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Investigation into the AlF₃ coating effect on the electrochemical behaviours in the LiNi_{0.5}Mn_{1.5}O₄//Li₄Ti₅O₁₂ full batteries by in-operando neutron powder diffraction and electrochemical characterization

Key words: lithium ion batteries, battery safety, output voltage, LiNi_{0.5}Mn_{1.5}O₄//Li₄Ti₅O₁₂ full battery, AlF₃ coating, in-operando, neutron powder diffraction, electrochemical performance

Lithium ion batteries (LIBs) with graphite anodes and LiCoO₂ cathodes have been widely used in our daily life. Since the operating voltage of graphite is close to that of the metal lithium dendrite formation, lowering the battery operating safety, Li₄Ti₅O₁₂ (LTO) anode is regarded as the promising alternative due to its excellent safety originating from its high working potential (~1.55V vs. Li/Li⁺) and superior structural stability ascribed to zero-strain lithium insertion. In order to enhance the output voltage of full batteries with LTO anode, the so-called 5V spinel LiNi_{0.5}Mn_{1.5}O₄ (LNMO) cathode is chosen. In the LNMO//LTO full battery, the LTO anode shows poor rate performance because of low intrinsic electrical conductivity and lithium-ion diffusion coefficient.

In this work, AlF₃ coating was applied on LTO to improve its rate capability in full batteries. The modified LTO anode exhibits significantly improved rate performance because of AlF₃ coating layer and parasitic Al doping (~3% onto the 16c crystallographic site of LTO structure) indicated by the joint refinement of X-ray diffraction (XRD) and neutron powder diffraction (NPD) data. In-operando NPD data also exhibits a smaller lattice parameter change of the modified LTO during lithiation and delithiation process. More interestingly, the AlF₃ coating on the anode LTO could also promote the rate of structural response of LNMO cathode shown by the in-operando NPD data of LNMO, suggesting faster delithiation and enhanced Li diffusion. We contribute this cathodic improvement to the protection of AlF₃ against HF and greater availability of lithium in the LNMO//AlF₃-coated LTO battery. Further details will be brought and discussed in the presentation.

Topic

Advanced Materials

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