Investigating the phase transitions of graphite by in situ neutron diffraction

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1. Stage transitions in graphite

Motivation:
1) Graphite in 90\% of today's batteries
2) Phase transitions show different C\texttextsuperscript{}rates [1]

Investigate phases by in situ XRD/NPD

graphite
stage 2L
stage 2
stage 1

Working hypothesis:
Graphite has distinct phases also at low state-of-charge

2. In situ cell

1) XRD: Pouch cell (polyimide and propylene window)
2) NPD: Cell with TiAl\texttextsuperscript{2} container with deuterated electrolyte LP30-D

new circular in situ NPD cell [4]

3. In situ x-ray and neutron powder diffraction

In situ XRD:

potential vs. Li / V

specific charge / mAhg

In situ NPD:

potential vs. Li / V

specific charge / mAhg

4. Results

Refinement of different phases:

Stage 1:

Y贵族
Y\texttextsuperscript{}caca
Y贵族-Y\texttextsuperscript{}calc
Bragg positions

Lattice parameter evolution:

C-C distance

C-C distance follows Vegard's law

graphene interlayer distance non-linear

Summary: In situ XRD:
1) less good method for Li-graphite system (low scattering of C, Li)
2) easy to redo at any synchrotron, very good electrochemistry in cell

In situ NPD:
1) very good results for Li-graphite diffraction
2) high overpotentials for 200 mg/cm\textsuperscript{2} loading and neutron sources needed

4) The first phase, proper determination of Li-in-plane concentration in disorder states

[C\texttextsuperscript{}]|C\texttextsuperscript{}|C


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