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Using 3D-ΔPDFs from electron diffraction data to determine local structure

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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 to quantitatively analyse the local structure of a material but the determination of three-dimensional local order principles requires complex modelling. For single crystal diffuse scattering data, 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].

To obtain 3D-ΔPDFs single crystals are needed which are suitable for the measurement with X-rays (approx. $(50\ \mu\text{m})^3$) or neutrons (approx. $(0.5\ \text{mm})^3$). Samples of these sizes are often hard to obtain for novel functional materials. Here, we demonstrate how the 3D-ΔPDF can be obtained from electron diffraction data which can be used on samples as small as $(10\ \text{nm})^3$.

For our proof of principle study, we use 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. By comparing the results from our electron ΔPDF to X-ray and neutron ΔPDFs we demonstrate the reliability of the 3D-ΔePDF. 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. 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 that are determined by local structure variations.

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

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