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In situ Neutron Diffraction Study on Layered Oxides Na0.5Ni0.25Mn0.75O2

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Layered oxides based on first-row transition metals dominate cathode materials for commercial batteries and remain highly interesting as well as challenging in their structural study during electrochemical reactions. Neutron diffraction is a powerful method to obtain periodic structural information complementary to that obtained by X-ray diffraction. Although inferior to X-ray diffraction in signal resolution, neutron diffraction reveals more reliable structural evolution as the whole bulk of materials are fluxed with neutron beam. Na0.5Ni0.25Mn0.75O2 is a potential sodium ion battery cathode due to its high operating voltage 3.2 V vs Na+/Na and high capacity 130 mAh/g. Its stoichiometry is designed to only utilize the redox couple Ni4+/Ni2+ to avoid the unstable redox couple Mn4+/Mn3+. The high voltage phase for this material has been under debate. The fact that sodium-containing layered oxides are highly hydroscopic, especially at low sodium content, makes it hard to study the final phase ex situ. In the work presented here, we have pushed the signal resolution of in situ neutron diffraction to the limit by loading the optimized material mass at the positive side and the corresponding amount of amorphous hard carbon at the negative side of a pouch cell. The result is the first robust proof of the reversible structural evolution from P3, O3 to O3s on charging and back to O3, P3 on discharging.

Speakers Gender

Level of Expertise

Student

Do you wish to take part in the poster slam

No

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