In Situ EXAFS Study of Tin Sulfide/Graphite Composite Anodes for Lithium-Ion Batteries

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Rapid growth applications of Lithium-ion batteries require significant improvement in their capacity, energy density, and cycle life. SnS_2 is a promising alternative of traditional graphite anodes which exhibits high theoretical initial capacity of 1231 mAh/g but still suffers from capacity and cycle life degradation. In this work, SnS_2/graphite composite with a capacity of 591 mAh/g after 50 cycles is synthesized using high-energy ball milling method to achieve enhanced electrochemical performance.

In order to have a better understanding of the improved performance and the reason of the capacity fading, in situ extended x-ray absorption fine structure (EXAFS) technique is developed to study the mechanism of lithiation/delithiation process using in situ vacuum-sealed pouch cells. The detailed local structural changes correlated to the electrochemistry are investigated by EXAFS modeling.

The enhanced performance of this material is attributed to the generation of the highly dispersed nanoscale SnS_2 in the matrix. The pristine crystalline phases of SnS_2/graphite composite are destroyed after cycling. Then a highly dispersed amorphous phase is generated under the help with graphite and Li_2S, the product of conversion reaction, which also acts as an active matrix. Graphite matrix increases electrical conductivity and prevents aggregation of Sn clusters to improve the reversibility of both conversion and alloying reactions. The conversion reaction in the amorphous tin sulfide phase is highly reversible while it is irreversible in the crystalline phase. Introducing low-cost graphite matrix and create highly dispersed samples by an easily repeatable ball milling method is a strategy to develop new battery materials in the future.