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Thermal structural stability of lithiated graphites

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Nowadays, 2H graphites are the most common anode materials in LIBs. Despite its overall popularity, the performance of LIBs is still limited by the capability of graphite electrodes to store lithium ions in its structure. Graphite builds up a layered hexagonal structure. During charging and discharging lithium ions are reversibly incorporated in the hexagonal structure resulting in the formation of lithiated graphite phases Li_xC_6 ($0 < x < 1$) of different kinds.

Despite the overall popularity there is a clear lack of information about the structural behaviour of Li_xC_6 at compositions of $x < 0.25$ [1, 2]. Even less information is available about the thermal stability of graphite anodes, which becomes more and more popular in the context of all-solid-state-batteries or fast charging.

In the current contribution, a temperature resolved diffraction study on variously lithiated Li_xC_6 samples is presented, where battery graphites were pre-lithiated to a desired lithiation grade in a Li-ion battery and then harvested. The thermal behavior of structural parameters was probed by using powder diffraction studies applying high-energy synchrotron radiation.

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