

XOP: A Multiplatform Graphical User Interface for Synchrotron Radiation Spectral and Optics Calculations.

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ABSTRACT

XOP (X-ray OPTics utilities) is a graphical user interface (GUI) created to execute several computer programs that calculate the basic information needed by a synchrotron beamline scientist (designer or experimentalist). Typical examples of such calculations are: insertion device (undulator or wiggler) spectral and angular distributions, mirror and multilayer reflectivities, and crystal diffraction profiles. All programs are provided to the user under a unified GUI, which greatly simplifies their execution.

The XOP optics applications (especially mirror calculations) take their basic input (optical constants, compound and mixture tables) from a flexible file-oriented database, which allows the users to select data from a large number of choices and also to customize their own data sets.

XOP includes many mathematical and visualization capabilities. It also permits the combination of reflectivities from several mirrors and filters, and their effect, onto a source spectrum. This feature is very useful when calculating thermal load on a series of optical elements. The XOP interface is written in the IDL (Interactive Data Language). An embedded version of XOP, which freely runs under most Unix platforms (HP, Sun, Dec, Linux, etc) and under Windows95 and NT, is available upon request (*srio@esrf.fr*, *dejus@aps.anl.gov*).

Keywords: graphical user interface, synchrotron sources simulation, optics modeling, interactive data analysis, x-ray optics database

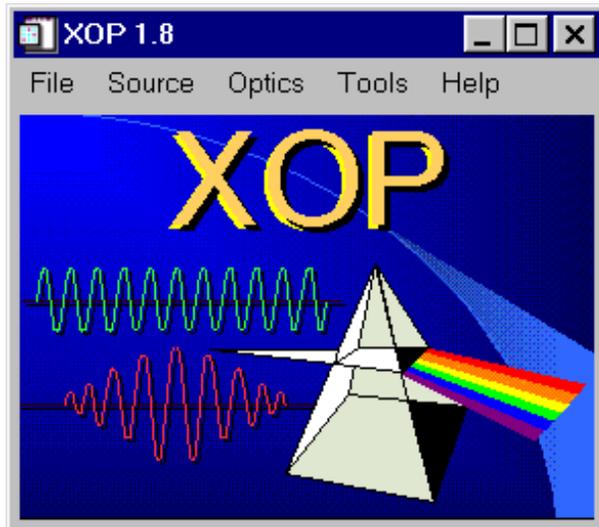


Figure 1. The main XOP window.

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1. INTRODUCTION

The basic calculations needed for synchrotron beamline design are related to the simulation of the source spectral characteristics and to the modeling of the optical elements (mirrors, crystals, etc.). The main difficulty arises from the fact that one often needs to combine the simulations of different programs, usually from different origins and authors, which sometimes run on different platforms. The goal of the XOP application is to overcome these difficulties and present to the user a flexible, unified, and reliable graphical user interface (GUI) to run such programs. The concept of including many applications under a single GUI was realized in 1994, when we released XOP version 1.0. At that time, the application was intended to be run internally at the ESRF and the APS. During the past years, more users became interested in running XOP, and new applications have increased the XOP's functionality. Currently we are releasing XOP version 2.0, a customizable and adaptable GUI for synchrotron users. A picture of the XOP main window is shown in Fig. 1. XOP's functionality has been expanded and now over 20 applications are available. It is used for synchrotron radiation simulations related to three different application groups:

- source simulations
- characteristics of optical elements
- multipurpose data analysis and visualization

The synchrotron source simulations include programs to calculate the radiation spectra (flux and power versus photon energy) of bending magnets, wigglers and undulators. The simulations consider the parameters of the storage ring (e.g., energy and emittances) and the characteristics of the insertion device (number of magnets, period length, magnetic field, etc.). In addition to the standard flux and power calculations, the undulator code *US* also computes other quantities, such as flux densities on a screen surface and polarization characteristics. An XOP window of the undulator part is shown in Fig. 2. The source models are not discussed in this paper; for information refer to the XOP on-line documentation and other publications.^{1,2}

The optics codes implemented in XOP can be classified into four groups: i) DABAX (DATAbase for X-ray applications) interface and related codes, ii) mirror and filter reflectivities, with the possibility to be coupled with the source models, iii) crystal diffraction profiles, and iv) multilayer reflectivities. The two first application groups are described in detail in the next paragraphs, whereas the other two groups are briefly described in Refs. 1 and 3.

The crystal diffraction codes available in XOP compute the diffraction profiles of perfect and mosaic crystals.³ The dynamical theory of the diffraction is used for these calculations. Two diffraction modes are allowed for all the codes: Bragg case (reflection mode) and Laue case (transmission mode). The perfect crystal codes can calculate diffraction profiles for flat crystals and also for bent crystals. Different theoretical methods are used for bent crystals, with different degrees of applicability and reliability. Approximated theories, such as the multilamellar model (for both Bragg and Laue crystals) and Penning-Polder (Laue crystals), are already implemented. A research program for calculating diffraction characteristics of bent and strained crystals is being developed and includes the numerical solution of the Takagi-Taupin differential equations using different algorithms. These codes will be available in a future release of XOP.

For multilayer calculations, XOP includes the program MLAYER, which is part of the ray-tracing package SHADOW.⁴ 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 XOP data visualization and analysis is performed by a module called XPLOT, which has been developed to serve as a common tool for many applications. It is in fact used for displaying the results of most XOP's applications. XPLOT can be used to perform operations on the data, for example integration of the source spectral power to obtain the total power, multiplication and convolution of diffraction profiles, etc. XPLOT is a general package for creating X-Y plots that also allows for sophisticated data visualization, processing, manipulation and analysis. Some of the XPLOT features are:

- Direct loading of data from multicolumn ASCII files. Multiple sets of data can be accessed from several files and merged together. Interactive action on data columns with the creation of new data from scratch or by manipulating existing data.

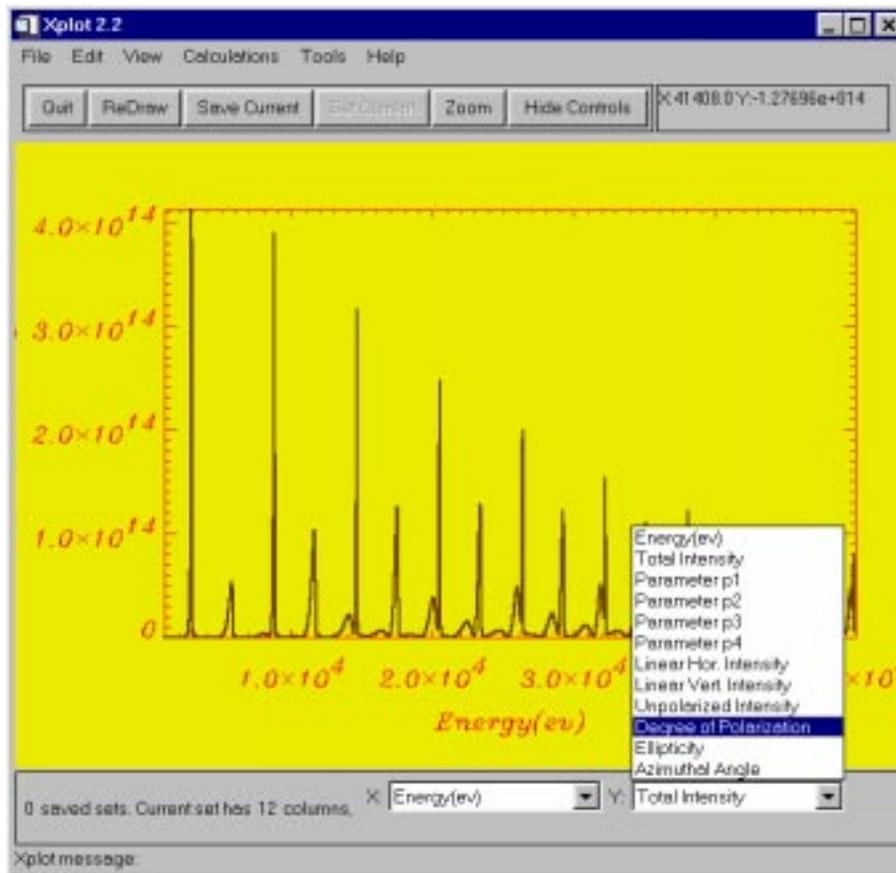


Figure 2. XPLOT window containing the result of an undulator calculation.

- Access to SPEC data files.⁵
- Direct printing from Unix workstations and PCs, and creation of PostScript and encapsulated PostScript files.
- Linear and logarithmic X- and Y-axes. Apply and change symbols, line styles, colors, thickness, fonts etc.
- Label, annotate, add legends, titles, etc. to the plots. Zoom, shift, switch columns, and over-plot data.
- Save and restore plots and attributes in a XPLOT backup file.
- Data analysis: extrema, moments, integrals, derivatives, CDFs, smoothing, user-defined operations, interactive Fourier filtering, interpolations, convolutions and correlations. It also includes several fitting routines: linear regression, polynomial fit, Gaussian fit and nonlinear fit (the gradient-expansion algorithm or the Powell method) with an on-line user-defined function.

XPLOT also includes some packages for specific data analysis. At present the XAID⁶ package for XAFS (X-ray Absorption Fine Structure) analysis is available. New applications and interfaces for data processing applied to different synchrotron techniques are under development, and they will be integrated in future releases.

2. MOTIVATION AND COMPUTER IMPLEMENTATION

The complete XOP interface is entirely written in the Interactive Data Language (IDL),⁷ using the built-in widget toolkit. IDL is a commercial package for interactive data reduction, analysis and display of vector-based variables. We have extensively used this toolkit for XOP together with the powerful mathematical and visualization capabilities

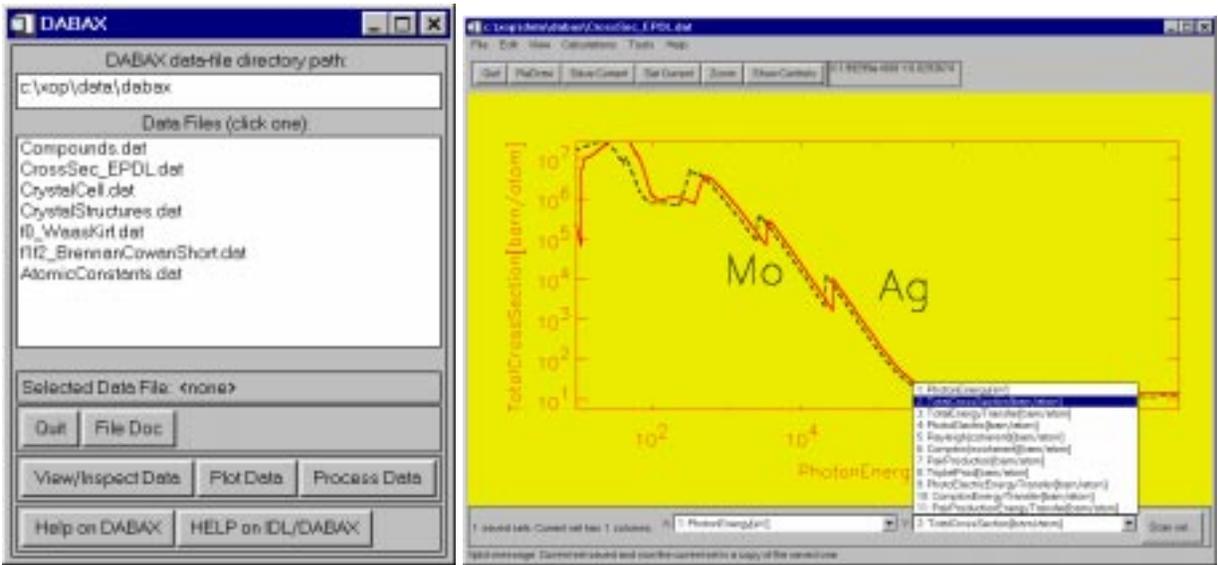


Figure 3. Main DABAX interface with a minimal set of files needed to run XOP (left). An example of data (right): The Ag and Mo total cross sections as stored in the EPDL dataset.

of IDL. The IDL code in XOP is platform independent. We have implemented and tested XOP under several Unix platforms (HP-Unix, Sun Solaris, Sun OS, Digital-Unix, Linux) and also under the Windows95 and WindowsNT operating systems.

Because XOP version 2.0 is available to users in the so-called embedded-IDL mode, the restrictive requirement that users have access to a machine with an IDL license is removed. Currently, the necessary IDL code and license validation are embedded in XOP.

The motivation to create XOP was the existence of many free *file-oriented* programs, which means that the program itself reads the input parameters from either an input file or the standard input, performs the calculations, and writes the output to a disk file (or several files). These programs are written in the most commonly used languages (FORTRAN, C) and are often portable to several platforms. However, these programs are in general not user friendly, because the user must, at a minimum, use a text editor to create the input file, know the command name to run the code, and use a graphics program to display the result, which (in most of the cases) requires data-format conversions. In order to overcome these difficulties, we created the XOP point-and-click interface that drives different programs from various origins and authors. It can, in addition, couple the calculations of several programs, for example it is easy to study the effect of a filter on the spectrum. The communication between XOP and the program is only done via disk files. The interface knows the parameters needed by the program, creates a window where all these parameters are presented simultaneously for editing, then writes the input file for the program, makes a system call (SPAWN) to run the program, and then passes the output files to the display routines.

3. THE DABAX DATABASE

DABAX (DAtaBAse for X-ray applications) is a compilation of tables for x-ray applications with a collection of computer programs to access, visualize, and process these tables.

DABAX was created to unify the tabulated data (e.g., scattering factors and x-ray atomic cross sections) for the different programs in XOP. In the first versions of XOP, each program included its own database, thus overloading disk space and avoiding direct comparison of the results. The XOP applications are presently being migrated from those using their own database to those using the DABAX.

The DABAX data files are well structured and customizable ASCII files. They are indexed to allow fast access. The data tables are often sorted by atomic number, nevertheless quantities referring to multi-atomic materials such as compounds and crystals may also be included.

The DABAX data directory in XOP contains a set of files that provides the basic data for photon-atom cross sections and scattering factors (dispersive and non dispersive components). It also contains files for atomic constants and atomic composition of compounds and crystals. The DABAX concept allows one the flexibility to include new data and to update existing data.

In addition to the minimum set of data files required by XOP (see Fig. 3 or Table 1) many other DABAX files are available either in the full XOP distribution or from the Internet.⁸ Therefore, an XOP user can add or change the files to ensure that the basic physical quantities correspond to the chosen model.

Table 1. List of all the DABAX files currently available. Files marked with (*) form the minimum set of default files for XOP.

Name of DABAX file	Description
f0_CromerMann.dat f0_CromerMann_old1968.dat (*) f0_WaasKirf.dat f0_mf_Kissel.dat f0_rf_Kissel.dat	f_0 data
f1f2_BrennanCowan.dat (*) f1f2_BrennanCowanShort.dat f1f2_Chantler.dat f1f2_EPDL.dat f1f2_Henke.dat f1f2_Sasaki.dat f1f2_Shadow.dat f1f2_asf_Kissel.dat	f_1 and f_2 data
(*) CrossSec_EPDL.dat CrossSec_XCOM.dat CrossSec_McMaster.dat CrossSec_Compton_Balyuzi.dat CrossSec_Compton_McMaster.dat CrossSec_Rayleigh_McMaster.dat	Atomic x-ray cross sections
XAFS_DATA_EXAFS_CHI.dat XAFS_DATA_XANES.dat XAFS_McKale.dat	X-ray Absorption Fine Structure files
(*) AtomicConstants.dat AtomicDensities.dat (*) Compounds.dat (*) CrystalCell.dat (*) CrystalStructures.dat EBindEner.dat XREmission.dat OptConst_Palik.dat	Miscellaneous files

DABAX can be used to store information from either theoretical computations or experimental measurements (for example, files with experimental XAFS spectra are available). Many other properties can be easily included in the database and accessed from the interface without changing the XOP code.

The full set of DABAX files already available contains about 30 data files (see Table 1) with different kind of information. They can be classified into three groups, which are discussed in the next sections.

3.1. Scattering Factors

The most commonly used parameter to characterize the scattering of photons by atoms is the so-called scattering factor f . It is defined as the factor by which the amplitude scattered by a single free electron is multiplied to yield

the total amplitude coherently scattered by a particular atom. The scattering factor is a function of the atomic number Z , the photon wavelength λ , and the scattering angle θ . It is usually written as:

$$f = f_0\left(\frac{\sin(\theta)}{\lambda}\right) + f_1(\lambda) + if_2(\lambda), \quad (1)$$

where f_0 is the atomic scattering factor far away from resonances, f_1 (also called f') and f_2 (or f'') are the real and imaginary parts (respectively) of the anomalous scattering factor.

The f_0 dependency on $\sin(\theta)/\lambda$ is usually parametrized as done by Cromer and Mann.⁹ The DABAX files `f0.CromerMann_old1968.dat` and `f0.CromerMann.dat` contain the coefficients of such parametrization as published in the original paper and in the International Tables for Crystallography,¹⁰ respectively. A new parametrization valid over a wider interval of $\sin(\theta)/\lambda$ was proposed more recently,¹¹ and the coefficients have been included in the file `f0.WaasKirf.dat`. Recent calculated tables (not parametrized) by Kissel *et al.*¹² of relativistic form factor and modified form factor are available in the files `f0_rf_Kissel.dat` and `f0_mf_Kissel.dat`, respectively.

The f_1 and f_2 components of the scattering factor are of special importance for calculating the electric susceptibility, complex index of refraction, surface and interface reflectivity, photoelectric attenuation, and crystal structure factors of materials. For such calculations, we need to have accurate data. We provide many different data files, which represents the present scenario for the theoretically calculated f_1 and f_2 data.

The first important and systematic calculations over a wide energy range were provided by Cromer and Liberman¹³ in 1970 and earlier. Currently, most simulation programs for x-ray applications are based on this theory. Computer programs from these authors and later modifications are generally available in different laboratories. Sasaki¹⁴ published tables calculated with Cromer and Liberman theory. He paid special attention to give data with a fine energy grid in the proximities of the absorption edges. The Sasaki tables are in the DABAX file `f1f2_Sasaki.dat`. Brennan and Cowan¹⁵ presented a program that calculates the anomalous scattering factor using the Cromer and Liberman theory. The tables calculated with this program are put in the DABAX files `f1f2_BrennanCowanShort.dat` and `f1f2_BrennanCowan.dat`. The first contains an equi-spaced energy grid on a logarithmic scale and the second contains this grid plus a fine grid close to the absorption edges (as used by Sasaki). Other classical references for anomalous scattering are the works of Henke *et al.*, first published in 1982¹⁶ and recalculated completely in 1993.^{17,18} The tables from the latter are in the DABAX file `f1f2_Henke.dat`.

Another source of f_1 and f_2 tables is the ray tracing code SHADOW,⁴ which uses data from Henke (1982)¹⁶ in the low energy range and from Cromer and Liberman (Sasaki) in the high energy range ($10 < E < 100 \text{ keV}$). These data are in the file `f1f2_Shadow.dat`.

Recent improved calculations have been published in 1995 in two papers, one by Chantler¹⁹ and the second by Kissel *et al.*^{12,20} The electronic tables from Chantler are sold by the Standard Reference Data Program at NIST.²¹ It is difficult to give a general rule of recommendation about which data file to use. We have performed a comparison test (see Fig. 4 for an example of Ni), and the conclusions are as follows. All the data sets provide comparable results far from the absorption edges and at photon energies larger than 1 keV . They are very different at energies below 1 keV . For those applications in which it is important to have enough data points close to the edges, files with a fine gridding, such as `f1f2_Sasaki.dat`, `f1f2_BrennanCowan.dat` or `f1f2_asf_Kissel.dat` should be used. The data by Chantler are good except close to the edges, but the difficulty is that they are not freely available. The data by Henke suffer from the limitations of their low upper energy (30 keV). The data by Brennan and Cowan sometimes present unphysical discontinuities at very high energies (e.g., f_1 of Au at $E > 100 \text{ keV}$). Thus, we can recommend the Kissel data before the Cromer and Liberman based data, because they are more recent and more accurate. However, in the interpolated electronic data provided by Kissel, many points are completely out of scale, requiring a particular filter before being used. Preliminary data for f_1 and f_2 which combine photo-ionization data from EPDL and photo-excitation data from Kissel (resolution broadened to remove singularities) are being investigated and will be available in a future release of XOP.²² To conclude, we will keep the conservative approach for XOP using the file `f1f2_BrennanCowanShort.dat`, containing data based on the theory by Cromer and Liberman, until the availability of corrected or better interpolated data.

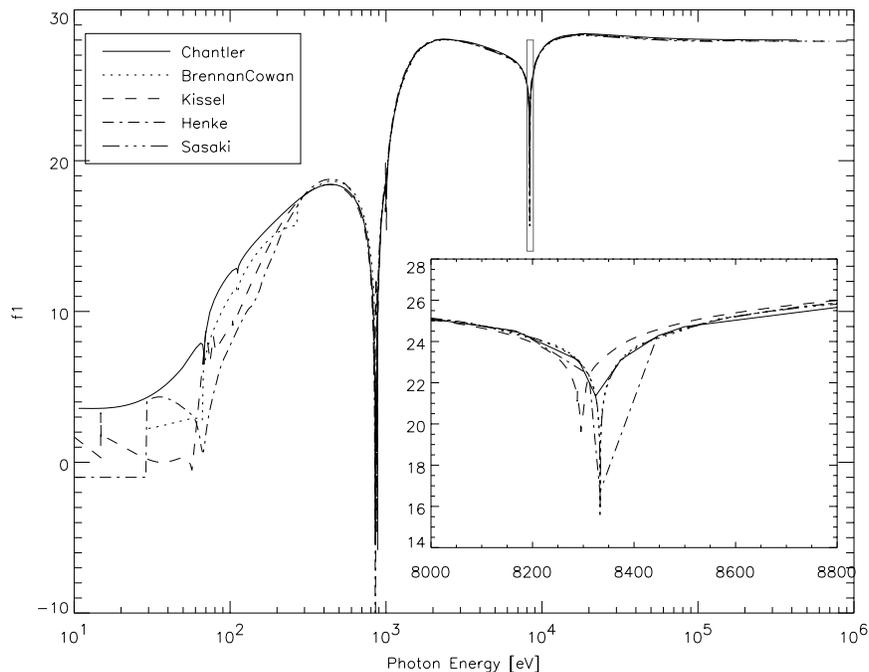


Figure 4. Comparison of f_1 values from different DABAX files for the Ni atom.

3.2. X-ray interaction cross sections and absorption coefficients

The attenuation of the x-rays by a filter is calculated from the weighted sum of the x-ray interaction cross sections of the elements that constitute the filter. The total interaction cross section is defined as:

$$\sigma = \sigma_{pe} + \sigma_R + \sigma_C + \sigma_{pp}, \quad (2)$$

where the subscript pe indicates the photo-electric cross section, R is the Rayleigh (or unmodified-elastic cross section), C is the Compton (inelastic) cross section and pp is the pair-production cross section. Other effects like triplet-production, etc., which occur at very high energies (in the MeV range) are not considered here. The DABAX files containing the tabulated cross sections are `CrossSec_EPDL.dat`, `CrossSec_XCOM.dat` and `CrossSec_McMaster.dat`. The first uses a subset of data from the EPDL²³ library and is the default in XOP. The second contains a tabulation created with the XCOM²⁴ program and the third uses data created by a program from McMaster.²⁵

3.3. Miscellaneous files

The typical atomic data found in almost any periodic table are stored in the `AtomicConstants.dat` file. Different values of atomic densities with their references can be found in `AtomicDensities.dat`. The electron binding energies for elements in their natural form are in `EbindEner.dat`, whereas the energies of the principal x-ray emission lines are in `XREmission.dat`. The file `Compounds.dat` contains the formulas and information of the most commonly used compounds and mixtures. It contains values of densities and the fractions in weight for each element that constitute the compound. Other files, such as `CrystalCell.dat` and `CrystalStructures.dat`, contain values of the unit cell of the most common crystals, together with the relevant information necessary to build the structure factors for crystal calculations.

Two DABAX files (`XAFS_EXAFS_CHI.dat` and `XAFS_XANES.dat`) contain a collection of experimental EXAFS and XANES spectra. These files were compiled from the collection of spectra recorded by Lytle.²⁶

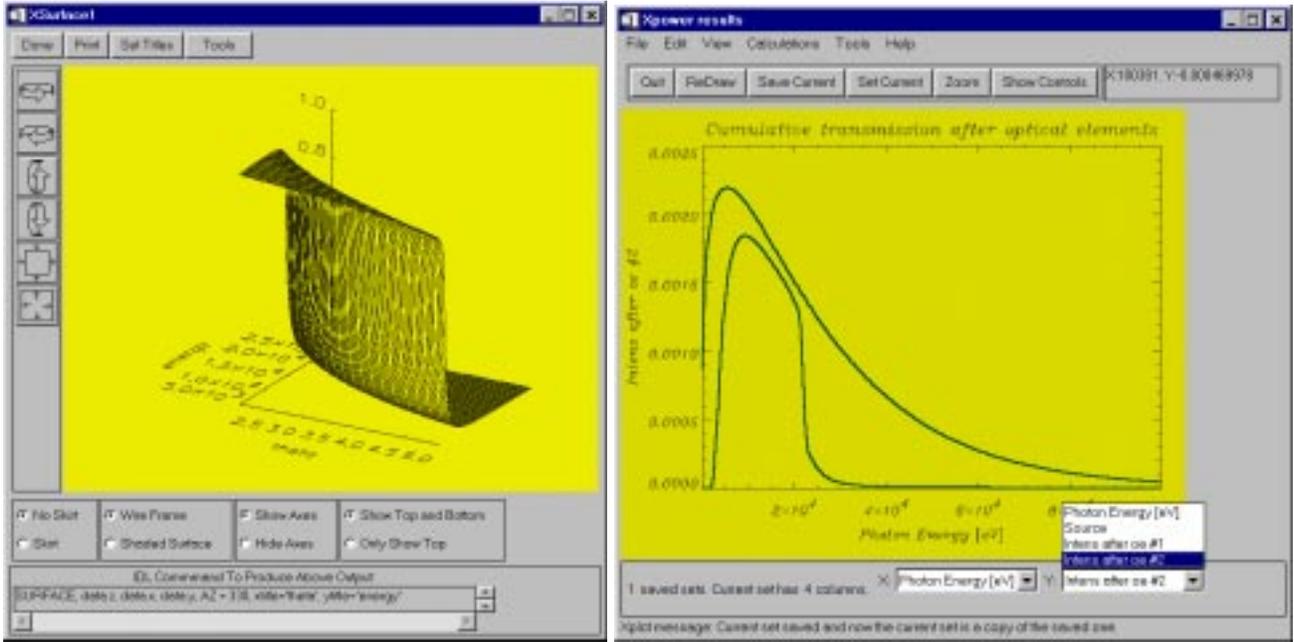


Figure 5. Left: Mirror reflectivity for Si as a function of grazing incidence angle and photon energy. Right: Transmission calculations for a bending magnet source and two optical elements: *Be* window (filter) plus *Rh* mirror.

4. MIRROR AND FILTER APPLICATIONS

X-ray mirrors are common devices that are found in most synchrotron radiation beamlines. They are used for deflecting, focusing, collimating, and/or filtering the x-ray beam. They usually work in the total reflection mode, which occurs for grazing incident angles θ smaller than the critical angle $\theta_c = \sqrt{2\delta}$, with δ being a part of the diffraction index n ($n = 1 - \delta - i\beta$). In the total reflection region, the mirror reflectivity is close to 1, and outside this region it drops as $(\theta_c/\theta)^4$. The calculation of the reflectivity profiles as a function of θ and/or the photon energy E is of crucial interest for the beamline scientist in charge of the design or operation of a beamline. For this purpose, XOP provides modules that allow the user to calculate mirror reflectivities and to apply them to the source spectra (see Fig. 5). From these calculations, it is straightforward to obtain the power absorbed and reflected by the mirrors. However, it is well known that the mirror design involves not only knowledge of the surface reflectivity but also an accurate study of the focusing properties, aberrations, surface errors, etc. For a complete simulation of the mirror optics, other programs, such as the ray-tracing code SHADOW,⁴ are more suitable. XOP can, nevertheless, always be used in a first phase to help in the definition of the incidence angles at the desired energies.

The reflectivity from ideal smooth surfaces can be calculated using the Fresnel formulas. The reflectivity is a function of the grazing angle θ and of the dielectric susceptibility ϵ ($\epsilon = 1 - \alpha - i\gamma$; $\alpha = 2\delta$ and $\gamma = 2\beta$), which depends on the material and on the photon wavelength.

For a material compound, the components of the dielectric susceptibility are related to the anomalous scattering factors by:

$$\alpha = \frac{r_e \rho \lambda^2 N_A}{\pi A} \sum_i n_i (f_1)_i; \quad \gamma = \frac{r_e \rho \lambda^2 N_A}{\pi A} \sum_i n_i (f_2)_i \quad (3)$$

with r_e the classical radius of the electron, λ the photon wavelength, N_A the Avogadro Number, A the compound molecular mass and ρ the material density. The summation index i extends over the different elements present in the compound, and n_i is the weight fraction of the i -th element.

The reflectivity of a surface of material when it is illuminated with σ -polarized radiation is:

$$R_\sigma = \frac{4\Lambda^2(\sin\theta - \Lambda)^2 + \gamma^2}{4\Lambda^2(\sin\theta + \Lambda)^2 + \gamma^2} \quad (4)$$

and for π -polarization:

$$R_{\pi} = R_{\sigma} \frac{4\Lambda^2(\Lambda \sin\theta - \cos^2\theta)^2 + \gamma^2 \sin^2\theta}{4\Lambda^2(\Lambda \sin\theta + \cos^2\theta)^2 + \gamma^2 \sin^2\theta} \quad (5)$$

with

$$\Lambda = \sqrt{\frac{1}{2}(\sin^2\theta - \alpha + \sqrt{(\sin^2\theta - \alpha)^2 + \gamma^2})}. \quad (6)$$

The usual approach to include surface roughness is based on a method developed by Debye²⁷ to analyze the thermal vibrations of a crystalline lattice when exposed to x-ray scattering. Although its applicability is only for a crystalline surface, the resulting formula may be used to model the roughness of any surface. Thus, the reflected intensity is often multiplied by a Debye-Waller factor DW to take into account the surface roughness (σ_{RMS}):

$$DW = \exp \left[- \left(\frac{4\pi\sigma_{RMS} \sin\theta}{\lambda} \right)^2 \right]. \quad (7)$$

In most beamlines, filters are used to decrease the beam intensity in a pre-defined spectral region or to separate different vacuum zones (e.g., *Be* windows). The filter transmission depends on its thickness and total attenuation coefficient μ , which is calculated from the total cross section given by Eq. 2. The transmission calculation is done in the XTRANS and XCROSSSEC applications of XOP. In addition, the XPOWER application can combine up to five optical elements (mirrors and filters) and combine their effects. These application have also been used to optimize sample thicknesses for XAFS experiments.

The filter transmission T is calculated from:

$$T = e^{-\mu t} \quad (8)$$

with μ being the total attenuation coefficient and t the filter thickness.

5. CONCLUSIONS

The XOP software provides a common interface to different useful codes for synchrotron radiation applications. It also contains a powerful and flexible material database as well as data analysis and visualization capabilities. It is being used at two of the third-generation synchrotron radiation facilities (ESRF and APS) and is gradually being used in other laboratories. The full distribution of the software is available under some limited conditions from the authors.

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