Determination of the magnetic structure of the spin-1/2 tetramer compound CuInVO5

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Two types of magnetic excitations exist in a magnetically ordered state. They are transverse-mode (T-mode) and longitudinal-mode (L-mode) excitations corresponding to fluctuations in directions perpendicular and parallel to ordered moments, respectively. The T-mode excitations are well known as spin wave excitations, whereas there are a few experimental observations on the L-mode excitations because of their weak intensity. According to the results of theoretical investigations, the L-mode excitations may be observed in an antiferromagnetically ordered state appearing on cooling in interacting antiferromagnetic (AF) spin-cluster compounds [1]. The shrinkage of ordered magnetic moments by quantum fluctuation is important for the appearance of the L mode. If the ground state (GS) of the isolated spin cluster is a spin-singlet state, the shrinkage of ordered moments can be expected in an ordered state generated by the introduction of intercluster interactions.

We focus on spin-1/2 tetramers [2]. The Hamiltonian of the spin tetramer is expressed as H = J1S2S3+J2(S1S2+S3S4). When J1 $>$ 0 and J2 $<$ 0, the GS is a spin-singlet state and an energy difference between GS and first-excited states (spin gap) is much smaller than J1 and |J2|. An ordered state with small ordered moments may be generated by weak intertetramer interactions in spin-1/2 tetramer compounds with J1 $>$ 0 and J2 $<$ 0.

We determined that the spin system of Cu2+ ions in CuInVO5 [3] was interacting spin-1/2 tetramers with J1 = 240 and J2 = -142 K [4]. We confirmed an AF transition at TN = 2.7 K in the specific heat and magnetic susceptibility. We will make single crystals of CuInVO5 and perform Raman scattering measurements to investigate the L-mode magnetic excitations. We will compare experimental results with calculated ones. We need the magnetic structure of CuInVO5 to calculate intensities of one-magnon Raman scattering in the interacting spin-1/2 tetramer model corresponding to CuInVO5.

In the previous measurements on CuInVO5 powder using the Echidna diffractometer (MI5686), we could determine the atomic positions at 5.0 K. However, we could not detect magnetic reflections. We succeeded in the determination of the magnetic structure of CrVMoO7 using the high-intensity powder diffractometer Wombat (P5174) [5]. Therefore, we measured neutron diffraction patterns of CuInVO5 powder using the Wombat diffractometer.

Figure 1 shows diffraction patterns at 1.8 and 5.1 K. The wavelength of neutrons is 0.431 nm. The two patterns overlap almost each other. We madethe difference pattern by subtracting the diffraction pattern at 5.1 K from that at 1.8 K. We could not obtain magnetic reflections, indicating that ordered magnetic moments were small as inferred. The signal to noise ratio is better in the TAIPAN triple-axis spectrometer. We submitted a proposal to determine the magnetic structure of CuInVO5 using the TAIPAN spectrometer (P6336).