

Structural evolution of a $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ cathode and a $\text{Li}_4\text{Ti}_5\text{O}_{12}$ anode in a functioning lithium-ion battery

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The relatively large penetration depth, sensitivity to light elements, and non-destructive sample interaction afforded by neutron scattering is combined with instrumentation allowing fast data-acquisition times to allow neutron powder diffraction (NPD) to be a powerful tool for studying the structural variation of cathode and anode materials during battery cycling [1-4]. In this study, a neutron-friendly battery comprised of a disordered $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ ($Fd\bar{3}m$) cathode, a $\text{Li}_4\text{Ti}_5\text{O}_{12}$ anode, deuterated electrolyte, and the relatively low-hydrogen polyvinylidene difluoride separator was used to research a battery chemistry not yet commercially available. This work tracks crystallographic changes, such as the variation of lattice parameters, lithium occupation, and oxygen positional parameters, of the $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ cathode and the $\text{Li}_4\text{Ti}_5\text{O}_{12}$ anode simultaneously with charge/discharge within a battery. Importantly, we find that the disordered $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ cathode has a solid-solution reaction associated with its lattice change and the $\text{Ni}^{2+}/\text{Ni}^{3+}$ redox couple, and a two-phase reaction, between $\text{Li}_x\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$ and $\text{Ni}_{0.25}\text{Mn}_{0.75}\text{O}_2$, that is related to the $\text{Ni}^{3+}/\text{Ni}^{4+}$ redox couple without a corresponding change in lattice. The details of these findings will be presented.

References:

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