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Elucidation of the complex (de-)lithiation reactions of SnO_2 in all-solid-state battery using operando X-ray photoelectron spectroscopy

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For the successful employment of Li-ion batteries at large scale, e.g. for electrical vehicles or stationary energy storage, a crucial point is to increase of energy density in the battery. In order to increase this parameter, anode conversion-alloy materials, such as SnO_2 with a specific capacity of ~ 1500 mAh/g, are a serious choice, in particular when mixed with graphite. Despite the theoretical predictions of the different SnO_2 conversion and alloy reactions during (de-)lithiation, the experimental identification of those electrochemical reactions and the formation of intermediate species (e.g. Li_aSnO_b, Li_xSn and Li_2O) is not fully understood,[1] mainly due to their possible relaxation and conversion to other byproducts during disassembling of the cycled cell in *post mortem* analysis.[2]

In this contribution we explore the capabilities of our recently developed *operando* X-ray photoelectron spectroscopy (o-XPS) to monitor in real time the evolution of the electrolyte-electrode interface and the (de-)lithiation processes of the active materials during solid state Li-ion battery operation.[3] In particular, we present the results of our study on the (de-)lithiation of the SnO_2 particles in a working electrode composed of SnO_2 nanoparticles, $(Li_2S)_3$-P_2S_5 (LPS)[4] solid electrolyte (SE) and Super P as conductive carbon cycled versus $InLi_x$ counter electrode (Figure 1a). The analysis of the Sn 3d (Figure 1b), Sn 4d, O 1s (Figure 1c) and Li 1s spectra reveals the progressive conversion of the SnO_2 particles to form Sn^0 and the simultaneous formation of the Li_xSn alloy. When the potential is below 0.4 V (vs. Li^+/Li), the Li_2O phase is formed and grows until the full lithiation at 0.01 V (vs. Li^+/Li), where the only species observed are Li_2O and Li_xSn. During the de-lithiation process, the partial reversibility of the conversion-alloy reactions takes place, where Li_xSn is converted to SnO_x at 2.5 V (vs. Li+/Li). The S 2p and P 2p core levels reveal the presence of reduced Li_2S byproduct species below 1.6 V (vs. Li+/Li), in accordance with previous studies.[4]

References:

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