Neutron scattering in O_2 adsorbent magnet

Takatsugu Masuda
International Graduate Schools of Arts and Sciences, Yokohama City University, 22-2 Seto, Kanazawa-ku, Yokohama, 236-0027

Oxygen molecule is a simple magnetic element that carries $S = 1$ spin. While metal ions are constituents of various types of magnetic compounds, O_2 based magnets has been restricted to monolayer O_2 molecule adsorbed on the surface of several materials such as Aluminum or graphite [1, 2]. The adsorbed O_2 forms spin framework that reflects the surface structure of mother compound. For example $S = 1$ trangular lattice is realized in the O_2 adsorbed graphite. However the small amount of the adsorbed spins makes the magnetic property measurement difficult. Hence the metal based compound has been major substances for the study of magnetism.

Recently the adsorption of O_2 molecule in the nanochannel of some microporous compounds were reported [3]. In contrast with the surface adsorption, the oxygen molecules are intercalated deep inside the host compound and the adsorption is realized in the bulk crystal. Hence the O_2 based magnet with the bulk size is experimentally realized. In this pioneering work we observed the magnetic excitation of O_2 $S = 1$ spins in the O_2 adsorbed microporous compound $[Cu(II)_2(bza)_4(pyz)]_n$ (bza and pyz are benzoate and pyrazine, respectively) by neutron scattering technique.

Crystal structure analysis by x-ray diffraction showed that the adsorbed O_2 molecule forms isolated trimer [3]. Preliminary magnetic susceptibility measurements is consistent with the spin trimer model with $J \sim 2.0$ meV [4]. If this is the case a narrow band excitation would be observed at $\hbar\omega \sim 2.0$, 4.0, and 6.0 meV with the intensity modulation in inelastic neutron scattering (INS). [5]. Hence we performed initial experiment at PONTA spectrometor installed at 5G beamline. However, we observed no intrinsic signal in the energy transfer range between 1 meV and 20 meV. This means that preliminary model is inconsistent with experiment. Then we performed the second experiment at HER spectrometer at C11 in guide hall. We repeat the measurements for both O_2 adsorbed and not adsorbed samples in the same experimental configuration.

Figure 1 shows a typical constant q scan. Well defined sharp peak was observed at $\hbar\omega = 0.40$ meV. We confirmed the disappearance of the peak in not adsorbed sample. The peak position was independent of q. The intensity decrease with the increase of q gradually and monotonically. The $\hbar\omega = 0.4$ meV mode is the only excitation that we observed in the energy range of 0.15 meV $< \hbar\omega <$ 20 meV. Furthermore we did not observe any sign for the intensity modulation.

The results mean that the observed peak is due to magnetic excitation from O_2 spins of $S = 1$. The q independence means that the spin system is isolated. The absence of the intensity modulation means that the interaction between O_2 spins is too weak to be detected in INS. The only possible explanation for the excitation is that a single ion anisotropy of an O_2 spin of $S = 1$.

In summary we succeeded in the observation of the magnetic excitation in O_2 adsorbent magnet.

References

[1] L. N. Mulay and L. K. Keys, J. Am. Chem. Soc. **8**6, 4489 (1964).
[2] Y. Murakami and H. Suematsu, Phys. Rev. B **5**4, 4146 (1996).
[3] S. Takamizawa, E. Nakata, T. Saito, T. Akatsuka, and K. Kojima, CrystEngComm, **6**, 197 (2004).
[4] S. Takamizawa, E. Nakata, and T. Akatsuka, Angew. Chem. Int. Ed. **4**5, 2216

(2006).
[5] U. Falk *et al.*, Phys. Rev. B **35**, 4893 (1987).

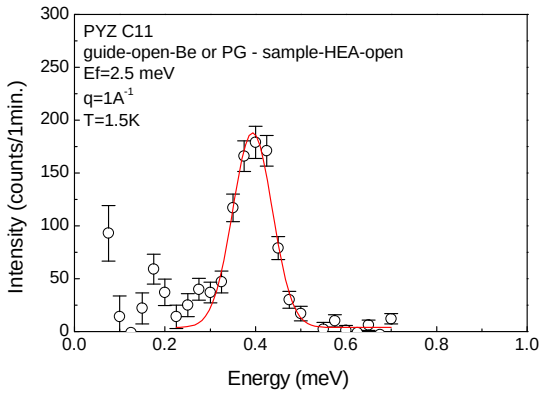

Fig. 1. Constant q scan in the O_2 adsorbed $[Cu(II)_2(bza)_4(pyz)]_n$.