Single crystal neutron diffuse scattering of layered ferromagnet $Fe_{3-x}GeTe_2$

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Gate-tunable magnetism has been recently demonstrated in few-layer-thin Fe_3GeTe_2 at room-temperature, suggesting great application potentials of this family of layered van der Waals materials towards low-dissipation spintronics. However, the magnetic properties of $Fe_{3-x}GeTe_2$ show a considerable dependence on the stoichiometry [1]. To better understand the effect of the Fe-deficiency, temperature dependent full three-dimensional diffuse neutron scattering data have been collected at the time-of-flight CORELLI spectrometer at SNS.

The Fe-deficient sample shows highly structured diffuse scattering patterns with a pronounced feature of half-moon decorated hexagons in the HK plane with a weak Q dependence along the L direction (Fig. 1 bottom). The cross-correlation analysis, using the unique statistical chopper at CORELLI, reveals that the diffuse scattering is mainly of a static origin. The temperature dependence indicates that nuclear scattering is the main contribution to the diffuse scattering. However, features from weak magnetic diffuse scattering are observed at low Q well above the Curie temperature, confirming the detrimental roles of vacancies on the long-range spin correlation. Monte Carlo simulations show that the features can be largely reproduced by considering short-range Fe-vacancy correlations on Fe(2) sites and correlated displacements of the nearest neighbors of the vacancies (Fig. 1 top). Interestingly, to explain the Q-dependence of the diffuse scattering intensity, it is necessary to consider a weak out-of-plane Fe(2)-vacancy occupational correlation besides strong in-plane correlations, consistent with the quasi-2D nature of the material.

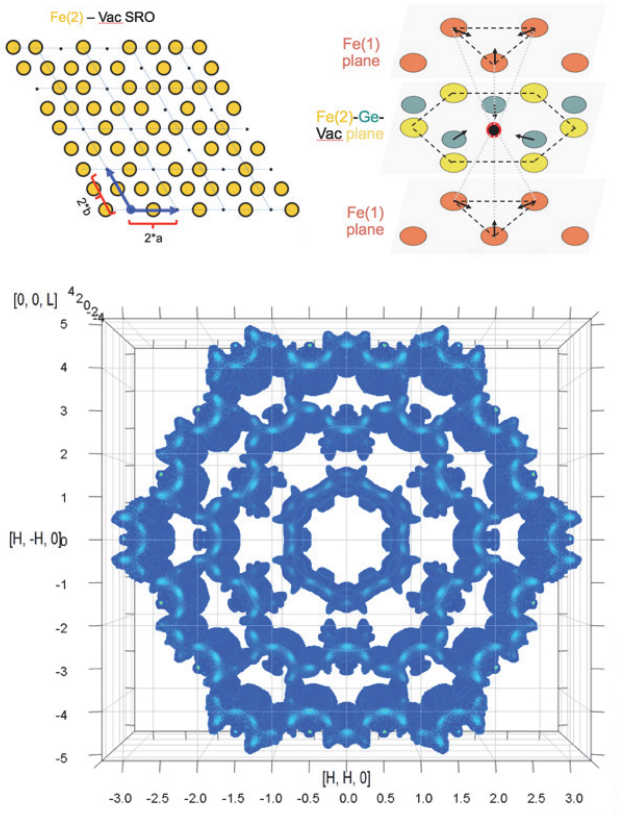

Fig. 1. (bottom) The major diffuse scattering features of a nonstoichiometric $Fe_{3-x}GeTe_2$, captured by computer-aided vision, highlights half-moon decorated hexagons. (top) The proposed minimal local-structural model consists of short-range Fe-vacancy correlations on Fe(2) sites and correlated displacements of the nearest neighbors of the vacant sites.

[1] May AF, Calder S, Cantoni C, Cao H, & McGuire MA, (2016) *Physical Review B* **93**, 014411.