

## **RIETVELD REFINEMENT OF LiCoO<sub>2</sub>-TYPE LAYERED STRUCTURES: SEMI-QUANTITATIVE ANALYSIS OF Li CONTENTS**

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Cathode materials based on the LiCoO<sub>2</sub> layered-type-structure are currently used in Li-ion cells and research regarding improvements to capacity are needed. One important aspect of these cells that requires characterization is the Li content of the cathode during various stages of charge and discharge. As the cell is charged, Li is extracted from the Li-O layer of the crystal structure resulting in a Li<sub>x</sub>CoO<sub>2</sub> composition. Upon discharge, the Li content in the cathode is returned to near LiCoO<sub>2</sub> composition.

Due to the low number of electrons, X-ray scatter of Li atoms is very limited. For an accurate measure of Li occupancy, neutron diffraction is a better alternative; but access to neutron sources is difficult to obtain and not routine. For LiCoO<sub>2</sub>-type materials the disadvantage of low x-ray scatter from Li can be partly overcome because the Li in this Rhombohedral crystal structure only occupies one crystallographic site. Additionally, due to the very large mole fraction of Li present in the formula (LiCoO<sub>2</sub>), Li still contributes a detectable amount to the peak intensities. Hence, we have successfully measured changes in Li site-occupancy for cathode materials at various states of charge using Rietveld analysis. Because of the large error associated with Li occupancies ( $\pm 10\%$ ) the analysis can only be considered semi-quantitative, but it can yield important information about the general state of charge/discharge for the cathode and thereby give the researcher an ability to track the very elusive Li atoms. Rietveld analysis performed on simulated powder patterns confirms our ability to detect varying Li contents semi-quantitatively ( $\pm 10\%$ ). Our results for Rietveld refinement will be presented along with supporting data from ICP measurements of Li content and electrochemical results of cell cycling.

\*Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.