

SHADOW

PRIMER 2.0

CXrL

August 25, 1998

Copyright ©1990 Center for X-ray Lithography

Permission to use and copy this software and its documentation for internal use of licensed user unless otherwise specified in written licensing agreement and without fee is hereby granted, provided that the above copyright notice appear in all copies and that both the copyright notice and this permission notice appear in supporting documentation, and that the name of the University of Wisconsin and Center for X-ray Lithography not be used in advertising or publicity pertaining to distribution of the software/documentation without specific, written prior permission. The University of Wisconsin makes no representations about the suitability of this software for any purpose. It is provided "as is" without express or implied warranty.

THE UNIVERSITY OF WISCONSIN DISCLAIMS ALL WARRANTIES WITH REGARD TO THIS SOFTWARE, INCLUDING IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS. IN NO EVENT SHALL THE UNIVERSITY OF WISCONSIN BE LIABLE FOR ANY SPECIAL, INDIRECT OR CONSEQUENTIAL DAMAGES OR ANY DAMAGES WHATSOEVER RESULTING FROM LOSS OF USE, DATA OR PROFITS, WHETHER IN AN ACTION OF CONTRACT, NEGLIGENCE OR OTHER TORTIOUS ACTION, ARISING OUT OF OR IN CONNECTION WITH THE USE OR PERFORMANCE OF THIS SOFTWARE.

Authors: Franco Cerrina, Chris Welnak, G.J. Chen, and M. Sanchez del Rio
Center for X-ray Lithography, University of Wisconsin

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 Capodiecici 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

1	INTRODUCTION	1
1.1	SHADOW structure	1
1.1.1	Data files:	3
1.1.2	Parameter Files:	3
1.1.3	Analysis Files:	3
1.2	Definitions and Nomenclature	3
2	OVERVIEW	7
2.1	HOW TO GET STARTED	7
2.2	SHADOW'S COMMAND LEVEL	9
2.2.1	HELP	9
2.2.2	SOURCE	9
2.2.3	TRACE	9
2.2.4	MENU	9
2.2.5	INIT	10
2.2.6	EXIT	10
2.3	INPUT MODES	10
2.4	PROMPT Mode Run	14
2.5	MENU Mode Run	30
2.6	BATCH mode run	42
3	OUTPUT FILES	45
4	PRELIMINARY PROGRAMS	49
4.1	BRAGG	49
4.2	PREREFL	50
4.3	PRESURFACE	50
4.4	MAKE_ID	50
5	ANALYSIS PROGRAMS	51
5.1	Basic	51
5.2	Advanced	53

6 Further Examples	55
6.1 Two Mirror Optical System	55
6.2 Diffraction Grating in Rowland Circle Mount	74
6.3 Power Density	90
6.4 Two Crystals I	109
6.5 Two Crystals II	136
 A Program Flow	 155
 B Glossary	 171

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

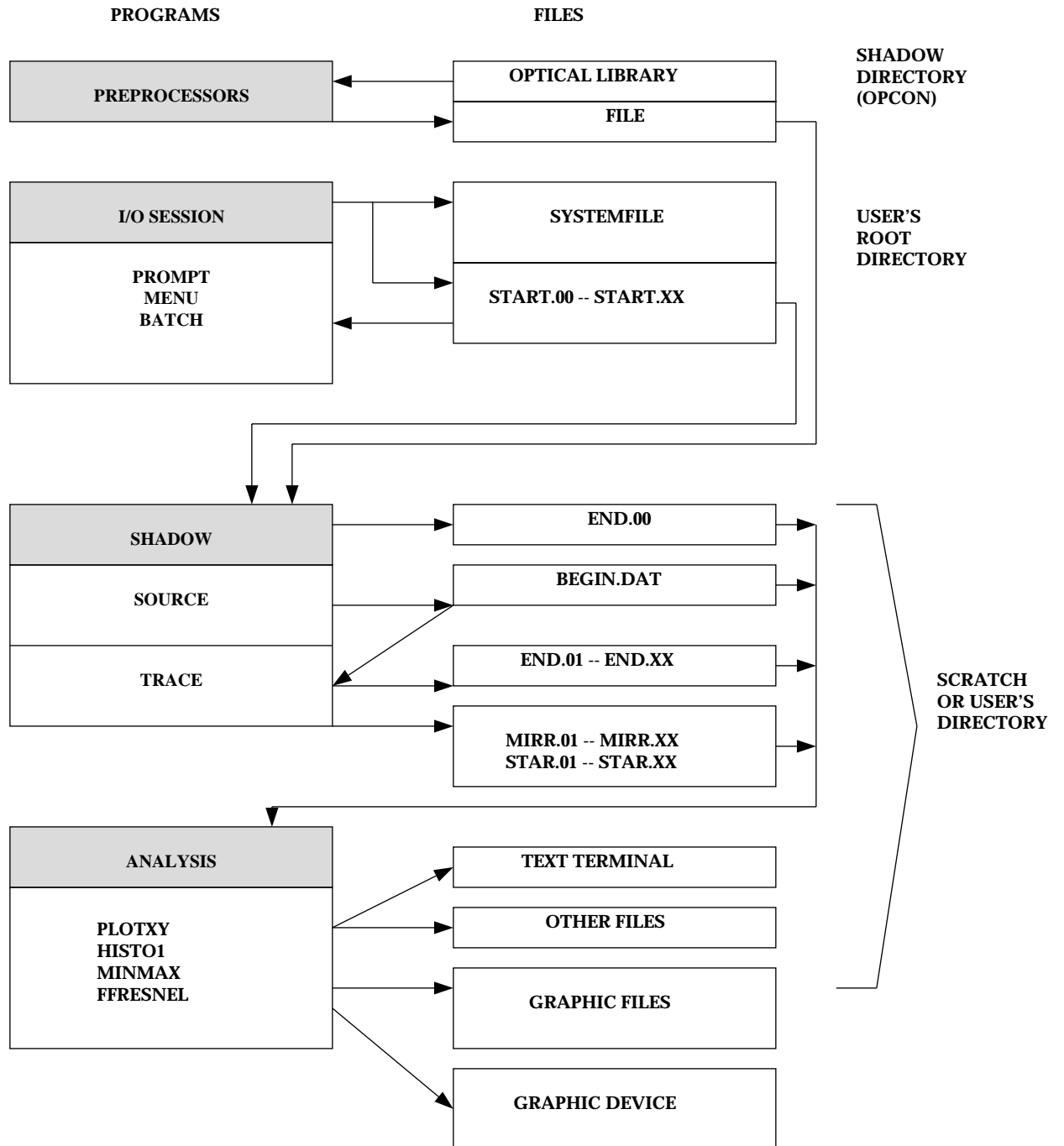


Figure 1.1: SHADOW structure

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 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',

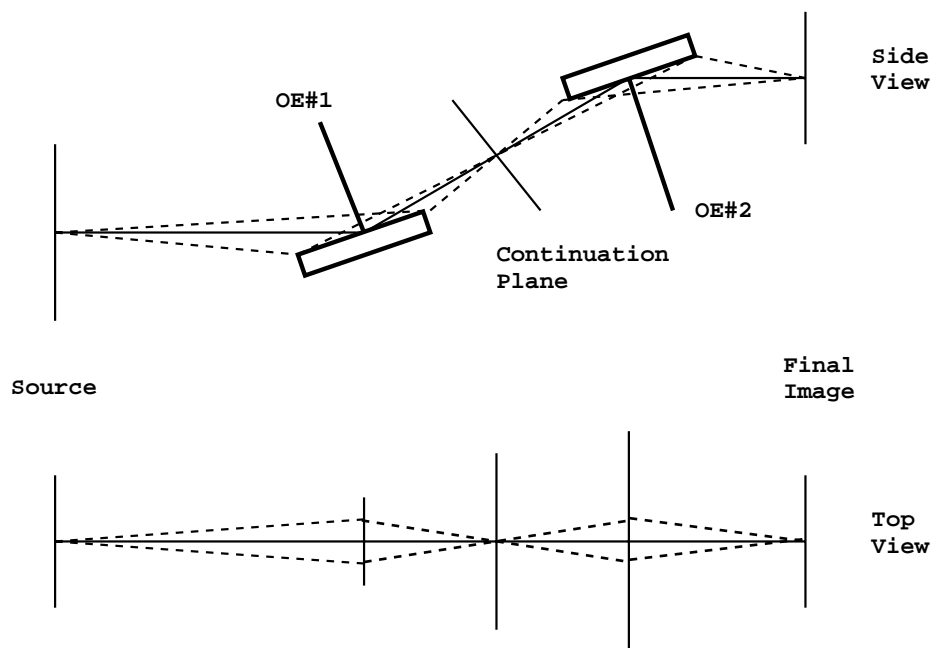


Figure 1.2: Two-mirrors Optical System

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 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.

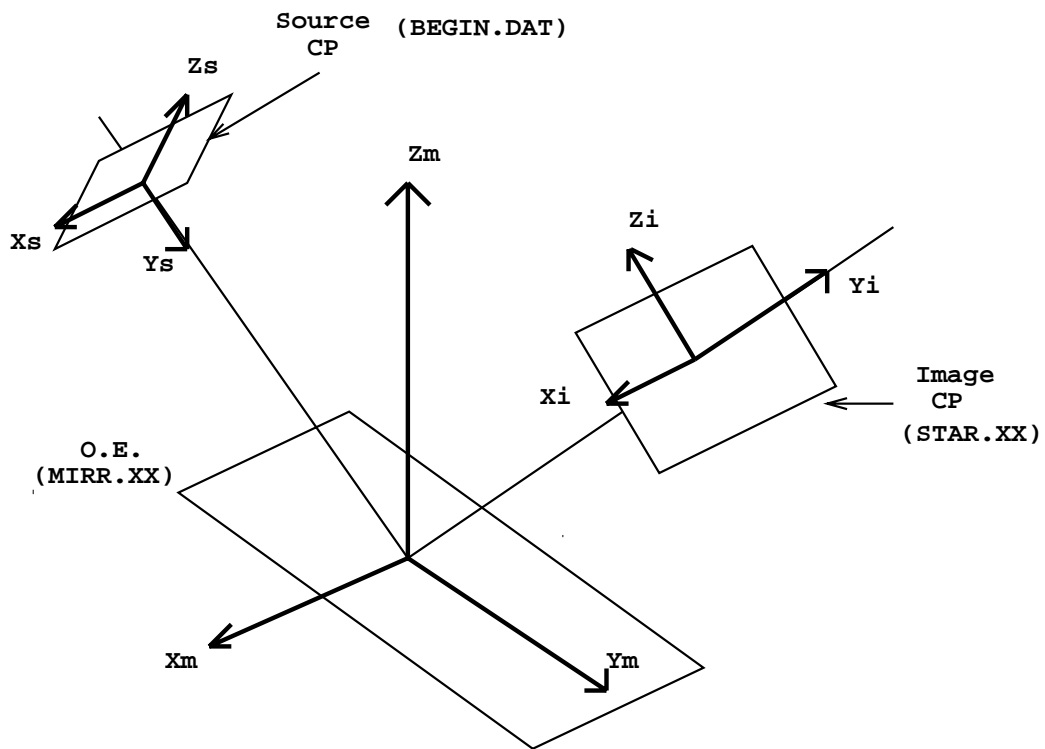


Figure 1.3: Optical Element Geometry and Continuation Planes

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.

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 (or TT:)	TT means the user's terminal in DEC's language.
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

\$ `DIR/SIZE/DATE/PROT *.DAT`

UNIX

% `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

\$ `@D0:[SHADOW]SETUP.COM`

UNIX

% `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

\$ `CREATE/DIRECTORY [.test]`

\$ `SET DEF [.test]`

UNIX

% `mkdir 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. An exception is the startup command GO.

¹For 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.

2.2 SHADOW'S COMMAND LEVEL

To access SHADOW programs from the system prompt level, enter 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	← 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.

↑, ↓	are used to move between the menu lines
<ctrl>P, <ctrl>N	UNIX command to move between lines
→, >	are used to enter a submenu or to move between OE's.
←, <	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.

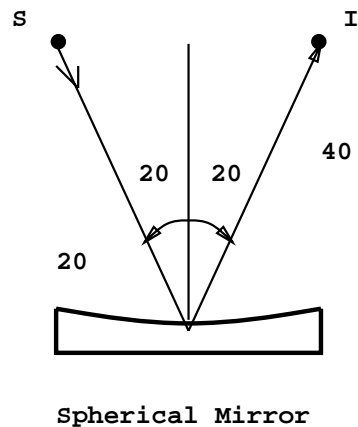


Figure 2.1: Spherical Mirror Geometry

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° 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

```

      ::::: :::  ::      ::: :::::      ::::  :::  ::  ::
      ::::: :::  ::      ::: :::::      :::::  :::  ::  ::
      :::      :::  ::      ::: : :::  ::: :::  :::  :::  ::
      :::      :::  ::      ::: :::  :::  :::  :::  :::  ::
      :::::  :::::      :::  :::  :::  :::  :::  :::  :::  ::
      :::::  :::::      :::  :::  :::  :::  :::  :::  :::  ::
      :::  :::  :::  :::  :::  :::  :::  :::  :::  :::  ::
      :::  :::  :::  :::  :::  :::  :::  :::  :::  :::  ::
      :::::  :::  :::  :::  :::  :::  :::  :::  :::  :::  ::
      :::  :::  :::  :::  :::  :::  :::  :::  :::  :::  ::
      :::  :::  :::  :::  :::  :::  :::  :::  :::  :::  ::
      :::  :::  :::  :::  :::  :::  :::  :::  :::  :::  ::
      :::  :::  :::  :::  :::  :::  :::  :::  :::  :::  ::
      :::  :::  :::  :::  :::  :::  :::  :::  :::  :::  ::
      :::  :::  :::  :::  :::  :::  :::  :::  :::  :::  ::
      :::  :::  :::  :::  :::  :::  :::  :::  :::  :::  ::

```

VMS/Ultrix/Sun/AIX VERSION 2.0

01 May 1993

Hit <RETURN> when ready:

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

UNIX

\$ %

/* This procedure generates a SOURCE for SHADOW.

```

Shadow:: 

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 ] ? : 

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 ? 

/* 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] ?
 How many rays [1 - 5 000] ?
 Seed [odd, 1000 - 1 000 000] ?
 Do you want to optimize the source ?

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

Then ?

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] ?

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] ?

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] ?

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

. [(-)x, rads] ?

```

Vertical          [ (+)z, rads ] ? 
.                  [ (-)z, rads ] ? 
Do you want a Photon energy [ Y/N ] ? 
Do you want to store the optical paths (OPD) [Y/N] ? 
Do you want to generate the A vectors (electric field) [Y/N] ? 

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 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

```
$ 
```

```
Directory D0:[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

```
% 
```

```
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

\$

```
/* 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 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 ?

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

```
/* self-explanatory
```

```
Defining Optical Element: 
```

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

```
/* 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 ? 
```

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 ? 
```

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 ? . //Degrees
```

```
Source Distance ? 
```

```
Reflection Angle? . //Degrees
```

```
Image Distance ? 
```

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

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

A: Is this a Kumakhov system? ☐

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

A: Is this mirror faceted [Y/N] ? ☐

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] ? ☐

Do you want to specify the mirror parameters ? ☐

Is the mirror Cylindrical ? ☐

Is this optical element a Fresnel Zone Plate ? ☐

Are we dealing with a Grating ? ☐

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

Is the mirror convex [Y/N] ? ☐

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] ? ☐

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] ?

Mirror Dimensions finite [Y/N] ?

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 $1/p + 1/q = 2/(R \cdot \cos(\theta))$ given p, q and θ . This will NOT affect in any way the placement of the mirror in the optical element.

Foci placed at continuation planes [Y/N] ?

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] ?

----- 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] ?

Distorted surface [Y/N] ?

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

Any screens in this OE [Y/N] ?

Slit at continuation plane [Y/N] ?

Extra Image plates [Y/N] ?
 File containing the source array ?

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 ?

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]

Shadow::

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

\$

\$

\$

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

```
% 
-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

```
$
$ 
PLOT> Input file? 
PLOT> Options --- Enter
PLOT> 0      for excluding the losses
PLOT> 1      for including only the losses
PLOT> 2      for including all the rays.
```

PLOT> Then ?

PLOT> Comment for plot [80 char] ?

UNIX

```
% 
```

```
PLOT> File read OK. Full specifications:
      D0:[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 ? 
PLOT>   for vertical axis   ? 
```

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

```
PLOT> Then ? 
```

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

```
PLOT> Then ? 
```

```
PLOT> Hairline at [ 0,0 ] ? 
```

```
PLOT> Overlay a mirror/slit ? 
```

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

```
PLOT> ? 
```

```
PLOT> Number of bins for X axis [default = 25] : 
```

```
PLOT> Number of bins for Y axis [default = 25] : 
```

VMS

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

```
PLOT> Do you want to save the TD command file ? 
```

UNIX

Display type:

[0] Xwindow

[1] Tektronix

[2] Postscript file

Terminal type:

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.

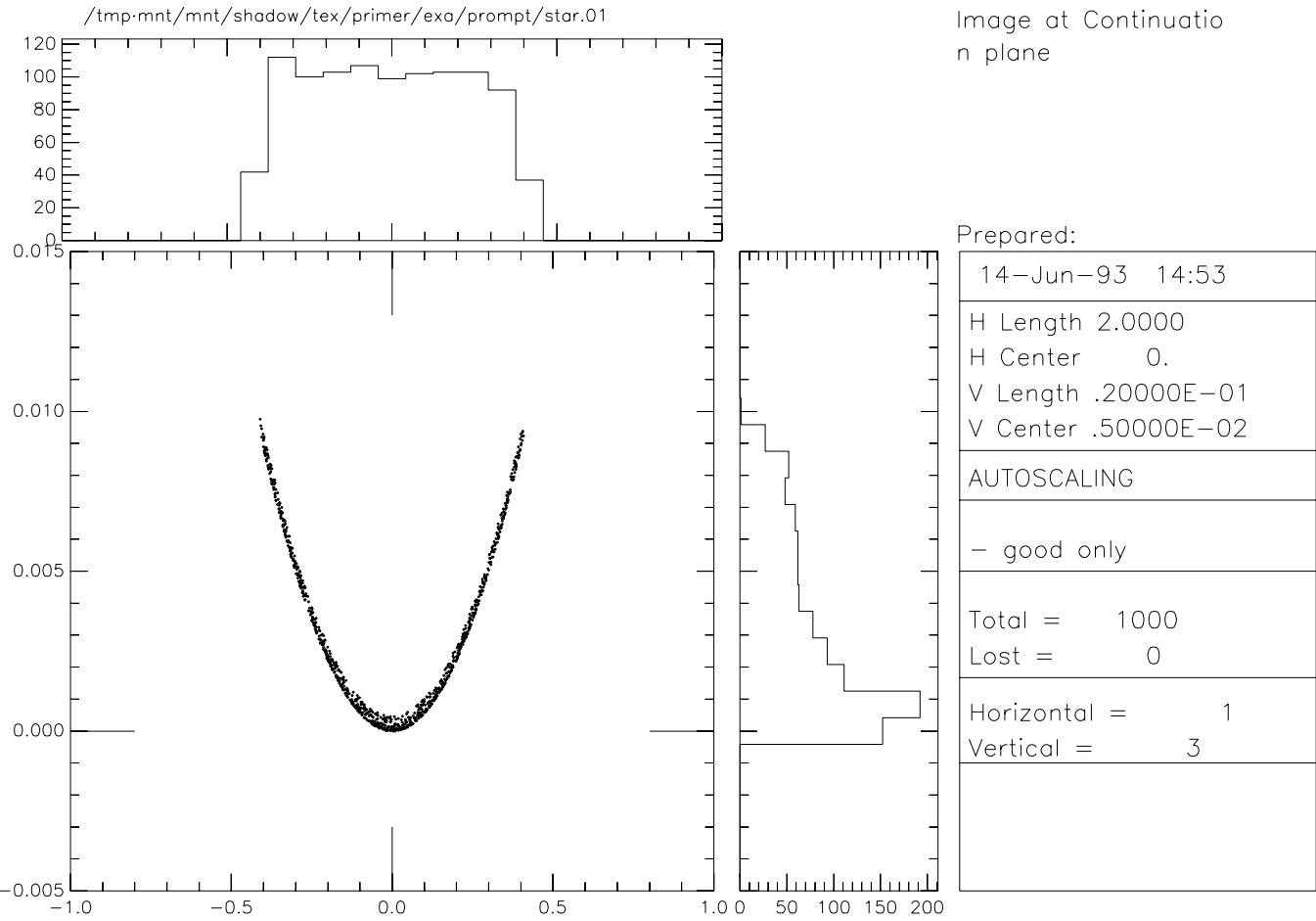
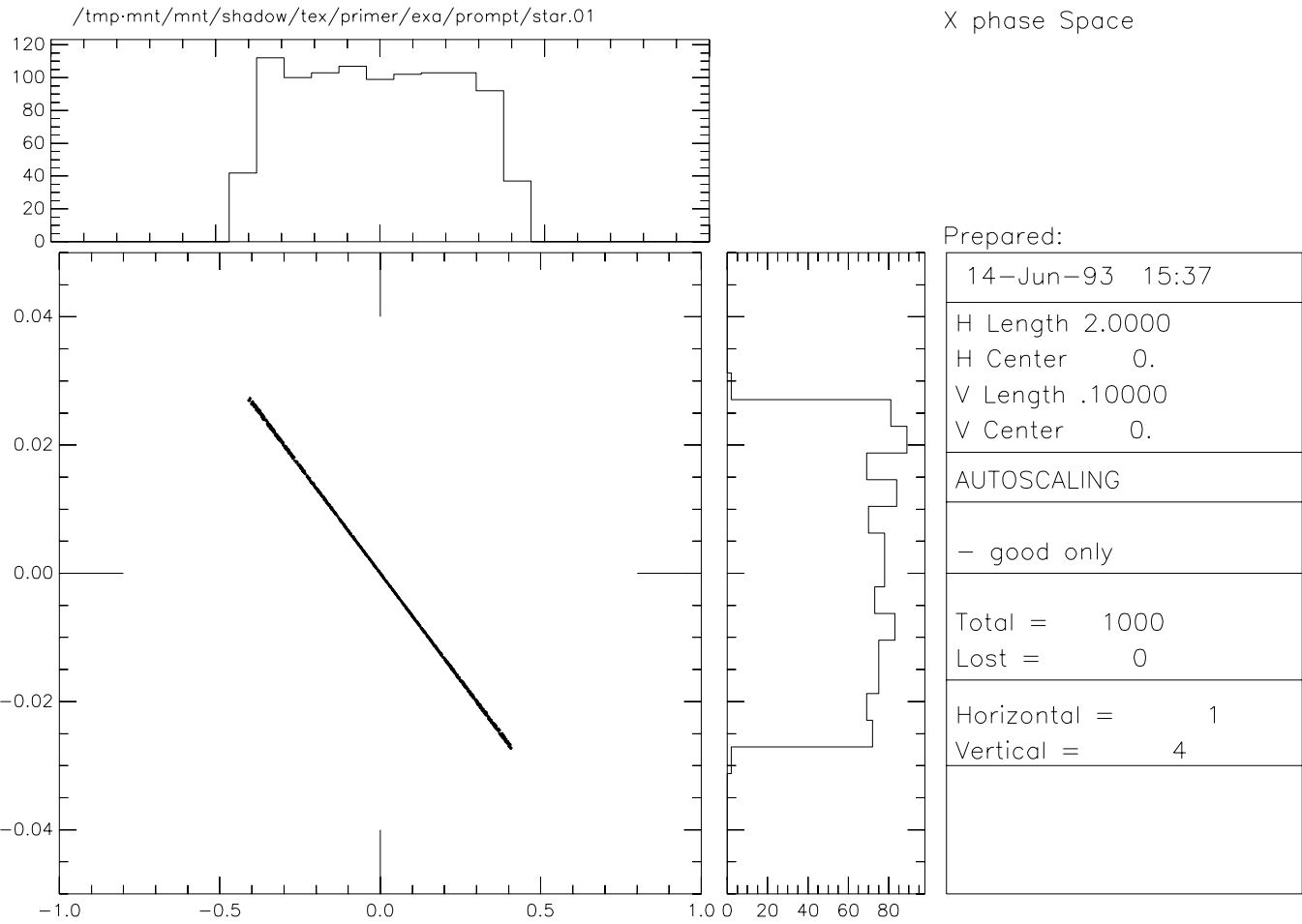


Figure 2.2: Image at continuation plane



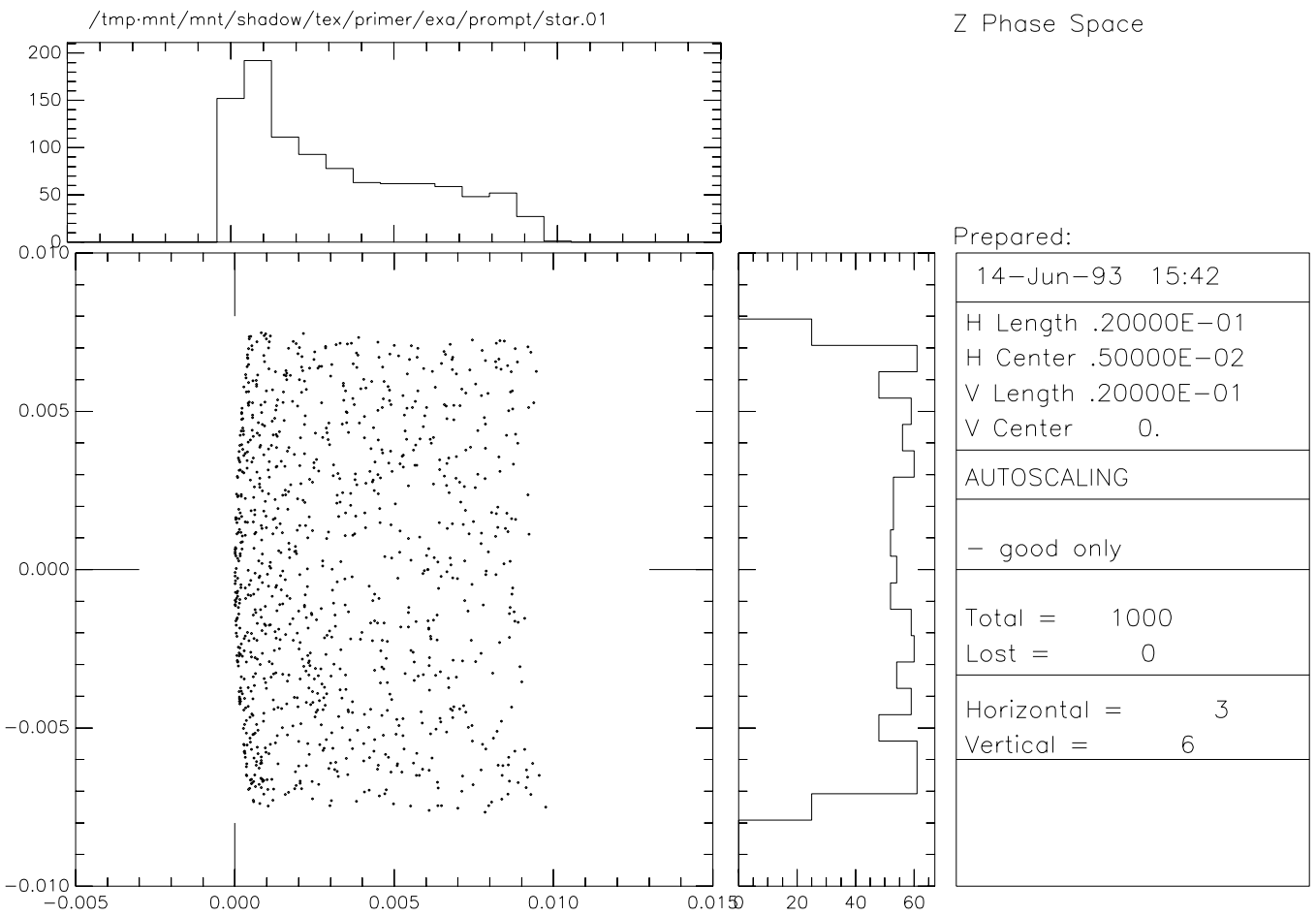


Figure 2.4: Z-phase space

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]	0.00000000000000E+00	
[(-)X]	0.00000000000000E+00	
Vertical divergence [(+)Z]	0.00000000000000E+00	
[(-)Z]	0.00000000000000E+00	
Cone internal half-aperture	n/a	0.00000000000000E+00
external	n/a	0.00000000000000E+00
Vertical Sigma [Z]	n/a	0.00000000000000E+00
Horizontal [X]	n/a	0.00000000000000E+00

```

/* Let's bring the cursor to the line
.      Horizontal divergence [(+)X]          0.00000000000000E+00  █
/* and then let's enter 0.05, without hitting <ret> yet.
/* The screen will show:
.      Horizontal divergence [(+)X]          0.00000000000000E+00  0.05
/* and, when we hit <ret> or any of the arrows, the field will be updated to
.      Horizontal divergence [(+)X]          0.50000000000000E-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]    0.50000000000000E-01
                             [(-)X]    0.50000000000000E-01
Vertical divergence  [(+)Z]    0.10000000000000E-01
                             [(-)Z]    0.10000000000000E-01
Cone internal half-aperture  n/a  0.00000000000000E+00
      external              n/a  0.00000000000000E+00
Vertical Sigma          [ Z ]  n/a  0.00000000000000E+00
Horizontal              [ X ]  n/a  0.00000000000000E+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:: EXIT
Source has not been SAVED.
Confirm EXIT [ Y/N ] ? N
/* we forgot to store the definition on disk and SHADOW reminds us.
/* We have then to enter:
Ready:: 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:: 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:: 
Ray Tracing Selected. Begin procedure.
Mode selected [ ? <ret> for HELP ] ? : 
MENU selected.
Execute existing SYSTEMFILE ? : 
```

...Prepare MENU

```
Ready:: 

Element: 
Ready:: 
Screen/Slit: 
Ready:: 
Number of Element: 
```

MAIN MENU	Optical Element 1
Files to write out	ALL
Source plane distance	0.00000000000000E+00
Image plane distance	0.00000000000000E+00
Incidence angle	0.00000000000000E+00
Reflection angle	0.00000000000000E+00
Mirror Orientation Angle	0.00000000000000E+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, if 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?

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   0.00000000000000E+00
Aperturing                   NO
Open slit/ solid stop        n/a SLIT
Aperture shape                n/a RECTANGULAR
Slit width/ x-axis           n/a 10.000000000000
Slit height/ z-axis          n/a 10.000000000000
Absorption                   NO
Thickness [ CM ]             n/a 0.00000000000000E+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 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 ?

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 to DCL

VMS

\$

\$

Directory D0:[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 : MIRRO1.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.

\$

\$

\$ 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] ? :

File containing source description [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::

Ray Tracing Selected. Begin procedure.

Mode selected [enter ? for HELP] ? :

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 ?

Input file [exit(Unix) or %EXIT(VMS) terminates OS] ?

```
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 ?

Input file [exit(Unix) or %EXIT(VMS) terminates OS] ?

```
/* 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 – PRE-REFL**].
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.Tirrell 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

- **FFRESNEL**

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.

- **HISTO2**

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.

- **RECOLOR**

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.

- **FILEX**

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

```
$ go source
```

UNIX

```
% 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 ?

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

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

Source type : [0] regular source

. [1] normal wiggler

. [2] undulator

. [3] elliptical wiggler

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

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

Magnetic Radius [m] ?

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] ? Do you want to include electron beam emittances [Y/N] ? Electron Beam Energy [GeV] ?

```

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

```

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::

Ray Tracing Selected. Begin procedure.

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

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 ?

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]

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

Optical Element definition:

Files to write out. Options:

All..... [0]

Mirror only.....[1]

Image at CP only.....[2]

None.....[3]

Then ?

Incidence Angle ?

Source Distance ?

Reflection Angle?

Image Distance ?

Reflector [0] or refractor [1] ?

A: Is this a Kumakhov system?

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

Mirror surface [1-9] ?

Do you want to specify the mirror parameters ?

Is the mirror Cylindrical ?

Is this optical element a Fresnel Zone Plate ?

Are we dealing with a Grating ?

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

Is the mirror convex [Y/N] ?

Reflectivity mode [0,1,2] ?

Orientation Angle [Alpha] ?

Mirror Dimensions finite [Y/N] ?

Focii placed at continuation planes [Y/N] ?

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

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

Distorted surface [Y/N] ?

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

Any screens in this OE [Y/N] ?

Slit at continuation plane [Y/N] ?

Extra Image plates [Y/N] ?

File containing the source array ?

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 ?

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]

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

Optical Element definition:

Files to write out. Options:

All..... [0]
 Mirror only.....[1]
 Image at CP only.....[2]
 None.....[3]

Then ?

Incidence Angle ?

Source Distance ?

Reflection Angle?

Image Distance ?

Reflector [0] or refractor [1] ?

A: Is this a Kumakhov system?

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

```

Mirror surface [ 1-9 ] ? 
Do you want to specify the mirror parameters ? 
Is the mirror Cylindrical ? 
Is this optical element a Fresnel Zone Plate ? 
Are we dealing with a Grating ? 
Are we dealing with a crystal [ Y/N ] ? 
Is the mirror convex [ Y/N ] ? 
Reflectivity mode [ 0,1,2 ] ? 
Orientation Angle [ Alpha ] ? 
Mirror Dimensions finite [ Y/N ] ? 
Focii placed at continuation planes [ Y/N ] ? 
Do you want to move the Source [ Y/N ] ? 
Do you want to move the mirror itself [ Y/N ] ? 
Distorted surface [ Y/N ] ? 
Do you want to include surface roughness [Y/N] ? 
Any screens in this OE [ Y/N ] ? 
Slit at continuation plane [ Y/N ] ? 
Extra Image plates [ Y/N ] ? 

```

Exit from INPUT

Tracing optical element # 2

Call to SETSOUR

.....

Exit from RESET

Do you want to change input mode ?

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]

End of session.

Procedure completed. Return to command level.

Shadow::

```
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 ? 
```

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

```
PLOT> Then ? 
```

```
PLOT> Hairline at [ 0,0 ] ? 
```

```
PLOT> Overlay a mirror/slit ? 
```

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

```
PLOT> ? 
```

VMS

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

```
Terminal type ? 
```

```
PLOT> Do you want to save the TD command file ? 
```

UNIX

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

```
Terminal type: 
```

The following four scatter plots include the plot completed above on file MIRR.01, and similarly on MIRR.02, STAR.01 and STAR.02.

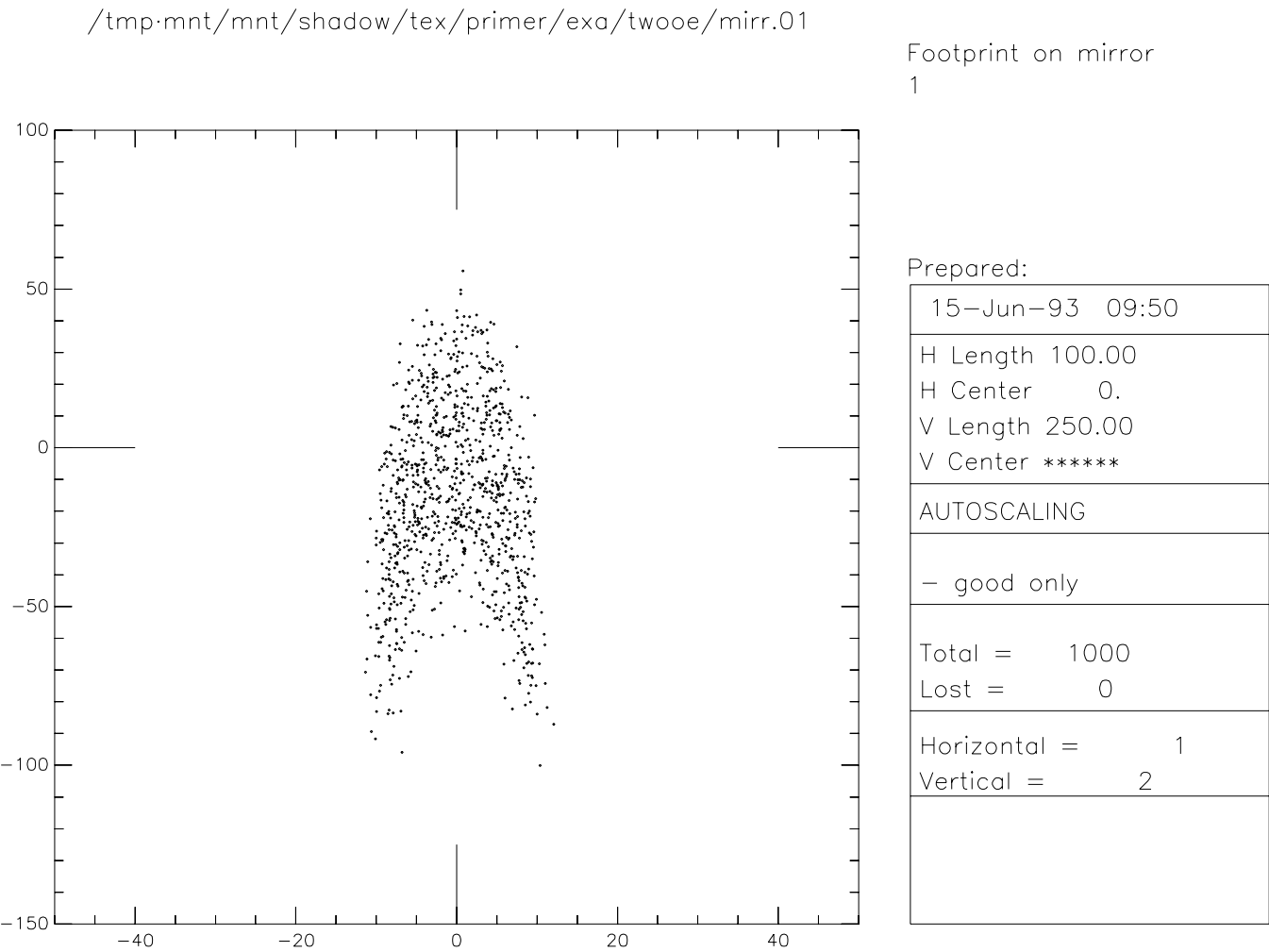


Figure 6.1: Footprint on mirror 1

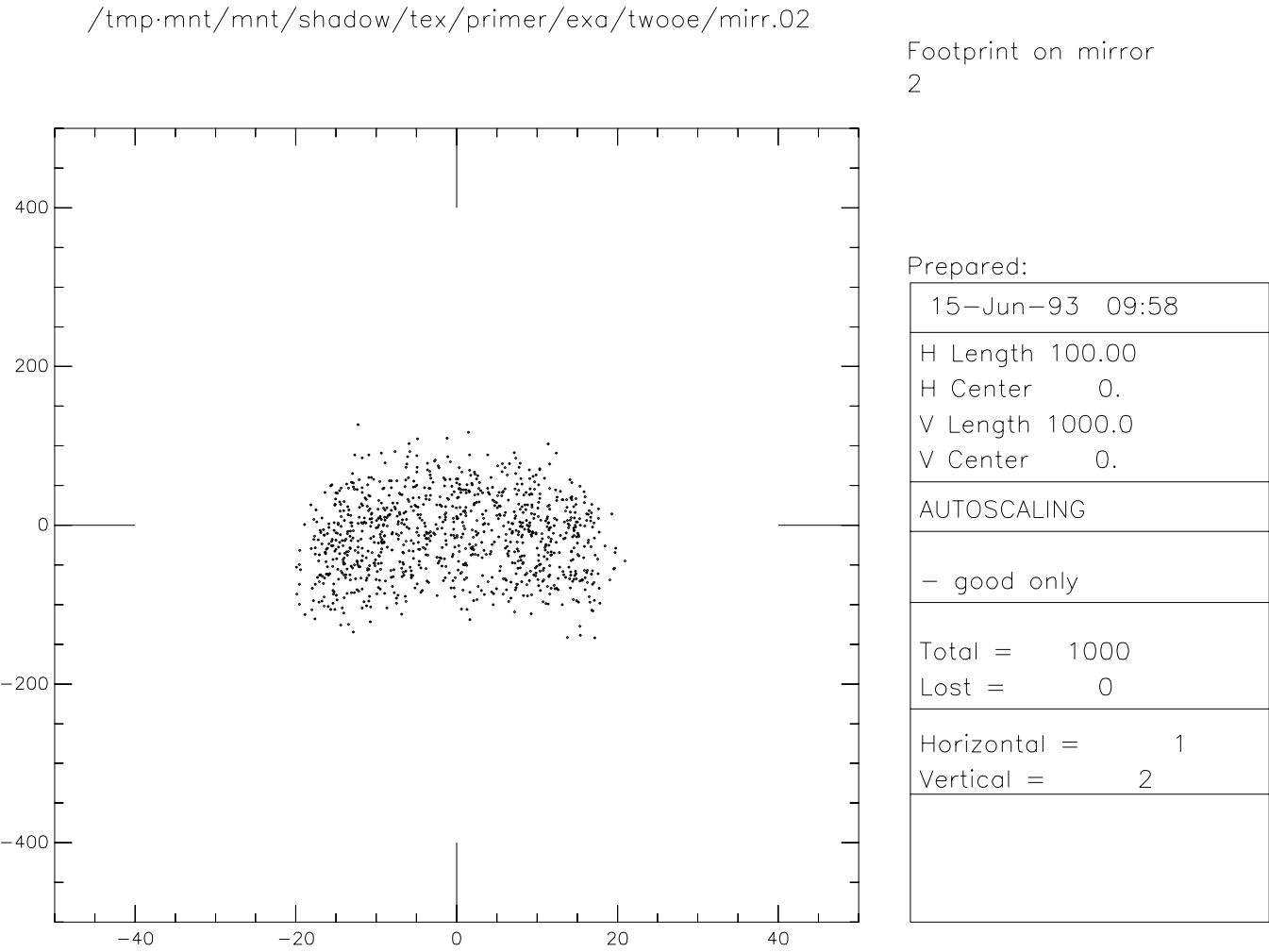


Figure 6.2: Footprint on mirror 2

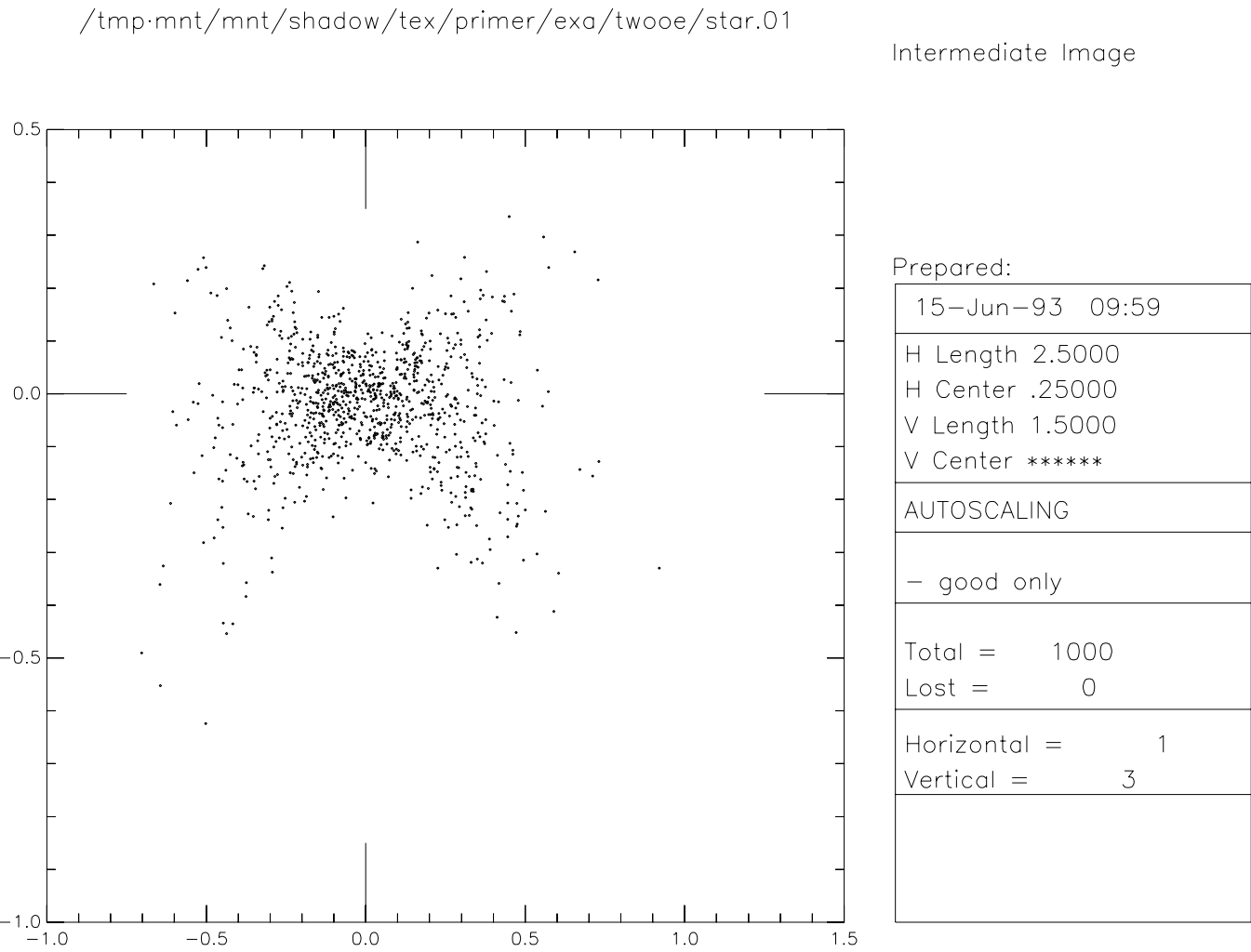


Figure 6.3: Intermediate Image

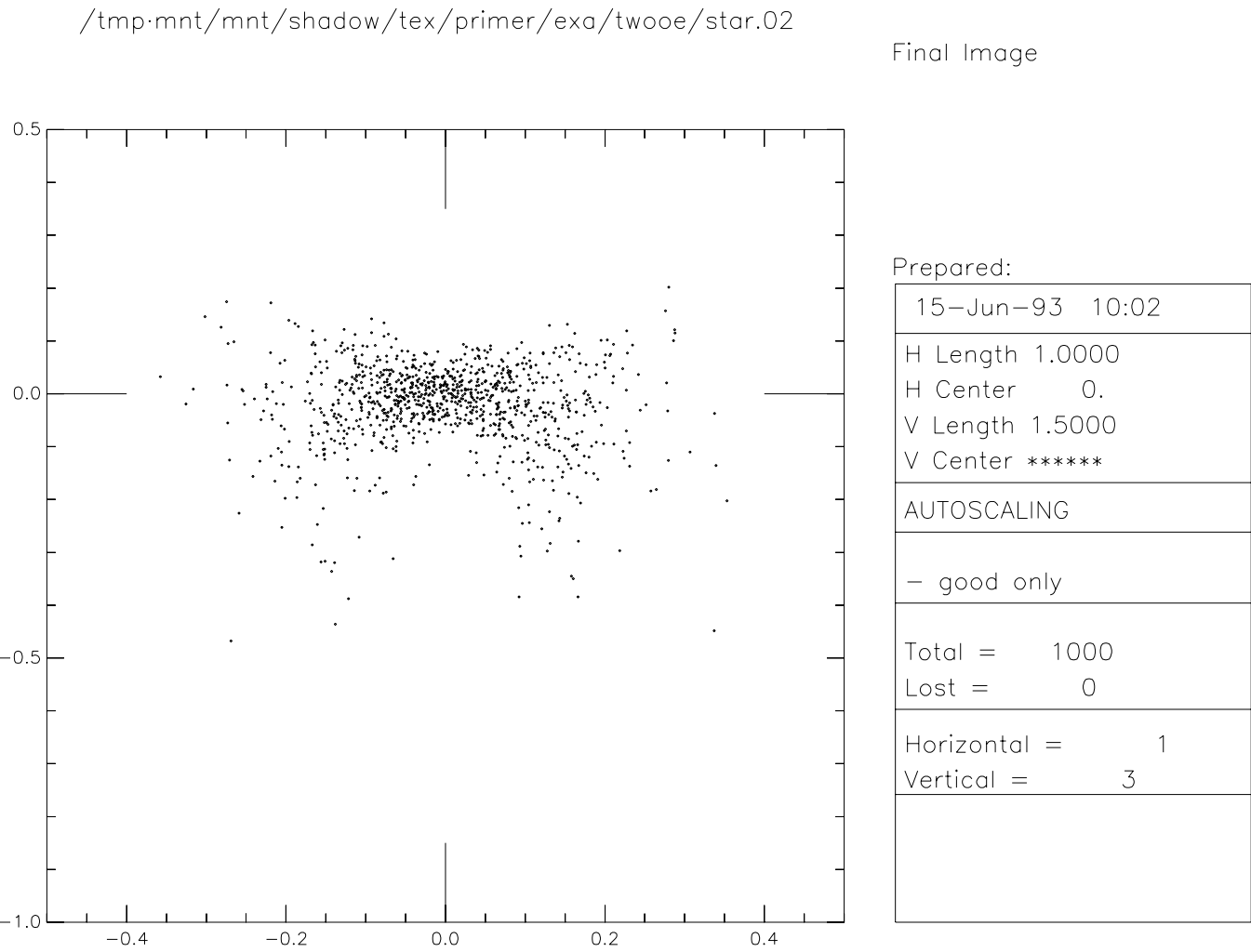


Figure 6.4: Final Image

We will use now the contouring capability of the program to generate a map of the ray's distribution.

```

$
$
$ 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. : 
PLOT> Vertical max. : 
PLOT> Plotting options :
      0   For scattered plot
      1   For connected plot
      2   For contour plot
PLOT> Then ? 
PLOT> Grid size [Nx by Ny] to prepare the contours.
PLOT> Nx : 
PLOT> Ny : 
PLOT> Number of contours : 
PLOT> Degree of polynomial used for joining [0=default] : 
PLOT> Included reflectivity ? 
PLOT> Data normalization :
      0   For no normalization
      1   For normalized to 1
      2   For normalized to total counts
PLOT> Then ? 
Smoothing [ Y/N ] ? 
Save grid file [ Y/N ] ? 
PLOT> Hairline at [ 0,0 ] ? 
PLOT> Overlay a mirror/slit ? 
PLOT> Ready for histograms. Enter:
      -1           to skip
       0   for same limits as plot
       1           3*stdev
       2           external
PLOT> ? 
```

VMS

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

UNIX

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

Terminal type:

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

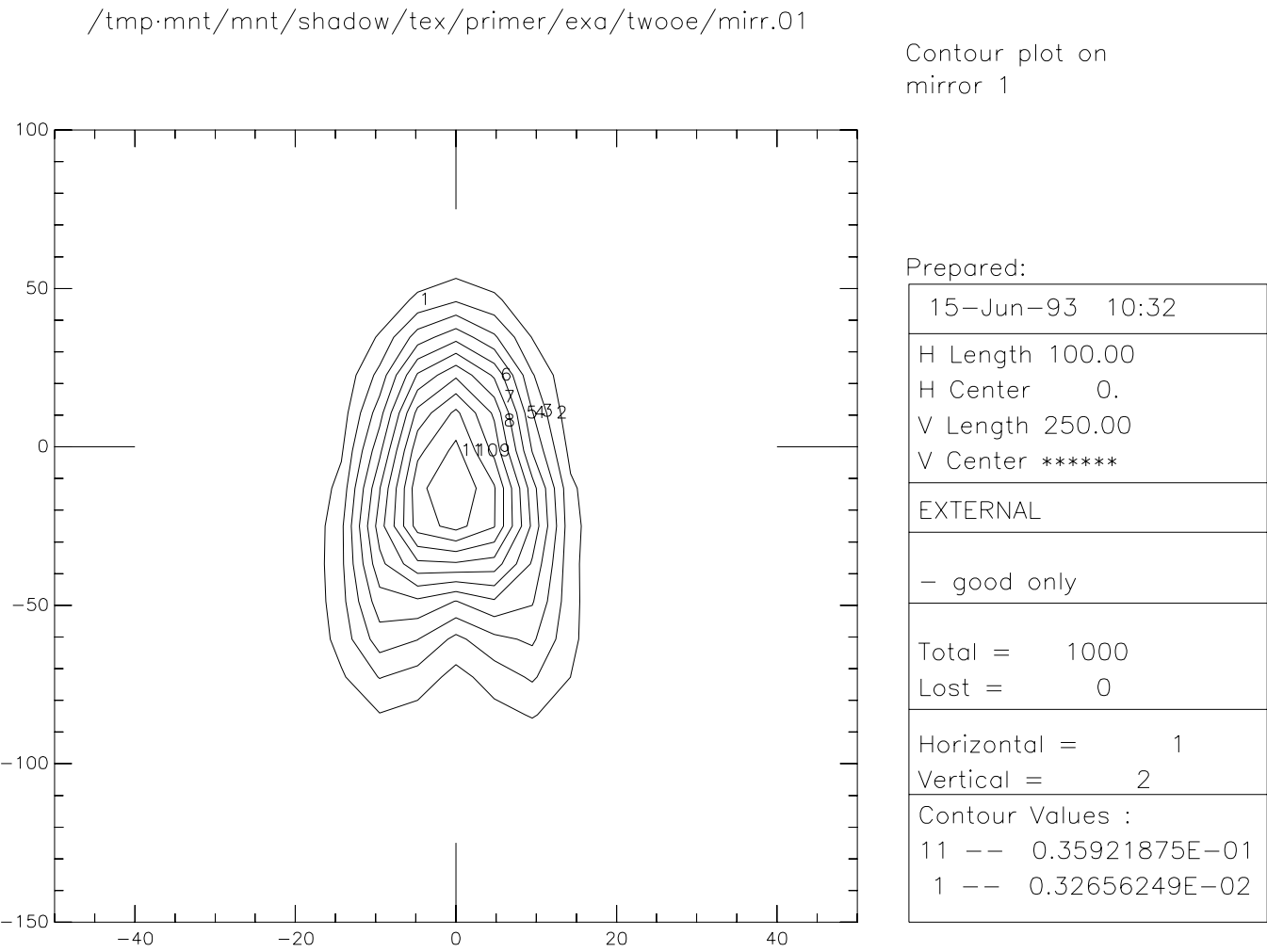


Figure 6.5: Contour plot of footprint on mirror 1

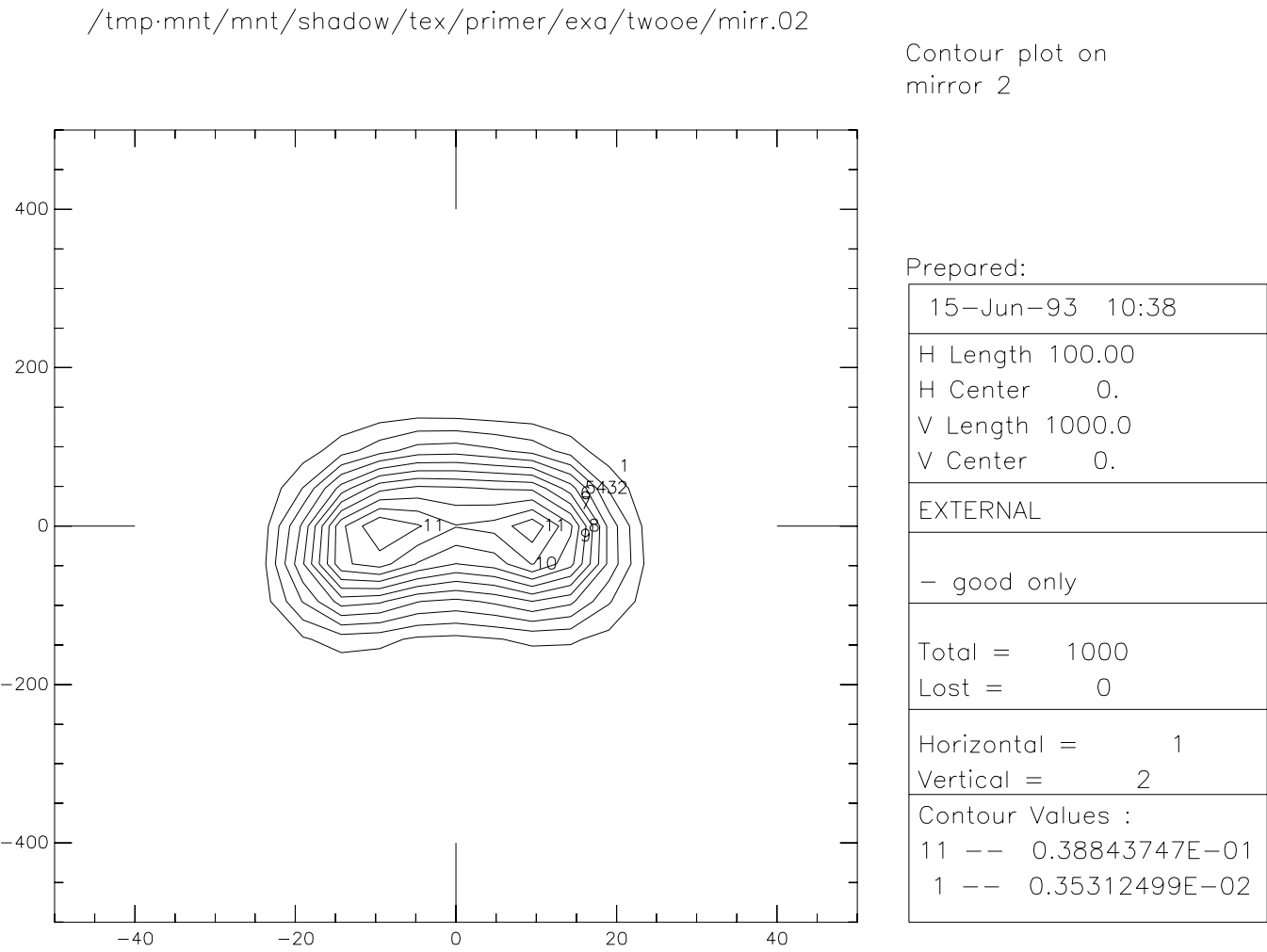


Figure 6.6: Contour plot of footprint on mirror 2

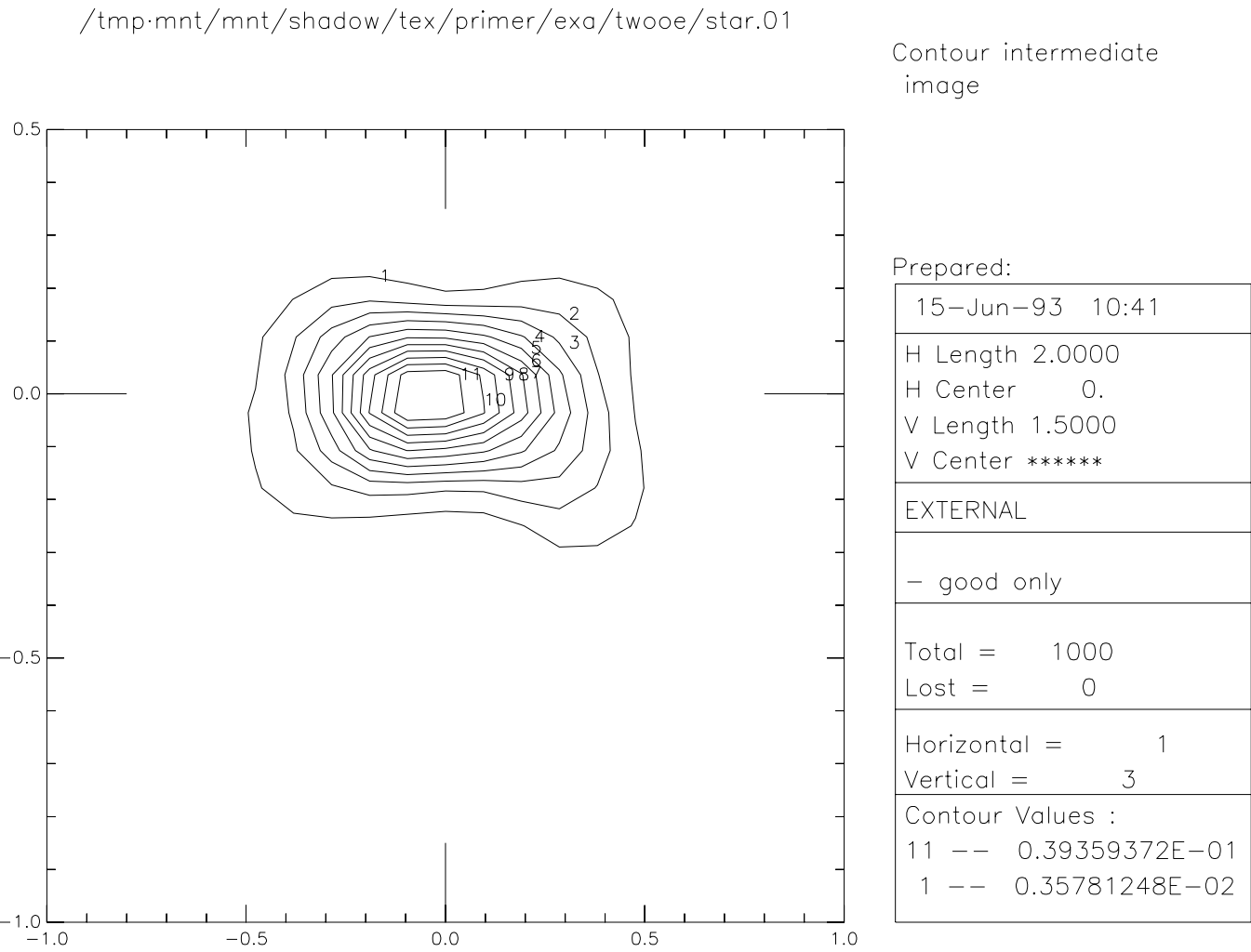


Figure 6.7: Contour plot of intermediate image

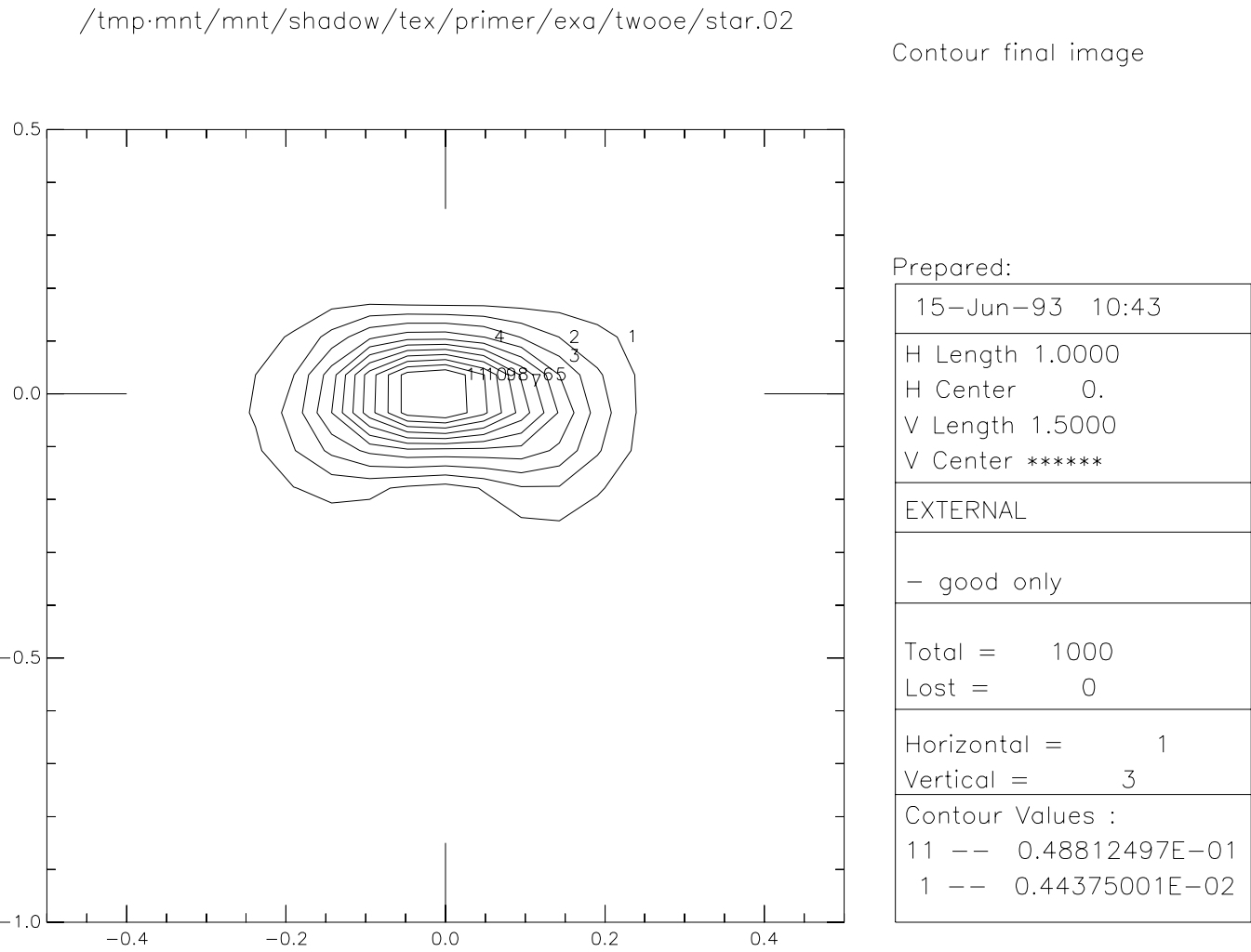


Figure 6.8: Contour plot of Final Image

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, $20\text{ }\mu\text{m}$ 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
```

```
----- 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:
```

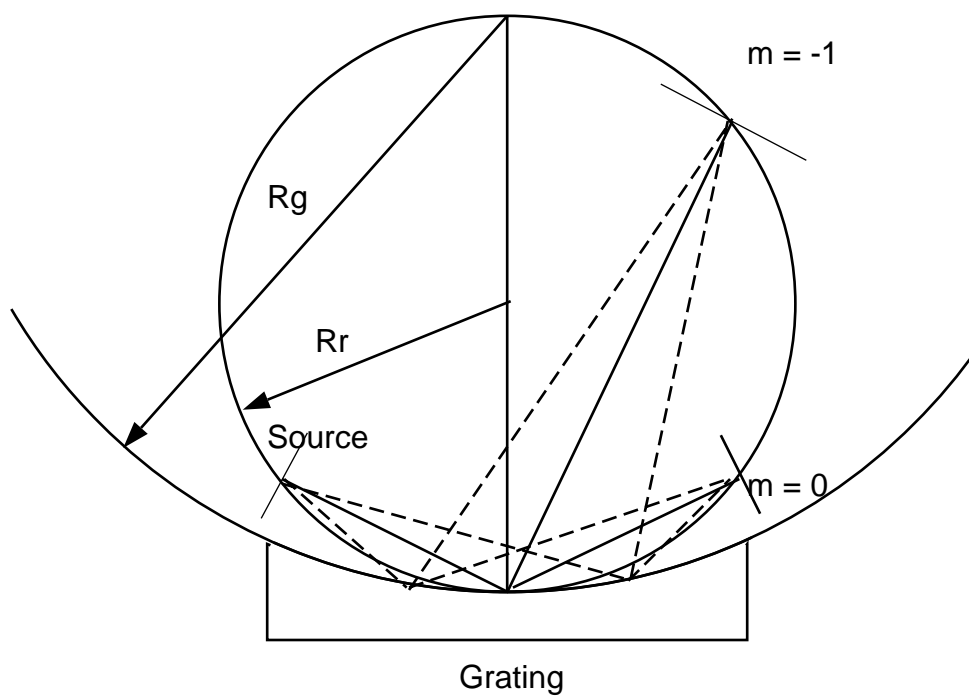


Figure 6.9: Rowland Circle Geometry

```

for YES answer Y, 1
for NO  answer anything else

```

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

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

```

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

```

```

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

```

Then ?

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

```

Source Width [ x ] ? 
. Height [ z ] ? 

```

Source Depth [1-4] ?

Source Angle Distribution [1-6] ?

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

. [(-)x, rads] ?

Vertical [(+)z, rads] ?

. [(-)z, rads] ?

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

Energy distribution [1-3] ?

Photon Energy [0] or Angstroms [1] ?

Energy [eV] ?

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

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

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:: 

Ray Tracing Selected. Begin procedure.

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

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 ? 

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

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

```

```

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

```

```

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

```

```

Is the mirror Cylindrical ? 
Is this optical element a Fresnel Zone Plate ? 
Are we dealing with a Grating ? 

```

```

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: 
Lines per CM ? 
Diffraction Order ? 
Auto Tuning of Grating [ Y/N ] ? 

```

```

/* 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 ] ? 
Reflectivity mode [ 0,1,2 ] ? 
Orientation Angle [ Alpha ] ? 
Mirror Dimensions finite [ Y/N ] ? 
Spherical Mirror Radius ? 

```

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

```
Exit from INPUT
```

```
Tracing optical element          #1
Call to SETSOUR
```

```
.....
Exit from RESET
```

```
Do you want to change input mode ? 
```

```
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 ] 
```

```
Shadow:: 
```

```
Return to DCL
```

```
Let's have a look at the image quality.
```

```
$ 
```

```
PLOT> Input file? 
```

```
PLOT> Options --- Enter
```

```
PLOT>  0   for excluding the losses
```

```
PLOT>  1   for including only the losses
```

```
PLOT>  2   for including all the rays.
```

```
PLOT> Then ? 
```

```
PLOT> Comment for plot [ 80 char ] ? 
```

```

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 ? 

```

```

PLOT>   for vertical axis ? 

```

```

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

```

```

PLOT> Then ? 

```

```

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

```

```

PLOT> Then ? 

```

```

PLOT> Hairline at [ 0,0 ] ? 

```

```

PLOT> Overlay a mirror/slit ? 

```

```

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

```

```

Then ? 

```

```

PLOT> X min : 

```

```

PLOT>   max : 

```

```
PLOT> Y min : 
PLOT>   max : 
```

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

```
PLOT> ? 
```

```
PLOT> Number of bins for X axis [default = 25] : 
```

```
PLOT> Number of bins for Y axis [default = 25] : 
```

VMS

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

```
PLOT> Do you want to save the TD command file ? 
```

UNIX

Display type:

```
[ 0 ] Xwindow
[ 1 ] Tektronix
[ 2 ] Postscript file
```

```
Terminal type: 
```

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.

```
$ 
```

```
File for input ? 
```

```
and for output ? 
```

```
Data ready. Read          2000 points.
```

```
Are you going to specify energies in eV [0] or wavelengths in angstroms [1] ? 
```

Available options :

```
1      single line
2      multi lines
3      box distribution
```

```
Then ? 
```

```
How many lines ? 
```

```
Line n.          1. Then ? 
```

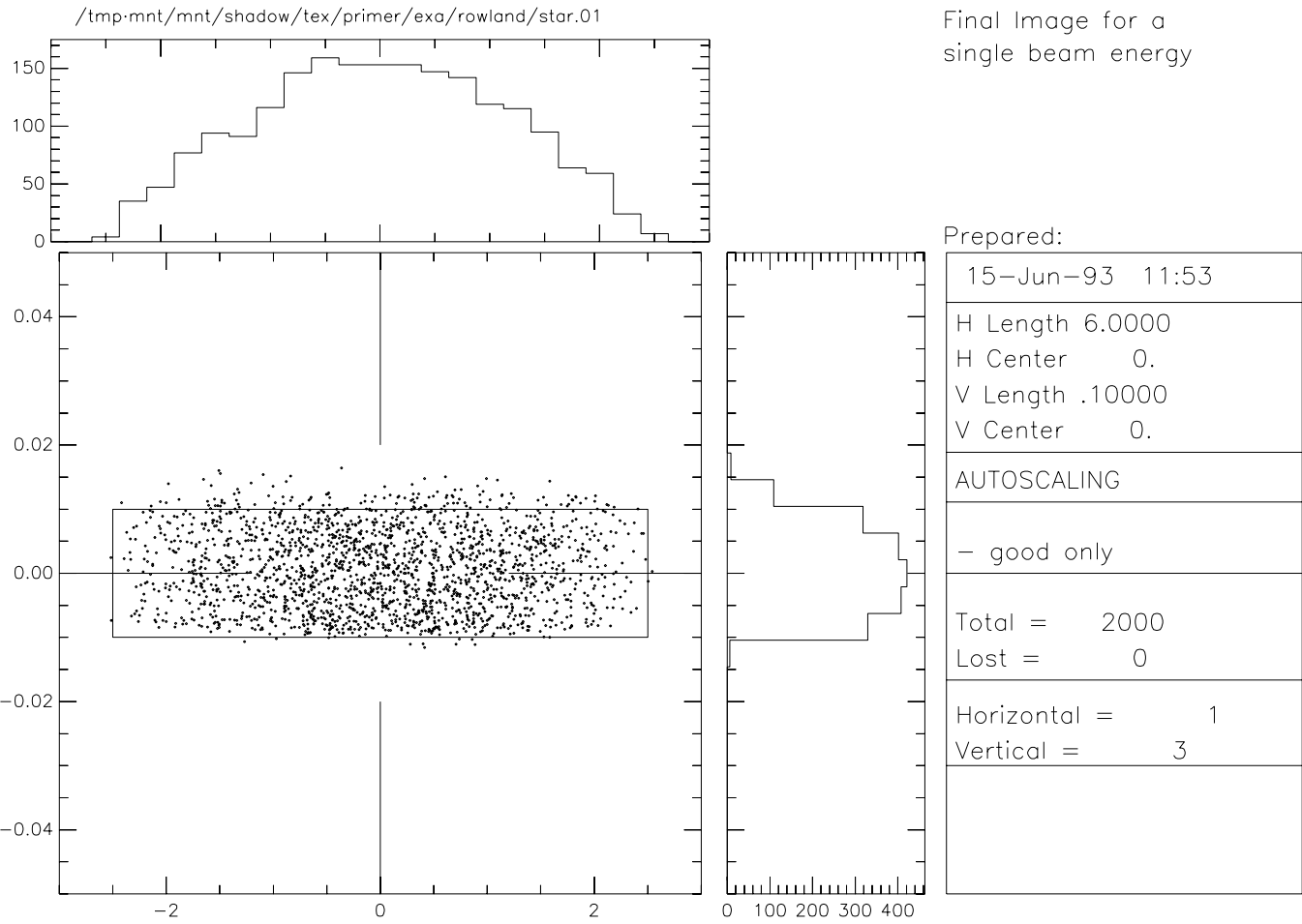


Figure 6.10: Final Image for a single beam energy

```

Line n.          2. Then ? 
Line n.          3. Then ? 
Enter seed for random number generator : 

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:

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

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.

```

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

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 ? 

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]

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

Optical Element definition:

Files to write out. Options:

```
All..... [ 0 ]
Mirror only.....[ 1 ]
Image at CP only.....[ 2 ]
None.....[ 3 ]
```

Then ?

Incidence Angle ?

Source Distance ?

Reflection Angle?

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

Image Distance ?

Reflector [0] or refractor [1] ?

A: Is this a Kumakhov system?

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

Mirror surface [1-9] ?

Do you want to specify the mirror parameters ?

Is the mirror Cylindrical ?

Is this optical element a Fresnel Zone Plate ?

Are we dealing with a Grating ?

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:

Lines per CM ?

Diffraction Order ?

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] ?

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

Photon Energy ?

TGM/SEYA 0

ERG 1

Con Inc Ang 2

Con Dif Ang 3

Hunter 4

Mount type ?

Is the mirror convex [Y/N] ?

Reflectivity mode [0,1,2] ?

Orientation Angle [Alpha] ?

Mirror Dimensions finite [Y/N] ?

Spherical Mirror Radius ?

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

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

Distorted surface [Y/N] ?

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

Any screens in this OE [Y/N] ?

Slit at continuation plane [Y/N] ?

Extra Image plates [Y/N] ?

File containing the source array ?

Exit from INPUT

Tracing optical element # 1

Call to SETSOUR

.....

Exit from RESET

Do you want to change input mode ?

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]

Shadow::

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.

\$

PLOT> Input file?

PLOT> Options --- Enter

PLOT> 0 for excluding the losses

PLOT> 1 for including only the losses

PLOT> 2 for including all the rays.

PLOT> Then ?

PLOT> Comment for plot [80 char] ?

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 ?

PLOT> for vertical axis ?

PLOT> Scaling options. Enter

0 For automatic scaling

1 For cartesian scaling

2 For external limits

PLOT> Then ?

```

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

```

```

PLOT> Then ? 

```

```

PLOT> Hairline at [ 0,0 ] ? 

```

```

PLOT> Overlay a mirror/slit ? 

```

```

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

```

```

Then ? 

```

```

PLOT> X min : 

```

```

PLOT>   max : 

```

```

PLOT> Y min : 

```

```

PLOT>   max : 

```

```

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

```

```

PLOT> ? 

```

```

PLOT> Number of bins for X axis [default = 25] : 

```

```

PLOT> Number of bins for Y axis [default = 25] : 

```

VMS

```

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

```

```

PLOT> Do you want to save the TD command file ? 

```

UNIX

```

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

```

```

Terminal type: 

```

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.

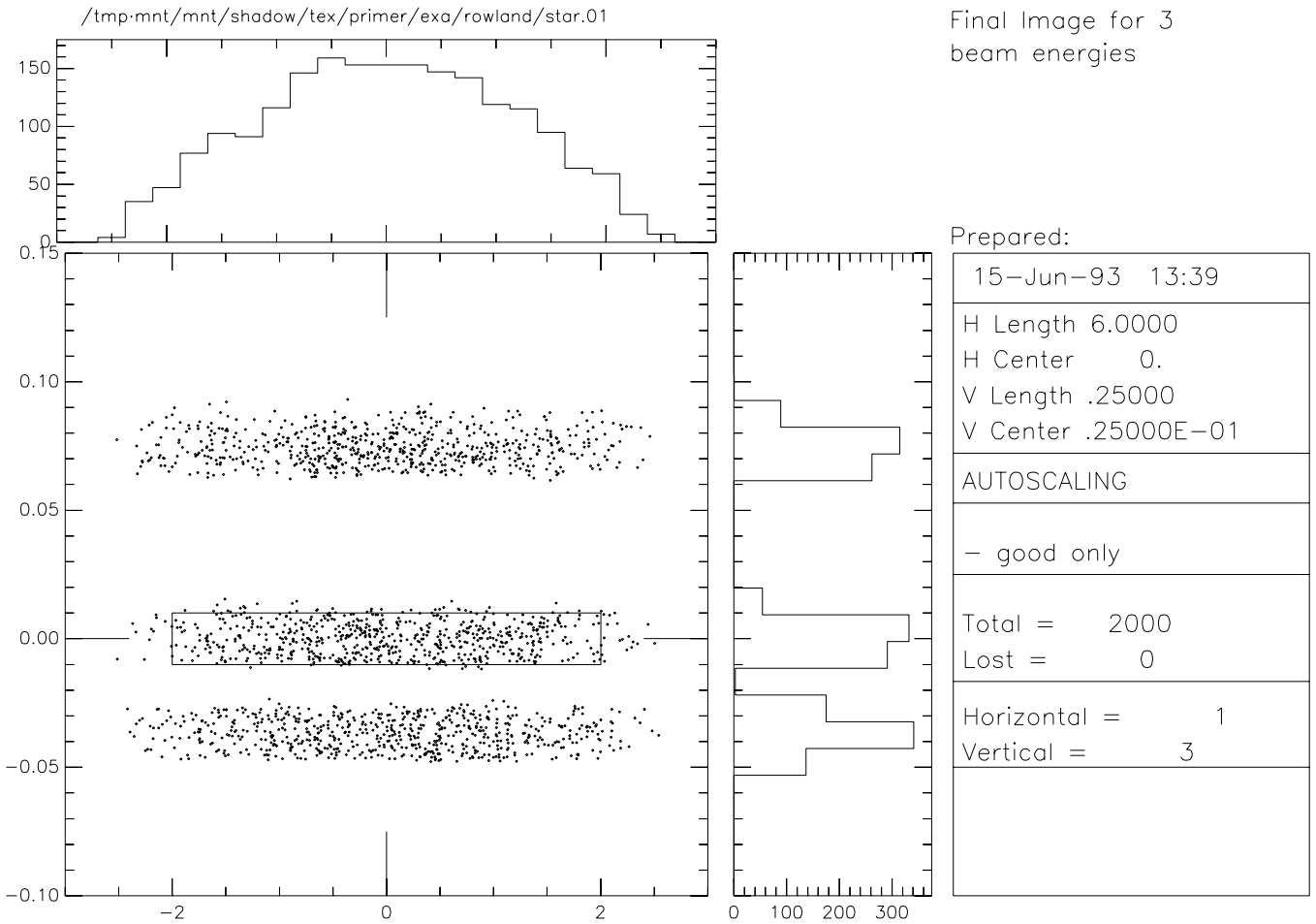


Figure 6.11: Final Image for three beam energies

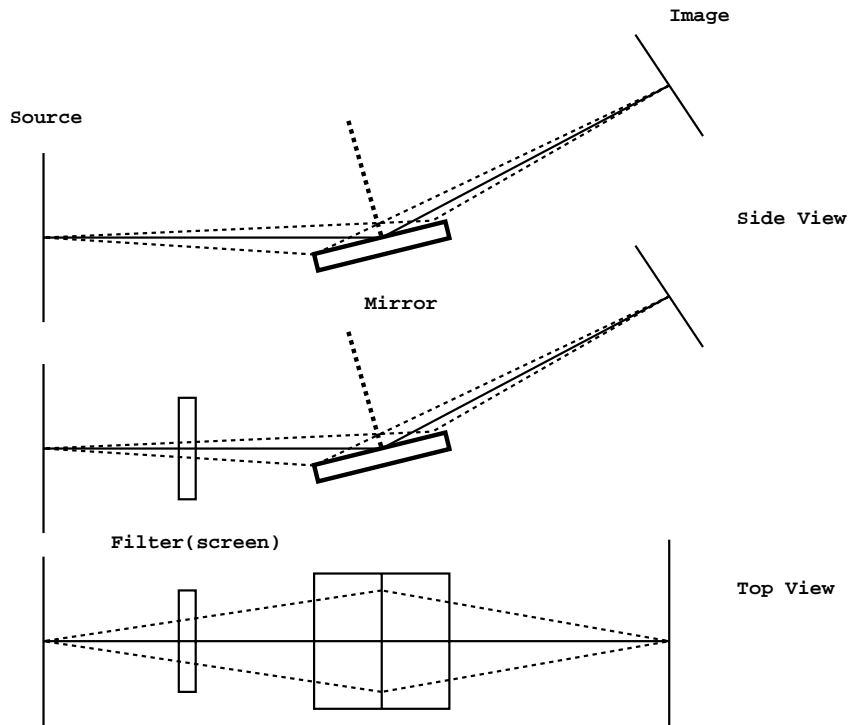


Figure 6.12: Optical System Consisting of a Gold Mirror With and Without a Filter

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] ? :

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 ?

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

Source modelling type [0-5] ?

How many rays [1 - 5 000] ?

Seed [odd, 1000 - 1 000 000] ?

Do you want to optimize the source ?

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

Then ?

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

Sigma along X ?

. Z ?

Source Depth [1-4] ?

Source Angle Distribution [1-6] ?

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

. [(-)x, rads] ?

Vertical [(+)z, rads] ?

. [(-)z, rads] ?

Magnetic Radius [m] ?

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

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

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

```

Exit from INPUT

```
Tracing optical element #          1
Call to SETSOUR
```

```
.....
Exit from RESET
```

```
Do you want to change input mode ? 
```

```
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 ] 
```

```
End of session
```

```
Procedure completed. Return to COMMAND level
```

```
Shadow:: 
```

```
Exit to DCL
```

```
$
```

```
$ 
```

```
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.

```
$ 
```

```
PLOT> Input file? 
```

```
PLOT> Options --- Enter
```

```
PLOT> 0 for excluding the losses
```

```
PLOT> 1 for including only the losses
```

```
PLOT> 2 for including all the rays.
```

```
PLOT> Then ? 
```

```
PLOT> Comment for plot [ 80 char ] ? 
```

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 ?

PLOT> for vertical axis ?

PLOT> Scaling options. Enter

0 For automatic scaling

1 For cartesian scaling

2 For external limits

PLOT> Then ?

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 ?

PLOT> Grid size [Nx by Ny] to prepare the contours.

PLOT> Nx :

PLOT> Ny :

PLOT> Number of contours :

PLOT> Degree of polynomial used for joining [0=default] :

PLOT> Included reflectivity ?

PLOT> Options :

- 0 Power density [J/area] reflected/transmitted
- 1 Power density [J/area] absorbed
- 2 Local reflectivity/transmission

PLOT> Then ?

PLOT> File to use for Io :

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 ?

Machine radius [m] ?

Machine energy [GeV] ?

Machine current[A] ?

milliradians of orbit ?

/* 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 ?

Total power accepted: 13.5220

Smoothing [Y/N] ?

Save grid file [Y/N] ?

PLOT> Hairline at [0,0] ? ☐

PLOT> Overlay a mirror/slit ? ☐

PLOT> Ready for histograms. Enter:

-1	to skip
0	for same limits as plot
1	3*stdev
2	external

PLOT> ? ☐

VMS

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

PLOT> Do you want to save the TD command file ? ☐

UNIX

Display type:

[0]	Xwindow
[1]	Tektronix
[2]	Postscript file

Terminal type: ☐

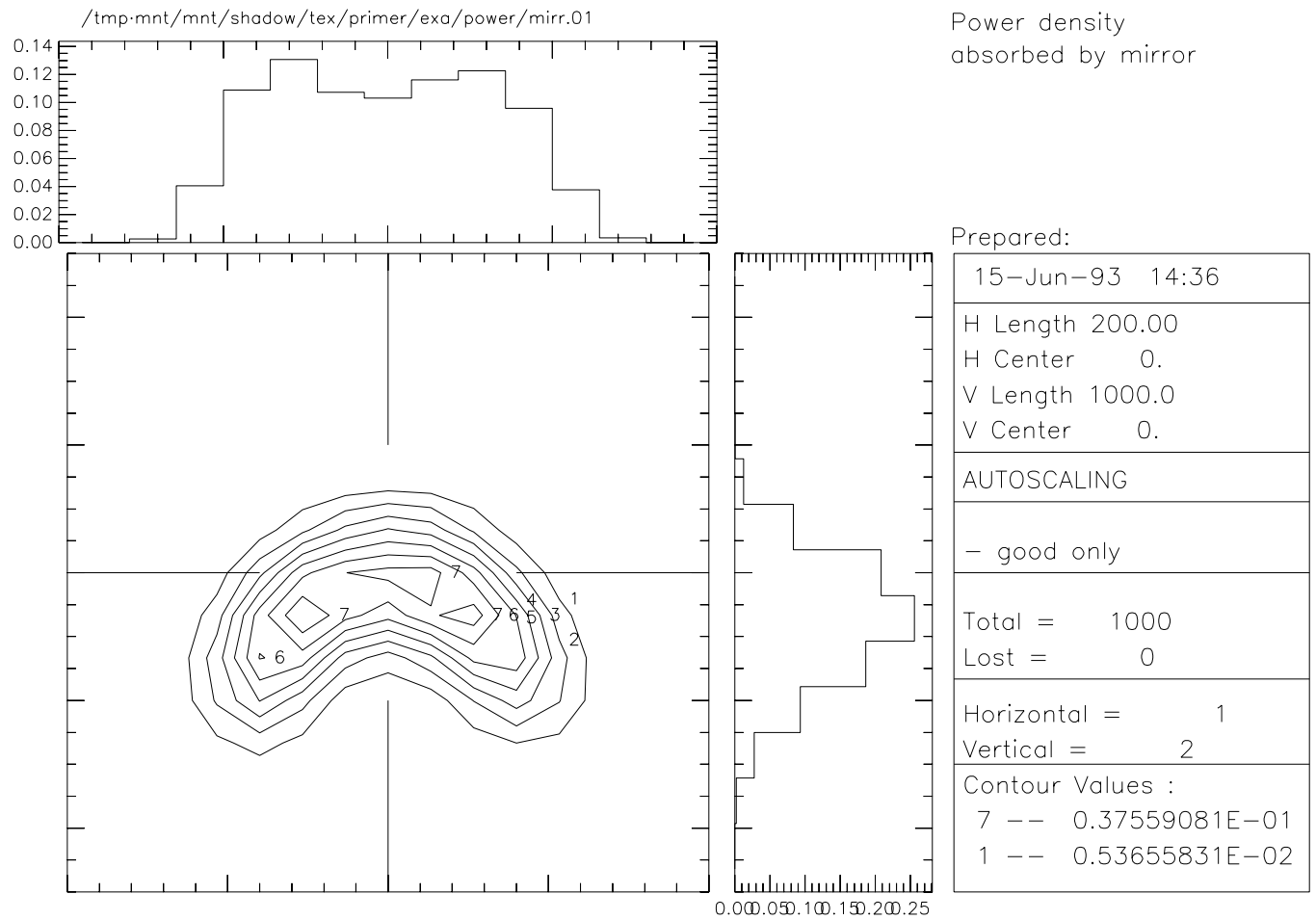


Figure 6.13: Contour plot of power density absorbed on first mirror

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.

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

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

```
$ 
```

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 ? 
```

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 ] 
```

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

Optical Element definition:

Files to write out. Options:

All..... [0]
 Mirror only.....[1]
 Image at CP only.....[2]
 None.....[3]

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

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

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 -----
May 1993                      F.Cerrina          CXrL/ECE - UW
```

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).

<?>

Scale to :

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

<?>

Output options :

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

Then ?

OK. Here we go !

Another run [Y/N] ?

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 ?

Column to analyze ?

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

<?>

Read : 1000 rays

Maximum :

Minimum :

Distribution center ?
width ?

Number of bins (odd, please) ?

Flag checks. Enter :

0 to exclude lost rays
1 to include lost rays too
2 to use only lost rays

<?>

Normalization kind. Enter :

0 for no normalization
1 to normalize to 1
2 area normalized to 1

<?>

Include reflectivity ?

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)

<?>

Scale to :

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

<?>

Output options :

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

Then ?

OK. Here we go !

Another run [Y/N] ?

File for analysis ?

Column to analyze ?

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

<?>

Read : 1000 rays

Maximum :

Minimum :

Distribution center ?

width ?

Number of bins (odd, please) ?

Flag checks. Enter :

- 0 to exclude lost rays
- 1 to include lost rays too
- 2 to use only lost rays

<?>

Normalization kind. Enter :

- 0 for no normalization
- 1 to normalize to 1
- 2 area normalized to 1

<?>

Include reflectivity ?

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)

<?>

Scale to :

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

<?>

Output options :

- [0] store histogram in a file
- [1] plot histogram on screen
- [2] both

Then ?

OK. Here we go !

Another run [Y/N] ?

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).

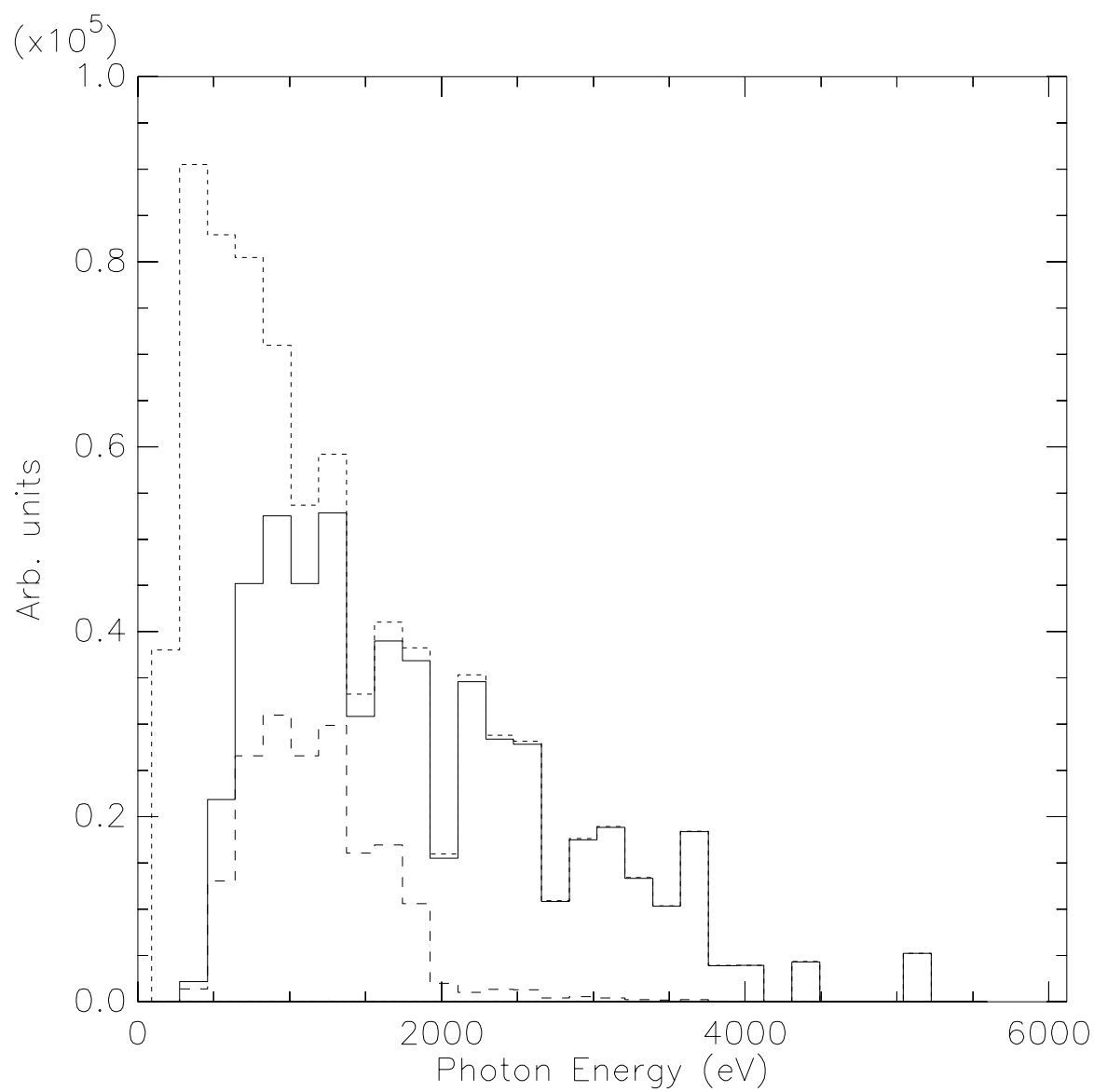


Figure 6.14: Overlay of histograms after source, filter, and mirror

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 α 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 surface¹. 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 misalignment 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 left unchanged. The source that we will be using will be a point source of single wavelength. The BRAGG condition

$$n \lambda = 2 d \sin \theta \quad (6.2)$$

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

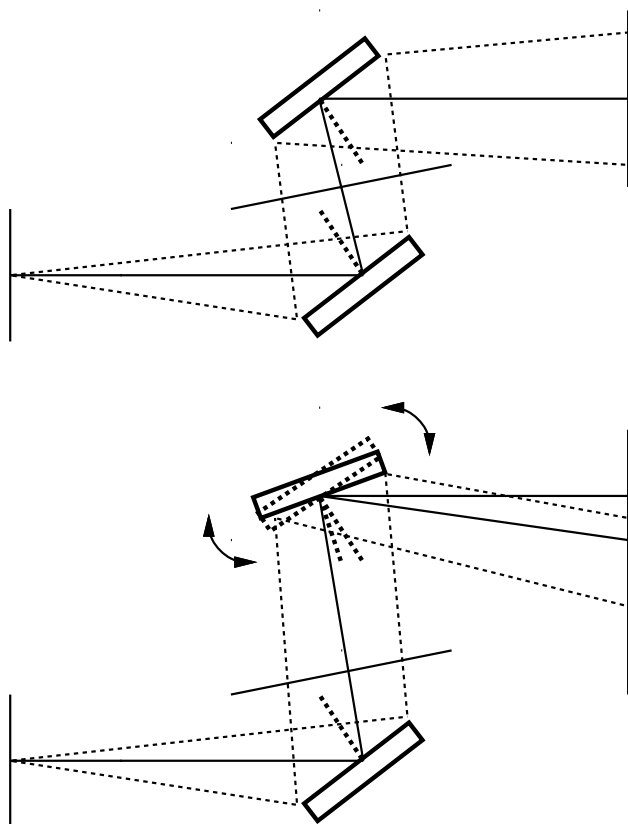


Figure 6.15: Two crystals monochromator with diverging radiation and antiparallel configuration: a)ideal case, b)misaligned second crystal.

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 for simple 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 ZINCBLLENDE 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 $f_0 + f' + if''$, where
 $f_0 = f_0(\sin(\theta)/\lambda)$ 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 :	<input type="text" value="0.14,27.162"/>
. , second set :	<input type="text" value="0.15,26.783"/>
. , third set :	<input type="text" value="0.16,26.406"/>
For atom B, first set :	<input type="text" value="0.14,28.742"/>
. , second set :	<input type="text" value="0.15,28.307"/>
. , third set :	<input type="text" value="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) :
 maximum photon energy (eV) :
 energy step (eV) :
 Do you want to include crystal absorption [1/0] ?
 Temperature (Debye-Waller) factor :

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

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

<?>

... at what energy (eV) ?

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 ?

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

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 :

How many points :

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

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

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

\$

VMS

\$

\$

Directory D13:[XRAYOP.XTAL]

GAAS.PAR;1 4 26-MAR-1987 14:17 (RWED,RWED,RE,RE)

ROCK_CURVE.P;1 20 26-MAR-1987 14:17 (RWED,RWED,RE,RE)

```

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

```

Total of 4 files, 47 blocks.

UNIX

```
% ls -al
```

```

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

```

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

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

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

```
$ TYPE GAAS.PAR
```

```

          0  1562378464.990918      3.2620290209213856E-08
          31          33  0.9790000000000000
(4.000000000000000,-6.8654264713317982E-17)
(4.000000000000000,6.8654264713317982E-17)
(8.4736075498395345E-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

```

11170.000000000000	-1.790085703926181	3.381267232438158
-2.524143733690788	0.5543032862233946	
11180.000000000000	-1.775082278683501	3.376457230615321
-2.536614203964387	0.5533865542912357	
11190.000000000000	-1.760078853440822	3.371647228792484
-2.549084674237986	0.5524698223590767	
11200.000000000000	-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    =     11160.000000000000      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] ? :

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 ?

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

Source modelling type [0-5] ?

How many rays [1 - 5 000] ?

Seed [odd, 1000 - 1 000 000] ?

Do you want to optimize the source ?

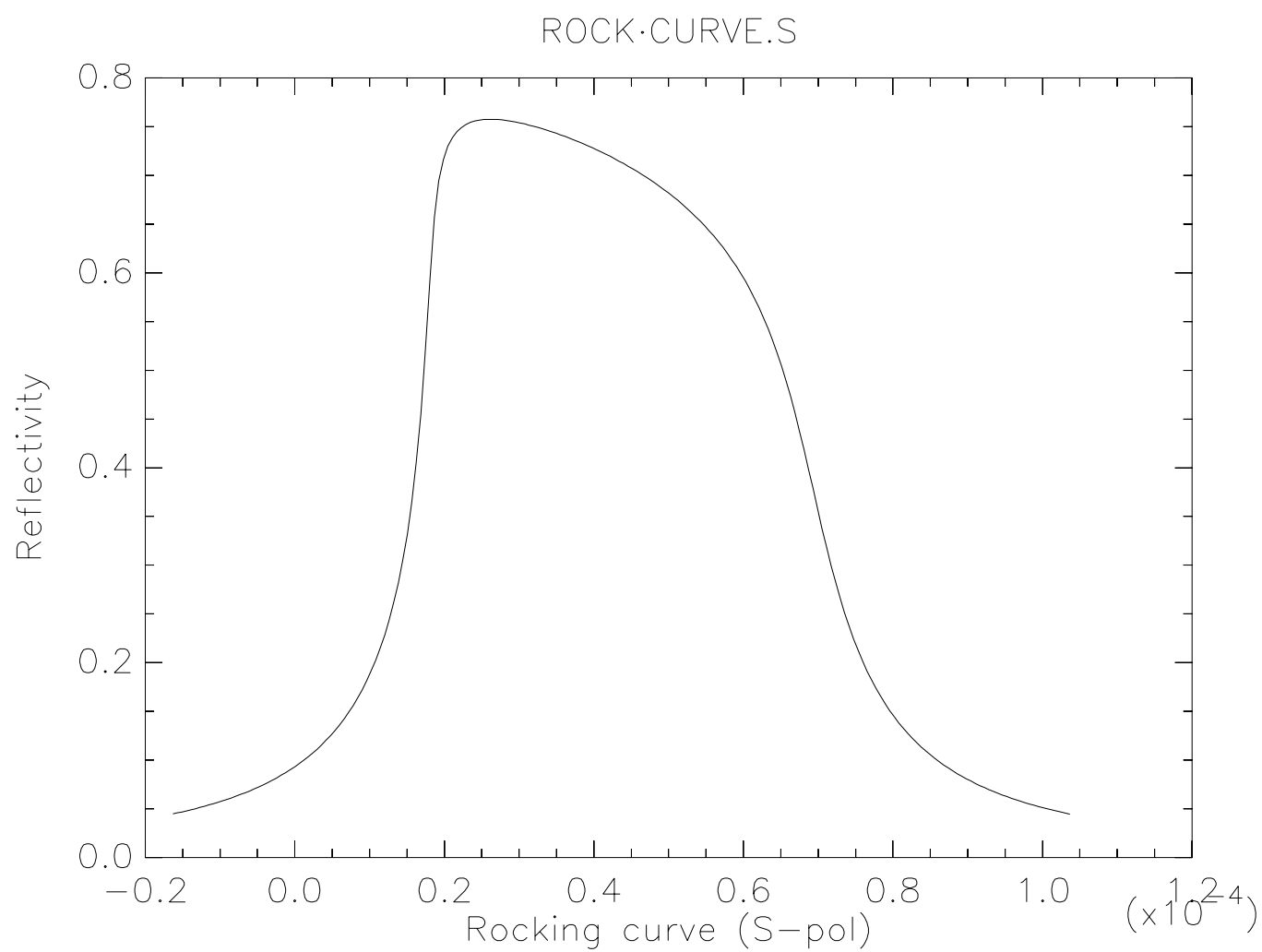


Figure 6.16: Rocking curve for S-polarization

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

Then ?

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

Source Depth [1-4] ?

Source Angle Distribution [1-6] ?

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

. [(-)x, rads] ?

Vertical [(+)z, rads] ?

. [(-)z, rads] ?

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

Energy distribution [1-3] ?

Photon Energy [0] or Angstroms [1] ?

Energy [eV] ?

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

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

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::

Ray Tracing Selected. Begin procedure.

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

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 ?

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]

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

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 ?

Optical Element definition:

Incidence Angle ?

Source Distance ?

Reflection Angle?

Image Distance ?

```
/* 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] ?

A: Is this a Kumakhov system?

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

Mirror surface [1-9] ?

Is the mirror Cylindrical ?

Is this optical element a Fresnel Zone Plate ? ☐

Are we dealing with a Grating ? ☐

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

* 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 ?

Is it a mosaic crystal [Y/N] ? ☐

Is the crystal asymmetric [Y/N] ? ☐

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

Automatic Tuning of Crystal [Y/N] ? ☒

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

Photon Energy ?

Is the mirror convex [Y/N] ? ☐

Reflectivity mode [0,1,2] ? ☐

Orientation Angle [Alpha] ? ☐

Mirror Dimensions finite [Y/N] ? ☐

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

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

Distorted surface [Y/N] ? ☐

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

Any screens in this OE [Y/N] ? ☐

Slit at continuation plane [Y/N] ? ☐

Extra Image plates [Y/N] ? ☐

File containing the source array ?

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]

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

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 ?

Optical Element definition:

Incidence Angle ?

Source Distance ?

Reflection Angle?

Image Distance ?

Reflector [0] or refractor [1] ?

A: Is this a Kumakhov system?

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

Mirror surface [1-9] ?

Is the mirror Cylindrical ?

Is this optical element a Fresnel Zone Plate ?

Are we dealing with a Grating ?

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

File containing crystal parameters ?

Is it a mosaic crystal [Y/N] ?

Is the crystal asymmetric [Y/N] ?

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

Automatic Tuning of Crystal [Y/N] ?

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

Photon Energy ?

Is the mirror convex [Y/N] ?

Reflectivity mode [0,1,2] ?

Orientation Angle [Alpha] ?

Mirror Dimensions finite [Y/N] ?

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

Do you want to move the mirror itself [Y/N] ?
 Distorted surface [Y/N] ?
 Do you want to include surface roughness [Y/N] ?
 Any screens in this OE [Y/N] ?
 Slit at continuation plane [Y/N] ?
 Extra Image plates [Y/N] ?

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]

End of session
 Procedure completed. Return to COMMAND level

Shadow::

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

VMS

\$

Directory D13:[XRAYOP.XTAL]

BEGIN.DAT;1	188	26-MAR-1987 14:22	(RWED,RWED,RE,RE)
EFFIC.01;1	1	26-MAR-1987 14:41	(RWED,RWED,RE,RE)
EFFIC.02;1	1	26-MAR-1987 14:48	(RWED,RWED,RE,RE)
END.00;1	6	26-MAR-1987 14:22	(RWED,RWED,RE,RE)
END.01;1	11	26-MAR-1987 14:41	(RWED,RWED,RE,RE)
END.02;1	11	26-MAR-1987 14:48	(RWED,RWED,RE,RE)
GAAS.PAR;1	4	26-MAR-1987 14:17	(RWED,RWED,RE,RE)
MIRR.01;1	188	26-MAR-1987 14:41	(RWED,RWED,RE,RE)
MIRR.02;1	188	26-MAR-1987 14:48	(RWED,RWED,RE,RE)
OPTAX.01;1	2	26-MAR-1987 14:40	(RWED,RWED,RE,RE)

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

Total of 23 files, 1089 blocks.

UNIX

```
% ls -al
```

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

Note the P-polarization has smaller average reflectivity, because of narrower width of the rocking curve (smaller value of 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                      150.000000000000
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 ?

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

PREPLOT> Row # 1 :

PREPLOT> 2 :

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 ?

VMS

Output options :

[0] store rays in a file
 [1] plot directly on screen
 [2] both

Then ?

PREPLOT> Output file ?

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

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:

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

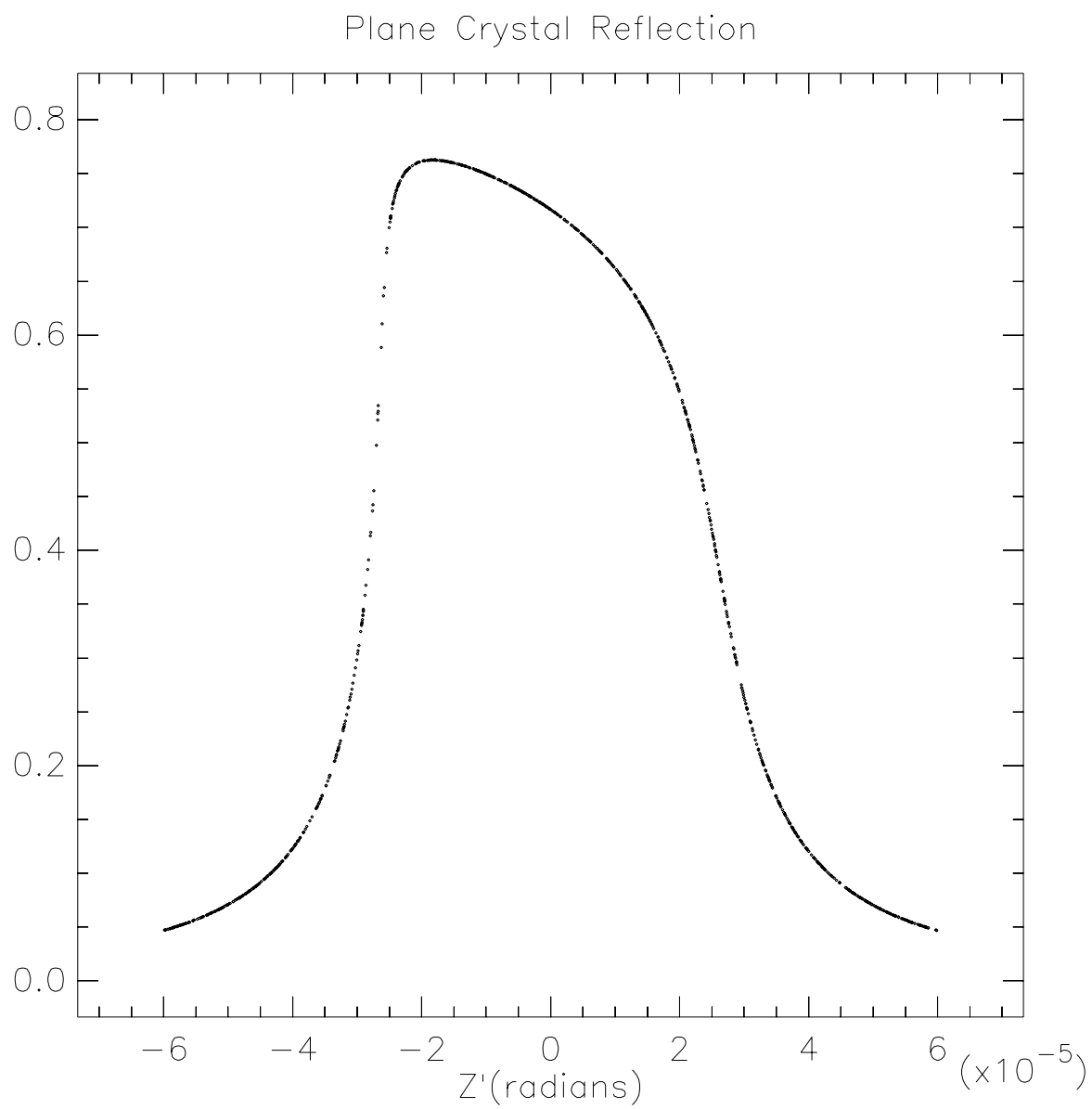


Figure 6.17: Plane Crystal Reflection

```
% 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
```

```
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: 
% 

```

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., $2.777\text{E-}3$ 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

```

$
$
$ 
$ 
$ 
$ 
$
$ 

```

UNIX

```

%
% 
% 
% 
% 
% 

```

Ray Tracing Selected. Begin procedure.

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

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 ?

Previous element number :

Image file of the previous OE ?

Do you want to change the input mode ?

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]

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

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 ?

Optical Element definition:

Incidence Angle ?

Source Distance ?

Reflection Angle?

Image Distance ?

Reflector [0] or refractor [1] ?

A: Is this a Kumakhov system?

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

Mirror surface [1-9] ?

Is the mirror Cylindrical ?

Is this optical element a Fresnel Zone Plate ?

Are we dealing with a Grating ?

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

File containing crystal parameters ?

Is it a mosaic crystal [Y/N] ?

Is the crystal asymmetric [Y/N] ?

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

Automatic Tuning of Crystal [Y/N] ?

Is the mirror convex [Y/N] ?

```

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

```

```

Exit from INPUT
Tracing optical element #           2
Call to SETSOUR

```

```

.....
Exit from RESET

```

```

Do you want to change input mode ? 
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 ] 

```

```

End of session
Procedure completed. Return to COMMAND level

```

```

Shadow:: 
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> Input file ? 

Read                1000 rays.
Each ray has        12 entries.

PREPLOT> How many columns to write out ? 

```

```

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 : 
PREPLOT>      2 : 

```

```

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 ? 

```

VMS

```

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

```

```

Then ? 

```

```

PREPLOT> Output file ? 

```

```

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

```

```

*****

```

```

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: 

```

```

% 

```

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

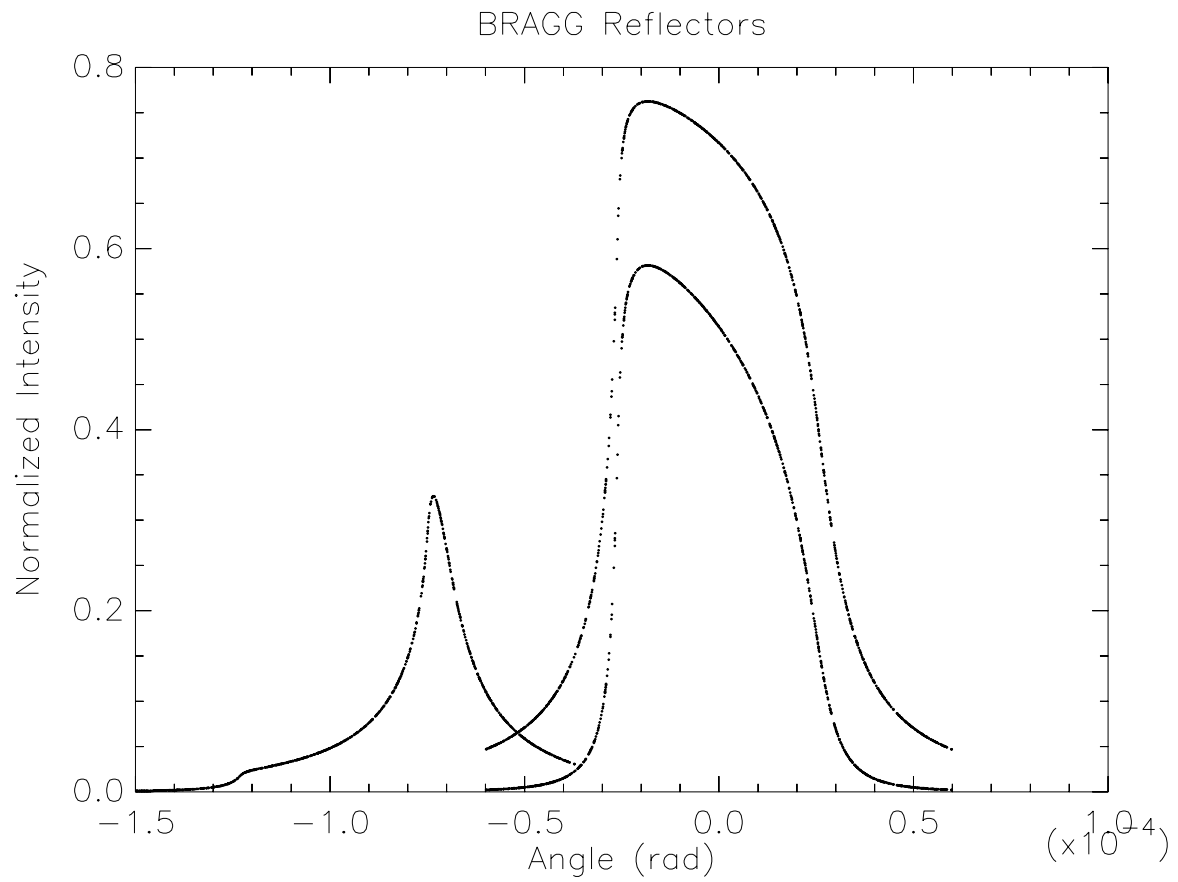


Figure 6.18: Comparison of BRAGG reflectors: offset and exact conditions

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.

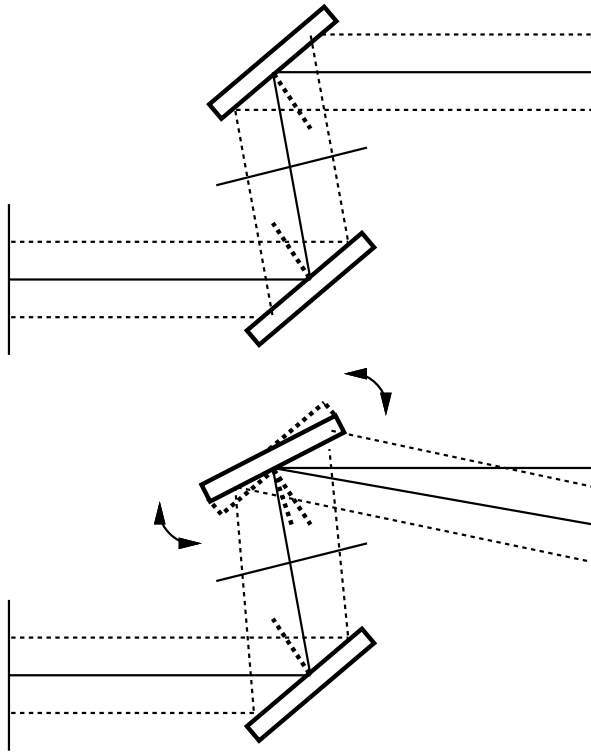


Figure 6.19: Two crystals monochromator in parallel radiation.

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

```
$ CREATE/DIRECTORY [.XTAL2]
$ SD [XRAYOP.XTAL2]
$ COPY [-]GAAS.PAR [*.*]
$ GO SOURCE
```

UNIX

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

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 ?

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

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

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

Then ?

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

Do you want to store the optical paths (OPD) [Y/N] ?
 Do you want to generate the A vectors (electric field) [Y/N] ?

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::

Ray Tracing Selected. Begin procedure.

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

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 ?

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

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 ?

Optical Element definition:

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

Slit at continuation plane [Y/N] ?

Extra Image plates [Y/N] ?

File containing the source array ?

Exit from INPUT

Tracing optical element # 1

Call to SETSOUR

.....

Exit from RESET

Do you want to change input mode ?

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]

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

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 ?

Optical Element definition:

Incidence Angle ?

Source Distance ?

Reflection Angle?

Image Distance ?

Reflector [0] or refractor [1] ?

A: Is this a Kumakhov system?

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

Mirror surface [1-9] ?

```

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 -----
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 to DCL

\$

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

\$

----- 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:

MINFO> File read correctly.

MINFO> Title ?

MINFO> Comment ?

MINFO> Output file ?

MINFO> Prepare output to file : 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                 149.89560000000000
Incidence Angle             80.19284670377978
Reflection/Diffraction Angle 80.19284670377978

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

```

VMS

\$ DIR

Directory D13:[XRAYOP.XTAL2]

```

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

```

```

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

```

Total of 17 files, 1012 blocks.

UNIX

```
% ls -al
```

```

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

```

```
$ PREPLOT
```

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

```

Read          1000 rays.
Each ray has   12 entries.

```

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

```

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

```

```

PREPLOT> Row # 1 : 
PREPLOT>      2 : 

```

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

```

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

```

```

PREPLOT> Then ? 

```

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 ? 

```

VMS

Output options :

```

[ 0 ] store rays in a file
[ 1 ] plot directly on screen
[ 2 ] both

```

```

Then ? 

```

```

PREPLOT> Output file ? 

```

```

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

```

```

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: 
% 

```

Now the second crystal will be offset.

VMS

```

$
$
$ 
$ 
$ 
$ 
$
$ 

```

UNIX

```

% 
% 
% 
% 
% 

```

Ray Tracing Selected. Begin procedure.

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

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 ?

Previous element number :

Image file of the previous OE ?

Do you want to change the input mode ?

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]

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

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 ?

Optical Element definition:

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

```

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

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

Do you want to change input mode ? 

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 ] 

End of session
Procedure completed. Return to COMMAND level

Shadow:: 

Exit to DCL

$ 

PREPLOT> Input file ? 

Read          1000 rays.
Each ray has   12 entries.

PREPLOT> How many columns to write out ? 

```

```

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 : 
PREPLOT>      2 : 

```

```

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

```

```

PREPLOT> Then ? 

```

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 ? 

```

VMS

Output options :

```

[ 0 ] store rays in a file
[ 1 ] plot directly on screen
[ 2 ] both

```

```

Then ? 

```

```

PREPLOT> Output file ? 

```

```

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: 

```

```

% 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
```

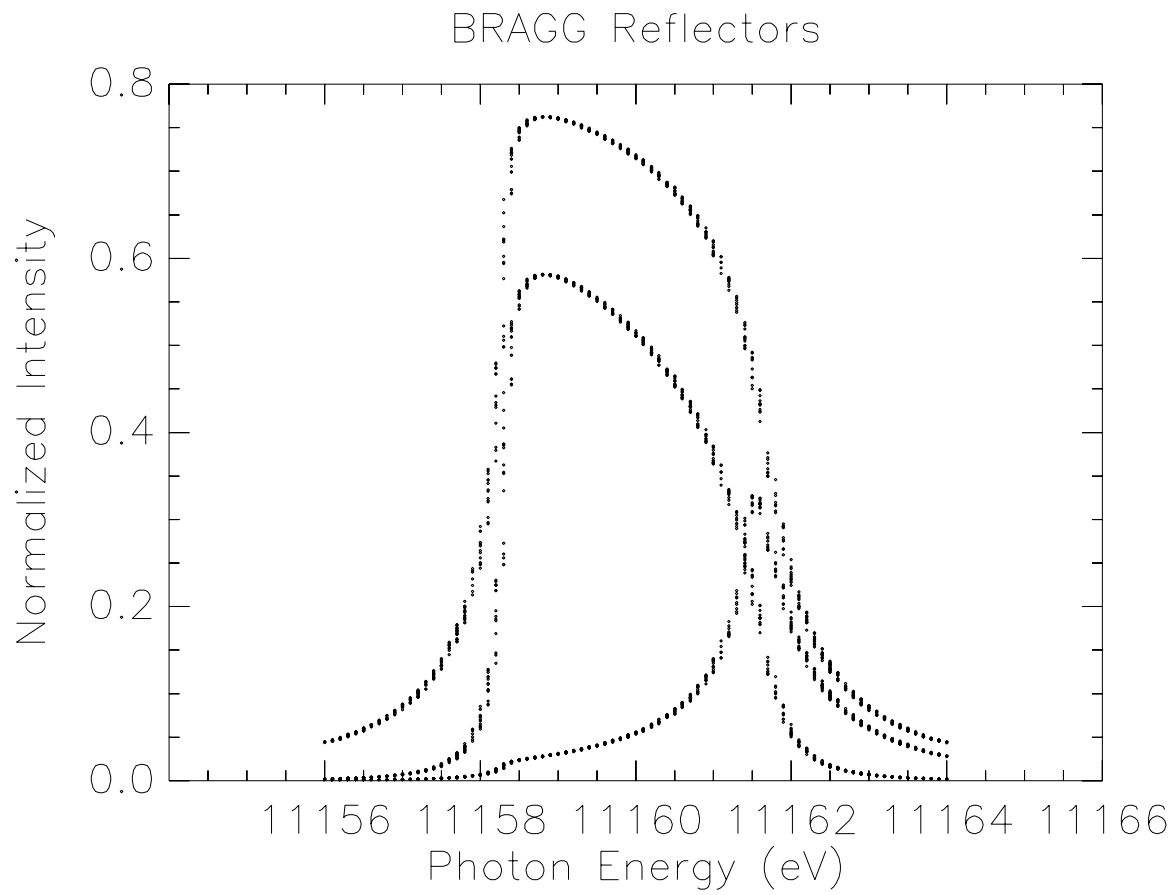


Figure 6.20: Comparison of BRAGG reflectors for continuous energy

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.

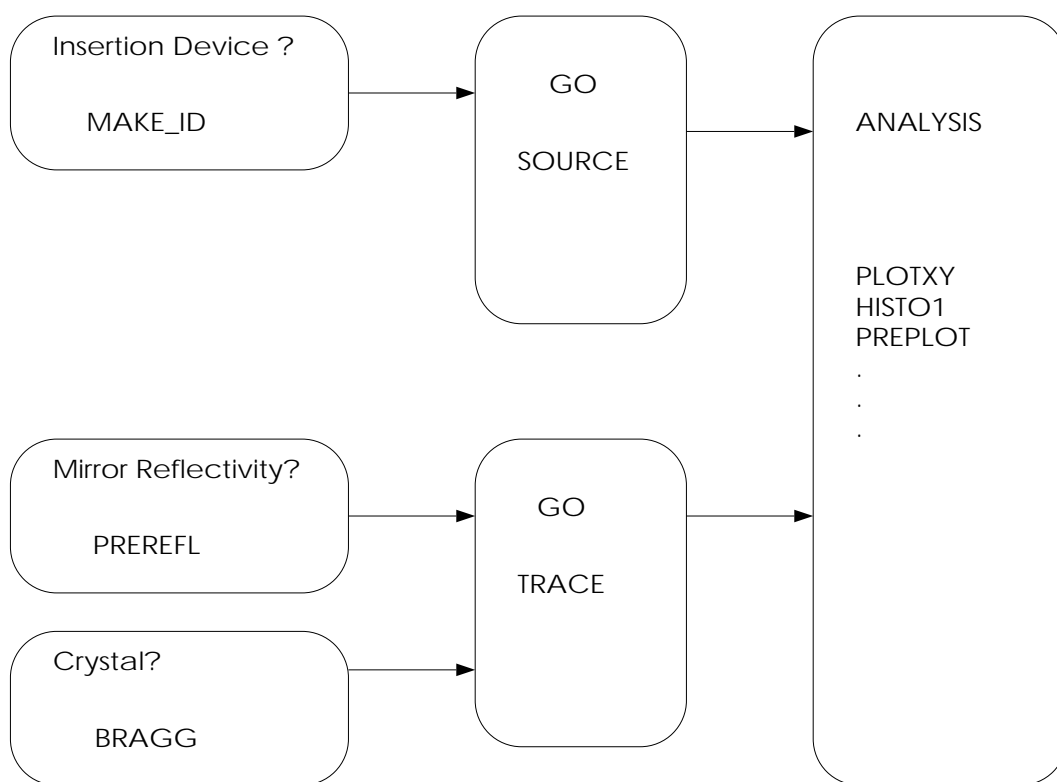
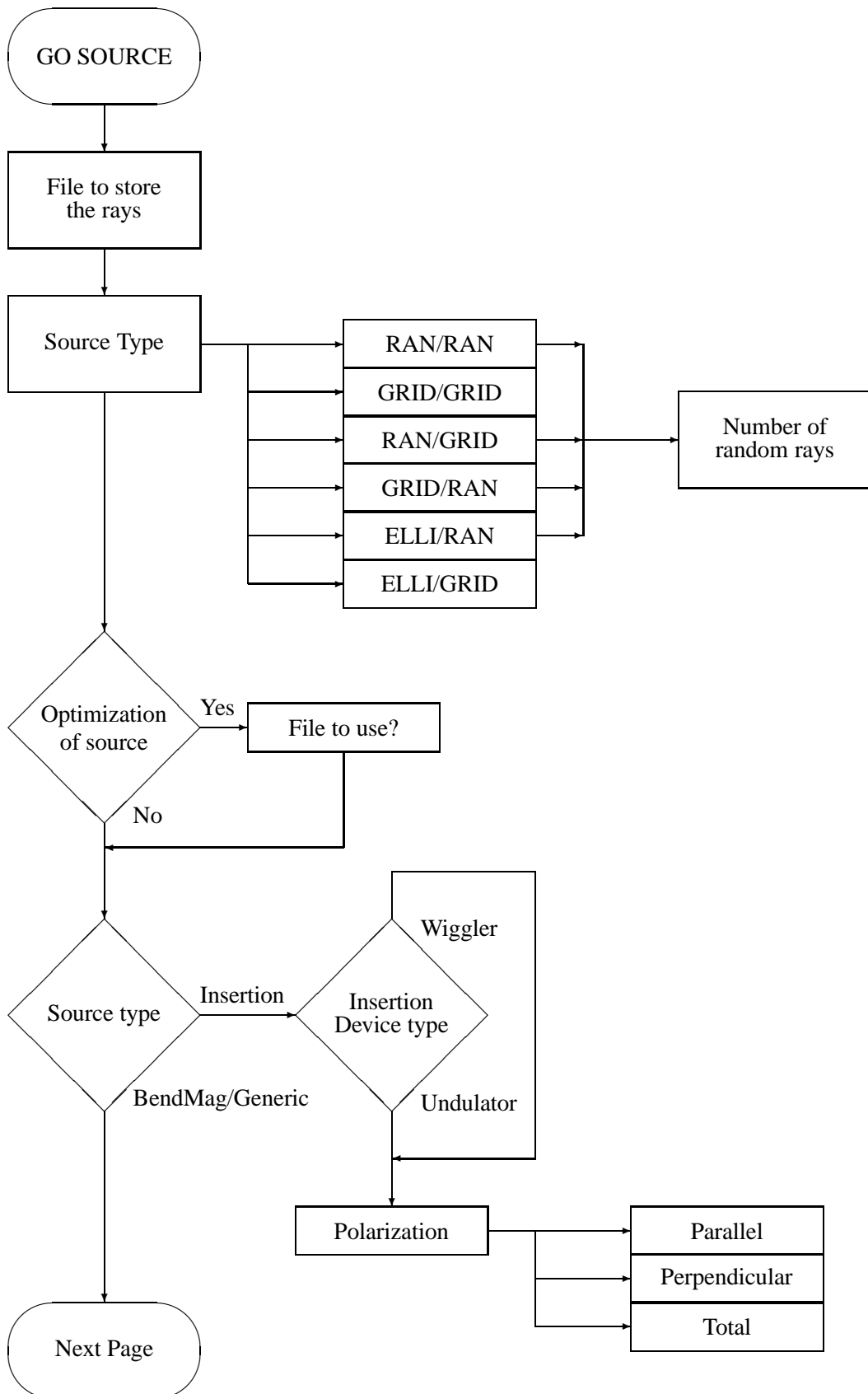
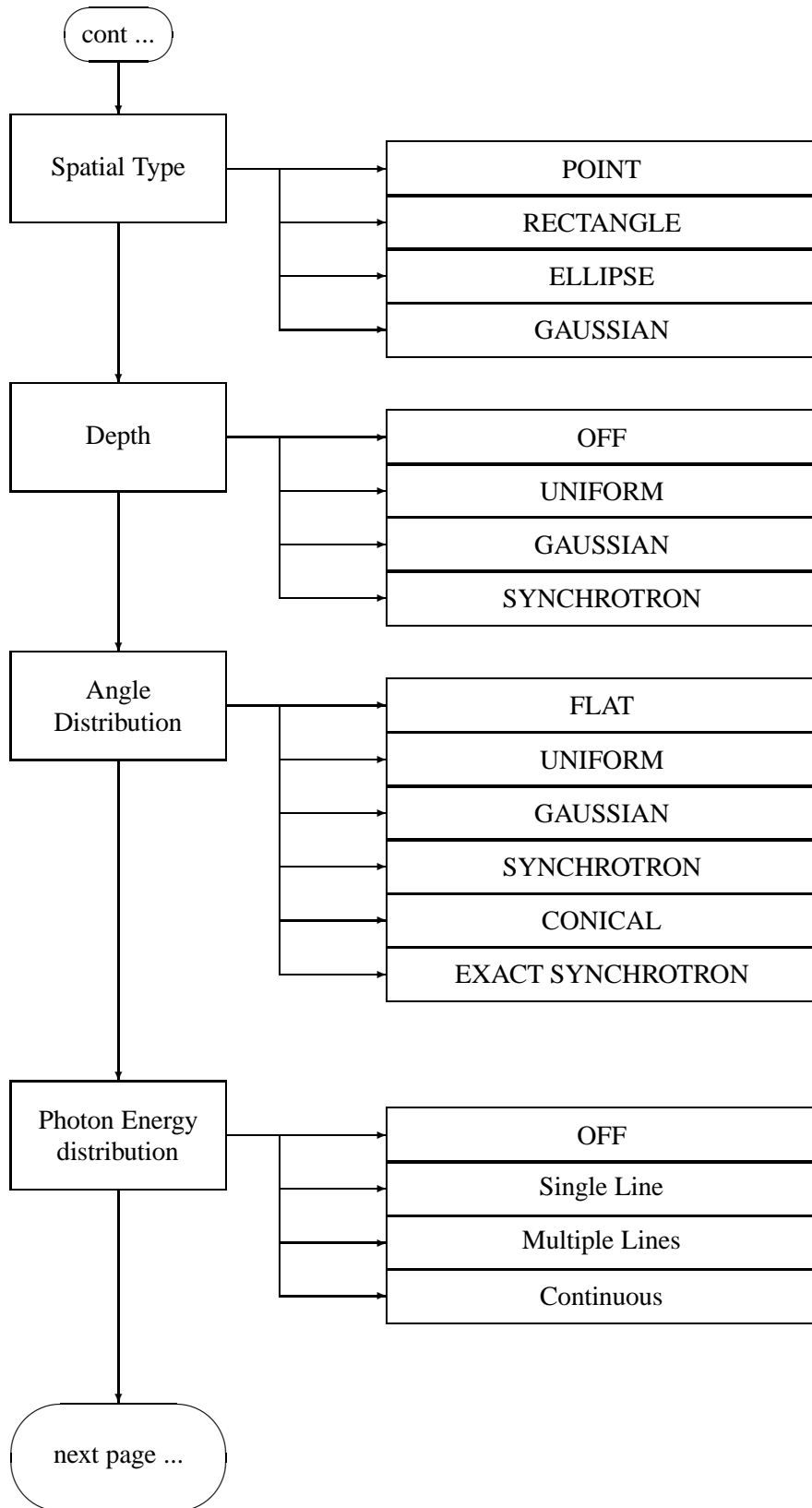
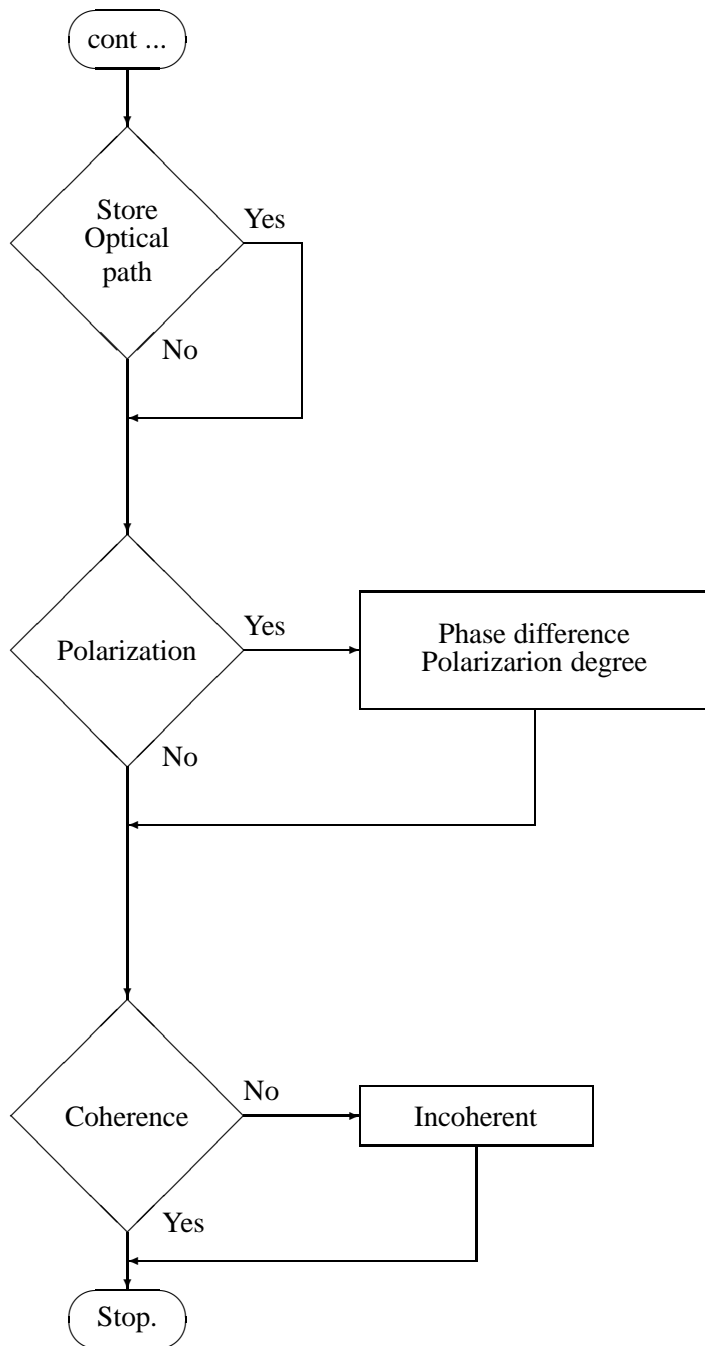
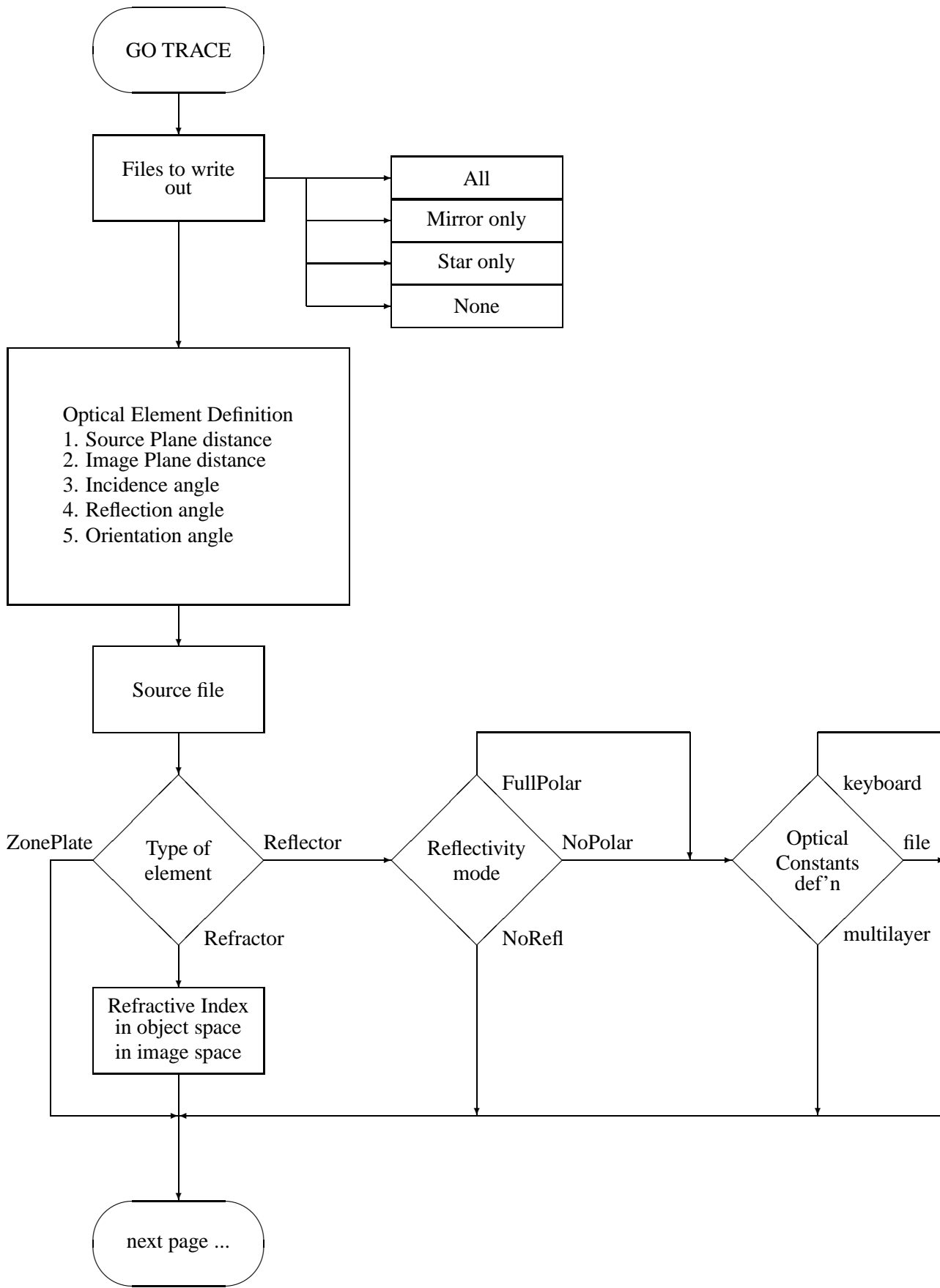


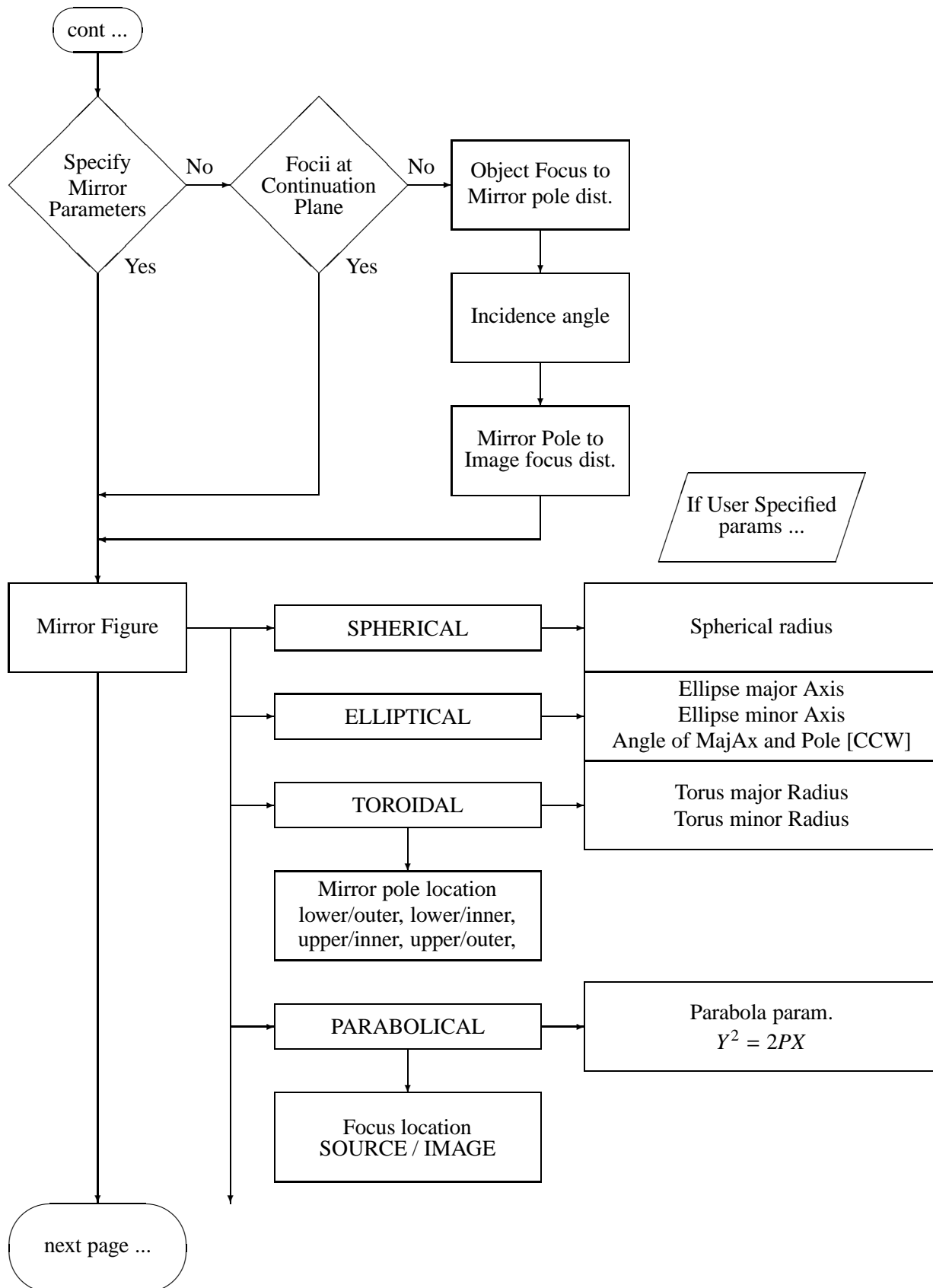
Figure A.1: Overview of program flow

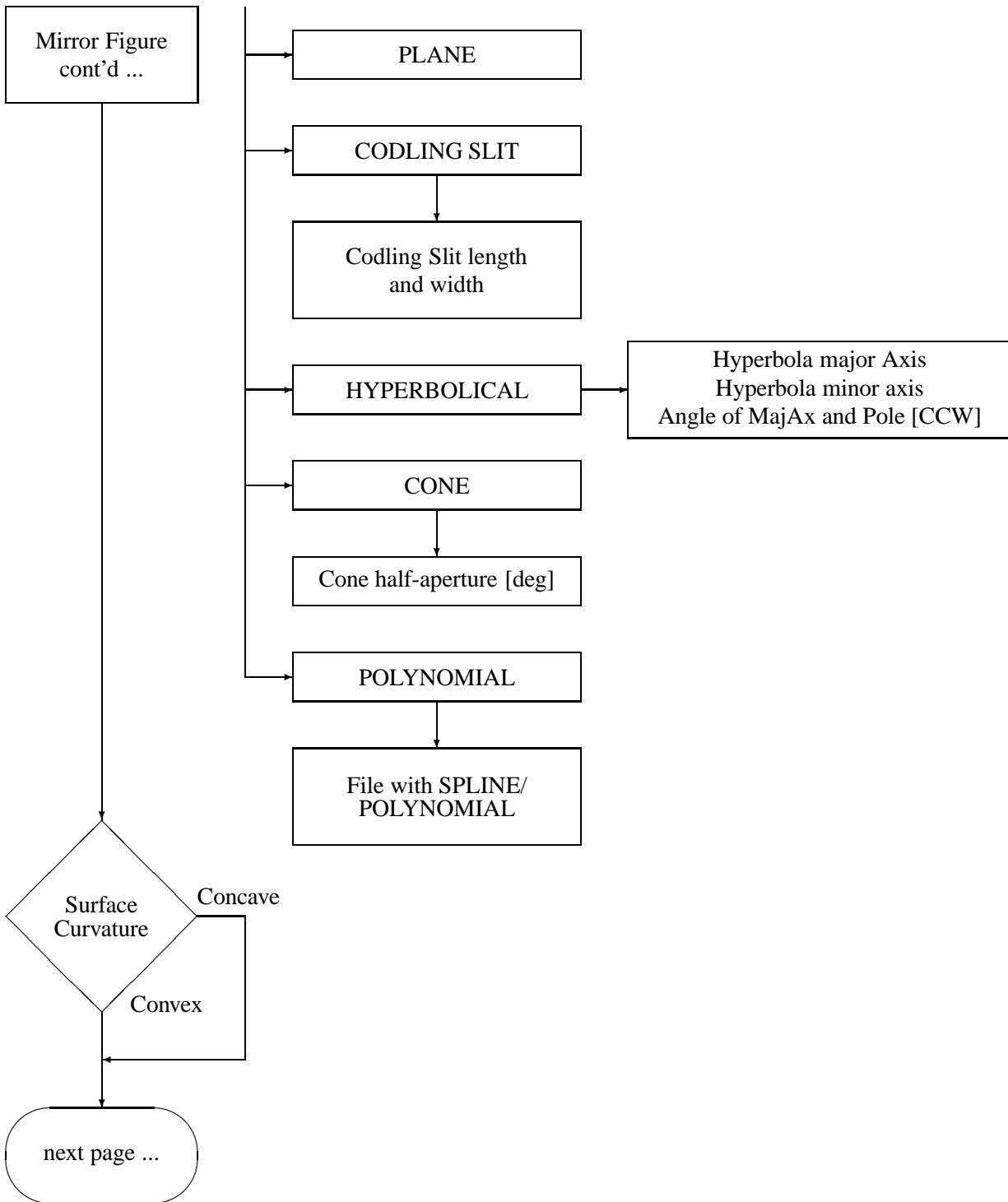


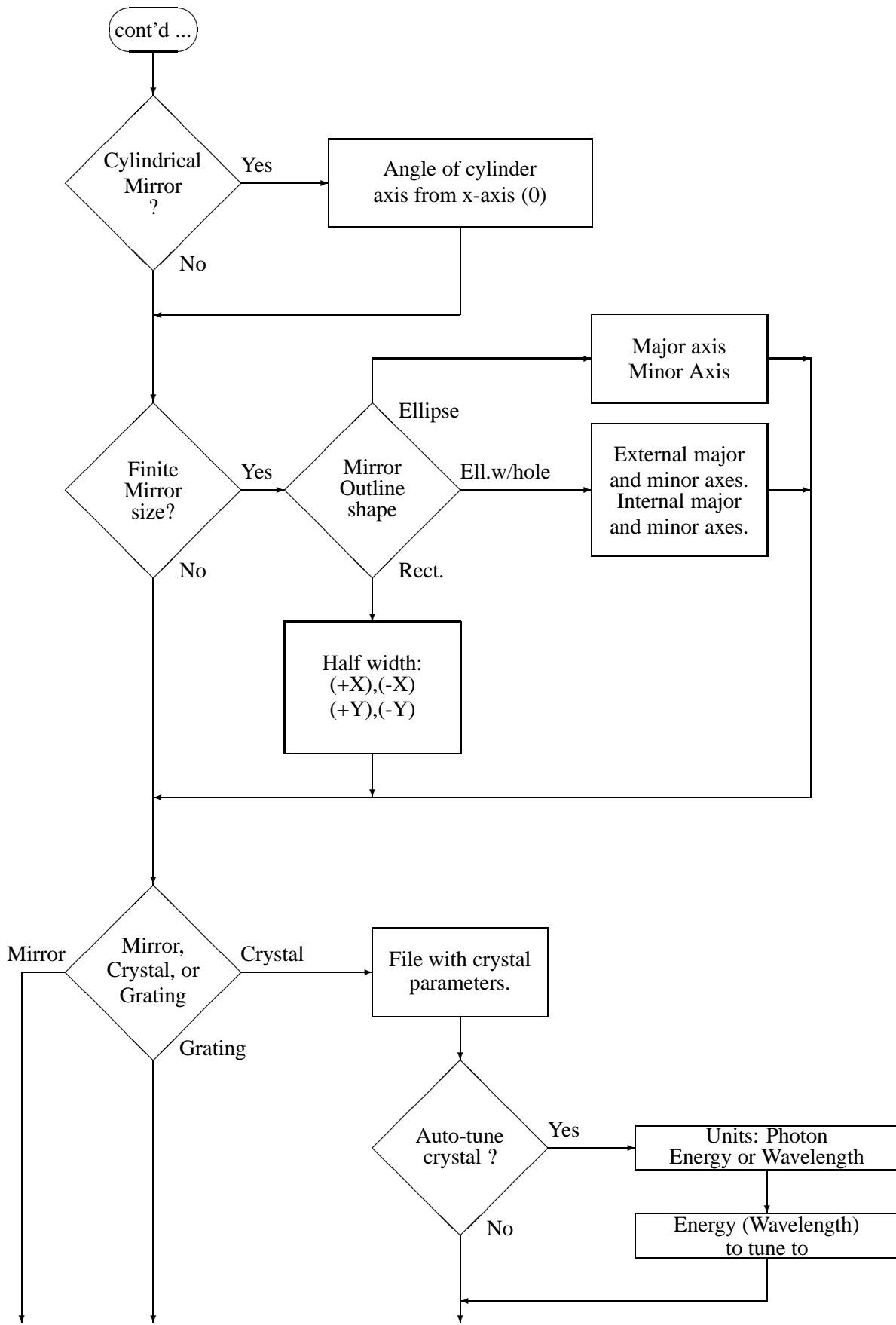








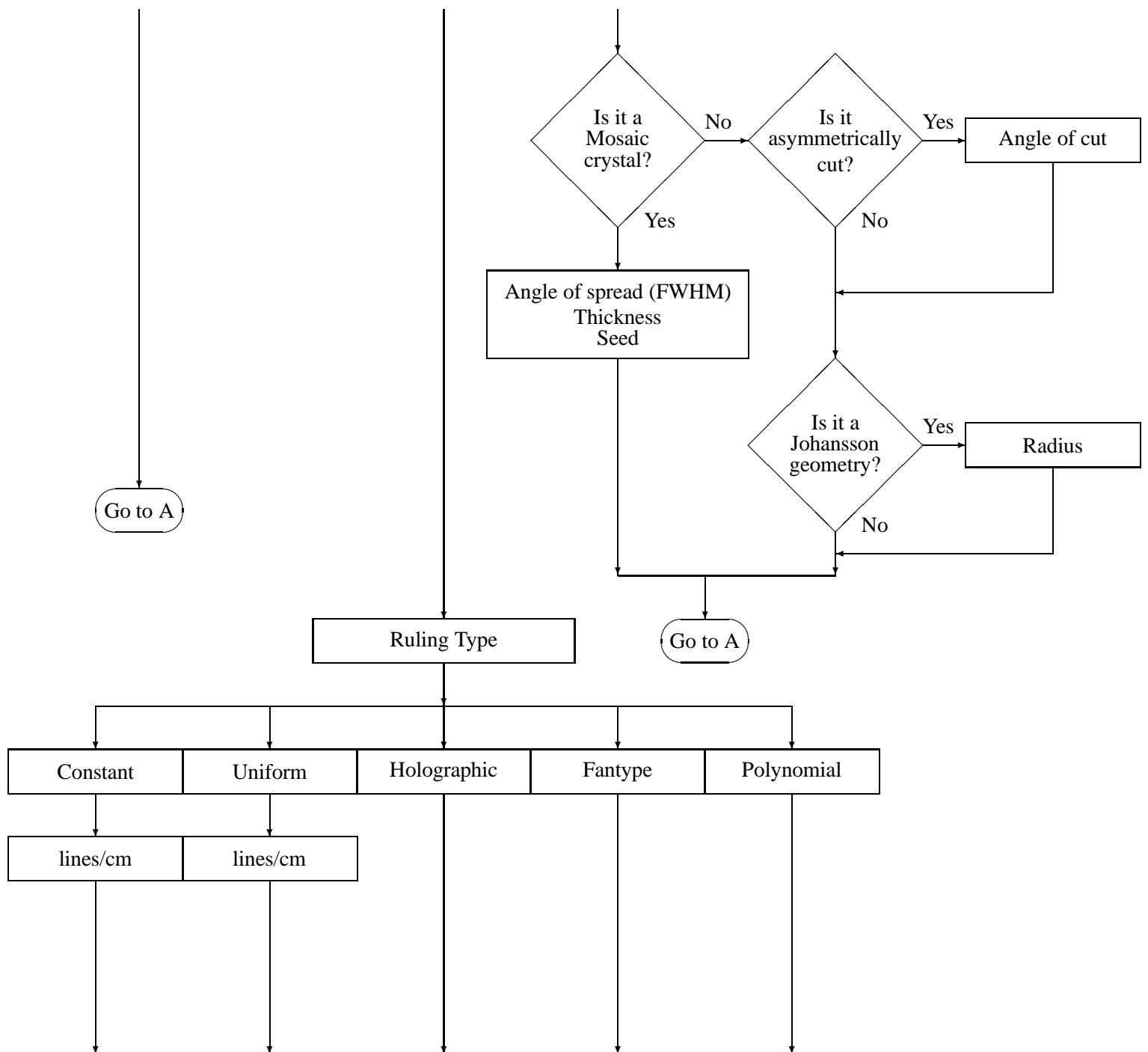




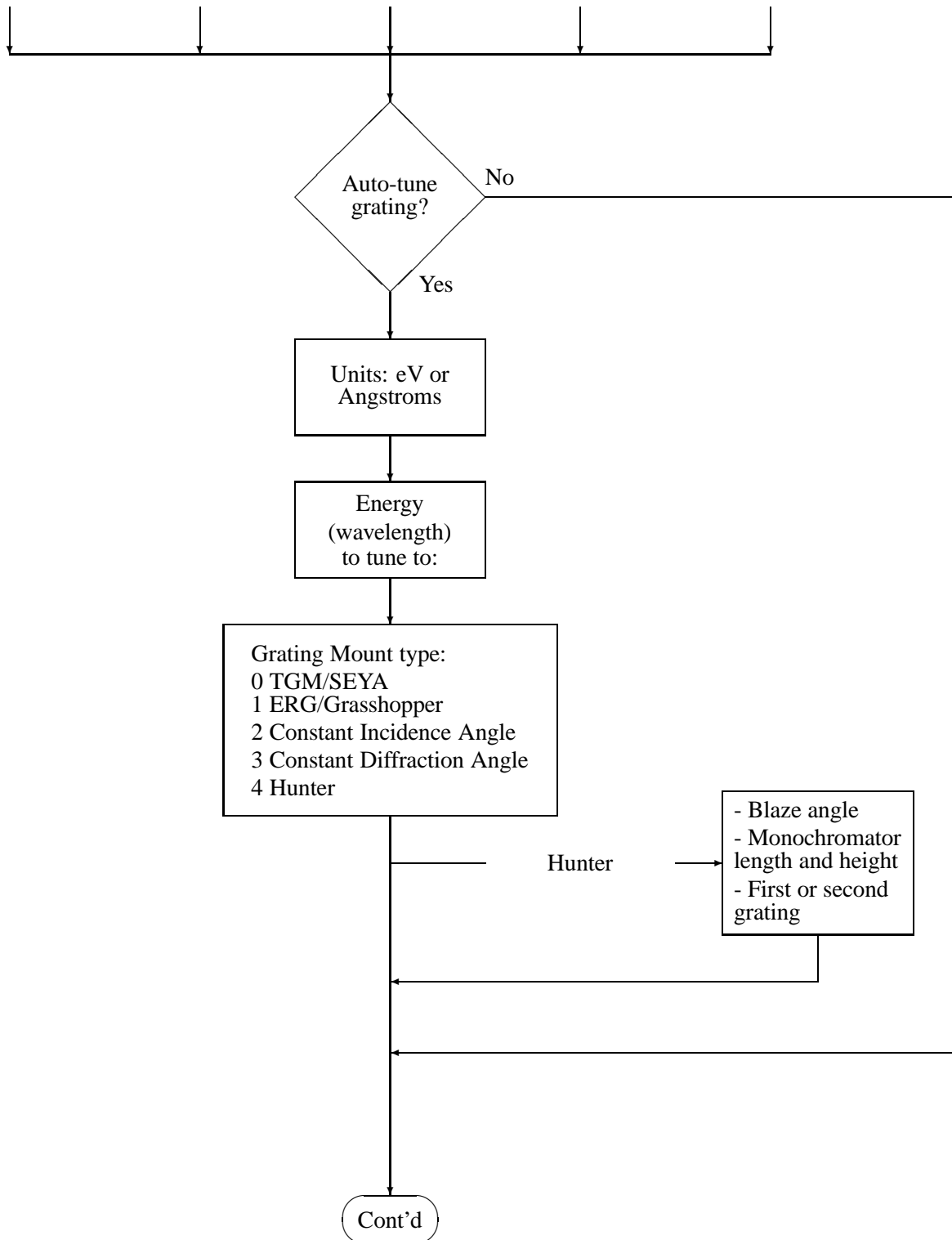
Mirror

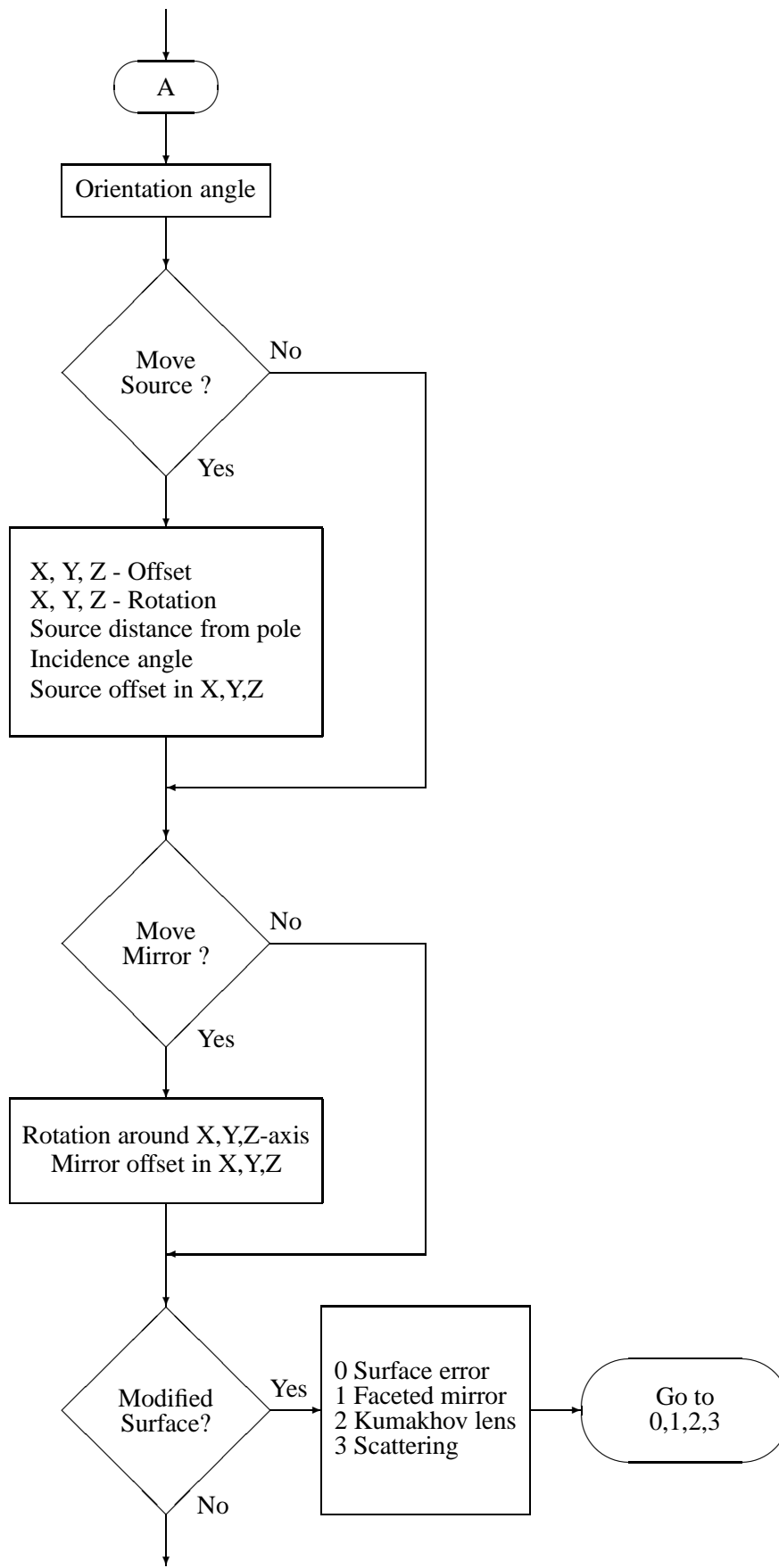
Grating

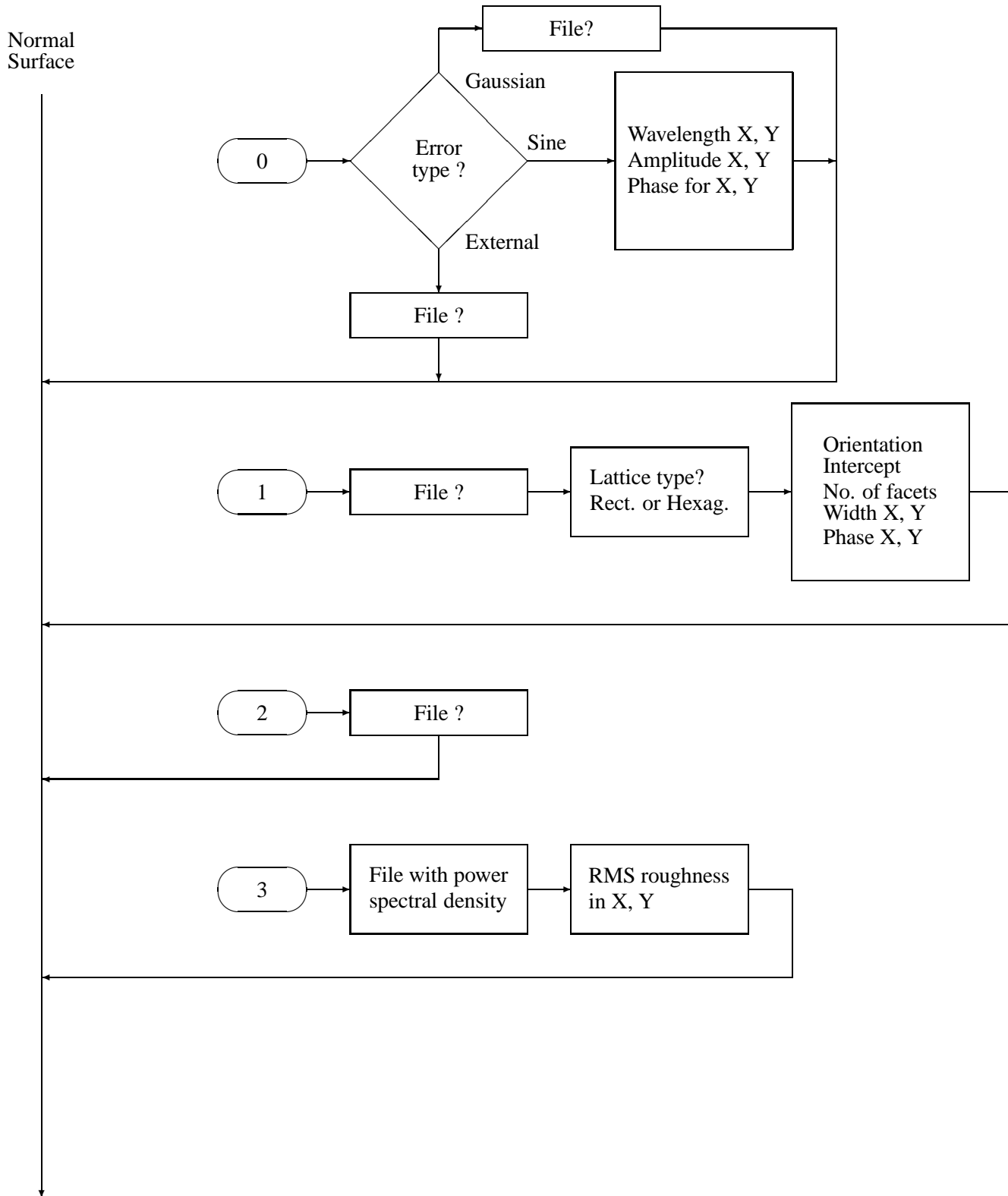
Crystal

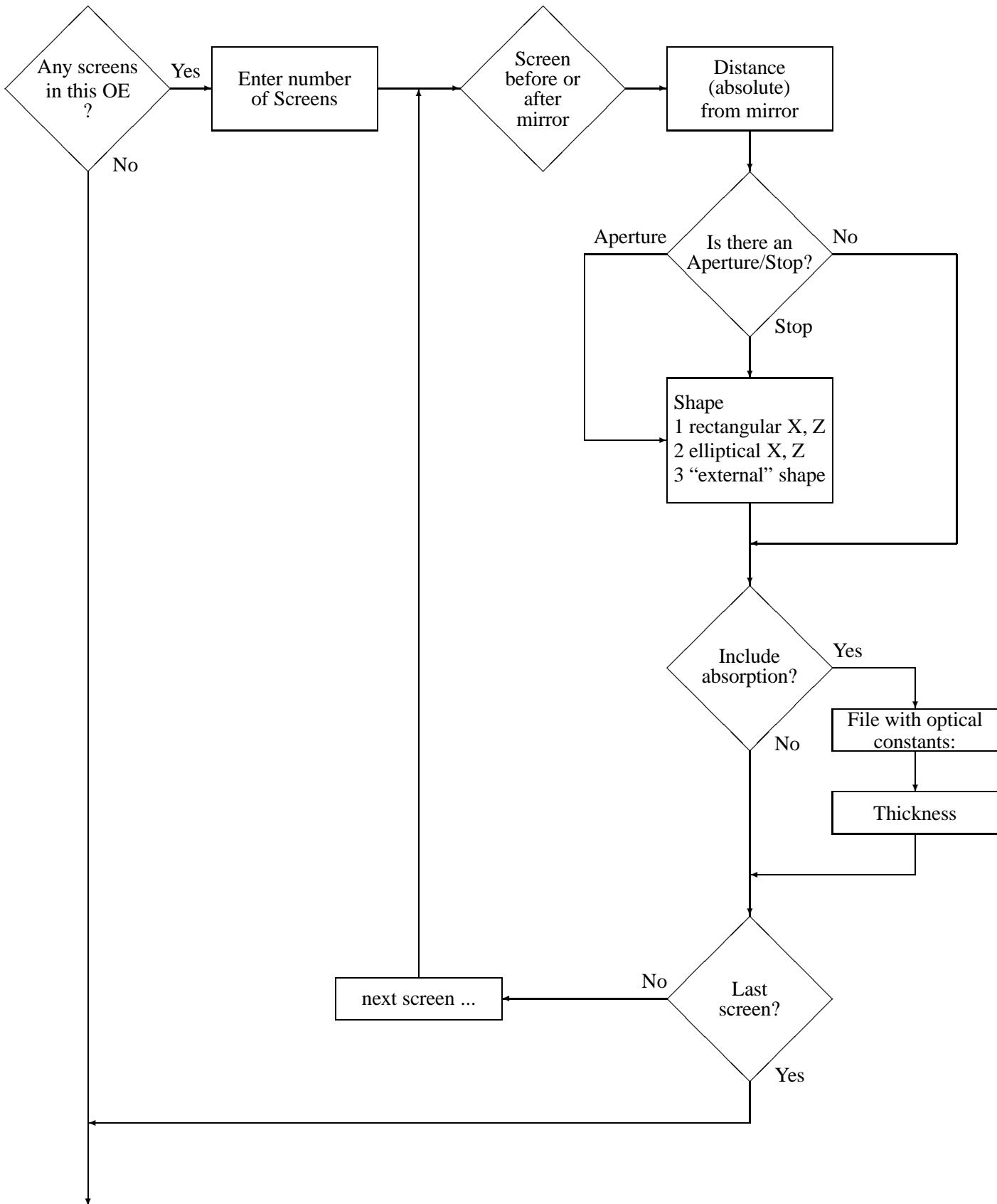


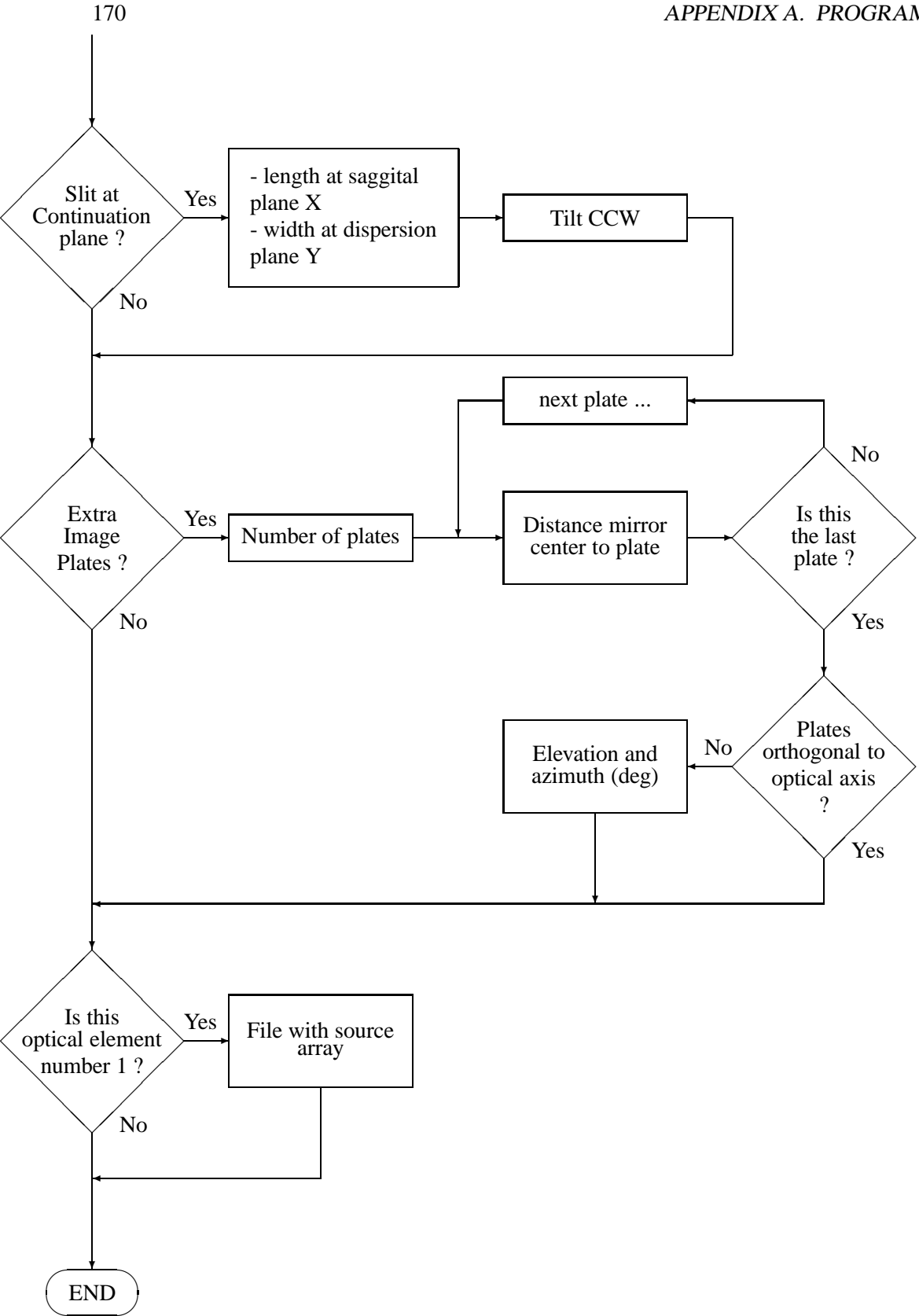
linear
quadratic
third power
fourth power











Appendix B

Glossary

<i>Active Surface</i>	A surface where the rays are reflected/refracted.
<i>Aligned System</i>	An optical system where nothing has been ‘moved’ when running SHADOW.
<i>Aperture</i>	A slit or hole at a screen that limits the latitude of the beam.
BATCH mode	Input mode that takes parameter files (START.xx, SYSTEM-FILE.DAT) generated by a previous input session and supplies them to SHADOW for a re-run. You will simply be prompted for these parameter file names.
<i>Beam</i>	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.
<i>Beamline</i>	The hardware implementation of an optical system used to relay with or without monochromatization the beam from source to sample.
<i>Bins</i>	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.
<i>Blaze</i>	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 <i>Gratings</i>).

<i>BOF</i>	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.
<i>Central Ray</i>	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.
<i>Collimated</i>	The condition of a beam in which all rays are parallel, i.e., the object/image is at infinity.
<i>Continuation Plane</i>	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.
<i>Cylindrical Figure</i>	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.
<i>DCL</i>	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.
<i>Diffraction Grating</i>	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.

<i>Diffraction Limit</i>	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: $\delta = \frac{\lambda}{2N.A.}$
<i>Diffraction Limited Optics</i>	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.
<i>Diffraction Order</i>	See Order.
<i>Element</i>	The part of an optical system that encloses an active surface.
<i>ERF</i>	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.
<i>External</i>	Pertaining to the definition of an optical element; the parameters are supplied by the user rather than being computed by SHADOW.
<i>Figure</i>	The mathematical function describing the surface of a mirror or of a lens. We speak of elliptical figure, etc.
<i>Figure Limited Optics</i>	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).
<i>Flag</i>	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.
<i>Footprint</i>	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:

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

where θ_i and θ_t are the angles of incidence and transmission respectively, and R_{\perp} and R_{\parallel} correspond to the reflectivities in the perpendicular (s-polarization) and parallel (p-polarization) directions with respect to the plane of incidence.

Geometrical Optics

The study of an optical system purely on the basis of geometrical relations between rays and surfaces.

GOTO

MENU mode command that allows the user to set the pointer to a particular OE. Useful for forgotten screens or if you're in the (good) habit of DEFINing all OEs at once and then using the SELECT command to input parameters.

Grating Horizon

The wavelength such that, for a particular incidence angle, the diffracted first order would be at -90° , i.e., diffracted back and tangent to the surface. Longer wavelengths would be diffracted 'inside' the surface, so that the grating behaves like a normal mirror for wavelengths beyond the horizon.

Grating Mount

The particular optical system configuration chosen to implement an instrument. A mount is specified by the geometry of the grating element and by focal conditions. Also used, more loosely, to indicate a type of scanning action, like in "TGM mount": this simply means a mount with constant included angle and rotation achieved by simple rotation of the grating.

Grazing Angle

An Incidence or Reflection angle in which the rays are nearly parallel to the optical surface.

Groove Shape

Refers to a grating's grooves. They can be generally divided in lamellar, triangular or sinusoidal.

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.
<i>Marginal Rays</i>	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.
<i>MENU mode</i>	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.
<i>Momentum Space</i>	The “space” which is occupied by the angles that the rays make with respect to the <i>Y</i> axis. The angles are expressed by their components in the <i>X</i> and <i>Z</i> 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.

<i>Monochromator</i>	An optical instrument capable of transmitting a very narrow band-pass of a white spectrum. Normally consisting of one or more gratings/crystals in a particular mount.
<i>Namelist</i>	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.
<i>Normal</i>	A vector which is perpendicular to the surface in question. Usually located at the geometric center of an optical surface.
<i>Numerical Aperture</i>	The sine of the angle formed by a ray with the optical axis.
<i>Optical Axis</i>	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.
<i>Optical Efficiency</i>	The ratio of the number of photons departing to the number incident on an optical element (or system).
<i>Optical Element or O.E.</i>	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.
<i>Optical Path</i>	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.

<i>Optical system</i>	The collection of optical elements under study.
<i>Orders</i>	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.
<i>Phase Space</i>	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' .

<i>Physical Optics</i>	The study of an optical system that explicitly includes physical aspects, such as reflectivity, diffractions, etc.
<i>Preprocessor</i>	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.
<i>PROMPT mode</i>	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.
<i>Ray</i>	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.
<i>Ray Index</i>	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.
<i>Real Space</i>	The ordinary geometrical space. The real space coordinates for a ray are in columns 1, 2, and 3 in the BOFs.
<i>Reflection Angle</i>	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.
<i>Roughness</i>	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 <i>MUST</i> 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.
<i>Seed</i>	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.
<i>Shape</i>	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 <i>Profile</i> .
<i>Sigma</i>	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.
<i>Source Depth</i>	The distribution of the source points in the <i>Y</i> direction.
<i>Source Distance</i>	The distance along the <i>Y</i> axis from the source or previous continuation plane to the next optical element in the system.
<i>Source Limited Optics</i>	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.
<i>Virtual Image</i>	Rays emerging from an OE or OS in image space are diverging, so image appears to exist in object space.
<i>Virtual Object</i>	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.