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3D-magnetic difference-PDF analysis of magnetic frustration in Bixbyite

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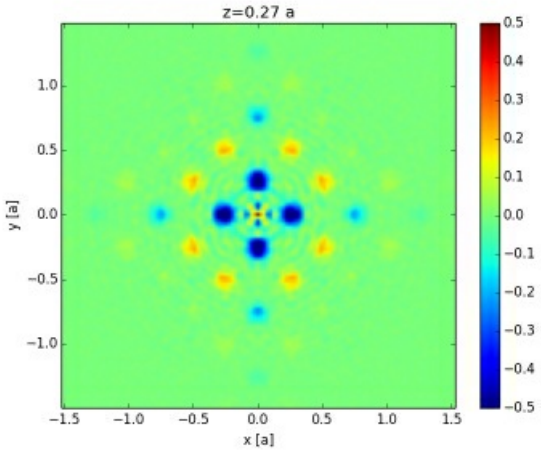
Magnetically frustrated materials are gaining a huge increase in interest due to exotic physical phenomena found in spin liquids and glasses. In order to obtain a better understanding of such magnetically disordered materials, magnetic diffuse neutron scattering can be measured and analyzed. For a long time, analysis mainly consisted of inspection of the wave-vector and temperature dependence of scattering, giving only limited information about the disorder. Recently, more advanced methods have been developed, such as modelling the scattering using reverse Monte-Carlo simulations for both powder and single-crystal data. Another recent approach has been to develop a magnetic pair distribution function analysis for powder neutron scattering. Such analysis gives a one-dimensional look at magnetic pairwise interactions, both ordered and disordered.

Here we show a new technique for single-crystal magnetic diffuse scattering analysis. The technique is analogous to the 3D-difference PDF pioneered by Weber and Simonov for X-ray scattering [1], as it takes the Fourier transform of only the magnetic diffuse scattering. The resulting 3D-magnetic difference-PDF gives a real-space view of the spin-spin correlation. As only the diffuse scattering is used, it is possible to get a view of the disordered part of the magnetic structure. This allows analysis of materials with an average magnetic structure containing some disorder without the ordered part dominating the result. In this way, it is possible to directly observe whether two moments tend to be more parallel or antiparallel aligned than the average structure.

We demonstrate the technique on the frustrated magnetic mineral Bixbyite, $FeMnO_3$. Data has been measured at the new instrument CORELLI at the Spallation Neutron Source, Oak Ridge national lab [2]. CORELLI allows for fast and accurate measurements of large volumes of reciprocal space with elastic/inelastic energy discrimination of unpolarized neutrons [2]. The scattering from Bixbyite is quite complex, as there is strong Bragg reflections, weak symmetry breaking reflections as well as both nuclear and magnetic diffuse scattering. We show how to separate out specifically the magnetic diffuse scattering in order to compute the 3D-magnetic difference-PDF. The analysis reveals that nearest neighbor metal atoms tend to prefer antiparallel alignment, next-nearest neighbors parallel alignment etc. and that correlations exist up to relatively long distances (> 10 Å).

[1] Weber, T. & Simonov, A. (2012) Z. Krist. 227, 238-247
[2] Rosenkranz, S. & Osborn, R. (2008) PRAMANA- Journal of Physics, 71, 4, 705-711.



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