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Neutron Depth Profiling and X-Ray Diffraction to Study Lithiation Mechanism of LiAl Electrodes

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Metal alloys, such as LiAl, are gaining more interest as anode materials for Li ion batteries because they exhibit a high theoretical capacity with 993 mAh/g while being inexpensive. During lithiation, aluminium begins to form a solid solution with Li, the so called alpha-LiAl phase. Once the solubility limit is reached upon lithiation, the alpha-LiAl undergoes a phase transition to the beta-LiAl phase.
Al electrodes were electrochemically lithiated to different state of charges in coin cells with Li metal as counter electrode. X-ray diffraction measurements were conducted on the disassembled anodes.The Rietveld refinements yield that the samples charged to SoC25 show a higher amount of alpha-LiAl. Simultaneously, the amount of beta-LiAl in the samples increases with higher SoC as expected.
Additional neutron depth profile measurements were performed in NPI CAS Rez at the CANAM infrastructure to determine the Li distribution throughout the lithiated samples. First results have confirmed that the lithiation of the aluminium starts at the surface where a higher Li concentration was identified. The higher charged sample also shows a stronger lithiation in the bulk of the Al anode. In the lower charged sample, no Li was detected near the backside of the anode, indicating that pristine Al is still present.
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