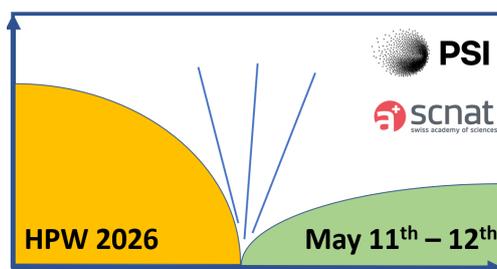


High Pressure Workshop



Contribution ID: 52

Type: Talk

The role of neutrons in understanding the behaviour of metal oxides at extreme conditions

Tuesday, 12 May 2026 15:30 (30 minutes)

Pearl is the dedicated high-pressure diffraction instrument at the ISIS Neutron and Muon Source. Using a series of examples from the user programme the current and developing capabilities of the instrument will be represented. In particular, we will demonstrate the pressure range and quality of different data we were able to measure. We will also showcase the technology we are using to provide access to a wide range of temperatures as well. Provided below are some of the science areas which will be used to highlight the instrument and technique capabilities.

The behaviour of the crystallography structure of more simple perovskites such as LaCoO_3 will be presented [1]. Highlighting changes in the polyhedral compression mechanism and indications as to the electronic configuration which can be extracted from such structural studies. We will then showcase the behaviour of BaTiO_3 as a function of pressure and temperature demonstrating the nature of the phase transitions which and the role in which neutron diffraction adds a unique insight into this material and even allowing estimation of the polarisation of the distorted material.

High pressure also provides the capability to prepare materials in previously inaccessible structural forms which can be recoverable to ambient pressure. One such recent study are metastable phases of FePO_4 which is a chemical analogue of orthorhombic (CrVO_4 -type, phase-II) SiO_2 . By preparing the metastable phase II of FePO_4 and recovering back to ambient pressure were able to infer the high-pressure behaviour of the equivalent crystalline phase of SiO_2 normally only observed as an amorphous solid by direct compression of the orthorhombic phase II of FePO_4 . [3]

Finally, we will show how with the application of pressure and temperature it is possible to prepare new perovskite related materials by taking the structure out of its stability field and preparing a series of perovskites which can be recovered back to ambient conditions. The example presented will be a series of perovskites in the solid solution $\text{SeCo}_{1-x}\text{Mn}_x\text{O}_3$ [4]. Neutron diffraction data will be presented on the structural behaviour of the solution and correlated to magnetic properties.

[1] M. Capone et al, High-Pressure Neutron Diffraction Study of LaCoO_3 , *Physica status solidi a*, (2019), 216, 1800736

[2] C. L. Bull et al, Comprehensive determination of the high-pressure structural behaviour of BaTiO_3 , *Materials Advances*, (2021), 2, 6094

[3] C.L. Bull et al, The distortion of two FePO_4 polymorphs with high pressure, *Materials Advances*, (2021), 2, 5096

[4] C. J. Ridley et al, Structure and physical properties of $\text{SeCo}_{1-x}\text{Mn}_x\text{O}_3$, *J. Physics: Condensed Matter* (2019), 31, 3195402

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