XOP: A graphical user interface for spectral calculations and x-ray optics utilities

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XOP: A graphical user interface for spectral calculations and x-ray optics utilities

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A graphical user interface, using the Interactive Data Language (IDL) widget toolkit, for calculation of spectral properties of synchrotron radiation sources and for interaction of x-rays with optical elements has been developed. The interface runs presently on three different computer architectures under the Unix operating system -- the Sun-OS, the HP-UX, and the DEC-Unix operating systems. The point-and-click interface is used as a driver program for a variety of codes from different authors written in different computer languages. The execution of codes for calculating synchrotron radiation from undulators, wigglers, and bending magnets is summarized. The computation of optical properties of materials and the x-ray diffraction profiles from crystals in different geometries are also discussed. The interface largely simplifies the use of these codes and may be used without prior knowledge of how to run a particular program.

I. INTRODUCTION

Quite often difficulties arise when performing computer calculations using applications from different origins by different authors. The XOP (X-ray OPtics utilities) graphical user interface provides a common interface for executing programs of interest to the synchrotron radiation community. We have chosen to use the Interactive Data Language (IDL)[1] widget toolkit, which includes graphical objects in Motif-style layouts for the X-window system using the Unix operating system, to implement this interface. In addition, mathematical and visualization capabilities are tightly integrated into IDL simplifying the data analysis and the presentation of results.

The programs available under the XOP interface have been naturally divided into two general categories (Fig. 1): sources for generation of synchrotron radiation spectra and power profiles for undulators, wigglers, and bending magnets; and optics for calculation of characteristics of optical elements, such as mirror reflectivities, filter transmissions, crystal diffraction profiles, and multilayer reflectivities for materials frequently used in beamline designs. The main programs, which have been collected from various authors, include codes for source generation from the Advanced Photon Source (APS)[2] and the ELETTRA synchrotron radiation source,[3] codes for crystal diffraction from the European Synchrotron Radiation Facility (ESRF),[4] and codes from the SHADOW ray-tracing package for materials' optical properties, crystal diffraction profiles, and multilayer reflectivities from the Center for X-ray Lithography (CXrL).[5]

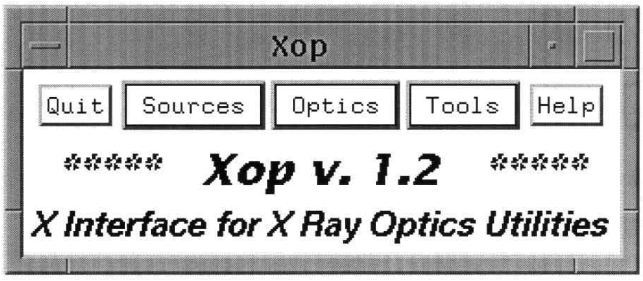

FIG. 1. The main menu of XOP. It contains two buttons, sources and optics, that create pop-up menus of different programs.

In this paper, we will give examples of the capabilities of the codes executed by XOP. Some of the codes are integrated so that the output of one program provides the input for another program. For example, the effect of filters and mirrors on the x-ray beam is studied by first generating the source spectrum and then letting it be incident on the optical elements.

II. SPECTRAL CALCULATIONS

A. Undulator radiation

The undulator code US calculates undulator spectra for an ideal planar undulator or an ideal elliptical undulator (including polarization in both cases) using the Bessel function approximation.[2,6] The code URGENT can also be used.[3] Several radiation quantities may be calculated with both of these codes, either with zero emittance or with a finite emittance of the stored particle beam. Figure 2 shows the pop-up menu for executing the code US.

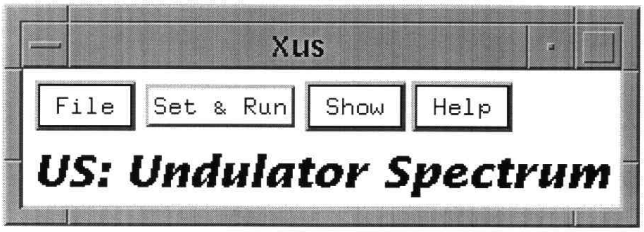

FIG. 2. Pop-up menu for the code US (Undulator Spectrum).

By clicking the Set&Run button, the input-dialog window appears in which the user enters input parameters and executes the code. The show button is used for displaying 2D and 3D graphics. All other codes discussed in this paper are used similarly.

As an example, the familiar single electron (zero emittance) radiation pattern at the energy of the third harmonic, 30 m from the source of Undulator A at the APS is shown in Fig. 3. The introduction of the finite emittance for the APS very dramatically modifies the appearance of this profile, smearing the sharp features and making the profile significantly broader.

By integrating over all energies, the smearing is even more pronounced and essentially insensitive to the beam emittance as is evident by the shape of the power density profile shown in Fig. 4.

The high on-axis power density, in excess of 100 W/mm^2, generated by undulators at high energy storage rings (APS 7.0 GeV, ESRF 6.0 GeV) has prompted intense research over the past years to solve the engineering problems associated with the high head loads deposited in windows and optical components.

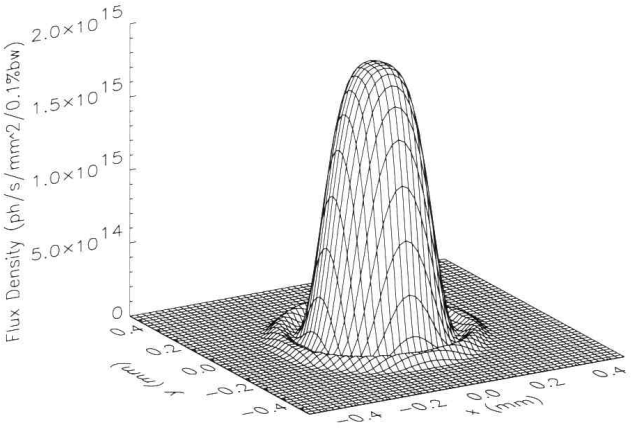

FIG. 3. Single electron radiation pattern in a plane perpendicular to the beam (x=horizontal, y=vertical) for the third harmonic (E3=18.6 keV) at 30.0 m for Undulator A at the APS (K=1.60).

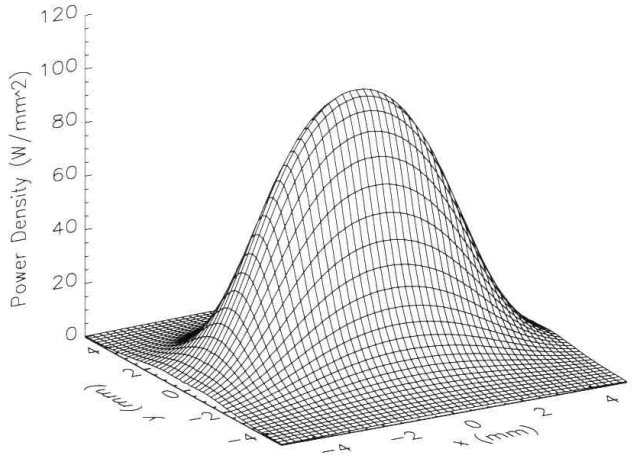

FIG. 4. Power density profile in a plane perpendicular to the beam (x=horizontal, y=vertical) at 30.0 m from the source for Undulator A at the APS (K=1.60).

B. Wiggler radiation

Two codes may be chosen for the wiggler radiation. The code WS (Wiggler Spectrum) is used to calculate the radiation spectra from an ideal sinusoidal magnetic field based on the modified Bessel functions.[7] The code WIGGLER_SPECTRUM from the SHADOW library calculates the particle trajectory and the emitted radiation from either a sinusoidal magnetic field or an asymmetric field entered from an external file or from a series of Fourier coefficients.

C. Bending magnet radiation

Similar to the calculations of the wiggler radiation, the bending magnet spectrum is calculated either from the modified Bessel functions or by using the SRCOMP routine from the SHADOW library.

III. OPTICS UTILITIES

The optical properties of materials, such as the dielectric function, the refractive index, the electron yield, and the scattering factors f' and f'', are calculated by the program ABREFC, and the effect of mirrors and filters on the source spectrum is computed by the code TRANSMIT, both from the SHADOW library. Codes for crystal diffraction profiles developed at the ESRF are also included in the interface.

A. Mirrors and filters

In many instances, it is important to be able to accurately calculate absorbed and transmitted powers by mirrors and filters. Figure 5 shows the input dialog menu for running the TRANSMIT program, which takes a source spectrum as input and transmits it through a series of beamline components. The effect of one Be window (750 μm thick) and a Pt-coated mirror are investigated in this case using incident radiation from Undulator A at the APS.

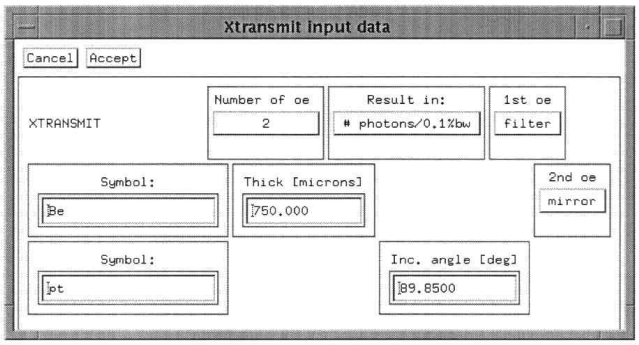

FIG. 5. Input dialog menu for the TRANSMIT program.

The effect of the beamline components are clearly seen in Fig. 6, which compares the undulator spectrum before and after the components. The x-ray spectrum is strongly attenuated at and below the first harmonic (6.2 keV) due to the highly absorbing Be window at low energies, and the high energy photons are poorly reflected due to the low reflectivity of Pt beyond 40 keV. Figure 7 shows a separate calculation of the reflectivities (from code ABREFC) for a Pt-coated and a Si-coated mirror. The Xplot interface (Fig. 6) is used for most graphic displays and contains commonly used mathematical operations (FWHM calculations, convolutions, fits, etc.) on the data.

B. Crystals

Two programs may be selected for diffraction from flat crystals. The program BRAGG from the SHADOW library calculates diffraction profiles of perfect and mosaic crystals in Bragg (reflection) and Laue (transmission) geometries using the dynamical theory of diffraction developed by Zachariasen.[8] The reflectivity of a thin Si (111) crystal in Bragg geometry at 8.0 keV calculated by BRAGG is shown in Fig. 8. The program INPRO (INtrinsic PROfiles) is similar and calculates diffraction profiles in Bragg and Laue geometries for flat perfect crystals.

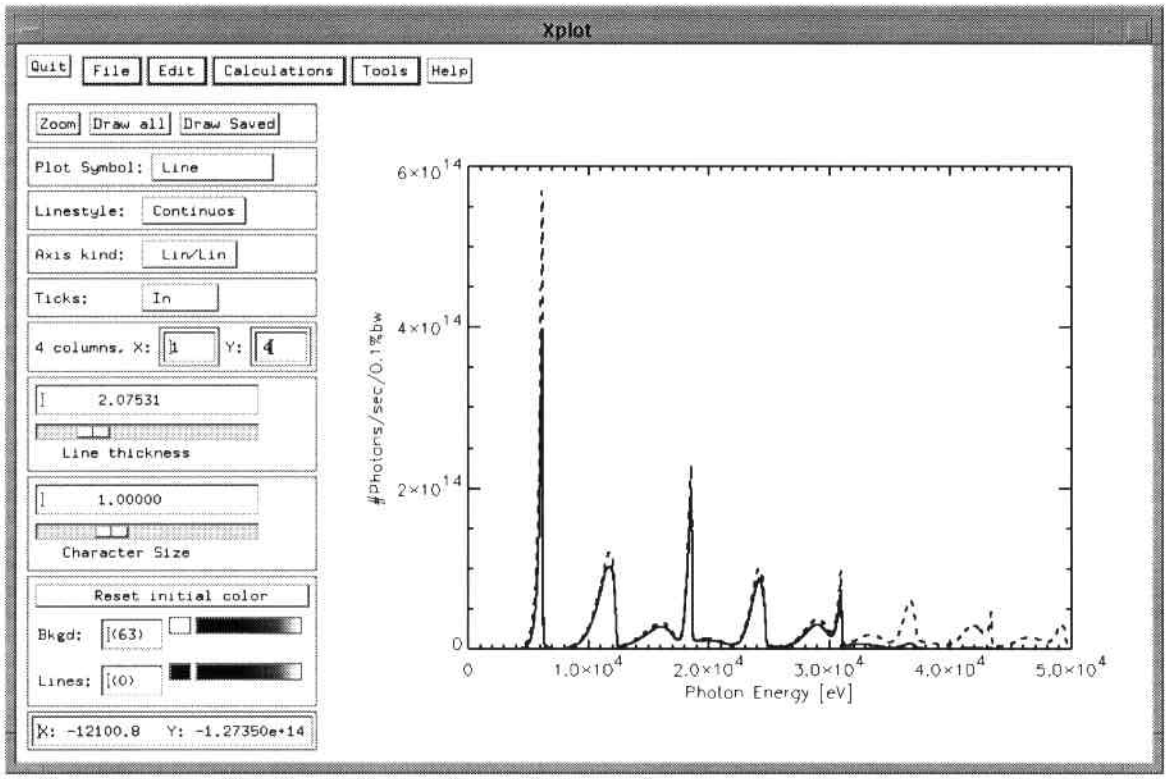

FIG. 6. The Xplot interface for 2D interactive graphics. Source spectrum of Undulator A at the APS (K=1.60) observed through a 2.5×1.0 mm aperture at 30 m (dashed curve), same spectrum attenuated by a 750-μm-thick Be window and reflected by a Pt-coated mirror at a 0.15° grazing incidence angle.

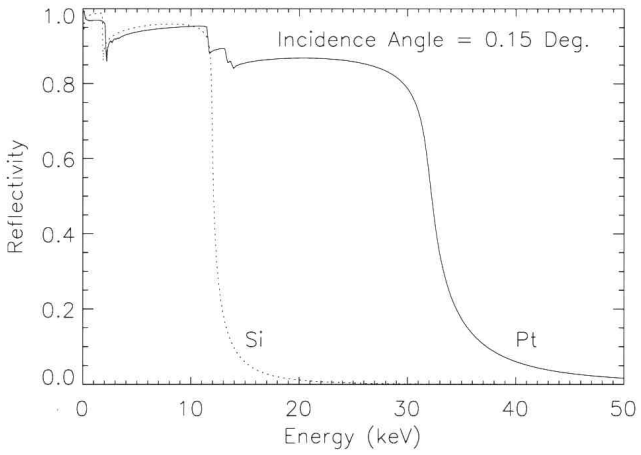

FIG. 7. Reflectivity curves for Pt (solid) and Si (dotted).

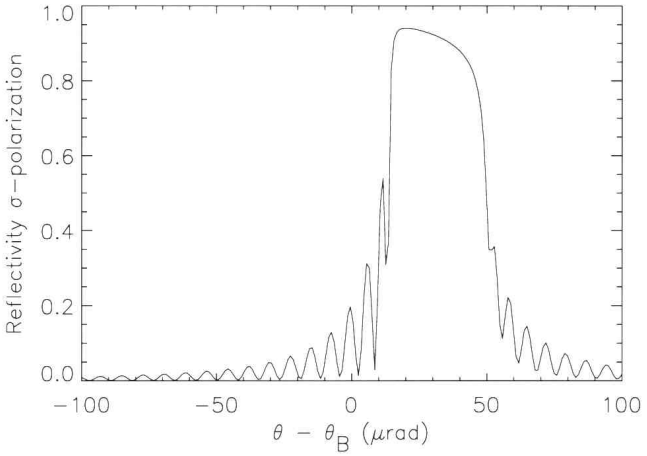

FIG. 8. Reflectivity for a thin (10 μm) Si (111) crystal in Bragg geometry at 8.0 keV.

The program REFLEX may be used to calculate diffraction profiles in Bragg or Laue geometries for either a flat perfect crystal or an elastically bent perfect crystal. As an example, Fig. 9 shows the diffraction profile for Si (111) in Bragg geometry at 8.0 keV using a bent crystal (R=0.20 m).

C. Multilayers

The program MLAYER, which is part of the SHADOW package, is used to calculate reflectivities and phase shifts of the scattered radiation for periodic or graded multilayers. The reflectivity of a periodic SiW multilayer is shown in Fig. 10.

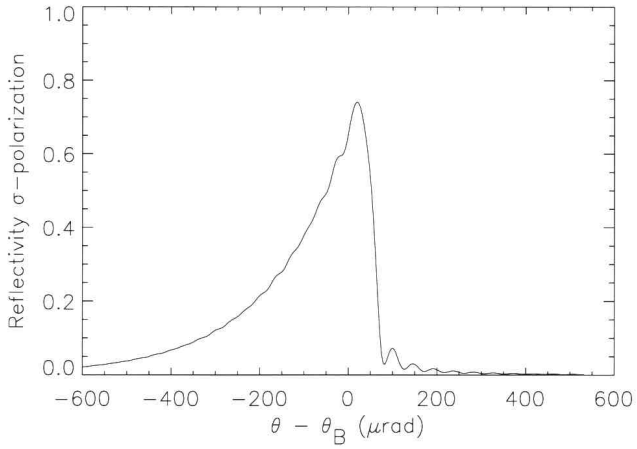

FIG. 9. Reflectivity for a 1.5-mm-thick Si (111) bent crystal (R=0.20 m) in Bragg geometry at 8.0 keV.

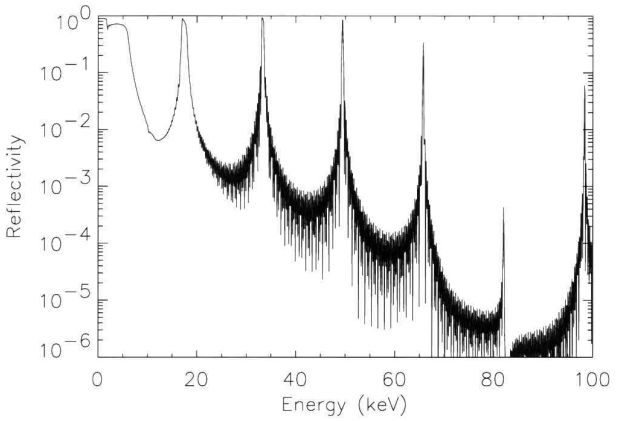

FIG. 10. Reflectivity for 100 pairs of a SiW multilayer at a grazing incidence angle of 0.42°. The thicknesses are 10 Å and 41 Å for the Si and W layers, respectively.

IV. DISCUSSION

The IDL interface runs on any workstation using the Unix operating system with little or no modifications. The computer programs called from the XOP interface are available on the Sun-OS, the HP-UX, and the DEC-Unix operating systems. The user needs however to have a valid IDL license to be able to run XOP.

The programs executed by the XOP interface have been customized at both the APS and the ESRF reflecting the facilities individual requirements and needs. A common version, which includes all codes, will be available in the future. The interface, which has been used extensively at the two newest third-generation synchrotron radiation facilities, has been proven to be a helpful tool during the beamline design stage.

The codes (the IDL codes, and the APS and ESRF source and binary codes) can be provided by the authors (dejus@aps.anl.gov and srio@esrf.fr). Some specific applications may be obtained by contacting their authors.

ACKNOWLEDGMENTS

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