Evaluation of the oxidation state and environment symmetry of transition metal in function of depth for cathode material with anionic substitution.

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1. 背景と研究目的

Materials for Lithium batteries are an active field of research. The anionic substitution to improve the battery performance is a path to improving battery performance. In this proposal, we measured the O and F K edges and the Ni and Mn $L_{2,3}$ edges in $LiNi_{0.5}Mn_{1.5}O_4$ (LMNO) using different detectors (TEY, TFY and AEY) to understand the influence of fluoirdation conditions in function of the depth.

2. 実験内容

The measurements of F-modified LNMO were prepared in dry-room box and transferred without contact to moisture to the measuring chamber. The O K-edge was measured separated from the rest of the elements. The scan step and time were optimized by a preliminary scan of these two groups of elements.

3. 結果および考察

The spectra of Mn and Ni L-edges exhibited no differences among the samples with fluoridation. However, in the case of the F K-edge, the signal was extremely noisy, rendering it impossible to extract any useful information. Conversely, when examining the O K-edge, significant disparities were observed among the samples. Notably, the pre-edge features (spectral components below 535 eV) were found to be strongly influenced by the fluoridation conditions, a phenomenon linked to the degeneracy of O 2p-Mn 3d states within distorted octahedral symmetries. Feff simulations are currently underway to gain a deeper understanding of the local symmetry within each sample.

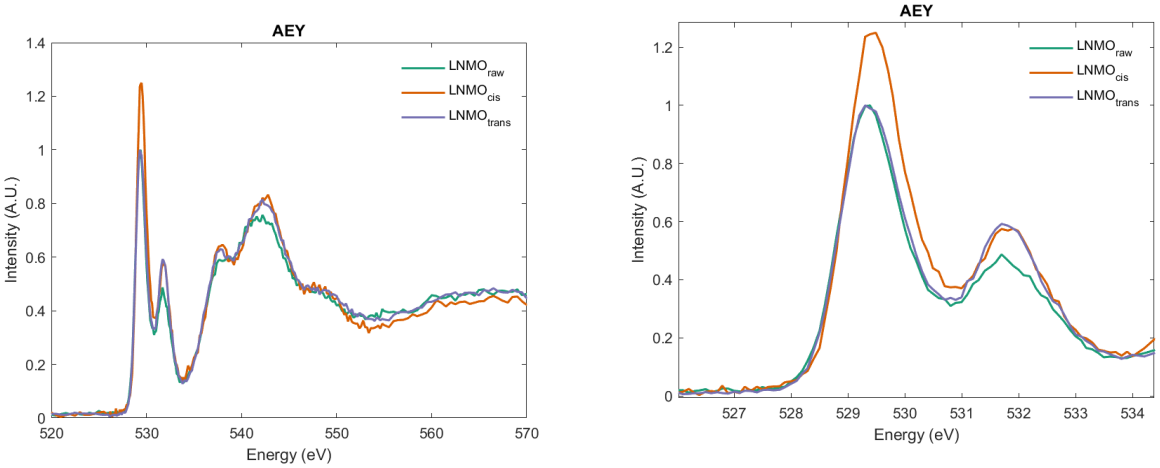

Fig 1 – Left: Oxygen K-edge in bare samples and with different XeF_2 treatments. Right: Idem with zoom on the pre-edge.

4. 参考文献

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