The Ordering Structure of Water Molecules in The Superconductor NaxCoO2.yD2O and The Magnetic Excitation in Na0.5CoO2

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Na0.3CoO2.1.3H2O exhibits the superconducting transition at 4.5 K[1]. Because strong magnetic fluctuation expected for correlated electrons on the 2-dimensional triangular lattice may play an important role in realizing superconductivity, the hydrated Co oxide, which may have such electrons have attracted much interest. We are also intersted in roles of the water intercalation in realizing the superconductivity of this system.
In the present work, two kind of neutron scattering studies have been carried out on aligned single crystals of Na0.5CoO2 and NaxCoO2.yD2O. First, we have investigated the intensity of magnetic excitation in Na0.5CoO2 which exhibits the magnetic transition at 87 K to compare to that in superconductor. Second, we have investigated the D2O ordering pattern in NaxCoO2.yD2O. This crystal contains superconducting phase (bilayer system, y˜1.3) and non-superconducting phase (non-deuterated system). The volume fractions of these systems were estimated to be 80% and 20%..
Neutron measurements were carried out using the spectrometer 5G with the triple-axis condition installed at JRR-3 in Tokai. The aligned crystals of Na0.5CoO2 were used with the [100] and [001] axes in the scattering plane. The crystal of NaxCoO2.yD2O was used with the [100] and [001] axes and [110] and [001] axes in the scattering plane.
In Na0.5CoO2, we carried out inelastic scattering along (h, 0, 3) and (1/2, 0, l) at 90 K for some transfer energies (E) between 2.5 and 15 meV. As the result, we observed peaks at Q = (1/2, 0, 3) which is the magnetic Bragg position. The E-dependence of spectral weight kai ”(Q, E) shows that these peaks are due to the magnetic fluctuation. In the neutron inelastic scattering on aligned crystals of NaxCoO2.yD2O with half of the molar number of Na0.5CoO2, no evidence has been found in the search for the ferromagnetic fluctuations in the superconducting phase [2]. These results indicate that magnetic fluctuations in NaxCoO2.yD2O are rather weak, if they exist. It can be said especially for ferromagnetic fluctuations and is consistent with the results of the NMR Knight shift reported by the present authors ’group[3, 4].
In NaxCoO2.yD2O, in the elastic scans along (1/2, 0, l), (3/2, 0, l) and (1/2, 1/2, l) at room temperature, we have observed a significant diffuse scattering contribution, which has an intensity modulation with a periodicity of c* of the bilayer system. The ordering is short-ranged along the c direction, while the in-plane correlation of D2O or the correlation length within a layer is almost infinite (at least more than 300 A), judging from the widths of the 1/21/20 reflection in the scan along (h, h, 0). Analyzing these data, we can find that scatterings originate from the intercalated D2O molecules. The ordering pattern is basically similar to the model proposed by Argyriou et al.[5]. Recently, it is shown that the transition temperature (Tc) changes with time for about 1000 hours after sample preparation by Barnes et al.[6]. We think that it is important to study the relationship between details of the D2O ordering pattern and Tc to clarify possible roles of the water intercalation in realizing the superconductivity of this system.

Reference

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