Experimental Thermodynamics and Phase Relations of New Electrode Materials for Li-Ion-Batteries

Joint DFG Project
within the
WeNDeLIB priority program

Conducted by
Dr. Damian Cupid, KIT, Karlsruhe
AO.Prof. Dr. Hans Flandorfer, University of Vienna
Doz. Dr. Torsten Markus, FZ-Jülich

Information to the research work in the
Karlsruhe Institute of Technology (KIT)

Local project manager: Dr. Damian M. Cupid
Project co-worker: Dr. Dajian Li

The goal of the project “Experimental Thermodynamics and Phase Relations of New Electrode Materials for Li-Ion Batteries” is the generation of accurate, self-consistent thermodynamic property and phase diagram data using both experimental and computational techniques for the promising (Co,Cu,Ni)-Li-Sn anode systems for lithium ion batteries. The project is arranged so that the experimental measurement of thermodynamic property data coupled with the experimental investigations of the multi-component phase diagram systems are performed by Subproject 2 (Prof. Hans Flandorfer, Siegfried Fürtauer University of Vienna) and Subproject 3 (Doz. Dr. Torsten Markus, David Henriques, Forschungszentrum Jülich). Subproject 1 focuses on the application of computational thermodynamics and the calculation of phase diagram (CALPHAD) method to develop thermodynamic descriptions of the multi-component systems based on the experimental data from Subprojects 1 and 2 and on a careful and critical assessment of the experimental literature data. The strength of the combined experimental and computational thermodynamics approach applied in the present priority project is that the self-consistency between all kinds of experimental phase diagram and thermochemical data (literature data as well as data obtained in the framework of the priority program) from various kinds of experimental methods can be checked. A second, key advantage is that the equilibrium open circuit voltages for the electrochemical cell as a function of the amount of transferred active species (the Li^+ ion) can be calculated and, in the absence of experimental data at the given conditions, even predicted. This data could then be used to aid in the development of lithium-ion batteries based on the (Co,Cu,Ni)-Li-Sn anode system.

This working method has already been already successfully implemented in the investigation of the binary Cu–Sn system. Here, a new thermodynamic description of the Cu–Sn binary system was developed based on new experimental phase diagram work performed in the framework of the priority program.