Poster Presentations

[MS27-P03] Crystal and magnetic structure of Fe_xO refined from total scattering data

Paul J. Saines[a], Anthony K. Cheetham[b] and Andrew L. Goodwin[a]

[a]*Department of Chemistry, University of Oxford*
[b]*Department of Materials Science and Metallurgy, University of Cambridge*
paul.saines@chem.ox.ac.uk

Wüstite, Fe_xO, is the most common non-silicate mineral in the earth and has an important effect on geological processes.[1] Despite its seemingly simple rock salt structure it is universally nonstoichiometric, significantly affecting its geologically relevant properties. It is known that its Fe deficiency leads to vacancies on the octahedral Fe sites and the formation of some tetrahedral interstitial Fe^{3+}, which are surrounded by octahedral vacancies. The precise nature of the local structure around these defects, and in particular how neighbouring defects interact with each other, has been debated for the last 50 years and remains unclear.[2] The role these defect clusters play in the magnetic ordering of Wüstite below ambient conditions is also unclear. In this work we present a detailed characterization of the local nuclear and magnetic structure of this seminal compound using Reverse Monte Carlo (RMC) refinements of neutron total scattering powder diffraction data, including pairdistribution function (PDF). This has been proven to be a powerful tool for examining a wide range of materials where complex deviations of the local structure from the average play a crucial role in the behaviour of the material. Here we have for the first time clearly characterised the bonding environments of both types of iron atoms in this mineral and re-examined the preferred cluster growth direction of the interstitial iron. Additionally we have shed new light on the fascinating magnetic structure of Fe_xO, revealing that the magnetic structure of the bulk octahedral iron is not only more complex than previous thought but also for the first time providing some clear characterisation of the magnetic correlations of the interstitial tetrahedral iron. This study not only reveals fascinating new insight into Wüstite but also represents one of the first well characterized examples of a study linking defect and magnetic structures; thereby highlighting the power of total scattering in understanding the structures of complex materials.

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2a) F. Koch *et al., Acta Cryst.* **B25**, 275 (1969); b) A.K. Cheetham *et al., J. Phys. C* **4**, 2160 (1971); c) T.R. Welberry *et al., Phys. Chem. Minerals* **24**, 24 (1997).

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