MM 61: Functional materials IV: Batteries III

Time: Thursday 15:45–16:45 Location: H52

MM 61.1 Thu 15:45 H52

From micro- to mesoscale: The impact of occupational disorder on Li ion mobility in $Li_4Ti_5O_{12}$ battery materials — •Hendrik H. Heenen, Christoph Scheurer, and Karsten Reuter — Chair for Theoretical Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany

Spinel-type lithium-titanium-oxide ($Li_4Ti_5O_{12}$) is an extraordinarily safe and long-living anode material employed in commercial lithium ion batteries. To complement experimental investigations, first-principles studies are often applied to gain microscopic insight into the underlying ion transport processes and the microscopic structure. This computationally demanding approach is however challenged by the treatment of the mixed occupancy of octrahedral sites by Li and Ti ions found in $Li_4Ti_5O_{12}$. The resulting vast configuration space is usually reduced to an idealized model, oversimplifying the investigated system. A numerically efficient, yet reliable, classical interatomic potential [1], allows for exploring the complex configuration space through extensive Monte-Carlo sampling and evaluating its electrochemical properties via molecular dynamics simulations. Our findings indicate a higher Li ion mobility with structural disorder, which is thermodynamically favored by high synthesis temperatures. We further assess the Markovian processes of the diffusion mechanism via a thorough microscopic analysis and elucidate the Li ion mobility in detail. This yields dynamic rates necessary for an extrapolation to kinetic Monte-Carlo simulations which pave the way for more quantitative predictions.

[1] M. Vijayakumar *et al*, J. Power Sources **196(4)**, 2211 (2011);

MM 61.2 Thu 16:00 H52

Characterization of an all solid-state thin-film battery — •Susann Nowak[1], Frank Berkemeier[2], and Guido Schmitz[1] — [1]Heisenbergstr. 3, 70569 Stuttgart — [2]Corrensstraße 46, 48149 Münster

In this talk an all solid-state thin-film battery is shown, which has been produced by ion beam sputtering of all parts, featuring LFP as the cathode material, LiPON as the solid electrolyte and tin as the anode material. The battery is characterized by means of cyclic voltammetry (CV), chronopotentiometry (CP) and transmission electron microscopy (TEM). From these measurements the capacity and its dependence on the cycle number is determined. Measurements at different scan rates (CV) and comparison of the peak currents yield kinetic information, which are compared to the parameters of the individual materials. In contrast to conventional battery cells, solid-state batteries can be operated at elevated temperatures. Experiments under variation of temperatures demonstrate that the capacity of the cell is significantly dependent on the temperature at which the cell is operated, pointing to a capacity loss due to kinetic restrains at room temperature. The obtained capacity after 100 cycles is starting at 20% of the LFP capacity (RT) and reaching 80% at 80°C. In contrast in a liquid cell the maximum capacity is already reached at room temperature.

MM 61.3 Thu 16:15 H52

Is it possible to achieve an all-solid-state thin-film Li-ion battery by laser assisted chemical vapor deposition (LA-CVD)? — •Christoph Loho[1], Azad Darbandi[1,2], Ruzica Djenadic[1,3], Oliver Clemens[1,2], and Horst Hahn[1,2,3] — [1]Joint Research Laboratory Nanomaterials, Darmstadt, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Helmholtz Institute Ulm, Ulm, Germany

Over the last decades a progressive miniaturization of electronic components took place. As a result there is an increasing demand for micro-sized power sources. In this respect an all-solid-state thin-film battery is desirable, since its excellent safety properties and easy integration in microelectronics are outstanding advantages. Furthermore, in the case of the garnet solid state electrolyte Li7La3Zr2O12, high voltage cathode materials and a lithium metal anode can be used to increase the energy density.

Chemical vapor deposition (CVD) is a suitable method to grow functional thin-films for Li-ion batteries, since it allows for homogeneous growth over large areas with high deposition rates and very high purity. Unique is also the capability of conformal, directional deposition in order to realize three-dimensional (3D) architectures.

In this contribution the successful deposition of LiCoO2 on different 3D architectures is reported. In addition, it is shown that the Li-ion conductivity of Li7La3Zr2O12 thin-films deposited by LA-CVD exceeds 10-6 S/cm. Finally, the assembly of an all-solid-state thin-film Li-ion battery is discussed.

MM 61.4 Thu 16:30 H52

$LiMn_2O_4$ as a thin-film battery electrode material — •Juliane Mürter, Susann Nowak, and Guido Schmitz — Institute of Materials Science, University of Stuttgart, Heisenbergstr. 3, 70569 Stuttgart, Germany

$LiMn_2O_4$ is a highly investigated cathode material for Li-ion batteries due to its low cost, low toxicity, and high voltage of over 4 V vs. Li. In this study, the material is deposited by ion-beam sputtering, with thicknesses ranging from 55 nm to 300 nm. Different post-deposition treatments are performed and the influence on capacity, cycle stability, and rate capability is studied. Excellent cycling stability over 500 cycles with almost no loss in capacity is achieved. X-ray diffraction (XRD) is used to determine the crystal structure. The electrochemical performance is investigated using chronopotentiometry (CP) as well as cyclic voltametry (CV).

Owing to the thin film geometry, the CV scan rate can be varied over 5 orders of magnitude presenting a consistent variation of peak current and overpotential. Using this data, experimental values are compared to kinetic models to determine the Li diffusion coefficient and the transfer coefficient through the surface.