Neutron total scattering studies of three multiferroic crystals

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Multiferroics are a class of materials where there are coupled phase transitions involving mostly ferromagnetic and ferroelectric ordering. The term ferroic implies that application of an electric field can switch the sign of the ordering (such as flipping the direction of the magnetisation), but in practice people consider types of magnetic ordering beside ferromagnetism. Here we consider three multiferroic materials, FeBiO3, CuO and YMnO3. We study these using neutron total scattering coupled with the Reverse Monte Carlo method. Our focus is purely on the structural components, ignoring completely for now the magnetic ordering. This is particularly good to look at what we call the local structure, namely how the atomic configurations on a short length scale fluctuate away from the average structure defined by the nominal average positions of atoms. The headline result from this work is that the local fluctuations are often so much larger than displacements associated with the ferroelectric distortions. We also see little obvious coupling between structural fluctuations and magnetic order. This point will be illustrated for each system.

Acknowledgements to Juan Du and Anthony Phillips (QMUL), David Keen and Matt Tucker (ISIS), and Donna Arnold (University of Kent)