Experience with ray-tracing simulations at the European Synchrotron Radiation Facility

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The ESRF is the first operational third-generation synchrotron radiation hard-x-ray source. Since the beginning of its construction (1988), the ray-tracing technique proved to be an essential computer tool for the beamline optics design. The optical systems of most beamlines have been simulated by ray tracing in order to optimize the optics, fully understand their properties, and check if operation performances were as expected. In this paper, a short compilation of the experience with ray tracing and optics simulation codes at the ESRF, as well as some other in-house developments, is presented. © 1996 American Institute of Physics.

I. INTRODUCTION

The construction of the ESRF synchrotron radiation source started in 1988 as a joint project of 12 European countries. The facility is designed and optimized to supply high brilliance x-rays from insertion devices. It consists of a 200-MeV electron LINAC, a 6-GeV fast cycling booster synchrotron and a 6-GeV low emittance storage ring. At present, 18 beamlines constructed by the ESRF and 4 built by the Collaborating Research Groups (CRG) are operational out of a total of 30 ESRF beamlines and an indeterminate number of CRGs foreseen by the end of 1998.

A number of simulation tools has been installed at the ESRF for the design of the beamline optical components. Designing software packages, such as CAD, finite element and ray-tracing programs, run on the ESRF computer systems. The network consists of UNIX workstations, which are also used to drive beamline instruments, perform the data acquisition, store experimental data as well as processing and analyzing experimental results. SHADOW\(^1\) is the main program used for ray-tracing calculations and is complemented by a large variety of simulation codes that are developed and available in this and other synchrotron radiation facilities. Effort has gone towards providing a user-friendly and documented environment so that the beamline responsibles can run the codes by themselves. This is complemented by a research activity that aims at developing computer models of optical elements and improving the existing ones. This is particularly important because we usually deal with new instruments. Indeed, almost all beamlines are equipped with very modern equipment, and many of the optical elements have been placed for the first time in such intense photon beams.

We present some cases in which the contribution of the ray-tracing program SHADOW has been essential, namely mirror and crystal optics. These two elements constitute the core of any hard x-ray optical system. The possibility of complementing and interfacing SHADOW with other available or developed codes is also discussed. SHADOW is suitable to perform accurate calculations of the beam point spread function at the sample position (or at any other position), the energy resolution of the monochromatized beam, and the flux or power transmitted by the beamline.

II. MIRROR OPTICS

Mirrors are used essentially to focus or collimate the x-ray beam. They can also be used as x-ray filters to avoid high heat load on other devices (monochromators) or as harmonic rejecters. The mirrors must operate at extreme grazing angles (typically tenths of a degree) in order to reflect efficiently the hard x-rays. This is known as the total reflection\(^2\) range. In this range, the grazing angle is smaller than the cut-off angle \(\theta_c\), which approximated value is \(\theta_c = \sqrt{2\delta}\), where \(\delta\) is associated with the refraction index \(n\) for a given photon energy: \(n = 1 - \delta + i\beta\). When using grazing incident angles, very long mirrors (typically 30-100 cm) are needed. Grazing angles also magnify the effect of geometrical aberrations and surface irregularities. These effects are difficult to study with fully analytical methods, and even more difficult is to analyze their combination with the geometrical and spectral characteristics of the synchrotron sources. Ray-tracing programs like SHADOW are the most indicated tools to perform reliable and accurate calculations of grazing incident mirrors under synchrotron radiation.

At the ESRF, most of the beamlines have at least two mirrors for focusing and/or collimating the x-ray beam. These mirrors are generally spherically bent (cylinders, spheres, and toroids). Although elliptical curvature would be ideal in most cases, spherical mirrors are usually preferred because of their lower cost and higher finishing quality.

SHADOW can model effectively the synchrotron radiation photon source (undulators, wigglers, and dipoles), when the electron beam parameters and emittances are known. Then the beam is sent to a mirror or combination of optical elements that may have any mathematical surface shape (ellipsoidal, spherical, toroidal, etc.). Given the source divergences, it is possible to calculate analytically the mirror dimensions needed to collect the full beam.\(^3\) SHADOW can, in addition, include the source size effects and calculate the footprint shape. It can calculate the acceptance of a mirror...
The quality of the mirror is limited by the technological manufacturing processes, as well as by heat load deformations. The surface errors can be classified in three families: (A) figure or geometry errors, (B) waviness, and (C) roughness. The limits between them are not clear and depend on the ratio between the imperfection characteristic lengths and the photon wavelength.

Figure errors are imperfections with characteristic length of the order of magnitude of the mirror dimensions. Typical cases are errors in curvature radius due to manufacturing tolerances, the bending effect of the gravity and/or mechanical clamping, thermal deformations, and calibration or other errors in adaptive mirrors. The thermal errors are due to the fact that the power absorbed by the mirror increases the temperature and thus deforms the mirror itself. Mirrors at the ESRF are refrigerated to reach the thermal equilibrium with a cooling medium. The beam heating produces two kind of thermal errors: (i) an additional longitudinal bending of the mirror caused by the differential expansion produced by the thermal difference between the surface and the cooling medium (this component may be reduced by cooling the mirror from the sides), and (ii) a thermal bump near to the center of the beam footprint on the mirror caused by the differences in power density on different points of the mirror surface. Figure errors can be studied with SHADOW by changing the input parameters (curvature radius, etc.) and adding an error surface shape to the main curved shape with the PRESURFACE utility. The error surface shape to be entered in SHADOW may come from different origins:

- it can be measured with different profilometer techniques;
- it can be calculated with finite element method (FEM) programs. In this aspect, SHADOW and the FEM are complementary. A first calculation of the power density on the mirror surface is done with SHADOW. Then this power mapping is used as input for the FEM calculations, which produce as output the deformed surface. Finally, the surface mapping is used by SHADOW to calculate the effect on the mirror focusing; and
- it can be simulated by using analytical or approximated formulae for the longitudinal bending and thermal bump.

All these options have been used at ESRF and a set of filters for file conversion between SHADOW and ANSYS have been written.

B. Waviness or slope error

Waviness or slope errors are generally associated with sinusoidal-like variations (or ripple) of the surface shape. The correlation lengths of these variations are much larger than the photon wavelength. Therefore, the geometric optics limit is valid for treating these errors. SHADOW has an option for including these effects, by overlapping a sinusoidal or a Gaussian profile on the main surface shape. Although this approximation is sufficient to give a rough estimation of the slope error effect, it is preferable to use measured profiles for ray-tracing calculations. These experimental profiles should give the best description of the optical surface. The problem is that such profiles are rarely or never available in the beamline design phase. At the ESRF, we compared the
results of the ray tracing performed by using measured profiles and sinusoidal modelled errors. It was observed that, for most cases, using a single sinusoidal error profile with a single characteristic length or frequency to describe the surface errors is not sufficient since it creates unrealistic intensity fluctuations in the image profile. It has been demonstrated\textsuperscript{12} that an adequate superposition of many sinusoidal signals can reproduce the exact calculations. An automatic mechanism of producing this kind of error signals (called WAVINESS\_GEN), which are introduced in SHADOW through the PRESURFACE utility, is systematically used to model the slope error of ESRF mirrors. Examples of SHADOW runs for the Microfocus beamline\textsuperscript{13} (BL1) at the ESRF are shown in Fig. 1. Typical values of slope errors (rms) at the ESRF mirrors range between 1 and 4 µrad.

C. Microroughness

Roughness is surface imperfections left by the machining and polishing processes. They have corrugation lengths of the order of magnitude of the photon wavelength that produces scattering or diffraction of the rays. A model\textsuperscript{14} has been implemented in SHADOW to treat the roughness imperfections. It starts with a file provided by the user containing the two-dimensional power-spectral-density function (PSD). This function is basically proportional to the square modulus of the Fourier transform of the mirror surface. Therefore, the PSD function presents peaks at the frequency values corresponding to the corrugation lengths of the surface. The integral of the PSD function gives the roughness rms value. This value defines the ratio between the probability that a ray is scattered or is specularly reflected. If the ray is scattered (diffracted), then a grating diffraction model is used. The ruling space is obtained from a Monte Carlo sampling method by using the PSD function as probability distribution function. The SHADOW utility JNTPSCALC prepares the PSD function in SHADOW’s format and can also generate Gaussian and other simplified PSD functions.

The systematic modelling of the roughness in ray tracing is not so critical as the slope errors, because the amount of scattered light with respect to the total flux can be easily estimated by using simple analytical formulae. Moreover, for the typical values of roughness rms of the ESRF mirrors (from 1 to 4 Å), the amount of scattered radiation is very low. In most cases, the diffused radiation is spread over a spot size that is slightly larger than the spot size that is obtained when considering real sources, aberrations, and waviness.

III. CRYSTAL OPTICS

Among the experimental techniques planned at the ESRF, only a few require white beam. Thus, the x-ray monochromator constitutes the core of the beamline optics. For hard x-rays, only crystal monochromators can be used, and most of the them are based on Si crystals (also Ge and diamond). There is, at the ESRF, a wide variety of monochromator designs and types due to the pluridisciplinary beamline requirements. The most commonly used is the double-crystal monochromator with sagittal bending of the second crystal and cryogenic cooling of the crystals.\textsuperscript{15} Other beamlines use specific monochromators, like crystals in transmission geometry (plane or bent), multiple crystal monochromators (i.e., SAXS cameras, high resolution monochromators), etc. SHADOW can simulate most of these systems. A collaboration between the ESRF and the CXrL is being carried out in order to implement in SHADOW new monochromator devices and crystals.

The application of SHADOW for crystal optics at the ESRF will be discussed in the following paragraphs: flat crystal optics and curved crystal optics. This presentation does not imply a focusing/nonfocusing monochromator classification. Any crystal diffraction – except the most conventional symmetric diffraction in reflection or Bragg mode – produces a change in the photon beam divergence and thus a focusing effect.

A. Flat crystal optics

Several ESRF beamlines use the well-known double-crystal Bragg monochromator, in either dispersive or non-dispersive configurations, or a combination of both. In addition, new flat crystal monochromators in transmission (Laue) geometry have been developed, built, and used at the ESRF. Thin perfect crystals (10-200 µm) of silicon or diamond diffracting photons in the hard x-ray range can produce an intense diffracted beam without involving high heat load. Moreover, the transparency of materials like diamond to the x-rays permits the use of both the diffracted

FIG. 1. Spot patterns for ESRF BL1 configuration produced with different mirror models: toroidal mirror without slope errors (top left), ellipsoidal mirror without slope errors (top right), ellipsoidal mirror with 0.8 arc sec slope errors and single sine waviness model (bottom left), and ellipsoidal mirror with 0.8 arc sec slope errors and multiple sine waviness mode (bottom right). Last case corresponds to the realistic one.
and transmitted beams to create multiple station beamlines. A computer model has been implemented in SHADOW to treat perfect crystals in transmission geometry. With this program, one can evaluate the focusing effect of the Laue crystals. On one hand, Laue crystals tend to focus polychromatic divergent photon beams when the beam divergence is much greater than the diffraction profile width. On the other, this focusing effect is not observed when the incident beam is monochromatic or almost collimated. This effect has been observed experimentally at the Troika beamline at the ESRF. The beam dimensions after the diffraction by an asymmetrically cut diamond crystal in transmission geometry have been recorded for several different crystal entrance slits. SHADOW simulations (Fig. 2) show a perfect agreement with the experimental results. This work has been helpful in understanding the focusing properties of these crystals as well as in demonstrating the reliability of the ray-tracing model. SHADOW is presently being used to complete the design of the remaining experimental stations of the Troika beamline and for the optical design of the Macromolecular Crystallography beamline (BL20).

B. Curved crystal optics

Curved crystals are used at the ESRF for several applications. They can focus the beam and combine the curvature effect with the intrinsic focusing effect of asymmetric crystals. The most common is the sagittal focusing of the photon beam in the horizontal plane. Other beamlines require bent-crystal monochromators, symmetrically or asymmetrically cut, like the Dispersive EXAFS Beamline (BL9) or the small angle x-ray scattering cameras at the BL 1. The curvature of the crystals can be modified or entirely originated by the effect of spurious bending. This is due to thermal load and anticlastic effects. Ray-tracing studies are very helpful for analyzing these combined effects. In double-crystal monochromators, one may suppose that the best system, in terms of density of flux at the sample position (high transmission plus high focalization), would be given by a tangentially bent first crystal and a second crystal sagittally bent. The curvature radius of the first crystal may be set either to focus the beam on the sample position or to satisfy the Rowland condition, giving an optimum transmission. Ray-tracing studies can show that the system in which the first crystal is bent to focus on the sample position deteriorates, in most cases, the transmitted flux. This is due to a bad coupling between the two crystals. Therefore, it is preferable to bend the first crystal in order to fit the Rowland condition or, even better, to use a first mirror to collimate the beam prior to the first flat monochromator crystal. This solution is adopted for many of the ESRF beamlines. Nevertheless, it is possible to modify the curvature of the tangentially bent first crystal in order to compensate the heat load and anticlastic effect on the monochromator crystals.

The thermal distortions of the monochromator crystals can be analyzed with SHADOW in the same manner as in the mirror case. That is, the deposited power on the silicon crystal is calculated using SHADOW and/or other programs like TRANSMIT or utilities available in XOP. Second, ANSYS is used to calculate the surface distortion due to the thermal load. Then, SHADOW calculates its effect on the spot size and flux transmission. Calculations of this type (Fig. 3) have been performed for the Materials Science beamline (BL2). In order to avoid anticlastic curvature, ribs can be cut in the crystal. The optical effect produced by the deformation in the crystal surface is originated by these ribs. This effect has been studied by coupled ANSYS-SHADOW calculations for BL13.
IV. SYSTEM IMPLEMENTATION AND OTHER DEVELOPMENTS

The package IDL\textsuperscript{24} has proved to be an extremely useful complement to SHADOW. IDL provides tools to create sophisticated graphical applications and widget interfaces. A library of SHADOW post-processors based on IDL has been developed at ESRF.\textsuperscript{25} This library permits one, for example, to make PLOTXY graphics where rays can be colored as a function of any given variable, animate the beam propagation, perform interactive fitting of SHADOW’s histograms, etc. IDL is also used systematically at the ESRF to create macros for multiple SHADOW runs (loops). This feature extends SHADOW’s number of rays limitation (5000) to an indeterminate number of them.

Another extremely advantageous feature of IDL is its widget tool facility, which allows one to create user interfaces. We have created an interface to run a customized SHADOW application for the ESRF BL3 (Fig. 4). This application presents screen menus in which a restricted set of SHADOW parameters are entered (the only ones that the user can modify). Some parameters, like the wiggler magnet gap, are pre-processed in order to calculate the parameters that SHADOW needs. This application can read mirror profile files that are measured on-line at the beamline. It performs all the necessary filtering and file format transfer in order to enter the mirror profile in SHADOW. It is thus possible, to compare the theoretical spot image with the one that is being monitored in order to optimize the alignment of the beamline elements. Calculations done with this application are in good agreement with experimental results.\textsuperscript{26}

Ray-tracing calculations can sometimes be tedious due to the high number of beamline parameters and combinations to analyze. The optimization of a single parameter can be done manually or automatically by sampling the parameter and performing a loop of SHADOW runs. However, to optimize simultaneously several parameters, an exhaustive search of the best value is impractical, and the only solution at present is the heuristic intuition of the developer. A feasibility study of the automation of such a global search of optimal parameters has been done at the ESRF.\textsuperscript{27} Two different approaches have been considered: genetic algorithms\textsuperscript{28} and simulated annealing.\textsuperscript{29} The conclusion of this study was that although both methods are suitable for optimizing the beamline parameters, the computer time needed for such optimization when a relatively large set of parameters are considered is extremely high for common UNIX workstations. In order to decrease this time, it would be necessary to work in two directions. First, the SHADOW main program structure has to be modified to accelerate systematic automatic calculations. In addition, pre- and post-processors should be written in order to calculate easily and flexibly the figure-of-merit function. For this purpose, we used IDL, but it was too slow for our needs. Second, we must find faster machines, which will certainly be widespread in a near future. An interesting option would be to use parallel machines, since the structure of genetic algorithms, simulated annealing and ray tracing is very suitable for parallel processing.

\begin{figure}[h]
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\includegraphics[width=\textwidth]{figure4.png}
\caption{Picture of some windows created by the ID09 IDL/SHADOW application.}
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