Contribution ID: **34** Type: **not specified**

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

Tuesday, 4 June 2024 18:00 (20 minutes)

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

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 necessary[1]. 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 ASSBs[2]. 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 $Li_{6-x}PS_{5-x}BrCl_x$ synthesized in-house[3] 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 Lithium[4], 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)
2. 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)

Primary author: ANIL KUMAR, Sreelakshmi (ILL Grenoble)

Co-authors: MASQUELIER, Christian (Laboratoire de Réactivité et de Chimie des Solides, Université de Picardie Jules Verne,); CHOTARD, Jean-Noël (Laboratoire de Réactivité et Chimie des Solides); SUARD, Emmanuelle (Institut Laue-Langevin); CROGUENNEC, Laurence (Univ. Bordeaux, CNRS, Bordeaux INP, ICMCB); Dr SHANBHAG, Dhanush (Laboratoire de Réactivité et Chimie des Solides)

Presenter: ANIL KUMAR, Sreelakshmi (ILL Grenoble)