22nd International Conference on
Diffusion in Solids and Liquids
22 TO 26 JUNE 2026 | RHODES, GREECE

ABSTRACT:

Cutting-Edge XRD Approaches for Battery Materials Characterization

The accelerating demand for high-performance rechargeable batteries has driven continuous innovation in materials characterization methods. X-ray diffraction (XRD) plays a pivotal role in understanding the crystallographic and structural evolution of electrode and electrolyte materials, both in- situ and in-operando. This presentation introduces state-of-the-art XRD methodologies developed at Rigaku for the comprehensive characterization of advanced battery systems — from raw material screening to complete cell evaluation.

We highlight the capabilities of Rigaku's SmartLab diffractometer platform, featuring high-flux sources, advanced optics, and detectors with excellent energy resolution, enabling high-sensitivity operando measurements of lithium-ion and all-solid-state batteries. These techniques allow real-time observation of phase transitions, lattice parameter changes, and valence variations during charge–discharge cycles. The integration of reflection and transmission geometries facilitates simultaneous analysis of cathode and anode materials within laminated and coin-cell configurations, while temperature- and pressure-controlled attachments provide insights into thermally driven phase behaviour and ionic transport phenomena.

Beyond conventional diffraction, we discuss total scattering and Pair Distribution Function (PDF) analysis, which extends structural resolution to disordered and amorphous phases-critical for understanding local structure in solid electrolytes such as $Li_7P_3S_{11}$ and argyrodite compounds. The combination of XRD with complementary X-ray fluorescence (XRF), X-ray emission spectroscopy (XES), and computed tomography (XCT) delivers a multi-scale perspective spanning atomic to macroscopic structures. Case studies include phase management in layered NCM cathodes, local structural mapping in sulfide electrolytes, and operando monitoring of structural degradation in full cells.

By integrating high-resolution diffraction, real-time operando analysis, and local structural probes, these cutting-edge XRD approaches provide an indispensable toolkit for accelerating the design and optimization of next-generation lithium and sodium batteries.