

Powder Neutron Diffraction Measurements of BaYb_2X_4 ($X = \text{S}, \text{Se}$)

H. Suzuki^A, T. Taniguchi^B, T. Onimaru^A

^A*AdSE, Hiroshima Univ.*, ^B*IMR, Tohoku Univ.*

Magnetically frustrated systems have attracted much attention in condensed matter physics. Magnetic frustration can give rise to a variety of exotic phenomena, including nonmagnetic ground states and magnetically ordered states with reduced magnetic moments. Geometrical frustration is commonly realized in crystal structures such as triangular and pyrochlore lattices.

A typical one-dimensional frustrated lattice is the zigzag chain. The $S = 1/2$ Heisenberg zigzag spin chain exhibits a nonmagnetic ground state due to strong quantum fluctuations [1]. In recent years, magnetic semiconductors and insulators containing Yb^{3+} ions with a $4f^{13}$ configuration have attracted considerable attention as frustrated magnetic systems, because the crystalline electric field often stabilizes an effective spin-1/2 ground state.

In this study, we focus on BaYb_2X_4 ($X = \text{S}$ and Se) [2]. These compounds contain two inequivalent Yb sites, each forming a zigzag chain. BaYb_2S_4 and BaYb_2Se_4 undergo magnetic phase transitions at 0.91 K and 1.15 K, respectively. The magnetic entropy at these transition temperatures is only about 20% of $R\ln 2$, indicating strong magnetic frustration in these compounds. To clarify their magnetic ground states, we carried out powder neutron diffraction measurements to determine their magnetic structures.

The samples were synthesized by the conventional solid-state reaction method. Powder neutron diffraction measurements were performed using the T1-3 HERMES diffractometer installed at JRR-3. Approximately 3 g of powder sample was used for each measurement. The incident neutron wavelength was $2.1974(2)$ Å. Diffraction patterns were collected at 0.7 K and 10 K using a 1 K refrigerator.

Figures (a) and (b) show the powder neutron diffraction patterns of BaYb_2X_4 measured at 0.7

K and 10 K. Because only one weak peak was observed at 8.7 deg., the magnetic propagation vector and magnetic structure could not be determined. This weak peak suggests that the ordered magnetic moment is strongly reduced because of magnetic frustration. Otherwise, this peak may originate from a magnetic impurity phase. To confirm whether it is an intrinsic reflection for BaYb_2X_4 , further neutron diffraction measurements should be carried out at lower temperatures using higher-purity samples with fewer magnetic impurities.

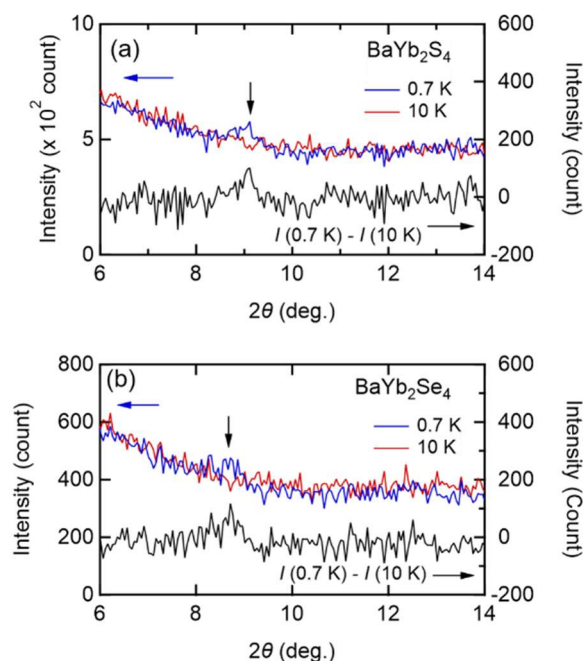


Fig. Powder neutron diffraction patterns of BaYb_2X_4 with (a) $X = \text{S}$ and (b) $X = \text{Se}$. The black solid lines show the difference between the patterns measured at 0.7 K and 10 K.

[1] K. Okunishi and T. Tonegawa, J. Phys. Soc. Jpn. **72**, 479 (2003).

[2] Y. Misawa *et al.*, J. Ceram. Soc. Jpn. **117**, 85 (2009).