Determination the local environment of Hf and Ta in $Li_{6.25}La_3(Zr, Hf, Sn, Ce, Nb, Sb, Ta)_2O_{12}$

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1. 背景と研究目的

Solid-state batteries (SSBs) with high energy density and excellent safety are expected to be the next-generation energy storage devices to replace traditional lithium-ion batteries (LIBs). In this proposal, we measured the local environment of Hf and Ta materials in $Li_{6.25}La_3(Zr, Hf, Sn, Ce, Nb, Sb, Ta)_2O_{12}$.

2. 実験内容

The measurements were performed at the Ta L_3 edge and Hf L_3 and L_2 edge in transmission mode.

3. 結果および考察

The comparison of the XANES spectra among the samples revealed differences in only one sample (4Hf: $Li_{6.25}La_3Hf_{1.25}Nb_{0.25}Sb_{0.25}Ta_{0.25}O_{12}$); the remaining samples did not show considerable differences.

In terms of k-space, the observed differences were more pronounced. The sample that exhibited a variation in the XANES spectra displayed a distinct feature at k~7 $Å^{-1}$. A similar feature was also observed in a second sample (6-ZSC: $Li_{6.25}La_3Zr_{0.75}Sn_{0.25}Ce_{0.25}Nb_{0.25}Sb_{0.25}Ta_{0.25}O_{12}$).

However, in the case of Hf L_3 and L_2 edges, no differences were observed in either the XANES or EXAFS region. Further in-depth studies will be conducted at the Ta edge to determine the structural origin of the observed feature.

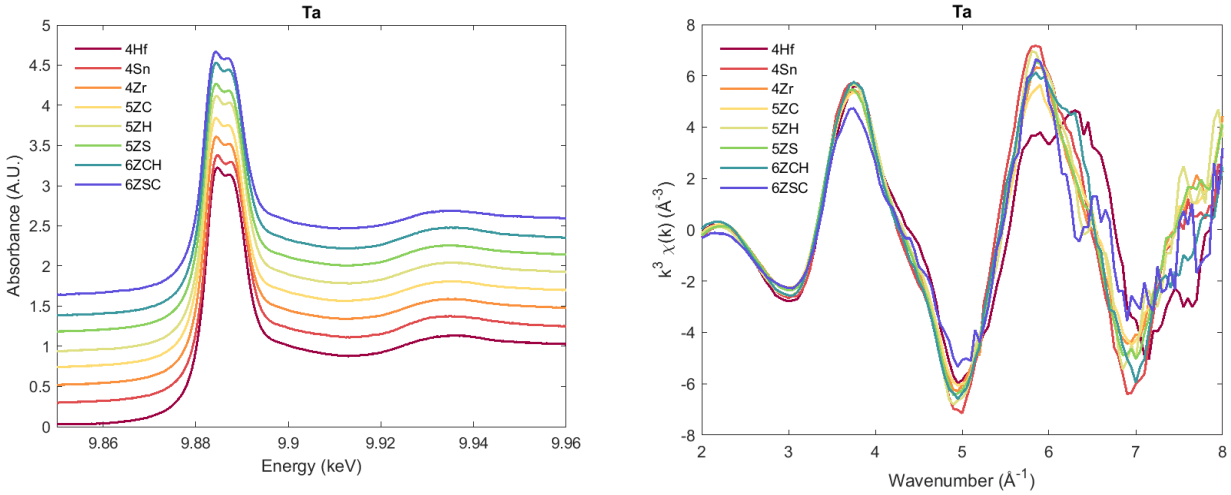

Fig 1 – Left) XANES spectra of Ta L_3 edge Right) k-space of Ta L_3 edge samples.

4. 参考文献

1. Jung, SK., Gwon, H., Kim, H. et al. “Unlocking the hidden chemical space in cubic-phase garnet solid electrolyte for efficient quasi-all-solid-state lithium batteries.” Nat Commun 13, 7638 (2022)