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

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Li-ion batteries (LIBs) have been used in various handheld devices like notebooks, cell phones or cameras, over many years. Their performance, however, in high power applications is still hampered by low capacity, energy density and cyclability. This is why new electrode materials are required for the next generation of powerful LIBs. Intermetallic materials, which show significantly higher theoretical capacities than the currently used graphite, are under consideration as anodes. Beside Si, also Sn is a candidate because there exist seven Li-Sn intermetallic compounds with $Li_{17}Sn_4$ as the highest lithiated one. It exhibits a rather high theoretical charge capacity of 842 mAh per gram of Sn compared to 339 mAh per gram of carbon. A serious problem, however, is degradation and thus low cyclability of such electrodes on lithiation starting from pure Sn. This is caused by the large volume changes on phase transformation. There are several proposals to solve this problem – a relatively simple and efficient way is the co-precipitation of a ductile phase together with the formation of the lithiated compounds. Trifonova et al. [1], for instance, proposed to use Sb-Sn alloys instead of pure tin which effects on lithiation the precipitation of Li-Sb alloys and Sn prior to the formation of the less stable Li-Sn alloys. In general, the thermodynamic investigation of related intermetallic alloy systems, in this case Li-Sb-Sn, is absolutely necessary for basic understanding of electrode processes and systematic electrode design. Therefore, experimental data, as well as CALPHAD modelling and theoretical calculations, are required. We investigated isothermal sections at 300 and 400 °C, the crystal structure of a new compound and the stability of the liquid phase in the ternary system Li-Sb-Sn. For this purpose XRD, thermal analysis and calorimetry were applied. Isothermal sections are presented, as well as the crystal structure of the new compound, which is structurally related to Li_8Pb_3.

[1] Trifonova A., Wachtler M., Winter M., Besenhard J.O., Ionics, 2002, 8(5-6), 321