

Quantification and Prediction of NMC Defect Concentrations

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Advanced neutron and synchrotron powder diffraction beamlines were utilized to accurately quantify important defects (anti-site, non-stoichiometry) for a large number of NMC cathode compositions, something that cannot readily be done using laboratory diffraction data. A comparison of defect concentrations obtained using neutron and synchrotron data gives good insights into the sensitivity of these methods. Based on these results, it is possible to make predictions about the anti-site defect concentration for arbitrary NMC compositions.