MM 58: Topical Session Battery Materials IV

Time: Thursday 15:45–17:30 Location: H6

Topical Talk MM 58.1 Thu 15:45 H6

Investigation of Microscopic Mechanisms and Mechanical Effects in Electrode Materials for Lithium-Ion Batteries — •Reiner Mönig — Karlsruhe Institute of Technology, Institute for Materials Research II, Postfach 3640, 76021 Karlsruhe, Germany

Lithium ion batteries are promising candidates for future electrical energy storage. Important components of batteries are the electrodes which critically determine energy and power density as well as reliability. In the electrodes, sufficiently high ionic and electronic conductivities often can only be achieved by using small particles. The small particles, which are often in the 100nm range, make detailed investigates complicated. For example, typical electrochemical characterization methods can only yield volume averaged data of a whole electrode. In this talk a technique for in situ scanning electron microscopy will be introduced. Observations recorded during Lithium insertion and extraction into individual Si nanowires and SnO_2 particles will be presented. The experiments give insight into the fundamental processes that control battery operation and reveal degradation mechanisms. Large volume expansions and the growth of cracks were frequently observed. In order to assess mechanical stresses arising from Li insertion/extraction, dedicated in situ substrate curvature experiments were performed. Mechanical stress seems to be an important factor controlling battery operation and degradation. In contrast to many chemical degradation mechanisms that can be suppressed by chemical means, mechanical stresses are inevitable and their consequences may be limiting factors for the applicability of novel battery materials.

MM 58.2 Thu 16:15 H6

Microscaopic investigation of Li-Ion Batteries and Quantitative Characterization of the Microstructure — •Carmen Hafner, Timo Bernthaler, Alwin Nagel, and Gerhard Schneider — Aalen University, Department Materials Science and Surface Engineering, Aalen, Germany

Lithium ion batteries are the most attractive candidates for mobile applications. The function of Li ion batteries is based on the change of active materials due to diffusion processes. Electrochemical and physical characterization techniques are well advanced and published. Unlike these techniques the microscopic visualization and quantification of the microstructure of the electrode materials are not state of the art. Cell performance and aging mechanisms depend strongly on the appearance and changes in the microstructure. Hence, the investigation and quantification of microstructures is of increasing importance for the understanding of battery materials. We present the potential of the combined microscopic techniques nano 3D-computed tomography, optical microscopy, scanning electron microscopy and image analysis to characterize cell designs and the microstructure of active materials. The process how to prepare and investigate Li ion batteries by these techniques will be described. For the measurement of specific microstructural features of the active materials methods of the quantitative microstructure analysis will be explained. Parameters like volume fraction of phases, homogeneity, pores, cracks, grain size and shape distribution and specific surfaces and interfaces will be discussed.

Topical Talk MM 58.3 Thu 16:30 H6

New materials for energy storage systems — •Margret Wohlfahrt-Mehrens — Zentrum für Sonnenenergie- und Wasserstoff-Forschung, Baden-Württemberg, Ulm

Electrochemical energy storage systems are the key components for mobile applications both in communication systems and in new car concepts as hybrid or full electric vehicles. The rechargeable lithium-ion battery system has become the dominant technology in the global battery market during the last decade. These batteries offer the highest energy density available to date. While commercially used lithium-ion batteries power mostly small devices as cellular phones, portable computers and other mobile electronic equipment, extensive world wide efforts are underway to develop this technology for much more demanding applications such as large batteries for electric vehicles.

The present status of rechargeable lithium-ion batteries, the requirements for various applications and the need for further development will be discussed. The focus of the presentation deals with the materials selection and the materials science principles that underlie the behaviour of advanced electrochemical storage systems. An overview of current electrode materials (anode and cathode) and electrolytes will be given and future research and development needs for new components will be discussed.

MM 58.4 Thu 17:00 H6

Metallocene-based nanocomposites as cathode materials in lithium batteries — •Raju Prakash, Clemens Wall, and Maximilian Fichtner — Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Lithium-ion batteries have been the most utilized batteries in the portable electronic market since many years. But their performance still lies behind the demands of the consumer. New electrode materials with high specific capacities are necessary to meet these demands. Metal fluorides have high theoretical specific capacity based on a novel conversion mechanism, making them promising cathode materials for high performance lithium-ion batteries. However, the metal fluoride cathodes are still hampered by loss of capacity and cyclic instability. Hence, a new approach such as encapsulation of active materials in nanotubes or carbon-coating, etc. is needed in order to improve their performance.

Herein, we present a simple method based on the thermal decomposition of a metallocene/LiF mixture to produce inexpensive cathode materials which exhibit a good cyclic stability and reversibility. The detailed structural investigations of the nanocomposites as well as their electrochemical performances will be presented.

MM 58.5 Thu 17:15 H6

The *ortho*–phosphate arrojadite as new material for cathodes in Lithium–ion batteries. — •Christoph Kallfass[1], Constantin Hoch[1], Hermann Schier[1], and Helmut Schubert[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisernbergstr. 1, D-70569 Stuttgart, — [2]Technische Universität Berlin, Institut für Werkstoffwissenschaften, Englische Str. 20, D-10587 Berlin

The investigation of the crystal structure of the iron- and manganese containing *ortho*–phosphate mineral arrojadite was extending over several years [1-3]. Single crystal diffraction using X–ray and neutron radiation combined with complete determination of all chemical constituents of the component result in a new structural model. The new model describes two different types of channels running along [010] and elucidates the occupancy of the atomic positions inside these channels. A novel chemical process offers the opportunity to modifiy the the elementar arrangement of the atomic positions inside the channels using methods of so–called “green chemistry”. When using Li^+ cations in this process a new material for cathodes can be made out of the mineral arrojadite. A lithium–ion battery made of an arrojadite cathode worked for more than 15.000 cycles ($2.0 \leq V \leq 4.5$) with minor loss in capacity. The novel chemical process and particularly the enrichement of Li^+ cations was verified by single crystal diffraction using neutron radiation and ^{6}Li–MAS–NMR–spectroscopy.

[1] Krutik, V. M. *et al.* *Sov. Phys. Crystallogr.*, **24**, 425–429, 1979.
[2] Moore, P. B. *et al.* *Am. Mineral.*, **66**, 1034–1049, 1981.
[3] Cámara, F. *et al.* *Am. Mineral.*, **91**, 1249–1259, 2006.