

The Role of Modeling in the Calibration of *Chandra's* Optics

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ABSTRACT

The mirrors flown in the Chandra Observatory are, without doubt, some of the most exquisite optics ever flown on a space mission. Their angular resolution is matched by no other X-ray observatory, existing or planned. The promise of that performance, along with a goal of achieving 1% calibration of the optics' characteristics, led to a decision early in the construction and assembly phase of the mission to develop an accurate and detailed model of the optics and their support structure. This model has served in both engineering and scientific capacities; as a cross-check of the design and a predictor of scientific performance; as a driver of the ground calibration effort; and as a diagnostic of the as-built performance. Finally, it serves, directly and indirectly, as the primary vehicle with which Chandra observers interpret the contribution of the optics' characteristics to their data. We present the underlying concepts in the model, as well as the mechanical, engineering and metrology inputs. We discuss its use during ground calibration and as a characterization of on-orbit performance. Finally, we present measures of the model's accuracy, where further improvements may be made, and its applicability to other missions.

Keywords: Chandra, AXAF, optics, modeling

1. INTRODUCTION

The *Chandra* X-ray observatory, launched in 1999, is the result of more than two decades of design, engineering, and manufacturing effort. At its heart is a set of four Wolter type I optics, fabricated of Zerodur and polished to a surface roughness of $1.3 - 3\text{\AA}$,¹ designed to provide better than $1''$ angular resolution. To a great degree, it has met, even exceeded, its specifications.^{2,3} *Chandra's* optics owe their spectacular performance to their designer and to the engineering and manufacturing teams which surmounted an amazing array of technical and practical hurdles to cast, grind, polish, align and assemble them into their final flight configuration.

From the outset there was a realization that to reach the performance goals a means of probing the characteristics of the as-built, soon-to-be-built, and might-be-built optical assembly was necessary. This required a flexible system for simulating the optics, applicable to both engineering and scientific analyses. The system was designed around the concept of tracing a ray through the system in a physically consistent manner, making as few approximations to the underlying physics as possible. All structures in the optical path would be modeled as per design and as-built blueprints, and would incorporate such materials, engineering and metrology data as were available. The geometry, dimensions, positions, and alignment of the optical elements and their support structures should be amenable to easy manipulation. The output would include not only summary information applicable to figure of merit analyses, but permit incorporation of realistic models of both the calibration detection systems as well as the on-orbit science instruments. The system should be able to simulate the assembly, integration, calibration, and on-orbit environments. Finally, the system should attain as high throughput as possible, with no limitations to the number of rays traced.

In this paper we provide an overview of the system and discuss the details of the software which integrates the physical models with the input data.

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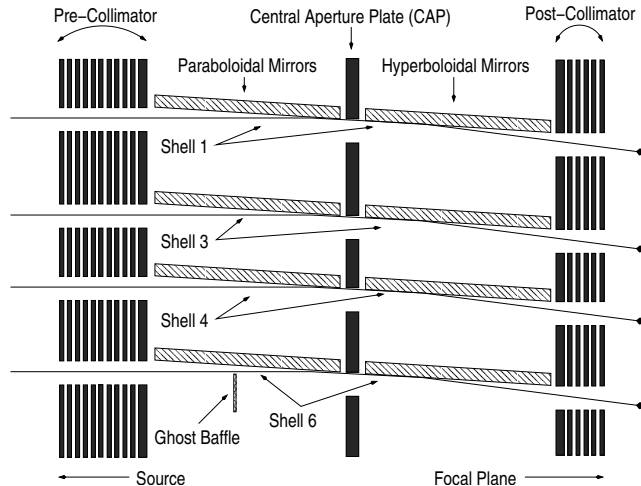


Figure 1. Schematic cut-away of the HRMA (less the mirror support sleeves). Not to scale.

2. THE OPTICS

Chandra's optics consist of 4 nested conical shells, each made up of two iridium coated Zerodur mirrors (the primary, paraboloidal; the secondary, hyperboloidal). Between the nested paraboloids and nested hyperboloids is a large aluminum plate known as the Central Aperture Plate (CAP). Twelve uniformly spaced support pads are bonded to the outer (non-reflecting) surface of each optic at its axial mid-plane. These are attached to the end of a cylindrical graphite epoxy mirror support sleeve (MSS), which extends to the CAP, where it is attached. Each mirror has its own MSS, and is thus independently secured to the CAP. A set of aperture plates (the pre-collimator) is attached at the input (front) end of the paraboloids; these serve as thermal and optical baffles. A similar set is attached at the output ends of the hyperboloids; these serve as optical baffles. The inner most mirror has an additional optical baffle midway along the paraboloid to help exclude ghost rays from the inner field of view. The optical path is more precisely defined in places by additional baffles (e.g. at the CAP) All of these structures make up what is known as the High Resolution Mirror Assembly, or HRMA. Fig. 1 presents a cut-away view of the optics.

3. THE SIMULATOR

The optics simulator is best described as the coupling of an extensive library of calibration data describing the optics' surfaces and their support structures with a suite of tools which implement the physics of the interactions with X-rays. The fidelity of the model of the optics is determined by the accuracy of the representation of the underlying physics and the descriptions of the deviations of the optical surfaces from their geometric prescriptions. The deviations may be the result of fabrication and assembly errors; technical limitations which prevent obtainment of the ideal figures even in the absence of errors; or the operational configuration (e.g., operations under Earth gravity, vertical or horizontal orientation of the shells).

Fig. 2 depicts a functional diagram of the simulator, with information flowing from left to right across the system. The various input data are combined into a description of the optical system, which is then used by the raytrace system to perform simulations and analyses.

3.1. Input Data

The input data describe the geometric positions and alignments of structures, and provide the basis for describing the deviations of the optics from their geometrical prescriptions. Because of the overall 1% calibration goal for *Chandra*, substantial effort was put into metrology, measurement, and modeling by other parts of the *Chandra* (then AXAF) project, resulting in a large, highly detailed, body of data. Among the data that were used are:

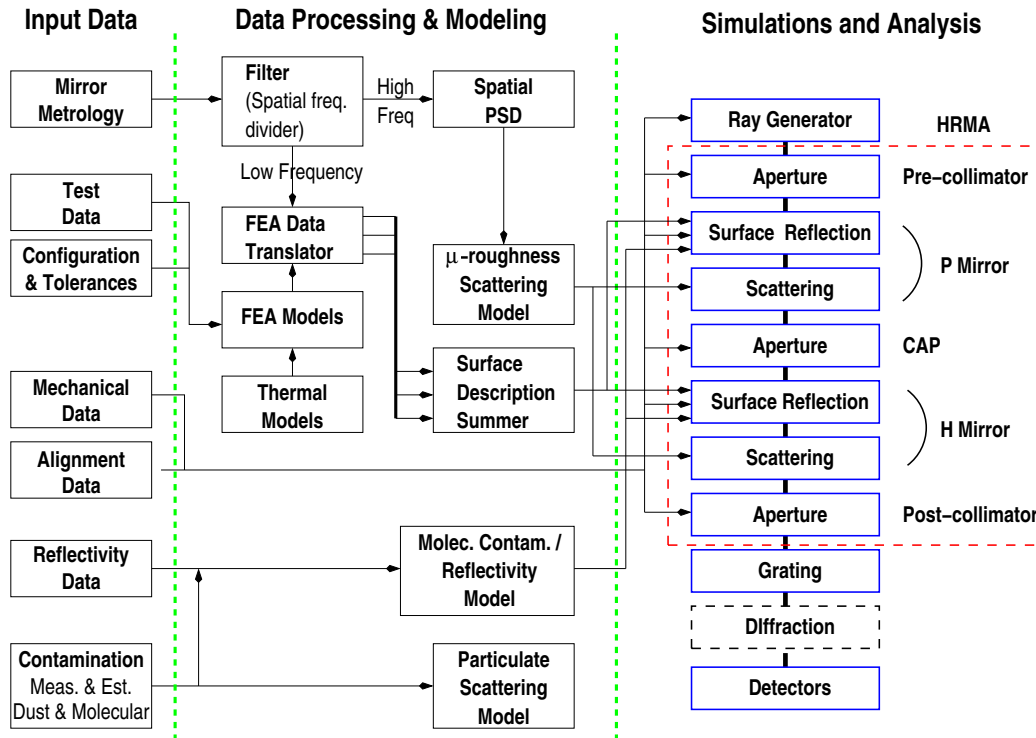


Figure 2. Functional overview of the *Chandra* optics' simulator

Mirror metrology

Measurements were made of the deviations of the optics' polished surface from their ideal figure (every $20\ \mu\text{m}$), as well as of their surface roughness.⁴

Mirror optical constants

High precision iridium optical constants were measured at Brookhaven National Lab's synchrotron and the Advanced Light Source at Berkeley.⁵

Mechanical and alignment data

Dimensions and positions of mechanical structures were determined at many stages of fabrication, assembly, and alignment. As-built values were used whenever available.

Measured dust contamination

Pull strips were used to determine the quantity and distribution of dust particles on the mirrors.

Mechanical tolerances

Positions and dimensions are subject to manufacturing and assembly tolerances; these were used to drive sensitivity analyses.

The input data also describe what is *not* known, especially before fabrication and subsequent calibration. Errors in fabrication or tolerances are at times not often reducible to a description of a physical structure, but must be introduced as an error term in some figure of merit.

3.2. Data Processing and Modeling

Some of the input data (such as positions and alignments) were directly usable in the simulations. Much of it, however, required reduction or incorporation into mechanical models to be of use. In particular, the descriptions of distortions in the optics evolved during the project. They were initially derived from error budgets and

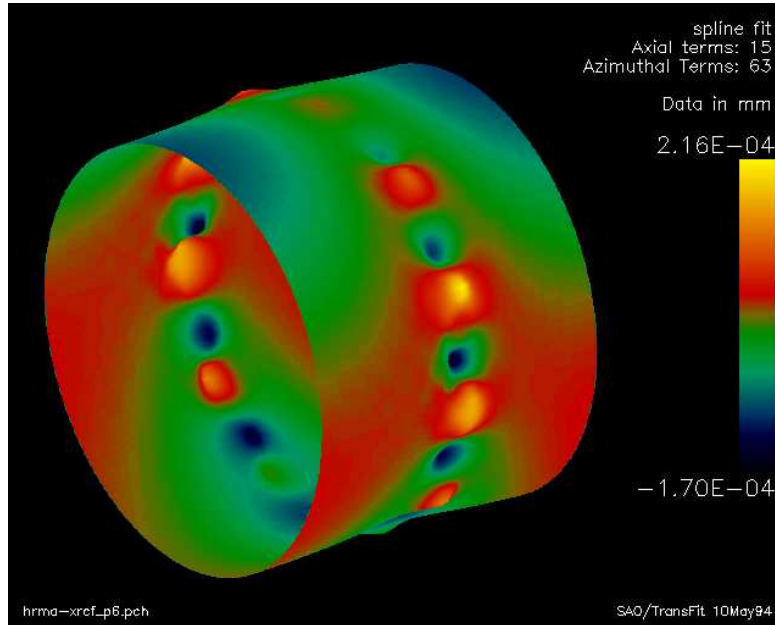


Figure 3. Example of stress on an optic due to gravity. Note the pronounced sag about the optic mid-plane, as well as the puckers at and between the twelve mount points.

presented either as a degradation of some figure of merit (such as encircled energy), or as a tolerance on a first or second order error in the optics (such as ΔR or $\Delta\Delta R$). Post fabrication measurements and metrology provided data more representative of the actual hardware.

All of these characterizations must be transformed into inputs suitable for raytracing. Most could be mapped onto a geometric realization of the HRMA, but some, such as surface roughness and dust contamination, were best represented as probabilistic in nature. Of note are the mirror errors and the measurements of surface reflectivity.

3.2.1. Mirror Errors

Metrology of the optics' surfaces were made on the unstressed mirrors prior to being bonded to their support structures. The data were filtered into low and high spatial frequency components. The latter were used to create a probabilistic description of the energy dependent X-ray scattering distribution, calculated similar to the treatment by Beckmann and Spizzichino.⁶ The low spatial frequency components were used to describe the surface deterministically. Further details are available in van Speybroeck¹ and references therein.

While rigid, the mirrors are still susceptible to deformations due to gravity and assembly strains (e.g., Fig. 3). The mirrors would be exposed to a variety of mechanical and thermal forces during their assembly, testing, and spacecraft integration in gravity, and in their final operating environment in orbit. To map from the distortion free optics to realistic operational scenarios, a detailed mechanical model of the optics and their support structures (the model has ~ 40000 elements) was constructed using ANSYS. The model was input to an in-house program (TRANSFIT⁷) which characterized the distortions to the optics via splines. Additional first and second order error terms were represented via Fourier-Legendre polynomials. These, along with the measured surface errors, were input to the raytraces.

3.2.2. Surface reflectivity

The optics' surfaces were coated with iridium over a thin layer of chromium. Ir optical constants were measured on witness flats coated alongside the flight optics as part of the overall *Chandra* calibration effort.⁵ The measurements resulted not only in the atomic data, but also in estimates of the layer thicknesses and coating boundary roughness.

3.3. Simulations and Analysis

The last component of the optics simulator is the suite of software which uses the input data and mechanical models to trace rays through the optical system and analyze their resultant properties. The system is based upon OSAC,⁸ a deterministic ray trace code for X-ray and conventional optics. Optics are modeled as conics, toroids, or flats, with deformations described by polynomials. OSAC was designed as a modular system with several independent executables, each of which performed a particular task. When tracing optics with multiple components (such as the two component shells in the HRMA), each component was traced separately, with incident rays read from a disk file, and exit rays written to disk. These exit rays served as the input for tracing the next optic.

OSAC was initially used without modification, but it became apparent that the details in the optical distortions revealed by the mechanical models were not well represented by the Fourier-Legendre polynomials available in OSAC. The code was modified to use spline deformation maps in addition to the polynomial prescriptions. Later modifications included the ability to read from and write to UNIX pipes, bypassing the disk altogether.

As OSAC concerns itself with optics only, it was necessary to introduce new modules to simulate the other elements in the HRMA, such as the baffles and support structures. Results from the iridium optical constants calibration program indicated the need for a more complex model of the reflecting surface than was available to OSAC. This led to the migration of the surface intersection functionality out of OSAC into its own program, and the addition of a module simulating reflection off of arbitrary multi-layer coatings. Probabilistic scattering of photons by surface micro-roughness was added as a separate module.

While the system has expanded greatly beyond the initial OSAC core, its fundamental concepts of modularity have been retained. The suite of programs, both new and derived, has over the years come to be known as SAOSac.

3.3.1. System Design

At the outset it was apparent that the simulator must serve the needs of both engineering and scientific staff. There was at first no designated software support staff, so implementation of new modules would be done by the users of the software. The advantages of the modularity of the original OSAC design (itself the product of the constraints of its original target system, an IBM 360 with 300kb of memory) were obvious: other than disk space, there was no inherent limit to the number of rays which could be traced. This was of immense importance given the complexity of the optics, and the need for a range of parameter sensitivity studies. Once the requirement that rays be read from and written to disk was removed, we were able to very quickly perform simulations with 10^9 rays using early 1990 UNIX workstations.

The modularity of the system was a boon in other aspects. With a user base comfortable with UNIX shell scripting and a set of programs compatible with the UNIX paradigm of programs acting as single purpose filters, a user could mix modules at will to create customized analysis tools, or probe the behavior of different aspects of the HRMA. The independence of each of the programs also meant that development could proceed on any aspect of the system without impacting other users or hampering other development. This would have been impossible to do had the simulator been a monolithic entity, given the software engineering skills of the users and the time frame available for development.

The overall design is straightforward. Programs may serve as ray sources, ray sinks, taps, or filters. They share a common interface to the ray stream and a common means of specifying program parameters.⁹ Various diagnostic programs are available which can be inserted into the ray stream at any point.

In order to maintain the efficiency of the system, rather than discarding rays whose probability of reflection from a surface is low, rays are assigned weights based upon that probability, and are allowed to reach the focal plane. Rays unfortunate enough to run right into something are not passed on.

The following sections present the programs which provide most of the end-to-end functionality of the system. There are many more.¹⁰

3.3.2. Ray generation

The system includes two ray generators, `raygen` and `genphot`.

`raygen` is the most flexible, designed to simulate complex (even astronomical) sources and directly fill the telescope aperture. It models the angular extent of sources as either simple geometric shapes or as a user-provided image. Multiple sources may be generated simultaneously and may have different spectra and fluxes; the output ray stream is the merged rays from each source, time tagged and sorted. Source specification is done via an embedded language, Lua.¹¹ Sources may be at a finite distance from the telescope's entrance aperture. Motion of the source (e.g. due to telescope dither) is not supported.

`genphot` is a much simpler tool designed to aid in diagnostics and design. It creates a parallel stream of rays emanating from sources of simple geometric shapes. The rays may be monochromatic or have energies sampled from a spectrum.

3.3.3. Intersections with optical surfaces

There are two programs which intersect rays with optical surfaces, `surface_intercept` and `flat`.

`surface_intercept` is a descendant of the OSAC DRAT program. It takes as input an ideal geometric prescription for an optic, as well as a description of deviations from that prescription. The latter can be expressed as either B-splines or as Fourier-Legendre polynomials. Unlike its predecessor, it no longer performs a reflection, but records the surface normals and tangents at the rays' intersection point with the optic.

`flat` models intersections of rays with an ideal flat surface.

3.3.4. Interactions with matter

Interactions of photons with matter which require a treatment of the physics (rather than just being stopped, as by a baffle) are modeled by `multi-layer_reflect` and `scatter`.

`multilayer_reflect` simulates the interaction of a photon with an arbitrary multi-layer coating. Boundary mixing (roughness) may be described using any of the Debye-Waller, modified Debye-Waller, or Nevot-Croce formalisms. It requires that rays have been projected to the reflecting surface and that surface normals have been determined.

`scatter` implements the probabilistic treatment of scattering by surface micro-roughness, using the probability distribution calculated from the high spatial-frequency surface errors derived from the mirror metrology.

3.3.5. Apertures and obstructions

Baffles, support structures and apertures are modeled by the program `aperture`. The program assembles apertures with complicated geometries by combining simple ones. An aperture may block as well as pass, may redirect rays (e.g. by scattering off of an aperture surface), or may re-emit one or more rays (e.g. by fluorescence). None of the currently implemented apertures actually perform the latter operations. Aperture descriptions are written in an embedded language, Lua.¹¹

Programs implementing simpler apertures suitable for diagnostic purposes (such as illuminating only an azimuthal wedge of a shell) are also available.

3.3.6. Detectors

There are a large number of detector models, ranging from the specific to the generalized.

`deticpt` is a generalized detector module which implements the intersection of rays with detectors which may have more than one detection element (such as an array of CCDs) positioned at arbitrary angles to the optical axis. This allows us to model detectors which are mounted so as to follow the focal surface of the telescope. `spatquant` is another generalized detector module which can be used to simulate the hexagonal pores and the grid of a multi-channel plate detector.

Some detectors models are abstracted for efficiency. For example, calibration of the two dimensional PSF during ground testing was performed by scanning a circular aperture backed by a non-imaging detector across the focused X-ray beam. To simulate this efficiently, we created a program, `pinhole`, which models a grid of circular apertures with a range of diameters simultaneously, allowing us to run a single raytrace and deduce the sensitivity of the results to aperture size and position.

3.4. Configuration of End-to-End simulations

During the early phases of the project when the knowledge of the as-built optics was minimal, maintaining control of the calibration data was relatively simple. As the sophistication of the modeling and analyses improved, and as the amount and range of calibration data grew, it became burdensome to the analyst to consistently specify each and every input parameter to the simulator's programs. A hierarchical version system was already in place to track revisions to the individual calibration data. What was needed was a mechanism to coordinate the inputs required for a simulation and to create the command pipeline required to realize it. At this point two major improvements were introduced: a formal description of all of the inputs for a particular HRMA configuration, and high level programs which could use these descriptions to create an end-to-end simulation of the HRMA.

The base program, `trace-shell`, implements a raytrace of a single shell. The higher level program, `trace-nest`, calls `trace-shell` for each shell, and merges the rays into a single stream. Both programs are written in Perl, and simply marshal the low-level programs described in §3.3. Running an end-to-end raytrace for a simple source now requires specifying at most a dozen, obvious parameters. It is now possible for users without a decade worth of experience with the simulator to consistently simulate the optics. While this may reek of a monolithic approach, the underlying design paradigm has not changed; it is just made more accessible to the casual user.

4. ROLE OF THE SIMULATOR IN THE CALIBRATION OF *CHANDRA*'S OPTICS

Calibration provides insight to the fundamental questions, *How should the system behave for this given set of conditions?* and *How much should we believe the answer?* It is never possible to completely determine a system's behavior; one must determine instead which sets of conditions will reveal the most about its fundamental characteristics, measure its performance in those conditions, and use the measurements to extrapolate behavior. The extrapolation is more problematic when the measured behavior is a composite response of many different subsystems, making it difficult to extract the behavior of any one element from the rest.

In this light, the optics' simulator provides the predictive piece of the calibration puzzle; the performance measurements made during ground testing at the Marshall Space Flight Center's X-ray Calibration Facility (XRCF) in 1996 and 1997 as well as those currently underway using on-orbit data provide the constraints which determine our level of trust in the model.

Over the course of the project, the simulator has lived up to its design goals of simulating the assembly, integration, calibration, and on-orbit environments. Just a few of the areas in which it has been used include:

- Predicting the performance of the first technology demonstration of the outermost shell
- Design evaluation of the support structures, baffle positions, effect of misalignments, and the thermal environment
- Independent validation of the EKC optics model
- Materials studies of epoxy shrinkage and creep
- Assembly and Alignment – It was used to model the double pass alignment procedure used during bonding of the shells into the support structure. It modeled the effects on optical performance of the progressive buildup of HRMA. When during the assembly Diagnosis of Shell 4 & 6 Axial Focus discrepancy itemize
- Ground calibration predictions – generation of the “HRMA Calibration Handbook”, presenting simulations of the effects of gravity (and the remediative efforts) on the calibration measurements at XRCF.
- Ground calibration test design – determining the optimal procedures and algorithms to perform measurements (such as centroiding, or focusing the telescope), as well as to prevent damage to detectors.
- Diagnosis of alignment errors discovered at the XRCF
- Detailed modeling of the interaction of the XRCF beam with the calibration detectors to understand and correct for systematic errors.
- Development of the on-orbit procedures for determining best focus for the science detectors
- Predictions of flight optical performance
- Interpretation and modeling of actual flight data

5. CONCLUSIONS AND FUTURE WORK

The simulator has proven itself to be an extremely valuable tool for both engineering and scientific analyses. It has also proven to be an accurate predictor of the PSF, effective area, and vignetting function.^{2,3,5,12-15} The only major discrepancy is in its under-prediction of the far PSF wings.¹³

There are, however, a number of weaknesses in the simulator which require addressing. The treatment of reflection and scattering should be unified, as physically they must be related. This may resolve some of the discrepancies in the wings. There are nagging discrepancies between measurements of the PSF and the models which may require adjustment of the mirror alignments.³ Our models over-predict the XRCF effective area, especially for the outermost shell at high energies^{13,14} (this does not affect the overall effective area significantly, as this shell contributes little in that region). Because our ray generator does not model telescope dither, comparison with on-orbit data is problematic.³

The success of the simulator in the *Chandra* program bodes well for its use in other grazing incidence missions. The largest software changes will be in the surface intercept program, the pipeline constructor (`trace-nest`), and the calibration data configuration management system, in order to accommodate the much larger numbers of segmented optics in the next generation of X-ray telescopes. Depending upon the quality of the optical surfaces an altogether new surface scattering model may need to be derived. Finally any decade old collection of code is in need of modernization of some of its cruftier corners; we look forward to the time when the SAOSac suite of tools will be available for download and use by the general public.

ACKNOWLEDGMENTS

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