Power Neutron Diffraction study on an iron-based magnet $BaFe_{12}Se_7O_6$

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Spin frustrated magnets attract much attention because of the emergence of exotic magnetic states. A typical geometrical spin frustration system is a triangular lattice with $d = 0$ and $z = 6$, where d and z represent the lattice depletion and bond number, respectively. This can be further extended to several types of triangle-based spin lattices, such as kagome ($d = 1/4$, $z = 4$) and honeycomb lattices ($d = 1/3$, $z = 3$)[1]. From a structural point of view, however, the design of real spin lattices with smaller d values is more difficult because long-period structures allowing ordered depletion sites are required. One such underexplored spin frustrated lattices is one with d = 1/9 and z = 4 and 6, so called, hexagram lattice, in which each hexagram is linked by corner sharing on the same plane (Figure 1).

Recently, we discovered a new iron-based magnet, $BaFe_{12}Se_7O_6$, that adopts a three-dimensionally connected hexagram spin lattice. Heat capacity and magnetic susceptibility measurements revealed three phase transitions at 160, 76, and 68 K, suggesting the presence of spin frustration. To clarify their origins, we performed powder neutron diffraction experiments using the HERMES diffractometer installed in JRR-3. The used wavelength was 2.20 Å. Figure 2 shows the temperature evolution of the neutron diffraction patterns of the iron oxyselenide. No extra peaks were observed down to 180 K. Upon further cooling, however, several new peaks, which could not be assigned to the nuclear structure, appeared, as indicated by dotted lines in Fig. 2. Upon further cooling from 70 to 5 K, additional peaks were observed. Unfortunately, the observed new peaks could not be reasonably assigned to simple k vectors. Single-crystal neutron diffraction studies are helpful for solving magnetic structures.

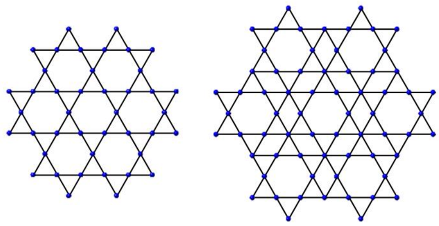

Fig. 1. (left) kagome lattice and (right) hexagram lattice.

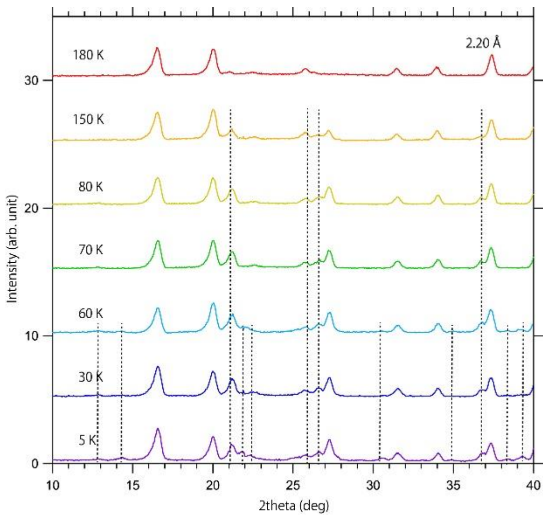

Fig. 2. Powder neutron diffraction patterns of $BaFe_{12}Se_7O_6$ collected at several temperatures.

[1] H. Lu *et al*., Dalton Trans. 47 (2018) 15303.