Polarized neutron scattering experiment on oxygen molecules adsorbed in deuterated CPL-1

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In some types of nanoporous metal complex, gas molecules can be adsorbed in its porous and a possibility of supercrystal was suggested. One of the most famous examples is a CPL-1 [1]. The O_2 molecules form ladder like structure in the porous, and $S = 1$ dimer system is expected. The dispersionless magnetic excitation was observed at 7.8 meV in inelastic neutron scattering experiments [2]. The neutron cross section was exlplained by singlet-triplet excitation of S = 1 dimer. This result indicates that a prototype of O2 supercrystal is realized in the porous compound. On the other hand, the intensity of the magnetic excitation decreases with decreasing temperature more drastically than expected from the dimer model. We expect that the observed excitation is not purely magnetic but is hybridized with the lattice vibration called phonon. In order to investigate such a hybridization, we did the inelastic neutron scattering at 5G spectrometer by using polarized neutron beam.

1.2 g of deuterated CPL-1 powder sample was used for the experiment. Specialized apparatus described in Ref. 2 was used for the induction of O2 gas. Temperature control down to 3 K was achieved by orange cryostat. We used half polarization setup to detect the interference of nuclear and spin; supermirror polarizer and PG analyzer were used. The polarization of the neutron spin was along the z-axis, perpendicular to the scattering plane. We measured the difference between the setups with the incident neutron spin up and down, which gives the interference of nuclear and spin scattering.

Figure 1 shows the constant-Q scans at $Q = 1$ Å^{-1} and $T = 3$ K. The magnetic excitation was observed at 8 meV, which is consistent with the previous study [2]. No difference was found between the measurements at the spin flipper for incident neutron on and off. We also measured the constant-Q scans at $Q = 1.5$ Å^{-1} for $T = 3$ K. Furthermore, the constant-Q scans at same Q point were carried out at 60 K. At 60 K, the intensity of the magnetic excitation decreases to one-fourth of that at 3 K. It is consistent with our previous results [3]. The signals in these scans do not depend on the spin state of the incident neutrons. These experiment results suggests that nuclear-magnetic interference term, which should be observed in this experimental setup, does not exist in this magnetic excitation. Another experiment with different polarization setup is needed for investigating the further details of this excitation.

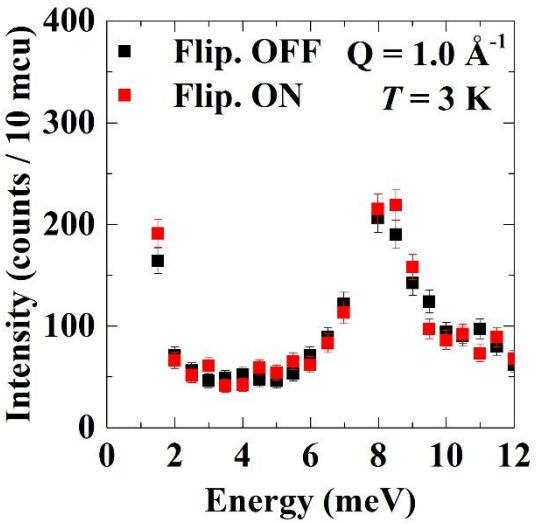

Fig. 1 constant-Q scans for O_2-adsorbed CPL-1 at $Q = 1$ Å^{-1} and $T = 3$ K.

[1] R. Kitaura *et al*., Science **298**, 2358 (2002).
[2] T. Masuda *et al*., J. Phys. Soc. Jpn. **77**, 083703 (2008).
[3]. S. Asai *et al*., JPS 74th annual meeting, 16pF304-3.