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Estimation of lithiated cathode loss for cycled 18650-type battery by in situ neutron powder diffraction

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18650-type cells comprising of LiNi0.54Co0.15Mn0.31O2 and LiNi0.87Co0.07Al0.06O2 as cathode and graphite as the anode are cycled at various SoC ranges. Inconsistent capacity fade is found, indicating that the medium SoC range cycling with less capacity loss behaves better than the high and low SoC ranges, while the low SoC range cycling tends to have nonlinear capacity fade. The non-destructive methods, in situ neutron powder diffraction (NPD) at SPODI, is used to obtain detailed structural information about the cathode and anode materials without opening the cell. The crystalline phases in the cell are identified and their lattice parameters and respective weight fractions are calculated. Loss of lithium inventory (LLI) is calculated by the relative weight ratio of LiC6 and LiC12, indicating that LLI is the dominating degradation factor for the inconsistent capacity fade of cells. The lithiated cathode loss is caused by the trapping of lithium in the cathode under the controlled battery cycling voltage window (2.5V - 4.2V), which leads to the mobile lithium and cathode material loss. Lithiated cathode loss is estimated by the observation of cathode unit volume change. The estimated lithiated cathode loss accounts for approximately half of the total LLI. The pulverization of the cathode particles is observed by SEM. The disintegration of the cathode particle causes the contact loss with active material inactivity, which is the main reason for the lithiated cathode loss.

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