Determination the environment of Ti and Si in $LiNi_{0.5}Mn_{1.5-x-y-z}O_4Ge_xTi_ySi_z$

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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 Ti and Si K edges in $LiNi_{0.5}Mn_{1.5-x-y-z}O_4Ge_xTi_ySi_z$ (LNMO) using CEY and TEYdetection mode to understand the position of Ti and Si in the lattice.

2. 実験内容

The samples for measurements of Ti, Si, Ge-modified LNMO with different compositions were done in dry room and transferred to the measuring chamber. The measurements were performed in normal XAS mode using CEY and TEY detection.

3. 結果および考察

The experimental measurements for both the Ti and Si K-edges revealed notably consistent spectra across all compositions of $LiNi_{0.5}Mn_{1.5-x-y-z}O_4Ge_xTi_ySi_z$. When closely examining the Ti edge, the XANES region did not display any significant variances, suggesting a uniform electronic environment for the titanium component. Conversely, the Si K-edge manifested some discernible features, which underscore differences in its surrounding environment. The observable alteration in the white line intensity for the Si K-edge can be interpreted as a shift in the local structural order. This shift might be attributed to the dampening effect on the Debye-Waller factor.

In the realm of k-space, both Ti and Si K-edges displayed an astonishing uniformity, revealing no major differences in their respective structural domains. To shed more light on the peculiarities detected in the Si XANES spectra, it is advisable to undertake additional computational analyses. These analyses might provide deeper insights into the origin and implications of these observed disparities.

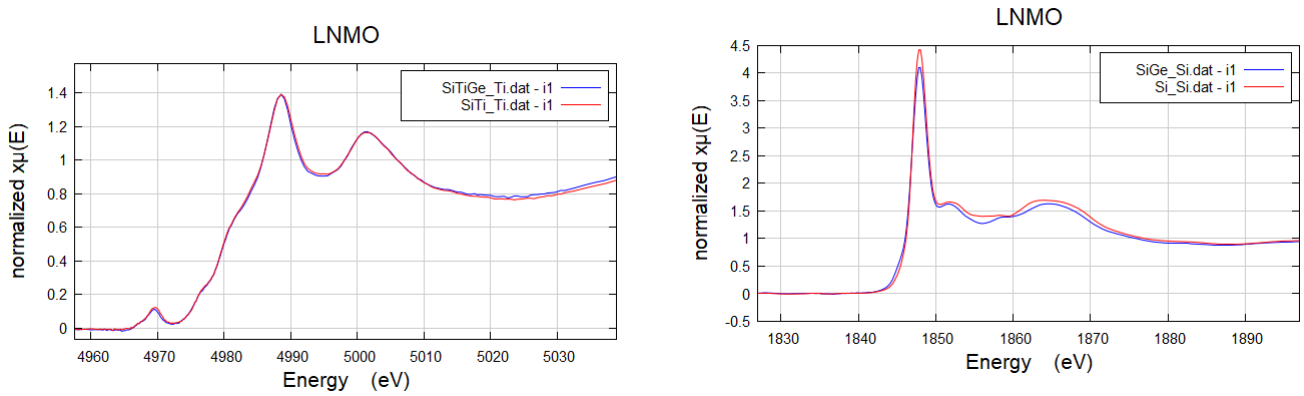

Fig 1 – Left) XANES spectra of Ti K-edge, right) XANES spectra of Si K-edge.

4. 参考文献

1. Ghigna et al., ACS Appl. Mater. Interfaces 2020, 12, 45, 50344–50354.