Magnetic structures of 1D frustrated chain compound NaCuMoO4(OH)

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In S = 1/2 one-dimensional frustrated chain with nearest-neighbor ferromagnetic interaction J1 and next-nearest-neighbor antiferromagnetic interaction J2, the ground state exhibits various quantum phases depending on the ratio between J1 and J2 [1]. Theoretical study predicted that applying magnetic field induces unconventional magnetic state, the spin multipole order, in the vicinity of the saturation field [2]. On the other hand, such a state has not been well identified in experimental researches because of too high saturation field and/or difficulty of obtaining a large crystal for the existing model compounds.

Recently a new model compound NaCuMoO4(OH) was reported [3]. Crystal structure is shown in Fig. 1(a) [4]. Cu2+ ions carrying S = 1/2 form one-dimensional chain through O2- ions along the crystallographic b direction. The magnetic transition temperature of 0.6 K, the saturation field of 26 T, and the synthesis of a large single crystal were reported [3]. Thus this compound is a good candidate for studying the quantum phases in the magnetic field. The ratio between J1 and J2 is estimated to be J1/J2 = -1.4 from the analysis of the magnetic susceptibility, which suggests helical magnetic order at low temperature in low magnetic field. We performed neutron diffraction experiment in order to investigate the ground state of NaCuMoO4(OH) experimentally.

Neutron diffraction experiment was performed on thermal neutron triple-axis spectrometer TAIPAN. We used dilution cryostat for measurement at low temperature. We used 1 g of deuterated polycrystalline sample synthesized by hydrothermal method. We chose the incident neutron energy of 14.87 meV.

Figure 1(b) shows a neutron diffraction profile at T = 1.2 K. We performed Rietveld refinement for the nuclear reflections and determined the positions of hydrogen atoms, which has not been investigated. We found that hydrogen atoms are located at 4c(0.243(4), 0.25, 0.030(4)). The positons of hydrogen atoms are shown in Fig. 1(a). It indicates that the hydrogen atom is bound to the one of the oxygen atom in the CuO2 chain. We observed no magnetic peaks below the transition temperature. Thus we couldn't determine the magnetic structure in this experiment.

References

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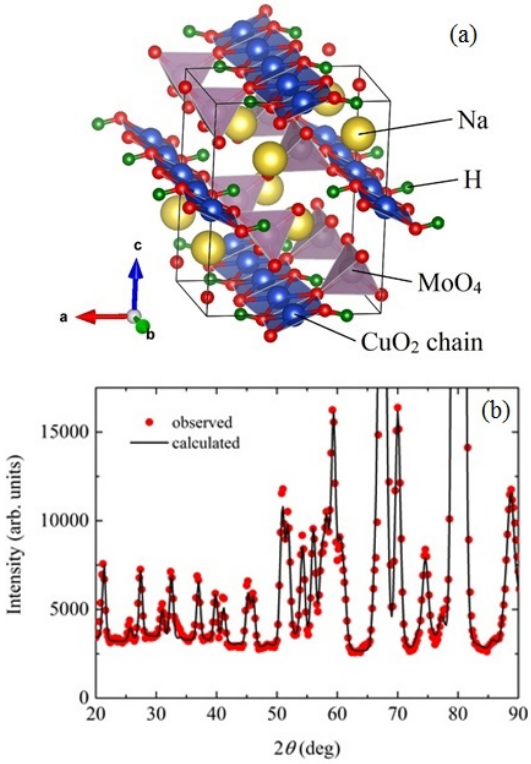

Fig. 1. (a) Crystal structure of NaCuMoO4(OH). The position of hydrogen was determined by this study. (b) Neutron diffraction profile of NaCuMoO4(OH) at T = 1.2 K.