A tabulation of x-ray optical constants is provided by the Center for X-ray Optics at Lawrence Berkeley National Laboratory, at this location[1]. This tabulation has been built up over the years first by Burt Henke and more recently by Eric Gullikson and collaborators. At Stony Brook, we have written routines to use this tabulation within the IDL[2] graphical programming package.

If you specify an element name or chemical compound and a density, the routines give you the real and imaginary parts of the refractive index δ and β (such that $n = 1 - \delta - i\beta$) for energies from 10 to 30,000 eV. One can then calculate the absorption coefficient using $(4\pi/\lambda)\beta$, and therefore calculate transmission of filters and so on. The routines also provide the complex number of electrons $(f_1 + if_2)$ used to obtain δ and β. Finally, the routines provide reflectivity in percent if you supply a grazing incidence angle in mrad. These various coefficients are available for further calculations in IDL.

1 Usage

For the most part, two routines are used:

1. `henke_array.pro`: This routine lets you load the optical constants for the entire accessible energy range for a given compound. For example, you can plot the attenuation length of water in micrometers with

```
IDL> henke_array
henke_array, compound_name, density, energies, f1, f2, delta, beta, $
    graze_mrad, reflect, inverse_mu=inverse_mu
  inverse_mu is 1/e absorption length in microns.
IDL> henke_array, 'water', rho, energies, f1, f2, delta, beta, $
    inverse_mu=inverse_mu
IDL> plot, energies, inverse_mu, xrange=[0,1000], $
    xtitle='eV', ytitle='Microns'
```

2. `henke.pro`: this routine works like the above, except that it will interpolate to give you the optical constants at a certain photon energy (e.g., 510 eV in this example):

```
IDL> henke, 'water', rho, 510., f1, f2, delta, beta, $
    inverse_mu=inverse_mu
```

These routines both refer to a file called `compound.dat` which looks like:

```
! This is the file COMPOUND.DAT for HENKE.  Entries are:
! compound  formula                     density (g/cc)
water       H2O                         1.0
protein     H48.6C32.9N8.9O8.9S0.6      1.35
```

[1]http://www-cxro.lbl.gov/optical_constants/
[2]http://www.rsinc.com

If there is not a a file compound.dat in the current working directory, the file in the system-wide directory is used. This directory is specified in compound.pro (this directory is also specified in read_henke.pro).

If the compound you want to use is not in compount.dat, you can add it with its density to that file. If you are only interested in a single element, you can just specify the element short name (e.g., 'Si' for silicon) when calling henke or henke_array, but you will have to give the density in the procedure call as well (density then changes from an output parameter to an input parameter).

2 Installation

To install the IDL routines and the data, you must get the file henke.zip[3]. Put this file in a directory according to your computer as follows:

Unix: the directory /usr/local/rsi/idl/lib/local/henke

Windows: the directory c:\rsi\idl60\lib\local\henke

Actually, you can unpack the henke package into any directory in your IDL path. The routines involved are:

compound.dat: as described above.

compound.pro: when given a text string of a chemical formula and a density, it builds an array z_array of how many atoms of each element there are in the specified molecule or compound.

henke.pro: as described above.

henke.xdr: the binary data file.

henke_array.pro: as described above.

henke_build.pro: used for building henke.xdr from the ASCII data files ".nff" provided by CXRO.

henke_extra.pro: to access the "extra" energies which provide further details on absorption edges. The routines henke.pro and henke_array.pro work only on the regularly-spaced energy points.

henke_read.pro: to read the binary data file henke.xdr.

zatwt.pro: given z_array such as calculated by compound.pro or zcompound.pro, zatwt.pro calculates the atomic/molecular weight of the compound.

zcompound.pro: a utility routine used by compound.pro

zshow.pro: lets one examine z_array

Note that for IDL 3 and 4 on Windows, you need to truncate the file names to 8 characters.

[3] http://xray1.physics.sunysb.edu/data/idl_programs/henke.zip

3 References

The first reference describes the tabulated data, and the second two references provide information on the physics and usage of the data.

1. B. L. Henke, E. M. Gullikson, and J. C. Davis, "X-ray Interactions: Photoabsorption, Scattering, Transmission, and Reflection at E=50–30,000 eV, Z=1–92," *Atomic Data and Nuclear Data Tables* **54**, 181–342 (1993).

2. B. L. Henke, "Low energy x-ray interactions: photoionization, scattering, specular and Bragg reflection," in D. T. Attwood and B. L. Henke, eds., *Low Energy X-ray Diagnostics* (American Institute of Physics Conf. Proc. **75**, New York, 1981), pp. 146–155.

3. R. E. Burge, "The interaction of x-rays," in A. G. Michette and C. J. Buckley, eds., **X-ray Science and Technology** (Institute of Physics, Bristol, 1993), Chapter 5, pp. 160–206.