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Investigation into the AIF3 coating effect on the electrochemical behaviours in the LiNi0.5Mn1.5O4//Li4Ti5O12 full batteries by in-operando neutron powder diffraction and electrochemical characterization

Key words: lithium ion batteries, battery safety, output voltage, LiNi0.5Mn1.5O4//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 LiNi0.5Mn1.5O4 (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

Primary author(s): Mr LIANG, Gemeng (PhD student, Institute for Superconducting and Electronic Materials (ISEM) Innovation Campus, University of Wollongong)

Co-author(s) : SOMANATHAN PILLAI SUSHAMAKUMARI AMMA, Anoop (University of Wollongong); Dr VANESSA, Peterson (ANSTO); Dr PANG, Wei Kong (University of Wollongong); Prof. GUO, Zaiping (University of Wollongong)

Presenter(s): Mr LIANG, Gemeng (PhD student, Institute for Superconducting and Electronic Materials (ISEM) Innovation Campus, University of Wollongong)

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