MM 50: Topical Session Battery Materials II

Time: Thursday 12:15–13:00 Location: H6

Topical Talk MM 50.1 Thu 12:15 H6

Hysteresis due to non-monotone material behaviour inside many particle systems — •Clemens Guhlke and Wolfgang Dreyer — Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany

Relying on two examples we study storage problems. The examples concern the storage of lithium in small iron phosphate particles constituting the cathode of a lithium-ion battery and the storage of air in elastic rubber balloons.

The two storage systems have in common: 1. The iron phosphate particles as well as the rubber balloons exhibit non-monotone constitutive behavior. 2. Phase transition and hysteresis during loading and unloading.

We describe the processes of loading and unloading by a kinetic equation of Fokker-Planck type. There are two small parameters that control whether the phase transition evolves along the Maxwell line or if they exhibit strong hysteretic behavior.

MM 50.2 Thu 12:45 H6

Thermodynamics and electronic structure of intrinsic point defects in $LiCoO_2$ — •Melanie Gröting and Karsten Albe — Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 32, D-64342 Darmstadt

A key problem of rechargable battery devices is their degradation. Various processes including microstructural changes, redox and intercalation reactions with the electrolyte, and particularly point defects in the active material are believed to play an important role in the degradation process. Therefore a detailed understanding of these mechanisms is important for improving the materials properties. In this study we present density-functional theory calculations (DFT) of intrinsic point defects in $LiCoO_2$ using the supercell approach. Formation energies are calculated and the electronic structures and density of states are examined in order to compare them with XPS data. Also, the thermodynamic stability of Li_xCoO_2 with lithium contents x = 1.0, 0.5 and 0 is determined with respect to the competing metal oxides. We consider lithium and cobalt vacancies, as well as oxygen vacancies and interstitials. An important finding is that besides oxygen defects cobalt vacancies can dominate under certain conditions.