

## ATOMS: crystallography for the X-ray absorption spectroscopist

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ATOMS is a user application providing crystallographic functionality useful to x-ray absorption spectroscopists. ATOMS is also a set of reusable, object-oriented software modules written in the Perl programming language providing crystallographic functionality and access to databases of absorption coefficients and anomalous scattering factors. The main use of the ATOMS program is to generate input data for the *ab initio*, multiple scattering, x-ray absorption spectroscopy code FEFF. However the code offers many additional features, including useful calculations involving absorption coefficients and simulations of Diffraction Anomalous Fine-Structure (DAFS) spectra. Command line, graphical, and web-based interfaces to the code are offered as part of the standard distribution. As Perl runs on a wide variety of common computer platforms, ATOMS itself is a cross platform application. All text presented to the user can be internationalized – support for four languages is currently included in the package. Development of ATOMS is active – a FEFF interface, structure visualization, and additional crystallographic calculations are among the future developments.

**Keywords:** FEFF; crystallography; object-oriented programming.

### 1. Introduction

X-ray Absorption Spectroscopy is often applied to problems of material science in conjunction with x-ray or neutron diffraction either because of the complementarity of the information provided by the two techniques or because the absorption data is interpreted in the context of the crystallographic structure of the material. In this paper I present ATOMS, a program which provides crystallographic functionality tailored for x-ray absorption applications.

ATOMS was originally conceived as a tool for generating input files of the form needed by FEFF, an *ab initio* multiple scattering code used to generate theoretical fitting standards for Extended X-Ray Absorption Fine Structure (EXAFS) analysis and simulation of X-Ray Absorption Near-Edge Structure (XANES) spectra. FEFF performs its calculation in real-space on a specified cluster of atoms and so requires a list of Cartesian coordinates of each atom in the cluster. The original purpose of ATOMS is to generate such a list from crystallographic structure data. The latest version of ATOMS performs this chore and also provides extensive additional functionality.

ATOMS is written entirely in the Perl (Wall *et al.*, 1996) programming language. Perl is an interpreted language used for both functional and object-oriented (OO) programming. Because the Perl interpreter has been ported to dozens of operating systems, including most Unix variants, all versions of Microsoft Windows, the Macintosh, VMS, BeOS, and many others, ATOMS can be used on many different platforms. To run ATOMS, one need only install the Perl interpreter, which is free of cost and can be downloaded from many sites on the Web. ATOMS itself is also free of cost and

distributed under the same license which covers the Perl interpreter.

The central algorithms in ATOMS are for interpreting space group symbols and constructing a description of a unit cell using space group symmetries and the input crystallographic data. These algorithms are implemented as a Perl module using OO principles. This makes the crystallographic functionality of ATOMS reusable, thus facilitating the development of new applications using crystal structure data.

In Sec. 2. I describe the algorithms for interpreting space group symbols and constructing unit cells and the use of these algorithms to generate input data for FEFF. In Sec. 3. I describe an OO interface to tables of x-ray absorption coefficients and anomalous scattering factors and the use of these data along with crystallography in applications. Finally in Sec. 4. I discuss the user interface to ATOMS and future directions of the development of the package.

### 2. Crystallographic Functionality

Each of the 230 space groups is identified by a symbol. However different notation systems, ambiguities in orthography, and ambiguities in crystal setting make identification of the space group from an input symbol difficult in practice. ATOMS reads from a database which contains, in part, all symbols using the Hermann-Maguin and Schoenflies conventions as given in the International Table for Crystallography (Hahn, 1992). The database includes Hermann-Maguin symbols in their short and long forms and all symbols for alternate settings of low symmetry space groups. The method used to parse the input symbol is insensitive to whitespace and to capitalization. It recognizes Schoenflies symbols using obsolete notation conventions, Hermann-Maguin symbols from the 1935 edition of The International Tables of X-Ray Crystallography, and the new Hermann-Maguin symbols used to denote double glide planes. Additionally the index of the space group from the International Tables can be used and nicknames for common space groups, e.g. "fcc" for  $F\bar{M}\bar{3}M$ , are recognized. The flexibility of the space group parser means that identification of the space group from the user-supplied symbol is rarely a problem.

Along with a space group symbol, ATOMS requires values for the non-obvious lattice constants and angles and coordinates of the unique atoms in the unit cell. It is not necessary to specify lattice constants and angles which can be intuited from the space group. For example, only the *a* lattice constant need be specified for cubic space groups and the value of the  $\gamma$  angle is always set to  $180^\circ$  for hexagonal space groups. Because all point and Bravais symmetries can be obtained from knowledge of the crystal space group, it is not necessary to specify the entire contents of the unit cell. From the coordinates of a representative atom of each crystallographic environment and the symmetries obtained from the space group symbol, ATOMS generates the coordinates of all atoms in the unit cell without regard to the size of the unit cell. This description of the contents of the unit cell is the basis for the cluster expansion used to generate the input file for FEFF.

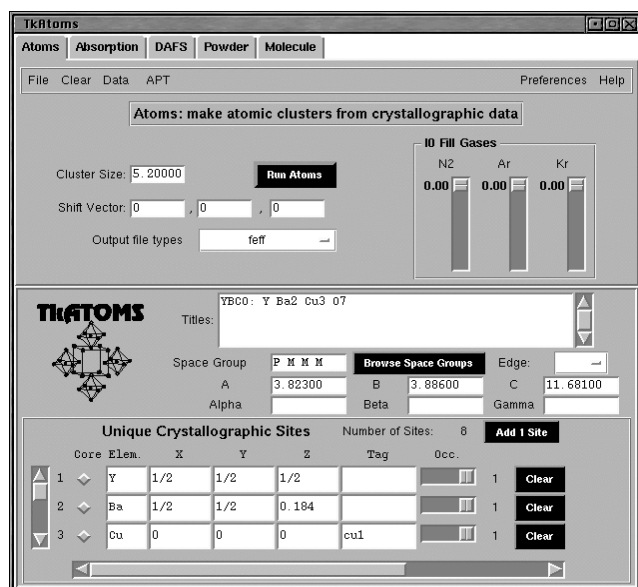
All crystallographic features are encoded in an OO manner in ATOMS. The unit cell is treated as an object, as are each of the unique crystallographic sites. Associated with each kind of object are data structures and methods for manipulating those data structures. The use of OO principles hides the implementation of the crystallography from the programmer, thus facilitating reuse of the crystallography module in other contexts, as described in Sec. 3.

The generation of the unit cell contents makes use of an interesting feature of Perl — run-time code evaluation. The symmetry operations of the space groups are encoded in the crystallo-

graphic database as statements in the Perl language. These commands are evaluated using the unique atom coordinates at run-time. This means that atom coordinates themselves can be expressed as numbers or as Perl statements, for instance as simple fractions or other math expressions.

Once the unit cell is entirely determined, a cluster is generated by repeating the unit cell in all three directions enough times to fill a rhomboidal volume which entirely encloses a sphere of a specified radius. The atoms which lie within the rhomboid but outside the sphere are discarded and the remaining atoms are sorted by radial distance. An atom of the species chosen as the absorber atom is selected and the coordinates of all atoms in the cluster are shifted to place the selected atom at the origin.

The radially sorted cluster is written to a file along with certain other information needed to run FEFF. Usually, FEFF can be run to completion without modifying the output from ATOMS. The exact format of the output file is determined from a template file read at run-time by ATOMS. Several useful template files come with the ATOMS distribution and new ones can be written by the user. The use of template-driven output allows for extensive user customization and provides sufficient flexibility to generate input files suitable for FEFF8 or for earlier versions of FEFF which uses slightly different input syntax. Indeed, the template driven output is sufficiently flexible that ATOMS can be used to generate output files in many interesting formats, including file formats used by popular ball-and-stick molecule viewers.



**Figure 1**

The main window of the TKATOMS application using the Tk graphical toolkit on a Linux computer. This figure shows the use of TKATOMS to generate a FEFF input file for  $\text{YBa}_2\text{Cu}_3\text{O}_7$ . The top panel is used to enter run-time parameters and the bottom panel is used to specify unique crystallographic sites.

### 3. Interface to X-Ray Absorption Databases

While generation of lists of atomic coordinates is a widely useful function, ATOMS is capable of performing a variety of calculations of interest to the absorption spectroscopist using the crystallographic objects. The features of ATOMS described in this section

all make use of tables of absorption coefficients and/or anomalous scattering factors via an OO interface.

Included with ATOMS are databases containing the absorption coefficient tables of McMaster (McMaster *et al.*, 1969) and Elam (Elam *et al.*, 2000) and the anomalous scattering factors of Henke (Henke *et al.*, 1993) and Chantler (Chantler, 1995). Also included with ATOMS are the Cromer-Lieberman (Cromer & Lieberman, 1970) scattering factors using the Brennan-Cowan (Brennan & Cowan, 1992) implementation adapted for use with Perl. Because the absorption function and the imaginary part of the anomalous scattering factor are related by the optical theorem (Cullity, 1978), all five databases can be used in a context requiring absorption coefficients.

ATOMS hides the details of accessing the various databases behind a uniform interface, thus simplifying their use at the programmatic level and allowing the user of ATOMS to choose at run-time which database to use for calculations. In this way the user can easily assess the effect of choice of database on any calculation. For calculations requiring the real part of the anomalous scattering factor, this is especially important. As has been noted by other authors (Sánchez del Río & Dejus, 1997), the Henke and Chantler tables are presented on overly sparse grids resulting in very poor behavior of the real parts near the resonant energies.

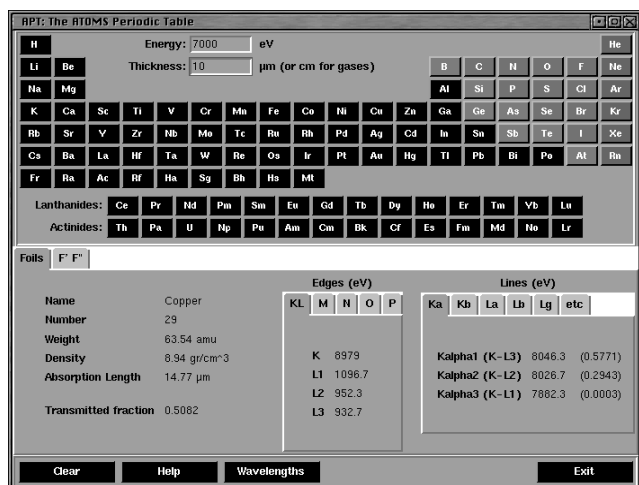
The crystallographic and absorption coefficient objects are combined in ATOMS to provide several interesting applications. One application computes a variety of quantities useful for preparing a sample for an EXAFS measurement and interpreting the results. The quantities include the total and unit-edge step absorption lengths of the crystal at the energy of the chosen central atoms and corrections for attenuations to the EXAFS data due to edge-step normalization and self-absorption in a fluorescence experiment. Another application simulates the smooth background to a Diffraction Anomalous Fine Structure (DAFS) spectrum given the Miller indices of a reflection. These objects can also be the basis of powder diffraction simulations and of a program for correcting the effect of self-absorption in a XANES spectrum, although those two applications have not yet been written.

### 4. User Interfaces and Future Developments

One of the great advantages of Perl is that it supports a variety of user interfaces. Consequently ATOMS exists in three forms. One form is a command line program which reads data from an input file and writes its output directly to disk. The second form is a graphical interface using the Perl/Tk (Walsh, 1999) graphical toolkit and is shown in Fig. 1. ATOMS is distributed with a second Perl/Tk application, a graphical periodic table of x-ray absorption edge and fluorescence line energies which is shown in Fig. 2. The third form is a CGI application (Stein, 1998) available on the World Wide Web. Thus the user benefits from a wide variety of user interaction models.

ATOMS is extensively customizable. Much of the run-time behavior can be determined by the user, including the language used for all text messages written to the screen by the command line version or to the graphical interface by the Tk version. Currently ATOMS supports English, Spanish, French, and German. With the introduction of Unicode support in the latest versions of Perl, the textual database used by ATOMS can be translated to virtually any language. Because the formats of all output files are template-driven standard output file formats are easily modified and new output file formats are easily created. Indeed, ATOMS is capable of generating input files suitable for GNXAS (Filipponi *et al.*, 1995).

ATOMS is under active development. I plan to extend its functionality as a front-end to FEFF. Currently, the input data for FEFF can be generated with graphical tools, either the TK application in Fig. 1 or the CGI version, however the user is required to use the FEFF command line interaction model to actually perform the FEFF calculation. A graphical tool is planned as a back-end to ATOMS for performing FEFF calculations using the input data generated by ATOMS and for displaying the results of the calculation. I also plan to provide structure visualization functionality. ATOMS could be used to generate input data for a ball-and-stick display of a crystal structure. That structure can be edited using graphical tools, then ATOMS can use the modified output to create new input data for FEFF.



**Figure 2**

The ATOMS Periodic Table, a graphical interface to x-ray absorption edges and line energies. It also computes absorption lengths and transmitted fractions of foils and gases and so is a useful beamline utility. This is an independent application built using the OO interface to tables of absorption data from ATOMS.

## 5. Conclusion

ATOMS is a flexible and powerful tool for manipulating crystallographic structure data in ways useful to the x-ray absorption spectroscopist. The primary function of ATOMS is to generate input data for the *ab initio*, multiple scattering, theory code FEFF. However, ATOMS performs other interesting chores such as simulation of DAFS spectra and various calculations using tables of x-ray absorption coefficients. The crystallographic functionality and the interface to the tables of x-ray absorption coefficients are written as

reusable, object-oriented modules. It is therefore easy to develop new applications. ATOMS can be used with a variety of interfaces — including a command line, a graphical interface, or a web-based interface — and on a variety of computer platforms. ATOMS is customizable and currently supports four languages. ATOMS is distributed without cost and using a license which encourages reuse, redistribution, and third party development.

The latest version of ATOMS (version 3.0alpha24 at the time of writing) is always available on the web at its home page <http://feff.phys.washington.edu/~ravel/software/atoms/>. A link on that page can be followed to the CGI version of ATOMS.

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