Invited Lecture

Using diffuse scattering from electron diffraction experiments to understand local order

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The utilization of structural flexibility in materials is a common strategy to enhance their properties. The intentional introduction of disorder locally disrupts the long-range order. Often disorder on a local scale is not random, and certain preferred local atomic configurations may significantly impact material properties [1]. In a diffraction these local ordering principles are manifested as single crystal diffuse scattering. However, functional materials in their applied stated are often not synthesized as large single crystals. Here, we demonstrate how to use three-dimensional electron diffraction experiments on sub-micron sized crystals to disentangle local order information.

The analysis of diffuse scattering is conventionally perceived as challenging. Here, we showcase two complementary approaches to address diffuse scattering. Firstly, we employ a mean-field approach to resolve diffuse scattering in rocksalt type structures, exemplified by battery materials such as $Li_{1.2}Mn_{0.4}Ti_{0.4}O_2$ (LMTO) and $Li_{1.2}Mn_{0.4}Zr0_{.4}O_2$ (LMZO), as previously investigated by Ji *et al*. [2] (see Figure 1). Secondly, we utilize the three-dimensional difference pair distribution function analysis (3D-ΔPDF) to elucidate experimentally observed diffuse scattering in yttria-stabilized zirconia ($Zr_{0.82}Y_{0.18}O_{1.91}$) [3].

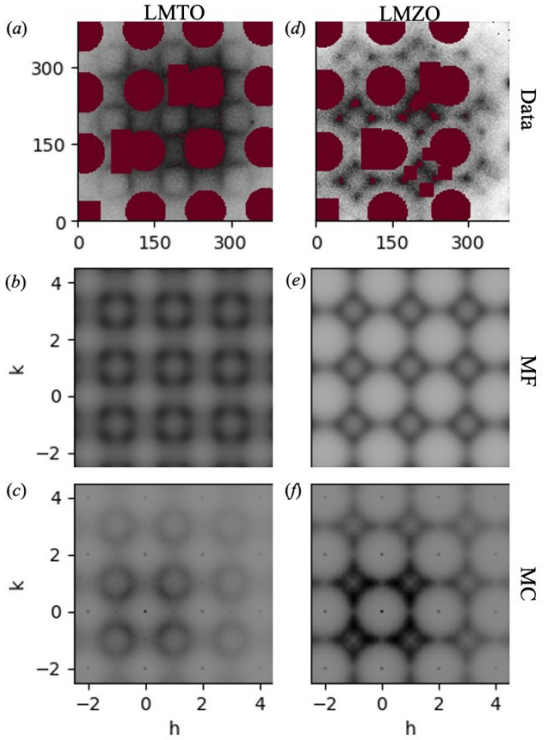

Figure 1. (a) Published LMTO diffuse scattering in the [001] zone axis by Ji *et al*. [2]. Red areas indicate masking of Bragg reflections and over-exposed pixels, as well as labels in the published data. Axis units correspond to pixels. (b) Results of the mean- field fit. (c) Diffuse scattering calculated from a Monte-Carlo simulation using the parameters determined by the mean-field fit. (d-f) Same as (a-d) for LMZO.

[1] Simonov, A. & Goodwin, A.L. (2020). *Nat. Rev. Chem.* **4**, 657–673.

[2] Ji, H. *et al.* (2019). *Nat. Commun.* **10**, 592.

[3] Schmidt, E.M. *et al.* (2023). *Nat. Commun.* **14**, 6512.