of the files containing OE descriptions. SYSTEMFILE.DAT is created when the SAVE SYSTEM command is issued at the menu command level. It can also be created by using an editor.

STOTxxxxx, SPARxxxxx,SPERxxxxx
These files contain the vertical distribution of an SR source, and thus are generated only when an exact SR source is chosen. The photon energy is specified by xxxxx.

RMIR.xx
Binary file generated when the "Move Mirror" option is chosen. Contains the intercepts of the beam at the moved mirror position.

ANGLE.xx
Ascii file containing information about the incidence and reflection angles for each ray for a given optical element. File contains: ray number, incidence angle, reflection angle, and whether the ray is good or lost. Only created if "Save incidence angle information" option is chosen.

These files are the most important ones. Once more, we urge the user to rename the START files to meaningful names, to avoid endless frustration during late-night runs.

Chapter 4

PRELIMINARY PROGRAMS

Following is a list of external files that the users may need to have before running SHADOW. They may be prepared by the user in the format SHADOW requires, or by preliminary programs described in detail in the USER's GUIDE (UsG).

1. Diffraction profile of a crystal [**UsG – BRAGG**]
2. Optical constants for calculating reflection coefficient of a mirror [**UsG – PREREFL**].
3. Optical constants for calculating absorption by a screen placed along the OS [**UsG – PREREFL**].
4. Specifications of surface errors introduced on a mirror surface [**UsG – PRESURFACE, or User Supplied**]
5. Coefficients to define a polynomial type mirror [**User Supplied**]
6. File with insertion device distribution – undulator or wiggler. [**UsG – MAKE_ID**].

Files of the type (1) and (2) are briefly described below, since they will be needed for the examples in Chapter 6. They both utilize the optical constant library based on B.Henke and G.Tirsell data for the energy range 10-10,000 eV and on Cromer compilation for the range 10,000-100,000 eV. For case (5) see the example supplied in the DEMO section.

4.1 BRAGG

This is a preliminary program which lets the users specify a crystal structure and write out the parameters in such a way that SHADOW can readily use it to compute the reflection coefficients. Dynamical diffraction calculation including crystal absorption is used following Zachariasen formalism for perfect crystals. Optional rocking curves can also be generated for immediate check (See the examples in Chapter 6 and the UsG for more information).

4.2 PREREFL

This is a preliminary program that generates the complex dielectric constant for the mirror (or filter) material from the atomic scattering factor library and data supplied from the user. The (unformatted) file is read by SHADOW and used to compute the local reflectivity based on Fresnel equations, as well as the phase shifts.

4.3 PRESURFACE

The program will read from a user-supplied file a mesh describing the surface. This can be either a surface error, in the sense of a small perturbation z = z(x,y) to the ideal mirror surface or a mirror surface in its own right (although it could always be interpreted as a perturbation to a plane surface). PRESURFACE generates the coefficients of a bicubic spline to be used by SHADOW in computing the intercepts. Due to the limited precision of these interpolations, we strongly suggest that PRESURFACE be used only for surface errors and pathological surfaces.

4.4 MAKE_ID

To generate sources that are insertion devices, we must do some preliminary calculations. MAKE_ID is the utility that generates the integrated probability distribution function for the undulators, and the CDF of photon emission for the wigglers. The files are binary and read in by the SOURCE in SHADOW. There are detailed examples in the User's Guide for the Source and for the Utilities.

Chapter 5

ANALYSIS PROGRAMS

SHADOW provides a set of programs to analyze the results of the calculations. Here are a few to get you started. In the following descriptions, BOF refers to a binary output file, i.e., a ray file generated by SHADOW. A BOF is unformatted thus unreadable by TYPing to the terminal whereas a formatted file is one you can TYPE to the terminal. All programs are launched by typing the name of the program unless otherwise specified.

5.1 Basic

- **PLOTXY**
  Generates a scatter, connected or contour plot using any two rows of the ray file (i.e., STAR.xx, MIRR.xx, BEGIN.DAT) as horizontal and vertical axes. Histograms are also available.

  ```
   Input:  binary output file.
  Output:  defined graphic display device, and
   Topdrawer command file TD.FIL on VMS,
   Primvs command file on Unix.
  ```

- **PREPLOT**
  Creates a two or three columns, formatted file from a binary output file. The user specifies which two or three columns of the ray file to use for output. The generated file is two or three column ascii.

  ```
   Input:  binary output file.
  Output:  defined graphic display device, and
   two or three column ascii file.
   Primvs command file on Unix.
  ```

- **TRANSLATE**
  Translates an unformatted BOF (i.e., BEGIN.DAT, MIRR.xx) into a formatted file. The twelve to eighteen rows of each ray are displayed in the output file as shown:

X	Y	Z	Spatial coordinate
X'	Y'	Z'	Direction
Asx	Asy	Asz	EM vector (s-)
FF	q	kk	Flag, wavenumber, ray index
opd	Fs	Fp	optical path length, phases
Apx	Apy	Apz	EM vector (p-)

```
 Input:  binary output file.
Output:  TT or user-named formatted file.
```

- **HISTO1**
  Creates the histogram describing the distribution of the rays within the limits specified by the user. The histogram can be displayed directly or the file can be written and later supplied to Topdrawer or Primvs. The histogram will exhibit the real intensity if the absorption of the OE has been taken into account, or will exhibit the geometrical image if the absorption has not been accounted for.

```
 Input:  a binary output file.
Output:  a two column file HISTO1.DAT.
         Defined graphic display device, and
 Primvs command file on Unix.
```

- **FMAX**
  This utility is useful in conjunction with PREPLOT. Scans a formatted, two column file and returns the extrema.

```
 Input:  any formatted two-column file.
Output:  TT.
```

- **MINMAX**
  This is a more general version of FMAX. Searches an unformatted data file (i.e., STAR.xx, MIRR.xx) and returns the extrema.

```
 Input:  binary output file.
Output:  TT and formatted file MINMAX.DAT.
```

5.2 Advanced

- **<u>FFRESNEL</u>**
  Takes a BOF (SCREEN.xxyy) and creates a file containing the diffracted image of this aperture. You must keep polarization and phase information (i.e., answer YES to POLARIZED source)

```
 Input:  a binary output file.
Output:  a formatted file FFPAR.DAT storing the
         responses to the input session needed
         to define the image. A formatted,
         two-column file FFRESNEL.DAT.
```

- **<u>HISTO2</u>**
  Creates a two-dimensional histogram of the ray distribution at a particular OE.

```
 Input:  a binary output file.
Output:  a Topdrawer command file or a three column file HISTO2.DAT.
```

- **<u>RECOLOR</u>**
  Takes a BOF and creates a new BOF with different wavelength conserving all the other coordinates. Useful for the analysis of monochromator systems where you may change the energy or the energy interval in the case of white (continuous) sources without altering the rest of the source.

```
 Input:  a binary output file.
Output:  a user-named binary output file NAME.DAT.
```

- **<u>FILEX</u>**
  Simple minded VMS version of AWK. Performs arithmetic operations on the SECOND column in a TWO column file only. Help is available by typing “ ? ” after the prompt FILEX>. Possible operations include exchanging the order of the columns in a file; arithmetic operations on column or between columns of two different files as well as operations of integration and differentiation. To represent a constant use the symbol “ % ” (e.g., file1.dat = file 2.dat + %12).

```
 Input:  any number of files containing two or
         three columns.
Output:  user-named file
```

- **INTENS**
  Generates a plottable file containing the locally absorbed or transmitted radiation across an OE from BOF (i.e., MIRR.xx).

```
 Input:  a binary ray file and "input IO file"
Output:  a user-named,formatted, two-column file
         NAME.DAT.
```

- **FOCNEW**
  Searches a BOF (i.e., MIRR.xx, STAR.xx) for a minimum in the waist (i.e., the best gaussian focus of the beam for both sagittal and tangential directions), and returns the optimum focal distance measured relative to the original image file. You have the option to generate a two-column plottable file of the waist size vs. position along the direction of propagation.

```
 Input:  a binary input file.
Output:  a formatted file FOCUS.DAT.
         a user-named, formatted, two column
         file NAME.DAT.
```

  Suggestions: To plot the beam variance file, use the TD command SCALE Y LOG. This creates a better plot.

- **H2KOL**
  Creates a one-dimensional histogram from a two column file. Useful with PREPLOT.

```
 Input:  a PREPLOTted, or a two-column file.
Output:  a two column file H2KOL.DAT.
 defined graphics display device, and
 Primvs command file on Unix.
```

Chapter 6

Further Examples

6.1 Two Mirror Optical System

As a simple example of the use of SHADOW with a realistic synchrotron source, let us consider the case of a two-mirror system to be installed at a machine like Aladdin to relay the radiation to the input slit of a monochromator. A pair of elliptical mirrors has been selected, with the goal of achieving an overall demagnification of a factor of 8. The parameters are as indicated in Fig. 1.2. These, together with the source specification, are the only input we need in order to trace the system. We will use, for brevity, the TERSE mode. If you are not sure of the question's meaning, compare with the VERBOSE example(s) of the former chapter. In this section we will then show how to:

- To define a Synchrotron Radiation source
- To trace an optical system formed by two optical elements
- To use PLOTXY to look at the results by scatter plots and by contour plots

Let us then begin by specifying the source; we select the case of Synchrotron source (the values used are NOT exactly those of Aladdin).

VMS	*UNIX*
\$ $\boxed{\text{go source}}$	% $\boxed{\text{GO source}}$

```
SOURCE selected. Begin procedure.

This procedure generates a SOURCE for SHADOW.

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

Call to INPUT
```

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

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


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

    ---------------- SOURCE SPECS ------------------

Source modeling type [ 0-5 ] ? [0]
How many rays [ 1 - 5 000 ] ?  [1000]
Seed [ odd, 1000 - 1 000 000 ] ?  [1111111]
Do you want to optimize the source ? [0]

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

Then ? [0]
X-Z plane source type [ 0-3 ] ? [3]
Sigma along X ?  [1]
.            Z ? [.2]
Source Depth [ 1-4 ] ?  [4]
Source Angle Distribution [ 1-6 ] ? [4]
Horizontal half-divergence [ (+)x, rads ] ?  [.005]
.                          [ (-)x, rads ] ?  [.005]
Vertical                   [ (+)z, rads ] ?  [.0025]
.                          [ (-)z, rads ] ?  [.0025]
```

NOTE: SHADOW calculates the correct vertical divergence for a synchrotron source <u>if</u> the user places a larger value here. Otherwise SHADOW cuts the vertical distribution to the selected values.

```
Magnetic Radius [ m ] ?  [2]

 Notice: the ORBIT radius MUST be in the same units as the rest
 of the optical system. Use negative ORBIT radius argument for CCW
 storage ring.

Orbit Radius [ same as other units ] ? [2000]
Do you want to include electron beam emittances [ Y/N ] ?  [0]
```

```
Electron Beam Energy [ GeV ] ?  1
Polarization Selected [ 1-3 ] ?  3
Distribution type [0,1] ? 0
Energy distribution [ 1-3 ] ?  1
Photon Energy [ 0 ] or Angstroms [ 1 ] ?  0
Energy [ eV ] ?  500
Do you want to store the optical paths (OPD) [Y/N] ?  0
Do you want to generate the A vectors (electric field) [Y/N]? 0

Exit from INPUT_SOURCE

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

SOURCE procedure completed.
```

The source has now been generated. We define and trace the Optical system.

```
Shadow:: trace

Ray Tracing Selected. Begin procedure.

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

PROMPT selected.
Call to RESET
Exit from RESET

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

Then ? 0

Call to INPUT_OE

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

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

```
for   NO   answer      anything else

Defining Optical Element:      1

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ]  <ret>
Do you want a verbose [ 1 ] or terse [ 0 ] output ? 0

Optical Element definition:

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

Then ?  0
Incidence Angle ?  88
Source Distance ?  2000
Reflection Angle?  88
Image Distance  ?  500
Reflector [ 0 ] or refractor [ 1 ] ?  0
A: Is this a Kumakhov system?  0
A: Is this mirror faceted [Y/N] ?  0
Mirror surface [ 1-9] ?  2
Do you want to specify the mirror parameters ? 0
Is the mirror Cylindrical ?  0
Is this optical element a Fresnel Zone Plate ? 0
Are we dealing with a Grating ?  0
Are we dealing with a crystal [ Y/N ] ?  0
Is the mirror convex [ Y/N ] ?  0
Reflectivity mode [ 0,1,2 ] ?  0
Orientation Angle [ Alpha ] ?  0
Mirror Dimensions finite [ Y/N ] ? 0
Focii placed at continuation planes [ Y/N ] ?  1
Do you want to move the Source [ Y/N ] ?  0
Do you want to move the mirror itself [ Y/N ] ?  0
Distorted surface [ Y/N ] ?  0
Do you want to include surface roughness [Y/N] ?  0
Any screens in this OE [ Y/N ] ?  0
Slit at continuation plane [ Y/N ] ?  0
Extra Image plates [ Y/N ] ?  0
File containing the source array ?  begin.dat
```

```
 Exit from INPUT

 Tracing optical element  # 1
 Call to SETSOUR                \* We have abbreviated the process of
    ........                    \* ray tracing as shown.
 Exit from RESET

/* The first element completed, SHADOW begins with the definition of the
/* second one. Before beginning, the program checks if the user wants
/* to change input mode.  This is useful if an optical system has
/* already been run once, so that START files are available and the user
/* wants to modify only a given OE. In the present case we will stay in
/* PROMPT mode.

 Do you want to change input mode ?  [0]

 Call to INPUT_OE

 ------------------------ S H A D O W  -----------------------------
 May 1993                               F.Cerrina     CXrL/ECE - UW
 Defining Optical Element:  # 2

 Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ]  [<ret>]
 Do you want a verbose [ 1 ] or terse [ 0 ] output ? [0]

 Optical Element definition:

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

 Then ? [0]
 Incidence Angle ?  [88]
 Source Distance ?  [1000]
 Reflection Angle?  [88]
 Image Distance  ?  [500]
 Reflector [ 0 ] or refractor [ 1 ] ?  [0]
 A: Is this a Kumakhov system? [0]
 A: Is this mirror faceted [Y/N] ?  [0]
 Mirror surface [ 1-9] ?  [2]
 Do you want to specify the mirror parameters ? [0]
```

```
Is the mirror Cylindrical ?  [0]
Is this optical element a Fresnel Zone Plate ? [0]
Are we dealing with a Grating ?  [0]
Are we dealing with a crystal [ Y/N ] ?  [0]
Is the mirror convex [ Y/N ] ?  [0]
Reflectivity mode [ 0,1,2 ] ?  [0]
Orientation Angle [ Alpha ] ?  [180]
Mirror Dimensions finite [ Y/N ] ? [0]
Focii placed at continuation planes [ Y/N ] ?  [1]
Do you want to move the Source [ Y/N ] ?  [0]
Do you want to move the mirror itself [ Y/N ] ?  [0]
Distorted surface [ Y/N ] ?  [0]
Do you want to include surface roughness [Y/N] ?  [0]
Any screens in this OE [ Y/N ] ?  [0]
Slit at continuation plane [ Y/N ] ?  [0]
Extra Image plates [ Y/N ] ?  [0]

Exit from INPUT

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


Do you want to change input mode ?  [0]

Call to INPUT_OE

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

Defining Optical Element:  3

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ]  [exit]

End of session.
Procedure completed.  Return to command level.

Shadow:: [exit]

Exit to DCL
$
$
```

The tracing has been completed and it is now time to have a look at the results. For this we will use PLOTXY, a general-purpose plotting program. We are interested in finding out the area of each mirror which is illuminated and the final and intermediate image. We start with a *scatter* plot of the radiation "footprint" on the mirrors. The image plots are generated in the same way. Notice how we use row {1,2} for the mirrors and rows {1,3} for the images.

```
 $ PLOTXY
 PLOT> Input file?   MIRR.01

 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
 PLOT> Comment for plot [ 80 char ] ?  Footprint on mirror 1

 PLOT> File read OK. Full specifications:
      D13:[XRAYOP.PRIMER.NEW.TEST]MIRR.01;1
      Was created : 17-MAR-1994 14:50

 PLOT> Found         1000 good points out of        1000

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

   1  X    -11.596         11.920       -0.42443E-01     5.7221
   2  Y    -117.67         58.162        -16.555         30.219
   3  Z     0.42904E-04     2.6775        0.61063        0.55759
   4  X'  -0.22132E-01    0.20109E-01  -0.81551E-04    0.10935E-01
   5  Y'    0.99922        0.99955        0.99940        0.00000E+00
   6  Z'    0.23097E-01    0.39218E-01    0.32703E-01    0.26625E-02
  11   Photon Energy  (eV)      500.00         500.00

/* This table tells the user some important statistical parameters of the
/* ray distribution, relative to each coordinate.

 PLOT> Rows to use for plot :

 PLOT>   for horizontal axis ?   1
 PLOT>   for vertical axis   ?   2

/*  The graph for MIRR.02 follows identically.  The procedure to
/*  plot the final image uses STAR.02 as the input file and 1 and
/*  3 as the horz. and vert. axis, respectively.
```

```
PLOT> Scaling options. Enter
      0   For automatic scaling
      1   For cartesian scaling
      2   For external limits

PLOT> Then ?   [0]

PLOT> Plotting options :
      0   For scattered plot
      1   For connected plot
      2   For contour plot

PLOT> Then ?   [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> ?   [-1]
```

VMS

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

Terminal type ? [2]
PLOT> Do you want to save the TD command file ?  [0]
```

UNIX

```
Display type:
  [ 0 ] Xwindow
  [ 1 ] Tektronix
  [ 2 ] Postscript file

Terminal type: [0]
```

The following four scatter plots include the plot completed above on file MIRR.01,and similarly on MIRR.02, STAR.01 and STAR.02.
We will use now the contouring capability of the program to generate a map of the ray's distribution.

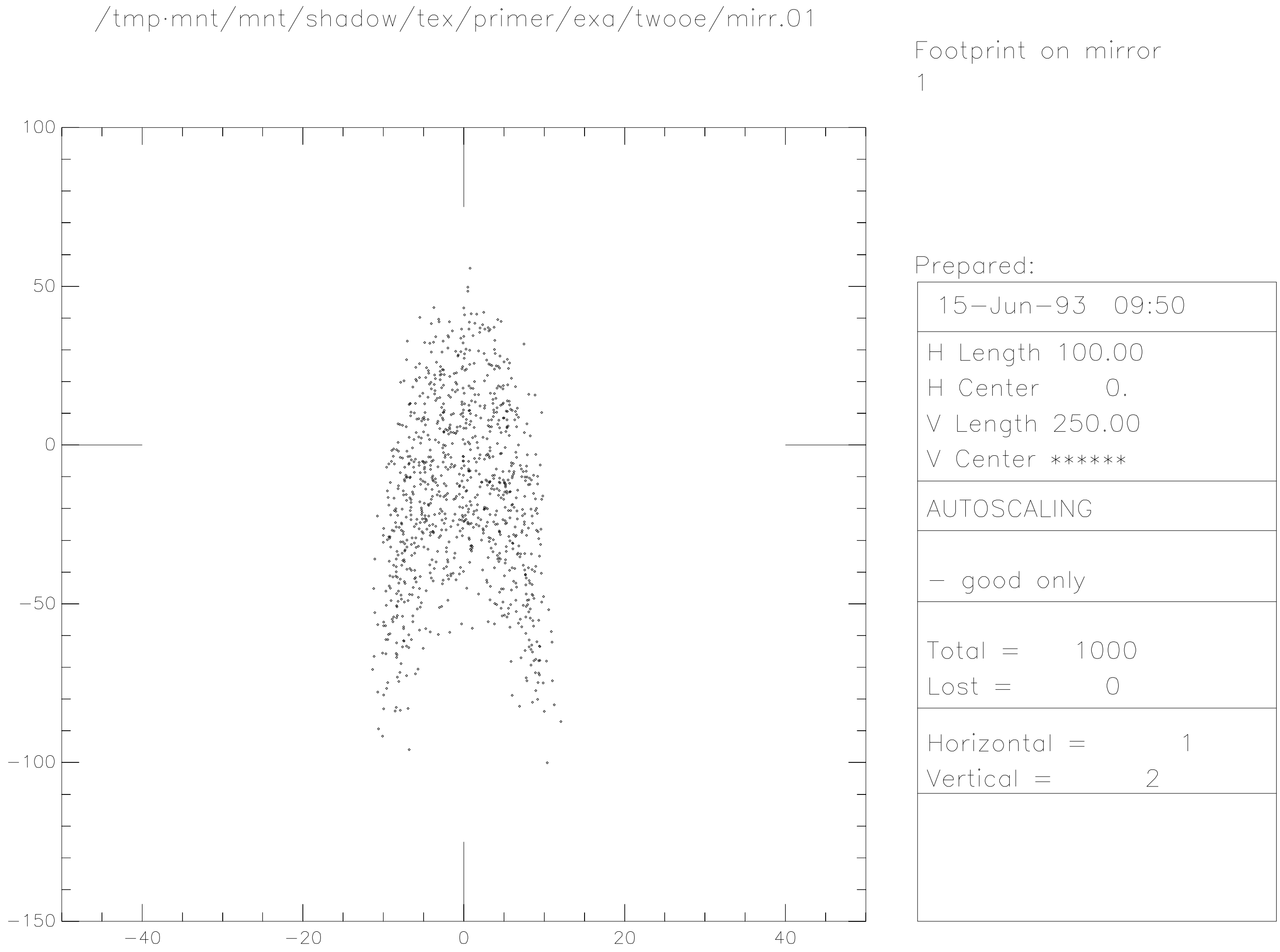

Figure 6.1: Footprint on mirror 1

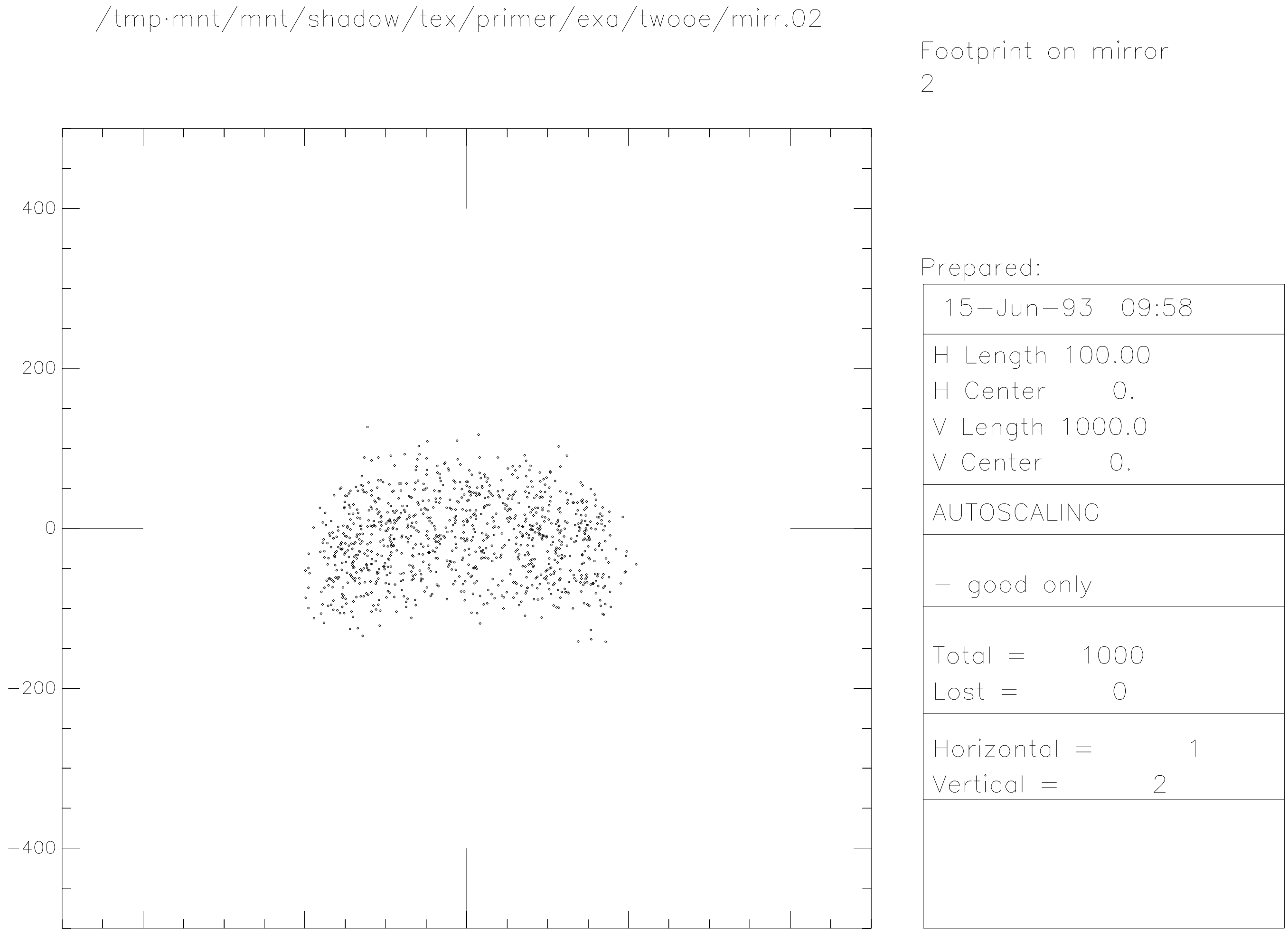

Figure 6.2: Footprint on mirror 2

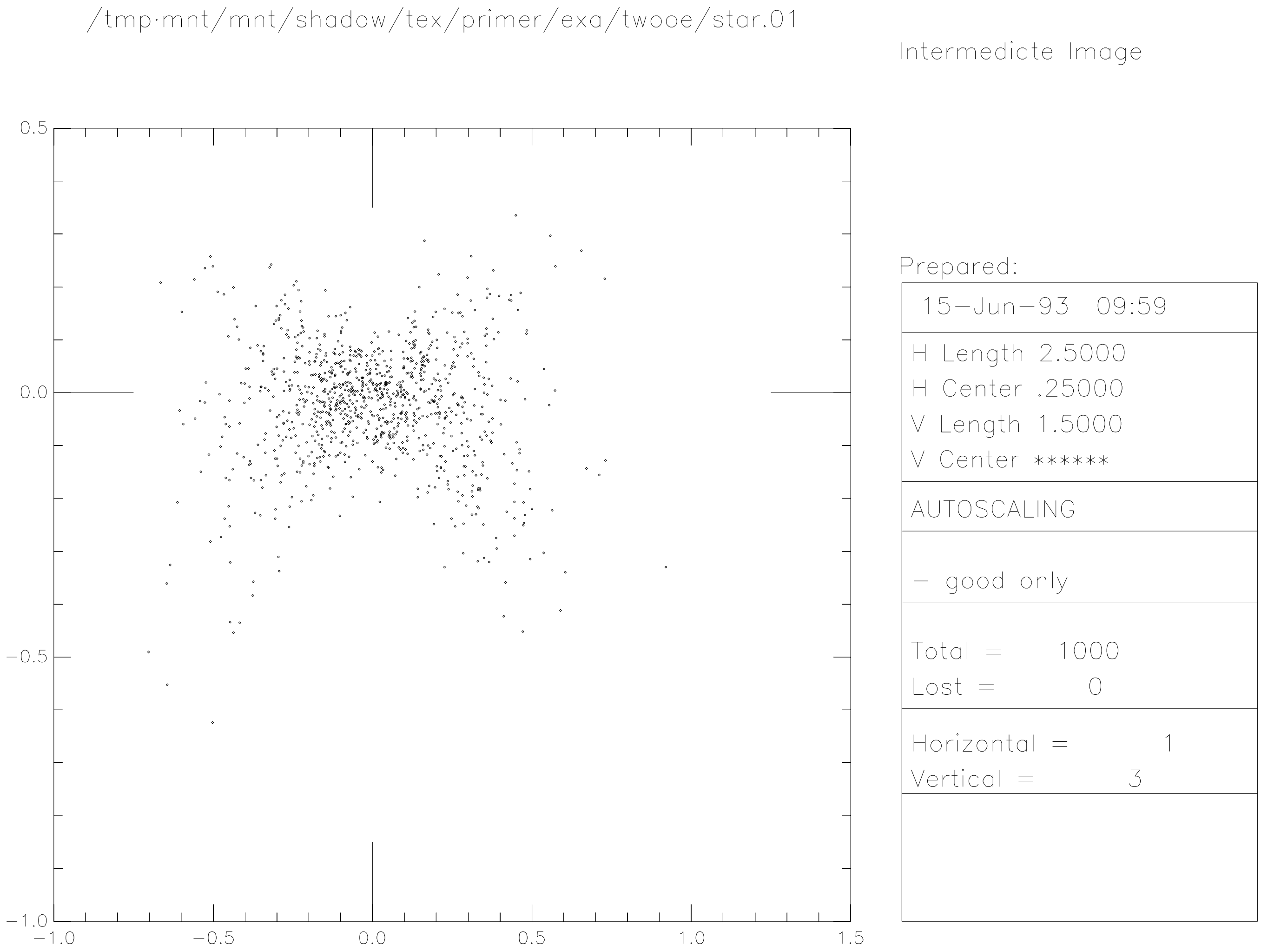

Figure 6.3: Intermediate Image

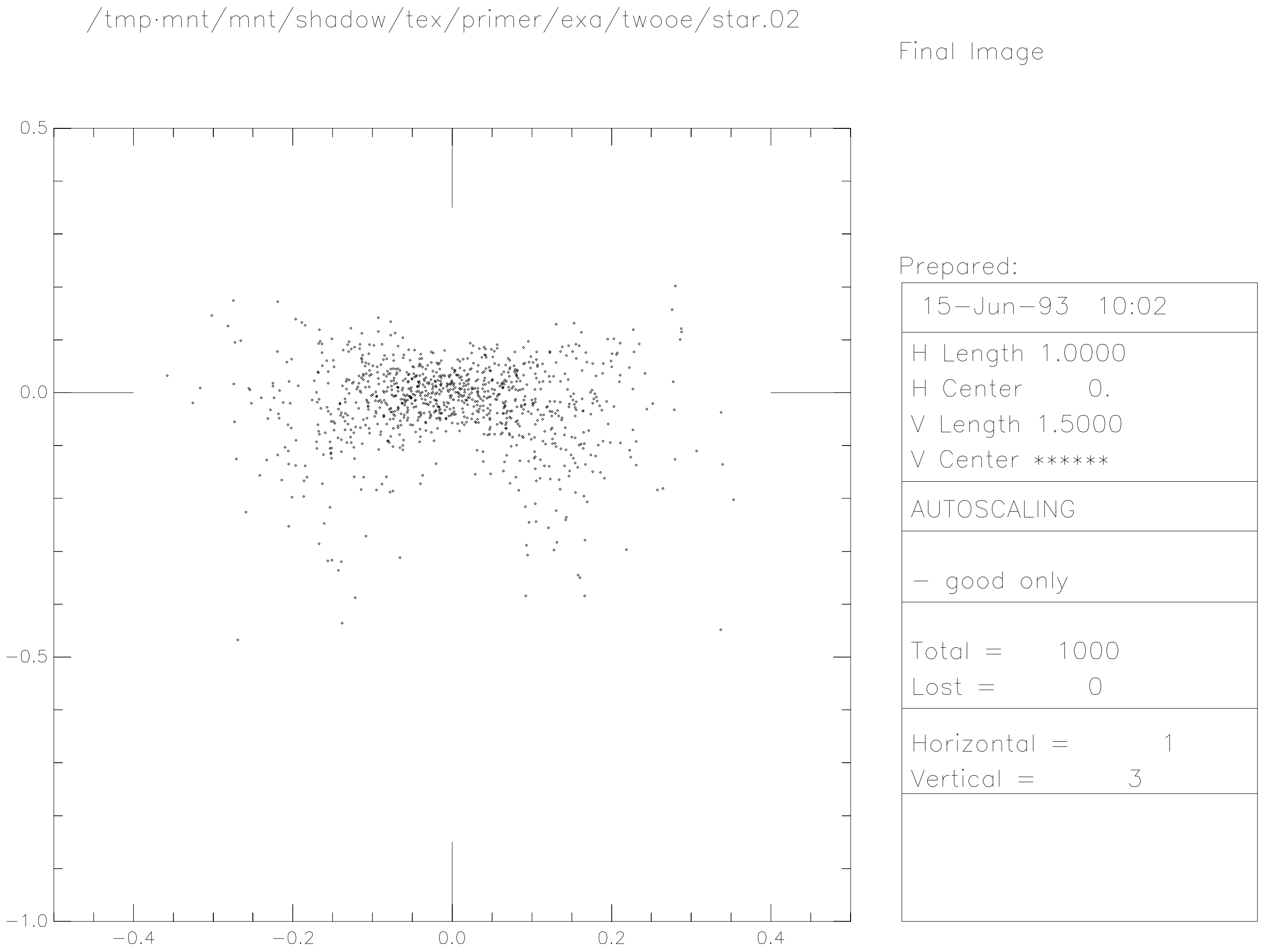

Figure 6.4: Final Image

```
$
$
$ [plotxy]
PLOT> Input file? [mirr.01]

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]
PLOT> Comment for plot [ 80 char ] ?  [Contour plot on mirror 1]

PLOT> File read OK. Full specifications:
      D13:[XRAYOP.PRIMER.NEW.TEST]MIRR.01;1
      Was created : 17-MAR-1994 14:50

PLOT> Found         1000 good points out of        1000

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

 1  X    -11.353        11.715       -0.57415E-01     5.7054
 2  Y    -114.29        55.666        -16.604         30.905
 3  Z    0.26519E-03    2.5488        0.60728        0.57589
 4  X'  -0.21421E-01   0.21403E-01   -0.22495E-04    0.10835E-01
 5  Y'   0.99922       0.99955        0.99940        0.12207E-02
 6  Z'   0.24061E-01   0.39219E-01    0.32718E-01    0.27935E-02
11   Photon Energy  (eV)      500.00         500.00

PLOT> Rows to use for plot :

PLOT>   for horizontal axis ?   [1]
PLOT>   for vertical axis   ?   [2]

PLOT> Scaling options. Enter
      0   For automatic scaling
      1   For cartesian scaling
      2   For external limits

PLOT> Then ?   [2]
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]
PLOT> Grid size [Nx by Ny] to prepare the contours.
PLOT> Nx :  [21]
PLOT> Ny :  [21]
PLOT> Number of contours :  [11]
PLOT> Degree of polynomial used for joining [0=default] : [0]
PLOT> Included reflectivity ?  [0]

PLOT> Data normalization :
      0   For no normalization
      1   For normalized to 1
      2   For normalized to total counts

PLOT> Then ?   [2]
Smoothing [ Y/N ] ?  [1]
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> ?   [-1]
```

VMS

```
PLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 :[2]
PLOT> Do you want to save the TD command file ?  [0]
```

UNIX

```
Display type:
  [ 0 ] Xwindow
  [ 1 ] Tektronix
  [ 2 ] Postscript file
```

```
Terminal type: 0
```

Entered here are four contour plots generated using the above procedure on the files, MIRR.01,MIRR.02,STAR.01 and STAR.02.

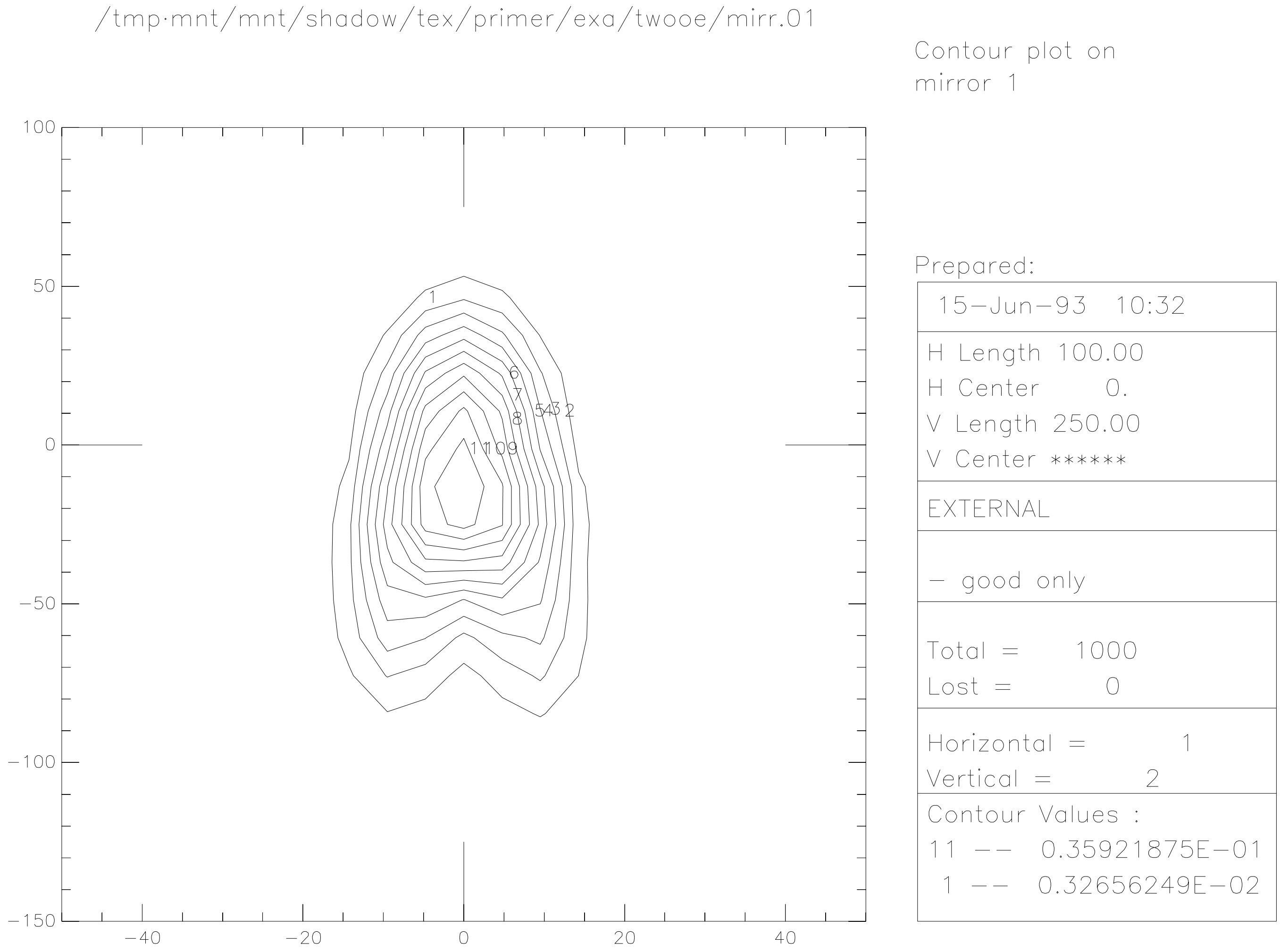

Figure 6.5: Contour plot of footprint on mirror 1

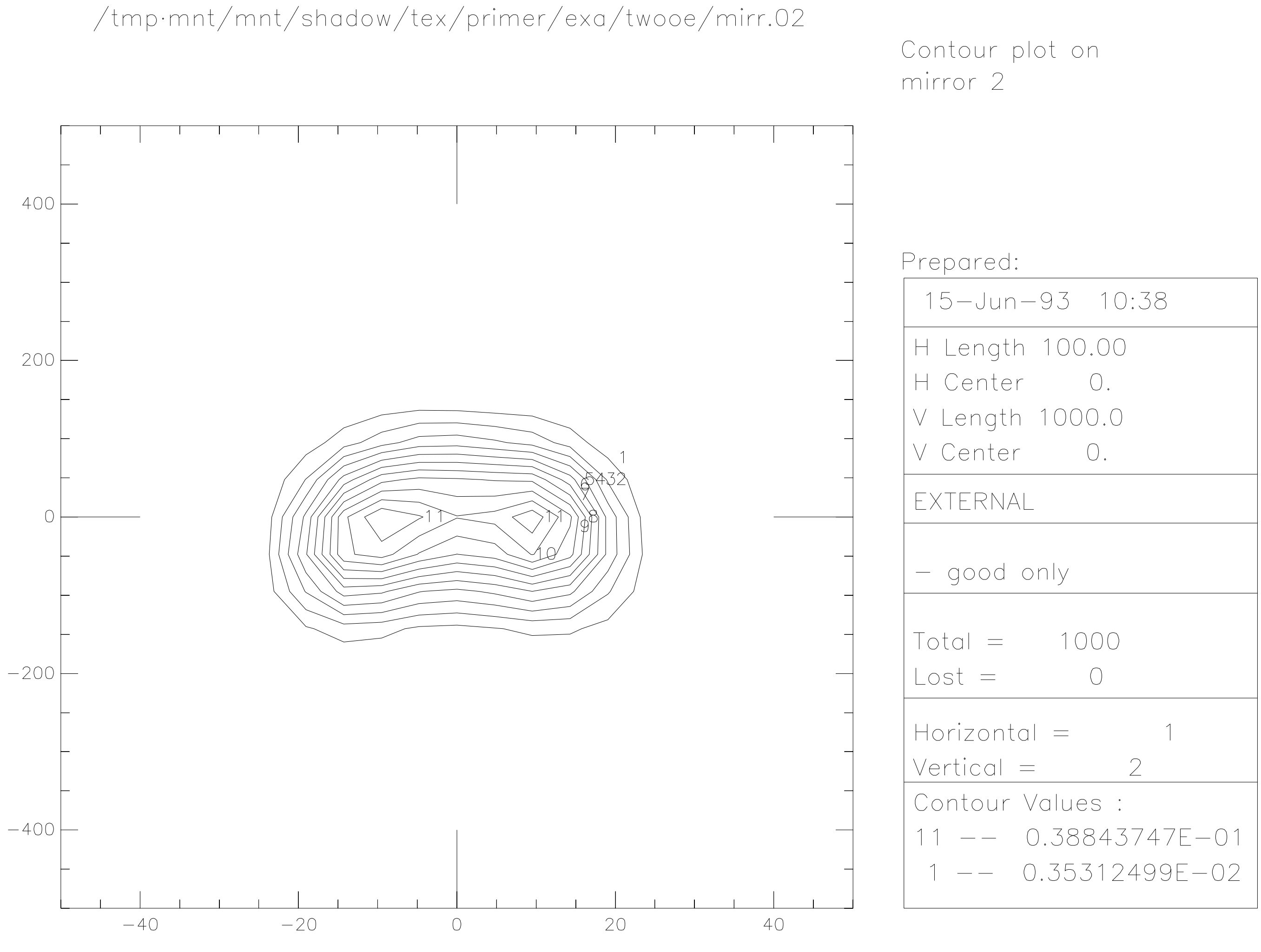

Figure 6.6: Contour plot of footprint on mirror 2

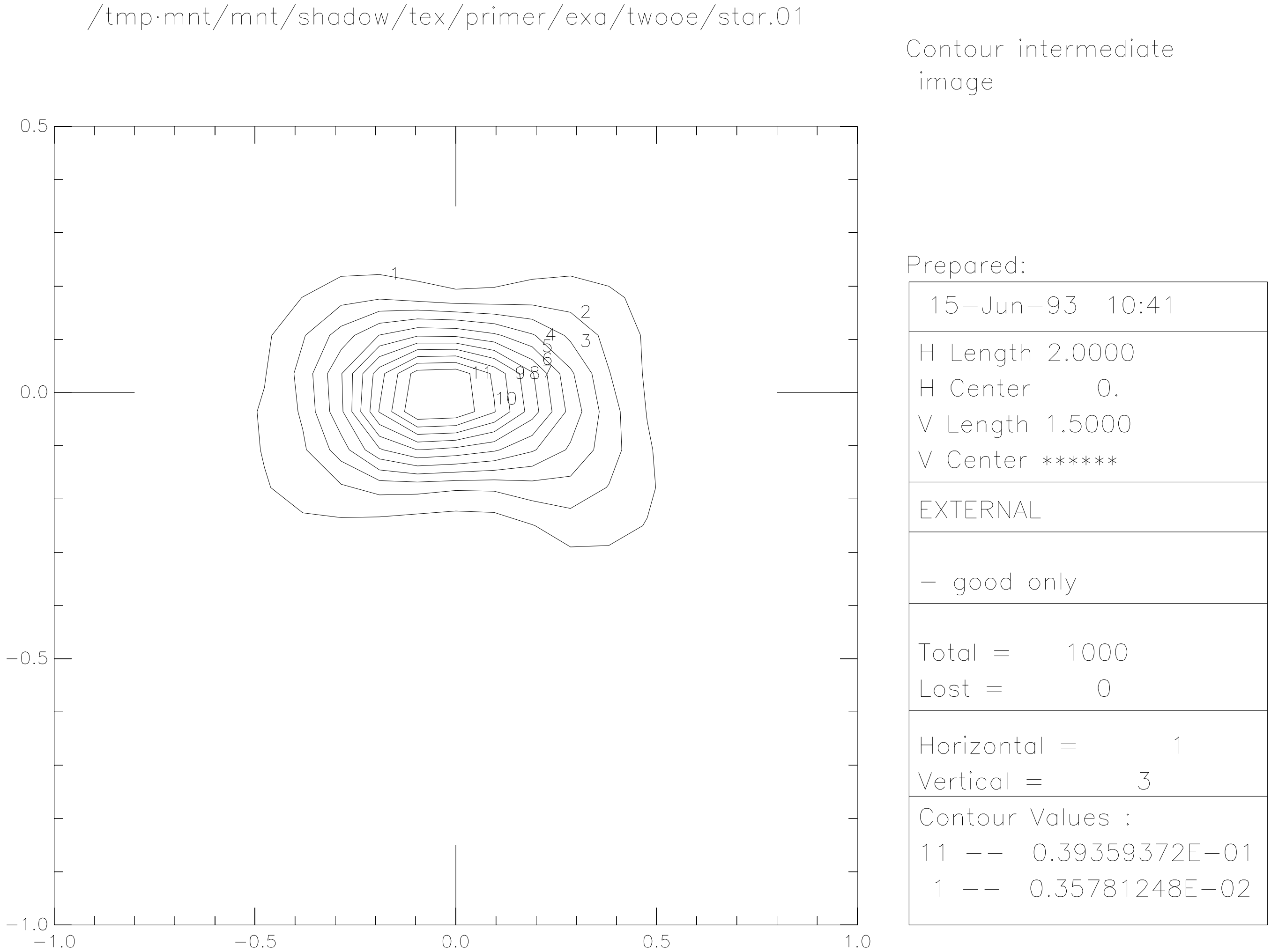

Figure 6.7: Contour plot of intermediate image

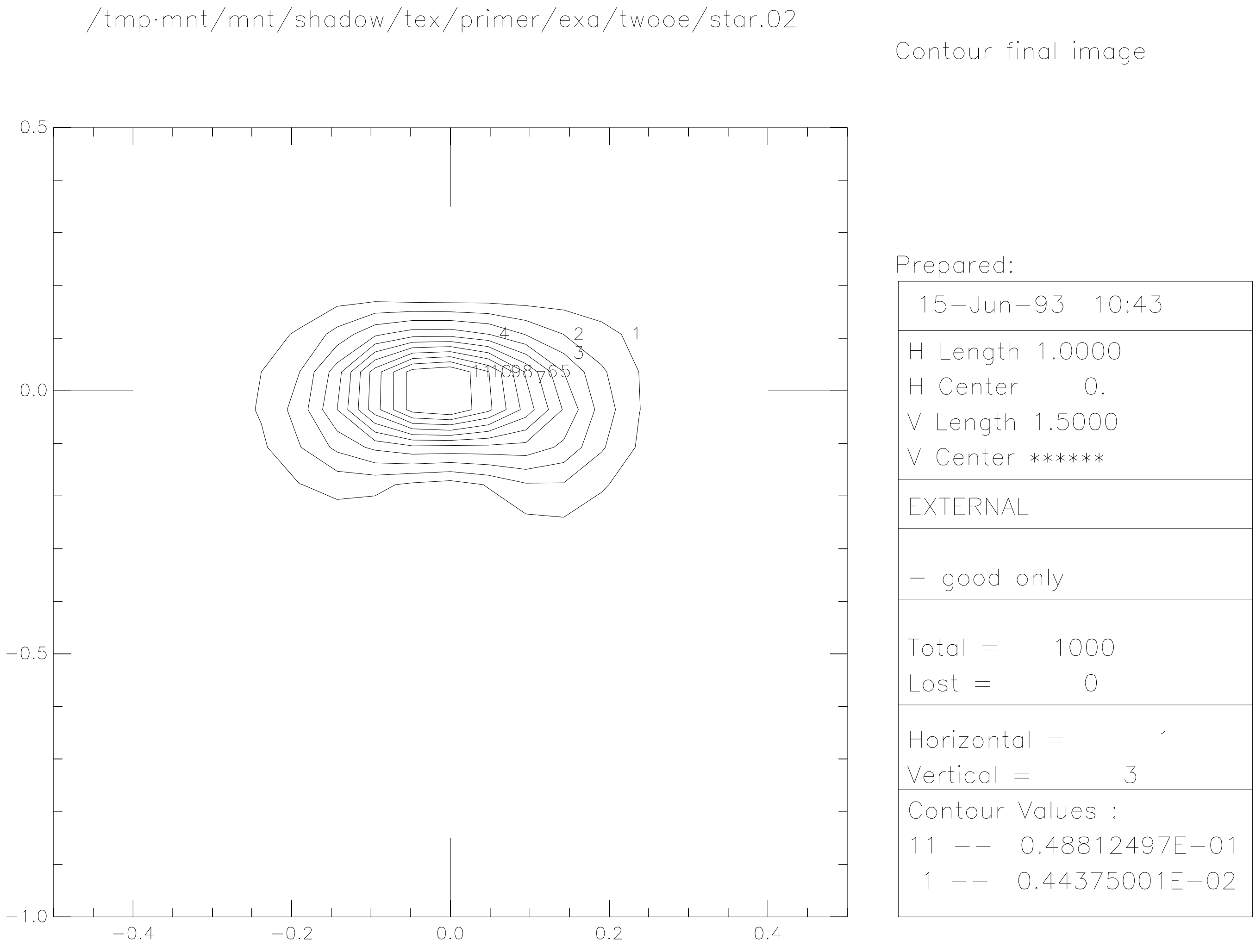

Figure 6.8: Contour plot of Final Image

6.2 Diffraction Grating in Rowland Circle Mount

The purpose of this section is to familiarize the user with the treatment of diffraction cases. The analysis of diffraction gratings is one of the central features of SHADOW. There are many different types of gratings and monochromator mounts. Here we will introduce the study of diffraction by having a look to the simple case of a spherical grating in the Rowland mount. We recall that a slit located on the Rowland circle will be imaged on the same circle, at unit magnification, at a position dependent on the wavelength. We will start with the case of a monochromatic rectangular source (slit) and then proceed to study the resolution of the grating by using a source with three different wavelengths. The procedure to be followed is typical of other systems.
One of the nice features of SHADOW is the capability of the program to figure out by itself the parameters of a mirror and/or diffraction grating. This extends to the calculation of the system geometry, since it is always annoying to have to compute the incidence and diffraction angles, etc. It is enough to request that SHADOW sets up the grating's angles to satisfy the particular mount geometrical conditions for a given wavelength. In this section we will then discuss how:

- to define an OE containing diffraction grating.
- to use the AUTOTUNE switch of SHADOW
- to use RECOLOR
- to use PLOTXY to study the resolution.

Let's assume that we want to study the behavior of a grazing angle 2m spherical grating, with a line density of 1200 lines/mm, to be used at 88° angle of incidence (typical Grasshopper) as shown in Fig. 6.9. The entrance slit is modeled by a rectangular source, 20 μm high and 2 mm wide, at a photon energy of 200 eV. At this energy, we have the geometry specified in the first run of TRACE. In the second, we simply tell SHADOW that the mount is a Rowland one, fixed angle of incidence, and let the program compute the angles.

```
$ go source

SOURCE selected. Begin procedure.

This procedure generates a SOURCE for SHADOW.

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

Call to INPUT

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```

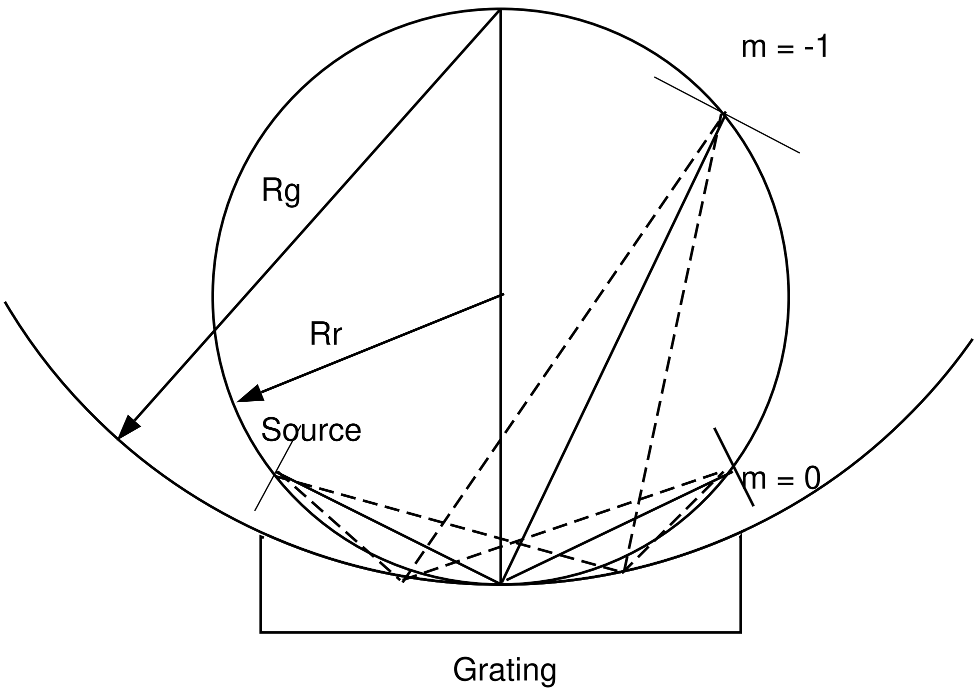

Figure 6.9: Rowland Circle Geometry

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


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

   ---------------- SOURCE SPECS ------------------

Source modelling type [ 0-5 ] ? 0
How many rays [ 1 - 5 000 ] ? 2000
Seed [ odd, 1000 - 1 000 000 ] ? 1000111
Do you want to optimize the source ? 0

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

Then ? 0
X-Z plane source type [ 0-3 ] ? 1
Source Width  [ x ] ? 2
.      Height [ z ] ? .02
Source Depth [ 1-4 ] ? 1
Source Angle Distribution [ 1-6 ] ? 1
Horizontal half-divergence [ (+)x, rads ] ? .005
.                          [ (-)x, rads ] ? .005
Vertical                   [ (+)z, rads ] ? .005
.                          [ (-)z, rads ] ? .005
Do you want a Photon energy [ Y/N ] ? 1
Energy distribution [ 1-3 ] ? 1
Photon Energy [ 0 ] or Angstroms [ 1 ] ? 0
Energy [ eV ] ? 200
Do you want to store the optical paths (OPD) [Y/N] ? 0
Do you want to generate the A vectors (electric field) [Y/N] ? 0

Exit from INPUT_SOURCE

Generated          250 rays out of         2000
                   500
                   750
                  1000
```

```
                   1250
                   1500
                   1750
                   2000
Exit from SOURCE
SOURCE => Source has been successfully generated.
SOURCE procedure completed.

 Shadow:: trace

Ray Tracing Selected. Begin procedure.

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

PROMPT selected.
Call to RESET
Exit from RESET

Mode selected is:
PROMPT

Options: to start anew              [ 0 ]
         to restart from a given OE [ 1 ]

Then ? <ret>

Call to INPUT_OE

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

Defining Optical Element:   # 1

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] <ret>
Do you want a verbose [ 1 ] or terse [ 0 ] output ? 0

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

```
Then ? [0]
Incidence Angle ? [88.0]
Source Distance ? [69.798]
Reflection Angle? [82.726]
Image Distance  ? [253.233]
Reflector [ 0 ] or refractor [ 1 ] ? [0]
A: Is this a Kumakhov system?  [0]
A: Is this mirror faceted [Y/N] ?  [0]
Mirror surface [ 1-9] ? [1]
Do you want to specify the mirror parameters ? [1]
```

```
/* Notice how we tell SHADOW that the mirror is fully user specified.
```

```
Is the mirror Cylindrical ? [0]
Is this optical element a Fresnel Zone Plate ? [0]
Are we dealing with a Grating ? [1]

Type of ruling.
0    ruling density constant on the X-Y plane
1    for ruling density constant onto the mirror surface.
2    for an holographic grating.
3    for an oriental-fan type
4    reserved
5    polynomial line density

Then: [0]
Lines per CM ? [12000]
Diffraction Order ? [-1]
Auto Tuning of Grating [ Y/N ] ? [0]
```

```
/* SHADOW knows that we are dealing with a grating and offers to 'align' it
/* at the right wavelength. For now, we decline.
```

```
Is the mirror convex [ Y/N ] ? [0]
Reflectivity mode [ 0,1,2 ] ? [0]
Orientation Angle [ Alpha ] ? [0]
Mirror Dimensions finite [ Y/N ] ? [0]
Spherical Mirror Radius ? [2000]
```

```
/* Had we not elected to specify the mirror/grating parameters, SHADOW would
/* not have asked this question.

 Do you want to move the Source [ Y/N ] ? 0
 Do you want to move the mirror itself [ Y/N ] ? 0
 Distorted surface [ Y/N ] ? 0
 Do you want to include surface roughness [Y/N] ?  0
 Any screens in this OE [ Y/N ] ? 0
 Slit at continuation plane [ Y/N ] ? 0
 Extra Image plates [ Y/N ] ? 0
 File containing the source array ? begin.dat

 Exit from INPUT

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

 Do you want to change input mode ? 0

 Call to INPUT_OE

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 Defining Optical Element:          2

 Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] exit
 Shadow:: exit
 Return to DCL
```

Let's have a look at the image quality.

```
$ plotxy

PLOT> Input file? star.01

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
PLOT> Comment for plot [ 80 char ] ? Final image for a single beam energy
```

```
PLOT> File read OK. Full specifications:
      D13:[XRAYOP.PRIMER.NEW.TEST]STAR.01;1
      Was created : 19-MAR-1987 11:34

PLOT> Found         2000 good points out of        2000

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

 1  X    -2.5075         2.5017        0.12543E-01     1.0864
 2  Y   -0.87826E-14    0.14889E-13    0.24403E-14    0.33340E-14
 3  Z   -0.11707E-01    0.15704E-01    0.64602E-03    0.59620E-02
 4  X'  -0.49934E-02    0.49976E-02    0.62109E-04    0.28411E-02
 5  Y'   0.99997         1.0000         1.0000        0.00000E+00
 6  Z'  -0.46417E-02    0.56025E-02    0.20221E-03    0.28685E-02
11   Photon Energy  (eV)      200.00         200.00

PLOT> Rows to use for plot :

PLOT>   for horizontal axis ? [1]
PLOT>   for vertical axis ? [3]

PLOT> Scaling options. Enter
      0   For automatic scaling
      1   For cartesian scaling
      2   For external limits

PLOT> Then ? [0]

PLOT> Plotting options :
      0   For scattered plot
      1   For connected plot
      2   For contour plot

PLOT> Then ? [0]
PLOT> Hairline at [ 0,0 ] ? [1]
PLOT> Overlay a mirror/slit ? [1]

PLOT> Mirror/Slit type:
      0 .... rectangular
      1 .... elliptical

Then ? [0]
PLOT> X min : [-2.5]
PLOT>   max : [2.5]
```

```
PLOT> Y min : -.01
PLOT>   max : .01

PLOT> Ready for histograms. Enter:
      -1        to skip
       0     for same limits as plot
       1                  3*stdev
       2                  external

PLOT> ? 0
PLOT> Number of bins for X axis [default = 25] : <ret>
PLOT> Number of bins for Y axis [default = 25] : <ret>
```

VMS

```
PLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 : 1
PLOT> Do you want to save the TD command file ? 1
```

UNIX

```
Display type:
   [ 0 ] Xwindow
   [ 1 ] Tektronix
   [ 2 ] Postscript file

 Terminal type: 0
```

After this first example, let us proceed to a more complex one. A monochromator is designed to separate wavelengths, so let us verify the resolution of this mount. We will now use RECOLOR to create a new source file with three different photon energies.

```
 $ recolor
 File for input ? begin.dat
 and for output ? begin.new

 Data ready. Read           2000 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 ? 2
 How many lines ? 3
 Line n.          1. Then ? 199
```

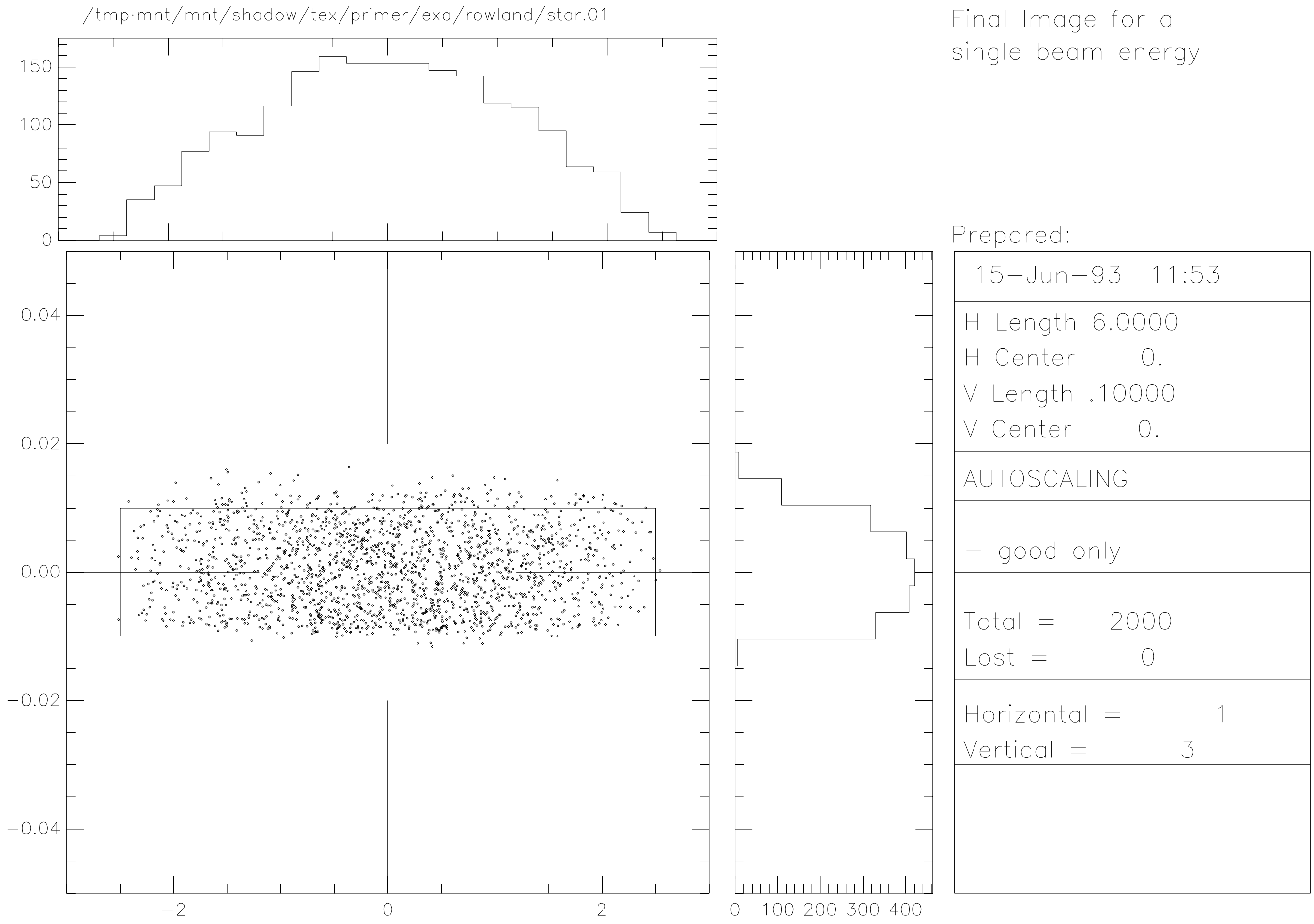

Figure 6.10: Final Image for a single beam energy

```
Line n.          2. Then ? 200
Line n.          3. Then ? 200.5
Enter seed for random number generator : 1000113

All done.
```

We will now run TRACE using BEGIN.NEW as source file to generate a new image file. In this case we will select the *autotuning* feature, and let SHADOW worry about figuring out diffraction angles. Since we are interested in a fairly simple case, we will keep the incidence angle constant and let SHADOW compute the "outgoing" diffracted beam angle. This corresponds to the case 2 in the "mount type" question. SHADOW recognizes several types of grating configurations (mounts). Starting from the grating equation:

$$sin(\alpha) + sin(\beta) = m\frac{\lambda}{d} \tag{6.1}$$

the mount used is specified by the relation between α, β. For instance, in the SEYA/TGM case the angle between incoming and outgoing central axis $(\alpha+\beta)$ is fixed so that SHADOW will figure out incidence and reflection angles that satisfy the grating equation at that particular wavelength. The user needs to specify only the included angle (this is done by using the zero order angles as the OE parameters angles) and SHADOW will rotate the grating by the correct amount. For the case of constant incidence angle (α fixed, β variable) SHADOW will simply compute the diffraction angle β that satisfies the grating equation, while keeping constant the incidence angle specified in the OE geometry. This is the case that we will be using.

```
$ go trace
Ray Tracing Selected. Begin procedure.
Mode selected [ ? <ret> for HELP ] ? : prompt

PROMPT selected.
Call to RESET
Exit from RESET

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

Then ? 0

Call to INPUT_OE
```

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

Defining Optical Element:  1

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] <ret>
Do you want a verbose [ 1 ] or terse [ 0 ] output ? 0
Optical Element definition:


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

Then ? 0
Incidence Angle ? 88.0
Source Distance ? 69.789
Reflection Angle? 10.00
```

Notice that the Reflection Angle will be computed by SHADOW, so that we do not need to specify it.

```
Image Distance  ? 253.233
Reflector [ 0 ] or refractor [ 1 ] ? 0
A: Is this a Kumakhov system? 0
A: Is this mirror faceted [Y/N] ? 0
Mirror surface [ 1-9] ? 1
Do you want to specify the mirror parameters ? 1
Is the mirror Cylindrical ? 0
Is this optical element a Fresnel Zone Plate ? 0
Are we dealing with a Grating ? 1

Type of ruling.
0    ruling density constant on the X-Y plane
1    for ruling density constant onto the mirror surface.
2    for an holographic grating.
3    for an oriental-fan type
4    reserved
5    polynomial line density

Then: 0
Lines per CM ? 12000
```

```
Diffraction Order ? [-1]
```

We will now instruct SHADOW to tune the grating to a photon energy of 200 eV; notice that there is no explicit relation between the energy tuning and the one used in specifying the source. Sometimes it may indeed be useful to have them different, for example when studying resolving power.

```
Auto Tuning of Grating [ Y/N ] ? [1]
Energy, in eV, [ 0 ] or wavelength, in Angs., [ 1 ] ? [0]
Photon Energy ? [200]

TGM/SEYA     0
ERG          1
Con Inc Ang  2
Con Dif Ang  3
Hunter       4

Mount type ? [2]
Is the mirror convex [ Y/N ] ? [0]
Reflectivity mode [ 0,1,2 ] ? [0]
Orientation Angle [ Alpha ] ? [0]
Mirror Dimensions finite [ Y/N ] ?[0]
Spherical Mirror Radius ? [2000]
Do you want to move the Source [ Y/N ] ? [0]
Do you want to move the mirror itself [ Y/N ] ? [0]
Distorted surface [ Y/N ] ? [0]
Do you want to include surface roughness [Y/N] ?  [0]
Any screens in this OE [ Y/N ] ? [0]
Slit at continuation plane [ Y/N ] ? [0]
Extra Image plates [ Y/N ] ? [0]
File containing the source array ? [begin.new]

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

Do you want to change input mode ? [0]

Call to INPUT_OE

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Defining Optical Element:  2
```

```
 Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] exit
 Shadow:: exit
 Return to DCL.
```

The tracing is completed and let's examine the result. Since we have used a source with three different wavelengths, we should observe three bands in the image plane.

```
$ plotxy

PLOT> Input file? star.01

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
PLOT> Comment for plot [ 80 char ] ? final image for 3 beam energies

PLOT> File read OK. Full specifications:
      D13:[XRAYOP.PRIMER.NEW.TEST]STAR.01;2
      Was created : 19-MAR-1987 11:59

PLOT> Found         2000 good points out of        2000

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

 1  X    -2.5075        2.5017        0.12543E-01     1.0864
 2  Y   -0.11266E-13   0.14475E-13    0.24527E-14    0.32827E-14
 3  Z   -0.47592E-01   0.92199E-01    0.13664E-01    0.47040E-01
 4  X'  -0.49934E-02   0.49977E-02    0.62108E-04    0.28411E-02
 5  Y'   0.99997        1.0000         1.0000        0.00000E+00
 6  Z'  -0.47882E-02   0.58971E-02    0.25365E-03    0.28727E-02
11   Photon Energy  (eV)      199.00         200.50

PLOT> Rows to use for plot :

PLOT>   for horizontal axis ? 1
PLOT>   for vertical axis   ? 3


PLOT> Scaling options. Enter
      0   For automatic scaling
      1   For cartesian scaling
      2   For external limits

PLOT> Then ? 0
```

```
PLOT> Plotting options :
      0   For scattered plot
      1   For connected plot
      2   For contour plot

PLOT> Then ? 0
PLOT> Hairline at [ 0,0 ] ? 0
PLOT> Overlay a mirror/slit ? 1

PLOT> Mirror/Slit type:
      0 .... rectangular
      1 .... elliptical

Then ? 0
PLOT> X min : -2
PLOT>   max : 2
PLOT> Y min : -.01
PLOT>   max : .01

PLOT> Ready for histograms. Enter:
      -1          to skip
       0      for same limits as plot
       1                      3*stdev
       2                      external

PLOT> ? 0
PLOT> Number of bins for X axis [default = 25] : <ret>
PLOT> Number of bins for Y axis [default = 25] : <ret>
```

VMS

```
PLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 : 1
PLOT> Do you want to save the TD command file ? 1
```

UNIX

```
 Display type:
   [ 0 ] Xwindow
   [ 1 ] Tektronix
   [ 2 ] Postscript file

 Terminal type: 0
```

Notice how the three wavelengths are well resolved. The box indicates the possible location of an exit slit. You may try to run again SHADOW using closer photon energies, e.g., 200.1 and 199.8 and see if they are still resolved. Another interesting exercise is to select a *continuous* source in RECOLOR, for example between 199 and 201 eV, rerun SHADOW and then PLOTXY. This time, select the 3 and 11 row to plot. You will have then a plot of the position at the exit slit plane versus the photon energy. The slope of that band of points is the grating dispersion; it is easy to obtain directly the photon energy bandpass transmitted by a given slit (Δz), just by drawing the lines corresponding to the slit down on the photon energy axis. For a more complete discussion, see the UG.

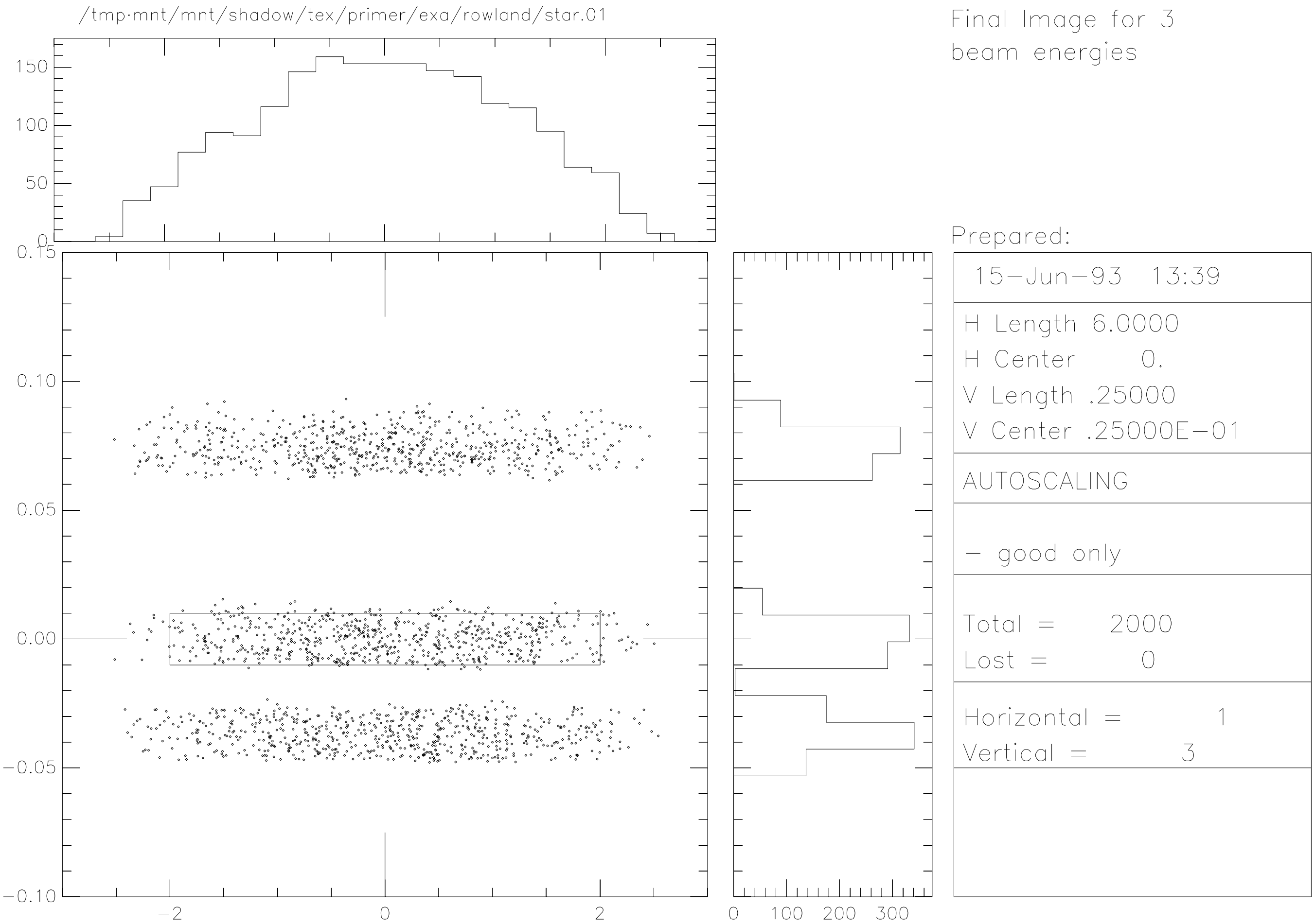

Figure 6.11: Final Image for three beam energies

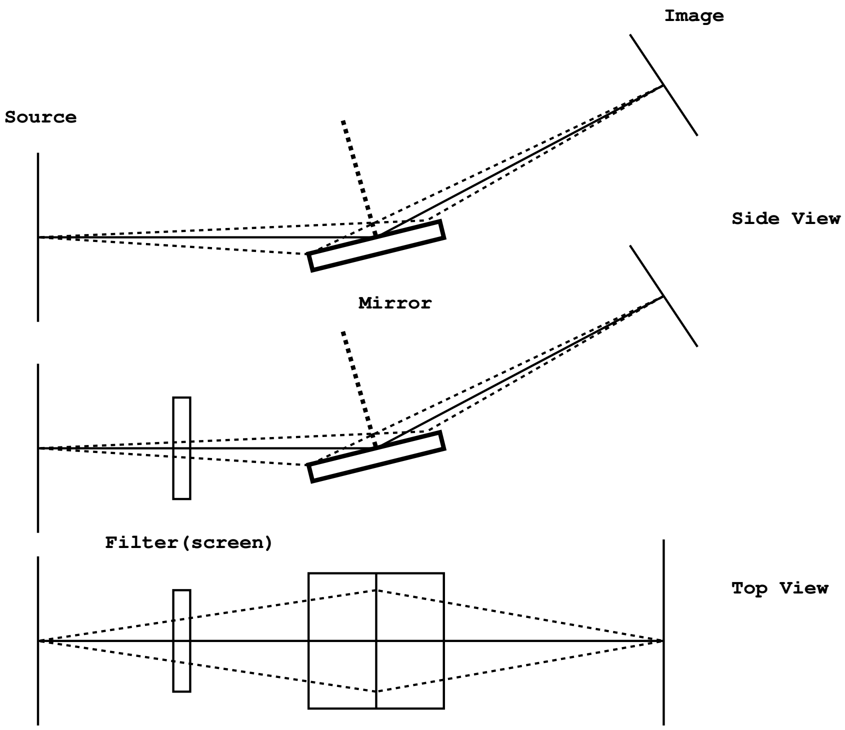

Figure 6.12: Optical System Consisting of a Gold Mirror With and Without a Filter

6.3 Power Density

One of the most important problems in synchrotron x-ray optics is that of the power loading of mirrors and other elements. In this section we will show how to deal with this problem and what insights can be obtained. We will demonstrate then how:

- To generate a Synchrotron source
- To use the program PREREFL
- To use the REFLECTIVITY switch in SHADOW
- To use PLOTXY to compute absorbed power density

We will consider the case of a gold mirror on a machine similar to Aladdin. See figure 6.12. We stress that NO approximations are made within SHADOW, and that both the source and the reflectivities are computed exactly. The source will cover the range 200-6000 eV, more than enough to model the system.

$ GO source

```
SOURCE selected. Begin procedure.

This procedure generates a SOURCE for SHADOW.

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


Call to INPUT

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

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


------------- SOURCE SPECS ------------------

Source modelling type [ 0-5 ] ? 0
How many rays [ 1 - 5 000 ] ? 1000
Seed [ odd, 1000 - 1 000 000 ] ? 10111
Do you want to optimize the source ? 0

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

Then ? 0
X-Z plane source type [ 0-3 ] ? 3
Sigma along X ? 1
.            Z ? .2
Source Depth [ 1-4 ] ? 4
Source Angle Distribution [ 1-6 ] ? 4
Horizontal half-divergence [ (+)x, rads ] ? .01
.                          [ (-)x, rads ] ? .01
Vertical                   [ (+)z, rads ] ? .005
.                          [ (-)z, rads ] ? .005
Magnetic Radius [ m ] ? 2.0833
```

```
 Notice: the ORBIT radius MUST be in the same units as the rest
  of the optical system.
 Use negative ORBIT radius argument for CCW storage ring.

 Orbit Radius [ same as other units ] ? 2083.3
 Do you want to include electron beam emittances [ Y/N ] ? 0
 Electron Beam Energy [ GeV ] ? 1
 Polarization Selected [ 1-3 ] ? 3
 Energy distribution [ 1-3 ] ? 3
 Photon Energy [ 0 ] or Angstroms [ 1 ] ? 0
 From photon energy or wavelength ...   ? 200
 ... to photon energy or wavelength :   ? 6000
 Do you want to store the optical paths (OPD) [Y/N] ? 1
 Do you want to generate the A vectors (electric field) [Y/N] ? 1


/* This step is essential. It directs SHADOW to generate and store the vectors
/* describing the amplitude of each ray's vector potential A. Normally SHADOW
/* does not generate this information, for space economy.

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

 SOURCE procedure completed.

 Shadow:: exit
 Exit to DCL
```

The source is now ready, but before we can run SHADOW we have to generate a file containing information about the optical properties of the material of the mirror surface. This is the purpose of PREREFL, that computes the complex dielectric function of the material. We recall that we cover all the elements in the range 30 – 100,000 eV.

```
 $ PREREFL

 Element [0] or compound [1] ? 0
 Density [ g/cm3 ] ? 19.3
 Enter 2-letters (capitalized) atomic symbol ? AU
 Enter starting photon energy,end and step
```

```
200
6000
100
Output file ? AUF1F2.OPT
```

All set to go. We can now trace the system.

```
$ GO trace


Ray Tracing Selected. Begin procedure.

Mode selected [ ? <ret> for HELP ] ? : prompt
PROMPT selected.
Call to RESET
Exit from RESET


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

Then ? 0

Call to INPUT_OE

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

Defining Optical Element:  1

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] <ret>
Do you want a verbose [ 1 ] or terse [ 0 ] output ? 0


Optical Element definition:

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

```
Then ? 0
Incidence Angle ? 88
Source Distance ? 5000
Reflection Angle? 88
Image Distance  ? 5000
Reflector [ 0 ] or refractor [ 1 ] ? 0
A: Is this a Kumakhov system? 0
A: Is this mirror faceted [Y/N] ? 0
Mirror surface [ 1-9] ? 3

Toroidal Selected.
Enter 0, if mirror pole is at the lower outer torus (usual case)
      1,                            lower inner
      2,                            upper inner
      3,                            upper outer

Mirror pole location ? 0
Do you want to specify the mirror parameters ? 0
Is the mirror Cylindrical ? 0
Is this optical element a Fresnel Zone Plate ? 0
Are we dealing with a Grating ? 0
Are we dealing with a crystal [ Y/N ] ? 0
Is the mirror convex [ Y/N ] ? 0
Reflectivity mode [ 0,1,2 ] ? 1
Optical Constant Source: [file=0,tt:=1], multilayer [2] ? 0
File with optical constants ? AUF1F2.OPT
Orientation Angle [ Alpha ] ? 0
Mirror Dimensions finite [ Y/N ] ? 0
Focii placed at continuation planes [ Y/N ] ? 1
Do you want to move the Source [ Y/N ] ? 0
Do you want to move the mirror itself [ Y/N ] ? 0
Distorted surface [ Y/N ] ? 0
Do you want to include surface roughness [Y/N] ? 0
Any screens in this OE [ Y/N ] ? 0
Slit at continuation plane [ Y/N ] ? 0
Extra Image plates [ Y/N ] ? 0
File containing the source array ? BEGIN.DAT


Exit from INPUT
Tracing optical element  #           1
```

```
Call to SETSOUR
   ........
Exit from RESET
```

`Do you want to change input mode ?` $\boxed{0}$

```
Call to INPUT_OE

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Defining Optical Element:  2
```

`Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ]` $\boxed{\text{exit}}$

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

`Shadow::` $\boxed{\text{exit}}$

```
Exit to DCL

$
```

`$` $\boxed{\text{type effic.01}}$

```
Of a total of   1000 rays, of which   1000 formed  the input set
     0 were out of the mirror N.    1
The mirror collects   1.0000     of the incoming flux.
The average reflectivities are :
S-pol                      0.57466
P-pol                      0.57103
Total                      0.57285
The overall efficiency of the mirror is : 0.57285
```

The tracing is completed. We have now to analyze the data in terms of power density. For that, we use PLOTXY.

`$` $\boxed{\text{PLOTXY}}$

`PLOT> Input file?` $\boxed{\text{MIRR.01}}$

```
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 ?` $\boxed{0}$

`PLOT> Comment for plot [ 80 char ] ?` $\boxed{\text{Power density absorbed by mirror}}$

```
PLOT> File read OK. Full specifications:
      D13:[XRAYOP.PRIMER.NEW.POWER]MIRR.01;1
      Was created :  1-APR-1987 22:36

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    -49.348        47.732        -1.7246         27.725
  2  Y    -311.50        195.35        -65.843         81.065
  3  Z    0.31349E-03    7.2126         2.2749         2.0296
  4  X'  -0.95526E-02   0.99813E-02   0.35168E-03    0.54279E-02
  5  Y'   0.99934       0.99946       0.99940        0.14648E-02
  6  Z'   0.31680E-01   0.36326E-01   0.34031E-01    0.85060E-03
 11   Photon Energy  (eV)      201.52         5222.8

/* notice the presence of the extra rows (13-18) and of the continuous photon
/* energy distribution.

PLOT> Rows to use for plot :

PLOT>   for horizontal axis ? [1]
PLOT>   for vertical axis   ? [2]

PLOT> Scaling options. Enter
      0   For automatic scaling
      1   For cartesian scaling
      2   For external limits

PLOT> Then ? [0]

PLOT> Plotting options :
      0   For scattered plot
      1   For connected plot
      2   For contour plot

/* 2 is the case that must be selected for power density.


PLOT> Then ? [2]
```

```
PLOT> Grid size [Nx by Ny] to prepare the contours.
PLOT> Nx : [15]
PLOT> Ny : [15]
PLOT> Number of contours : [7]
PLOT> Degree of polynomial used for joining [0=default] : [2]
PLOT> Included reflectivity ? [1]
PLOT> Options :
      0   Power density [J/area] reflected/transmitted
      1   Power density [J/area] absorbed
      2   Local reflectivity/transmission
PLOT> Then ? [1]
PLOT> File to use for Io : [BEGIN.DAT]
Scaling options:
No scaling                          [ 0 ]
Scaling with user-supplied number   [ 1 ]
Auto-scaling for SR source          [ 2 ]

/* This point is important. Beam current is not supplied in the SHADOW
/* data files.
/* PLOTXY needs this extra information in order to have realistic
/* modelling.

PLOT> Then ? [2]
Machine radius [ m ] ? [2.0833]
Machine energy [ GeV ] ? [1]
Machine current[ A ] ? [.1]
milliradians of orbit ? [20.0]

/* This was the source divergence we used.  See, for example SOURCE run.

We need the conversion factor from the units used in the
calculations to CM. e.g., if mm were used, enter .1
Then ? [.1]
Total power accepted:    13.5220
Smoothing [ Y/N ] ? [1]
Save grid file [ Y/N ] ? [1]
PLOT> Hairline at [ 0,0 ] ? [1]
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> ? $\boxed{0}$

VMS

PLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 : $\boxed{2}$

PLOT> Do you want to save the TD command file ? $\boxed{1}$

UNIX

```
Display type:
  [ 0 ] Xwindow
  [ 1 ] Tektronix
  [ 2 ] Postscript file
```

Terminal type: $\boxed{0}$

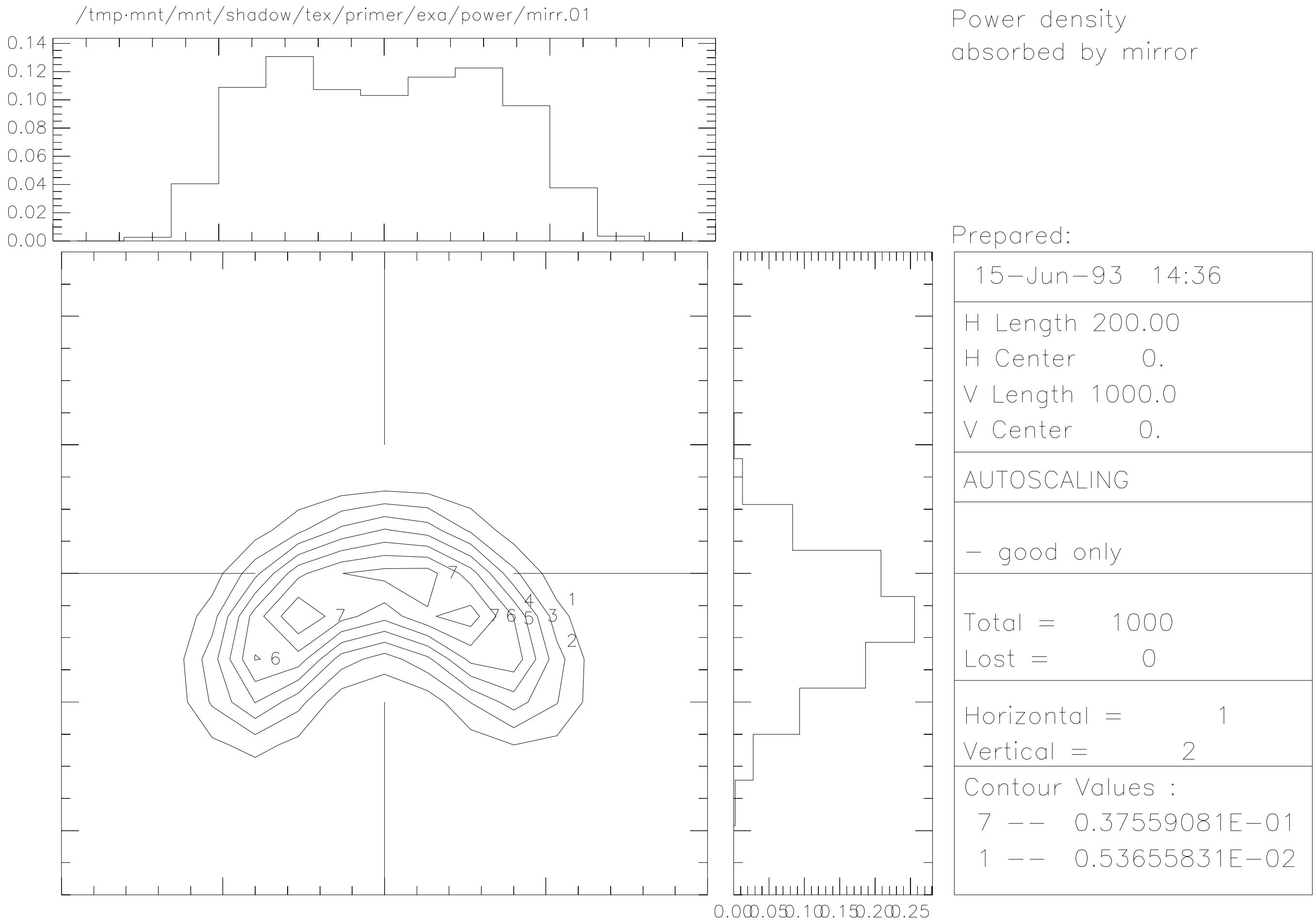

Figure 6.13: Contour plot of power density absorbed on first mirror

Mirror-Filter Combination

In this case we will examine the effect on the spectrum of the radiation of a filter and of a mirror together. We will trace a beamline with a beryllium filter in front of a gold mirror. We could plot as done above the power density at the filter and at the mirror, but we will leave that to the reader. Let us begin by generating the file with the constants of Be.

```
$ PREREFL
Element [0] or compound [1] ? 0
Density [ g/cm3 ] ? 1.845
Enter 2-letters (capitalized) atomic symbol ? BE
Enter starting photon energy,end and step 200,6000,100
Output file ? BEF1F2.OPT
```

Since the source already exists, we can proceed directly with the calculations.

```
$ GO trace

Ray Tracing Selected. Begin procedure.

Mode selected [ ? <ret> for HELP ] ? : PROMPT
PROMPT selected.
Call to RESET
Exit from RESET

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

Then ? 0

Call to INPUT_OE

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

Defining Optical Element:  1

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] <ret>
Do you want a verbose [ 1 ] or terse [ 0 ] output ? 0

Optical Element definition:
```

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

Incidence Angle ? 88
Source Distance ? 5000
Reflection Angle? 88
Image Distance  ? 5000
Reflector [ 0 ] or refractor [ 1 ] ? 0
A: Is this a Kumakhov system? 0
A: Is this mirror faceted [Y/N] ? 0
Mirror surface [ 1-9] ? 3

Toroidal Selected.
Enter 0, if mirror pole is at the lower outer torus (usual case)
      1,                           lower inner
      2,                           upper inner
      3,                           upper outer

Mirror pole location ? 0
Do you want to specify the mirror parameters ? 0
Is the mirror Cylindrical ? 0
Is this optical element a Fresnel Zone Plate ? 0
Are we dealing with a Grating ? 0
Are we dealing with a crystal [ Y/N ] ? 0
Is the mirror convex [ Y/N ] ? 0
Reflectivity mode [ 0,1,2 ] ? 1
Optical Constant Source: [file=0,tt:=1], multilayer [2] ? 0
File with optical constants ? AUF1F2.OPT
Orientation Angle [ Alpha ] ? 0
Mirror Dimensions finite [ Y/N ] ? 0
Focii placed at continuation planes [ Y/N ] ? 1
Do you want to move the Source [ Y/N ] ? 0
Do you want to move the mirror itself [ Y/N ] ? 0
Distorted surface [ Y/N ] ? 0
Do you want to include surface roughness [Y/N] ? 0
Any screens in this OE [ Y/N ] ? 1
How many in this OE [ total ] ? 1
```

```
Screen N.           1

Is this screen before mirror [ Y/N ] ? 1
Distance from mirror [ absolute ] ? 2500
Is Screen Carrying an Aperture Stop [ Y/N ] ? 0
Include absorption [ Y/N ] ? 1
File with optical constants ? BEF1F2.OPT
Thickness of film [ cm ] ? 2.0E-4


/* This is a 2 microns BE filter.

Slit at continuation plane [ Y/N ] ? 0
Extra Image plates [ Y/N ] ? 0
File containing the source array ? BEGIN.DAT

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

Do you want to change input mode ? 0

Call to INPUT_OE

----------------------- S H A D O W  ------------------------------
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Defining Optical Element:  2

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] exit

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

Shadow:: exit

Exit to DCL
```

The data have been generated. In order to analyze the output, we will need to know the power per eV in the spectrum. This can be achieved by using HISTO1 on the files BEGIN.DAT, SCREEN.0101, MIRR.01. They represent the source, the beam after the filter and after the mirror. By computing the *transmitted* flux at each one, we can follow the progression of the spectrum along the beamline. By using FILEX, one could also obtain the system transmission function from the HISTO1 files. Notice that the flux units (eV/sec), are used because we are not interested in absolute fluxes for which we should know more about the machine; PLOTXY would be better suited in that case.

```
 $ [HISTO1]
 File for analysis ? [BEGIN.DAT]
 Column to analyze ? [11]


/* 11 is the position where the photon energy of the ray is stored. We want
/* then to perform a binning operation based on it.

 Options : [0] Angstroms
         : [1] eV
         : [2] cm-1

 <?> [1]

 Read    :         1000 rays

 Maximum :     [5222.791]
 Minimum :     [201.5226]
 Distribution center ? [2750]
              width  ? [5500]
 Number of bins (odd, please) ? [31]

 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

/* We must not normalize.

 <?> [0]
 Include reflectivity ? [1]

 Options. Enter:
 0        to use |A| as weighing factor
 1        to use |A|**2 as weighing factor (transmitted)
```

```
 2        to use 1-|A|**2 as weighing factor (absorbed )

/* Simply use the intensity (amplitude squared).

 <?> 1

 Scale to :
   0      no scaling (cm-1)
   1      Watt
   2      eV/sec.

 <?> 2

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

 Then ? 0

 OK. Here we go !

 Another run  [ Y/N ] ? 1
```

For Unix users, you may want to exit out of HISTO1 in between files and rename the histo1.dat's to something useful. Otherwise they will be overwritten by subsequent runs.

```
 File for analysis ? SCREEN.0101
 Column to analyze ? 11

 Options : [0] Angstroms
         : [1] eV
         : [2] cm-1

 <?> 1

 Read    :         1000 rays

 Maximum :    5222.791
 Minimum :    201.5226
 Distribution center ? 2750
              width  ? 5500
 Number of bins (odd, please) ? 31

 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 ? 1

Options. Enter:
0        to use |A| as weighing factor
1        to use |A|**2 as weighing factor (transmitted)
2        to use 1-|A|**2 as weighing factor (absorbed )

<?> 1

Scale to :
  0      no scaling (cm-1)
  1      Watt
  2      eV/sec.

<?> 2

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

Then ? 0

OK. Here we go !

Another run  [ Y/N ] ? 1
File for analysis ? MIRR.01
Column to analyze ? 11

Options : [0] Angstroms
        : [1] eV
        : [2] cm-1

<?> 1

Read    :         1000 rays

Maximum :     5222.791
Minimum :     201.5226
Distribution center ? 2750
             width  ? 5500
Number of bins (odd, please) ? 31
```

```
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 ? 1

Options. Enter:
0        to use |A| as weighing factor
1        to use |A|**2 as weighing factor (transmitted)
2        to use 1-|A|**2 as weighing factor (absorbed )

<?> 1

Scale to :
  0      no scaling (cm-1)
  1      Watt
  2      eV/sec.

<?> 2

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

Then ? 0

OK. Here we go !

Another run  [ Y/N ] ? 0

Return to DCL
$
$
$
```

The three histograms can be plotted together using TopDrawer or Primvs. The command files for both are shown, and the histograms plotted in figure 6.14.
VMS

```
$ TYPE HISTO.COM
  @HISTO1.DAT;1
  @HISTO1.DAT;2
  @HISTO1.DAT;3
  HISTO
  TITLE BOTTOM 'Photon Energy (eV)'
  TITLE LEFT   'Arb. units'
```

UNIX

```
% more histo.com
  initpage(xwin)
  regionr(0.1,0.1,0.9,0.9,1.0)
  xyrange(0.00, 0.61187500E+04, 0.000, 1.0E+06)
  linestyle(2)
  plotl("begin.hist")
  linestyle(1)
  plotl("screen.hist")
  linestyle(3)
  plotl("mirror.hist")
  linestyle(1)
  box("bcnst",0,0,"bcnstv",0,0)
  label("Photon Energy (eV)","Arb. units","")
  exit
```

Notice how the Be filter cuts the low energies, while the Au mirror cuts the high ones. FILEX can be used to study the total power progression (by integrating the HISTO1 files) or the beamline transmission (by taking the ratio of HISTO1.DAT;3 to HISTO1.DAT;1).

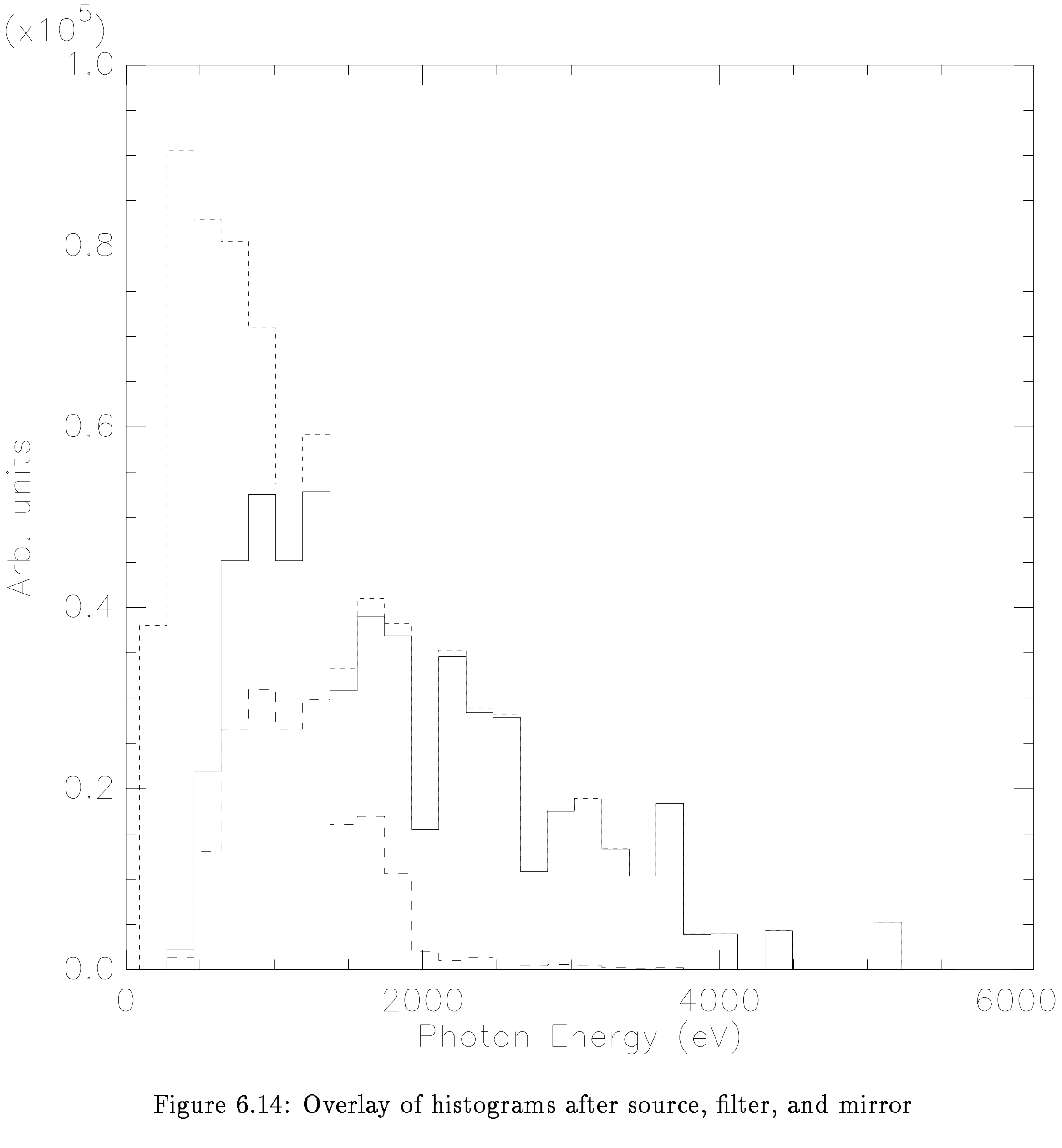

Figure 6.14: Overlay of histograms after source, filter, and mirror

6.4 Two Crystals I

The main purpose of this section is to demonstrate how to ray-trace a crystal monochromator. SHADOW needs a data file prepared by BRAGG to ray trace a crystal. In addition, BRAGG may allow the user to visualize the diffraction patterns or rocking curves of the crystal in consideration. SHADOW deals with crystals in both reflection (Bragg) and transmission (Laue) mounting. Two crystal models are allowed in SHADOW: perfect crystals (i.e. Silicon, Diamond) and mosaic crystals, where the crystal block is made by an agglutination of small microcrystals (i.e. graphite, beryllium). Perfect crystals may be symmetric (the Bragg planes are parallel to the crystal surface in Bragg mounting, and perpendicular in Laue mounting) and asymmetric, when the crystal planes form an arbitrary angle alfa with the crystal surface. Mosaic crystals can only be symmetrical in SHADOW. Ground-bent crystals (the so-called Johansson geometry) for perfect crystals are also allowed in SHADOW. We remind the reader that a symmetric perfect crystal in Bragg mounting is essentially a mirror with a very narrow bandwidth in energy or angle, determined by its rocking curve or diffraction pattern. An asymmetric crystal does not act as a mirror, but as a grating, where the "grating ruling" is provided by the intersection lines between the Bragg planes and crystal surface[1]. In addition,the rocking curve determines the energy or angular acceptance, as in symmetric crystals. In all the crystal cases of three-dimensional Bragg scattering, only the rays close to the Bragg condition will be diffracted; the other ones will be *absorbed* by the crystal. For this reason, to only look at the scatter plot of the reflected (outgoing) beam, like we did in the case of the grating, is not enough. This is because of the way SHADOW carries the intensity information; to each ray is associated the vector potential A that contains, in its modulus, the intensity (and polarization) information. For this reason a simple scatter plot does not convey any information on the *intensity* of the rays; it is necessary then to use either the facilities provided by PLOTXY in the CONTOUR mode (two dimensional case), or make use of the INTENSITY flag in PREPLOT (one dimensional case). Since PLOTXY has already been demonstrated, we will concentrate on PREPLOT. In this example we will then show how to:

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

The case that we will consider is that of a two-crystal monochromator in an antiparallel configuration. After considering the ideal case, we will introduce some rotational misalignement and study its effect on the transmitted spectrum. See figure 6.15 below. In order to do that, we will restart the calculations at the second OE, since the first one will have been

[1]M. Sanchez del Rio, et. al, Review of Scientific Instruments 63(1), 1992

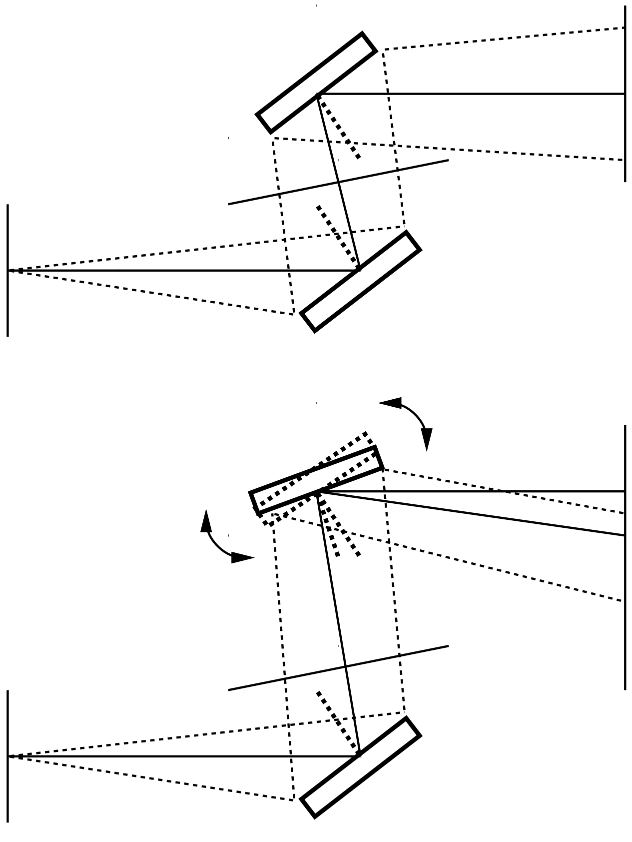

Figure 6.15: Two crystals monochromator with diverging radiation and antiparallel configuration: a)ideal case, b)misaligned second crystal.

left unchanged. The source that we will be using will be a point source of single wavelength. The BRAGG condition

$$n\,\lambda \;=\; 2\,d\,sin\theta \tag{6.2}$$

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

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

In order to prepare BRAGG it is necessary to have a table of the real part of the atomic scattering coefficients in function of $sin(\theta)/\lambda$. An exhaustive table can be found in the *International Tables of X-Ray Crystallography, Vol.III, Sect.2.2, Table 2.2A, p.72.* A shorter version can be found in *X-ray Diffraction*, by B.E. Warren, Addison-Wesley, 1969. BRAGG will prompt about the coefficients.
BRAGG is the program that generates the crystal parameters in a format suitable for input to SHADOW. Let us use the GaAs (111) plane, with incident energy of 11160 eV.

```
$ BRAGG

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

Then ? 0
Lattice constant (Angs) ? 5.65
Index of crystal plane of reflection H,K,L : 1,1,1


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

```
Enter 2-letters (capitalized) atomic symbol for atom A : GA
Enter 2-letters (capitalized) atomic symbol for atom B : AS

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

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

For atom A, first set  : 0.14,27.162
.         , second set : 0.15,26.783
.         , third set  : 0.16,26.406
For atom B, first set  : 0.14,28.742
.         , second set : 0.15,28.307
.         , third set  : 0.16,27.877

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

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

minimum photon energy (eV) : 11100
maximum photon energy (eV) : 11200
energy step (eV) : 10
Do you want to include crystal absorption [1/0] ? 1
Temperature (Debye-Waller) factor : 0.979
```

This is the value of the Debye-Waller coefficient,

$$e^{-\frac{1}{3}G^2u^2}$$

where G is the scattering vector and u the rms atomic displacement. If in doubt, enter 1.0. This will ignore then DW effects.

```
 Output file name (for SHADOW) : GAAS.PAR
 Do you want to generate a rocking curve [1/0] ? 1
 What do you want to calculate ?:
 [1] Diffracted beam in Transmission (Laue) geometry
 [2] Diffracted beam in Reflection (Bragg) geometry
 [3] like [2] using thick crystal approximation
  <?> 3
 ... at what energy (eV) ? 11160


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

 Do you want to calculate a mosaic crystal ? 0
 Do you want an asymmetrical cut [1/0] ? 0

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

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


 +/- how many microradians : 60
 How many points : 200
 Do you want to use sec [1/0] ? 0
 Do you want the R.C. not centered [1/0] ? 0
 Do you want to try another energy [1/0] ? 0
 $
```
VMS
```
 $
 $ DIR
```

```
Directory D13:[XRAYOP.XTAL]

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

Total of 4 files, 47 blocks.
```

UNIX

% ls -al

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

GAAS.PAR will be the input parameter file to SHADOW. At the end of the file GAAS.PAR is a table of:

eV $f'(Ga)$ $f''(Ga)$ $f'(As)$ $f''(As)$

which form the optical constant library. The user can edit this file if more accurate values are available, especially near an absorption edge.

$ $\boxed{\text{TYPE GAAS.PAR}}$

```
          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 11160 eV, which are a function of the real part of Ss and Sp (for the S- and P-polarization). For this case, Ss = 25.541 and Sp = 24.060 microradians.

$ TYPE ROCK_CURVE.PAR

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

```
/*  Plot out the rocking curve for S-polarization.
```

VMS

$

$ TD_NEW

```
Top Drawer 08/11/82
```

@rock_curve.s

title bottom 'Rocking curve (Ss)'

join 1

end

UNIX

```
% primvs
```

Primvs> initpage(xwin)

Primvs> regionp(0.1,0.1,0.9,0.9)

Primvs> autoscale

Primvs> plotl("rock_curve.s")

Primvs> box("bcnst",0,0,"bcnstv",0,0)

Primvs> exit

Things seem to be reasonable, so we can run SHADOW (finally). To check things out, let us use a monochromatic source with only vertical divergence.

$ GO SOURCE

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

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

Call to INPUT

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

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

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

------------- SOURCE SPECS ------------------

Source modelling type [ 0-5 ] ? 0
How many rays [ 1 - 5 000 ] ? 1000
```

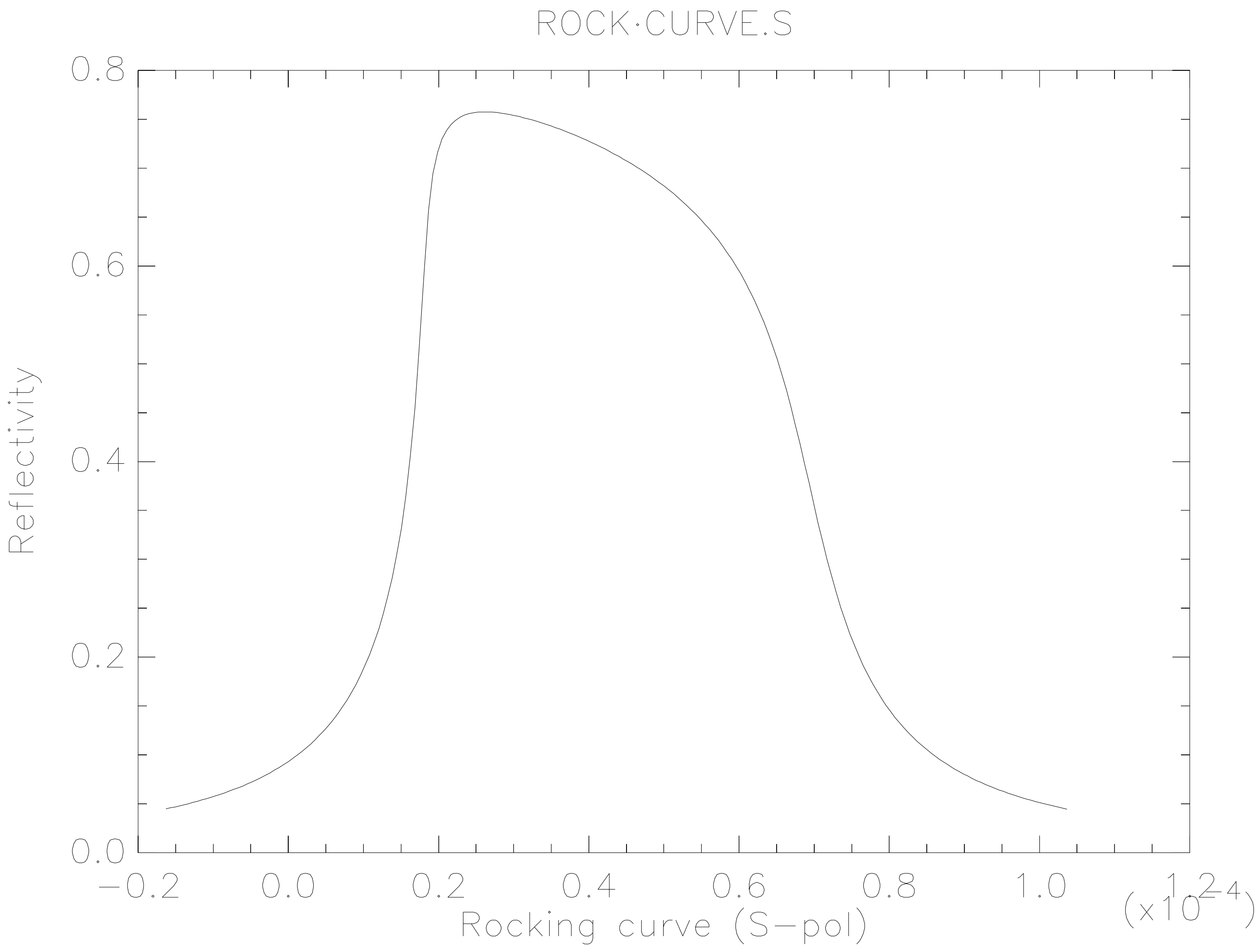

Figure 6.16: Rocking curve for S-polarization

```
Seed [ odd, 1000 - 1 000 000 ] ? 12345
Do you want to optimize the source ? 0

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

Then ? 0
X-Z plane source type [ 0-3 ] ? 0
Source Depth [ 1-4 ] ? 1
Source Angle Distribution [ 1-6 ] ? 2
Horizontal half-divergence [ (+)x, rads ] ? 0
.                          [ (-)x, rads ] ? 0
Vertical                   [ (+)z, rads ] ? 60E-6
.                          [ (-)z, rads ] ? 60E-6
Do you want a Photon energy [ Y/N ] ? 1
Energy distribution [ 1-3 ] ? 1
Photon Energy [ 0 ] or Angstroms [ 1 ] ? 0
Energy [ eV ] ? 11160
Do you want to store the optical paths (OPD) [Y/N] ? 0
Do you want to generate the A vectors (electric field) [Y/N] ? 0


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

Shadow:: trace

Ray Tracing Selected. Begin procedure.

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

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

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

 Then ? 0

 Call to INPUT_OE

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

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

 Defining Optical Element:  1

 Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] <ret>
 Do you want a verbose [ 1 ] or terse [ 0 ] output ? 0

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

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

 Then ?  0

 Optical Element definition:

 Incidence Angle ? 10
 Source Distance ? 5000
 Reflection Angle? 10
 Image Distance  ? 150

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

```
Reflector [ 0 ] or refractor [ 1 ] ? 0
A: Is this a Kumakhov system?  0
A: Is this mirror faceted [Y/N] ?  0
Mirror surface [ 1-9] ? 5
Is the mirror Cylindrical ? 0
Is this optical element a Fresnel Zone Plate ? 0
Are we dealing with a Grating ? 0
Are we dealing with a crystal [ Y/N ] ? 1
```

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

```
File containing crystal parameters ? GAAS.PAR
Is it a mosaic crystal [ Y/N ] ? 0
Is the crystal asymmetric [ Y/N ] ? 0
Are we working in Johansson geometry [Y/N] ? 0
Automatic Tuning of Crystal [ Y/N ] ? 1
Energy, in eV, [ 0 ] or wavelength, in Angs., [ 1 ] ? 0
Photon Energy ? 11160
Is the mirror convex [ Y/N ] ? 0
Reflectivity mode [ 0,1,2 ] ? 0
Orientation Angle [ Alpha ] ? 0
Mirror Dimensions finite [ Y/N ] ? 0
Do you want to move the Source [ Y/N ] ? 0
Do you want to move the mirror itself [ Y/N ] ? 0
Distorted surface [ Y/N ] ? 0
Do you want to include surface roughness [Y/N] ? 0
Any screens in this OE [ Y/N ] ? 0
Slit at continuation plane [ Y/N ] ? 0
Extra Image plates [ Y/N ] ? 0
File containing the source array ? BEGIN.DAT

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

Call to INPUT_OE
```

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

Defining Optical Element:  2

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] <ret>
Do you want a verbose [ 1 ] or terse [ 0 ] output ? 0

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

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

Then ?  0

Optical Element definition:

Incidence Angle ? 10
Source Distance ? 150
Reflection Angle? 10
Image Distance  ? 5000
Reflector [ 0 ] or refractor [ 1 ] ? 0
A: Is this a Kumakhov system?  0
A: Is this mirror faceted [Y/N] ?  0
Mirror surface [ 1-9] ? 5
Is the mirror Cylindrical ? 0
Is this optical element a Fresnel Zone Plate ? 0
Are we dealing with a Grating ? 0
Are we dealing with a crystal [ Y/N ] ? 1
File containing crystal parameters ? GAAS.PAR
Is it a mosaic crystal [ Y/N ] ? 0
Is the crystal asymmetric [ Y/N ] ? 0
Are we working in Johansson geometry [Y/N] ? 0
Automatic Tuning of Crystal [ Y/N ] ? 1
Energy, in eV, [ 0 ] or wavelength, in Angs., [ 1 ] ? 0
Photon Energy ? 11160
Is the mirror convex [ Y/N ] ? 0
```

```
Reflectivity mode [ 0,1,2 ] ? 0
Orientation Angle [ Alpha ] ? 180
Mirror Dimensions finite [ Y/N ] ? 0
Do you want to move the Source [ Y/N ] ? 0
Do you want to move the mirror itself [ Y/N ] ? 0
Distorted surface [ Y/N ] ? 0
Do you want to include surface roughness [Y/N] ? 0
Any screens in this OE [ Y/N ] ? 0
Slit at continuation plane [ Y/N ] ? 0
Extra Image plates [ Y/N ] ? 0

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

Call to INPUT_OE

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

Defining Optical Element:  3

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] exit

End of session
Procedure completed. Return to COMMAND level

Shadow:: exit
```

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

VMS

```
$ DIR

Directory D13:[XRAYOP.XTAL]

BEGIN.DAT;1            188  26-MAR-1987 14:22  (RWED,RWED,RE,RE)
EFFIC.01;1               1  26-MAR-1987 14:41  (RWED,RWED,RE,RE)
EFFIC.02;1               1  26-MAR-1987 14:48  (RWED,RWED,RE,RE)
END.00;1                 6  26-MAR-1987 14:22  (RWED,RWED,RE,RE)
END.01;1                11  26-MAR-1987 14:41  (RWED,RWED,RE,RE)
```

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

Total of 23 files, 1089 blocks.
```

UNIX

% $\boxed{\text{ls -al}}$

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

```
-rw-rw-r--   1 shadow      4451 Jun 10 12:41 start.01
-rw-rw-r--   1 shadow      4466 Jun 10 12:41 start.02
-rw-rw-r--   1 shadow        30 Jun 10 12:41 systemfile.dat
```

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

```
 $ type effic.01

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

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

```
 $ mirinfo

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

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

 MINFO> Please input filename: end.01

 MINFO> File read correctly.

 MINFO> Title ? plane crystal reflection
 MINFO> Comment ? to test SHADOW computation of the rocking curve.
 MINFO> Output file ? mirr.inf

 MINFO> Prepare output to file : mirr.inf

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

 $
 $
 $ type mirr.inf
```

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

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

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

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

```
$
$
$ PREPLOT
PREPLOT> Input file ? STAR.01

Read                 1000 rays.
Each ray has           12 entries.

PREPLOT> How many columns to write out ? 2

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

PREPLOT> Row # 1 : 6
PREPLOT>       2 : 23

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

PREPLOT> Then ? 0
```

VMS

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

Then ? 2
PREPLOT> Output file ? STAR01.PLT
PREPLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 : 1

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

UNIX

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

```
Display type:
  [ 0 ] Xwindow
  [ 1 ] Tektronix
  [ 2 ] Postscript file
Terminal type:  0
```

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

```
% mv preplot.dat star01.dat
```

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

```
$ PREPLOT
PREPLOT> Input file ? STAR.02

Read                 1000 rays.
Each ray has           12 entries.

PREPLOT> How many columns to write out ? 2

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

PREPLOT> Row # 1 : 6
PREPLOT>       2 : 23

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

PREPLOT> Then ? 0
```

VMS

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

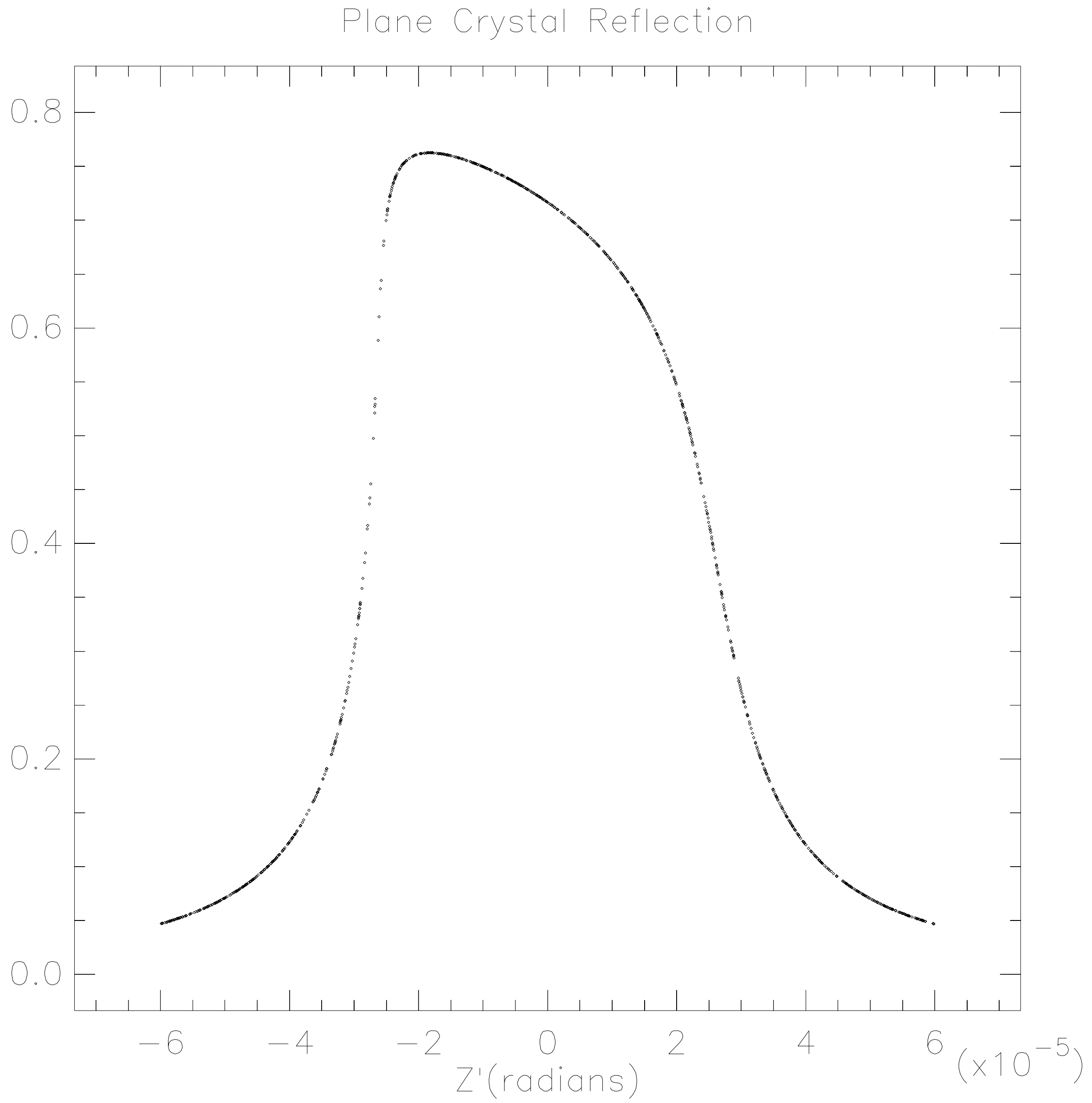

Figure 6.17: Plane Crystal Reflection

```
Then ? 0
PREPLOT> Output file ? STAR02.PLT
PREPLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 : 1

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

UNIX

```
Found   1000 good points out of  1000
Display type:
  [ 0 ] Xwindow
  [ 1 ] Tektronix
  [ 2 ] Postscript file
Terminal type:   0
% mv preplot.dat star02.dat
```

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

VMS

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

UNIX

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

```
$ GO TRACE

Ray Tracing Selected. Begin procedure.

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

PROMPT selected.
Call to RESET
Exit from RESET

Mode selected is:
PROMPT
```

```
 Options: to start anew                 [ 0 ]
            to restart from a given OE [ 1 ]

 Then ? [1]
 Previous element number : [1]
 Image file of the previous OE ? [STAR.01]
 Do you want to change the input mode ? [0]


 Call to INPUT_OE

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 Defining Optical Element:  2

 Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] [<ret>]
 Do you want a verbose [ 1 ] or terse [ 0 ] output ? [1]

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

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

 Then ?  [0]

 Optical Element definition:

 Incidence Angle ? [80.1956244]
 Source Distance ? [150.0]
 Reflection Angle? [80.1900690]
 Image Distance  ? [5000]
 Reflector [ 0 ] or refractor [ 1 ] ? [0]
 A: Is this a Kumakhov system?  [0]
 A: Is this mirror faceted [Y/N] ?  [0]
 Mirror surface [ 1-9] ? [5]
 Is the mirror Cylindrical ? [0]
 Is this optical element a Fresnel Zone Plate ? [0]
 Are we dealing with a Grating ? [0]
```

```
Are we dealing with a crystal [ Y/N ] ? 1
File containing crystal parameters ? GAAS.PAR
Is it a mosaic crystal [ Y/N ] ? 0
Is the crystal asymmetric [ Y/N ] ? 0
Are we working in Johansson geometry [Y/N] ? 0
Automatic Tuning of Crystal [ Y/N ] ? 0
Is the mirror convex [ Y/N ] ? 0
Reflectivity mode [ 0,1,2 ] ? 0
Orientation Angle [ Alpha ] ? 180
Mirror Dimensions finite [ Y/N ] ? 0
Do you want to move the Source [ Y/N ] ? 0
Do you want to move the mirror itself [ Y/N ] ? 0
Distorted surface [ Y/N ] ? 0
Do you want to include surface roughness [Y/N] ? 0
Any screens in this OE [ Y/N ] ? 0
Slit at continuation plane [ Y/N ] ? 0
Extra Image plates [ Y/N ] ? 0

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

Do you want to change input mode ? 0

Call to INPUT_OE

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Defining Optical Element:  3

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] exit

End of session
Procedure completed. Return to COMMAND level

Shadow:: exit
Exit to DCL
$
$
```

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

```
$ PREPLOT
PREPLOT> Input file ? STAR.02

Read                 1000 rays.
Each ray has           12 entries.

PREPLOT> How many columns to write out ? 2

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

PREPLOT> Row # 1 : 6
PREPLOT>       2 : 23

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

PREPLOT> Then ? 0
```

VMS

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

Then ? 0
PREPLOT> Output file ? STAR02.PLT
PREPLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 : 1

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

$
```

UNIX

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

```
Display type:
  [ 0 ] Xwindow
  [ 1 ] Tektronix
  [ 2 ] Postscript file
Terminal type:  0
% mv preplot.dat star02.dat
```

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

```
$
$ TD_NEW

@[-]star01.plt          \* these are the ones from the "above" directory.
@[-]star02.plt
@star02.plt
plot
title top 'BRAGG reflectors'
title bottom 'Angle (rad)'
title left 'Normalized Intensity'

$
$
```

UNIX

```
% primvs
Primvs> initpage(xwin)
Primvs> regionp(0.1,0.1,0.9,0.9)
Primvs> xyrange(-.00015,0.0001,0.0,0.8)
Primvs> plotp("./../star01.dat")
Primvs> plotp("./../star02.dat")
Primvs> plotp("star02.dat")
Primvs> box("bcnst",0,0,"bcnstv",0,0)
Primvs> label("Angle (rad)","Normalized Intensity","BRAGG Reflectors")
Primvs> exit
```

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

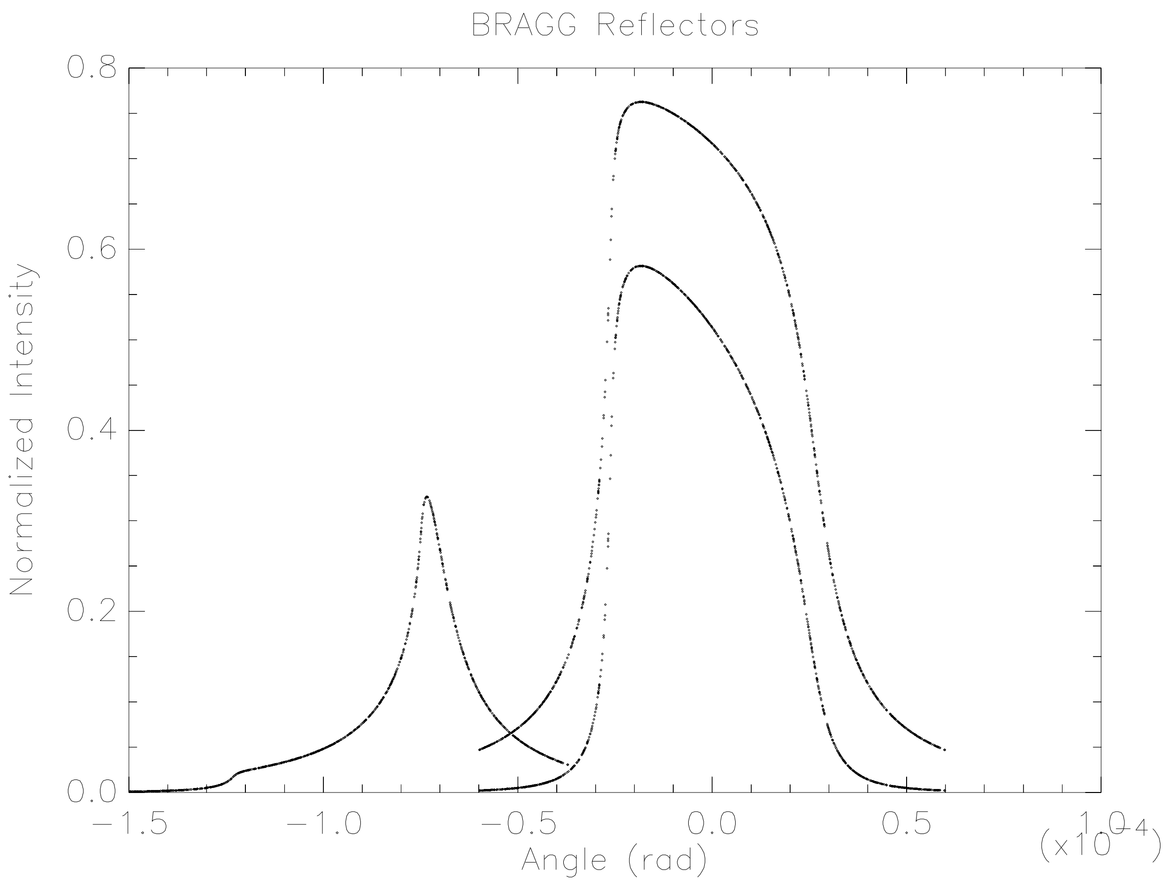

Figure 6.18: Comparison of BRAGG reflectors: offset and exact conditions

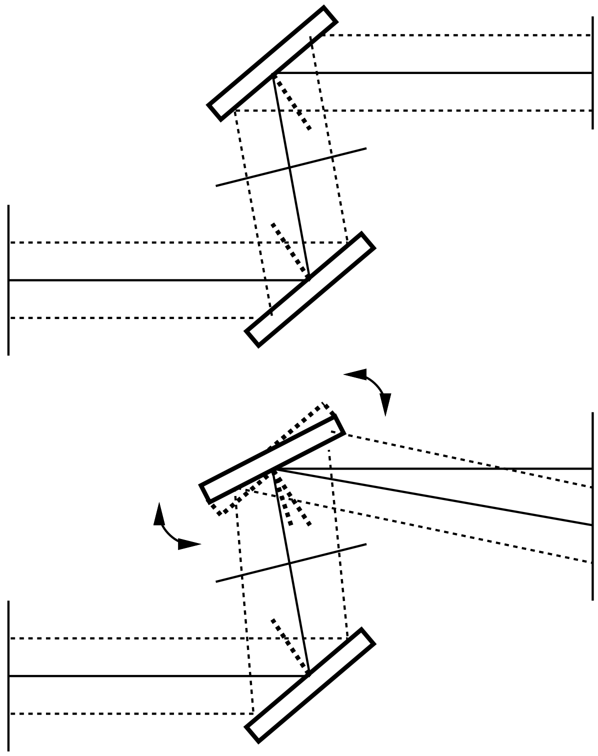

Figure 6.19: Two crystals monochromator in parallel radiation.

6.5 Two Crystals II

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

VMS	*UNIX*
$ CREATE/DIRECTORY [.XTAL2]	% mkdir ./xtal2
$ SD [XRAYOP.XTAL2]	% cd ./xtal2
$ COPY [-]GAAS.PAR []*.*	% cp ./../gaas.par .

$ GO SOURCE

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

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

Call to INPUT

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


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


------------- SOURCE SPECS ------------------

Source modelling type [ 0-5 ] ? 0
How many rays [ 1 - 5 000 ] ? 1000
Seed [ odd, 1000 - 1 000 000 ] ? 12345
Do you want to optimize the source ? 0


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

Then ? 0
X-Z plane source type [ 0-3 ] ? 1
Source Width  [ x ] ? 1
.      Height [ z ] ? 1
Source Depth [ 1-4 ] ? 1
Source Angle Distribution [ 1-6 ] ? 1
Horizontal half-divergence [ (+)x, rads ] ? 0
.                          [ (-)x, rads ] ? 0
Vertical                   [ (+)z, rads ] ? 0
.                          [ (-)z, rads ] ? 0
Do you want a Photon energy [ Y/N ] ? 1
Energy distribution [ 1-3 ] ? 3
Photon Energy [ 0 ] or Angstroms [ 1 ] ? 0
From photon energy or wavelength ...  ? 11156
```

```
... to photon energy or wavelength : ? [11164]
Do you want to store the optical paths (OPD) [Y/N] ? [0]
Do you want to generate the A vectors (electric field) [Y/N] ? [0]


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

Shadow:: [TRACE]

Ray Tracing Selected. Begin procedure.

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

PROMPT selected.
Call to RESET
Exit from RESET

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

Then ? [0]

Call to INPUT_OE

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

Defining Optical Element:  1

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] [<ret>]
Do you want a verbose [ 1 ] or terse [ 0 ] output ? [0]
```

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

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

Then ? $\boxed{0}$

Optical Element definition:

Incidence Angle ? $\boxed{10}$
Source Distance ? $\boxed{5000}$
Reflection Angle? $\boxed{10}$
Image Distance ? $\boxed{149.8956}$
Reflector [0] or refractor [1] ? $\boxed{0}$
A: Is this a Kumakhov system? $\boxed{0}$
A: Is this mirror faceted [Y/N] ? $\boxed{0}$
Mirror surface [1-9] ? $\boxed{5}$
Is the mirror Cylindrical ? $\boxed{0}$
Is this optical element a Fresnel Zone Plate ? $\boxed{0}$
Are we dealing with a Grating ? $\boxed{0}$
Are we dealing with a crystal [Y/N] ? $\boxed{1}$
File containing crystal parameters ? $\boxed{\text{GAAS.PAR}}$
Is it a mosaic crystal [Y/N] ? $\boxed{0}$
Is the crystal asymmetric [Y/N] ? $\boxed{0}$
Are we working in Johansson geometry [Y/N] ? $\boxed{0}$
Automatic Tuning of Crystal [Y/N] ? $\boxed{1}$
Energy, in eV, [0] or wavelength, in Angs., [1] ? $\boxed{0}$
Photon Energy ? $\boxed{11160}$
Is the mirror convex [Y/N] ? $\boxed{0}$
Reflectivity mode [0,1,2] ? $\boxed{0}$
Orientation Angle [Alpha] ? $\boxed{0}$
Mirror Dimensions finite [Y/N] ?$\boxed{0}$
Do you want to move the Source [Y/N] ? $\boxed{0}$
Do you want to move the mirror itself [Y/N] ? $\boxed{0}$
Distorted surface [Y/N] ? $\boxed{0}$
Do you want to include surface roughness [Y/N] ? $\boxed{0}$

```
 Any screens in this OE [ Y/N ] ? 0
 Slit at continuation plane [ Y/N ] ? 0
 Extra Image plates [ Y/N ] ? 0
 File containing the source array ? BEGIN.DAT

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

 Do you want to change input mode ? 0

 Call to INPUT_OE

 ------------------------ S H A D O W  ------------------------
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 Defining Optical Element:  2

 Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] <ret>
 Do you want a verbose [ 1 ] or terse [ 0 ] output ? 0

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

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

 Then ?  0

 Optical Element definition:

 Incidence Angle ? 10
 Source Distance ? 149.8956
 Reflection Angle? 10
 Image Distance  ? 5000
 Reflector [ 0 ] or refractor [ 1 ] ? 0
 A: Is this a Kumakhov system?  0
 A: Is this mirror faceted [Y/N] ?  0
 Mirror surface [ 1-9] ? 5
```

```
Is the mirror Cylindrical ? [0]
Is this optical element a Fresnel Zone Plate ? [0]
Are we dealing with a Grating ? [0]
Are we dealing with a crystal [ Y/N ] ? [1]
File containing crystal parameters ? [GAAS.PAR]
Is it a mosaic crystal [ Y/N ] ? [0]
Is the crystal asymmetric [ Y/N ] ? [0]
Are we working in Johansson geometry [Y/N] ? [0]
Automatic Tuning of Crystal [ Y/N ] ? [1]
Energy, in eV, [ 0 ] or wavelength, in Angs., [ 1 ] ? [0]
Photon Energy ? [11160]
Is the mirror convex [ Y/N ] ? [0]
Reflectivity mode [ 0,1,2 ] ? [0]
Orientation Angle [ Alpha ] ? [180]
Mirror Dimensions finite [ Y/N ] ? [0]
Do you want to move the Source [ Y/N ] ? [0]
Do you want to move the mirror itself [ Y/N ] ? [0]
Distorted surface [ Y/N ] ? [0]
Do you want to include surface roughness [Y/N] ? [0]
Any screens in this OE [ Y/N ] ? [0]
Slit at continuation plane [ Y/N ] ? [0]
Extra Image plates [ Y/N ] ? [0]

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

Do you want to change input mode ? [0]

Call to INPUT_OE

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

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] [exit]


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

```
Shadow:: [EXIT]

Exit to DCL

$ [TYPE EFFIC.01]

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

$ [MIRINFO]


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

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

MINFO> Please input filename: [END.01]
MINFO> File read correctly.
MINFO> Title ? [PLANE CRYSTAL REFLECTION 2]
MINFO> Comment ? [<ret>]
MINFO> Output file ? [MIRR.INF]

MINFO> Prepare output to file : MIRR.INF

$ [TYPE MIRR.INF]


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

Surface figure was defined as:       PLANE
```

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

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

VMS

$ $\boxed{\text{DIR}}$

```
Directory D13:[XRAYOP.XTAL2]

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

```
OPTAX.02;1                 3  30-MAR-1987 14:05  (RWED,RWED,RE,RE)
STAR.01;1                188  30-MAR-1987 14:03  (RWED,RWED,RE,RE)
STAR.02;1                188  30-MAR-1987 14:05  (RWED,RWED,RE,RE)
START.00;1                 6  30-MAR-1987 14:01  (RWED,RWED,RE,RE)
START.01;1                11  30-MAR-1987 14:03  (RWED,RWED,RE,RE)
START.02;1                11  30-MAR-1987 14:05  (RWED,RWED,RE,RE)

Total of 17 files, 1012 blocks.
```

UNIX

```
% ls -al

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

```
$ PREPLOT
PREPLOT> Input file ? STAR.02


Read                  1000 rays.
Each ray has            12 entries.

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

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

PREPLOT> Row # 1 : 11
PREPLOT>       2 : 23
```

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

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

PREPLOT> Then ? 1

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

PREPLOT> Then ? 0
```

VMS

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

Then ? 0
PREPLOT> Output file ? STAR02.PLT
PREPLOT> Terminal type: [0] VT240, [1] TEK 40xx, [2] HIREZ, [3] TEK 4107 : 2

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

UNIX

```
Found   1000 good points out of  1000
Display type:
  [ 0 ] Xwindow
```

```
  [ 1 ] Tektronix
  [ 2 ] Postscript file
Terminal type: 0
% mv preplot.dat star02.dat
```

Now the second crystal will be offset.

VMS

```
$
$
$ CREATE/DIRECTORY [.OFFSET2]
$ SD [.OFFSET2]
$ COPY [-]STAR.01,GAAS.PAR [ ]
$ COPY [-]OPTAX.01 [ ]
```

UNIX

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

```
$ GO TRACE

Ray Tracing Selected. Begin procedure.

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

PROMPT selected.
Call to RESET
Exit from RESET

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

Then ? 1
Previous element number : 1
Image file of the previous OE ? STAR.01
Do you want to change the input mode ? 0

Call to INPUT_OE

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Defining Optical Element:  2

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] <ret>
Do you want a verbose [ 1 ] or terse [ 0 ] output ? 0
```

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

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

 Then ? 0

 Optical Element definition:

 Incidence Angle ? 10
 Source Distance ? 149.8956
 Reflection Angle? 10
 Image Distance  ? 5000
 Reflector [ 0 ] or refractor [ 1 ] ? 0
 A: Is this a Kumakhov system?  0
 A: Is this mirror faceted [Y/N] ?  0
 Mirror surface [ 1-9] ? 5
 Is the mirror Cylindrical ? 0
 Is this optical element a Fresnel Zone Plate ? 0
 Are we dealing with a Grating ? 0
 Are we dealing with a crystal [ Y/N ] ? 1
 File containing crystal parameters ?GAAS.PAR
 Is it a mosaic crystal [ Y/N ] ? 0
 Is the crystal asymmetric [ Y/N ] ? 0
 Are we working in Johansson geometry [Y/N] ? 0
 Automatic Tuning of Crystal [ Y/N ] ? 1
 Energy, in eV, [ 0 ] or wavelength, in Angs., [ 1 ] ? 0
 Photon Energy ? 11160
 Is the mirror convex [ Y/N ] ? 0
 Reflectivity mode [ 0,1,2 ] ? 0
 Orientation Angle [ Alpha ] ? 180
 Mirror Dimensions finite [ Y/N ] ? 0
 Do you want to move the Source [ Y/N ] ? 0
 Do you want to move the mirror itself [ Y/N ] ? 1
 Rotation around X axis [ degrees ] ? 2.777E-3
 .               Y.                 ? <ret>
```

```
.               Z.                 ? <ret>
Mirror Offset. In X ? <ret>
.                 Y ? <ret>
.                 Z ? <ret>
Distorted surface [ Y/N ] ? 0
Do you want to include surface roughness [Y/N] ? 0
Any screens in this OE [ Y/N ] ? 0
Slit at continuation plane [ Y/N ] ? 0
Extra Image plates [ Y/N ] ? 0
Exit from INPUT

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

Do you want to change input mode ? 0

Call to INPUT_OE

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

Defining Optical Element:  3

Continue ? [ exit(Unix) or %EXIT(VMS) to terminate OS ] exit

End of session
Procedure completed. Return to COMMAND level

Shadow:: EXIT

Exit to DCL

$ PREPLOT

PREPLOT> Input file ? STAR.01

Read                  1000 rays.
Each ray has            12 entries.

PREPLOT> How many columns to write out ? 2

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

```
PREPLOT> Row # 1 : [11]
PREPLOT>       2 : [23]

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

PREPLOT> Then ? [1]

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

PREPLOT> Then ? [0]
```

VMS

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

Then ? [0]
PREPLOT> Output file ? [STAR01.PLT]

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

UNIX

```
Found   1000 good points out of  1000
Display type:
  [ 0 ] Xwindow
  [ 1 ] Tektronix
  [ 2 ] Postscript file
Terminal type:   [0]
% [mv preplot.dat star01.dat]

$
$
$ [PREPLOT]

PREPLOT> Input file ? [STAR.02]
```

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

PREPLOT> How many columns to write out ? [2]

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

PREPLOT> Row # 1 : [11]
PREPLOT>       2 : [23]

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

PREPLOT> Then ? [1]

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

PREPLOT> Then ? [0]
```

VMS

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

Then ? [0]
PREPLOT> Output file ? [STAR02.PLT]

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

UNIX

```
Found   1000 good points out of  1000
Display type:
  [ 0 ] Xwindow
```

```
   [ 1 ] Tektronix
   [ 2 ] Postscript file
Terminal type:  0
% mv preplot.dat star02.dat
```

VMS

```
$ T STARPLOT.COM

@star01.plt
@star02.plt
@[-]star02.plt
plot
title top'BRAGG reflectors'
title bottom 'Photon Energy (eV)'
title left 'Normalized Intensity'

$ TD_NEW

TOP DRAWER (10/10/80) NOW EXECUTING

@STARPLOT.COM
END
$
$
$
```

UNIX

```
% primvs

Primvs> initpage(xwin)
Primvs> regionp(0.1,0.1,0.9,0.9)
Primvs> xyrange(11154,11166,0.0,0.8)
Primvs> plotp("star01.dat")
Primvs> plotp("star02.dat")
Primvs> plotp("./../star02.dat")
Primvs> box("bcnst",0,0,"bcnstv",0,0)
Primvs> label("Photon Energy (eV)","Normalized Intensity","BRAGG Reflectors")
Primvs> exit
```

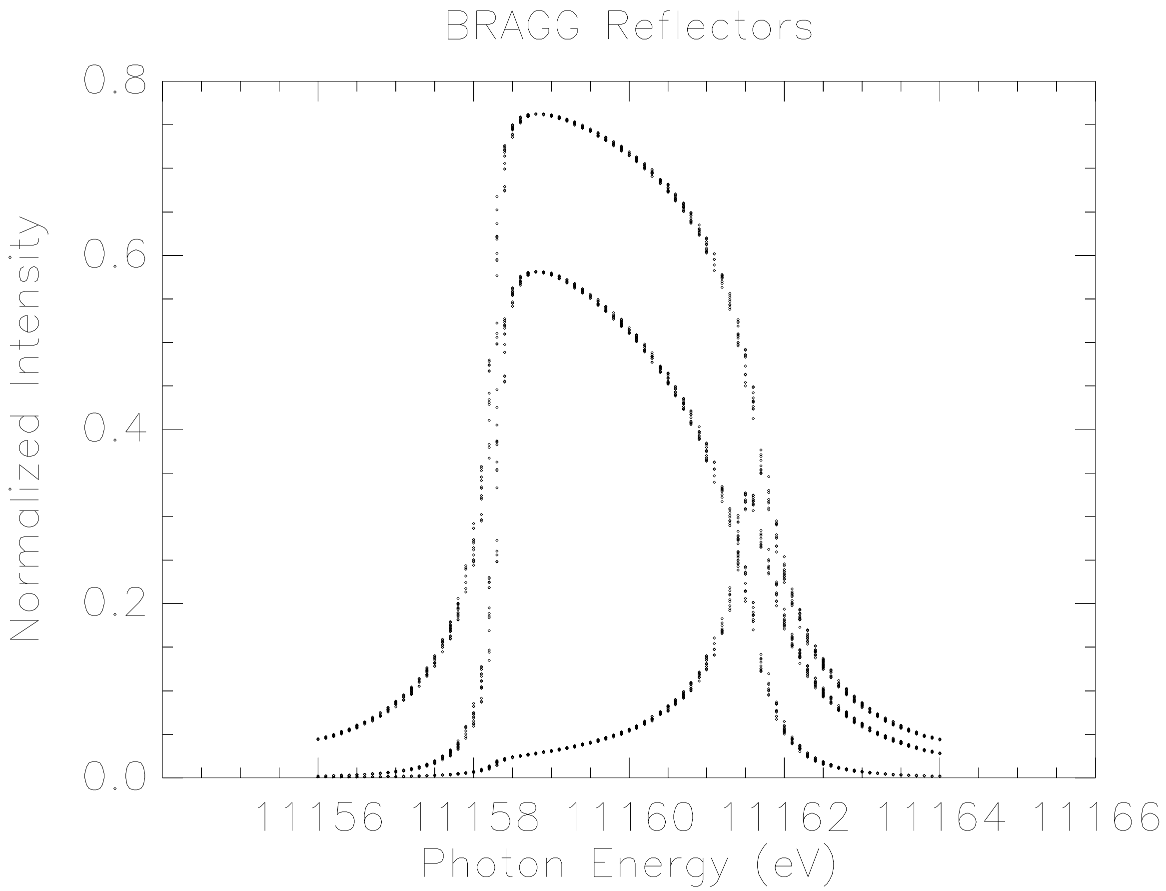


Figure 6.20: Comparison of BRAGG reflectors for continuous energy

Appendix A

Program Flow

The following pages describe graphically the options available to the user of SHADOW during the I/O session. They will be fully discussed in the User's Guide; for now they should be considered as a map to the possible cases that SHADOW recognizes. The structure of a flow-chart is natural in SHADOW, since the program branches depending on the user's answers. The plots should be self-explanatory.

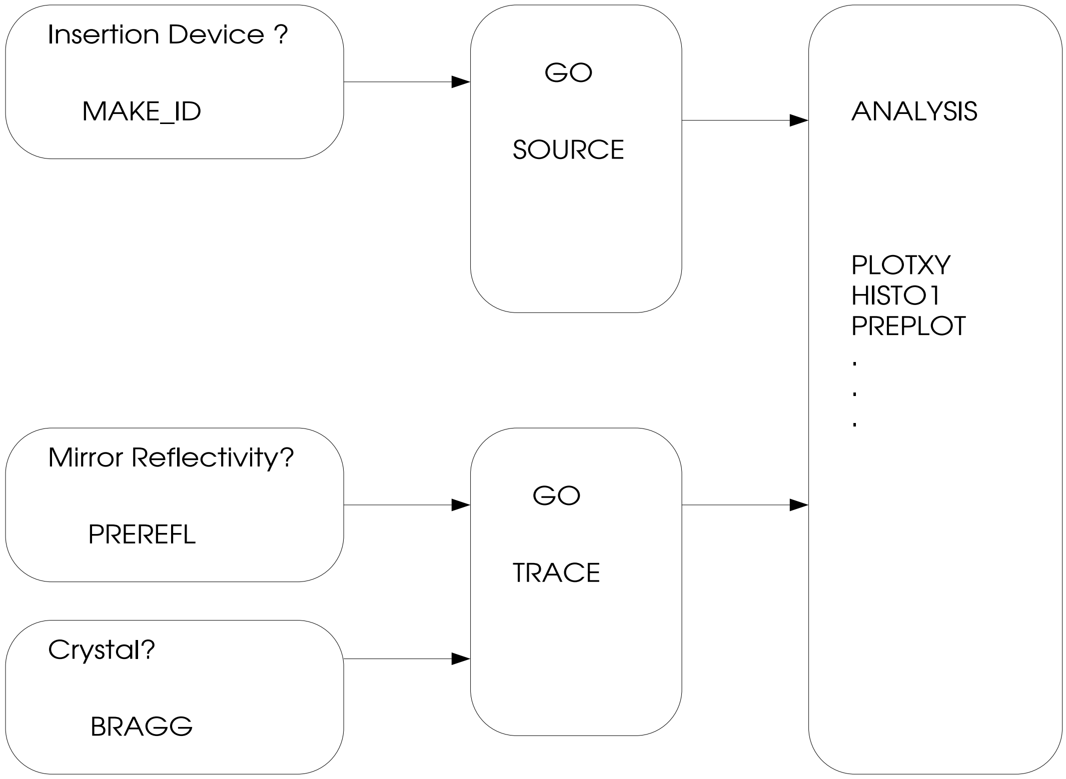
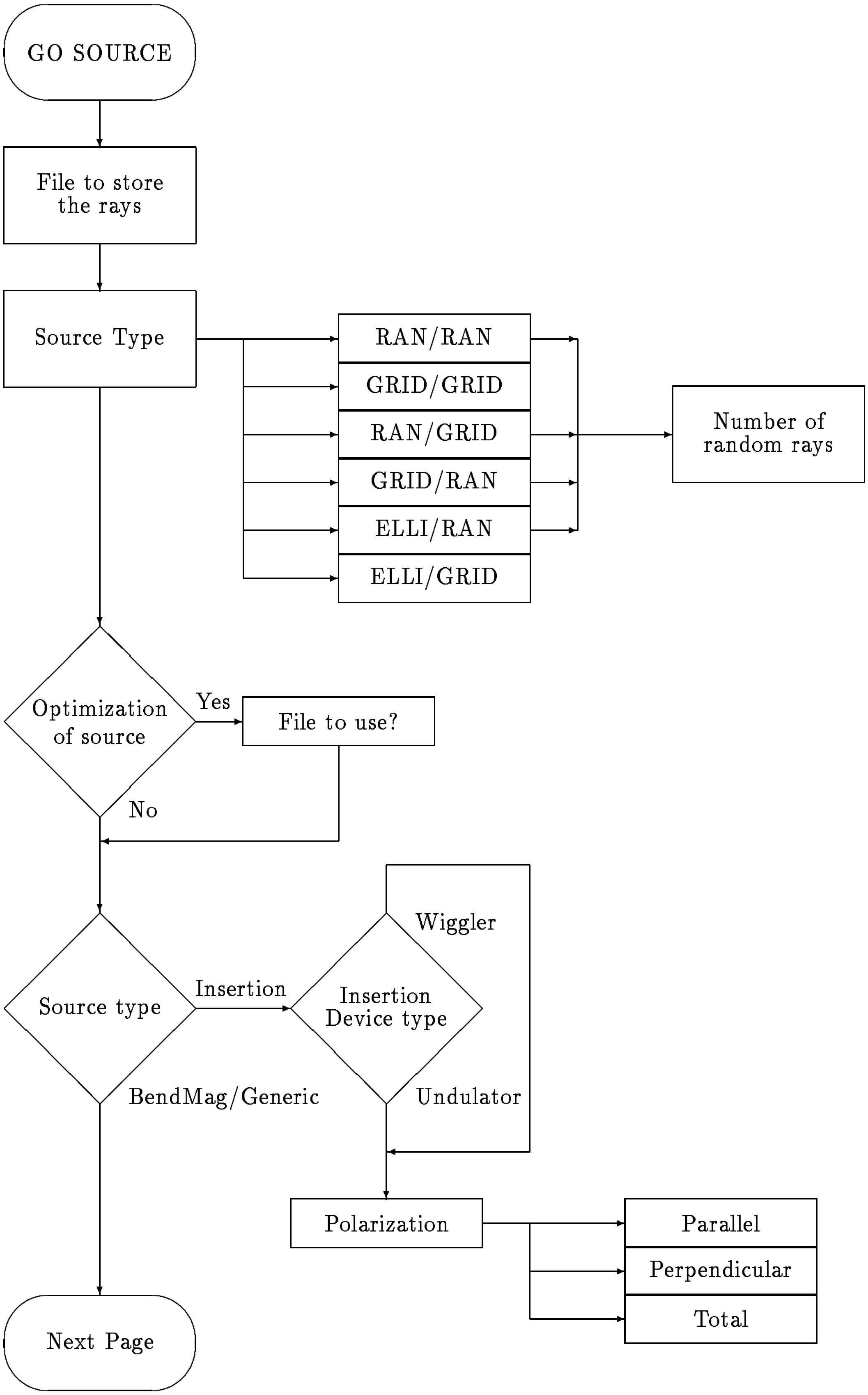
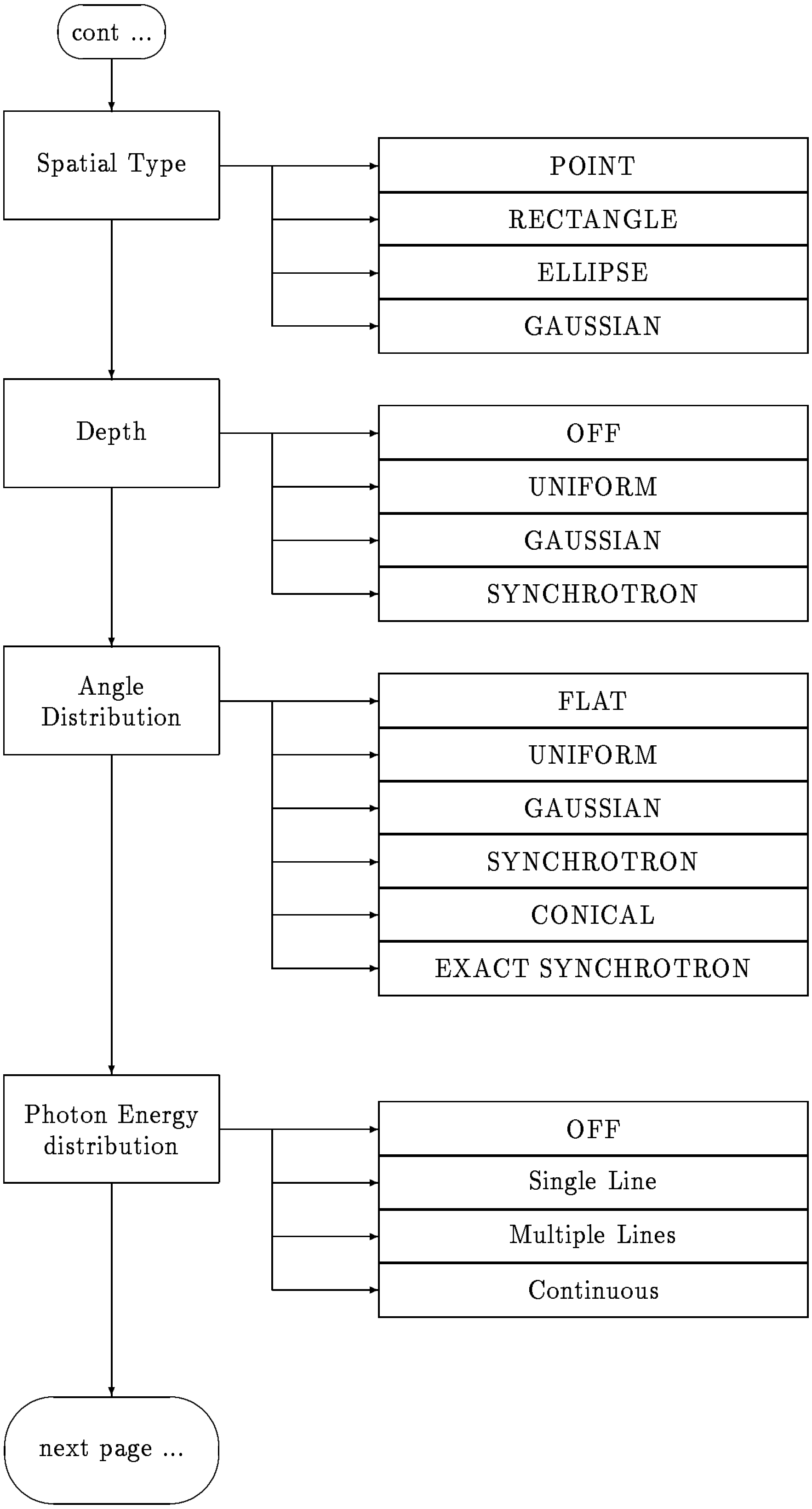
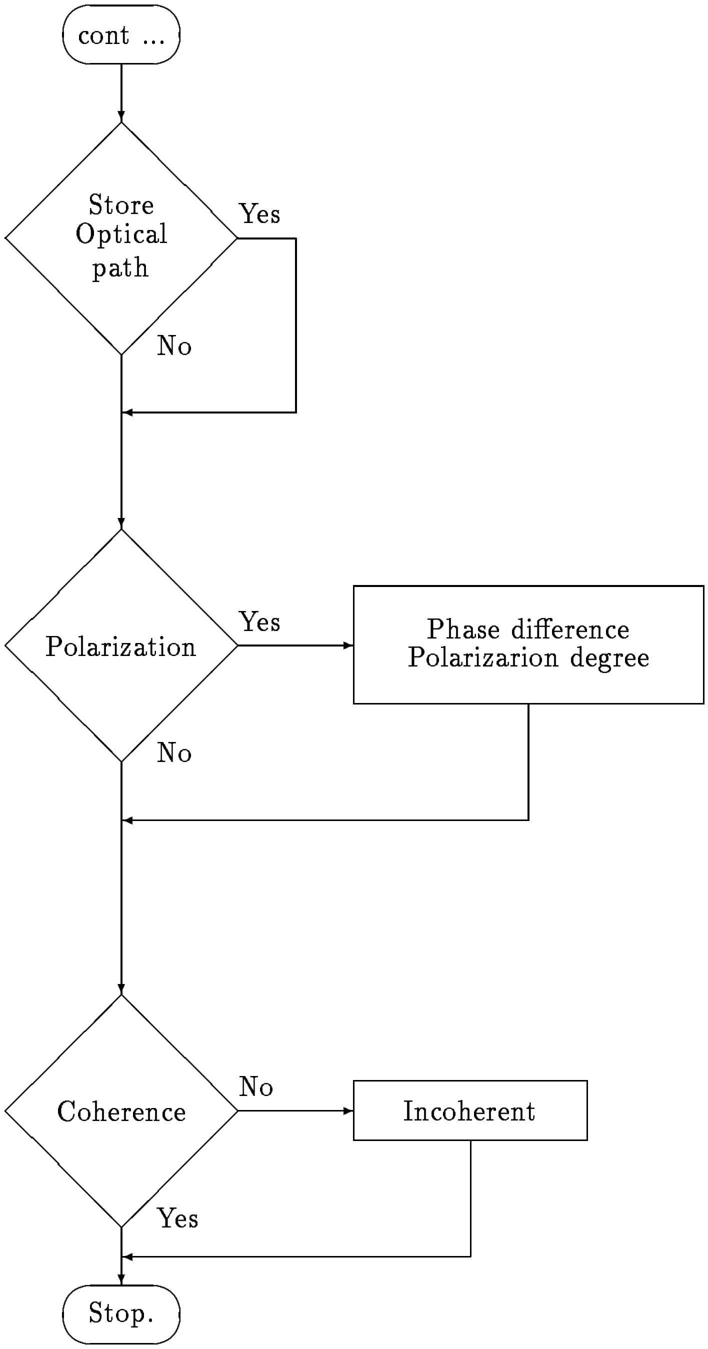
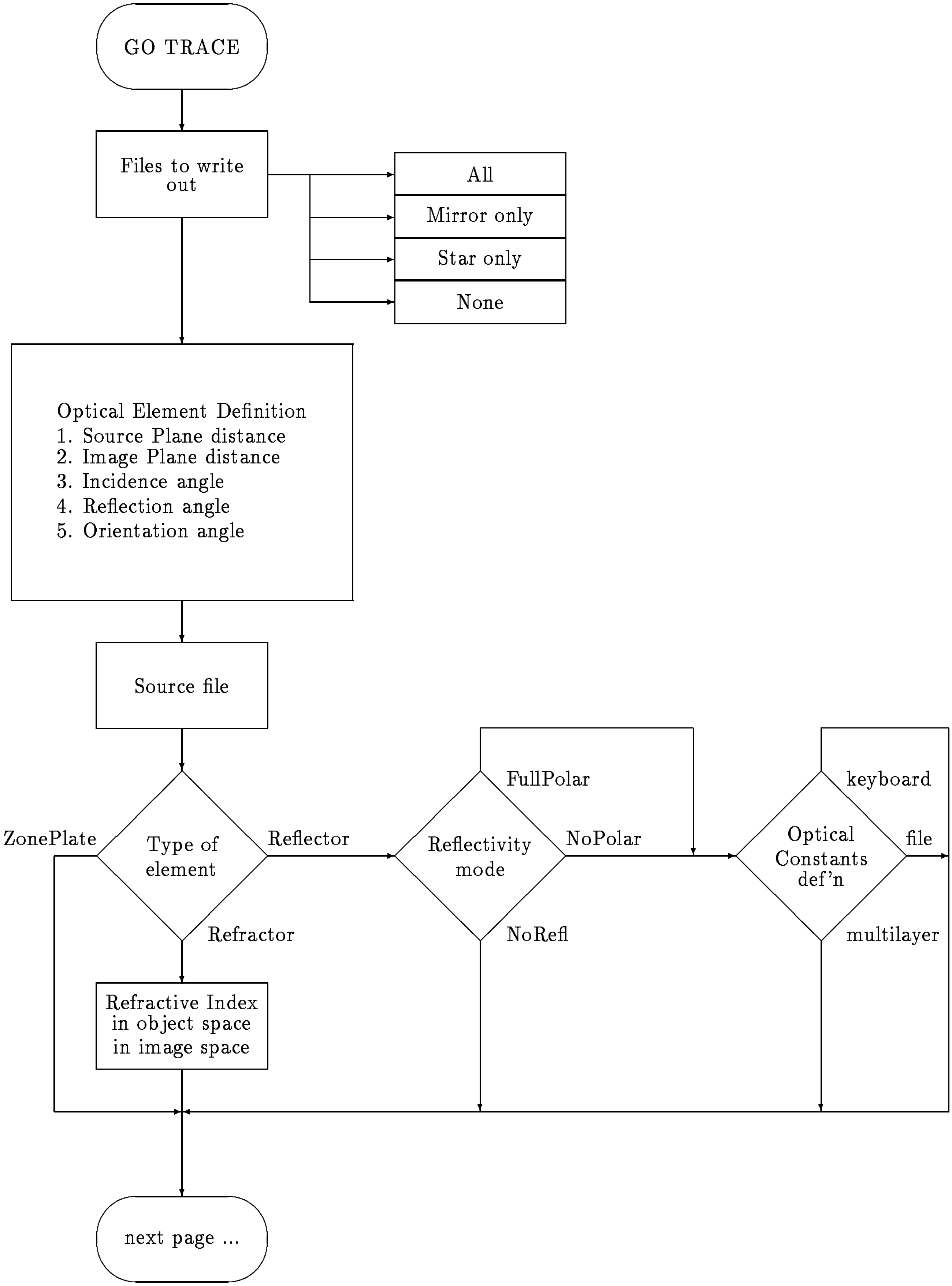


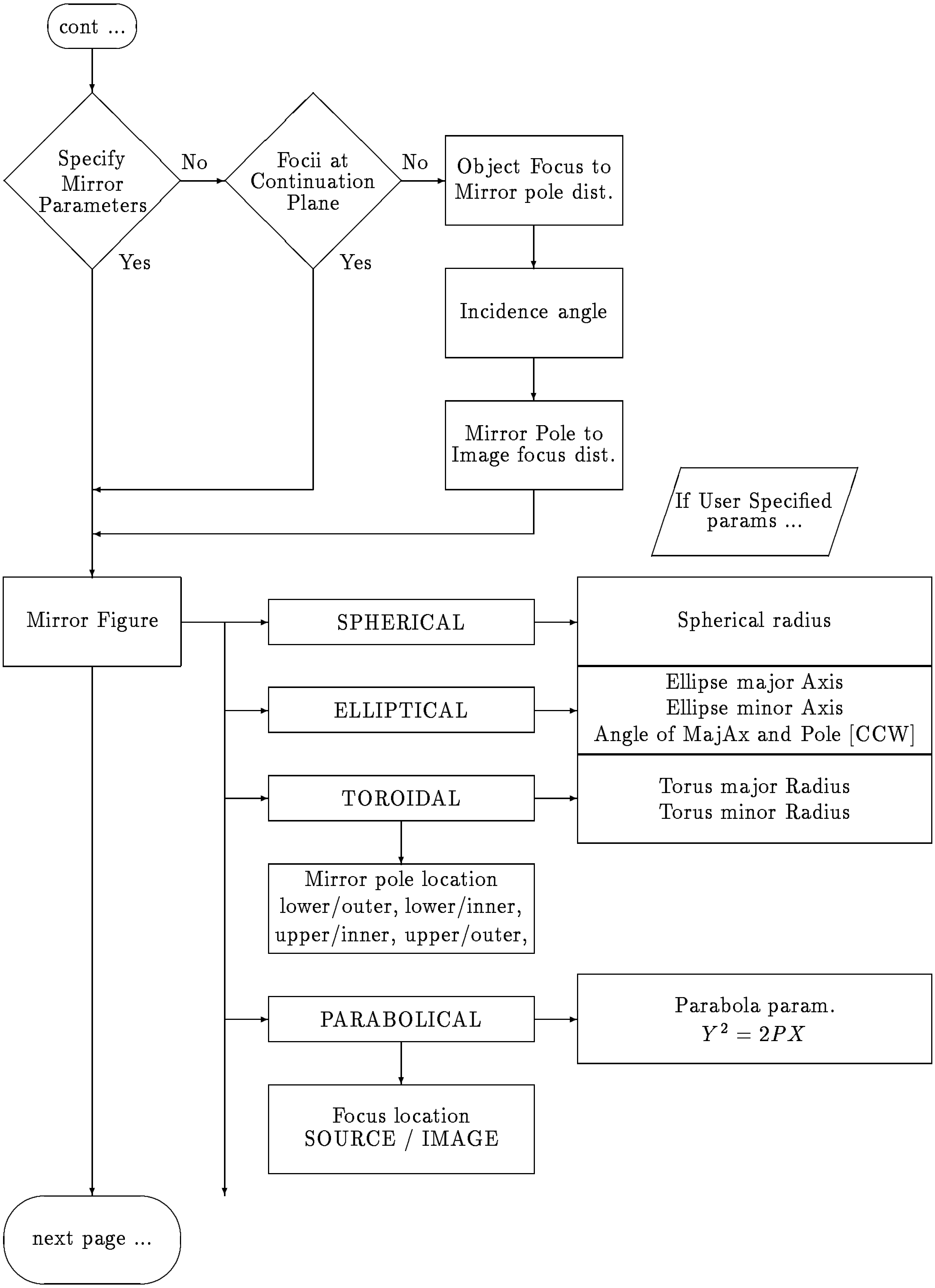
Figure A.1: Overview of program flow

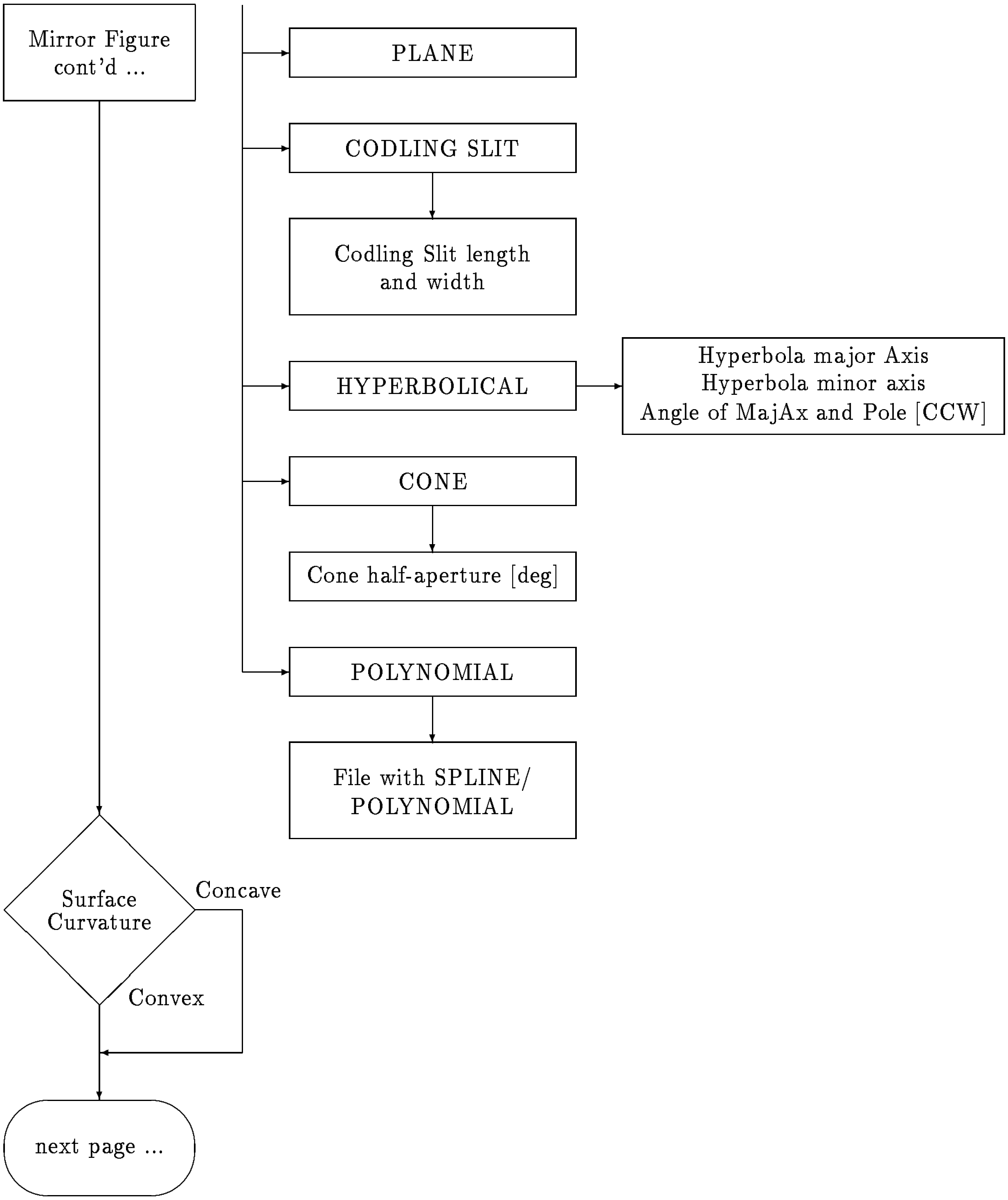

GO SOURCE
File to store the rays
Source Type
RAN/RAN
GRID/GRID
RAN/GRID
GRID/RAN
ELLI/RAN
ELLI/GRID
Number of random rays
Optimization of source
Yes
File to use?
No
Source type
Insertion
Insertion Device type
Wiggler
Undulator
BendMag/Generic
Polarization
Parallel
Perpendicular
Total
Next Page

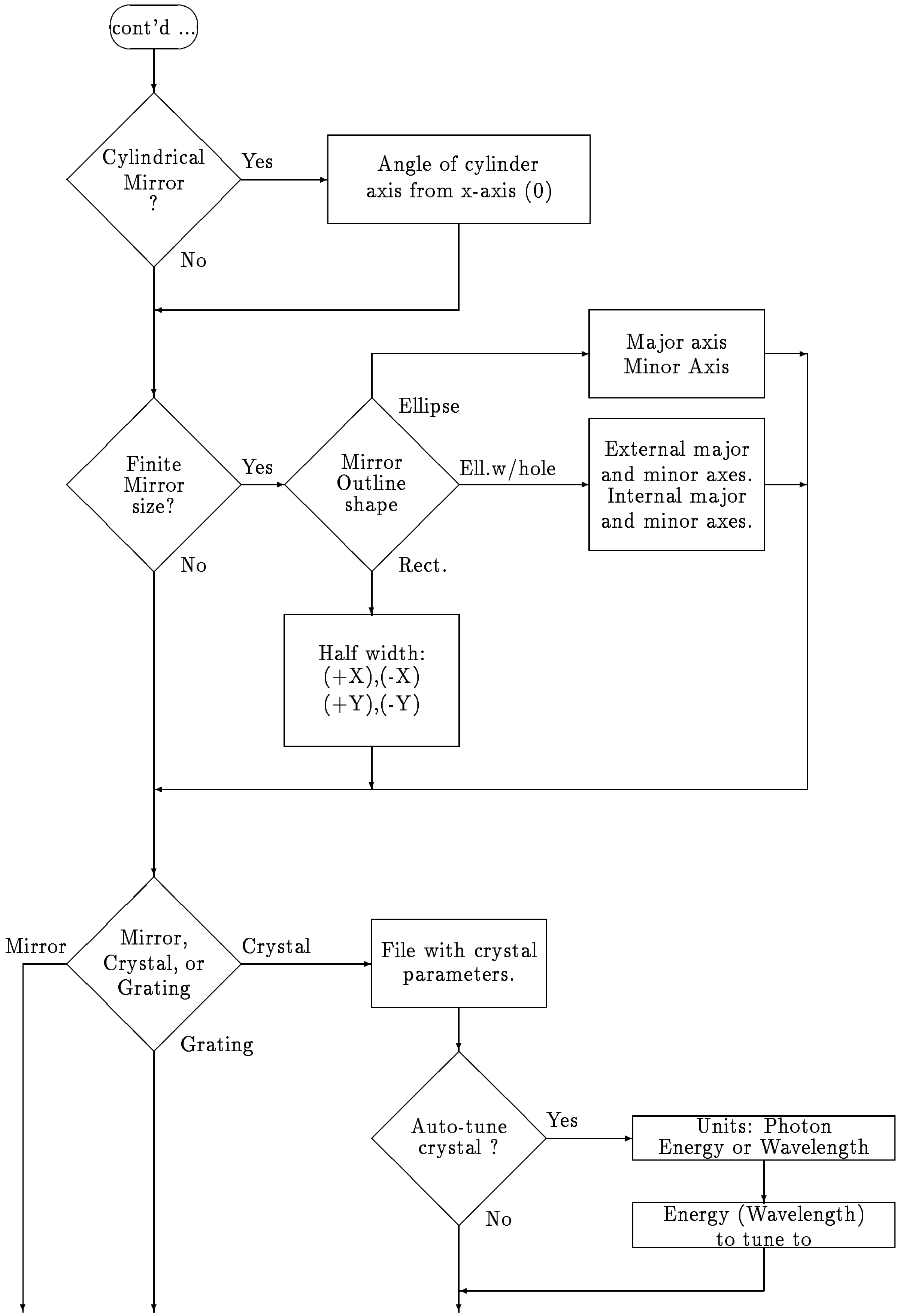

cont ...
Spatial Type
POINT
RECTANGLE
ELLIPSE
GAUSSIAN
Depth
OFF
UNIFORM
GAUSSIAN
SYNCHROTRON
Angle Distribution
FLAT
UNIFORM
GAUSSIAN
SYNCHROTRON
CONICAL
EXACT SYNCHROTRON
Photon Energy distribution
OFF
Single Line
Multiple Lines
Continuous
next page ...

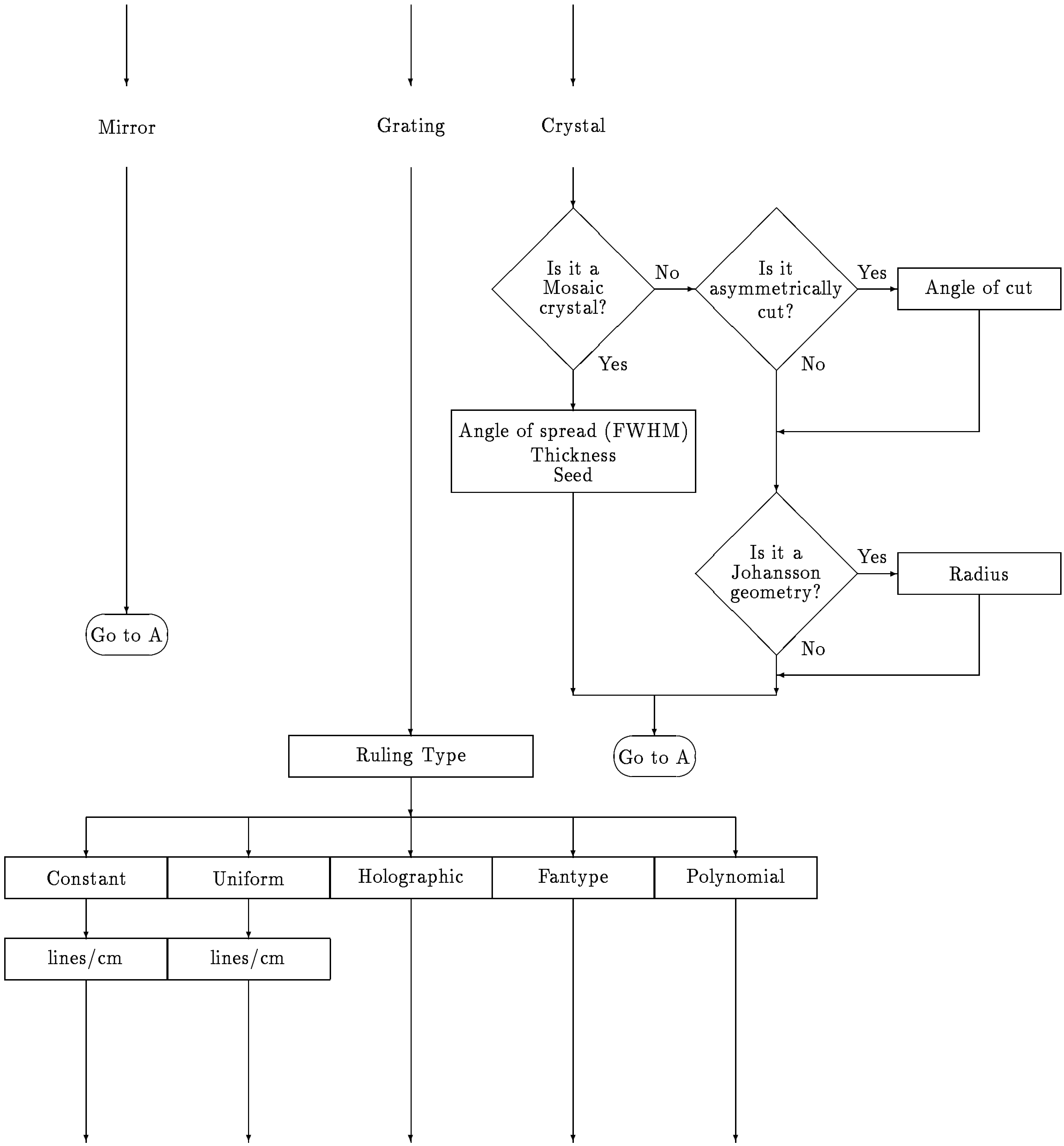

cont ...
Store
Optical
path
Yes
No
Polarization
Yes
Phase difference
Polarizarion degree
No
Coherence
No
Incoherent
Yes
Stop.

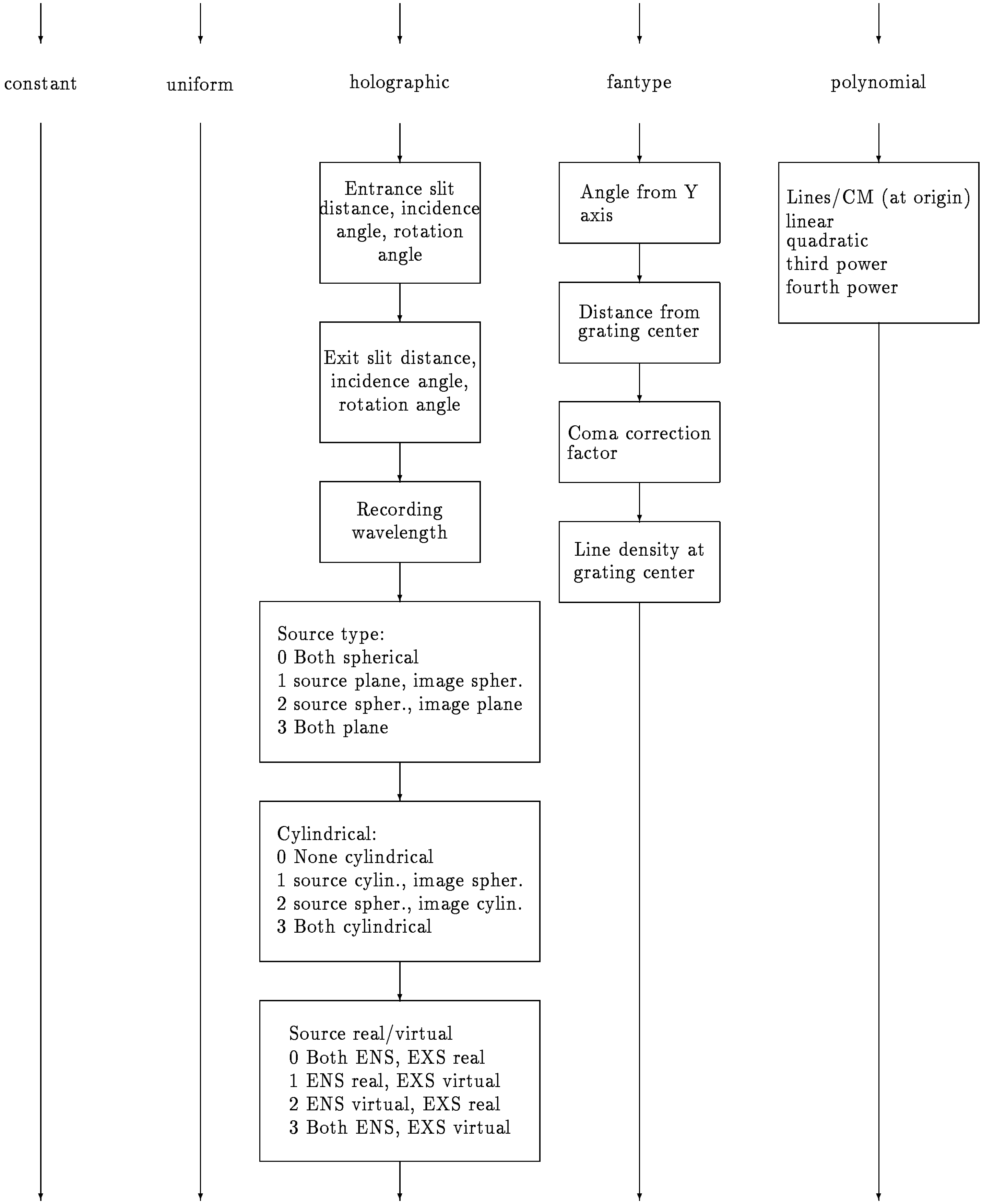

GO TRACE
Files to write out
All
Mirror only
Star only
None
Optical Element Definition
1. Source Plane distance
2. Image Plane distance
3. Incidence angle
4. Reflection angle
5. Orientation angle
Source file
ZonePlate
Type of element
Reflector
Refractor
Refractive Index
in object space
in image space
FullPolar
Reflectivity mode
NoPolar
NoRefl
keyboard
Optical Constants def'n
file
multilayer
next page ...

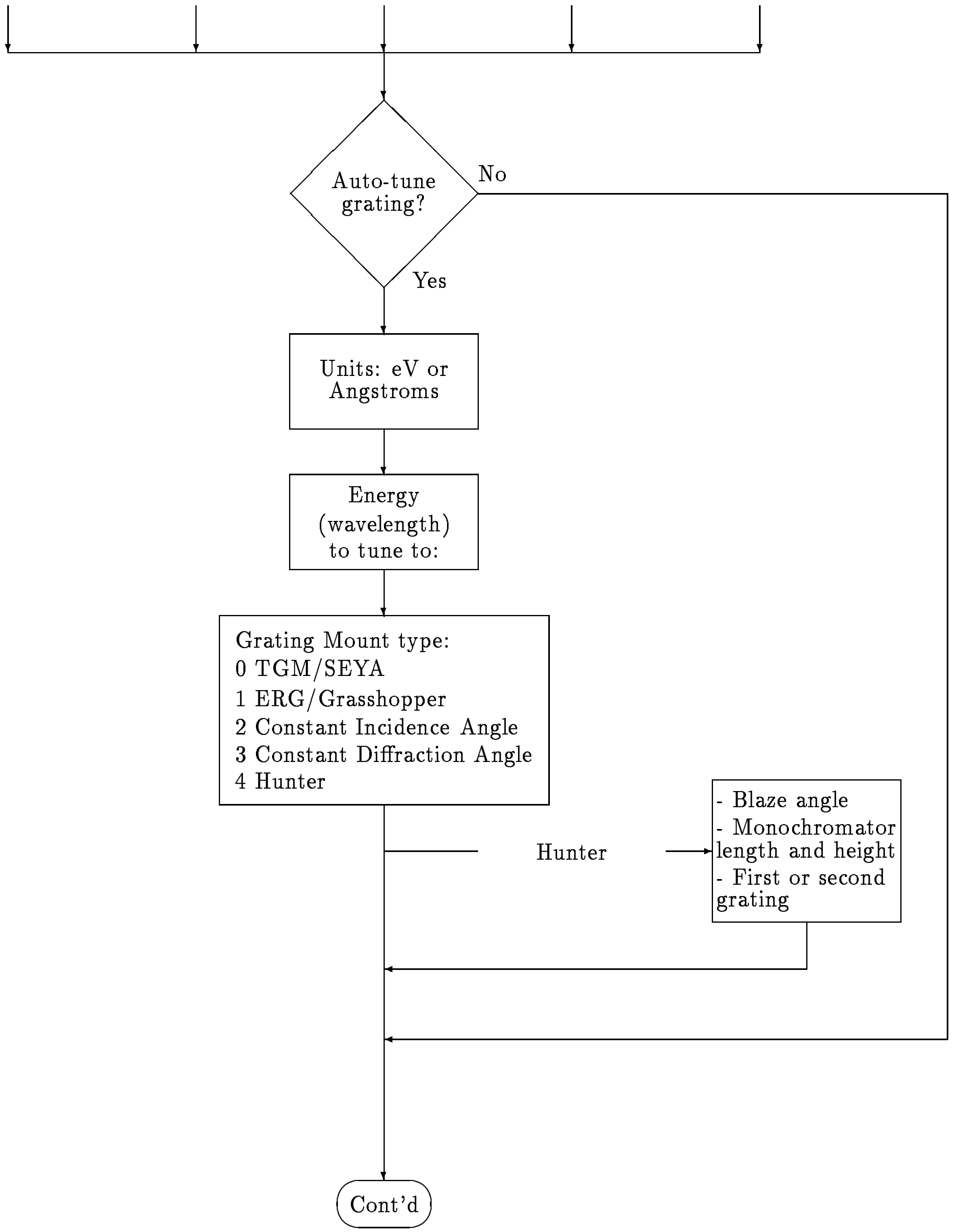

cont ...
Specify Mirror Parameters
No
Yes
Focii at Continuation Plane
No
Yes
Object Focus to Mirror pole dist.
Incidence angle
Mirror Pole to Image focus dist.
If User Specified params ...
Mirror Figure
SPHERICAL
Spherical radius
ELLIPTICAL
Ellipse major Axis
Ellipse minor Axis
Angle of MajAx and Pole [CCW]
TOROIDAL
Torus major Radius
Torus minor Radius
Mirror pole location lower/outer, lower/inner, upper/inner, upper/outer,
PARABOLICAL
Parabola param. $Y^2 = 2PX$
Focus location SOURCE / IMAGE
next page ...

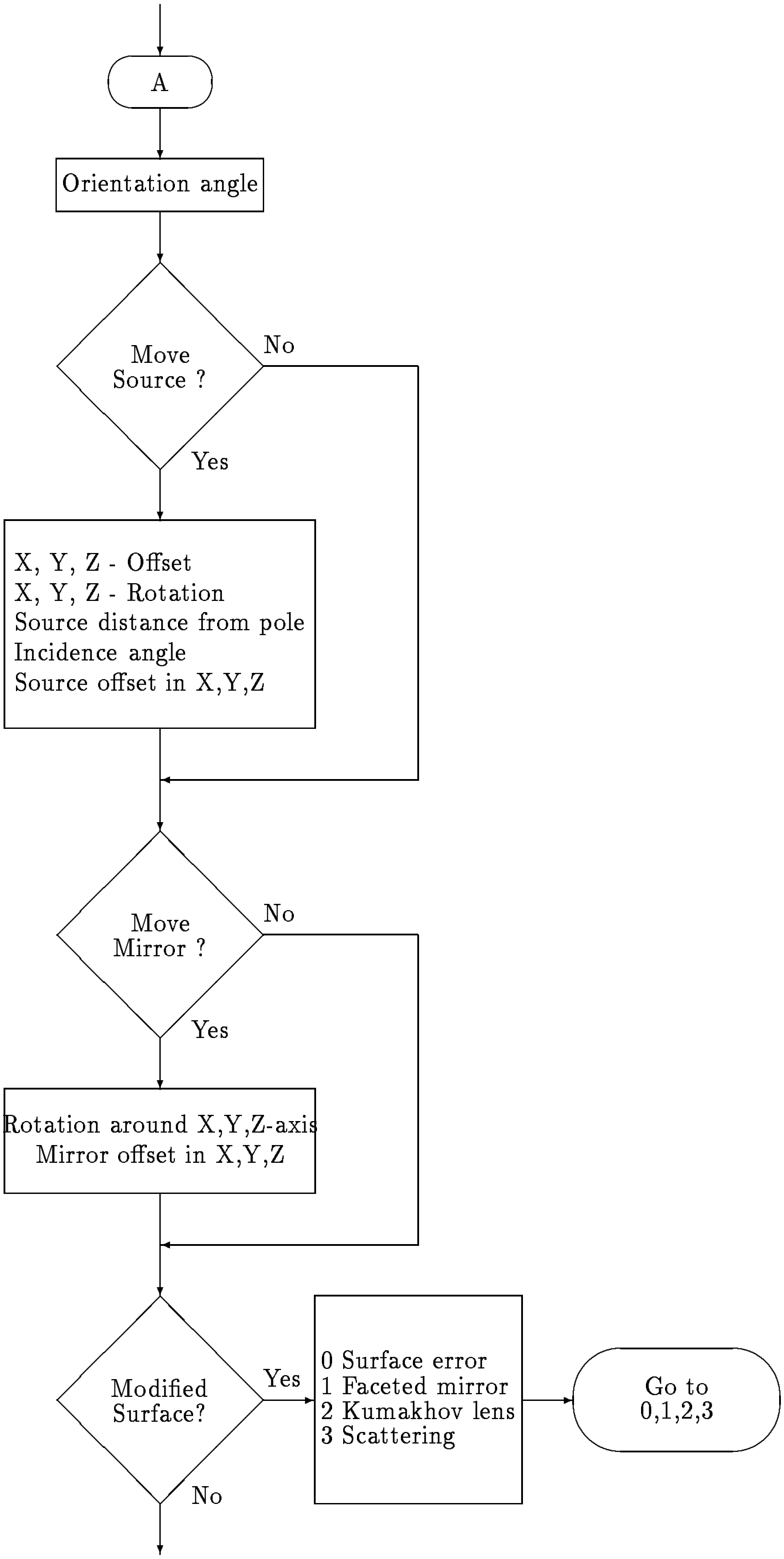

Mirror Figure cont'd ...
PLANE
CODLING SLIT
Codling Slit length and width
HYPERBOLICAL
Hyperbola major Axis
Hyperbola minor axis
Angle of MajAx and Pole [CCW]
CONE
Cone half-aperture [deg]
POLYNOMIAL
File with SPLINE/ POLYNOMIAL
Surface Curvature
Concave
Convex
next page ...

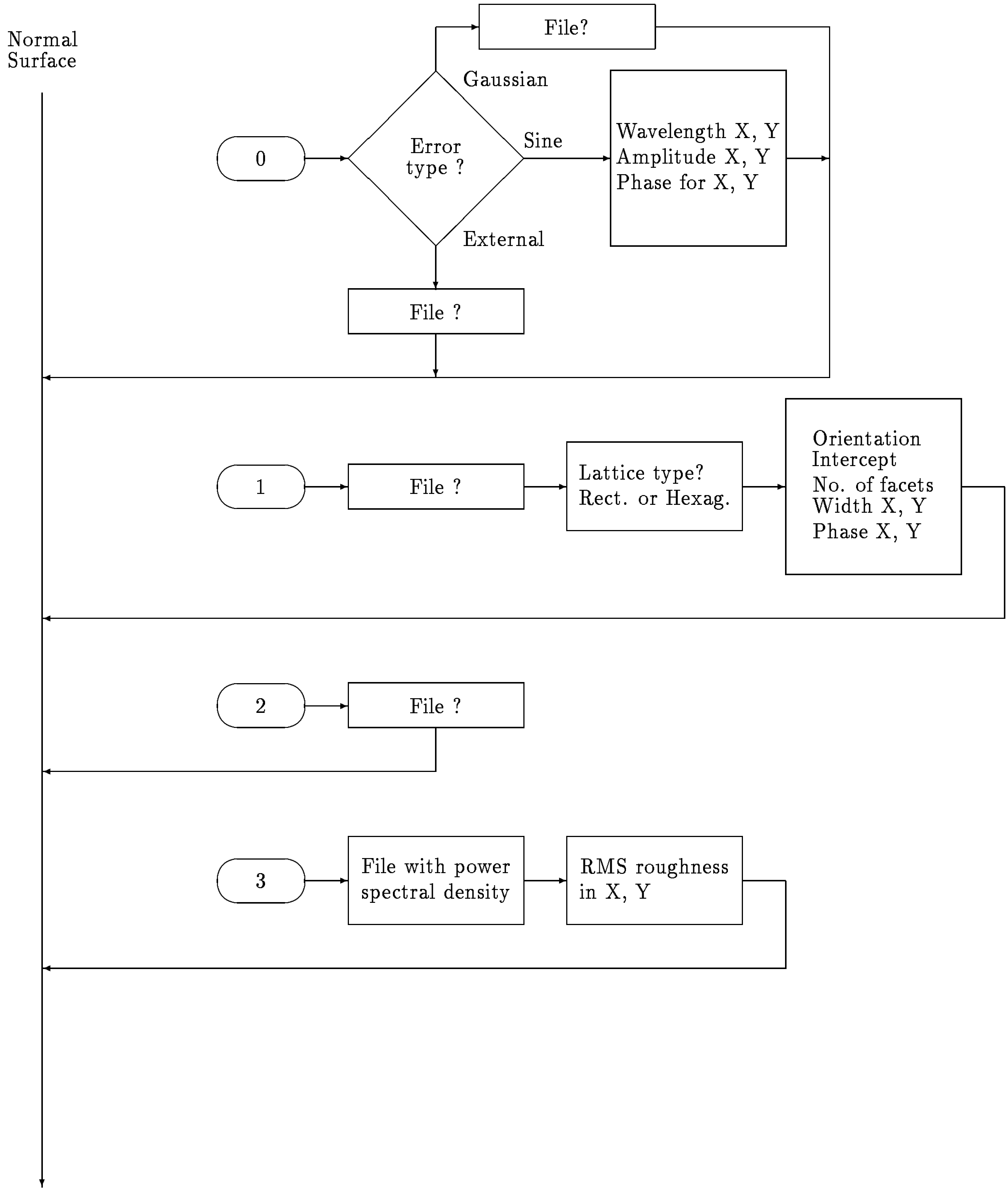

cont'd ...
Cylindrical Mirror ?
Yes
Angle of cylinder axis from x-axis (0)
No
Major axis Minor Axis
Ellipse
Finite Mirror size?
Yes
Mirror Outline shape
Ell.w/hole
External major and minor axes. Internal major and minor axes.
No
Rect.
Half width: (+X),(-X) (+Y),(-Y)
Mirror
Mirror, Crystal, or Grating
Crystal
File with crystal parameters.
Grating
Auto-tune crystal ?
Yes
Units: Photon Energy or Wavelength
No
Energy (Wavelength) to tune to

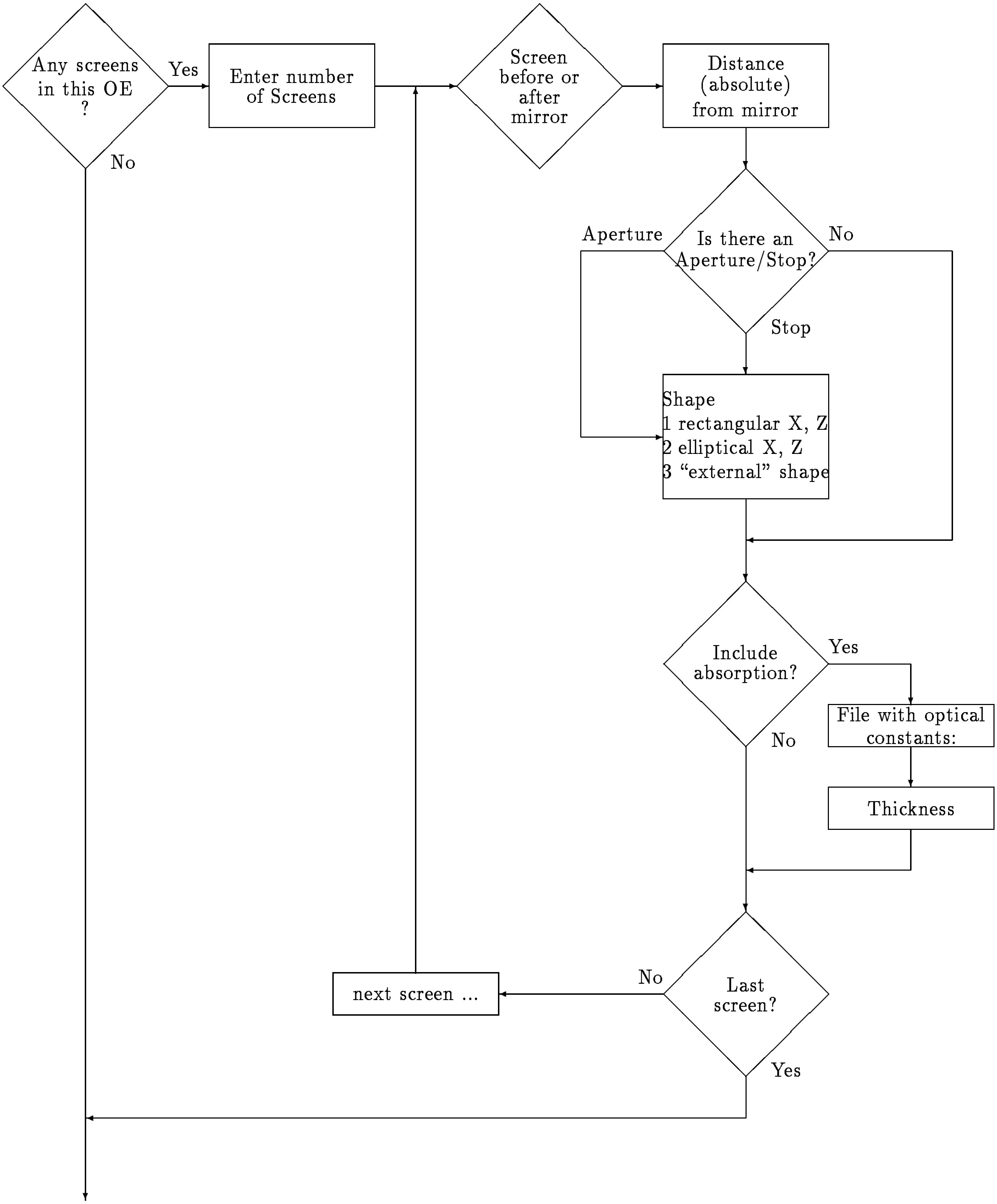

Mirror
Grating
Crystal
Is it a Mosaic crystal?
No
Yes
Is it asymmetrically cut?
Yes
No
Angle of cut
Angle of spread (FWHM)
Thickness
Seed
Is it a Johansson geometry?
Yes
No
Radius
Go to A
Go to A
Ruling Type
Constant
Uniform
Holographic
Fantype
Polynomial
lines/cm
lines/cm

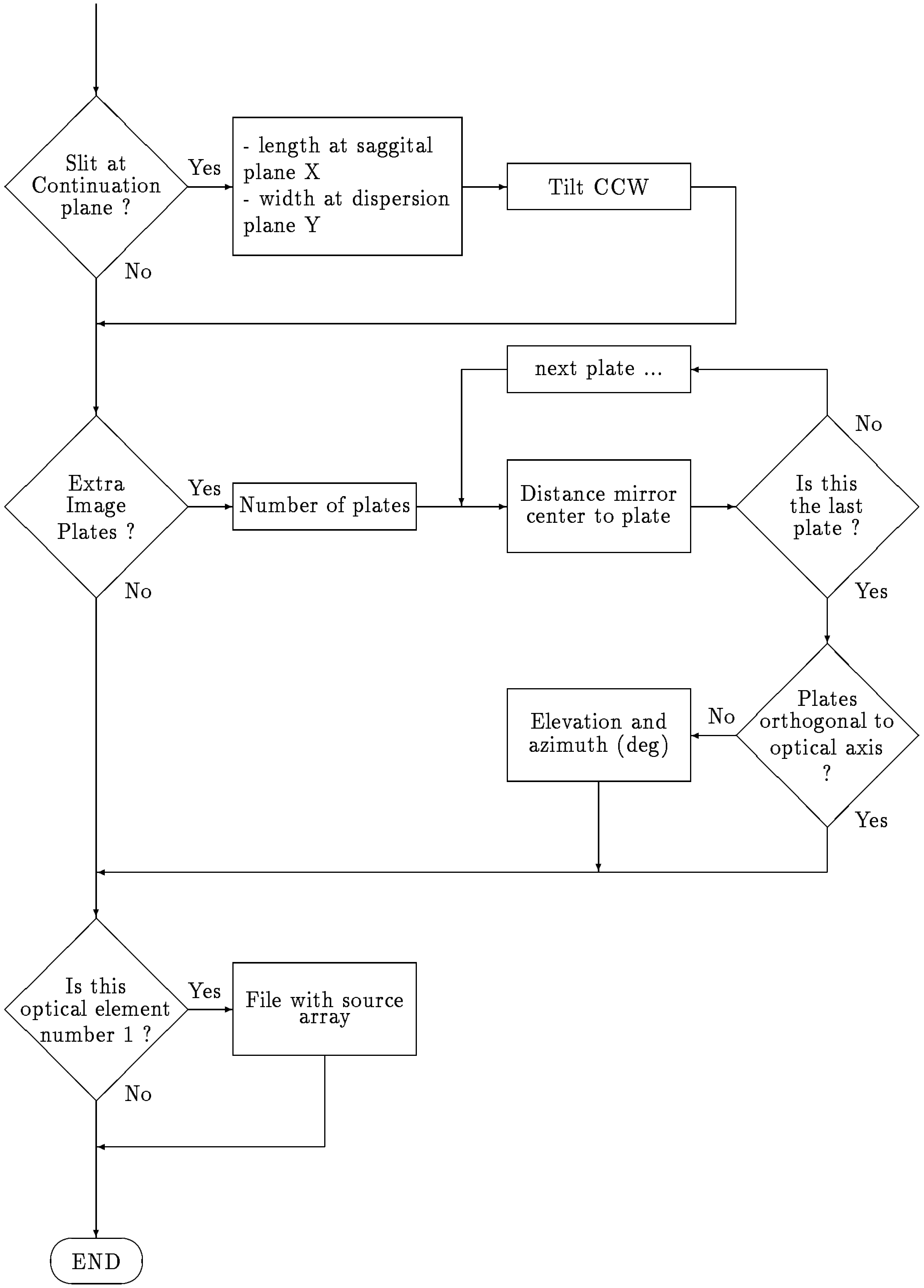

constant
uniform
holographic
fantype
polynomial
Entrance slit distance, incidence angle, rotation angle
Exit slit distance, incidence angle, rotation angle
Recording wavelength
Source type:
0 Both spherical
1 source plane, image spher.
2 source spher., image plane
3 Both plane
Cylindrical:
0 None cylindrical
1 source cylin., image spher.
2 source spher., image cylin.
3 Both cylindrical
Source real/virtual
0 Both ENS, EXS real
1 ENS real, EXS virtual
2 ENS virtual, EXS real
3 Both ENS, EXS virtual
Angle from Y axis
Distance from grating center
Coma correction factor
Line density at grating center
Lines/CM (at origin)
linear
quadratic
third power
fourth power


Auto-tune grating?
No
Yes
Units: eV or Angstroms
Energy (wavelength) to tune to:
Grating Mount type:
0 TGM/SEYA
1 ERG/Grasshopper
2 Constant Incidence Angle
3 Constant Diffraction Angle
4 Hunter
Hunter
- Blaze angle
- Monochromator length and height
- First or second grating
Cont'd


A
Orientation angle
Move Source ?
No
Yes
X, Y, Z - Offset
X, Y, Z - Rotation
Source distance from pole
Incidence angle
Source offset in X,Y,Z
Move Mirror ?
No
Yes
Rotation around X,Y,Z-axis
Mirror offset in X,Y,Z
Modified Surface?
Yes
No
0 Surface error
1 Faceted mirror
2 Kumakhov lens
3 Scattering
Go to 0,1,2,3


Normal
Surface
File?
Gaussian
0
Error
type ?
Sine
Wavelength X, Y
Amplitude X, Y
Phase for X, Y
External
File ?
1
File ?
Lattice type?
Rect. or Hexag.
Orientation
Intercept
No. of facets
Width X, Y
Phase X, Y
2
File ?
3
File with power
spectral density
RMS roughness
in X, Y


Any screens in this OE ?
Yes
No
Enter number of Screens
Screen before or after mirror
Distance (absolute) from mirror
Is there an Aperture/Stop?
Aperture
No
Stop
Shape
1 rectangular X, Z
2 elliptical X, Z
3 "external" shape
Include absorption?
Yes
No
File with optical constants:
Thickness
Last screen?
No
Yes
next screen ...


Slit at Continuation plane ?
Yes
- length at saggital plane X
- width at dispersion plane Y
Tilt CCW
No
next plate ...
Extra Image Plates ?
Yes
Number of plates
Distance mirror center to plate
Is this the last plate ?
No
Yes
No
Elevation and azimuth (deg)
No
Plates orthogonal to optical axis ?
Yes
Is this optical element number 1 ?
Yes
File with source array
No
END

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, SYSTEMFILE.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 used to relay with or without monochromatization the beam from source to sample.
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 generate 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.

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 B.O.F. 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 autocorrelation 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:

$$R_\perp = \frac{\sin^2(\theta_i - \theta_t)}{\sin^2(\theta_i + \theta_t)}, \qquad R_{||} = \frac{\tan^2(\theta_i - \theta_t)}{\tan^2(\theta_i + \theta_t)}$$

where θ_i and θ_t are the angles of incidence and transmission respectively, and $R_\perp$ and $R_{||}$ 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.

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.

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.

HELP	Evokes the help facility at the SHADOW command level and provides some on-line description of the local commands and their purposes.
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 in VMS, "." for Unix; 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 "space" which is occupied by the angles that the rays make with respect to the Y axis. The angles are expressed by their components in the X and Z directions, thus for any ray: $x'^2 + y'^2 + z'^2 = 1$. The coordinates in momentum space for a ray are in columns 4, 5, and 6 in any B.O.F.

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.

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'.
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 12,13, or 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 random errors left on a surface by machining or coating. Included in SHADOW using the Power Spectral Density function mapped onto the surface of the element. See Demo for more details.

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 SYSTEMFILE.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 or other random processes.

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. Same as *Profile.*

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.

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.

Zero order The beam reflected by a grating without scattering, whereby it acts like a simple mirror.