Weak Trimerization in 2D Heisenberg Antiferromagnet

Detailed neutron scattering studies revealed fragile trimerization in an almost perfect 2D Heisenberg Antiferromagnet.

The 2D-THA systems are of particular interest owing to their geometric frustration and potential for novel spin states. The material investigated, $Lu_yY_{1-y}MnO_3$, belongs to the family of hexagonal $RMnO_3$ compounds, where *R* represents a rare-earth ion. It has been studied for its multiferroic properties and intriguing magnetic behavior. $Lu_yY_{1-y}MnO_3$ adopts *P*6₃cm symmetry; Shinichiro Yano (NSRRC) and his collaborators focused on the six irreducible representations as candidates of magnetic structures of $Lu_yY_{1-y}MnO_3$ and its high-resolution spin dynamics.

Yano utilized neutron powder diffraction at **WOMBAT** in ANSTO to determine the magnetic structure of $Lu_yY_{1-y}MnO_3$, which was described as a mixture of two magnetic space groups at different compositions. He especially focused on y = 0.3, where x_{Mn} is close to the 1/3; therefore, an almost perfect triangular lattice is realized by the system. This approach, combined with temperature variation, gave insight into the system's trimerization and exchange interactions.

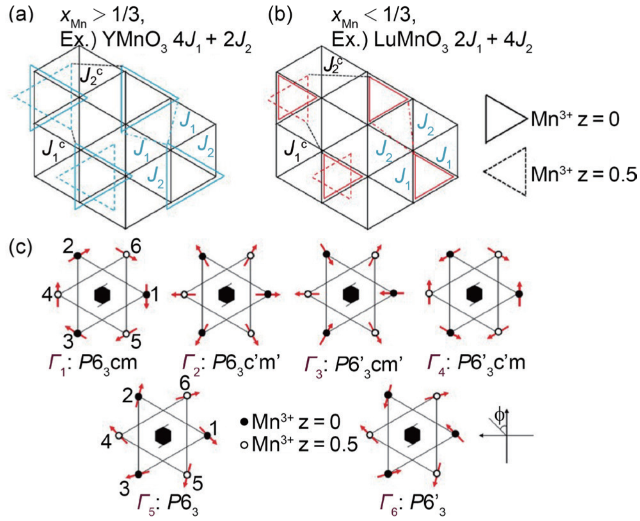

Fig. 1: (a,b) Exchange interactions in the plane. Mn position (x_{Mn}, 0, 0) x ~ 1/3 is a critical parameter because there are four J_1 and two J_2 when x_{Mn} > 1/3, while there are two J_1 and four J_2 when x_{Mn} < 1/3. These are the next nearest neighbour J_1 and the subsequent nearest neighbour J_2. (c) There are six candidates of magnetic structure under P63cm symmetry, Γ_1 to Γ_4 are one-dimensional irreducible representations and Γ_5 and Γ_6 are two-dimensional irreducible representations. [Reproduced from Ref. 1]

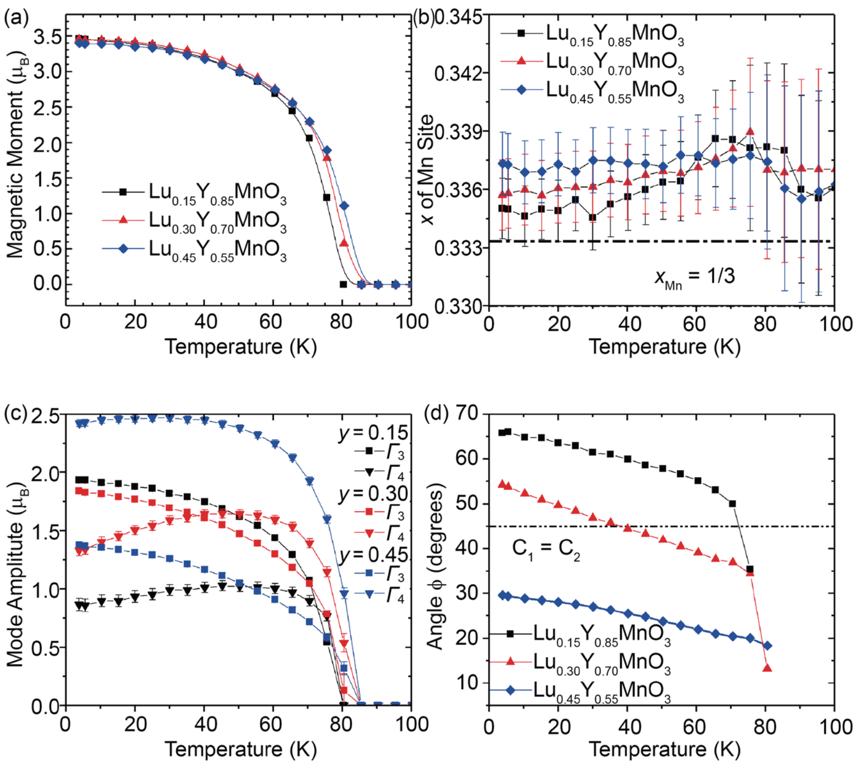

Fig. 2: Neutron power diffraction data revealed the detailed crystal and magnetic structures. (a) Magnetic phase transition temperatures are determined for y = 0.15, 0.30, and 0.45. (b) Trimerization at manganese *x* position was not observed, and x_{Mn} remains at a constant temperature below 100 K. (c) It was found that two irreducible representations Γ_3 and Γ_4 are needed to describe the magnetic structures. (d) Temperature dependence is observed for the ratio of the linear combination of the two irreducible representations Γ_3 and Γ_4. [Reproduced from Ref. 1]

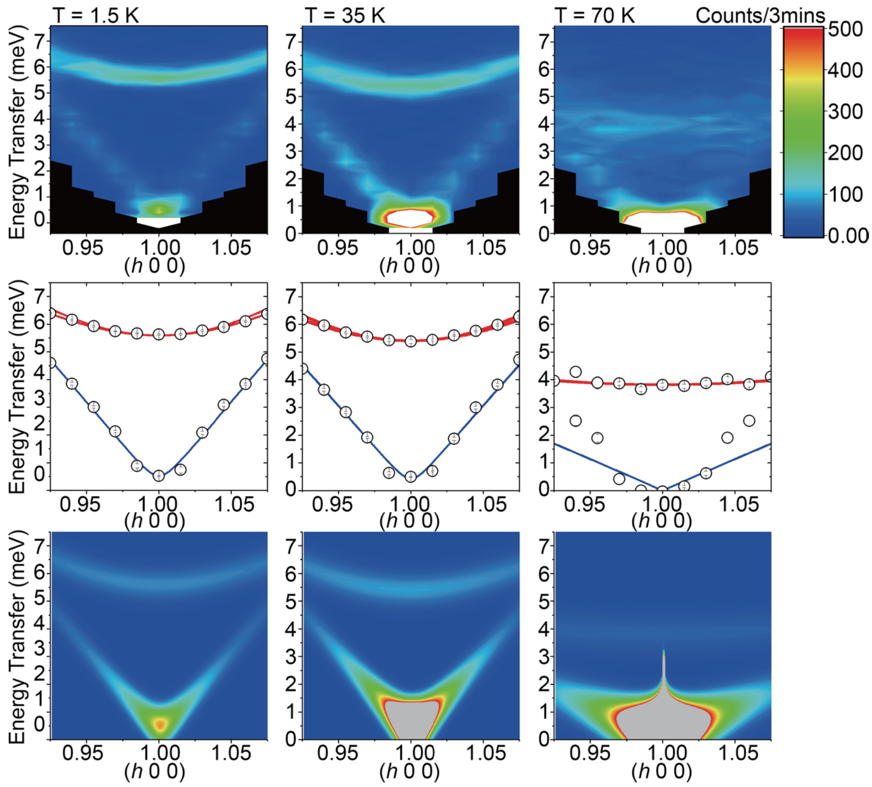

Fig. 3: Low energy side of spin wave dispersion at T = 1.5, 35, and 70 K using a cold triple axis spectrometer **SIKA**. These data allow the team to determine the exchange parameters J_1 and J_2 with high resolution. [Reproduced from Ref. 1]

Their research delves into the complexities of the magnetic and crystal structures of $Lu_yY_{1-y}MnO_3$, outlining how various compositions affect these structures. It discusses the temperature-dependent atomic positions of Mn and how these shifts relate to the magnetic ordering and trimerization of the system. The results indicate a subtle yet noticeable impact on the magnetic structure and behavior of the material depending on the temperature and the (Lu,Y) composition. This may help to further understand the underlying physics of 2D-THA systems. Particularly, their work has revealed that using two irreducible representations may be necessary to solve the magnetic structures of other 2D-THA systems.

To understand the magnetic structures and dynamics further, inelastic neutron scattering studies were conducted using **SIKA** in ANSTO. These experiments allowed for a detailed investigation of the spin-wave dispersion and the magnetoelastic excitations. The team noted that the composition $Lu_{0.3}Y_{0.7}MnO_3$ was an ideal candidate to investigate these phenomena due to its near-ideal parameters for examining trimerization and frustrated magnetism.

Furthermore, their study extensively discusses the spin-wave dispersion. The research showed that the trimerization effect upon cooling was not noted at the manganese atomic position x_{Mn}, highlighted by changes in the nearest-neighbor exchange interaction as shown in **Fig. 3**. This is referred to as "weak trimerization."

In summary, their research offers a detailed exploration of the weak trimerization observed in $Lu_yY_{1-y}MnO_3$ and its implications for understanding the materials' magnetic and structural properties. Through comprehensive structural analysis and magnetic excitation studies, the research contributes valuable insights into the complex behaviors of 2D-THA systems, with broader implications for the field of condensed matter physics. (Reported by Shinichiro Yano)

This report features the work of Shinichiro Yano and his collaborators published in Phys. Rev. B ***107****, 214407 (2023).*

ANSTO SIKA – Cold Neutron Triple-axis Spectrometer
ANSTO WOMBAT – High-intensity Powder Diffractometer

- Neutron Inelastic Scattering
- Materials Science, Condensed-matter Physics

Reference

1. S. Yano, C.-W. Wang, J. S. Gardner, W.-T. Chen, K. Iida, R. A. Mole, D. Louca, Phys. Rev. B **107**, 214407 (2023).