More Silicon for more Miles? - A way to High-Energy Lithium-Ion Batteries through finishing the Silicon-Anode with Fluorinated Aromatic Isocyanates (FAI)

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The ongoing demand for Lithium-Ion Batteries (LIB) for automotive application led recently to a boost in research & development of large batteries. The usage in hybrid vehicles as the most promising short-term commercial scenario focus high-power batteries (HP) with the ability to store and release high energy amounts in short time-intervals (regenerative braking, supporting the combustion engine during acceleration).

To extend the applications-range of LIBs to Full-Hybride and native electric drive, the availability of storage systems with increased volumetric and gravimetric energy density (high-energy batteries, HE) is a precondition. Advanced oxidic *cathode materials* like NMC or NCA introduced the race to higher energy densities, but widely in combination with the fast but capacity-limited anode material graphite.

Introducing the next evolutionary leap ahead effective *anode materials* like silicon with its unique lithium-storage capability state the future material of choice. A way to handle challenging material properties such as dilatation during charging/discharging are revealed by using special *electrolyte additives* forming surface-films with special impact on silicon.

By using amorphous [1-2] or nano-sized [3-5] silicon, undesired Si_xLi_y two-phase areas with different molar volumes are avoided, whereas the design of flexible SEI-layers states a challenge. The novel additive class of Fluorinated Aromatic Isocyanates (FAI) discloses a solution.

In the course of the presented work the cycling performance, the chemical and morphologic properties of anodic films generated on Si-surfaces in FAI-containing electrolytes [6] beside electrochemical methods were studied using SEM, HATR/FTIR-spectrometry and Ion-Exchange-Chromatography (Figure 1 and 2).

Acknowledgment

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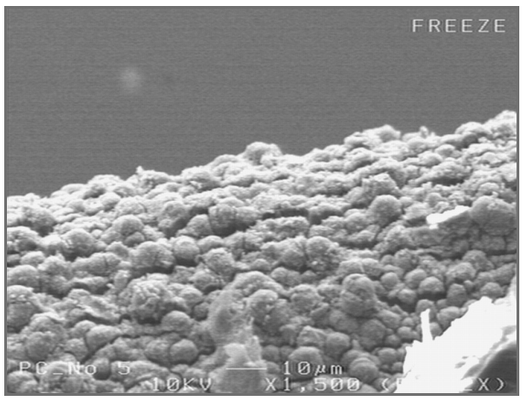

Figure 1: SEM image of the filmed anode on a folding edge after 300 cycles with 1C in EC:DEC 3:7, 1 M $LiPF_6$ + 2% (w/w) 4 - fluorophenyl isocyanate (4-FP, magnification 1500).

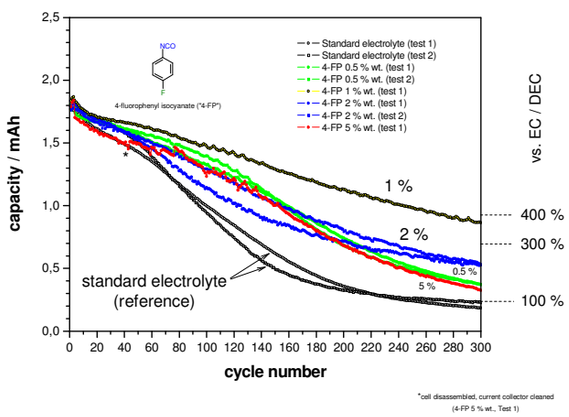

Figure 2: Discharge capacities of a Si/$LiCoO_2$-system in EC:DEC 3:7, 1M $LiPF_6$+x% (w/w) 4 - fluorophenyl isocyanate additive.

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