Neutron diffraction study on hyperkagome antiferromagnets

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A hyperkagome lattice is a 3D corner-sharing triangular network. When magnetic ions with antiferromagnetic interactions form such a triangle-based lattice, the system cannot attain a stable magnetic state due to the competition of the interactions. Such a state is called geometrical frustration, which leads to unusual magnetic ordering and thermodynamic phases. Recently, we have topochemically synthesized new hyperkagome antiferromagnets $Zn_2Mn_3O_8$ and $Co_3V_2O_8$. The heat capacity C_p of $Zn_2Mn_3O_8$ has a sharp peak at $T_N = 5.6$ K, and the magnetic susceptibility χ decreased slightly at the same temperature [1]. The Curie-Weiss temperature fit of the inverse χ provides $\Theta_{CW} = -56$ K. The Θ_{CW} for $Co_3V_2O_8$ was –2.3 K, and relatively smaller than that for $Zn_2Mn_3O_8$. Nevertheless, $Co_3V_2O_8$ showed apparent evidence for the antiferromagnetic transition at $T_N = 2.6$ K, besides another small anomaly around 5 K. The interesting point of these compounds is the temperature dependence of the heat capacity in the antiferromagnetic phase. While the heat capacity of general antiferromagnets with a 3D structure is proportional to the cube of temperature, $Zn_2Mn_3O_8$ and $Co_3V_2O_8$ has the temperature dependence of $\sim T^2$, which suggests the realization of a 2D magnon-like dispersion in the 3D hyperkagome lattice.

In this study, we have performed the neutron powder diffraction (NPD) experiments on $Zn_2Mn_3O_8$ and $Co_3V_2O_8$ to elucidate the magnetic change caused by the phase transition given above. The NPD measurements were conducted the diffractometer HERMES installed in the guide hall at JRR-3. The powder sample was mounted on the cold head of the 4K GM refrigerator for $Zn_2Mn_3O_8$ and of the ^{3}He refrigerator for $Co_3V_2O_8$.

Figure 1 shows the temperature dependence of the NPD pattern of $Zn_2Mn_3O_8$. The NPD pattern at 15 K represents only the nuclear Bragg peak, corresponding to the paramagnetic phase. Below the antiferromagnetic transition temperature of 5.6 K, other peaks were observed to develop at a different position from the nuclear Bragg peak, and the first magnetic ordering was observed in hyperkagome antiferromagnets. The analysis of this pattern revealed that it has a magnetic wavenumber vector k = (1/4, 1/4, 1/4) and a magnetic space group R_I32. This four-fold periodic magnetic structure is interesting because it is different from the magnetic structure expected from previous theoretical studies. The measurements of $Co_3V_2O_8$ also showed that the ground state has the same magnetic wave vector and magnetic space group as $Zn_2Mn_3O_8$. This result suggests that this magnetically ordered structure may be common in hyperkagome antiferromagnets.

[1] S. Kitani *et al*., Phys. Rev. Materials **5**, 094411 (2021).

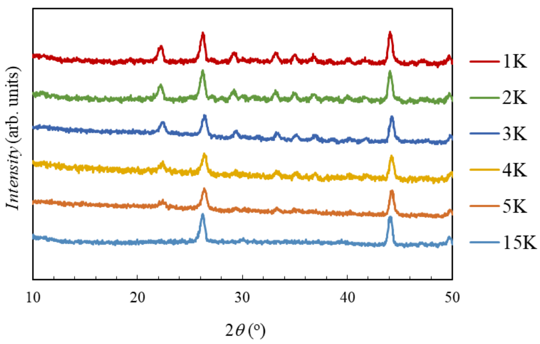

Fig. 1. Temperature dependence of neutron diffraction pattern of $Zn_2Mn_3O_8$.