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Aging in Li-ion cells examined with neutron diffraction, electrochemical analysis and physico-chemical modeling

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Aging in 18650-type NMC/C cells, produced under commercial conditions, has been experimentally characterized by *in situ* neutron diffraction and electrochemical analysis. The comparison of discharge capacity of an uncycled cell with that of a cell which has undergone 1000 cycles under ambient conditions, shows a capacity fade of 21% on cycling. Neutron diffraction of the uncycled and cycled cell, in their charged state, shows a reduction in the weight fraction of the LiC6 phase as well as an increase in the weight fraction of the LiC12 phase on aging, from which a cyclable lithium loss corresponding to a capacity loss of 23% can be extracted. In spite of this large capacity loss, both the anode and cathode materials are scrutinized to be structural stable and no evidence of active material loss is observed in the evaluation of these neutron diffractograms. Thus, other aging mechanisms could be excluded from these measurements, within the experimental accuracy of the method. A physico-chemical aging model, which attributes capacity fade solely to loss of cyclable lithium in the growth of a continuous solid electrolyte interface (SEI) film on the anode surface, is developed to reconsider aging contributions. This model is first validated by reproducing the obtained experimental aging and voltage profiles which confirms cyclable lithium loss into SEI layer growth as the sole aging mechanism. It also predicts a reduction or shift in x = 0:18 for anode stoichiometry LixC6 (0 < x < 1), for the cycled cell. This is in good agreement with the anode stoichiometry shift of x = 0:20 for the cycled cell as obtained from neutron diffraction experiments.

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