Electronic structure of $LiCoO_2$ and $LiNiO_2$ bulk materials and thin films prepared by magnetron sputtering

David Ensling, Qi-Hui Wu, Javier Fernandez-Madrigal, Andreas Thißen, Wolfram Jaegermann

Institute of Materials Science, Surface Science Division,
Darmstadt University of Technology
Petersenstr. 23, D-64287 Darmstadt, Germany

$LiCoO_2$ and $LiNiO_2$ are most promising materials for applications as cathode materials in thin film battery devices.

In this work bulk powder samples and thin films deposited by magnetron sputtering have been used to study the electronic structure of the stoichiometric compounds and during Li-deintercalation and intercalation in order to elucidate its relation to electrochemical parameters like battery voltages.

Commercial $LiCoO_2$ and $LiNiO_2$ powders have been pressed to pellets to improve handling in the vacuum system. Different vacuum preparation techniques like Ar^+-ion etching and annealing in different oxygen partial pressures have been used to obtain clean and stoichiometric sample surfaces. The effects of the different preparation steps on surface contaminations and oxygen and lithium content in the samples has been investigated systematically.

$LiCoO_2$ thin films have been prepared by magnetron sputtering. First results on the effect of different sputtering parameters like argon and oxygen partial pressure and sputtering voltages and frequencies will be presented.

The crystal structures and sample morphologies have been studied by X-ray diffraction (XRD), scanning electron (SEM) and atomic force microscopy (AFM).

X-ray induced photoelectron spectroscopy (XPS) has been used to determine chemical composition and stoichiometry of the samples and the oxidation states of the different elements in the compound. UV-light induced photoelectron spectroscopy (UPS) and resonant photoemission (ResPES) has been used to study the electronic structure. While UPS reveals information on work function and band bending, ResPES allows the assignment of valence band emissions to O2p-, Co3d- or Ni3d-like states. Thus, the partial valence band density of states (PVBDOS) can be derived.

First results on electrochemical measurements performed in a battery setup for the powder samples and for the thin films will be presented. Ex-situ cycling of the cells influences the chemical and electronic properties of the cathode materials studied by XPS.