



Determination of substituting elements environment in LLZO garnet structure by Anomalous X-Ray scattering (AXS).

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1. 背景と研究目的

Materials for solid electrolyte in batteries are an active field of research. Since the first study around 2007, $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) attracted much scientific attention as a solid electrolyte for 'Beyond Li-Ion Battery' concepts such as Li-air and Li-S batteries. The implementation of LLZO as solid-state electrolyte requires the stabilization of cubic phase with higher Li-ion conductivity with respect to tetragonal phase.

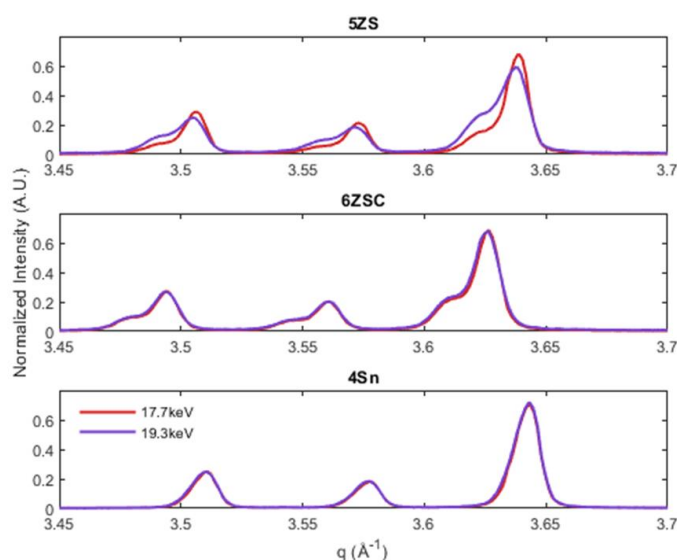
The strategy to stabilize the cubic phase is mainly based in cationic substitution. In our case we introduced Zr, Ce, Hf, Sn, Nb, Sb, and Ta. AXS is a powerful tool to determine the of each cation in the lattice.

2. 実験内容

8 samples with composition $\text{Li}_7(\text{La Ce, Hf, Sn, Nb, Sb, Ta})_3\text{Zr}_2\text{O}_{12}$ were measured close to the Zr (17778eV) and Nb (19296eV) edge in transmission mode using 0.3 mm capillary.

3. 結果および考察

All the samples showed the LLZO reported structure as previously confirmed using conventional XRD in the lab. The samples with Sn in the composition (see composition details *ut infra*) showed significant differences in the



peak shape as observed in Fig 1.

The sample 4Sn showed a diffraction pattern in agreement with a cubic structure, while the 5ZS and 6ZSC showed a symmetry brake which can be attributed to a tetragonal distortion.

The most significant results are observed in sample 5ZS, which showed, at difference from 6ZSC, instead of showing a symmetric decrease of the peaks intensity, it shows an asymmetric change in peak intensity. AXS on the other edges are being planned to understand this behaviour.

Fig 1 Diffraction patterns of LLZO, **5ZS**: $\text{Li}_{6.25}\text{La}_3\text{Zr}_{1.00}\text{Sn}_{0.25}\text{Nb}_{0.25}\text{Sb}_{0.25}\text{Ta}_{0.25}\text{O}_{12}$, **6ZSC**: $\text{Li}_{6.25}\text{La}_3\text{Zr}_{0.75}\text{Sn}_{0.25}\text{Ce}_{0.25}\text{Nb}_{0.25}\text{Sb}_{0.25}\text{Ta}_{0.25}\text{O}_{12}$ and **4Sn**: $\text{Li}_{6.25}\text{La}_3\text{Sn}_{1.25}\text{Nb}_{0.25}\text{Sb}_{0.25}\text{Ta}_{0.25}\text{O}_{12}$

4. 参考文献

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