Insertion and extraction mechanisms of lithium in aluminum model electrodes studied by in-situ XRD: A comparison with gold

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Lithium ion batteries (LIBs) are nowadays widely used for low power applications in a wide range of consumer electronics. For future high power applications such as electromobility considerable improvements of the performance are still required. This need of progress has triggered fundamental research efforts to gain insight into the atomic-scale mechanisms during charging and discharging. In-situ techniques are often required in such studies due to the high reactivity and possible metastable phases occuring during the mostly ambient temperature processes [1,2].

We investigated the electrochemically driven insertion and extraction of Li by several techniques including lab-based characterization as well as synchrotron-based in-situ X-ray diffraction. Here we used Al poly-crystals, Au thin films prepared by PVD, as well as Au single crystals and ultra-thin nanoporous Au foils. For our measurements we used as electrolyte a 0.3 M solution of the Li salt LiTFSI in the ionic liquid 1-Butyl-1-methyl-pyrrolidinium-bis(trifluormethane)-sulfonylimide (Pyr_{14}TFSI). The Au model electrodes were polarized galvanostatically at a rate of 2.5C, the Al sample at 5C. During the lithiation/ delithiation of the gold electrodes two metastable AuLi alloy phases are involved which appear in all of the different Au model electrodes. In the case of Al the situation is different. Here only one phase is involved which forms during lithiation and dissolves during delithiation. Moreover the observed phase is exactly the AlLi phase with 1:1 composition known from the phase diagram. In contrast to Au the lithiation of Al involves only one thermodynamically stable phase.

[1] F. U. Renner, H. Kageyama, Z. Siroma, M. Shikano, S. Schöder, Y. Gründer, O. Sakata, Gold model anodes for Li-ion batteries: Single crystalline systems studied by in situ X-ray diffraction, Electrochimica Acta 53 (21), 6064-6069 (2008).

[2] P. Bach, A. Seemayer, U. Rütt, O. Gutowski, F. U. Renner, in prepartion