Direct Localization of Atoms in Nanoporous Powders by Resonant Contrast Diffraction

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Based on the experimental improvement of data collection achieved for DAFS spectroscopy and applied using the MAD principles, a methodology has been developed for powder sample analysis in order to optimise the use and the interpretation of anomalous information. By using a zeolite example[1] our aim was to validate the resonant scattering method for contrast studies in complex powders with mixed occupancy sites. On one hand we show that even in powder samples with considerable reflection overlap and with a basically known framework the use of "***dispersive difference***" electron density maps allows an easy localisation of resonant atoms. On the other hand, the use of "***anomalous difference patterns***" enables good agreement factors to be achieved for accurate localisation. These two specific difference tools can also be used in powders containing several phases. The application of these methods can be extended to materials in geology, industry, environmental studies to localize transition metals or RE atoms. It can also give their valence by the use on powders of Diffraction Anomalous Near Edge Structure spectra. The extension of resonant contrast diffraction to in situ measurements can be foreseen to analyse the evolution of atomic order during chemical reactions.

[1] Palancher H. et al., *Angew. Chem. Int. Ed.*, 2005, **117**, 1753.

Keywords: anomalous diffraction, resonant scattering, zeolites