Determination of the spin system in $Ni_2V_2O_7$ using neutron diffraction in magnetic fields

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Neutron diffraction has made great contribution to studies of magnetism because magnetic structures can be determined. We can also study magnetism in paramagnetic states by combing neutron diffraction and magnetic fields. Magnetic moments are induced by magnetic fields and generate magnetic reflections. In a magnet with plural crystallographical magnetic-ion sites, we can evaluate a field-induced magnetic moment (magnetization) on each site from analyses of the magnetic reflections.

Our objective in this study is to show that neutron diffraction in magnetic fields is a powerful tool to determine spin systems. We investigated $Ni_2V_2O_7$ as an example. We briefly summarize the magnetism of $Ni_2V_2O_7$ [1]. Magnetic phase transitions occur at $T_{N1} = 6.7$ and $T_{N1} = 5.7$ K. The magnetic structures have not been determined. A 1/2 quantum magnetization plateau was observed between 8 and 30 T at 2 K. There are two crystallographical Ni^{2+}-ion sites having spin-1. There are three types of short Ni-Ni pairs having antiferromagnetic exchange interactions. A few sets of the values were reported and were inconsistent with one another [1,2].

In order to determine the spin system (the values of the exchange interactions) in $Ni_2V_2O_7$, we performed neutron diffraction experiments on $Ni_2V_2O_7$ pellets using the WOMBAT diffractometer and the AVM-1 magnet. We can see several magnetic reflections in a difference pattern made by subtracting a neutron powder diffraction pattern at 10 K in 0 T from that at 1.8 K in 0 T. We infer an incommensurate magnetic structure from the positions of the magnetic reflections.

Figure 1 shows a difference pattern made by subtracting a neutron powder diffraction pattern at 20 K in 10 T from that at 1.8 K in 10 T. As described, the 1/2 quantum magnetization plateau appears above 8 T at low temperature. Therefore, the state at 1.8 K in 10 T is a kind of paramagnetic state (without magnetic long-range order). We can see several magnetic reflections generated by field-induced magnetic moments. The red circles indicate intensities of magnetic reflections calculated in the case that M2/M1 = 5. Here, M1 and M2 are the magnitude of field-induced magnetic moments on Ni1 and Ni2 sites, respectively. The calculated intensities seem consistent with the experimental ones. Several reflections indicated by triangles, however, cannot be explained by the field-induced magnetic moments. The magnetic reflections at 1.8 K in 0 T seem to remain, suggesting the coexistence of the two phases.

We measured difference patterns at 1.8 K in several magnetic fields. As the magnetic field increases, the intensities of the magnetic reflections at 1.8 K in 0 T and those generated by field-induced magnetic moments decrease and increase, respectively. We can see magnetic reflections that are different from those in 0 and 10 T at 1.8 K. Probably, the indices of the magnetic reflections are integers. The intensity of the magnetic reflections increases with increasing magnetic field and is strongest around 6 to 8 T, suggesting another magnetic long-range order in finite magnetic fields below the magnetization-plateau fields. The magnetic reflections disappear in 10 T.

We will determine the magnetic structures in zero and finite magnetic fields and evaluate M1 and M2 at 1.8 K in 10 T. We will be able to determine the spin system (the values of the exchange interactions).

[1] Z. W. Ouyang et al., Phys. Rev. B. 97, 144406 (2018).

[2] Y. C. Sun et al., Eur. Phys. J. Plus 131, 343 (2016).

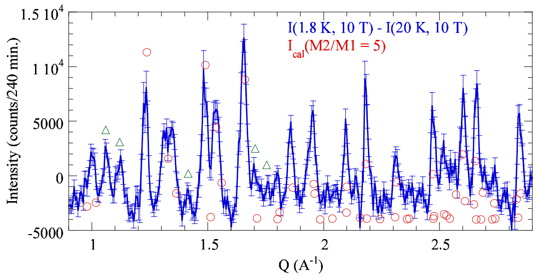

Fig. 1. A difference pattern made by subtracting a neutron powder diffraction pattern at 20 K in 10 T from that at 1.8 K in 10 T.