Intermetallics for anodes in Li-ion batteries: The system Sb-Sn-Ti

H. Flandorfer[a], P. Berger[a], C. Schmetterer[b], H.S. Effenberger[c]

[a]Department of Inorg. Chemistry – Functional Materials, University of Vienna, Austria
[b]Department of Physical Chemistry, University of Vienna, Austria
[c]Department of Mineralogy and Crystallography, University of Vienna, Austria

Li-ion batteries (LIBs) are most frequently used in various handheld devices like notebooks, cell phones or cameras. For high power applications like load leveling or electro-mobility their capacity, energy and power density as well as cyclability is not sufficient. New electrode materials are required for the next generation of LIBs. Among possible candidates for improved anodes are intermetallics which show significantly higher theoretical capacities than the graphite currently used. Many metals and alloys are able to form intermetallic phases with Li, e.g. there are several Li-Sn compounds where Li17Sn4 is the highest lithiated one. It exhibits a theoretical charge capacity of 842 mAh per gram of Sn (compare to 339 mAh per gram of carbon). A serious drawback, however is degradation and thus low cyclability of such electrodes caused by the large volume changes on lithiation/delithiation starting from pure Sn. One possibility to overcome this phenomenon is the co-precipitation of a matrix phase together with the formation of the lithiated compounds. Using for instance SbSnTi alloy instead of the pure metals Sb or Sn lithiation finally leads to the formation of active Li_3Sb and Li_7Sn_2 phases together with Ti which is inert against Li and also forms nano-crystalline Sb-Ti and Sn-Ti compounds on delithiation [1,2]. The latter are able to buffer crack formation by volume change. Generally, the investigation of related intermetallic alloy systems is indispensable for systematic understanding of electrode processes and electrode design. This comprises experimental data as well as CALPHAD modelling and theoretical calculations. As a first step we studied the phase relations and crystal structures in the ternary Sb-Sn-Ti subsystem of Li-Sb-Sn-Ti by means of XRD, thermal analysis and SEM/EDX. Isothermal sections at different temperatures are presented as well as the crystal structures of two new compounds.

---

[1] Sougrati M.T., Fullenwarth J., Debenedetti A., Fraisse B., Jumas J.C., Monconduit L., J. Mater. Chem., 2011, 21, 1069

[2] Marino C., Sougrati M.T., Gerke B., Pöttgen R., Huo H., Menetrier M., Grey C.P., Monconduit L., Chem. Mater., 2012, 24, 4735