The xraylib library for X-ray—matter interactions

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Introduction

X-ray based analytical techniques have seen a surge in popularity over the last decades. This had led to an increased interest in interaction cross sections and other atomic parameters, which are of fundamental importance in both quantitative and qualitative analysis. In X-ray fluorescence (XRF), for example, quantification using either the fundamental parameter method or Monte-Carlo simulations is only possible if accurate data of X-ray interactions with matter are available. Such data can be obtained in two ways: experimental and computational through quantum mechanical calculations. Several authors have published databases and tabulations in the literature, but none of them are presented in the form of freely available library functions, which can be easily included in software applications for X-ray techniques.

In an effort to solve the problem of interfacing the data to the user, Brunetti et al.[1] designed a software package called xraylib based on a shared ANSI C language library. In this work we will present the features and datasets offered by the most recent release of the xraylib package, but also introduce some recent additions [2]. In order to increase the library’s usability and adoption, we have added bindings to several popular programming languages, and have created packages compatible with all major operating systems and architectures.

We have launched a website, hosted at [http://xraylib-web.dawnsci.org](http://xraylib-web.dawnsci.org), that relies on xraylib’s PHP bindings to provide access to all of its databases while simultaneously giving developers assistance on how to extend their software with the application programming interface. xraylib is released under the BSD license.

References


Usage

The function prototypes are defined in the xraylib.h header. Example for partial photoionization cross sections:

```c
double CS_Photo_Partials(int Z, int shell, double E);
```

with Z: atomic number, shell: atomic shell (xraylib macro) and E: photon energy.

Partial photoionization cross sections

The xraylib library contains the partial and total photoionization cross section database calculated by L. Kissel (see Ba example). Usage of these cross sections lead to more reliable XRF production cross sections compared to those calculated with the jump factor calculated by L. Kissel (see Ba example). Usage of these cross sections leads to more reliable XRF production cross sections compared to those calculated with the jump factor calculated by L. Kissel (see Ba example).

Available functions

**Cross sections (including differential)**

- Absorption cross sections
- Photoionization CS
- Partial photoionization CS
- Rayleigh CS, DCS and DCSP
- Compton CS, DCS and DCSP
- Klein-Nishina CS, DCS and DCSP
- Thomson DCS and DCSP
- X-ray fluorescence production CS with or without (non-)radiative cascade contributions

**Crystal diffraction parameters**

- (Partial) structure factors
- Bragg angle
- Unit cell volume
- d-spacing
- Atomic factors
- Q scattering amplitude

**Cascade effect corrected XRF production cross sections**

The cascade effect occurs when the excitation energy is sufficiently high to excite multiple shells of a constituent element. Its influence is seen in the boosted XRF production cross sections, which in turn has a severe impact on XRF quantification procedures such as the FPM and Monte Carlo based methods.

Features

- xraylib provides convenient access to several databases (Elam, Kissel, Krause, Hubbell, Cullen, Larsson, Deslattes, Biggs, Campbell, Papp, Chen and Crasemann) through over 60 functions in a shared ANSI C library, directly callable from C, C++ and Objective-C
- Provides bindings to programming languages such as Python, Perl, IDL, Java, Fortran and C
- Supported on virtually every architecture: Linux, Mac OS X, Windows (32/64-bit), Solaris, FreeBSD...
- xraylib is an open source project hosted on Github at [www.github.com/tschoonj/xraylib](http://www.github.com/tschoonj/xraylib)

**Available functions**

- Absorption edge energies
- Fluorescence line energies
- Fluorescence yields
- Jump ratios
- Radiative transition probabilities
- Auger transition probabilities
- Coster-Kronig transition probabilities
- Atomic level widths
- Electron configurations

**Miscellaneous**

- Atomic form factor for Rayleigh scattering
- Incoherent scattering function for Compton scattering
- Momentum transfer for X-ray photon scattering
- Anomalous scattering

**Data Analysis Workbench (DAWN)**

- Data Analysis Workbench (DAWN) is an Eclipse based workbench for doing scientific data analysis. It implements sophisticated support for:
  1. Visualization of data in 1D, 2D and 3D
  2. Python script development, debugging and execution
  3. Processing and Workflows for visual algorithms analyzing scientific data
- DAWN is not a rocket scientist tool, but it has clear cut goals. It was developed by and for the synchrotron community foremost but has strong overlap with other communities like neutron scattering, photon science and any scientific communities with the above or similar needs.
- The DAWN 2.0 ships with xraylib's new pure java implementation, providing the essential foundation for many new and exciting features, such as new data processing operations, new tools for data visualization and interpretation and more!
- See [www.dawnsci.org](http://www.dawnsci.org) for downloads and documentation.

**XRF Analysis Tool**

- Identify quickly fluorescence lines, escape peaks and pile-up

**XAS Sample Calculation Tool**

- Generate transmittance and optical depth profiles, as well as XRF spectra including scatter for a given sample and excitation conditions