Probing the Reversibility of Silicon Monoxide Electrodes

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Silicon is a high capacity anode material that attracts much attention. However, large volume changes during lithiation and delithiation lead to mechanical issues such as particle fracture, binder failure and electrode delamination. One method to improve the stability of silicon is to incorporate oxygen into the lattice. Silicon monoxide (SiO) can give a capacity of about 1250 mAh g^{-1} with better cycle performance than Si. Though, the formation of Li-Si-O compounds leads to a low first cycle efficiency (FCE).

Here, we would like to study the factors affecting the reversibility of SiO during first and subsequent cycles. Three types of samples (1 µm SiO, 5 µm SiO and 5 µm SiO with carbon coating) are initially tested. The materials are mixed with acetylene black (AB) and carboxymethyl cellulose (CMC) binder in a weight ratio of 6:1:2 to form into electrodes. The electrodes are made into 2032 coin cells with 1M $LiPF_6$ in fluoroethylene carbonate (FEC) and diethyl carbonate (DEC) electrolyte. While the 1 µm SiO and 5 µm SiO materials give an initial charge capacity of about 1250 mAh g^{-1} which a FCE of 68%, carbon coating increases the charge capacity and FCE to 1700 mAh g^{-1} and 77%, respectively. Though, cycle stability decreases with increasing particle size and carbon coating (Fig. 1).

The causes of the differences in FCE and cycle performance are probed from two perspectives: chemical and mechanical. First, we study the role of the oxygen by thermal disproportionation and chemical reduction. While higher capacity can be obtained after thermal disproportionation, cycle stability is reduced. Second, the thickness changes of the SiO electrodes during charge and discharge are monitored by in-situ dilatometry to correlate between mechanical properties and cycle performance. In addition, we are performing tests on carbon-coated and polymer-coated SiO, and the results will be presented at the meeting.

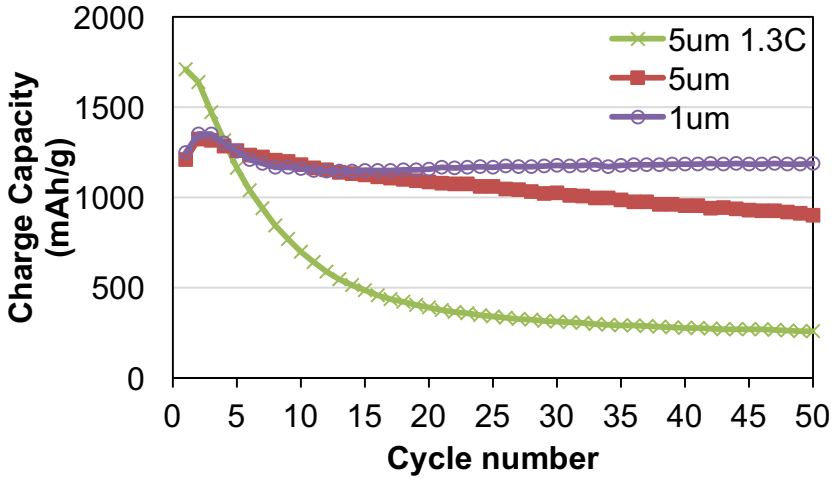

Fig. 1. Cycle performance of various SiO materials.