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Final Report

SOFTWARE TO MODEL AXAF-I IMAGE QUALITY

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Appendix 1: "Software to Model the Performance of X-Ray Telescopes", a copy of the paper presented at the SPIE Aerosense Conference, April 1995.

Appendix 2: The Command Mode GRAZTRACE (GT2) User Manual*

Appendix 3: The Convolve User Manual*

Appendix 4: The GRAZTRACE Software Reference Manual*

* The user manuals listed as appendices 2,3 and 4 consist of several hundred pages and, therefore, are not being distributed to everyone. The copies of these manuals have been supplied to the COTR at MSFC. Other interested persons can obtain a copy of these manuals from the authors listed on the cover page.

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ABSTRACT

This final report describes the work performed under the delivery order number 117 from May 1994 through June 1995. The scope of work included a number of software development tasks in support of the AXAF-I program. The objective of these tasks was to continue the development of the integrated optical performance modeling software for AXAF-I. A number of new capabilities and functions have been added to the GT2 software, which is the command mode version of the GRAZTRACE software, originally developed by MSFC.

Main body of the software consists of more than 10,000 lines of source code written in FORTRAN 77. The IMSL mathematical and statistical library has been used for the data analysis functions. The new PV-WAVE graphics package is used for producing the 2-D, 3-D, color, and shaded plots to depict modeling results. More than 70 routines have been developed to cover the user interface, data management, data interface, ray-trace, image characterization, and convolution modeling. Currently the software is running on SUN/SPARC station (ZEUS) at MSFC Optical Design Branch.

① The software is under the management of source code control system (SCCS) to keep track of any updates that are made, and prevent accidental deletion. More than 110 commands are available to manipulate the data, perform ray-trace, modeling and analysis, set system parameters, and execute the utilities. The 3-character mnemonic commands are used for all functions. Automatic command syntax prompt has been provided if the exact command input format is not known. On-line help has also been provided to obtain a detailed explanation of the commands.

More than 60 routines are accessible in the library to allow the users to write their own FORTRAN programs and perform specific analyses. Makefile, makerules, and user routine templates are provided for the users to program, compile, and link their customized programs.

Up to 50 surfaces in series with grazing incidence conic or flat shape are allowed in the analysis. The deformation data interface and deformation ray trace allow performance predictions for structural and thermal distortions of the mirrors. Up to 200,000 rays with up to 15 energy levels can be traced simultaneously with various ray patterns, in addition to tracing a single ray.

The result can be saved in ray file with intercept coordinates, ray directions, entrance coordinates, and accumulated weights for all energy levels. Statistical image analysis can be performed to obtain the centroid and RMS of the image. The refocus feature allows the user to find the best focal plane location.

The Image characterization and plotting capabilities consist of: Encircled Energy Distributions, Spot Diagrams, Point Spread Functions, and Point Spread Function Contour Plots. The convolution analysis capability has been provided to convolve the image with the x-ray source geometry, surface scattering, and detector scan patterns. Linear scattering distribution, random

scattering distribution, and various other scattering patterns can be used. Rectangular and circular detectors with various scan patterns can also be modeled.

Macro or sequential commands are allowed in the command mode operation. The command log and/or output log are automatically saved, and are available for later use, if needed. The operating system shell is provided so the user can execute system commands without quitting the program. The variable and array inquiry have been provided to check the value of any parameter for the system under analysis.

A structural data interface has also been developed for the EAL (old SPAR) finite element analysis FEA program, which is being used by MSFC Structural Analysis group for the analysis of AXAF-I. This interface utility can read the structural deformation file from the SRAR program, and convert the data to a suitable format that can be used for the deformation ray-tracing to predict the image quality for a distorted mirror.

A technical paper describing the modeling software developed under this contract was presented at the SPIE's Aerosense '95 conference held at Orlando, FL in April 1995. A copy of this paper is included with this report as appendix 4.

1. INTRODUCTION

Marshall Space Flight Center (MSFC) is involved in overseeing the design, development, construction and testing of the Advanced X-ray Astrophysics Facility-Imaging (AXAF-I). The High Resolution Mirror Assembly (HRMA) will collect and focus the x-rays to the 0.5 arc-second resolution level. The HRMA will include the recently completed four pairs of nearly cylindrically-shaped mirrors, which are assembled in Wolter type I configurations. The largest of these mirrors has a diameter of approximately 1.2 meters, and the smallest mirror is about 0.6 meters in diameter. The x-rays will graze off the inside surfaces of the nested mirror pairs and will be directed to the system focus about 10 meters behind the center of the HRMA. The mirrors are constructed from Zerodur glass and the optical surfaces will be coated with iridium.

Specialized optical analysis software has been used by MSFC and the AXAF-I contractors in order to design, tolerance, interpret ground test data, and predict the on-orbit image quality. This software largely consists of in-house collections of programs developed at the various institutions and companies involved with the AXAF-I program. The commercially available optical analysis and design programs, such as CODE V and SYNOPSIS, are optimized only for the normal-incidence optics, and are not suitable for modeling the performance of grazing-incidence x-ray systems.

A modular user-friendly computer program for the modeling of grazing-incidence type x-ray optical systems has been developed. This comprehensive computer software GRAZTRACE covers the manipulation of input data, ray tracing with reflectivity and surface deformation effects, convolution with x-ray source shape and x-ray scattering. The program also includes the capabilities for image analysis, detector scan modeling and graphical presentation of the results. A number of utilities have been developed to interface the predicted mirror structural and thermal distortions with the ray-trace.

There is no commercially available (or published) program tailored for the analysis of grazing-incidence type optical systems. The GRAZTRACE program has the analysis and graphics capabilities similar to those of the standard design and analysis programs (CODE V and SYNOPSIS) for normal-incidence optical systems. This software is written in FORTRAN 77 and runs on a SUN/SPARC station. An interactive command mode version and a batch mode version of the software have been developed.

2. PROGRAM STRUCTURE AND SYSTEM REQUIREMENTS

The GRAZTRACE software currently can run on a SUN/SPARC station 10 with 64 MB physical memory (RAM) and 176 MB virtual memory (disk swap space). The software structure, management and the two operating modes of the program are briefly described as follows:

2.1 Software structure

The main body of the software is written in FORTRAN 77. The data analysis part of the software uses the IMSL mathematical and statistical library. The graphics part uses the PV-WAVE graphics package. The main body of the software consists of the user interface, system data management, structural, thermal, and metrology interface, ray-trace routines, image characterization, and image convolution and detector modeling. The on-line help system and documentation are also available. The total number of routines is more than 70, with over 10,000 lines of source code.

2.2 Software management

The source code of the software is managed by source code control system (SCCS), which monitors all modifications. The source files are protected by allowing only one person at a time to make changes, by maintaining a record of all changes, and by rebuilding any previous version when necessary. Regular backups are also being used for the software management during the development process.

GT2 input command sequence files are being generated for analysis cases similar to those studied for AXAF-I, VETA-I, AXAF-S, and SXI systems. The results from GT2 are compared to the results of running the original GRAZTRACE/CONVOLVE software. The cases tested exercise most of the program options on actual or proposed x-ray systems for which there is already a knowledge base. Any time that changes are made to GT2, these test cases can be rerun as a check to the program.

2.3 Operation modes

Two operation modes are available: interactive command mode and a batch program mode. In the interactive command mode, more than 100 commands are available to manipulate optical prescription data, perform various ray-trace and performance analyses, set system parameters, and utilize some utilities. The 3-character mnemonic commands are used for all functions. The command syntax will automatically prompt if the exact command input format is not known. In batch program mode, more than 60 user routines are accessible to allow the users to write their own programs and to perform specific analyses.

3. PRIMARY PROGRAM FUNCTIONS

3.1 Help function

On-line help is available in the interactive command mode version of the GT2 program. The users can type *help* or "?" mark followed by the command mnemonic to obtain a detailed explanation of the command. If a user types *help* or "?" mark followed by a non-existent command, a list of valid commands is displayed. By typing *help* or "?" mark only, the information about the current or latest input command can be obtained. The *Help* file for the on-line help function is a plain ASCII text

file. A help function routine has been developed to match the command mnemonics and to search for the related explanatory text.

3.2 Optical system prescription

A total of 50 surfaces are allowed in the analysis. The available surface types for the ray-trace are grazing incidence conic or flat type of surfaces. The conic types are: (i) a direct calculation with no deformation; (ii) an iteration including the deformation file data; and (iii) a direct calculation followed by an iteration including the deformation file data.

The permissible surface aperture types are an annular (circular) aperture defined by the minimum and maximum radii and a rectangular aperture defined by the width, height, and orientation. The surface aperture can also be limited by defining the minimum and maximum axial limits of the surface. The allowed surface obscuration types are annular (circular) and rectangular.

3.3 Structural/thermal interface

A structural and thermal data interface has also been developed to extract deformation data from the standard output of COSMOS/M and NASTRAN finite element analysis programs. The deformation data is then used in the ray-trace to predict the performance of the mirror due to the structural and thermal distortions. No restriction is placed on the number of nodes for the structural analysis. The nodes can be in a random order and randomly spaced to optimize the structural analysis. Interactive options are provided for the coordinate transformation, coordinate shift, scaling, and axial length change.

The FEA to GRAZTRACE data conversion program now consists of the following subroutines:

<code>drinfea.f</code>	main interactive conversion program
<code>spa.f</code>	SPAR data extraction
<code>mas.f</code>	NASTRAN data extraction
<code>rcos.f</code>	COSMOS/M data extraction
<code>extend.f</code>	extend data 30 degrees
<code>modify.f</code>	modify data by shifting the coordinates and scaling

Currently, all these files and executable code are in the directory `/export/home/chen/stru/spar/drinfea` on ZEUS.

The new `spa.f` utility can read the node location and structural deformation data without any header restrictions (i.e. the header lines do not need to be identified by `$` and `*` symbols). Up to 20 lines of the header information from both of these files are echoed on the screen for the user information to ensure that the correct files have been read.

The data extraction, conversion and interpolation are processed in one program. The input data files for this utility are the EAL/SPAR output files consisting of the node location file and the node

deformation file, or one single file with both the node locations and deformations (as for the NASTRAN and COSMOS). The output file is the *.dfm for input to the GRAZTRACE.

Some other features of this conversion utility are summarized as follows:

1. The header of the *.dfm file can be keyed in by the user.
2. The symmetric data is automatically checked and mirrored to generate a complete data set if the input file consists of half of the data.
3. The output file can be for the parabola only, hyperbola only, or a combination of the parabola and hyperbola.
4. The mirror shell center, shell length, intersection location, and scale can be defined by the user. The default length of the shell is 100% of length used in the input data file.
5. A file existence check has been added for the output file to allow the user to overwrite the output file, if desired.

3.4 Ray tracing

A number of special methods and options have been provided for ray tracing due to the special nature of x-ray optical system. These options and features are described briefly in the following sections:

3.4.1 Wheel spoke ray pattern, random ray pattern, and individual rays

Because of the highly annular nature of aperture in the grazing-incidence optics, a rectangular grid can not be used to generate the rays for the ray-trace. Three wheel spoke and one random ray pattern generators are available. One wheel spoke ray pattern has a constant radial increment and a constant azimuthal increment arranged on the first surface annulus. The other modified wheel spoke ray pattern has a varying radial increment or a varying azimuthal increment to obtain a uniform area for each ray. A total of up to 200,000 rays can be generated and traced.

A single surface to surface ray-trace can also be performed for a specific ray for the given entrance coordinates and directions. This capability is useful for pin-pointing the vignetting or any other ray failure problem. It is also useful for exactly laying out the aperture stop and other parts of the system.

3.4.2 Source definition

Two types of x-ray source position definitions are provided to satisfy different preferences. A source position can be defined by the azimuth, elevation, and distance to the first surface center. The source

can also be defined as x, y, and z coordinates relative to the center of the first surface of the system.

3.4.3 Ray weights, energy levels, and delbets

Unlike any commercially available ray-trace program, the telescope entrance area, field angle, surface reflectivities and number of rays are used in the x-ray ray-trace in the GT2 program to calculate the intensity of each ray. The surface reflectivity for the grazing- incidence x-ray is a function of the incident angle and the x-ray energy dependent complex index of refraction for the surface coating. The ray weight is the effective area or collecting area for the traced ray. The ray weights are calculated for up to 15 x-ray energy levels. The complex indices of refraction as represented by the delbet parameters must be supplied for each energy level.

3.4.4 Focusing and image plane shift

A refocus function is used to find the focus position for the minimum RMS image radius. The ray intercept data and net focal plane shift are updated for the new evaluation plane. The image plane can also be shifted by any amount to perform a *through focus* performance evaluation. The ray intercept data and net focal plane shift are updated and the image statistics are recalculated.

3.4.5 Ray storage files

The ray-trace data can be saved to a ray file for further analysis. Up to 200,000 rays can be saved to a ray file with the ray intercept coordinates x, y and z, the ray directions dx/dz and dy/dz, the entrance coordinates x and y, and the ray weights for all energy levels. The header information, number of rays, number of energy levels, focal shift, focal length, and the number of header text lines are also saved.

3.5 Image characterization

Several basic image characterization functions are provided in this program to evaluate the x-ray system performance. The graphical plots and analytical data can be simultaneously displayed in the *X-Windows* environment as shown in Figure 1. Moreover, the GT2 program allows to display multiple windows simultaneously to depict the modeling results as shown in Figure 2. Some of the image characterization functions of GT2 software are briefly discussed as follows:

3.5.1 Centroid and RMS

A statistical image performance analysis is available to obtain the centroid of the image and the RMS image size. The extreme ray locations are also reported with a maximum and a minimum in both

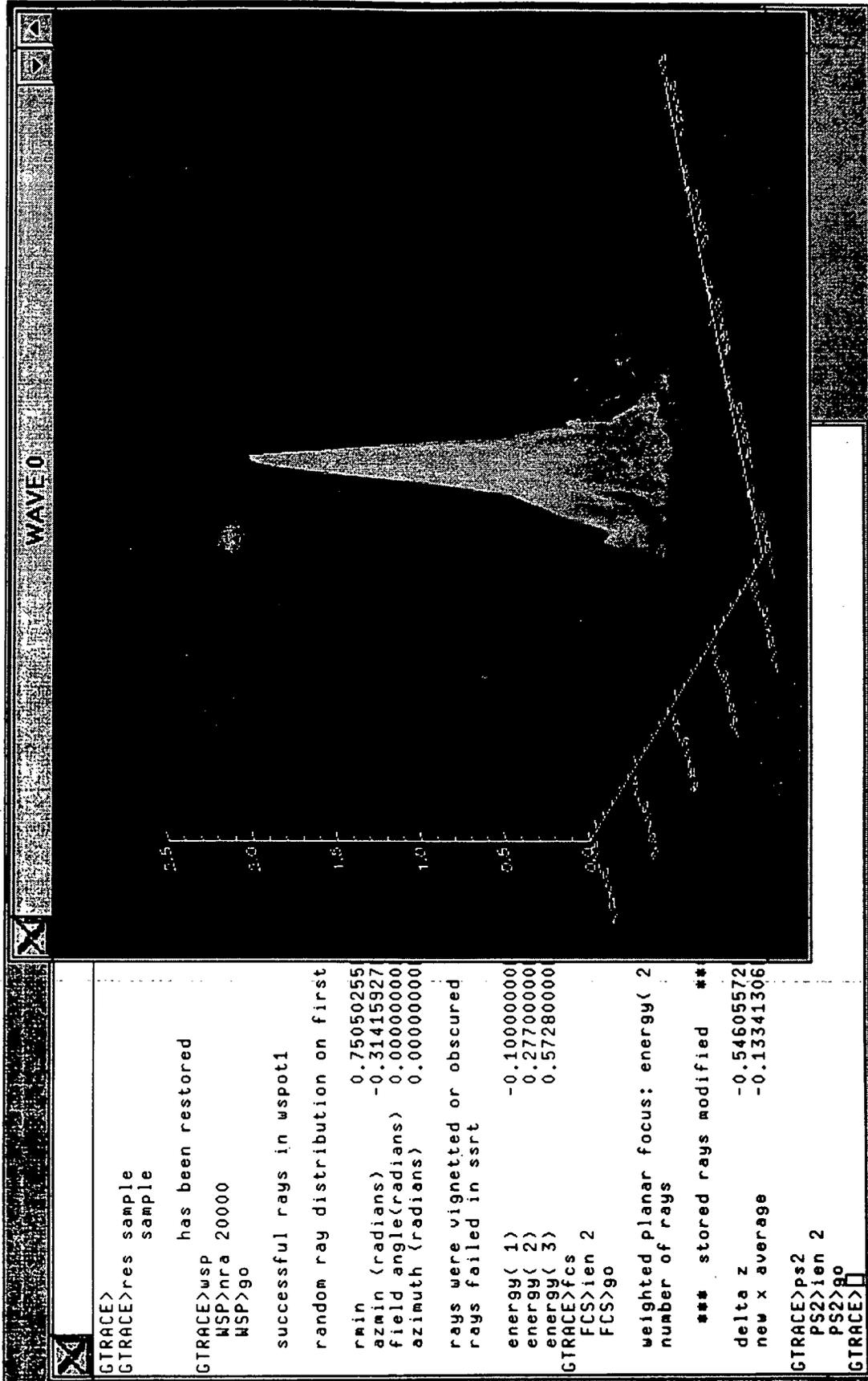


Figure 1. A sample GT Screen Display Showing the Graphical and Numerical Data Simultaneously

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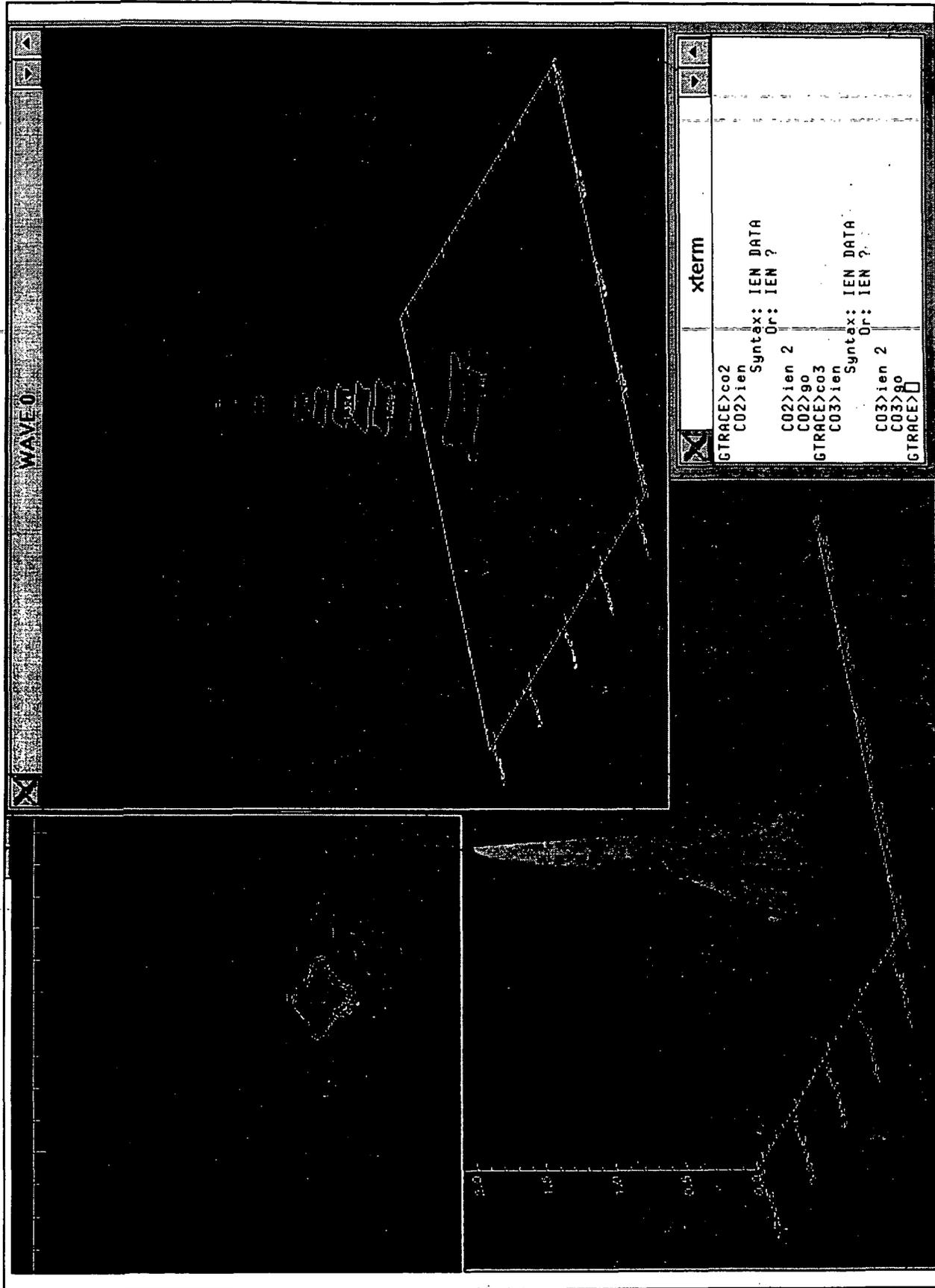


Figure 2. Multiple Windows Can Display the Modeling Results in Several Forms Simultaneously.

x and y directions. The statistics in arc-second units are also given. The RMS values in each direction and the total RMS value are also provided.

3.5.2 Encircled energy

The encircled energy distribution function is available to compute the radial energy distribution on the image plane. The function is in the form of a series of radii in the image plane within which certain fixed percentages of x-ray energy are contained. The table gives the circle radii which enclose 5%, 10%, ... 100% of the energy or any other defined percentage of the energy.

3.5.3 Spot diagram and PSF plots

Like any other optical analysis program, the spot diagram plots are used to check the result of the geometrical ray-trace. Figure 3 depicts a typical spot diagram for 20,000 rays traced through a sample x-ray system. Because of the weighted ray-trace nature of the GT2 program, the point spread function (PSF) plots are the primary form of visual presentation of the performance. Both 3-D mesh and 3-D color shaded PSF surface plots provide detailed information about the image performance. The meshed and shaded PSF plots produced by this program are shown in Figure 4. The 2-D, 3-D, and 3-D color contour plots are also provided to quantify the image quality as illustrated in Figure 5.

3.6 Convolution image analysis

The convolution capability has been provided to perform image analysis with x-ray source geometry, surface scattering, and detector scan patterns. These program features are briefly described as follows:

3.6.1 Convolution of image with rough surface scattering and other effects

To predict the performance of an x-ray system under the real operating conditions, the convolution analysis capability has been provided for the image to include the effects of rough surface scattering and other effects. The image ray data obtained by ray-trace is convolved with a predicted scattering distribution.

A general linear scattering distribution is prepared by a separate program called EEGRAZ. This data is stored in a file and is then read into the GT2 program to convolve it with the ray-trace image data or pre-stored image data from a ray data file.

The ray image data from the GT2 or ray file includes the x and y positions of the ray at the first surface so that the tangential and sagittal ray scatter directions can be determined. Some other distribution models are also available to generate the random distribution for the modeling of

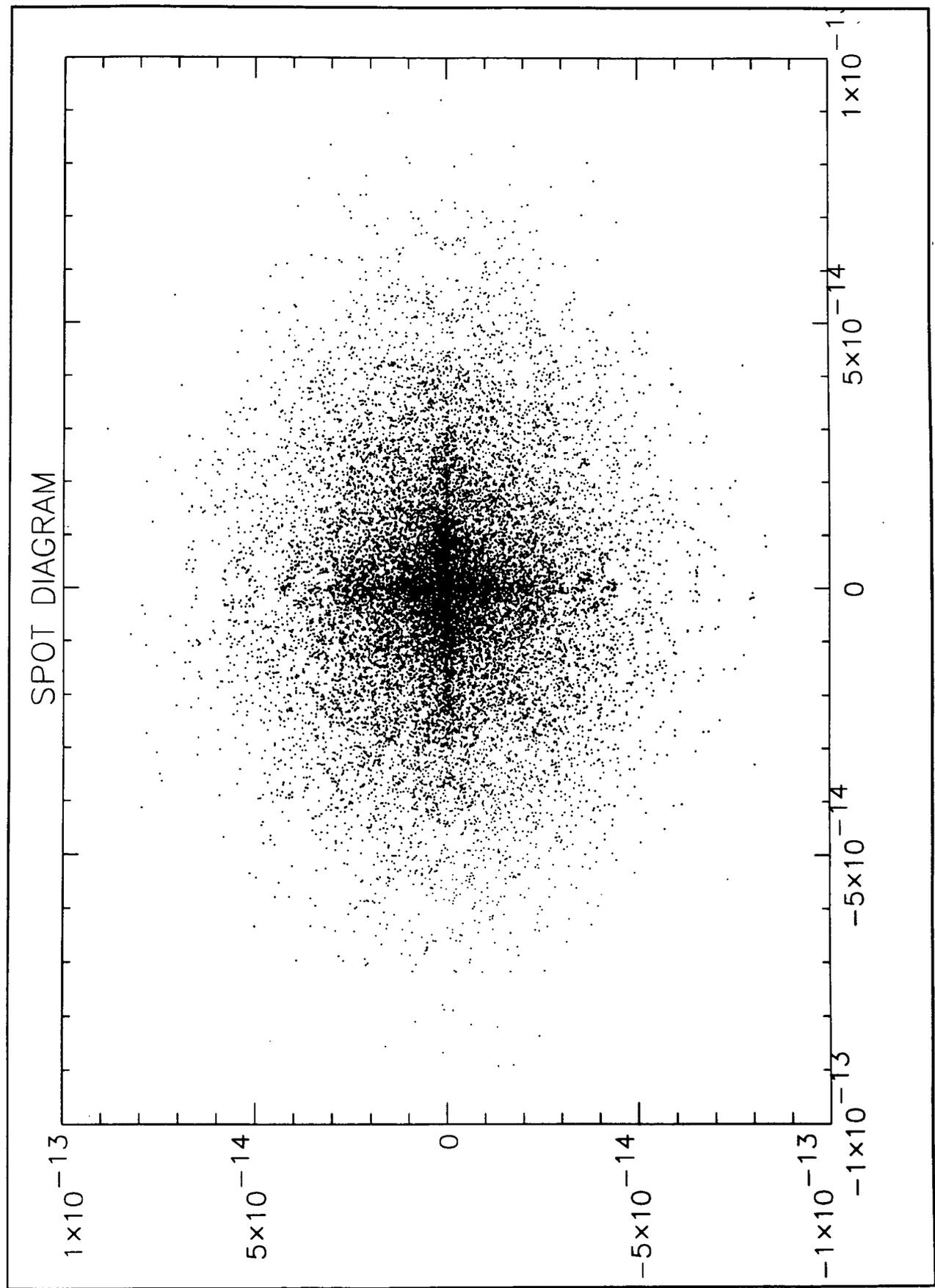


Figure 3. A Typical Spot Diagram for 20,000 Rays Produced by GT2

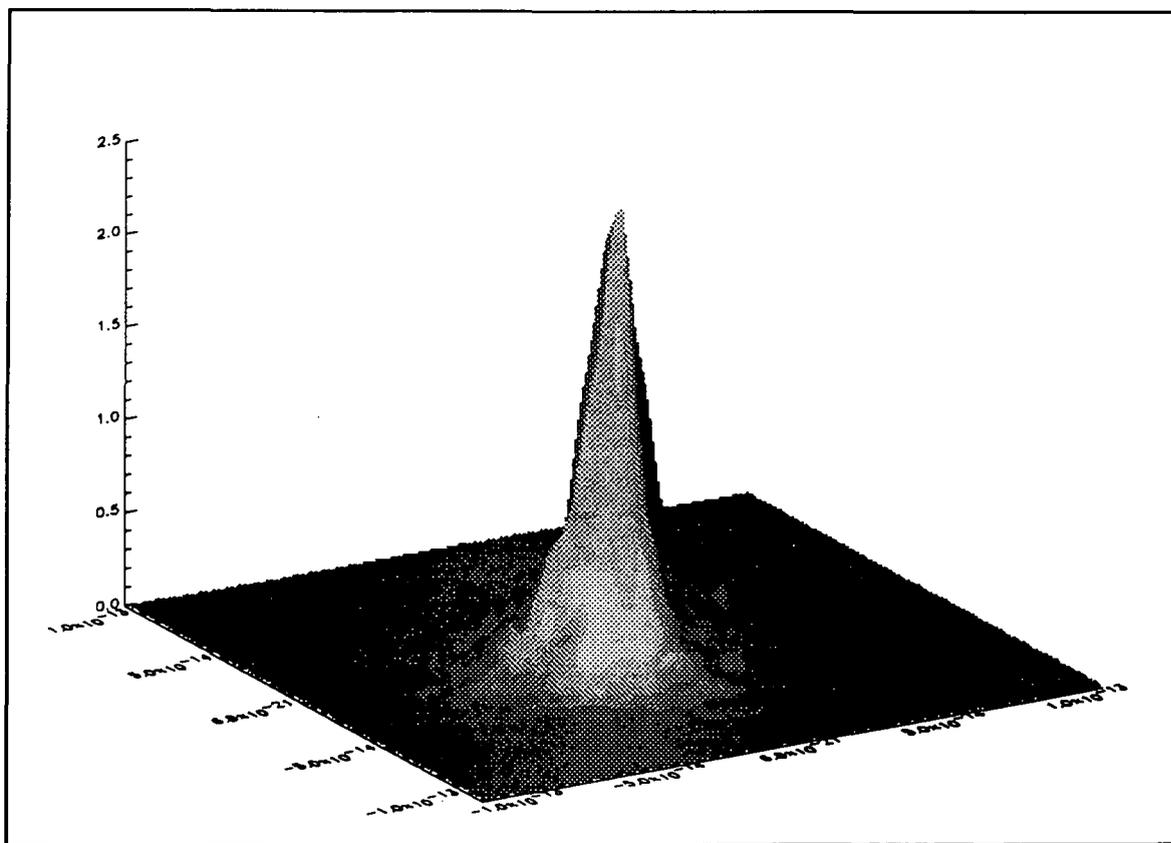
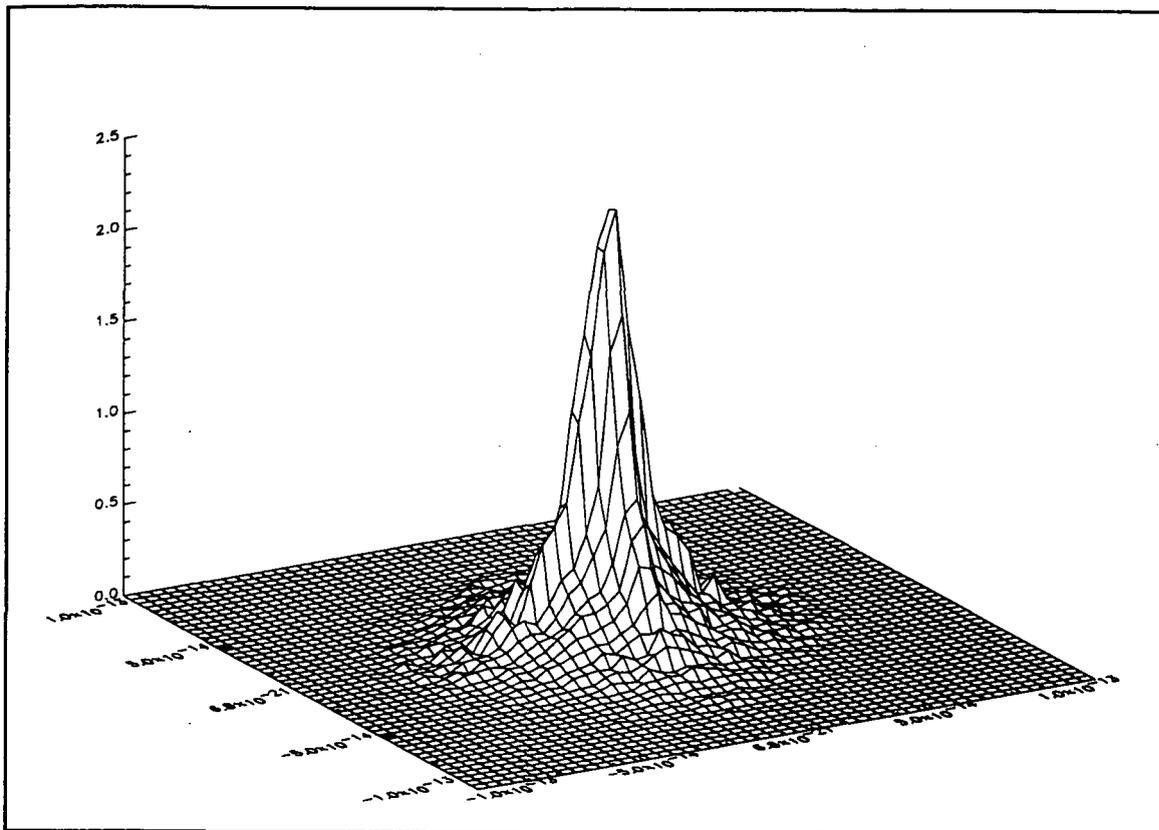


Figure 4. The Point Spread Function Plots Produced by GT2 Program; a Meshed Plot (top) and a Shaded Plot (bottom)

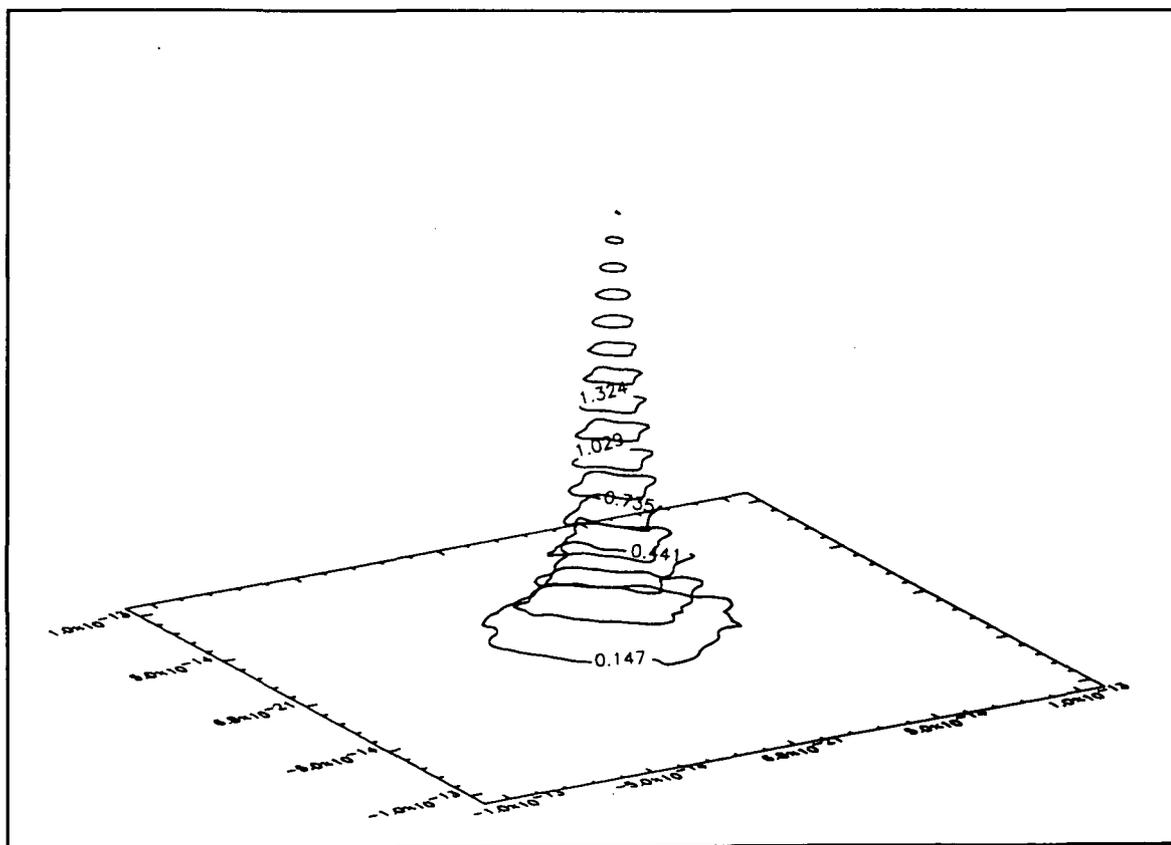
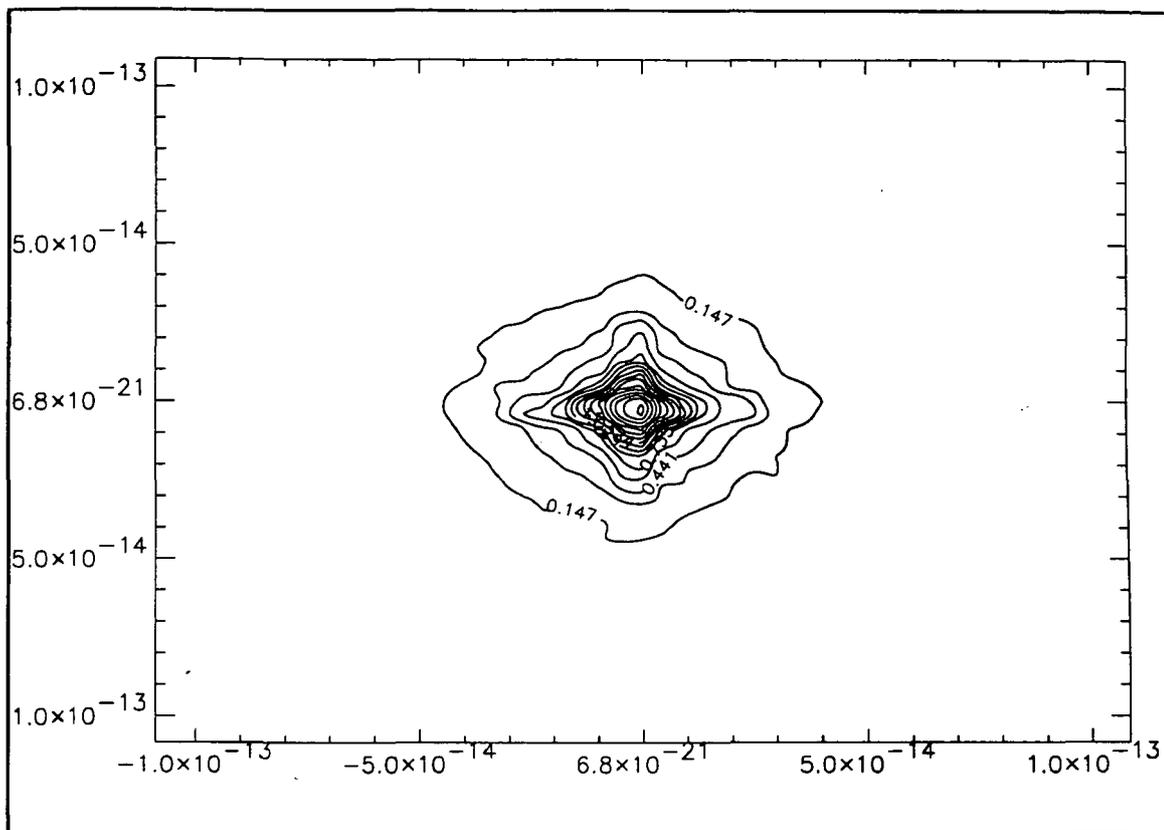


Figure 5. The Point Spread Function Contour Plots Produced by GT2 Program; a 2-D Plot (top) and a 3-D Plot (bottom)

scattering or for the x-ray source geometry. The rectangular, disc, and double-gaussian scattering distributions can also be modeled. The convolved image can also be checked by plotting the point spread function. Compared with the *ray-trace only* point spread function, the convolved point spread function provides a visual evaluation of the effect of the surface scattering and other effects.

3.6.2 Convolution with detector aperture size and shape

The convolution analysis has also been used in the detector scan modeling to characterize the image energy distribution. Various detector scans can be modeled. A circular detector of a given diameter can be scanned through the image with a specified range, center coordinates, and scan direction. A rectangular detector of a given width, height, and orientation can also be scanned through the image with a specified range, center coordinates, and scan direction. The resulting detector response data is displayed in tabular form, and can also be viewed by x-y plots showing the signal vs. location information. Figure 6 shows the collected energy of an image scanned by a rectangular detector. The encircled energy distribution of the convolved image can be easily obtained by convolving the image with detector aperture of varying diameter as shown in Figure 7.

3.7 Other program features

The command mode GT2 allows the users to interactively run the program. Macro or sequential commands are also furnished for running the program. The command log and output log are also available, if needed. An operating system shell is provided to perform the operating system operations without leaving the program. The system run time parameters and controls can also be checked and set, including the ray-trace status and ray trace iteration criterion.

4. SUMMARY AND FUTURE RECOMMENDATIONS

Much of the original ray-trace and image convolution software has now been documented and can be run in a command mode fashion as described above. A number of graphics features have been provided to review and interpret the results of modeling more easily. The software needs to be exercised further before it can be released to allow evaluation of ease of use, flexibility, and robustness. The program will be checked as it is used for the initial predictions for the image of the AXAF-I HRMA before the HRMA construction begins later this year.

A number of additional capabilities must be added to GT2 to perform additional modeling tasks. The capability to model the cumulative image from multiple mirror shells is needed. The ability to read the mirror surface metrology maps directly from Flexible Image Transport System (FITS) format files will be added. A program to convert the mirror surface-height power-spectral-density (PSD) files into files readable by MSFC's version of the EEGRAZ x-ray scattering program is needed.

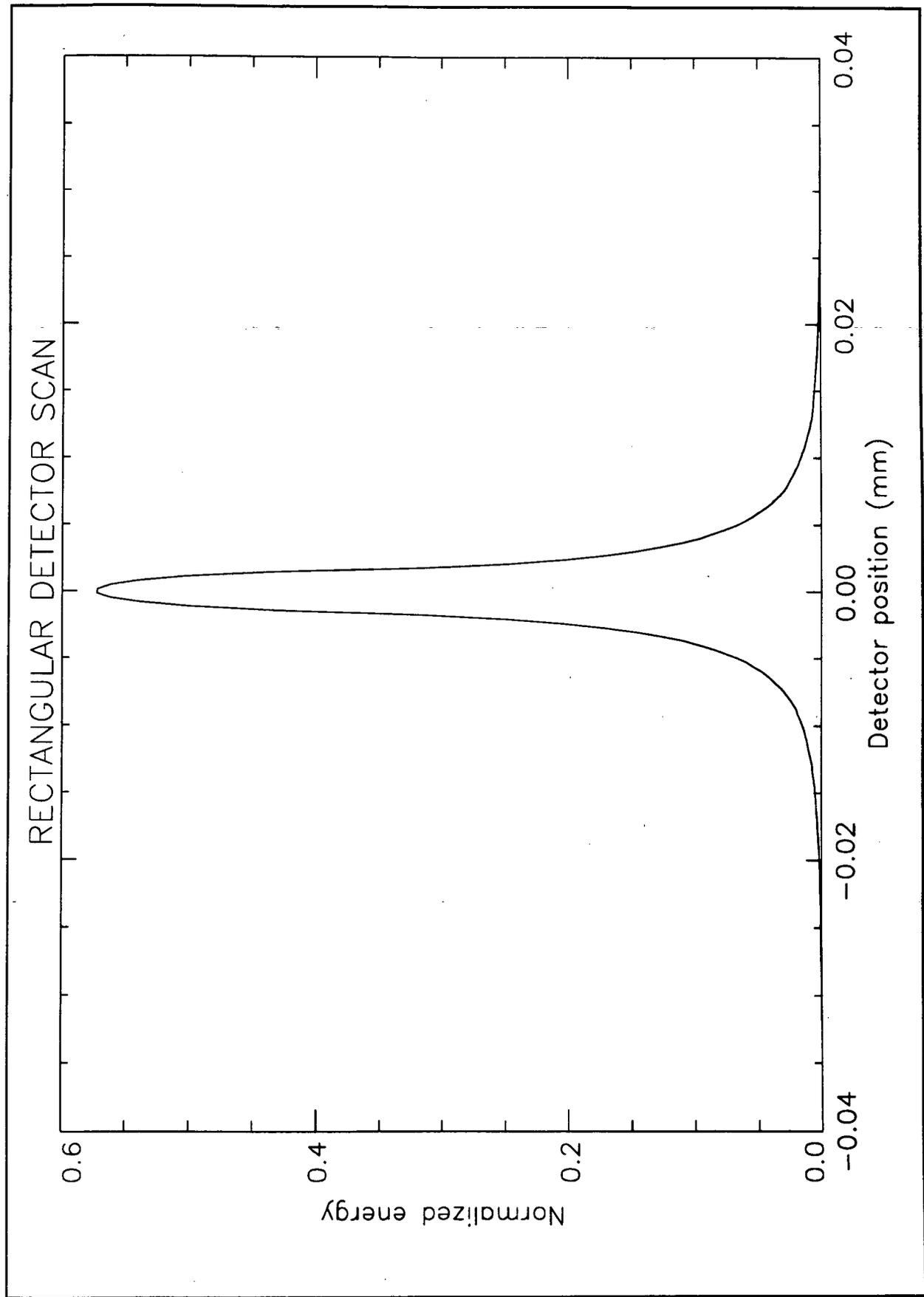


Figure 6. Collected Energy for an Image Scanned by a Rectangular Detector

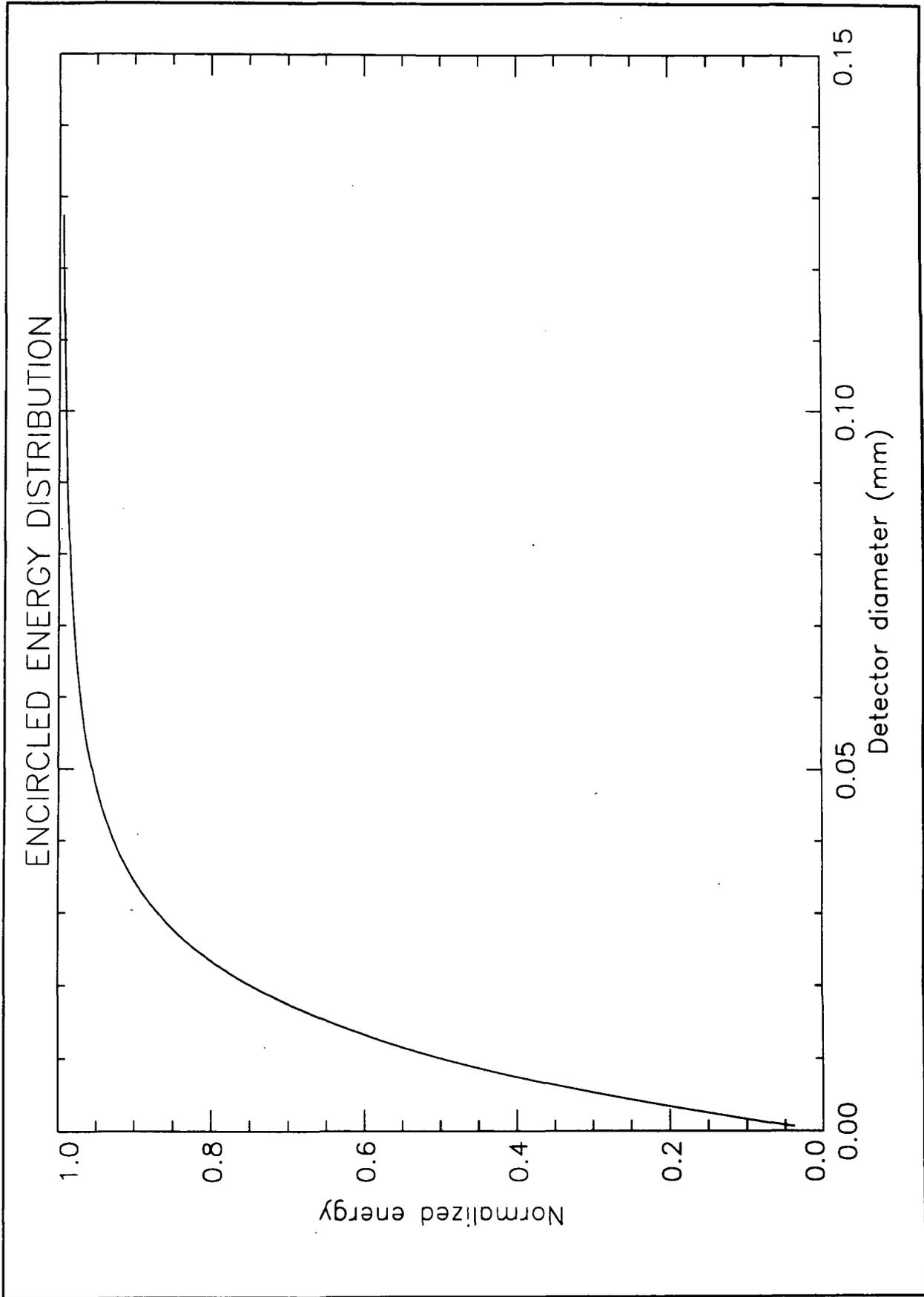


Figure 7. Encircled Energy Distribution for an Image Convolved with Detector Apertures of Varying Diameter

Spatial-frequency cuts must be made from the PSD data files, the transition regions between various PSD measurements must be smoothed, and PSD plots must be made. Routines to plot the image RMS, x-ray collecting area, image encircled-energy diameters, and image encircled energy-fractions vs. field angle must also be developed.

We need to add a utility to generate the mirror surface deformation files based on Fourier-Legendre polynomial coefficients. Software to scale and add together the mirror surface deformation files must be added to GT2. The deformation file plot routine and the deformation file print routine need to be upgraded. Testing of the program must be completed and the existing features of the GT2 program must be refined based on the feedback from the users. Also, it would be desirable to add the effects of dust scattering to the x-ray system modeling. MSFC's version of the EEGRAZ x-ray scattering program needs the addition of surface-height autocovariance (ACV), PSD, and image encircled-energy plots.

APPENDIX 1

Software to Model the Performance of X-Ray Telescopes

(Copy of the paper presented at the SPIE Aerosense Conference, Orlando, FL, April 1995)

Software to model the performance of x-ray telescopes

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ABSTRACT

A modular user-friendly computer program for the modeling of grazing-incidence type x-ray optical systems has been developed. This comprehensive computer software GRAZTRACE covers the manipulation of input data, ray tracing with reflectivity and surface deformation effects, convolution with x-ray source shape and x-ray scattering. The program also includes the capabilities for image analysis, detector scan modeling and graphical presentation of the results. The utilities have been developed to interface the predicted mirror structural and thermal distortions with the ray-trace.

There is no commercially available (or published) program tailored for the analysis of grazing-incidence type optical systems. The GRAZTRACE program has the analysis and graphics capabilities similar to those of the standard design and analysis programs (CODE V and SYNOPSIS) for normal-incidence optical systems. This software is written in FORTRAN 77 and runs on a SUN/SPARC station. An interactive command mode version and a batch mode version of the software have been developed. The application of GRAZTRACE for the image modeling of AXAF-I (Advanced X-ray Astrophysics Facility- Imaging) telescope is also discussed.

Keywords: X-ray optics, x-ray telescopes, grazing-incidence optics, integrated system modeling, ray tracing, optical analysis, convolution analysis, finite-element analysis, interactive software, AXAF

1. INTRODUCTION

1.1 Background

Marshall Space Flight Center (MSFC) is involved in overseeing the design, development, construction and testing of the Advanced X-ray Astrophysics Facility-Imaging (AXAF-I). The High Resolution Mirror Assembly (HRMA) will collect and focus the x-rays to the 0.5 arc-second resolution level. The HRMA will include the recently completed four pairs of nearly cylindrically-shaped mirrors, which are assembled in Wolter type I configurations¹. The largest of these mirrors has a diameter of approximately 1.2 meters, and the smallest mirror is about 0.6 meters in diameter. The x-rays will graze off the inside surfaces of the nested mirror pairs and will be directed to the system focus about 10 meters behind the center of the HRMA. The mirrors are constructed from Zerodur glass and the optical surfaces will be coated with iridium.

Specialized optical analysis software has been used by MSFC and the AXAF-I contractors in order to design, tolerance, interpret ground test data, and predict the on-orbit image quality. This software largely consists of in-house collections of programs developed at the various institutions and companies involved with the AXAF-I program. Highly-developed commercially available optical analysis and design programs, such as CODE V and SYNOPSIS, are optimized only for normal-incidence optics.

MSFC has been involved in the development of other x-ray telescopes such as the Soft X-ray Telescope (SXT) and Solar X-ray Imager (SXI). SXT is a small grazing-incidence telescope on the Japanese Solar-A satellite for the study of solar flares. United Technology Optical Systems (UTOS) built the SXT mirror pair from a common substrate. The SXI telescope will be flown on a GOES weather satellite primarily as a solar radiation warning device. The SXI project is largely a MSFC in-house project. The SXI mirror fabrication was started by UTOS, but now is being completed largely by MSFC. MSFC is also developing the capability to design and build electroplated nickel replicated (ENR) optics. This effort was initiated with the work (now cancelled) on the development of AXAF-Spectroscopic (AXAF-S). The work is being continued with an eye toward other future multiple mirror systems. The design optimization of a polynomial-prescription multiple mirror system with a relatively large field of view has been accomplished. Also, a small 1/10th scale ENR version of the smallest AXAF-I mirror may be used for testing the detector for the HRMA testing. Recently, the effects of gravity deformations on the image quality of this mirror have been modeled.

1.2 Description of GRAZTRACE and CONVOLVE software

The collection of x-ray optical ray-trace programs developed at MSFC is called GRAZTRACE. The collection of programs developed at MSFC to convolve the ray-trace image with the x-ray scattering, x-ray source distribution, and detector geometry is called CONVOLVE. This software was used originally to predict the image quality for the Verification Engineering Test Article-I (VETA-I) x-ray ground test at MSFC of the largest pair of AXAF-I mirrors². The image modeling for VETA-I included the surface prescription, alignment, x-ray source size, mirror surface metrology data, roughness specification, and thermal/structural deformations along with a set of randomly distributed rays input to the system. The surface prescription included the conic section formula as well as parameters for average-radius and average-slope errors. The alignment was specified by surface tilts and displacements.

The mirror metrology data (fabrication errors) and thermal/structural model (gravity deformation) information were input to GRAZTRACE as mirror surface radius errors interpolated onto a finely spaced grid over the mirror surfaces. The roughness specification was used in the x-ray grazing-incidence scattering program EEGRAZ³ to compute the x-ray scattering. The x-ray scattering distribution and x-ray source size was convolved with the traced rays by adding randomly distributed displacements to the ray intercepts. The detector was modeled by computing the number of rays entering the detector aperture. The effective area is computed by computing the ray weights which take into account the telescope entrance area, field angle, surface reflectivity, and the number of input rays. Predicted image centroid, RMS, and encircled-energy distribution values were computed. Predicted image point spread functions (PSF) were plotted.

Although the software was already written to do the modeling for VETA-I, it was not documented and required the user to do FORTRAN programming in order to exercise the various program options. Therefore, it could only be used by one or two people intimately familiar with the program source code. It was decided that the program should be documented and should not require the user to do FORTRAN programming. The new version of the software GT2 still requires some basic knowledge of grazing-incidence optical systems. The flexibility inherent in the original version of the program has also been maintained for expert users.

1.3 Reorganization and documentation of the software

The original software has been reorganized to make the development of the program easy. The huge source code files have been split and recombined into several small source files. A user library has been built for the users to develop their customized programs. The *makefile*, *makerules* and *user routine* templates are provided for the users to compile and link their customized program. The source files, which are under development are placed under the management of source code control system(SCCS) to prevent accidental deletion, to keep track of changes, and to allow more than one person to modify the files. An interactive command mode version of the software called GT2 has been implemented. A user manual for the command mode GRAZTRACE program has been compiled. A reference manual for the library routines has also been documented for the users to customize their own program.

2. PROGRAM STRUCTURE AND SYSTEM REQUIREMENTS

The GRAZTRACE software currently can run on a SUN/SPARCstation 10 with 64 MB physical memory (RAM) and 176 MB virtual memory (disk swap space). The software structure, management and the two operating modes of the program are briefly described as follows:

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The main body of the software is written in FORTRAN 77. The data analysis part of the software uses the IMSL mathematical and statistical library. The graphics part uses the PV-WAVE graphics package. The main body of the software consists of the user interface, system data management, structural, thermal, and metrology interface, ray-trace routines, image characterization, and image convolution and detector modeling. The on-line help system and documentation are also available. The total number of routines is more than 70, with more than 10,000 source code lines.

2.2 Software management

The source code of the software is managed by source code control system (SCCS), which monitors all modifications. The source files are protected by allowing only one person at a time to make changes, by maintaining a record of all changes, and by rebuilding any previous version when necessary. Regular backups are also effectively used in the software management during the software development.

GT2 input command sequence files are being generated for analysis cases similar to those studied for AXAF-I, VETA-I, AXAF-S, and SXI systems. The results from GT2 are compared to the results of running the original GRAZTRACE/CONVOLVE software. The cases considered exercise most of the program options on actual or proposed x-ray systems for which there is already a knowledge base. Any time that changes are made to GT2, these cases can be rerun as a check on the program.

2.3 Operation modes

Two operation modes are available: interactive command mode and a batch program mode. In the interactive command mode, more than 100 commands are available to manipulate optical prescription data, perform various ray-trace and performance analyses, set system parameters, and utilize some utilities. The 3-character mnemonic commands are used for all functions. The command syntax will automatically prompt if the exact command input format is not known. In batch program mode, more than 60 user routines are accessible to allow the users to write their own programs and to perform specific analyses.

3. PRIMARY PROGRAM FUNCTIONS

3.1 Help function

On-line help is available in the interactive command mode version of the GT2 program. The users can type *help* or "?" mark followed by the command mnemonic to obtain a detailed explanation of the command. If a user types *help* or "?" mark followed by any non-existent command, a list of valid commands is displayed. By typing *help* or "?" mark only, the information about the current or latest input command can be obtained. The *Help* file for the on-line help function is a plain ASCII text file. A help function routine has been developed to match the command mnemonics and to search for the related explanatory text.

3.2 Optical system prescription

A total of 50 surfaces are allowed in the analysis. The available surface types for the ray-trace are grazing incidence conic or flat type of surfaces. The conic types are: (i) a direct calculation with no deformation; (ii) an iteration including the deformation file data; and (iii) a direct calculation followed by an iteration including the deformation file data.

The surface data to describe the mirror surface are:

S ₁	radius ρ at $z = 0$ (z is along the optical axis)
S ₂	subnormal at $z = 0$
S ₃	$1 - e^2$ (e is the eccentricity)
S ₄	full mirror length
S ₅	zero-peak sag error (mirror ends fixed)
S ₆	average ρ error
S ₇	delta ρ error

The sag equation used is:

$$\rho = \sqrt{s_1^2 + 2s_2z - s_3z^2} - 4s_5 \left[\left(\frac{z}{s_4} \right)^2 - \frac{1}{4} \right] + s_6 - s_7 \frac{z}{s_4}$$

The surface thickness is defined as the separation to the next surface. The displacements are allowed to define a linear translation of the surface along all three coordinate axes. The tilts are allowed to define an angular rotation of the surface about all three axes in the sequence specified by the user.

The permissible surface aperture types are an annular (circular) aperture defined by the minimum and maximum radii and a rectangular aperture defined by the width, height, and orientation. The surface aperture can be also limited by defining the minimum and maximum axial limits of the surface. The allowed surface obscuration types are annular (circular) and rectangular. Figure 1 shows the geometry used in the software to define a typical Wolter type I x-ray mirror. The inset on this figure shows a 3-D sectional view of a typical single shell x-ray mirror.

The surface mode is set for distinguishing a reflection surface from a reference surface. Two modes are available: 'refl' is for the reflection surface; and 'thru' is for the dummy surface for reference.

3.3 Structural/thermal interface

The structural deformation plots from the COSMOS/M finite element analysis program for an x-ray mirror are shown in Figure 2. This one-piece prototype mirror for SXI was produced by ENR process, and is about 6" in diameter and 4" long has a wall thickness of only 1 mm. The mirror is supported at six equally spaced points on the intersection plane between the paraboloid and hyperboloid sections of the mirror.

A structural and thermal data interface has also been developed to extract deformation data from the standard output of COSMOS/M and NASTRAN finite element analysis programs. The deformation data is then used in the ray-trace to predict the performance of the mirror due to the structural and thermal distortions. No restriction is placed on the number of nodes for the structural analysis. The nodes can be in a random order and randomly spaced to optimize the structural analysis. Interactive options are provided for the coordinate transformation, coordinate shift, scaling, and axial length change.

3.4 Ray tracing

A number of special methods and options have been provided for ray tracing due to the special nature of x-ray optical system. These options and features are described briefly in the following sections:

3.4.1 Wheel spoke ray pattern, random ray pattern, and individual rays

Because of the highly annular aperture in grazing-incidence optics, a rectangular grid can not be used to generate the rays for the ray-trace. Three wheel spoke and one random ray pattern generators are available. One wheel spoke ray pattern has a constant radial increment and a constant azimuthal increment arranged on the first surface annulus. The other modified wheel spoke ray patterns have a varying radial increment or a varying azimuthal increment to obtain a uniform area for each ray. A total of up to 200,000 rays can be generated and traced.

A single surface to surface ray-trace can also be performed for a specific ray with the given entrance coordinates and direction. This capability is useful for pin-pointing the vignetting or any other ray failure problem. It is also useful for exactly laying out the aperture stop and other parts of the system.

3.4.2 Source definition

Two types of x-ray source position definitions are provided to satisfy different preferences. A source position can be defined by the azimuth, elevation, and distance to the first surface center. The source can also be defined as x, y, and z coordinates relative to the center of the first surface of the system.

3.4.3 Ray weights, energy levels, and delbets

Unlike any commercially available ray-trace program, the telescope entrance area, field angle, surface reflectivities and number of rays are used in the x-ray ray-trace in the GT2 program to calculate the intensity of each ray. The surface reflectivity for the grazing-incidence x-ray is a function of the incident angle and the x-ray energy dependent complex index of refraction for the surface coating. The ray weight is the effective area or collecting area for the traced ray. The ray weights are calculated for up to 15 x-ray energy levels. The complex indices of refraction as represented by the delbet parameters must be supplied for each energy level.

3.4.4 Focusing and image plane shift

A refocus function is used to find the focus position for the minimum RMS image radius. The ray intercept data and net focal plane shift are updated for the new evaluation plane. The image plane can also be shifted by any amount to perform a *through focus* performance evaluation. The ray intercept data and net focal plane shift are updated and the image statistics are recalculated.

3.4.5 Ray storage files

The ray-trace data can be saved to a ray file for further analysis. Up to 200,000 rays can be saved to a ray file with the ray intercept coordinates x , y and z , the ray directions dx/dz and dy/dz , the entrance coordinates x and y , and the ray weights for all energy levels. The header information, number of rays, number of energy levels, focal shift, focal length, and the number of header text lines are also saved.

3.5 Image characterization

Several basic image characterization functions are provided in this program to evaluate the x-ray system performance. The graphical plots and analytical data can be simultaneously displayed in *X-Windows* environment as shown in Figure 3. Some of these functions are briefly discussed as follows:

3.5.1 Centroid and RMS

A statistical image performance analysis is available to obtain the centroid of the image and the RMS image size. The extreme ray locations are also reported with a maximum and a minimum in both x and y directions. The statistics in arc-second units are also given. The RMS in each direction and the total RMS are also provided.

3.5.2 Encircled energy

The encircled energy distribution function is available to compute the radial energy distribution on the image plane. The function is in the form of a series of radii in the image plane within which certain fixed percentages of x-ray energy are contained. The table gives the circle radii which enclose 5%, 10%, ... 100% of the energy or any other defined percentage of the energy.

3.5.3 Spot diagram and PSF plots

Like any other optical analysis program, the spot diagram plots are used to check the result of the geometrical ray-trace. Figure 4 depicts a typical spot diagram for 20,000 rays traced through a sample x-ray system. Because of the weighted ray-trace nature of the GT2 program, the point spread function (PSF) plots are the primary form of visual presentation of the performance. Both 3-D mesh and 3-D color shaded PSF surface plots provide detailed information about the image performance. The meshed and shaded PSF plots produced by this program are shown in Figure 5. The 2-D, 3-D, and 3-D color contour plots are also provided to quantify the image quality as illustrated in Figure 6.

3.6 Convolution image analysis

Convolution has been used to perform image analysis with x-ray source geometry, surface scattering, and detector scan patterns. These program features are briefly described as follows:

3.6.1 Convolution of image with rough surface scattering and other effects

To predict the performance of an x-ray system in the real world, the convolution analysis has been used for the image to include the effects of rough surface scattering and other effects. The image ray data obtained by ray-trace is convolved with a predicted scattering distribution.

A general linear scattering distribution is prepared by a separate program called EEGRAZ. This data is stored in a file and is then read into the GT2 program to convolve it with the ray-trace image data or pre-stored image data from a ray data file. The ray image data from the GT2 or ray file includes the x and y positions of the ray at the first surface in order that the tangential and sagittal ray scatter directions can be determined.

Some other distribution models are also available to generate the random distribution for the modeling of scattering or for the x-ray source geometry. The rectangular, disc, and double-gaussian scattering distributions can also be modeled. The convolved image can be also checked by plotting the point spread function. Compared with the ray-trace only point spread function, the convolved point spread function provides a visual evaluation of the effect of the surface scattering and other effects.

3.6.2 Convolution with detector aperture size and shape

The convolution analysis has also been used in the detector scan modeling to characterize the image energy distribution. Various detector scans can be modeled. A circular detector of a given diameter can be scanned through the image with a specified range, center coordinates, and scan direction. A rectangular detector of a given width, height, and orientation can be scanned through the image with a specified range, center coordinates, and scan direction. The resulting detector response data is displayed in tabular form, and also can be viewed by x-y plots showing the signal vs. location information. Figure 7 shows the collected energy of an image scanned by a rectangular detector. The encircled energy distribution of the convolved image can be easily obtained by convolving the image with detector aperture of varying diameter as shown in Figure 8.

3.7 Other program features

The command mode GT2 allows the users to interactively run the program. Macro or sequential commands are also furnished for running the program. The command log and output log are also available, if needed. An operating system shell is provided to perform the operating system operations without leaving the program. The system run time parameters and controls can also be checked and set, including the ray-trace status and ray trace iteration criterion.

4. SUMMARY AND FUTURE DEVELOPMENT PLANS

Much of the original ray-trace and image convolution software has now been documented and can be run in a command mode fashion as described above. The software needs to be exercised further before it can be released to allow evaluation of ease of use, flexibility, and robustness. The program will be checked as it is used to develop the initial predictions for the image of the AXAF-I HRMA before the HRMA construction begins later this year.

A number of additional capabilities are planned to be added to GT2. The capability to model the net image of multiple mirror shells is needed. The ability to read the mirror surface metrology maps directly from Flexible Image Transport System (FITS) format files will be added. A program to convert the mirror surface-height power-spectral-density (PSD) files into files readable by MSFC's version of the EEGRAZ x-ray scattering program is needed. Spatial-frequency cuts must be made from the PSD data files, the transition regions between various

PSD measurements must be smoothed, and PSD plots must be made. Routines to plot the image RMS, x-ray collecting area, image encircled-energy diameters, and image encircled energy-fractions vs. field angle are needed.

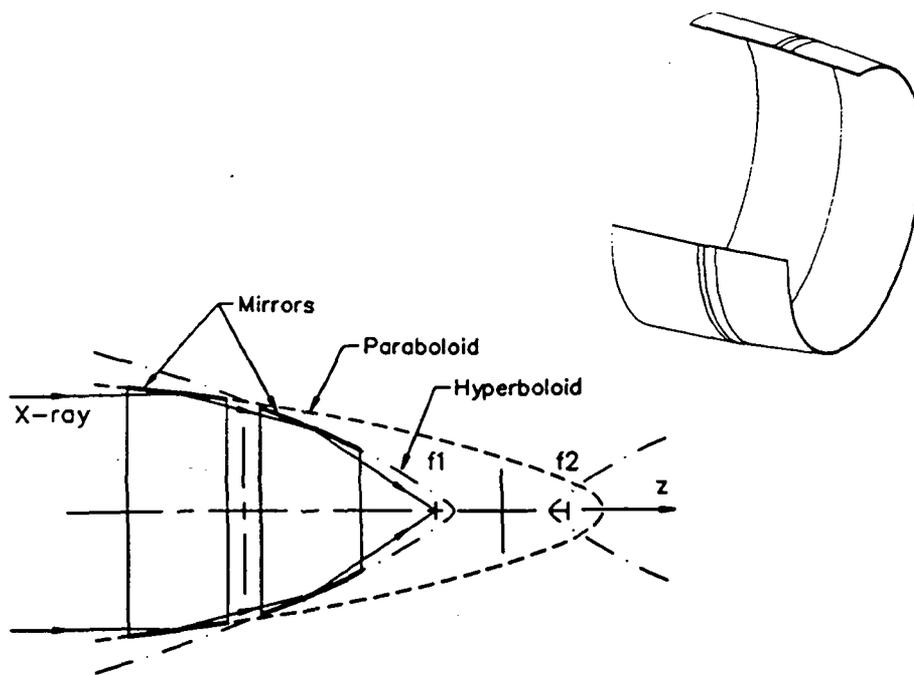
We need to add a utility to generate the mirror surface deformation files based on Fourier-Legendre polynomial coefficients. Software to scale and add together the mirror surface deformation files must be added to GT2. The deformation file plot routine and the deformation file print routine need to be upgraded. Testing of the program must be completed and the existing features of the GT2 program will be refined. Also, it would be desirable to add the effects of dust scattering to the x-ray system modeling. MSFC's version of the EEGRAZ x-ray scattering program needs the addition of surface-height autocovariance (ACV), PSD, and image encircled-energy plots.

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f1: The system focus and one of the hyperboloid foci
 f2: The paraboloid focus and the other hyperboloid focus

Figure 1: The geometry required to define an x-ray mirror in GT2 software. The inset (top right) shows a 3-D section of a typical x-ray mirror.

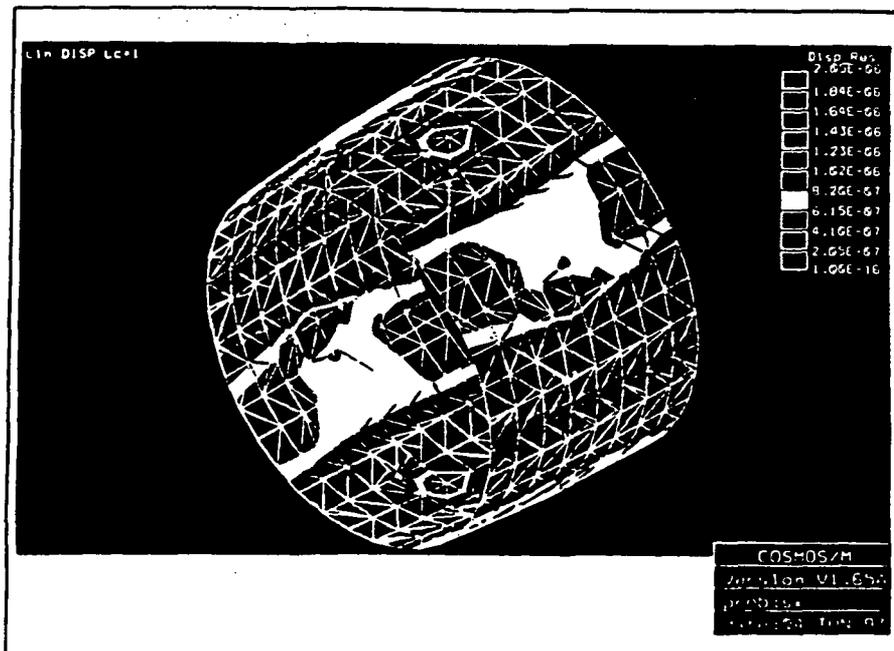


Figure 2: Structural deformation plot for a thin shell x-ray mirror.

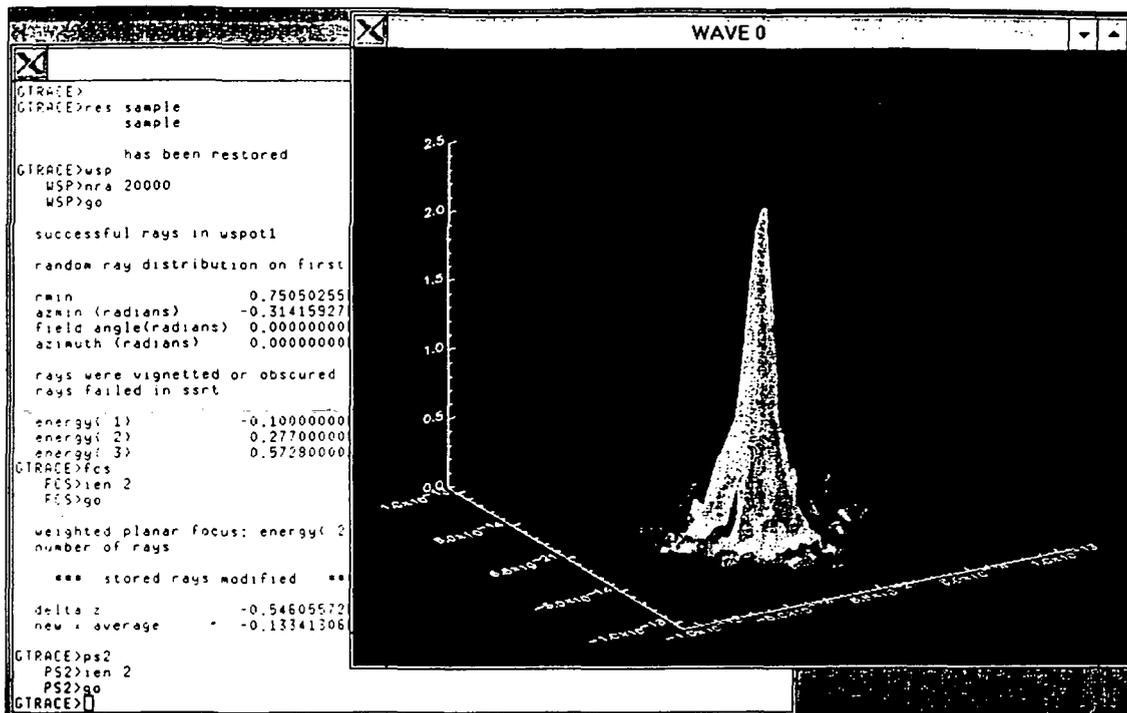


Figure 3: A sample GT2 screen display showing the graphical and numerical data

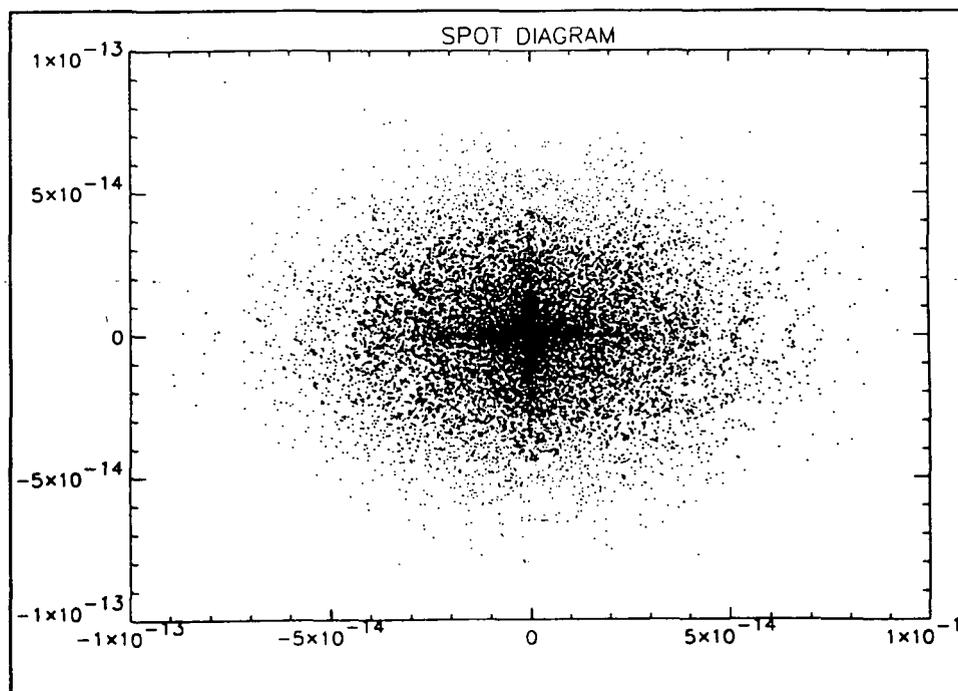


Figure 4: A typical spot diagram produced by GT2 program

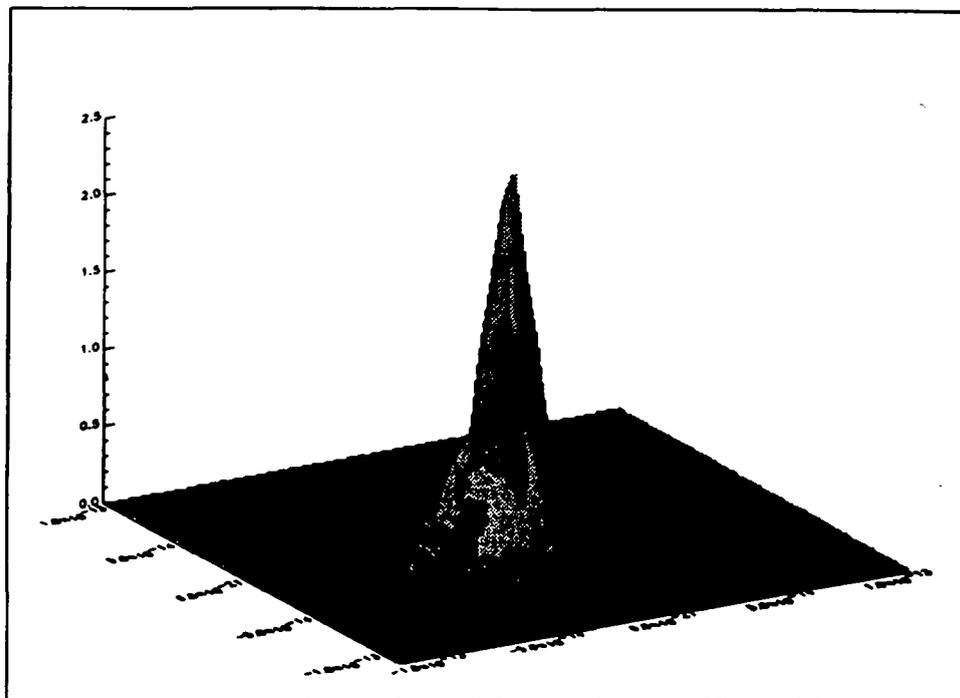
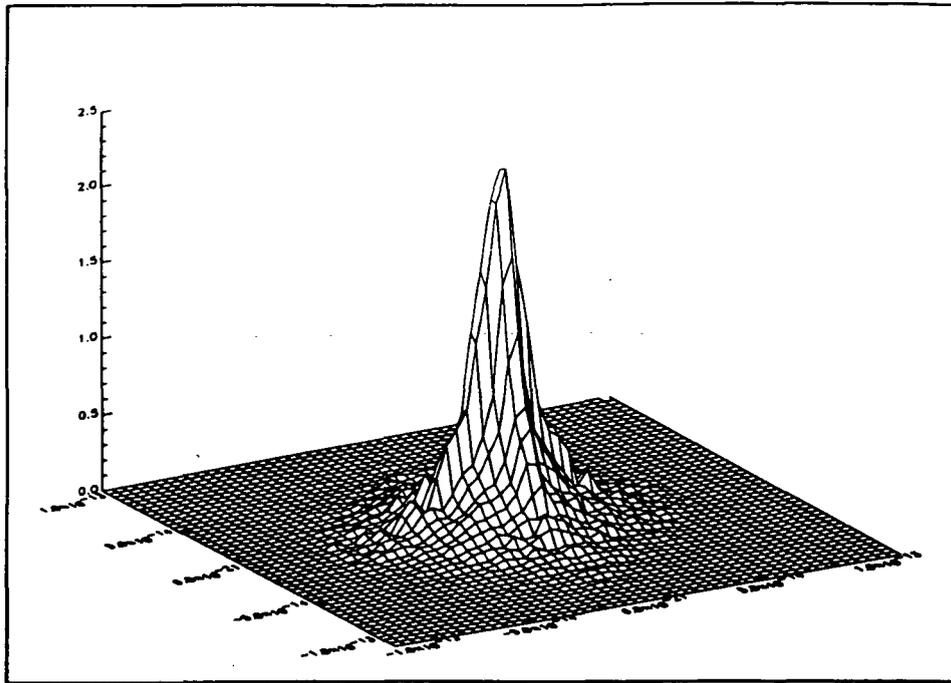


Figure 5: The point spread function plots produced by GT2 program; a meshed plot (top) and a shaded plot (bottom)

Report Document Page

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