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Role of native oxide layer in silicon anodes for Li/S batteries

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Lithium/sulfur (Li/S) and Lithium/air systems are possible candidates for future electrochemical energy storage, due to higher gravimetric density compared to conventional Li-ion batteries. In these systems, a lithiated silicon (Si) electrode often replaces the Li metal anode, used as a Li ions reservoir. Detailed studies on lithiation and delithiation of Si anodes are of fundamental importance in understanding capacity fading effects. Silicon crystals are used with the native silicon dioxide (SiO2) layer: upon lithiation and delithiation, Li ions interact first with the SiO2, and subsequently intercalate in the Si crystal forming a Li/Si alloy. Due to the negative scattering length density of Li, neutron reflectometry is a powerful technique for investigating lithiation and delithiation of Si anodes. Two different Li/Si cells were prepared, one with and one without native oxide layer (removed using HF etching) on the Si anode. Both were measured at the reflectometer V6 at the BER II neutron source, to shade some light on the role of the SiO2 native layer formation and its (ir-)reversibility using both electrochemical (CV, EIS, charge/discharge) and in situ/operando neutron reflectometry measurements.

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