Intercalation of lithium into disordered graphite in a working battery - DTU Orbit
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Intercalation of lithium into disordered graphite in a working battery
The structural transformations occurring during the intercalation of lithium into disordered graphite in a working battery were studied in detail by operando X-ray powder diffraction (XRPD). By using a capillary-based micro-battery cell, it was possible to study the stacking disorder in the initial graphite as well as in lithium-doped graphites. The micro-battery cell was assembled in its charged state with graphite as positive electrode and metallic lithium as counter electrode. The battery was discharged until a stage II compound (LiC12) was formed. The operando XRPD data reveal that the graphitic electrode material retains a disordered nature during the intercalation process. A DIFFaX+ refinement based on the initial operando XRPD pattern shows that the initial graphite generally has an intergrown structure with domains of graphite 2H and graphite 3R. However, the average stacking sequence of the initial graphite also contains a significant concentration of AA-type stacking of the graphene sheets. DIFFaX+ was further used to refine structure models of a stage III type compound and the final stage II compound. The refinement of the stage II compound showed that it is dominated by $\text{A}_2\text{A}_3\text{A}_2\text{A}_3$ stacking, but that it also contains a significant concentration of $\text{A}_2\text{A}_3\text{B}_2\text{B}_3$-type slabs in the average stacking sequence.

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