3D- ΔPDF from electron diffraction data

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Many functional materials seem to have surprisingly simple average structures with some disordered components. To understand the relationship between the structure of a material and its complex physical properties, a full description including local order is necessary. Hence, the diffuse scattering has to be analysed. The recently established three-dimensional delta pair distribution function (3D- PDF) maps local deviations from the average structure and allows a straightforward interpretation of local ordering mechanisms [1].

Many functional materials can only be grown as powders. While powder X-ray and neutron diffraction experiments can give limited insight into disordered structural arrangements, electron diffraction techniques allow to capture large portions of reciprocal space even for nanocrystals. Here, we demonstrate how the 3D- PDF can be used with electron diffraction to understand the complete local structure of the ion conductor calcium stabilized zirconia ($Zr_{0.82}Y_{0.18}O_{1.91}$).

$Zr_{0.82}Y_{0.18}O_{1.91}$ crystallizes in the fluorite structure and shows composition disorder on both the metal and oxygen site. Due to the vastly different bond lengths of Y-O and Zr-O, strongly structured diffuse scattering is observed alongside the Bragg reflections (see Figure (a)). By employing the 3D- PDF to electron diffraction data, we can directly interpret the local correlations (see Figure (b)).

Large single crystals of $Zr_{0.82}Y_{0.18}O_{1.91}$ that are suitable for X-ray and neutron measurements were investigated. By comparing the results from our electron PDF to X-ray and neutron PDFs we demonstrate the reliability of the 3D- ePDF.

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.

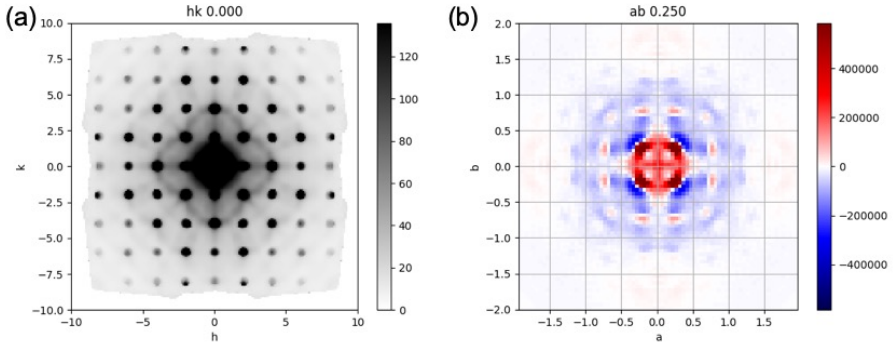

Figure 1. (a) hk0 reciprocal space section with diffuse scattering and Bragg reflections. (b) 3D- ePDF in the ab0.25 layer showing the relaxation of metal-oxygen bond lengths around (0.25,0.25,0.25).

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

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