

Lithium Transport through Nanosized Amorphous Silicon Layers

Thursday, 19 September 2013 14:30 (30 minutes)

The talk presents an approach to use neutron reflectometry (NR) to measure non-destructively lithium transport through nanometer thin layers of, e.g., relevant electrochemical materials. Such experiments are interesting for research on nanostructured electrode materials to understand and improve high energy density lithium batteries. Beside the important role of Li diffusion for the insertion and removal of Li at electrodes, the determination of the Li permeability through ultrathin films is also of interest. This is especially true for devices where selective diffusion of Li is required. The selective filtering of Li is especially important for lithium-air batteries, Li ion selective electrodes, and sensors [1].

The methodology is demonstrated for 10 nm thin amorphous silicon layers covered by solid Li tracer reservoirs [2]. A multilayer with a repetition of five [Si / natLiNbO₃ / Si / ⁶LiNbO₃] units is used for analysis. Two types of NR Bragg peaks are detectable. One type of Bragg peaks originates from LiNbO₃/Si chemical contrast, the other one from ⁶Li/⁷Li isotope contrast. Diffusion annealing reduces the intensity of the Bragg peak resulting from the ⁶Li/⁷Li isotope contrast but not that from the LiNbO₃/Si chemical contrast. This demonstrates that the Bragg peak decrease is a measure of the ⁶Li and ⁷Li transport through the Si layer.

These results open the possibility to determine the rate determining step (diffusion controlled or interface reaction controlled) of the Li transport process and to quantify Li transport parameters (diffusivity and permeability) in nanometer thin layers as a function of (i) chemical composition, (ii) film structure (amorphous or nanocrystalline), (iii) confinement (thickness of the layer) and (iv) temperature (e.g. to determine activation energy).

References:

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- [2] E. Hüger, L. Dörrer, J. Rahn, T. Panzner, J. Stahn, G. Lilienkamp, and H. Schmidt, Lithium-Transport through Nanosized Amorphous Silicon Layers, *Nano Lett.* 2013, 13, 1237.

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