X-ray diffraction and total scattering characterization of battery materials

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X-ray diffraction, scattering and imaging are powerful tools for the study of battery materials. In this work we describe combined X-ray diffraction and total scattering methods that can provide a wealth of information about new materials used in battery applications. By using X-ray diffraction (XRD) it is possible to identify the different crystallographic phases, and with the Rietveld method it is possible to refine the crystallographic structures of the different materials and quantify the amount of each phase in the bulk material. Improvements in high energy radiation (Mo or Ag X-ray anodes) optics and detectors for laboratory instruments facilitate in operando XRD of battery cells and Pair Distribution Functional (PDF) analysis using total X-ray scattering analysis of new battery cathode materials. Combining these approaches is valuable because disorder in the short-range structure revealed by PDF can explain the loss of performance in some batteries during cycling. In addition, the short-range structure of crystalline, nano-crystalline and amorphous materials can be studied with the Pair Distribution Function method (PDF), based on a total scattering approach.