Status of XOP: an x-ray optics software toolkit

Manuel Sánchez del Río[a*] Roger J. Dejus[b]

[a]ESRF, BP 2002, F-38043 Grenoble Cedex
[b]APS, Argonne National Lab. 9700 S. Cass Avenue, Argonne, IL 60439

ABSTRACT

XOP is a user-friendly computer environment for performing calculations of interest to the synchrotron radiation community. It provides codes for: i) modeling x-ray sources (e.g., synchrotron sources, such as undulators and wigglers), ii) calculating characteristics of optical elements (mirrors, filters, crystals, multilayers, etc.), and iii) multipurpose data visualization and analyses. The XOP functionality can be extended with external plug-ins (extensions). We describe the status of XOP including recent developments in the current version (XOP 2.11). Plans for the future will also be presented.

Keywords: Synchrotron radiation, insertion device, optics modeling, x-ray optics database, graphical user interface

1. INTRODUCTION

X-ray oriented programs (XOP) is a graphical user-interface environment for computer codes of interest to the synchrotron radiation community. It has been widely distributed at synchrotron facilities and research laboratories. It can be downloaded from the XOP web site [1]. Today, we count over 400 registered users.

XOP was written with the aim of combining, in a user-friendly software environment, many utilities for calculating basic properties of synchrotron radiation that are useful for beamline designers and experimentalists. The main applications are source simulations (mainly spectral properties—but also angular and spatial distributions of bending magnets and insertion devices), and x-ray optics calculations (response of optical elements, such as crystals, mirrors and multilayers, to x-rays). XOP includes also a database (DABAX) with atomic and electronic properties and photon-atom interactions (cross sections and scattering factors) for the elements. A number of applications are included to process and visualize the DABAX database and for general visualization and data analysis purposes.

2. OVERVIEW OF XOP'S FUNCTIONALITY

The functionality of the applications can be divided into four groups:

1. x-ray sources
2. x-ray optics
3. databases and tools
4. Additionally, packages can be plugged into XOP (as "extensions") that typically would belong to any of the precedent three groups too.

For a more complete description of XOP and its applications, and for the latest information on XOP, the reader is referred to the XOP web site and documentation. We summarize in this section the main functionality of these four groups of applications.

* srio@esrf.fr; phone +33 476 882 513

2.1 X-ray source simulation

XOP has several independent tools to simulate different x-ray sources. The majority of them are for characteristics of synchrotron radiation. Other programs simulate the emission spectra of x-ray tubes. Two programs are interfaced into XOP to evaluate the spectral emission of x-ray tubes over a particular energy interval [2,3], i) XTUBE_W for tungsten anodes from 30 to 140 keV, and ii) XTUBES for Mo, Rh and W anodes from 18 to 42 keV. Both use the "gold standard" experimental spectra as the starting point in the interpolation algorithm. Another application is for computation of spectral distributions of the well-known Planck distribution (thermal radiation from a black body).

Several codes are available for computing characteristics of synchrotron sources —spectral emission, angular and spatial distributions, etc., of bending magnet sources, and wigglers and undulators—. The bending magnet code BM computes the spectral flux and power for a given angular emission angle, or integrated over an angle interval, or integrated over the full vertical angle. It uses the formalisms described in refs. [4,5]

Two models are available for calculating the spectral flux emitted by a wiggler. The first, XWIGGLER, calculates the full emission of a wiggler by computing the electron trajectory (usually sinusoidal, but also non-sinusoidal trajectories for the so-called asymmetric wigglers), and then, for each point along the trajectory, it computes the local radius of curvature to calculate the emitted dipole radiation (as for a bending magnet source). The total integrated flux is calculated as the integral of the local emissions over the whole length of the electron trajectory. This model was adapted from the wiggler code in reference 6. The second program, WS, calculates the emission at each grid point of a receiving aperture using the Eq. 3.12 described by Kim [7]. (Both programs produce the same results when a large enough aperture is chosen in WS.) None of these programs include the effect of the finite size and divergence (emittance) of the electron beam, and none can generate power distribution maps. For these kinds of calculations, it is sometimes possible to enter the wiggler parameters into the provided undulator programs.

By far, the most common synchrotron source calculations for third-generation facilities are for plane and helical undulators. Two programs, XUS and URGENT [8] are used to compute spectral properties, angular and spatial emission maps, and on-axis brilliances. The functionality of the programs overlaps, but both are maintained in XOP because different users have different preferences.

2.2 X-ray optics and Photon-atom interactions

The application programs in this group calculate interactions of x-ray beams with optical elements or components. Typical cases are mirrors, multilayers and crystals. All applications require the calculation of the index of refraction and the attenuation coefficient of the materials in use. These calculations cannot be done quickly from first principles; therefore we have compiled a database (DABAX, DAtaBAse for X-ray applications) with tabulations of these parameters. One of the advantages of DABAX is the decoupling of the data from the calculations. It is easy to change the data files in the database without the need to change the programs. Furthermore, in most programs, a menu is included that allows the user to choose the preferred data file.

The DABAX application is a front-end graphical user interface to the DABAX data files. It allows one to i) inspect data files, ii) download new data files to your local XOP installation, iii) consult file documentation, iv) view numerical data and, v) plot the data files. From this interface, it is also possible to start applications that make post-processing of the DABAX data to calculate different parameters for beamline experiments: i) XF1F2 for anomalous scattering factors, index of refraction, and material reflectivity, ii) xCrossSec for photon-atom cross sections and attenuation coefficients, iii) xFh for crystal structure factors, and iv) XF0 for elastic scattering functions.

Attenuation coefficients can be calculated from the tabulated cross sections using the xCrossSec program. (XF1F2 calculates the photoelectric attenuation coefficient, but it is not recommended for attenuation calculations at high photon energies or for high-atomic number elements because it ignores inelastic scattering.) The reflectivity of thick reflecting surfaces (mirrors) versus photon energy, incidence angle, or both, is computed by XF1F2 using the Fresnel formulas, which use the index of refraction obtained from the DABAX database. (The reflectivity is energy dependent because the index of refraction depends on the photon energy.) The application XPOWER imports a previously calculated x-ray

spectrum and calculates the effect of optical elements (up to five attenuators and mirrors placed in the beam) on the spectrum. XPOWER could handle monochromatots using a very simple formalist described in [9].

Crystals are used as x-ray monochromators. Almost all x-ray monochromators in synchrotron beamlines use perfect crystals like silicon or germanium. For describing the crystal diffraction by perfect crystals, the dynamical theory of diffraction should be used. Several calculation algorithms are implemented in XOP crystal applications to treat different kind of crystals. For flat, perfect crystal diffraction profiles, e.g., Si, Ge or diamond, the code XCRYSTAL can be used. It calculates angular scans for a given photon energy or energy scans for a given incident beam angle. Any crystal structure defined in DABAX may be used as input. It includes a simple model for the temperature factor. (The reflectivity of mosaic crystals can also be computed using XCRYSTAL.)

The diffraction profiles of curved crystals are in general different from the profiles of flat crystals. Several models are available in the program XCRYSTAL_BENT for curved crystals [10]. A program for displaying multiple reflections and calculating umweganregung patterns (MAMON) is also included. It is valid for cubic lattices only, and it uses a simplified model (no dynamical theory) for the line intensities.

A basic program for multilayer calculations (MLAYER) is included. It calculates the multilayer reflectivity (for a periodic or graded multilayer) versus photon energy (for a fixed incidence angle) or versus incidence angle (for a fixed energy). It is limited to atomic elements (no compounds), and it does not take into account the effect of the roughness at the interfaces on the reflectivity. Users interested in more advanced multilayer modeling and fitting to experimental data can use the code IMD [11], which is available as an XOP extension. A program called CRL for calculating the focusing effect of compound refractive lenses using a simplified ray-tracing model is also available.

2.3 General purpose tools

A number of tools are available in XOP to create graphics from the numerical results. In some cases they are built into the applications, but our goal has been to create general tools that are shared by several utilities and that can be used generically in the area of visualization, number crunching and data analysis. With this aim in mind, the XPLOT tool was created—an XY-data analysis and visualization generic tool with several options to make overplotting, fitting, high-quality customized graphics, etc.

An application called EXODUS has been recently integrated in XOP. It can be used to import multiple sets of data from either SPEC files or multiple ASCII files, and permits to interpolate, average, operate and display these sets of data in a very flexible way.

An imaging tool called XPLOT2D is targeted for scientific image display. It can import data in a variety of formats (ESRF data format, MAR CCD, TIFF, etc) and allows different selection of region of interest (ROI), masking data, radial and azimuthal integrations, etc. It has been applied to the analysis of image plates with X-ray diffraction data. It permits the calibration of some detector parameters (position of the center of the beam and distance sample-detector), and it allows overplotting on top of the recorded image the Debye-Scherrer rings of a known material.

2.4 XOP extensions

An XOP “extension” is a software package that is not part of the XOP standard distribution but can be optionally installed and run under the XOP interface. The complete list of extensions, download instructions, tutorial, and installation procedures is available from the XOP web page. Some of the currently supported XOP extensions are:

SHADOWVUI: Visual User Interface for the SHADOW [8] ray-tracing package.
IMD [11]: Specular and nonspecular (diffuse) optical functions of an arbitrary multilayer structure.
NOP [12]: Optics for beams of thermal neutrons.
XAID [13]: A few data analysis tools for x-ray absorption spectroscopy.
INES: For data analysis of inelastic scattering data.

RECENT IMPROVEMENTS AND PERSPECTIVES

The development of XOP can be classified in three groups: i) technical development, in order to be compatible with the newest versions of operating systems, ii) application development, with the aim of improving the functionality of the existing applications, and write new applications, iii) user's support.

Regarding the technical development, we recently embedded XOP 2.11 using the IDL version 6.0. A distributed version will be available very soon from the XOP web page. It will run on most Unix platforms, including Linux, Windows (XP and 2000) and also Mac OS X.

Many applications have been updated and debugged. For example, the bending magnet radiation code BM has been upgraded to compute the spectral flux and power for a given angular emission angle, or integrated over an angle interval, or integrated over the full vertical angle. The calculation of the crystal structure factor in XFH can be now be done as a function of the energy, and allows displaying useful quantities like the Darwin width or intrinsic resolution. The code MAMON, which calculates multiple crystal diffraction has been debugged and extended to neutron diffraction. New applications for data analysis have been included, like XPLOT2D and EXODUS.

User's support is done via the maintenance of an updated web page, from where they can download the code. A mailing-list also exists, where the users can address problems and tricks. All mails sent to the mailing-list are stored in a database accessible by the web. The on-line documentation has been improved and is provided in PDF format. A generic documentation set was created that will help users select the most appropriate application for a particular task from the pool of applications that XOP offers. A user guide of XPLOT is also available.

For users getting started with XOP, a new and efficient way of learning is provided. A tutorial formed by a collection of tasks on practical exercises of x-ray sources and optics is available. Hints to solve the exercises (and solutions), including XOP input files are also available. The tutorial includes also some aspects of the XOP extensions IMD and SHADOW.

For the future, we plan to maintain and extend XOP as much as possible. However, XOP has grown a lot in the last years, and it is now a large computer package that can be used for many different x-ray sources and optics simulations, and many experimental techniques. Therefore, it requires a lot of work to maintain, and much more work to improve and extend. As manpower and resources are limited, we plan to extend XOP only in some directions that are compatible with the author's current tasks. For instance, we developed an XOP extension to deal with neutron scattering [12], and we are working in some applications for the analysis of X-ray fluorescence and X-ray diffraction data. Users are always welcome to give us feedback on their use of XOP, and perhaps contribute with their software to the extension of XOP.

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