T13: Hard X-ray total scattering

Hard X-ray total scattering is a hard X-ray characterization technique based on measurement of elastic scattering in a large volume of reciprocal space (up to 20–30 A^{-1}), so that Pair Distribution Function (PDF) and Rietveld analysis are possible and give reliable information about the atomic structure of the amorphous or crystalline materials consisting the battery. Such characterization is achieved by using high energy X-rays at advanced light sources (synchrotrons) and large 2D detectors. The advantage over the more traditional XRD approach is that all materials inside the battery (even amorphous, liquid and with XRD peak overlap) can be characterized at the same time, with high temporal resolution and in operando conditions.

In a typical experiment, a battery is placed in the path of the X-ray beam and elastically scattered X-rays are collected behind the sample with a large 2D detector. The use of high energy results in more condensed reciprocal space therefore accessing large momentum transfer (q). During the measurement the battery condition can be changed (charge/discharge) and atomistic processes happening in all the materials can be followed. The diffraction patterns need to be further analyzed by Rietweld and/or PDF analysis to obtain the atomic structure of the materials. The information about the atomic structure often is the key to understand the processes leading to loss of activity and degradation and form the base for material development and assessment of stability.

Typically, all battery materials can be characterized as following:

- Electrodes - Atomistic characterization and information about the fundamental processes during charge and discharge cycles, phase transitions and degradation.
- Electrolytes - Following the changes in the structure of electrolytes during charge/discharge, aging of electrolytes.
- SEI formation - development of SEI during conditioning of the cell.
- Holistic studies of synergy between all materials of the cell in operando conditions.