Xcoeff_new

Xcoeff_new is designed to calculate weighting factors of each atomic correlation for neutrons and x-rays. It is known that neutron scattering length is constant while x-ray atomic form factor has a Q dependent. This software can manage both calculations.

Please refer the following article for neutron scattering length.
V. F. Sears,Neutron News **3**, 26(1992).
Please refer the following article for x-ray atomic form factor.
D. Waasmaier and A. Kirfel, Acta Cryst. A51, 416-431 (1995).
Atomic form factors are available at the following web site.
http://lipro.msl.titech.ac.jp

The following example is SiO_2 case.

How to execute the code

WinNFLP menu「Useful」, 「DATA programs」 execute「Xcoeff_new」

1. X-ray case (Q dependent)

Number of atom types > 2 ! Si and O
Kind of radiation (X/N) > x ! type "x" for x-rays, "n" for neutrons
Calculation at (O)ne energy or (D)ifference calculation at two energies
(O/D) > O ! In the case of normal x-ray diffraction, type "O"

Type 1
Fractional concentration > 1
Atom/ion symbol > Si
Form factor parameters (a1,b1,..,a5,b5,c):
5.275329 2.631338
3.191038 33.73073
1.511514 0.8111900E-01 ! the parameters for Si

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   1.356849       86.28864
   2.519114       1.170087
  0.1450730
Energy dependent parts of the SI atomic form factor
d f'                      > -0.0137      ! f' for Si at E=61.43keV
d f''                     > 0.0049       ! f'' for Si at E=61.43keV

Type     2
 Fractional concentration > 2
 Atom/ion symbol          > O
 Form factor parameters  (a1,b1,..,a5,b5,c):
   2.960427       14.18226
   2.508818       5.936858
  0.6378530      0.1127260
  0.7228380       34.95848
   1.142756      0.3902400
  0.2701400E-01
 Energy dependent parts of the O atomic form factor
 d f'                     > -0.0055      ! f' for O at E=61.43keV
 d f''                    > 0.004        ! f'' for O at E=61.43keV
Options for coefficients are:
   1 - Use as calculated
   2 - Divide by <f**2>
   3 - Divide by <f>**2
 Choose option            > 3            ! The normalization of I(Q)
                                           1:I(Q)
                                           2: normalize by <f^2>
                                           3 normalize by <f>^2

Input file               > sio04sqo.dat ! file name of S(Q) data
 Output file             > sio04sq.dat  ! the name of new file
Fortran Pause -Enter command<CR> or <CR >to continue
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Type return for exit

Neutron case

Number of atom types > 2

Kind of radiation (X/N) > n ! type “n” for neutron

You choose the weight calculations for thermal neutrons!

Type 1

Fractional concentration > 1

Atom/ion symbol > Si

Isotope abundance of this element is the same as in the natural one? (y/n) >y

! Usually y

Parameters of the 'SI' element for natural isotope abundance:

Bound coherent scattering length: 4.153 +i* 0.000 [fm]

Total scattering cross-section : 2.171 [barn]

Absorption cross-section : 0.1710 [barn]

Type 2

Fractional concentration > 2

Atom/ion symbol > O

Isotope abundance of this element is the same as in the natural one? (y/n) >y

Parameters of the 'O' element for natural isotope abundance:

Bound coherent scattering length: 5.803 +i* 0.000 [fm]

Total scattering cross-section : 4.232 [barn]

Absorption cross-section : 0.1900E-03 [barn]

Neutron absorption cross-section : 0.5712667E-01 [barn]

Neutron total scattering cross section : 3.545000 [barn]

consists of coherent cross section : 3.467742 [barn]

incoherent cross section : 0.7725835E-01 [barn]

Weights (<b><b*>_ij) [barn/sterad] showed in 1-2, 1-3,..,1-n, 2-2,2-3,.. format
:

0.1916748E-01 0.1071208

0.1496658

Weights are normalised to |1.0| and showed in 1-1, 1-2, 1-3,..,1-n, 2-2,2-3,..
format:

0.6945894E-01 0.3881834 ! weighting factor for Si-Si, and Si-O

0.5423576 ! weighting factor for O-O

Fortran Pause -Enter command<CR> or <CR >to continue

Type return for exit