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Operando Investigation of NMC622/Argyrodite based All-Solid-State Battery using Neutron Diffraction

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All-solid-state batteries (ASSBs) are gaining increased attention due to their potential for enhanced safety and higher energy density compared to conventional metal-ion batteries. They are particularly suited for industrial applications like oil wells, where battery operation at high temperatures is necessary¹. A deep understanding of the assembly and electrochemical cycling mechanisms of ASSBs is still needed to assess reactivity and structural evolution of the active materials. The positive electrode material, LiNi0.6Mn0.2Co0.2O2 (NMC622), currently utilized in commercial Li-ion batteries for its balance of high energy density, safety, and durability, is being considered for ASSBs². Additionally, mixed-halide argyrodite solid electrolytes are recognized for their high ionic conductivity and softness, despite their relatively high chemical instability and reactivity.

We investigated operando the solid-state battery system comprising of NMC622 and a mixed-halide solid electrolyte $\text{Li}_{6-x}\text{PS}_{5-x}\text{BrCl}_x$ synthesized in-house³ which possesses a RT ionic conductivity of 10^{-2} S.cm⁻¹ thus allowing to build very thick ASSBs. Due to the high penetration power of the neutron beam and its sensitivity to light elements such as Lithium⁴, neutron diffraction (ND) is the method of choice. By combining ex situ and operando ND techniques, we analysed the reactivity at the solid-solid interfaces and thus the stability of each component (NMC622, Argyrodite), and more generally all the mechanisms involved upon electrochemical operation, at room temperature and upon increasing temperature (100°C)⁵.

Operando ND measurement of ASSB

References

- 1. R. R. Kohlmeyer, et al. "Pushing the thermal limits of Li-ion batteries." Nano Energy 64, (2019)
- O. Dolotko, et al. "Understanding structural changes in NMC Li-ion cells by in situ neutron diffraction." J. Power Sources 255, 197-203 (2014)
- 3. J. Auvergniot, C. Masquelier, V. Viallet, D. Shanbhag, World Patent WO2023/247531A1 (2023)M.
- 4. Bianchini, et al., "A new null matrix electrochemical cell for Rietveld refinements of in-situ or operando neutron powder diffraction data." J. Electrochem. Soc. , 160(11), A2176 (2013)
- 5. MG. Boebinger, et al. "Understanding transformations in battery materials using in situ and operando experiments: progress and outlook." ACS Energy Letters, 5, 335-345 (2020)

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