



## 2. 実験方法及び結果(つづき) Experimental method and results (continued)

### Results

From the neutron diffraction patterns measured using SuperHRPD, it was confirmed that  $\text{LiMn}_{1/3}\text{Ni}_{1/3}\text{Co}_{1/3}\text{O}_2$ -based materials had a single phase of the layered rock-salt structure (S. G.;  $R-3m$ ). On the other hand, it was demonstrated that some specimens of the  $\text{LiNi}_{0.8}\text{Co}_{0.2}\text{O}_2$  system had an impurity phase of  $\text{Li}_2\text{CO}_3$  although such an extra phase could not be detected by laboratorial X-ray diffractions. The  $\text{Li}_2\text{CO}_3$  amounts seemed to depend on the preparation process, that is, a synthesis method and a heat-treatment condition. Because cycle performances of Li-ion batteries using samples with the extra phase as the cathode were inferior, it can be concluded that the  $\text{Li}_2\text{CO}_3$  had a negative influence on the cathode characteristics.

In order to discuss the crystal structures in more detail, we performed the Rietveld analysis using the diffraction data on some  $\text{LiMn}_{1/3}\text{Co}_{1/3}\text{Ni}_{1/3}\text{O}_2$ -based samples, which were prepared by means of the solution method and then heat-treated under controlled gas conditions. The Rietveld analysis could be performed successfully by assuming the space group as  $R-3m$ . An occupancy of the Ni at the Li site (i.e., an amount of a cation mixing) was below 10 %, regardless of the specimens. In the analyses, a site occupancy of the oxygen was also refined. As a result, it was suggested that the sample heat-treated in air had no oxygen vacancy in the case of  $\text{LiMn}_{1/3}\text{Ni}_{1/3}\text{Co}_{1/3}\text{O}_2$  system.