



Ex-situ monitoring the oxidation state and fine structures of mixed anion cathode materials during charge/discharge process in-operando conditions

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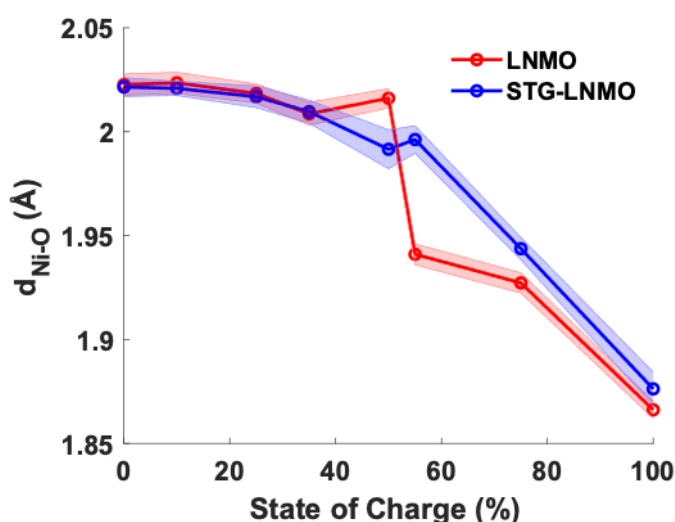
1. 背景と研究目的

Materials for Lithium batteries are an active field of research. The cationic substitution to improve the battery performance is a path to improving battery performance. In this proposal, we measured the Ni and Mn K edges in $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (LNMO) and $\text{LiNi}_{0.5}\text{Mn}_{1.4}\text{Si}_{0.033}\text{Ti}_{0.033}\text{Ge}_{0.033}\text{O}_4$ (STG-LNMO) to understand the influence of cationic substitution in battery performance.

2. 実験内容

The LNMO and STG-LNMO cathodes were prepared at different State of Charge (SoC), the coin cells were opened in glove box, and the cathode material was protected from exposure to air using Kapton tape.

3. 結果および考察



The fitting information obtained from the MnK-edge showed no differences between the LNMO and STG-LNMO samples, while the Ni K-edges provided interesting insights as shown in Fig 1.

The initial and final $d_{\text{Ni-O}}$ obtained for LNMO and STG-LNMO were the same, indicating that the cation substitution does not affect these two states. The differences between LNMO and STG-LNMO in the $d_{\text{Ni-O}}$ were observed around 50% SoC. This change in the $d_{\text{Ni-O}}$ can be attributed to the change in the oxidation state of Ni atoms, which would increase the coulombic interaction between the Ni and the O atoms and shorten the bond distances. In this regard, the cationic substitution would make less abrupt changes in the Ni oxidation state.

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Fig 1 – Distance of the first coordination shell ($d_{\text{Ni-O}}$) obtained from fitting of LNMO and STG-LNMO.

4. 参考文献

1. Narumi et al. "Tailoring charge/discharge reaction mechanisms in ordered spinel $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ cathodes by multi-element doping" Chem. Comm. Submitted.