16. XRO

XRO—X-ray optics—calculates the reflectance, reflectance phase, thin-film transmittance, conductivty, dielectric function, and complex refractive index at X-ray wavelengths.

The scattering functions f_1 and f_2 for atomic constituents are those of Henke (1993)*, with new KK transforms for f_1. The data are embedded in the `xro.exe` file; auxiliary files are not needed.

You will need to specify the formula, e. g., `YBa2Cu3O6.93`. Fractional subscripts are fine. Case matters: cobalt (Co) is not carbon monoxide (CO)! XRO does not do very complicated parsing of formulae, so a material with a formula of $(La_{0.5}Pr_{0.5})_{0.67}Ca_{0.33}MnO_3$ would be reported as `La0.335Pr0.335Ca0.33MnO3`.

You will also need to specify either V, the volume per formula unit in cubic Angstroms, or the density, in grams/cc. Here, V is the volume of the formula unit, typically V_{cell}/Z as specified by the structural paper. Z is the number of formula units in the unit cell. For example, NaCl is fcc with a lattice constant of 5.64 Å. The unit cell volume is 179.4 Å^3 but $Z = 4$, so $V = 44.8$ Å^3. Note that density always works. You get the same xro data using the density of 2.165 g/cm^3 for NaCl or Na_4Cl_4. The volumes V would be 44.8 and 179.4, respectively.

Examples:

```
XRO YBa2Cu3O6.93 /v186
XRO silver /fAg /r10.49 /P
```

In the first, XRO calculates for YBCO, using a cell volume of 186 Å^3. In the second the reflectance and the phase are computed for Ag, based on a density of 10.49 g/cm^3. The output file is silver.XRP.

Switches:

`/F<formula>`	— Chemical formula
`/V`*nnn*	— Volume/formula unit is *nnn*
`/D`*nnn* `/R`*nnn*	— Density is *nnn*
`/E`	— Energy in eV rather than cm^{-1}
`/P`	— Write also the phase; 3 columns data
`/S1`	— Write conductivity, $\sigma_1(\omega)$
`/E1`	— Write dielectric const, $\epsilon_1(\omega)$
`/I`	— Write Index (n and κ) rather than $\mathscr{R}$ and (with `\P`) ϕ
`/T`	— Write Transmittance, $\mathscr{T}$
`/X`*nnn*	— For $\mathscr{T}$: the thickness (in Å) is *nnn*
`/F`	— Write f_1 and f_2 (for the *first* atom in the formula)
`/q`	— Fewer questions

Switches may be introduced with '/' or '-', have optional spaces between them, and may be in upper or lower case.

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* 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).

You may enter the formula on command line, as in `XRO YBa2Cu3O6.93 ...` or using the `/F` switch. The output file is <formula>.XRO. If you enter a non-formula on the command line, that will be the name of the output file and you will need to use the `/F` switch or answer the prompt for the formula. (Be careful here! YBCO is shorthand for the 123 superconductor, but it also is yttrium boron carbon oxide. Lower case, e. g., ybco, is always safe.)

XRO calculates the dielectric function using the original atomic scattering factor data developed by Henke. Some information about this is at `http://henke.lbl.gov/optical_constants/`.*

The dielectric function† is

$$\epsilon = 1 - \sum_j \frac{4\pi n_j e^2}{m\omega^2}(f_1^j - if_2^j) \tag{74}$$

where the sum runs over atoms j at number density n_j and with complex scattering factor f^j. Note that this has the right limiting high-frequency behavior, because $f_1^j \to Z^j$ (with Z^j here the atomic number)‡ and $f_2 \to 0$, so that $\epsilon \to 1 - \sum_j 4\pi n_j Z^j e^2/m\omega^2$

The refractive index is $N = \sqrt{\epsilon}$ and the reflectance is calculated from the usual equation, Eq. 57. The transmittance is calculated from Eqs. 59–64.

* XRO uses the first version of the scattering data because it is sampled at identical photon energies for each atom; the newer version is not.

† Henke—and the website above—write an equation for the refractive index $N = 1 - (nr_0\lambda^2/2\pi)(f_1 + if_2)$ with $r_0 = e^2/mc^2$ the classical radius of the electron and $\lambda = 2\pi c/\omega$ the wavelength. This is clearly an expansion of $N = \sqrt{\epsilon}$.

‡ There is a small relativistic correction.