Structure and Delithiation/Lithiation of the Lithium-Rich Layered Oxide $\text{Li}[\text{Li}_{0.23}\text{Ni}_{0.15}\text{Mn}_{0.62}]\text{O}_2$ as Cathode Material

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doi: 10.20964/2017.09.25

Received: 29 April 2017 / Accepted: 5 July 2017 / Published: 13 August 2017

The typical lithium-rich layered oxide $\text{Li}[\text{Li}_{0.23}\text{Ni}_{0.15}\text{Mn}_{0.62}]\text{O}_2$ is synthesized via a solid state reaction, and is used as the cathode material for lithium-ion batteries. *In situ* X-ray diffraction analyses reveal the formation process of $\text{Li}[\text{Li}_{0.23}\text{Ni}_{0.15}\text{Mn}_{0.62}]\text{O}_2$ crystallites with $C2/m$ monoclinic symmetry. The $\text{Li}[\text{Li}_{0.23}\text{Ni}_{0.15}\text{Mn}_{0.62}]\text{O}_2$ cathode delivers an initial discharge capacity of 221 mAh g^{-1} and keeps a reversible capacity of 174 mAh g^{-1} after 50 cycles. A large capacity loss and the unique charge curve during the first cycle both indicate that $\text{Li}[\text{Li}_{0.23}\text{Ni}_{0.15}\text{Mn}_{0.62}]\text{O}_2$ was changed into $\text{Ni}_{0.2}\text{Mn}_{0.8}\text{O}_2$ due to irreversible oxygen loss and “rich lithium” extraction. The cathode’s high capacity results from the reversible conversions between $\text{Ni}_{0.2}\text{Mn}_{0.8}\text{O}_2$ and $\text{LiNi}_{0.2}\text{Mn}_{0.8}\text{O}_2$. Both $\text{Ni}_{0.2}\text{Mn}_{0.8}\text{O}_2$ and $\text{LiNi}_{0.2}\text{Mn}_{0.8}\text{O}_2$ keep a stable framework during cycling due to two suggested reasons: (1) some transition metal atoms migrate into the lithium layers and play as the supports between the transition metal layers; (2) $1/4 \text{ Mn}$ keeps a stable tetravalent state during cycling and then weakens the Jahn-Teller effect of Mn^{3+} . The predicted reversible capacity of $\text{Li}[\text{Li}_{(1-2x)/3}\text{Ni}_x\text{Mn}_{(2-x)/3}]\text{O}_2$ ($0 < x < 0.5$) increases from 229 to 280 mAh g^{-1} with increasing x value, and fairly coincides with the experimental results in this work and literature.

Keywords: Lithium-rich layered oxide; cathode; lithium-ion battery

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