Solving The Magnetic Structures in The Complex In-field Phase Diagram of Ymn$_6$sn$_{6-\chi}$ge$_\chi$ Using Single Crystal Neutron Diffraction

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The **B** || *ab*-plane in-field magnetic phase diagram of $\mathrm{YMn_6Sn_6}$ has recently garnered attention due to the coexistence of a large topological Hall effect with one of the phases namely, a transverse conical spiral magnetic phase [1]. This spin texture can be directly related to the observation of the real-space Berry curvature arising from a fluctuation-driven mechanism. Generally, the crystal structure of magnetic compounds forming the $\mathrm{HfFe_6Ge_6}$- type structure (*P*6/*mmm* and shown in Fig. 1(a)) lays much of the foundation for the interesting physics observed. For example, the topological Hall effect in $\mathrm{YMn_6Sn_6}$ originates from parametrically frustrated interplanar exchange interactions that arise due to the particular stacking sequence of the Mn kagome planes. It is also this frustrated interplanar exchange and delicate balance of energy scales with the inclusion of an in-plane applied magnetic field that leads to the complex magnetic phase diagram shown in Fig. 1(b).

Recently, we have explored what happens when the stacking of the Mn planes is tuned via Ge doping [2]. For $\mathrm{YMn_6Sn_4Ge_2}$, Ge preferentially replaces the Sn at the 2*c* Wyckoff position, which is in the same layer as the Y atoms. This results in the J_1 and J_p exchange interactions (Fig. 1(a)) essentially staying constant, whereas J_2 and J_3 switch signs and change in magnitude, leading to a quite different in-field phase diagram. Additionally, even a subtle change to the zero-field ground state magnetic structure influences the fermiology making $\mathrm{YMn_6Sn_4Ge_2}$ more conductive along the *c*-axis.

Crucially, single crystal neutron diffraction was required to solve the magnetic structures of $\mathrm{YMn_6Sn_{6-\mathit{x}}Ge_\mathit{x}}$ ($x = 0, 2$) in the *B*-*T* magnetic structure phase diagram. The intimate relationship between the electronic structure and magnetic structure in $\mathrm{YMn_6Sn_{6-\mathit{x}}Ge_\mathit{x}}$ required knowledge of the spin textures which could only be gained from neutron diffraction. This talk will discuss the practical details of experiment planning, magnetic neutron diffraction, and interpreting the $\mathrm{YMn_6Sn_{6-\mathit{x}}Ge_\mathit{x}}$ results via Rietveld refinement.

{1} Ghimire et al., Sci. Adv. ***6****, eabe2680 (2020).*
{2} Bhandari et al. (2023) (in preparation).

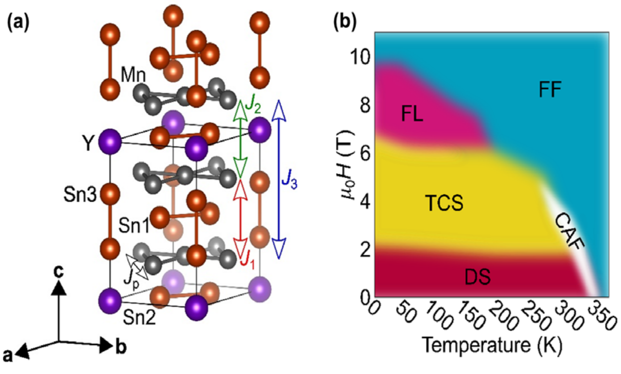

Figure 1. (a) The crystal structure and exchange interaction pathways (J_p, J_1, J_2, and J_3) for $\mathrm{YMn_6Sn_6}$. (b) Magnetic structure phase diagram for an applied field within the ab-plane of $\mathrm{YMn_6Sn_6}$. The phases shown are distorted spiral (DS), transverse conical spiral (TCS), fan-like (FL), forced ferromagnetic (FF), and canted antiferromagnet (CAF).

Figure 1