Amorphous SnCo-Carbon Anode: Understanding the Reaction Mechanism


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Amorphous tin-cobalt based anode, which possesses much better electrochemistry than traditionally used graphite, has attracted considerable interest since it was first introduced by SONY in 2005. The combination of intercalation and conversion reactions (crossover material) appear to offer a great potential for increasing its gravimetric and volumetric capacities. However, a rational elucidation of the fundamental mechanisms is required to build a roadmap for developing future crossover materials. In this work, nanostructured SnCo embedded in carbon matrix is considered as a model system, where both intercalation reaction forming Li2SnCo and a subsequent conversion reaction to give Li0.5SnCo products could occur. We investigate how the nano-SnCo alloy reacts with lithium in an electrochemical cell by 7Li MAS NMR, STEM, in-situ X-ray absorption, Raman spectroscopy, in-situ small-angle x-ray scattering (SAXS), and magnetic studies. Co displacement upon Li insertion is confirmed by the magnetic properties, SAXS and STEM. Since the corresponding Li NMR spectra revealed only a small shift, indicating a diamagnetic Li environment, we are further investigating the possible existence of Li2SnCo using ex-situ pair distribution function analysis.

Understanding Electrochemical Mechanism of Amorphous SnCoC is Key to the Development of Low-cost Sn-based Anodes

Need
- Safe, low cost
- High capacity

Current anode materials
- Graphite: low potential vs. Li/Li+, dendrite growth
- Limited capacity, gravimetric as well as volumetric
- 300-400% volume expansion if bulk Sn is used

Possible Reaction Mechanism

Intercalation

SnCo + xLi ⇌ LixSnCo

Conversion

SnCo + Li ⇌ Li0.5Sn + Co

Intercalation/Conversion

SnCo + yyLi ⇌ yLi0.5Sn + Sn1-yCo

y > 0.5, bulk: Ferromagnetic

Magnetization Susceptibility Measurements

- Region I: M increases not change up to 40% SOC → Li intercalation
- Region II: M increases linearly between 40 and 80% SOC → Co displacement
- Region III: M increases gradually → possibly due Li intercalation in graphite carbon

SnCo-C Anode STEM/EELS

Co accumulates upon cycling, particles stay small

Conclusions

- Solid State NMR reveals that the Li is probably in a diamagnetic environment
- The magnetic results show an increase of the magnetization above 40% lithiation, and an increase in the size of the superparamagnetic particles from 1.6 to 2.5 nm
- The porod length increases from 1.7 to 2.3 nm upon lithiation as observed from the in-situ SAXS.
- In-situ XAS supports the observation that the peak corresponding to the Sn-Co bond decreases upon delithiation, but does not disappear
- The results suggest a reaction mechanism in which a Co-rich alloy, Sn0.5Co, is formed.