Poster Presentation

MS55.P13

Local order in wüstite. Fe1-xO, using a PDF approach

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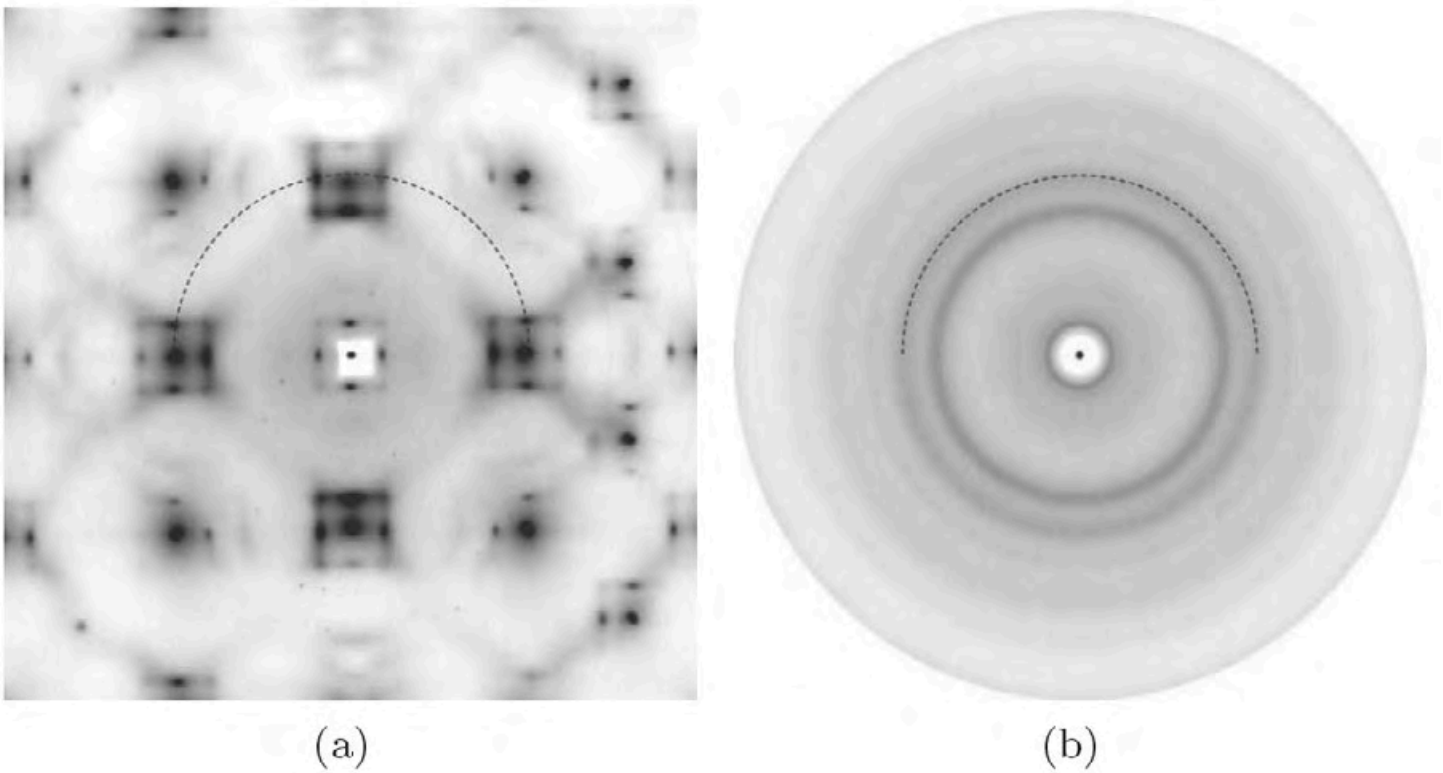
Many minerals (and materials more widely) show evidence of strong and complex local structural ordering. This local ordering can affect a material's mechanical properties, its transport properties (for example, how vacancies relate to oxygen transport through the structure) and its thermodynamics, and so is clearly of prime importance. For crystalline materials the analysis of single crystal diffuse scattering (SCDS) is the most definitive way of determining local structure but for many minerals (and materials more widely) single crystals of a sufficient size for such studies are often not readily obtainable and powder diffraction data must suffice. While conventional powder XRD (e.g. using Rietveld refinement) can provide information about the average crystal structure, total scattering (TS) – which includes both Bragg peaks and diffuse scattering – is needed if information about the local structure and short-range order is to be gained. The pair distribution function (PDF) analysis of such total scattering data has become a widely used technique for extracting such local structural information from a wide variety of materials including crystalline powders, nano-materials, amorphous materials, glasses and liquids. The aim of the present work is to explore the sensitivity of the PDF methodology to various aspects of disorder and short-range order for a mineral system for which the local structure has been characterised previously using SCDS. The system chosen for this study is the non-stoichiometric iron oxide wüstite, (Fe1−xO, x = 0.057). The X-ray diffraction patterns obtained from a single crystal of wüstite show strong and richly structured diffuse scattering (see Fig. 1). This has enabled a detailed model of the defect structure to be established. The aim is to assess to what extent this defect structure model could have been established using PDF analysis of powder diffraction data.



Keywords: Single crystal diffuse scattering, Pair Distribution Function, Wüstite