Singel-crystal neutron diffraction study of a spin-frustrated antiferromagnet $BaFe_{12}Se_7O_6$

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Geometric spin frustration based on triangular lattices continues to be a central topic in magnetic physics because it is expected to generate non-trivial magnetic states. Recently, many compounds with two-dimensional frustrated lattices with periodically introduced lattice defects (d), including the Kagome (d = 1/4) and honeycomb (d = 1/3) lattices, have been newly synthesized,[1] and various magnetic states have been observed depending on temperature, pressure, magnetic field and so on. Controlling bonds (z) between magnetic ions also allows us to design complex spin lattices, such as '*hexagram*' lattice (d = 1/8, z = 4+ 6) Although a few theoretical studies are reported, there have been yet no model substances to be examined. a new oxyselenide $BaFe_{12}Se_7O_6$, which we have recently synthesized by flux method, is a candidate of a modified hexagram lattice model. It exhibits complex magnetic phase transitions at T_{N1} = 158, T_{N2} = 73, and T_{N3} = 67 K. We previously investigated the magnetic states by neutron powder diffraction using the HERMES diffractometer. Several magnetic reflections were successfully observed below 180 K, but the propagation vectors could not be assigned.

In this study, to determine the magnetic propagation vectors, we performed single-crystal neutron diffraction experiments using the FONDER diffractometer installed at JRR-3. The wavelength was 1.2464 Å. As a result of scanning a number of possible q vectors at 10 K, a $(-2, -1, -0.5)_h$ or $(-1.5, 0.5, 1.5)_r$ reflection was detected. h and r stand for hexagonal and rhombohedral notation, respectively. This peak disappeared above 160 K, which is consistent with T_{N1}. It should be noted that the integrated intensity showed jumps at around T_{N3} and T_{N2}, suggesting changes in magnetic structures. To determine the propagation vector for the high-T magnetic phase ($T_{N2} < T < T_{N1}$), exhaustive scanning of possible q vectors was conducted at 100 K. As a result, we observed many magnetic reflections that can be described by $k = (1/2\ 1/2\ 1/2)_r$. This result also explains the magnetic peaks observed in the powder diffraction data in the T range from 70 to 150 K. Our preliminary magnetic structure analysis revealed the spin orientation of Fe magnetic moments $(m_a, m_b, m_c)_{Fe1}$ = (-3.10 -3.10 2.22) with $|m|_{Fe1} = 3.8\ \mu_B$ and $(m_a, m_b, m_c)_{Fe2}$ = (0.25 0.57 -0.53) with $|m|_{Fe2} = 0.72\ \mu_B$. Furthe study is needed for full characterization of the magnetic structures of three magnetic states.

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

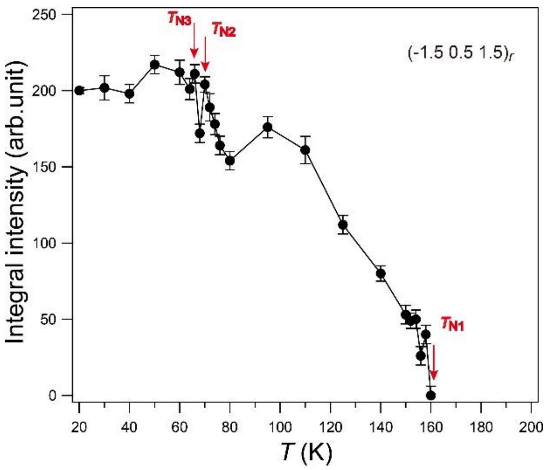

Fig. 1. Temperature dependence of integral intensities of the magnetic Bragg peak corresponding to $(-1.5\ 0.5\ 1.5)_r$.