MS38 Computations with/for Pair Distribution Functions

MS38-04

Direct visualization of magnetic correlations in frustrated spinel $ZnFe_2O_4$

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Abstract

Magnetic materials with the spinel structure (AB_2O_4) form the core of numerous magnetic devices, but $ZnFe_2O_4$ constitutes a peculiar example where the nature of the magnetism is still unresolved [1,2]. Here the Fe atoms sit on the octahedral sites which constitutes a pyrochlore lattice whose geometry, a network of corner-sharing tetrahedra, is very conducive to exotic magnetic ground states. Using a combination of AC and DC susceptibility measurements in conjunction with heat capacity data we have established the presence of a spin-glass phase in $ZnFe_2O_4$ at low temperature.

Recently, we introduced the magnetic 3D-ΔPDF method, which through a model-free approach allowed us to directly reconstruct the magnetic correlations in magnetically disordered systems [3]. We have collected Single crystal neutron scattering patterns down to 1.5K which revealed clear structured diffuse scattering showing that despite the lack of long-range order, the spins are correlated on short length scales. The elastic diffuse scattering signal was isolated which enabled the use of 3D-mΔPDF analysis to determine the local magnetic correlations present in $ZnFe_2O_4$ at low temperatures which clearly shows the nature of the magnetic frustration in the compound.

Integration of the peaks in the 3D-mΔPDF revealed the behaviour of the individual correlations, and thus also the correlation length, with temperature. The correlations can be rationalized by orbital interaction mechanisms for the magnetic pathways giving insight into the underlying magnetic exchange mechanisms. Using the 3D-mΔPDF results in conjunction with the magnetic exchange considerations a preferred spin-cluster around any given Fe atom has been proposed.

Our study demonstrates how analysis of the detailed 3D single crystal neutron diffuse scattering offers a means to build microscopic understanding of magnetic exchange mechanisms in magnetically disordered materials, which is not possible from merely the Bragg scattering.

References

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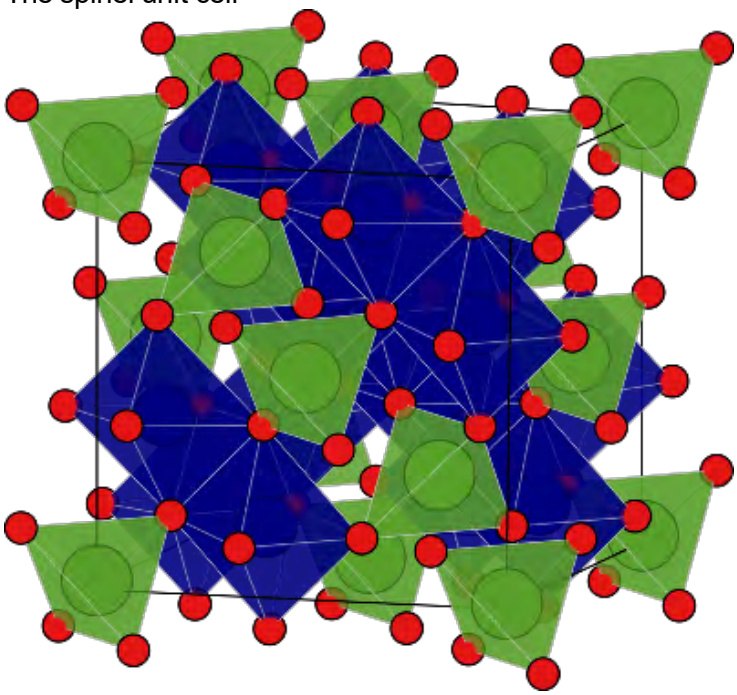
[2] Kremenovč, A., Antič, B., Vulič, P., Blanuša, J. & Tomic, A., *J. Magn. Magn. Mater.* 426, 264-266 (2017).

[3] Roth, N., May, A. F., Ye, F., Chakoumakos, B. C. & Iversen, B. B., *IUCrJ* 5, 410-416 (2018)

The spinel unit cell



Isolated diffuse scattering at 1.5 K