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X-ray Diffraction Studies on the Lithiation of LiAl Electrodes for Lithium Ion Batteries

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Metal alloys as anode material for lithium ion batteries such as LiAl offer a high theoretical capacity in relation to their low cost. Compared to the conventional graphite anode, aluminium has an almost three times higher specific capacity with 993 mAh/g. During lithiation, aluminium first forms a solid solution with lithium called the alpha-LiAl phase until the solubility limit is reached. Subsequently, the alpha-LiAl will transform to the beta-LiAl upon further lithiation near the electrolyte-electrode interface.

Here, phase identification via x-ray diffraction (XRD) measurements was performed in order to help the understanding of the lithiation mechanism. First results have shown that both alpha-LiAl and beta-LiAl are present within the sample. Higher lithiated phases such as Al₂Li₃ could not be identified. For both SOC 25 and SOC 50 however, LiOH could be determined as an additional phase whereas the percentage was higher for samples charged to SOC 50. Similarly, a higher amount of beta-LiAl was identified while the samples charged to SOC 25 showed an increased percentage of alpha-LiAl. Operando XRD measurements are planned that will minimize the ambient air related formation of LiOH and allow the measurement of alpha- and beta-LiAl nucleation directly under protective conditions.

This work is performed as a collaboration between TUM (Heinz Maier-Leibnitz Zentrum, FRM II) and RWTH Aachen (ISEA) in the frame of the BMBF project ExcellBattMat cluster.

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