Magnesium and Magnesium-Silicide coated Silicon Nanowire composite Anodes for Lithium-ion Batteries

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Abstract

We synthesized composites consisting of silicon nanowires (SiNWs) coated with magnesium and magnesium silicide (Mg_2Si) for lithium-ion battery anodes and studied their electrochemical cycling stability and degradation mechanisms. Compared to bare SiNWs, both Mg and Mg_2Si coated materials show significant improvement in coulombic efficiency during cycling, with pure Mg coating being slightly superior by ~1% in each cycle. XPS measurements on cycled nanowire forests gave quantitative information on the composition of the SEI layer and showed lower Li_2CO_3 and higher polyethylene oxide content for coated nanowires, thus revealing a passivating effect towards electrolyte decomposition. Extensive characterization of the microstructure before and after cycling was carried out using scanning- and transmission electron microscopy aided by focused ion beam cross-sectioning. The formation of large voids between the nanowire assembly and the substrate during cycling, causing the nanowires to lose electrical contact with the substrate, is identified as an important degradation mechanism.