Structural and magnetic phase transitions in oxides and mixed-anion materials

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The properties of functional materials are determined in large part by their crystal structures (and symmetries), and so powder diffraction is a key technique for their characterisation. However, diffraction data alone, or data collected at a single point in the phase diagram, don’t always allow a complete understanding of a material’s properties. Exploring how structure and properties change in response to stimuli (e.g. temperature, applied magnetic field) and the nature of phase transitions can give a better understanding of the origins of functionalities including magnetic, dielectric and electronic properties.

This presentation focuses on structural and magnetic phase transitions (and transitions in which these are coupled) in transition metal oxides and mixed-anion materials including perovskite-related phases, corundum-derived systems and layered oxychalcogenides. The presentation the additional insight gained from neutron and x-ray powder diffraction experiments carried out as a function of temperature or applied magnetic field, and the importance of complementary techniques.

Figure 1. (a) Schematic illustrating phase transitions of Pr$_2$O$_2$MnOSe$_2$ (in zero field) with temperature; (b) the higher $d$-spacing region Rietveld refinement profiles of NPD data (1.5 K, $M = \text{Fe}$) emphasizing magnetic reflections (black line).