Neutron diffraction on breathing pyrochlore antiferromagnet LiInCr₄S₈

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The pyrochlore lattice, where regular tetrahedra are connected by sharing corners, is one of the well-known spin systems that exhibits magnetic frustration. It is known that it does not order in the classical Heisenberg model at finite temperatures [1]. The breathing pyrochlore lattice, where alternating tetrahedra with different magnetic interactions are connected, lies between the pyrochlore lattice and isolated tetrahedral spin systems. Theoretical calculations based on the classical Heisenberg model propose four different magnetic states as the ground state depending on the sign of the interactions [2].

The spinel compound LiInCr₄S₈ is a model compound which realizes a breathing pyrochlore lattice [3]. In theoretical calculations, the magnetic interactions that form the tetrahedra in this material are both ferromagnetic, and their magnitudes are significantly different [4]. This combination of magnetic interactions is unique in the related materials. The calculation suggests that the collinear magnetic structure with the magnetic propagation vector Q = (1, 0, 0) r. l. u. [4]. In addition, a large contraction of the lattice near antiferromagnetic the transition temperature of 30 K has also been reported [5], which indicates the magnet-lattice coupling. On the other hand, magnetic ground state has not been investigated yet.

In this study, we conducted powder neutron diffraction experiments using the HERMES diffractometer installed at JRR-3 to investigate the magnetic structure realized in this material. Conventional vanadium cylinder was used for holding the sample. 2.197 Å was used for the wavelength of neutron. We used GM cryostat for achieving a low temperature down to 4.2 K. The diffraction patterns were measured at various temperatures.

Figure 1 shows the neutron diffraction at 4.2



Fig. 1. Neutron diffraction patterns on $LiInCr_4S_8$ at 4 and 35 K. Red arrows indicates the magnetic peaks.

and 35 K. Above the transition temperatures, the diffraction patterns are well reproduced by the previous crystal structure model [3]. Below 26 K, four magnetic peaks indicated by the red arrows were observed. The magnetic propagation vector Q = (1/2, 1/2, 0) r.l.u. were determined by indexing these peaks. It indicates that the realized magnetic structure is different from the calculated one [4]. The magnetic structure analysis with the combination of irreducible representation analysis and Rietveld analysis is in progress.

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