Neutron scattering study on the molecular magnet Mn6Sb2

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Mn_6Sb_2 is a molecular magnet. Mn^{2+} ions with $s = 5/2$ are forming a approximately eqational hexagon and coupled by ferromagnetic exchange interaction between nearest neighbor ions, and the ground state is $S = 15$.

We performed inelastic neutron scattering experiments and succeeded to observe the magnetic excitations. There were two inelastic peak at 0.26 and 0.54 meV in the inelastic neutron scattering spectrum at 1.5 K. They are confirmed to be magnetic excitations from their temperature dependences and Q dependences. On the other hand, magnetic susceptility result expects that the first excitation mode from $S = 15$ to 14 exists at 0.52 meV. We measure the Q-scans at the peak energies 0, 0.26 and 0.54 meV, and at two temperatures 1.5 and 6.0 K. Fig. 1 shows the temperature subtractions of the obtained Q-scans. The Q dependence of 0.26 meV is different from that of 0.54 meV. Thus, the inner-cluster Heisenberg Hamiltonian cannot explain the peak at 0.26 meV. At the elastic position, diffuse scattering was observed shown in Fig. 1, and its shape is good agreement with the Q dependence of 0.26 meV. This fact suggests that a short-range correlation is developed at low temperature and have the excitation mode at 0.26 meV.

The peak of diffuse scattering is at $Q = 0.2$ A^{-1}, corresponding to $2\pi/0.2 \sim 30$ A in real space which is comparable with the distance between Mn_6Sb_2 clusters. We suppose that there are antiferromagnetic interaction between cluster spins ($S = 15$), resulting in the diffuse scattering. The origin of the inter-cluster interactions may be the dipole and/or exchange interactions. D, the constance of a dipole interaction is $(g\mu_B)^2/R^3 = 0.028$ μeV, and thus the dipole interaction cannot account for the peak at 0.26 meV. Hence we add the innter-cluster exchange interaction between Mn_6Sb_2 cluster with $S = 15$ as a perturbation to inner-cluster Heisenberg model. Taking account of the layered triangular structure of the Mn_6Sb_2 system, we found that antiferromagnetic short-range-spin correlations on the triangular lattice reproduce the observed diffuse scattering pattern. The Q dependence of the 0.26 meV peak is also reproduced as the elementary excitation in the short-range ordered cluster spins. Thus the inter-cluster interaction can explain not only the diffuse scattering but also the peak at 0.26 meV.

Ferromagnetic inter-cluster interactions have been know in the magnetic molecules, such as in Mn_{12} where inter-cluster interactions give rise to the long-range magnetic order. However, the antiferromagnetic interactions were quite rare; Mn_6Sb_2 is the first system in which antiferromagnetic interactions are confirmed by the neutron spectroscopy. The inter-cluster interaction is the second-dominant term which does not perturb the inner-cluster ferromagnetic coupling (i.e., $S = 15$ is the ground state even with the inter-cluster coupling). Since the cluster spin forms 2D triangular net, the intrinsic geometrical frustration may prohibits the long-range order in the Mn_6Sb_2 system.

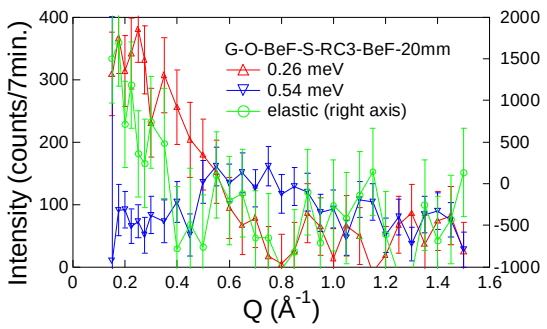

Fig. 1. The subtractions of Q dependency at 6.0 K from that at 1.5 K of 0.26, 0.54 and 0 meV