

Subproject 14.1

Li intercalation at a-Li_xSi electrodes probed by isotope exchange and SIMS depth profiling

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The aim of the joint projects 14.1 and 14.2 is the quantitative description of lithium intercalation at negative electrodes of lithium ion batteries, using amorphous silicon as a model system. This goal will be reached by using a combination of complementary experimental methods (see Fig.1). They comprise neutron reflectometry (NR) and neutron diffractometry (see subproject 14.2) and standard electrochemical methods (like GITT, PITT, CV, EIS) which detect charge transport and/or electrical potential variations, whereas the electrochemical quartz crystal microbalance (EQCM) allows quantifying mass and charge transport simultaneously. Further, EIS permits to differentiate between ionic and electronic conductivities (with blocking electrodes). Neither of the above mentioned two methodological “families” will, however, be able to supply direct concentration profiles on a length scale beyond about a hundred nanometers without using models. In this situation SIMS based tracer diffusion experiments are a highly versatile complementary approach to gather direct data on mass transport and phase formation. For our investigations a small classical three-electrodes electrochemical cell (see subproject 14.2, Fig. 1) will be used, which allows to apply standard electrochemical techniques as described above. With this experimental setup we will perform the following types of experiments with sputtered a-Si anode layers:

- Tracer diffusion of ⁶Li from a constant ⁶Li-enriched electrolyte at equilibrium potential into a-Li_xSi will yield the tracer diffusion coefficient D_{Li}^* and, in general, an interface exchange reaction rate constant.
- The same experiment as described above but at non-equilibrium potential will yield the chemical diffusion coefficient \tilde{D} (and a “chemical” exchange reaction rate constant).
- Standard electrochemical measurements (PITT, GITT etc.) in order to get \tilde{D} and thus also information on the thermodynamic factor $\phi = \partial \ln a_{Li} / \partial \ln c_{Li} = \tilde{D}_{Li} / D_{Li} \approx \tilde{D}_{Li} / D_{Li}^*$ (if Fickian diffusion is assumed to be rate controlling, otherwise “apparent” values will be obtained).

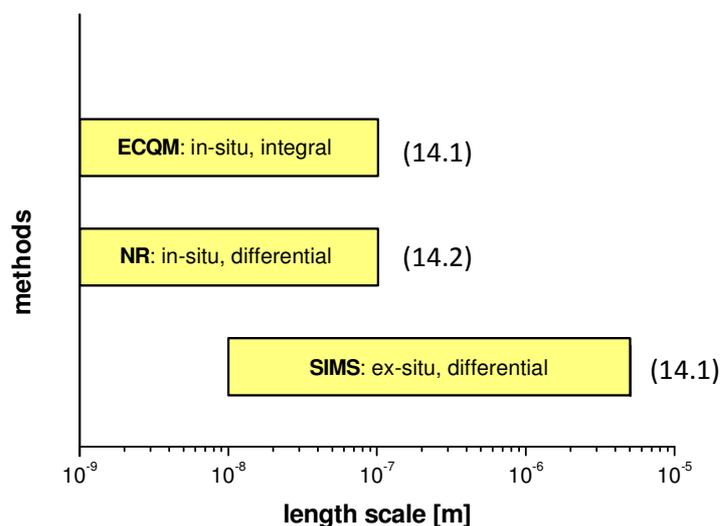


Fig. 1 The main complementary methods to be used for measuring mass transport and their respective length scales.