Resonant elastic scattering treatment by multipolar oscillator model revisited

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Treatment of resonant elastic scattering, also known as anomalous dispersion, is usually done using a dipole approximation of the induced oscillation of electrons and generally assuming polarization corrected scattering corresponding to Thomson scatterers. The physical basis of the solution of the underlying model using Waller’s dispersion formula, as done in the work of Hönl, Eisenlohr and Müller and Wagenfeld [1-3], results in a leading term that is consistent with a forward-scattering dipole approximation. However, this corresponds to a truncation of the series after the first element. In the present work the calculations are repeated without approximations that were used in the referenced work due to limited available computational power. We also implemented higher orders of resonance in the calculation process to investigate angular and energetic dependence of these higher moments of anomalous dispersion corrections, especially at energies where the higher moments of oscillation are more significant. Structural investigations where precise and detailed results are desired, for example quantum crystallographic studies or the refinement of structures with heavy scatterers, where strong resonant effects are observable would benefit most from these.

Fig. 1 shows an example of a theoretical difference density obtained by Fourier synthesis for the resonant scattering with and without considering higher angular moments and their respective angular dependency referenced against the scattering power of a Thomson scatterer.

The newly implemented models of resonant scattering were used for the refinement of crystal structures with heavy elements at different wavelengths and the comparison of refinement statistics, residual density maps and the features of their distribution are considered to judge whether consideration of higher angular moments of resonant scattering is advisable when refining high-quality and high-resolution diffraction data.


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