

Thermodynamic Modelling and Experiments in Systems Evaluated in the WENDELIB Priority Program for Li-ion Batteries

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ABSTRACT

Materials thermodynamics play a key role in the development of electrode materials for lithium ion batteries with improved performance. The priority program “Materials with New Design for Improved Lithium Ion Batteries (WeNDeLIB)” funded by the German Research Foundation promotes scientific research on the relationships between thermodynamics, kinetics, crystal chemistry and micro-/nanostructures of new materials for lithium ion batteries. Several candidate materials systems are investigated and key experiments are combined with a CALPHAD-based thermodynamic modeling to produce self-consistent thermodynamic descriptions which reproduce the measured thermochemical, phase diagram, and electrochemical data. At the last GTT meeting, we reported on work in the Li-Cu-O system for conversion electrodes and on the Cu-Sn and Li-Sn systems for intermetallic anodes. In this presentation, we will highlight our progress in the last year of research. Our results on high temperature oxide solution calorimetry to determine the enthalpies of formation of Li-Mn-O compounds have been used in a CALPHAD-based thermodynamic assessment of the system. With this description, we can predict open circuit voltages as a function of lithium content at different operating temperatures. We have also made progress in our work on the intermetallic systems. The Cu-Li system has been re-assessed and a preliminary description for the Cu-Li-Sn system based on the three sub-binaries, all re-optimized in the framework of WeNDeLIB, has been created. The enthalpies of mixing of the ternary liquid calculated based on the Muggianu extrapolation method are compared to experimental calorimetry data in the Cu-Li-Sn system, which was also measured in the framework of WeNDeLIB.