Neutron Diffraction Study on La$_{2-x}$Ca$_x$CoO$_4$

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Perovskite Co oxide, La$_{1-x}$AxCoO$_3$ (A=Ca, Sr, Ba), has attracted considerable interest because of their fascinating physical properties. F. Fauth et al. reported the diffraction and transport properties of La$_{0.5}$Ba$_{0.5}$CoO$_3$ [1]. From the neutron and synchrotron diffraction powder studies, they have observed the Jahn-Teller (JT) distortion of the CoO$_6$ octahedra below $T_c$. The JT-effect is favored for the intermediate spin state (IS) configuration, ($t_2g$)$_5$($eg$)$_1$. Thus, they concluded that ferromagnetic transition and IS state are strongly correlated each other in La$_{0.5}$Ba$_{0.5}$CoO$_3$.

Recently, we reported neutron diffraction experiments of La$_{1.5}$Ca$_{0.5}$CoO$_4$ and CE-type spin and charge configurations are probably realized. In the CE-type spin configuration, double-exchange interaction between Co$^{2+}$ (HS) and Co$^{3+}$ (IS) is realized and it is expected that JT-distortion is formed below $T_N$. In order to clarify the JT effects in a half-doped material, we performed neutron powder diffraction experiments using the diffractometer, HERMES, installed on T1-3 port of JRR-3M reactor. La$_{1.5}$Co$_{0.5}$O$_4$ has two-magnetic domains, so we use a single magnetic domain of La$_{1.85}$Ca$_{0.15}$CoO$_{4.17}$ which is an almost half doped material.

The structure analysis for La$_{1.85}$Ca$_{0.15}$CoO$_{4.17}$ at 7, 50 and 100K concluded that its space group is P4/mmm which corresponds to the isotropic oxygen displacement model ($\theta$ 2atet $\theta$ 2atet $\theta$ c). Figure 1 shows the temperature dependence of Co-O apical oxygen distance. In neutron experiments of La$_{1.5}$Sr$_{0.5}$CoO$_4$, it is found that Co$^{2+}$-O distance is longer than Co$^{3+}$-O distance [2]. We assumed that the Co(1)-O(2) and Co(3)-O(5) distances correspond to that of Co$^{2+}$-O and Co$^{3+}$-O, respectively. As can be seen in Fig.1, temperature dependence of the apical oxygen distortion coincides with that of the antiferromagnetic order. This result suggests that magnetic transition and JT-distortion are also strongly related each other in La-Ca system. Magnetic diffuse peaks due to an antiferromagnetic ordering of Co$^{2+}$ are observed at (0.5, 0, 0.5) and (0.5, 0, 2.5). These peaks are indexed in the crystallographic unit cell. This indicates that the magnetic peaks are two-dimensional Bragg diffraction because of the layered crystal structure.

References