**MS24 3D electron diffraction**

MS24-02
Using 3D-ΔPDFs from electron diffraction data to determine local structure
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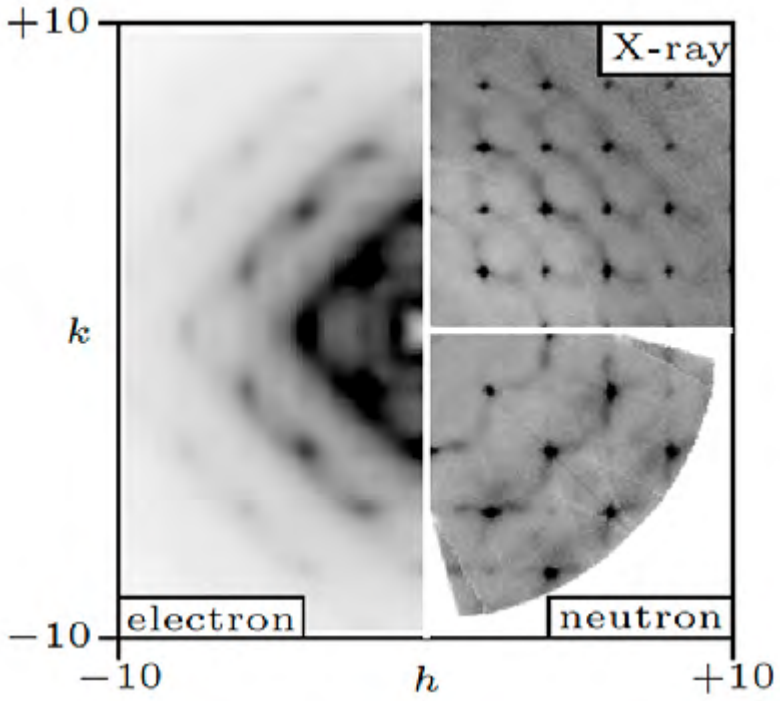
Abstract
Many functional materials have surprisingly simple average structures, but often partially occupied sites indicate disorder. To understand structure property relationships in complex ordered materials a description including local order is needed. Powder pair distribution functions are often used quantitatively to analyse the local structure of a material. While the experimental setup is very simple, the determination of three-dimensional local order principles requires complex modelling. Experimentally the analysis of single crystal diffuse scattering is more complex, but the recently established three-dimensional delta pair distribution function (3D-ΔPDF) is the perfect tool to map local deviations from the average structure and provides a straightforward interpretation of local ordering principles [1].
Here, we demonstrate how the 3D-ΔPDF can be obtained from electron diffraction data to understand the complete local structure of the high temperature ion conductor yttrium stabilized zirconia $Zr_{0.82}Y_{0.18}O_{1.91}$ (YSZ). YSZ crystallizes in the fluorite structure and shows composition disorder on both the metal and oxygen site. The substitution of $Y^{3+}$ for $Zr^{4+}$ on the metal site results in oxygen vacancies for charge compensation. Locally, $O^{2-}$ ions relax towards the vacancies, while the metal-ions relax away from them.
Single crystals of YSZ were investigated with electron, X-ray and neutron diffraction. Highly structured diffuse scattering is observed alongside the sharp Bragg reflections (see Figure 1). By comparing the results from our electron ΔPDF to X-ray and neutron ΔPDFs we demonstrate the reliability of the 3D-ΔePDF (see Figure 2). A detailed analysis of the intensity distribution in the 3D-ΔPDF in the vicinity of the nearest neighbour inter-atomic vectors allows us to quantify the local structure relaxations.
To our knowledge, this is the first 3D-ΔePDF ever reported and this proof of principle is an important step towards the full description of a disorder model. This has important implications for the large variety of disordered materials of which single crystals for X-ray or neutron techniques are not available. In those cases, the 3D-ΔePDF will pave the way to understanding and tailoring physical properties.

References
[1] Weber, T., & Simonov, A. (2012). Z. Kristallogr., 227(5), 238-247.

hk0 layer




3D-ΔPDF in the ab0.25-layer