with nominal composition $Pb_2(Pb,Li,Na,K,Rb,Re)_{1-x}Nb_5O_{15}$ ($0 \leq x \leq 0.15$, Re = rare earth). Interestingly, many of these compounds also exhibit a large SHG response. These workers proposed a new parameter, called local distortion index *m*, to evaluate the degree of local distortion of these compounds. Please refer to the Supporting Information of Ref. 1 for the definition of local distortion index *m*. **Figure 2** shows the distribution of the SHG response and local distortion index *m* of several NLO materials. The SHG response evidently tends to be strengthened with the enhancement of local distortions.

In summary, the analysis of the local structure unveiled that the structural vacancies at the A1-site strengthen the local distortion and local dipole moments of nearby NbO_6 octahedra and significantly improve the NLO effect. Lin's work is a perspective for the search and design of new materials with an effective NLO performance. (Reported by Chin-Wei Wang)

This report features the work of Kun Lin and his collaborators published in J. Am. Chem. Soc. ***142****, 7480 (2020).*

ANSTO ECHIDNA – High-resolution Powder Diffractometer

- NPD, XRD, Total Scattering
- Materials Science, Chemistry

Reference

1. K. Lin, P. Gong, S. Chu, Q. Li, Z. Lin, H. Wu, Q. Wang, J. Wang, M. J. Kim, K. Kato, C.-W. Wang, X. Liu, Q. Huang, J. Chen, H. Zhu, J. Deng, X. Xing, J. Am. Chem. Soc. **142**, 7480 (2020).

Magnetic Frustration Induces Liquid-Like Short-Range Ordering in Cubic $Mn_{1.5}Cr_{1.5}O_4$

Short-range magnetic correlation manifested by the liquid-like structure factor is observed at temperatures well above T_N in the title compound.

Neutron diffraction is a powerful tool to study magnetic phenomena. It is the best method to determine the magnetic structure and can detect the short-range magnetic correlation between magnetic spins. It is known that competing antiferromagnetic interactions among the magnetic spins on a regular lattice could lead to geometrically magnetic frustration, resulting in the absence of long-range magnetic order or extremely low ordering temperatures. In such systems, the diffuse scattering and unconventional spin dynamics could be observed in a neutron-scattering experiment. Spinel compounds of formula AB_2O_4 have been studied for a long time. The B-site (16*b* of space group *F d* -3 *m*) cations form a regular corner-sharing tetrahedral network, which is potentially geometrically frustrated. Hsiung Chou (National Sun Yat-sen University) and his coworkers maintain a great interest in spinel compounds and recently conducted the powder neutron experiments on $Mn_{1.5}Cr_{1.5}O_4$, employing both high-resolution diffractometer **ECHIDNA** and high-intensity diffractometer **WOMBAT** of ANSTO.

This work determined the cation distribution and magnetic structure of $Mn_{1.5}Cr_{1.5}O_4$, using the high-resolution NPD data (**Fig. 1(a) and 1(b)**). The magnetic structure is collinear ferrimagnetic; the uncompensated A- and B-site sublattice produces a net magnetization. The magnetic order parameter obtained from neutron diffraction (**Fig. 1(a)**) matches satisfactorily with the spontaneous magnetization for the transition temperature and the critical exponent (**Fig. 1(a)**), but the deviation from the Curie-Weiss behavior occurs at a much higher temperature, $T' \sim 170$ K, indicating that diffuse scattering might be detectable in neutron-diffraction experiments. Detailed temperature-dependent measurements were hence conducted employing HIPD WOMBAT (**Fig. 2(a)**). **Figure 2(a)** shows that modulation of the background intensities develops below T' before it eventually collapses onto the magnetic Bragg reflections at T_N. The diffuse magnetic scattering weakens but continues to co-exist with the ferrimagnetic phase below T_N. The difference between the diffraction patterns collected at 163 K and 63 K clearly reveals the modulation (**Fig. 2(b)**). Because of the *Q* dependence of the instrument resolution, the oscillation at higher *q* is smeared out and becomes shallower, but the oscillation persists. Chou suggested that the liquid-like short-range order develops because of the presence of magnetic frustration in the system.

This observation of diffuse scattering above the magnetic-ordering temperature is neither the first time reported nor a rare case. For example, magnetic diffuse scattering of the textbook example, MnO, was reported in the 1940s.[2] The broad diffuse

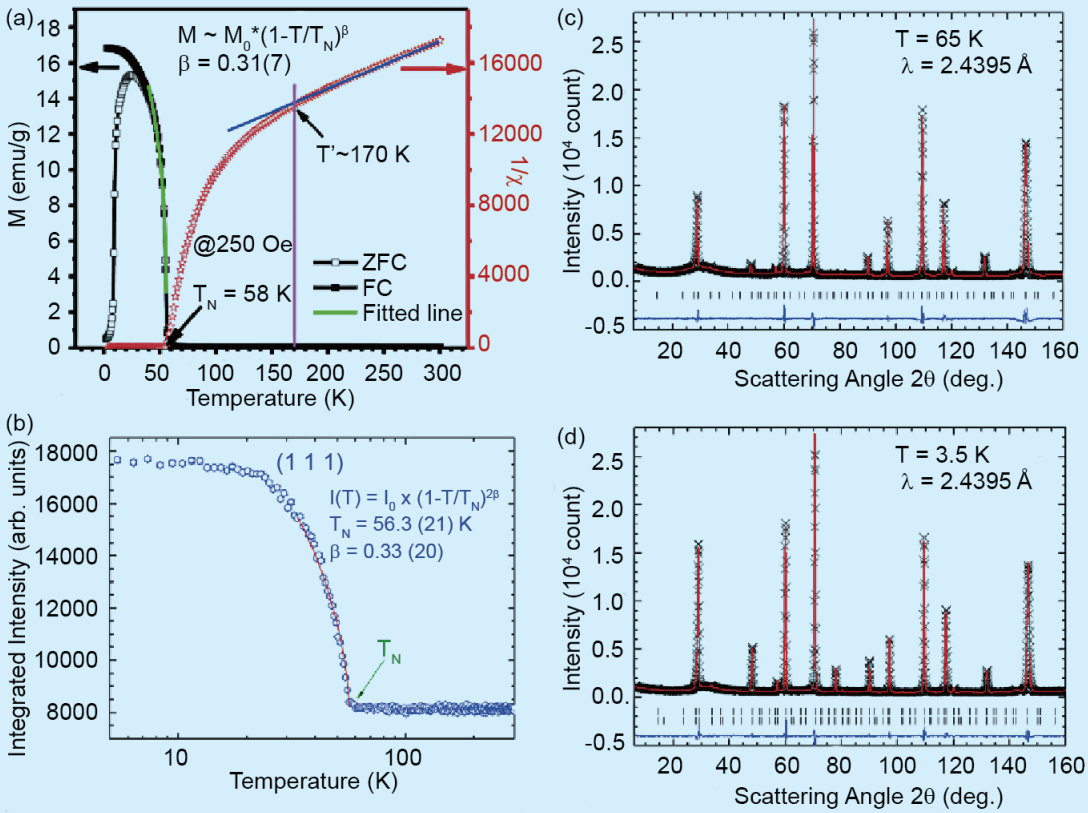

Fig. 1: (a) Left axis shows ZFC and FC M(T) curves of $Mn_{1.5}Cr_{1.5}O_4$ under applied magnetic field 250 Oe. The right axis represents an inverse magnetic-susceptibility curve. (b) Magnetic order parameter of $Mn_{1.5}Cr_{1.5}O_4$ manifested by the integrated intensity of signal (1 1 1). Rietveld plot of $Mn_{1.5}Cr_{1.5}O_4$ neutron powder-diffraction (NPD) data at (c) 65 K and (d) 3.5 K. [Reproduced from Ref. 1]

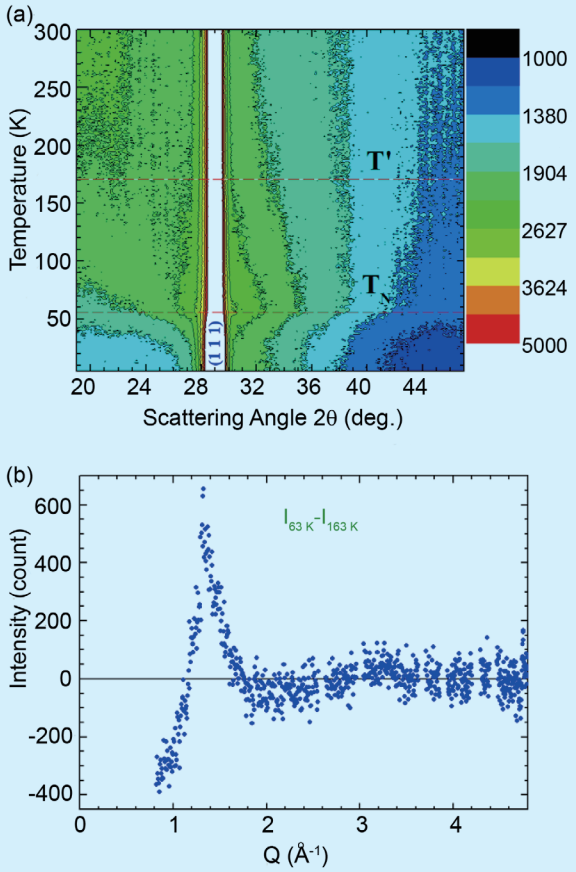

Fig. 2: (a) Small-angle view of the 2D plot of the temperature-dependent diffraction pattern around the (111) signal shows that the background intensity diffuses below 170 K and then concentrates around the (111) signal below T_N. (b) Residual magnetic signal obtained from the difference of diffraction patterns at 163 K and 63 K. [Reproduced from Ref. 1]

signals above the ordering temperature are generally regarded as the precursor of long-range magnetic order; the inverse signal width reflects the magnetic correlation length or the size of the magnetic clusters. Chou and his coworkers demonstrated the oscillatory nature of the magnetic diffuse-scattering intensities in $Mn_{1.5}Cr_{1.5}O_4$, which could lead to various physical pictures. The ferromagnetic magnetic correlation above T_N could refer to the Griffiths phase; the local minimum in the oscillation might refer to a pinch point in the context of spin ice. This work has indeed triggered a motivation to grow single-crystal samples and to expand the neutron-scattering investigations of spinel compounds. (Reported by Chin-Wei Wang)

This report features the work of Hsiung Chou and his collaborators published in Appl. Phys. Lett. ***116****, 182406 (2020).*

ANSTO WOMBAT – High-intensity Powder Diffractometer
ANSTO ECHIDNA – High-resolution Powder Diffractometer

- NPD
- Condensed-matter Physics

References

1. G. D. Dwivedi, C. W. Wang, S. M. Kumawat, H. Chou, Appl. Phys. Lett. **116**, 182406 (2020).
2. C. G. Shull, J. S. Smart, Phys. Rev. **76**, 1256 (1949).