Materials Science & Engineering Thesis Defense

Energetics and Stability of NiMnCo (NMC) Cathode Materials

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Abstract

Lithium nickel manganese cobalt oxides (NMCs) are layered oxide cathode materials which are becoming increasingly popular as the demand for lithium-ion batteries increases. Lithium-ion batteries are used to power modern vehicles and for other battery applications. To better understand the structure and energetics of NMCs, various molar ratios of these compounds were synthesized via a sol-gel method and characterized with powder X-ray diffraction profile fitting. Lattice constants for the nickel, manganese, and cobalt solid solutions were determined. High temperature oxide melt solution calorimetry was used to determine the enthalpies of formation and mixing. All but Li2MnO3 had the same space group as LiCoO2 (R-3m). The lattice constants approximately followed a linear fit with cobalt mole fraction (R2average= 0.973) for the cobalt series. As the molar ratio of cobalt increased the lattice constants decreased. The nickel series was less linear (R2average=0.733) and had an opposite lattice constant trend to cobalt. The manganese series possessed a roughly linear trend when excluding the outlier Li2MnO3 (R2average=0.282). The formation enthalpy of the cobalt series becomes more negative as more cobalt is added. A second order polynomial fit could be used to model the enthalpies of mixing for the series. NMC2.5,2.5,5 exhibited the most stable energetics.

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