Thermal structural stability of lithiated graphites

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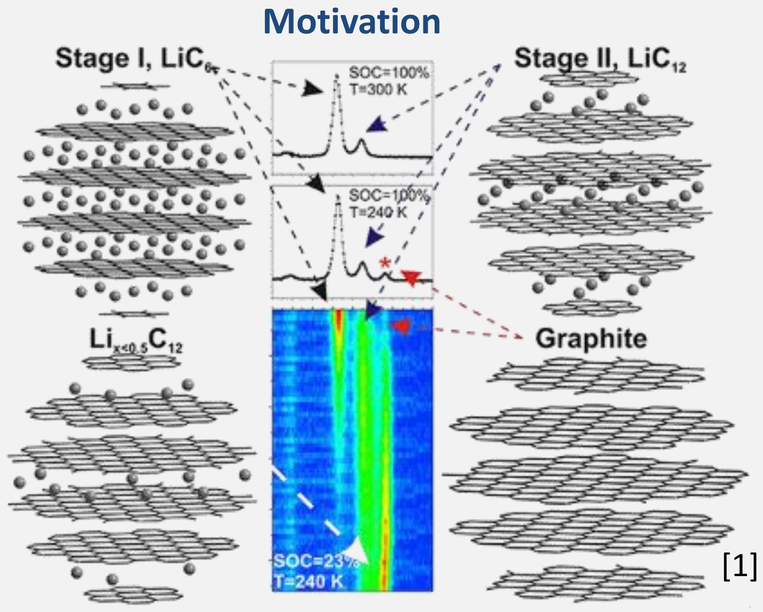
Aim and results

1. Probing thermal phase stability of differently lithiated graphites
2. Clarification of lithiated graphite phase evolution on the level of phase diagram
3. Information about high temperature stability of lithiathed graphites
4. Correlation with counter electrode thermal behavior

→ Motivation and selected results for a series of commercial NCR18650GA-type cells

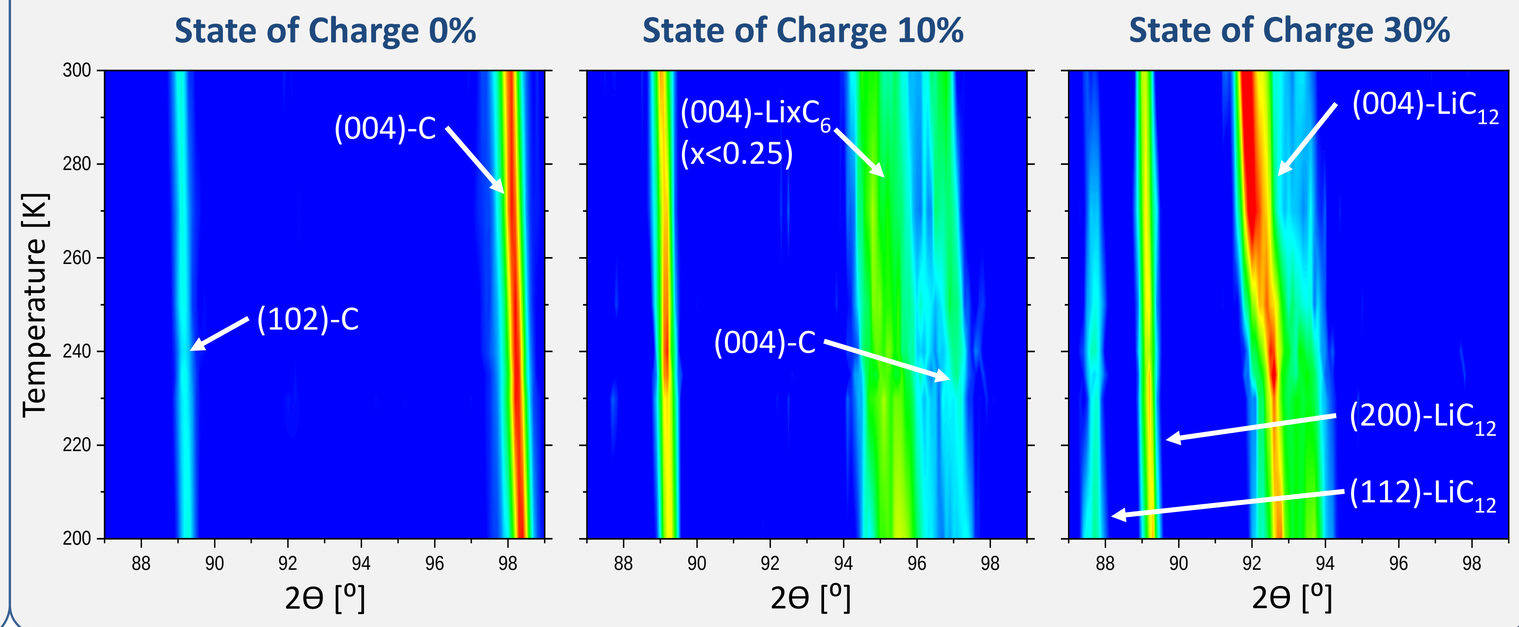
Motivation



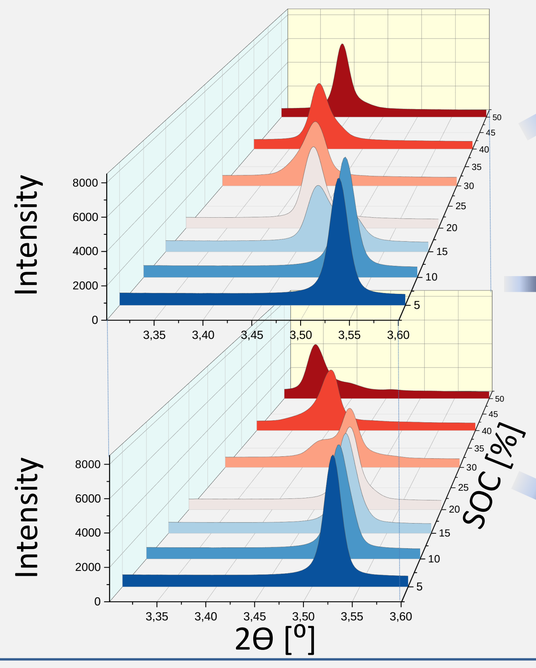
[1]

→ Different lithiated graphite stages in the scope of various state of charges and temperatures

High-resolution neutron powder diffraction of differently intercalated graphite phases



High- resolution x-ray powder diffraction



Temperature: 500K

Blue: (002)-Graphite
Red: (002)-LiC_{12}

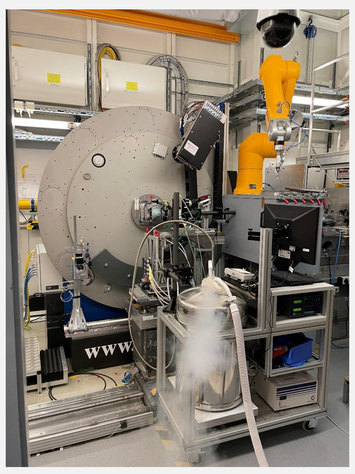
Temperature: 180K

Discussion and outlook

1. Motivation
   - Ongoing debates about the complex phase diagram of Li_xC_6, especially for small x
   - Temperature resolved phase stability is studied poorly and results are often controversial due to anomalous structural changes and inconsistencies in the temperature stability of Li_xC_6
   - Diffraction signature of lithium pathways between LiC_{12} and C has been found different at a set of temperatures, indicating structural instability for Li_xC_6 with $x < 0.25$
2. Measurements:
   - Exploratory temperature dependent ex-situ XRD studies on differently intercalated graphite samples that were precharged in commercial NCR18650GA-type batteries
   - Identification of graphite phases by full-profile Rietveld refinement and analysis of temperature resolved structural stability
3. Outlook:
   - Temperature dependent *ex-situ* XRD measurements at DESY of intercalated graphites with Li_xC_6 compositions where $x < 0.25$ in a temperature range from 180K to 500K
   - Further neutron measurements at SPODI with higher sensitivity to detect Li ions

→ For better battery performances the mechanisms of thermal induced structural behavior of negative, as well as positive cell electrodes has to be further investigated. Such structural data will clarify the phase diagram in the above-mentioned temperature region. Furthermore, it will provide information about high temperature stability of Li-ion batteries at higher temperatures, which become especially relevant in the scope of so-called asymmetric temperature modulation actively discussed with regard to fast charging [2]

Methods



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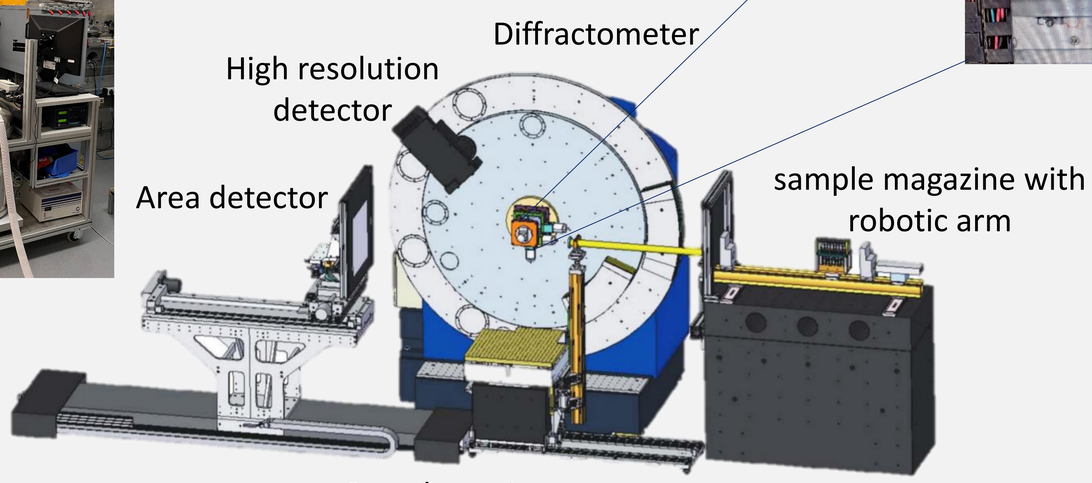
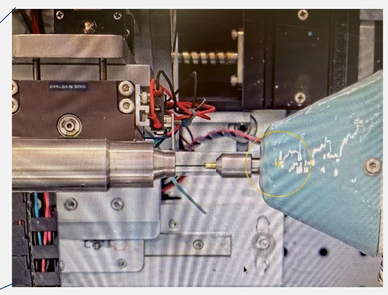
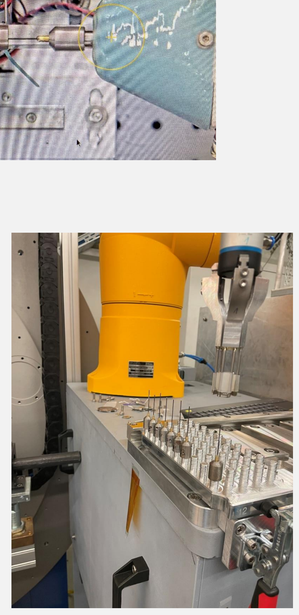
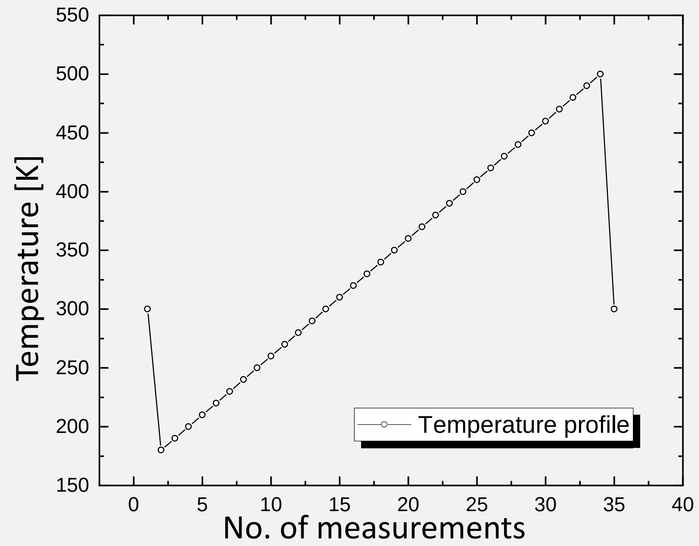
X-Ray Powder Diffraction
Beamline P02.1 Petra III, DESY
Experimental setup







Temperature profile maintained by Oxford Cryostream



→ Temperature profile covering 180K to 500K with start and stop at 300K

Quellen

[1] A. Senyshyn, M. J. Mühlbauer, O. Dolotko, and H. Ehrenberg, Journal of Power Sources **282**, 235-240 (2015)
[2] X. G. Yang, T. Liu, Y. Gao, S. Ge, Y. Leng, D. Wang, C.-Y. Wang, Joule **3,** 3002-3019 (2019)
[3] A. C. Dippel, H. P. Liermann, J. T. Delitz, P. Walter, H. Schulte-Schrepping, O. H. Seeck, and H. Franz, Journal of synchrotron radiation **22**(3), 675-687 (2015)

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