

# Lithium-Ion Batteries from a Neutron Point of View

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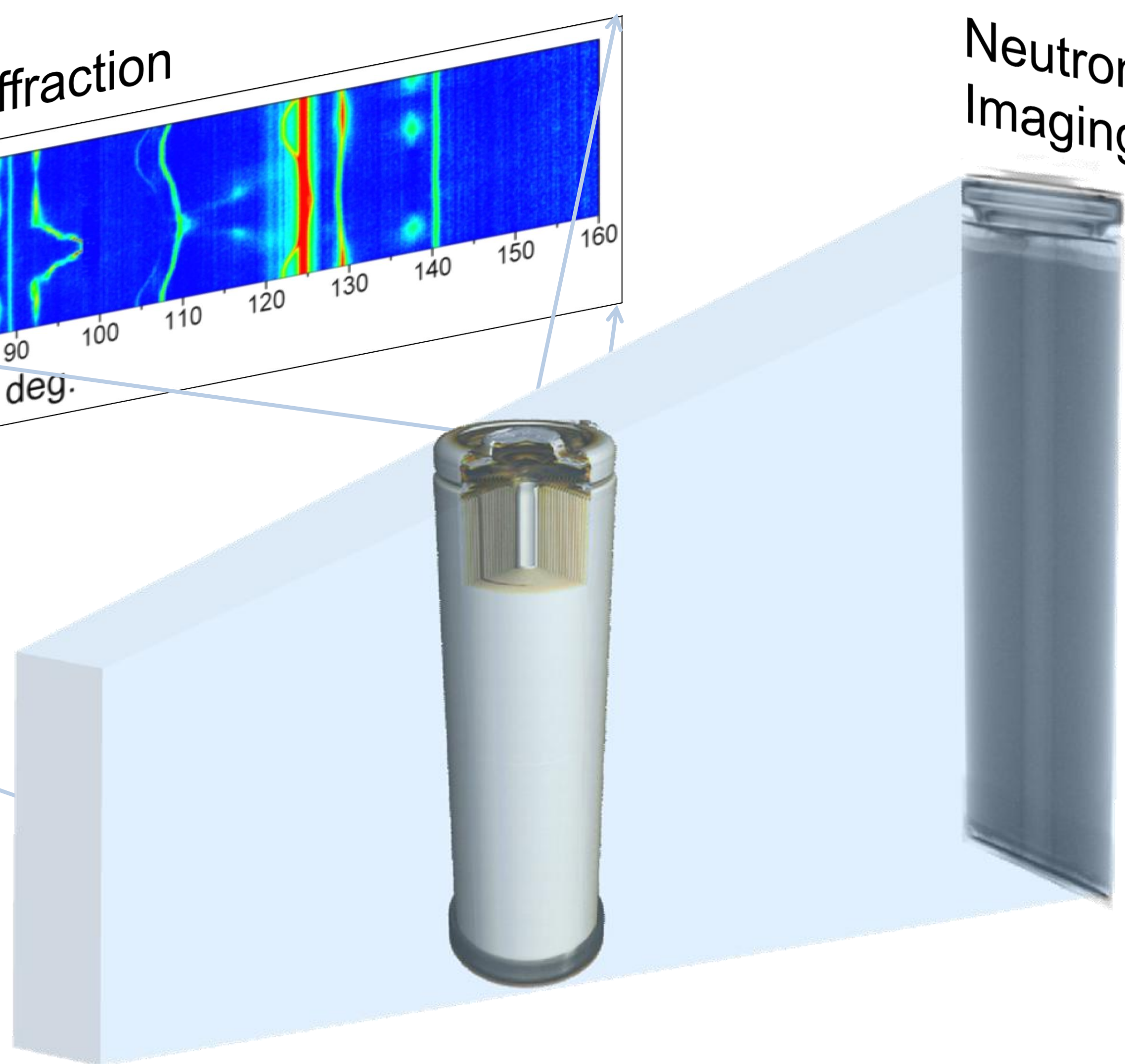
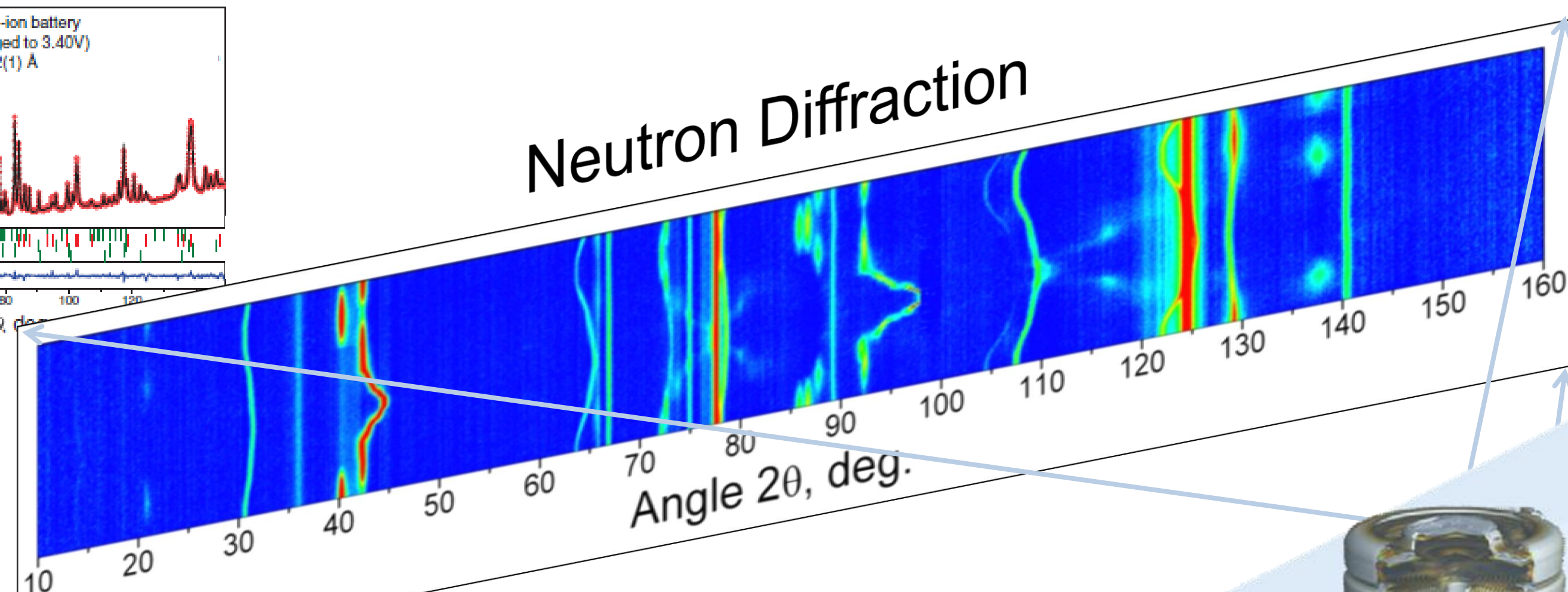
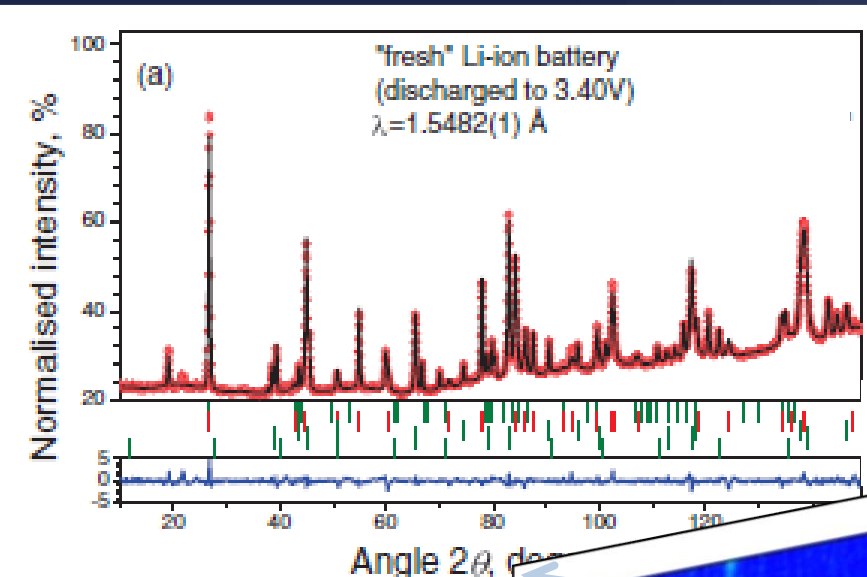
## Motivation and objectives

- The improvement of Lithium-ion batteries needs new materials and advanced cell concepts.
- Complex interactions between components require a characterization of materials at least on cell level.
- Life-time modelling and safety issues need to be considered on complete devices.
- Proceeding of fatigue can only be studied by non-destructive methods.



- Multi-phase refinements of the underlying crystal structures, including light elements and microstructure parameters.
- Improving spatial resolution in order to resolve components on a length scale of ~10-100  $\mu\text{m}$ .
- Correlation of state-of-charge (SOC) and state-of-health (SOH) with structural details.
- Revealing working and fatigue mechanisms.
- Establishing comprehensive life-time models and failure scenarios (supported by complementary methods)

## Approach



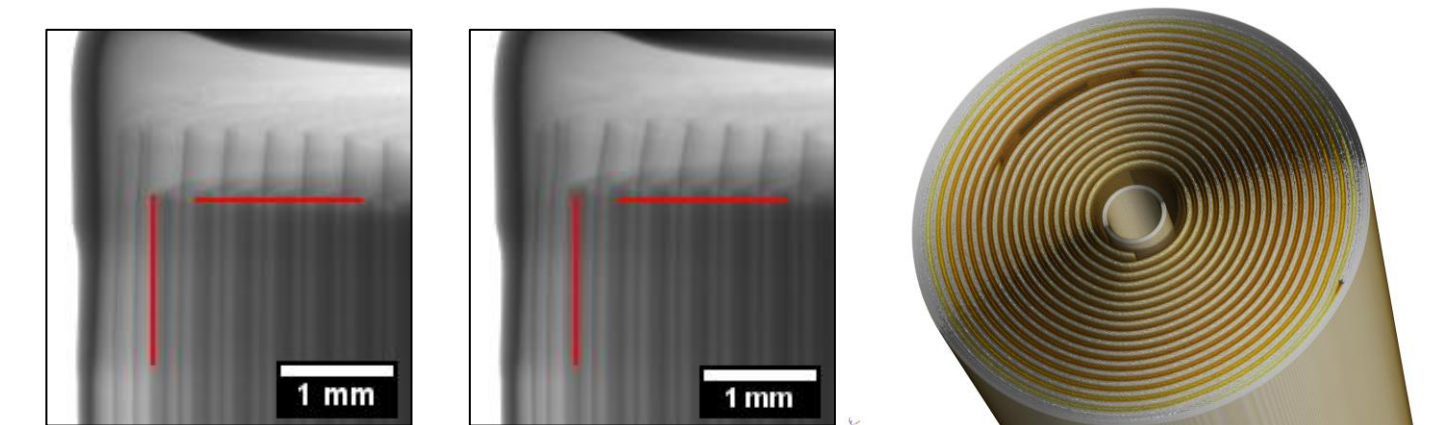
### Neutron Imaging:

- Sensible for changes on a length scale of micrometers
- Deep penetration of neutrons into the matter
- meV energy for epithermal neutrons
- High absorption cross section for lithium; sufficient absorption contrast for transition elements
- 3D representation of the whole sample volume

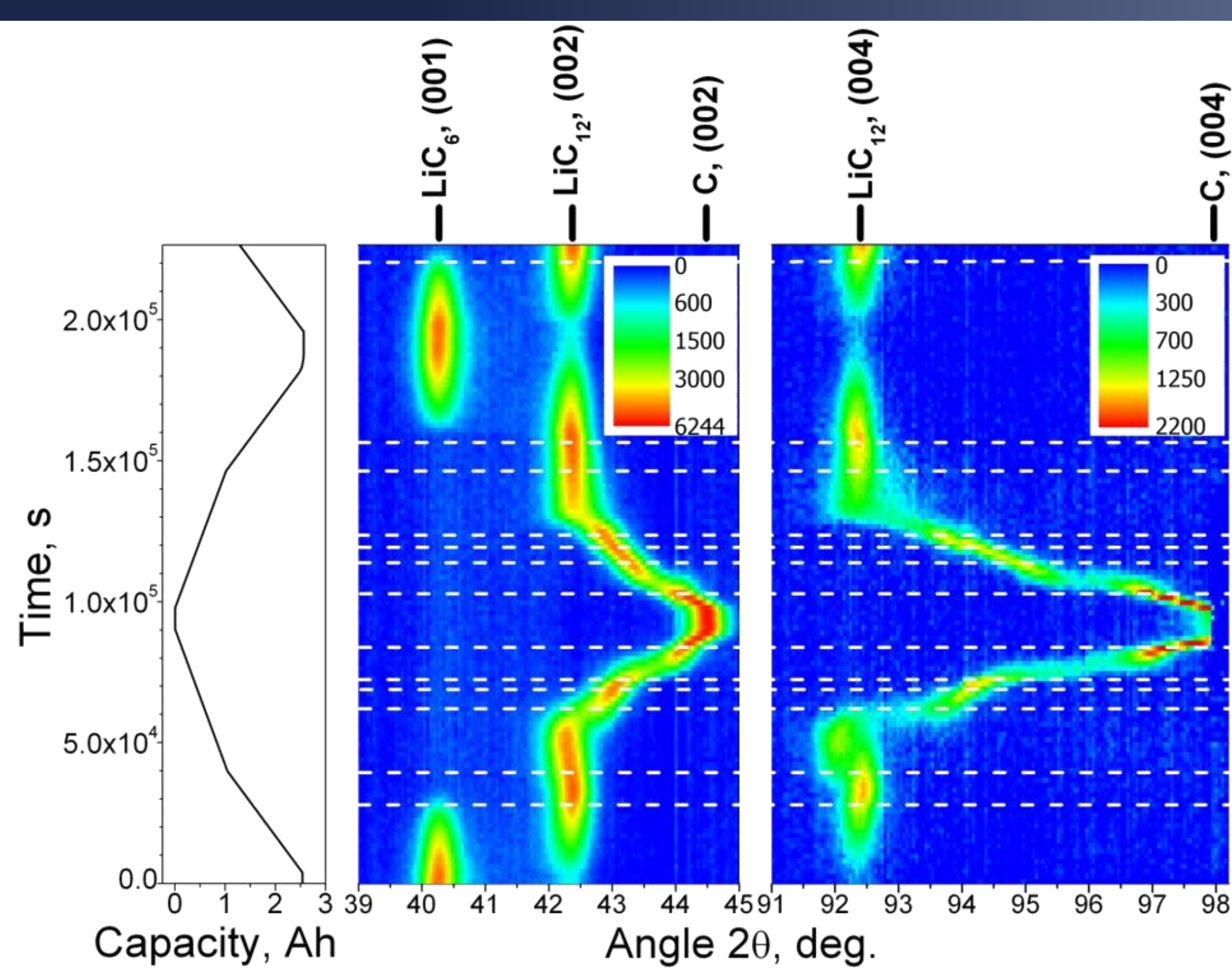
### Neutron Diffraction:

- Sensible for changes on an atomic length scale
- Sensitivity to light atoms; discrimination of transition elements
- Accurate determination of atomic positions and Debye-Waller factors
- Averaging over sample volume

Complementary X-ray data for details of cell geometry

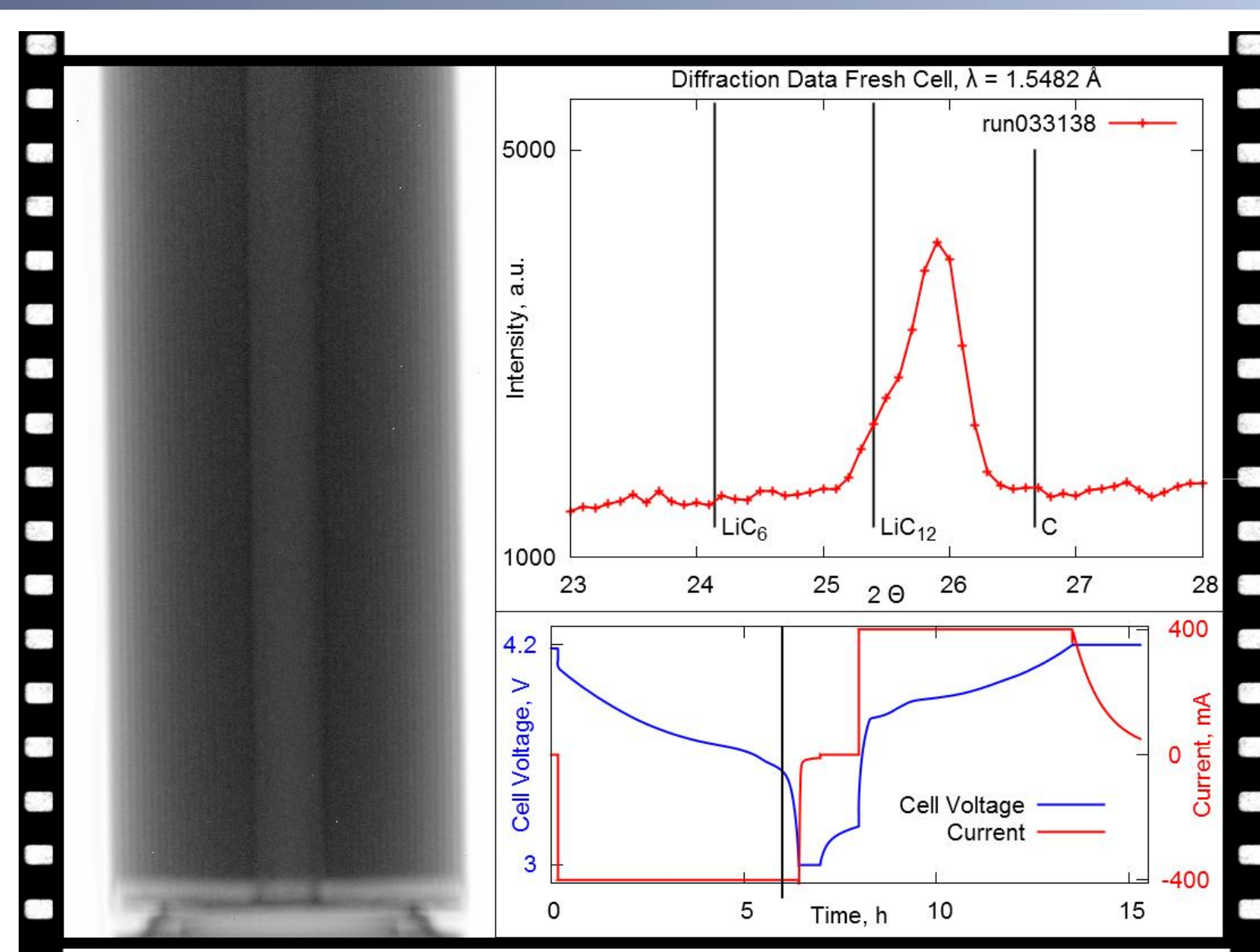


## Results

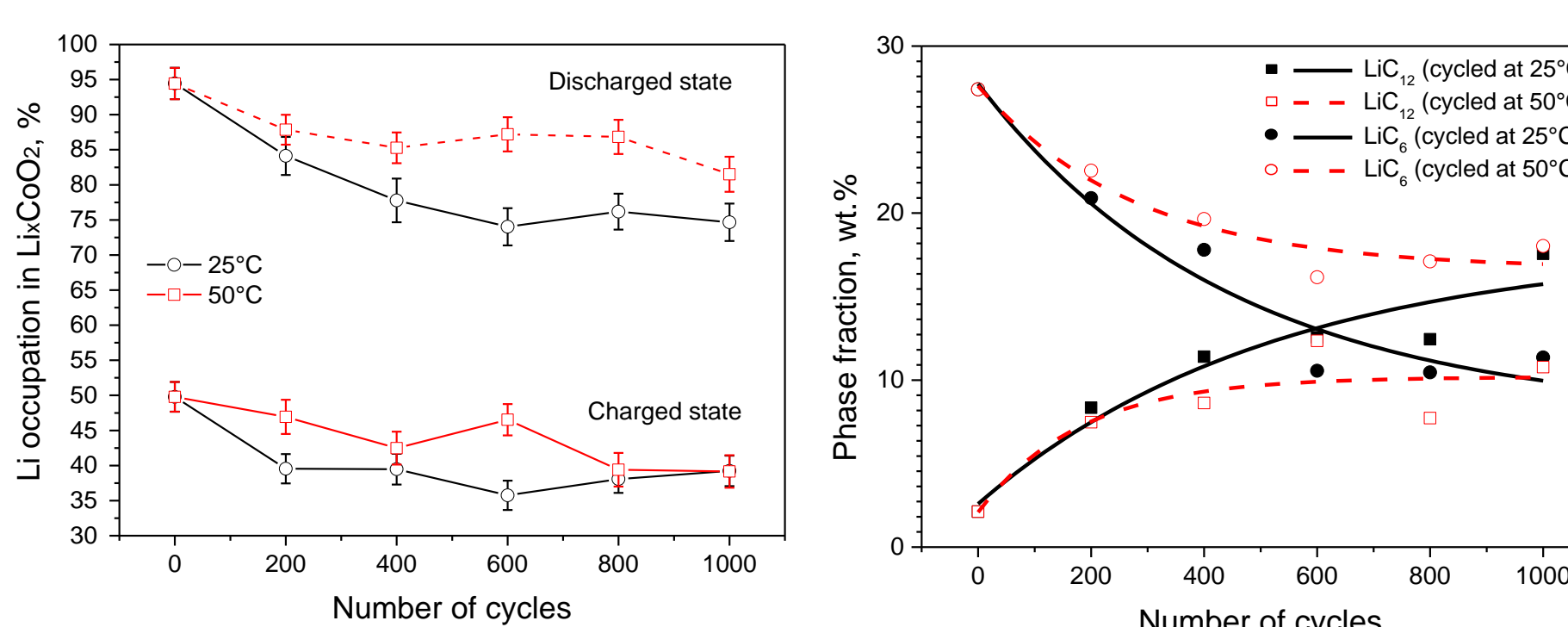


Time resolved neutron diffraction revealing an asymmetry in lithium intercalation

A. Senyshyn, O. Dolotko, M.J. Mühlbauer, K. Nikolowski, H. Fuess, H. Ehrenberg, *Journal of The Electrochemical Society*, 160 (5) A3198-A3205 (2013)

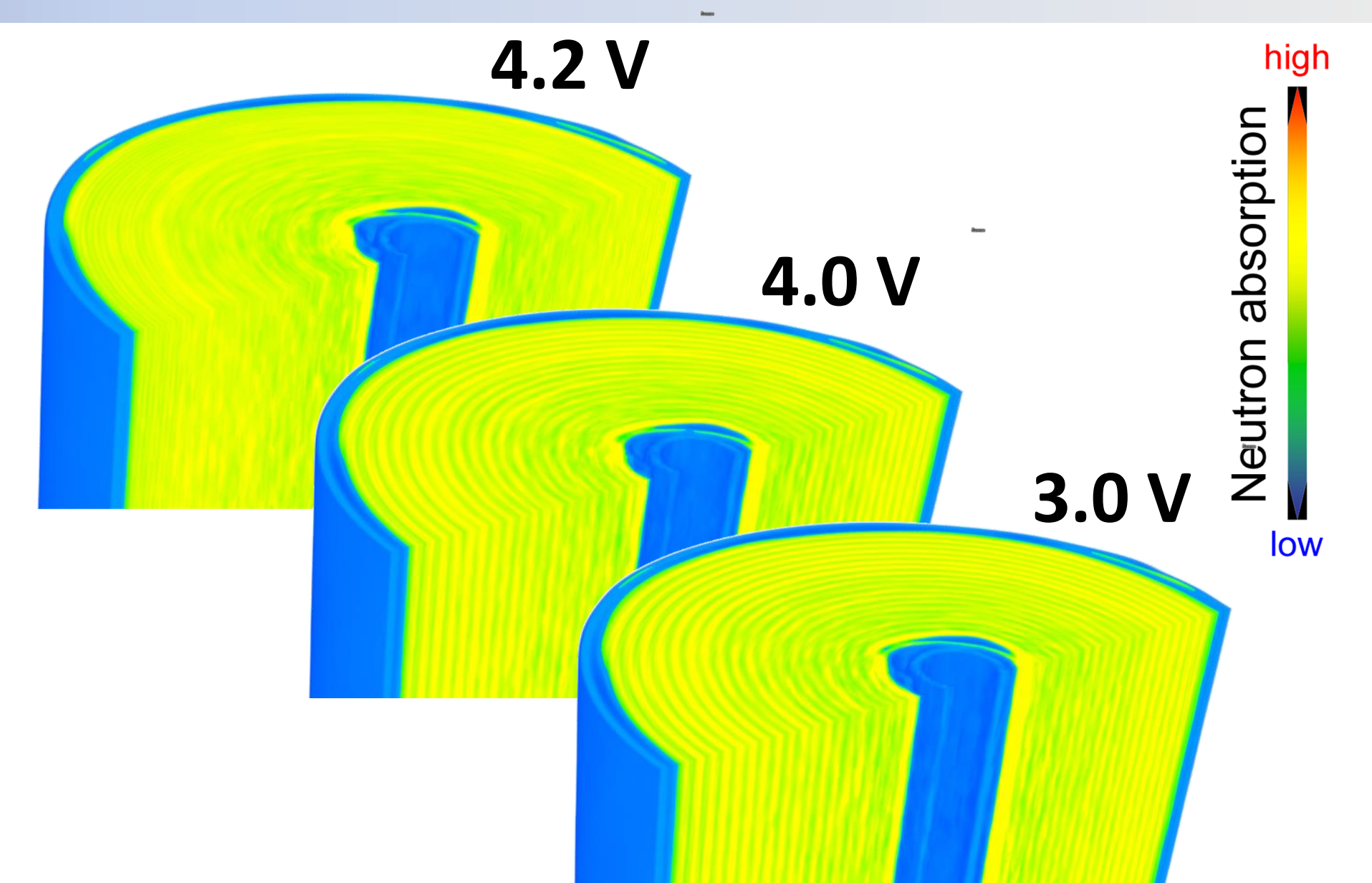


Charge and discharge of cells with simultaneous acquisition of neutron diffraction and imaging data



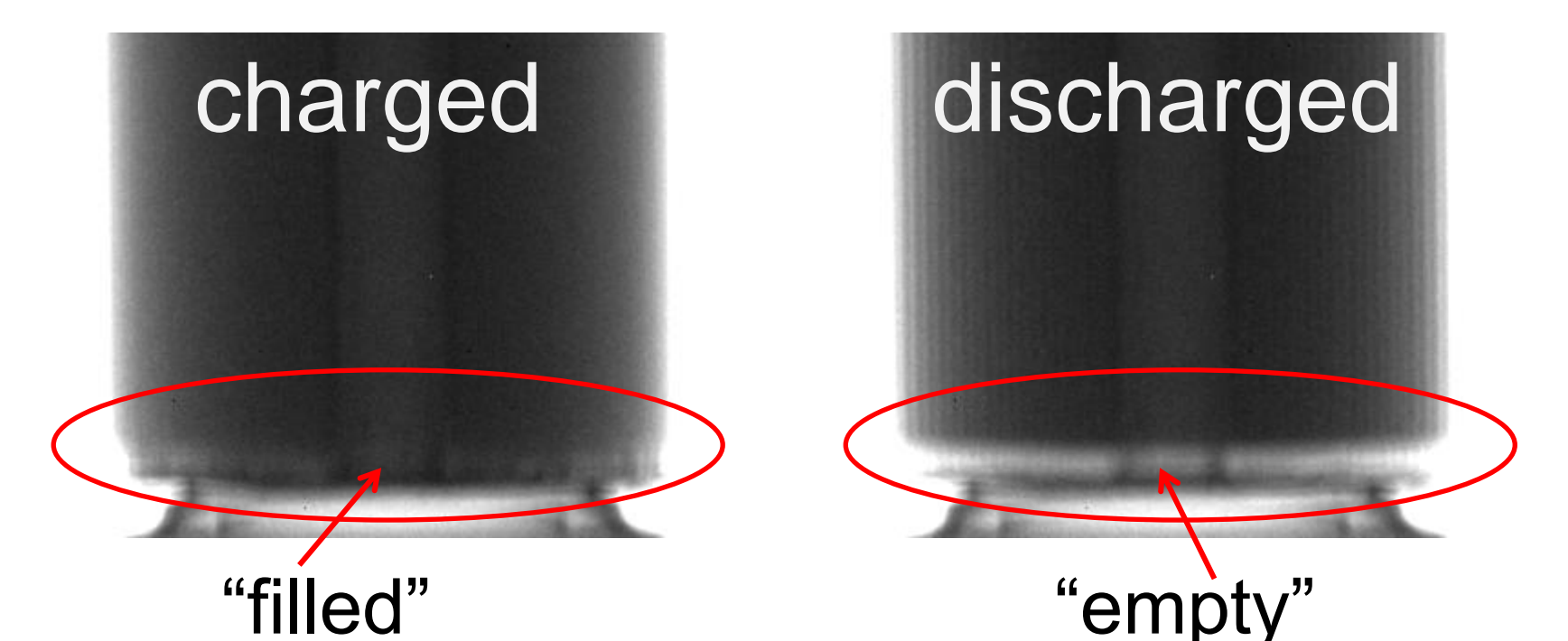
Lithium occupation of cathode and anode for different states of fatigue

O. Dolotko, A. Senyshyn, M.J. Mühlbauer, K. Nikolowski, F. Scheiba, H. Ehrenberg, *Journal of The Electrochemical Society*, 159 (12) A1-A7 (2012)

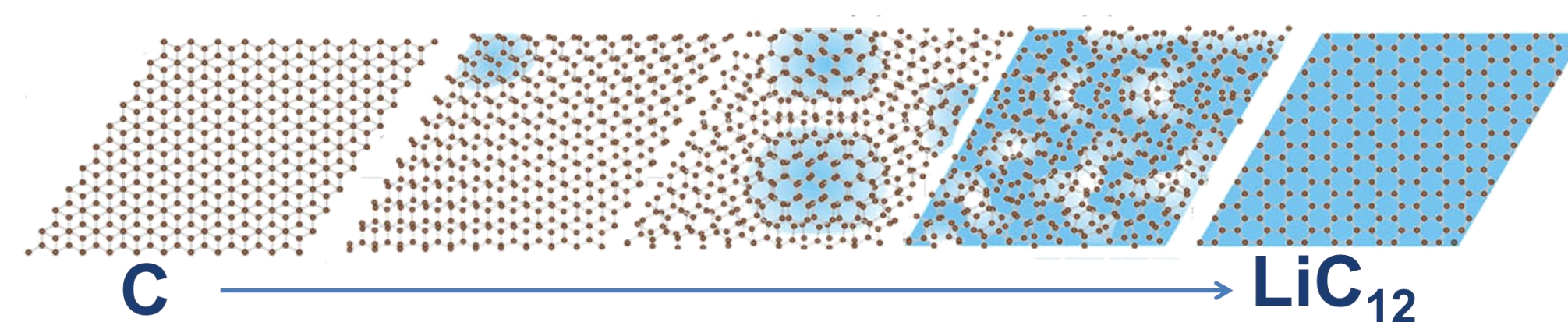


Exchange of lithium causes the neutron attenuation to change according to the state of charge

A. Senyshyn, M.J. Mühlbauer, K. Nikolowski, T. Pirling, H. Ehrenberg, *J. Power Sources* 203 (2012) 126-129



Due to volume change of the electrodes the electrolyte level inside the reservoir is altered



Deviation from the expected stage formation of lithiated graphites at low lithium content