

XOP: Recent Developments

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ABSTRACT

XOP (X-ray OPTics utilities) is a graphical user interface (GUI) to run computer programs that calculate basic information needed by synchrotron radiation beamline scientists and engineers. It can also be used as a front end for specific codes or packages for data analysis and data reduction (XAFS, surface crystallography, etc.). XOP contains a customized database for optical and atomic constants. It has a flexible design and new applications may be added.

The capabilities of XOP, including those related to simulations of crystal diffraction profiles and multilayer reflectivities, are summarized. We discuss the most recent developments to be included in XOP version 2.0. A few other examples of typical calculations are: insertion device (undulator and wiggler) spectra and angular distributions, mirror and multilayer reflectivities, and crystal diffraction profiles. The computer programs are executed and the results are analyzed within the GUI, which makes them fast and easy to use.

The XOP interface is written in the Interactive Data Language (IDL) from Research Systems Inc., and it runs on the Unix (HP, Sun, Linux, DEC-Alpha, and Silicon Graphics), and on the Windows 95/NT operating systems. It has been built with an IDL license embedded and is available under some limited conditions free of charge from the authors.

Keywords: synchrotron radiation, insertion device, optics modeling, x-ray optics data base, graphical user interface, interactive data analysis

1. INTRODUCTION

XOP is a software toolkit for calculating basic quantities useful for synchrotron beamline designers and experimentalists. The main calculations include simulation of source characteristics and modeling of optical elements (mirrors, crystals, etc.). Basic data analyses and visualizations are also available, and more specialized modules, e.g., XAFS and surface crystallography data analyses, can optionally be plugged into XOP.

Synchrotron radiation users have usually faced difficulties when they need to combine results from different computer programs, which very often are from different origins and come from different authors, and which sometimes even must run on different computers. XOP arose from such considerations, and the main purpose of XOP was to overcome these difficulties and to provide a flexible, unified, and yet reliable graphical user interface (GUI), written in IDL,¹ to run such programs.

The first distributed version of XOP (version 1.9, which should be considered a beta-test release) was released in January of 1998, and the demand has been encouraging - we have received over 100 installation requests within the first 6 months of its initial release date. Currently, we are working on the first production release (version 2.0), which includes many improvements over the present version. For example, new features have been added (most based on users requests), the distribution and installation procedures have been updated and simplified, the on-line help system has been improved, and new applications have been developed.

The XOP main window (shown in Fig. 1) is the front-end window to start the applications in XOP. The menus in this window are fully customizable to allow for local modifications. XOP's functionality has been expanded since

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its inception and there are now more than 20 main applications and 5 "extensions" available. The simulations can be divided into three different application groups:

- Source simulations
- Characteristics of optical elements
- Multipurpose data analysis and visualization

The synchrotron source simulations include programs to calculate radiation spectra (flux and power versus photon energy) of bending magnets, wigglers and undulators. The simulations take into account the parameters of the storage ring, e.g., beam energy and emittances, and the characteristics of the sources (number of magnetic periods, period length, magnetic field strength for insertion devices). In addition to common flux and power calculations, the undulator codes also compute other quantities, such as angular and spatial flux distributions, and polarization characteristics.

The optics applications can be divided into three subgroups:

- Mirrors and filters (described in Ref. 2)
- Crystals (described in Ref. 3)
- Other elements (multilayers and compound refractive lenses)

XOP uses the DABAX database for many of its optics applications. DABAX (DAtaBAse for X-ray applications) is a compilation of data tables needed for x-ray optics applications, and it also contains a collection of computer programs to access, visualize, and process the tables. DABAX was created to unify tabulated databases, e.g., scattering factors and x-ray atomic cross sections, and to simplify their accessibility and use in XOP. The XOP applications are presently converted to use the DABAX database rather than an inherent database that came with the applications themselves. DABAX can be used to store information from either theoretical computations or from measurements, e.g., experimental XAFS spectra are available. Many other properties can be included in the database and accessed from XOP without the need to modify any of the codes. We have also most recently made available a new database for atomic x-ray cross sections and anomalous scattering factors, which contains data over a wide energy range, 1.0 eV to 1.0 MeV (upper energy was set to 1.0 MeV for inclusion in XOP). The data were derived from the Evaluated Photon Data Library, the '97 version by Cullen *et al.*⁴ Anomalous scattering factors from Chantler⁵ can be available in DABAX, but a user license from NIST⁶ is required. The inclusion of improved Chantler data in XOP is under consideration.

We have introduced the concept of "extensions" in XOP because we needed a mechanism to include larger applications. Generally, the applications distributed with XOP require only small resources and small amounts of disk space and are relatively easy to use. However, there are other applications suitable for XOP that require larger software resources. Their functionality is typically well suited to the philosophy of XOP and is related to the synchrotron radiation field. In addition, many of them have been designed using the data libraries of XOP. However, because of their somewhat limited use and functionality, we have chosen to treat such applications as "extensions". This concept simply means that the standard distribution of XOP can optionally be extended, but it requires a special user installation. After installation, such applications behave and function the same as those applications of the standard distribution. At present, the following packages are available as XOP extensions:

- SHADOWVUI: a visual user interface to the ray-tracing package SHADOW⁷
- RODGUI: a graphical user interface to the program ROD⁸ for surface crystallography modeling and fit
- PROW: a data integration program based on profile fitting for the evaluation of weak and/or overlapped two-dimensional macromolecular diffraction patterns by Bourgeois⁹
- IMD: a program for generation and analysis of multilayer structures by Windt¹⁰
- Other programs: such as TOPO for surface texture analysis by Windt¹¹ and GEDET, a multistrip Ge detector simulation program¹²

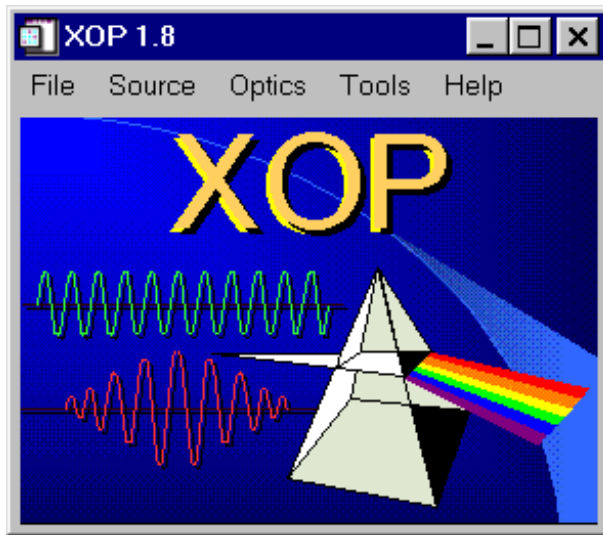


Figure 1. The main XOP window.

2. SOURCE SIMULATIONS

Recent developments in undulator fabrication technology (including magnetic phase shimming) have resulted in devices that behave almost as ideal radiation sources, and, in most practical applications, the deviation from ideal may be neglected. The deviation is further shadowed by the particle beam emittance and energy spread, and computer codes based on ideal devices are therefore adequate under most circumstances. From a computational point of view, this presents a tremendous speed increase - typically a 100-fold to 1000- fold reduction in execution time.

There are two codes in XOP for simulating ideal undulators (no magnetic field errors or tapering allowed) based on the same formalism - the Bessel function approximation. The first code (URGENT) was developed by Walker and Diviacco¹³ and was subsequently rewritten by Dejus¹⁴ and released as code US. Both codes calculate undulator spectral characteristics, angular distributions, and emitted power and power density profiles for planar and elliptical devices. The high accuracy of the US code for modeling of undulator sources was discussed in a paper by Ilinski *et al.*¹⁵ where a comparison was made with experimental results obtained at the Advanced Photon Source (APS). Excellent agreements were found versus absolute flux measurements, and the small discrepancies found could be attributed to small magnetic field errors present in the real device.

The code US has also formed the foundation for other codes under development, e.g., tuning curve programs. These programs calculate the on-axis brilliance or the flux through an aperture versus a change of the K value (or the harmonic energy). The program YAUP¹⁶ has been included to provide for calculations of tapered undulators - its usefulness is being reviewed in the context of incorporating other codes that use a measured or simulated non-ideal magnetic field profile as input.

XOP also includes two codes for simulating wiggler spectra. One is XWIGGLER, obtained from the SHADOW⁷ package, which calculates flux generated by a standard planar (sinusoidal) wiggler or an asymmetric wiggler versus the photon energy, integrated over all emission angles. The electron trajectory is calculated along the device, and, for each point in the trajectory, the radiation is computed using the instantaneous bending magnet radius in the well-known bending magnet formulas. The other code, called WS, is also based on the bending magnet formalism but allows for many more calculational modes, for instance, flux spectrum through a finite size aperture, angular flux density distributions, and power and power density profiles. Radiation from a simple bending magnet is also available, and a number of new modes have been implemented. For a recent review on characteristics of synchrotron radiation sources, see Ref. 17.

Some users have expressed interest in conventional sources (x-ray tubes) and would like to have such a modeling capability in XOP. However, since the work starting with Kramers¹⁸ in 1923, there have been many attempts to

reliably model spectra from x-ray tubes. To this date, there has not been a consensus reached on a theoretical model that is applicable under different voltage conditions and anode materials. An interpolation method using measured "gold standard" x-ray spectra has been proposed by Boone and others^{19,20} and applied successfully to *W* anodes¹⁹ in the photon energy interval 30 to 140 keV and to *Mo* and *Rh* anodes²⁰ from 4.5 to 38.5 keV. The supplied codes have been interfaced to XOP and calculated spectra can be used with other XOP applications, for example XPOWER can be used to compute the effect on the beam by mirrors and filters.

3. CHARACTERISTICS OF OPTICAL ELEMENTS

The optics codes implemented in XOP can be classified into four groups: i) the DABAX (DATAbase for X-ray applications) interface and related codes, ii) filter and mirror reflectivities, with the possibility to be coupled with the source models, iii) crystal diffraction profiles, and iv) other elements (multilayer reflectivities and compound refractive lenses). The first two application groups were described in detail in Ref. 2, and the crystal models were fully described in Ref. 3.

3.1. Crystal codes

Two main crystal codes are available in XOP to compute diffraction profiles. XCRYSTAL calculates the diffraction profiles for plane crystals, whereas XCRYSTAL_BENT simulates the diffraction by bent crystals.

XCRYSTAL computes diffraction profiles of perfect and mosaic crystals. For perfect crystals it codes the dynamical theory of diffraction as described in the book of Zachariasen.²¹ This allows one to simulate crystal diffraction patterns for two geometries: Bragg (reflection mode) and Laue (transmission mode). Its general implementation allows one to simulate accurately crystals of any thickness. Diffraction in almost-normal incidence is also allowed. XCRYSTAL also simulates mosaic crystals using the theory of Zachariasen²¹ in both the Bragg and Laue cases.

For bent crystals, the code XCRYSTAL_BENT implements several theoretical approaches. They are fully described in Ref. 3. The models have different degrees of applicability and reliability. The multilamellar model, although available for both Bragg and Laue geometries, only gives acceptable results for most of the cases in Bragg geometry. To improve the accuracy in modeling Laue crystals, we coded the Penning-Polder²² theory. More precise calculations will be required to solve numerically the Takagi-Taupin^{23,24} equations, a coupled set of differential equations. For that, an experimental code is available in XOP. Good results have been obtained in several Laue cases.

3.2. Multilayers

For multilayer calculations XOP includes the program MLAYER, written by Underwood,²⁵ which was extracted from the SHADOW⁷ package. It computes reflectivities and phase shifts as a function of either the grazing incidence angle or the photon energy for either a periodic or a graded multilayer.

The MLAYER code is relatively simple, and the applications are limited. For users who need a complete program for multilayer simulations and fitting capabilities to experimental data, the code IMD¹⁰ is recommended. The IMD program is available as an extension to XOP.

3.3. Compound Refractive Lenses

Compound refractive lenses (CRLs) have been proposed and successfully used²⁶⁻²⁸ to focus hard x-rays. A new software application for simulating compound refractive lenses has been written and integrated into XOP. It computes both the main parameters of a CRL (focal distances, gains, etc.), and the beam profiles and phase space at the image plane. The latter calculations are performed using a pseudo-ray tracing method described in Ref. 28.

3.4. The SHADOW Visual User Interface

Although XOP provides the basic tools for making calculations to obtain a preliminary design of a synchrotron beamline (source spectra simulations and characteristics of optical elements), an accurate simulation of the beamline optics requires ray-tracing simulations. The *de facto* standard code for these simulations in the synchrotron radiation community is SHADOW.⁷ It is a complete package for simulating x-ray sources using the Monte Carlo method and ray traces the source sequentially over the beamline components (mirrors, crystals, gratings, multilayers, etc.). SHADOW is available from Ref. 29, and it runs directly using its command mode or by using its

graphical user interface. We have developed applications in IDL to do the SHADOW postprocessing (visualization, histogramming, statistics). These functions have been integrated in a global visual user interface for SHADOW called SHADOWVUI,³⁰ which allows the user to exploit all of the SHADOW capabilities from a simple point-and-click interface and to visualize the results using applications based on the IDL graphics. SHADOWVUI was designed using the same concepts used in XOP and is available as an extension to XOP.

4. DATA ANALYSES

XOP data visualization and basic analyses are performed by the module called XPLOT, which has been developed to serve as a common tool for many applications. It is used for displaying the results of most XOP's applications. XPLOT can be used to perform operations on the data, for example, integrating the source spectral power to obtain the total power, multiplication and convolution of diffraction profiles, etc. XPLOT is a general package for creating and manipulating X-Y plots.

XOP can also include packages for specific data analyses. A few of these extensions are:

- XAID³¹: A package for XAFS (x-ray absorption fine structure) analysis. It performs basic operations for background removal and Fourier transform and filtering.
- RODGUI³²: A graphical user interface for the program ROD.⁸ ROD is a data analysis and fitting program written by Vlieg⁸ and commonly used in surface crystallography. It is used at ESRF as a standard tool at several beamlines. In order to make the program more user friendly and to improve the graphics, it was decided to create a GUI on the top of ROD. This interface was written under IDL, and it uses many of the existing programming tools designed for XOP. The user can now run ROD from a point-and-click environment. The interface also allows direct typing of ROD commands and allows for automatic creation of macros that are editable and executed in future working sessions. The first version is currently available as an XOP extension.
- PROW³³: A data integration program based on profile fitting for the evaluation of weak and/or overlapped two-dimensional macromolecular diffraction patterns. A new technique⁹ has been developed for the integration of weak and/or spatially overlapped two dimensional diffraction patterns. The program, named PROW (Profile fitting for Overlapped and Weak data) can be used for the evaluation of either Laue or monochromatic data.

5. CONCLUSIONS

The XOP graphical user interface provides a common interface to a wide variety of computer codes for synchrotron radiation applications. It also contains a flexible materials database, as well as data analysis and visualization capabilities. It is now in use in more than 50 laboratories world wide, and new applications are being added based on user demand. The full distribution of the software is available under some limited conditions from the authors.³⁴

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