

CALCULATION OF ATOMIC SCATTERING AND DEBYE-WALLER FACTORS: STEP TOWARD ACCURATE ESTIMATION FOR X-RAY POLARIZABILITY

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Recently, the phase-sensitive techniques are intensively developing for the solving of crystal structures in material sciences and biology. Most of these studies uses x-ray radiation with variable wavelength, like synchrotron or parametric x-ray radiations, which give more degree of freedom than conventional sources with fixed frequency. However, the quality of obtained information depends on the methods and theories used for data interpretation, where the calculation of x-ray polarizability of real crystals is the start point for developing of further approximations. Thus, the reliability of simulated x-ray reflectivity, diffracted or diffused intensity depends strongly on the correctness of calculated x-ray polarizability for arbitrary wavelength and real crystallographic elementary cells.

We developed new analytical method and software for calculation of atomic scattering factors, which make important contribution to x-ray polarizability dependence on wavelength. Usually, Cromer-Mann tabulated coefficients are used to interpolate Hartree-Fock formfactors within the limited interval of moment transfer s . We have completed an alternative tabulation based on analytical approximation for wavefunctions of atoms and ions. The atomic factors being calculated by our approach agree well with ones by Cromer-Mann method. However, the approach proposed has a certain advantages: (i) atomic factors can be calculated for arbitrary value of s (Cromer-Mann's table is valid in interval $0 < s < 2$), and (ii) method permits to takes into account the anisotropy of atomic factors caused by external and internal electromagnetic fields in crystal influencing the outer electron shells. The second term contributing to precision of polarizability calculations is the Debye-Waller factor (DWF). Presently, the most rigorous approach to estimate the DWF uses experimental data for spectral density of phonons. However, this data are available only for elementary crystals and few compounds. We realized an universal method for calculation of DWF for arbitrary crystallographic unit cell, taking into account its anisotropy. The method uses the analytical approximation for atomic wavefunctions and experimental data for Debye temperature of elementary crystals. Numerical examples and comparison with conventional techniques are presented.