PAUL SCHERRER INSTITUT

ELECTROCHEMISTRY LABORATORY

BATTERIES

supported by BASF The Chemical Company

Modification of High Energy NCM $Li_x(Ni_aCo_bMn_c)O_2$

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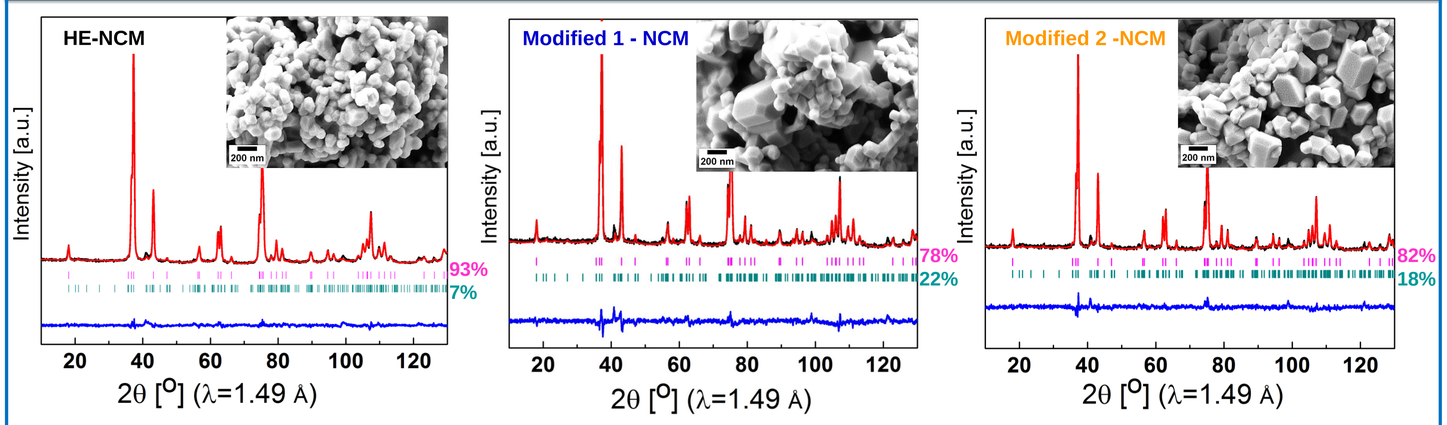
Motivations and challenges

Layered materials $Li_x(Ni_aCo_bMn_c)O_2$ (HE-NCM) → + : high voltage, high specific charge: 250 mAh/g

→ - : ageing (voltage drop, specific charge fading)

Goals:
1. Increase cycling stability
2. Mitigate voltage drop

Neutron diffraction

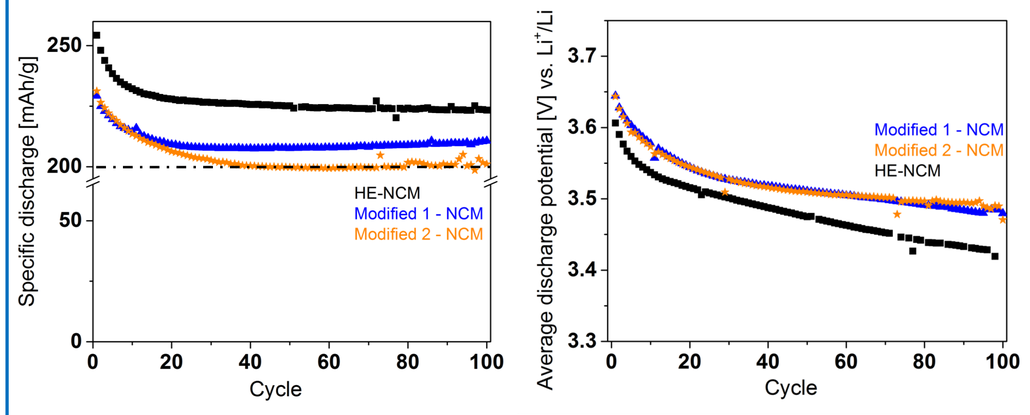


Structure maintained by modification of NCM, 2 phases *R-3m* / *C2/m*

Increase of lattice volume when NCM is modified

Electrochemistry 1 – Performance

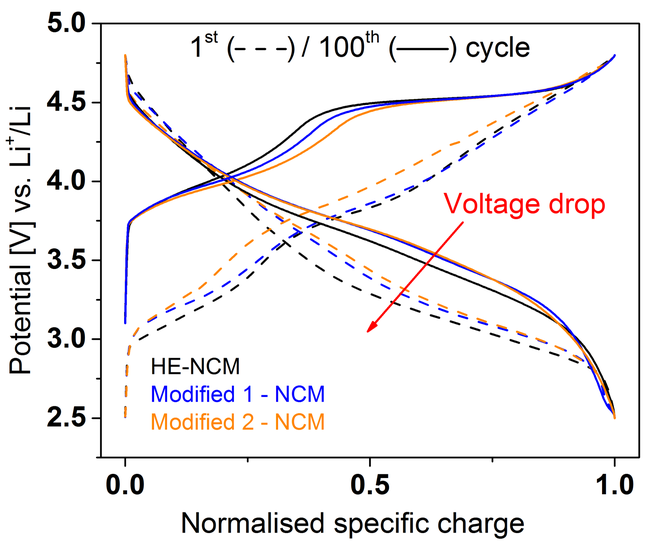
Half cells, 1M $LiPF_6$ in EC:DMC 1:1, 2 – 4.8 V vs. Li^+/Li, C/10



> 200 mAh/g after 100 cycles

Mitigation of potential drop for modified - NCM

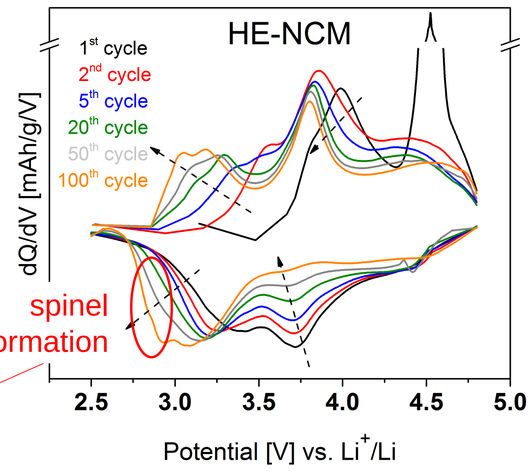
Electrochemistry 2 - Load curves

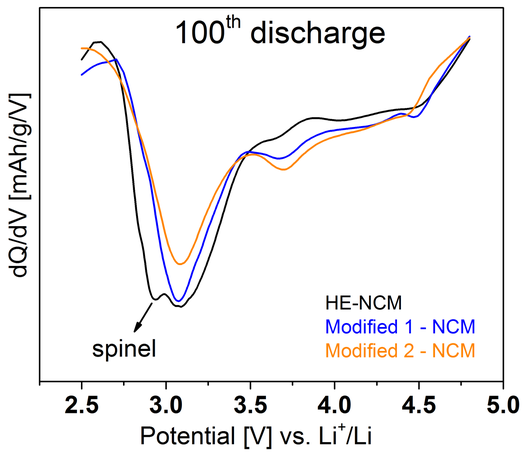


Overpotential for modified-NCM compounds in discharge

Larger hysteresis for Modified 2 - NCM

Potential plateau at ~ 3.0 V in discharge only for HE-NCM (spinel)

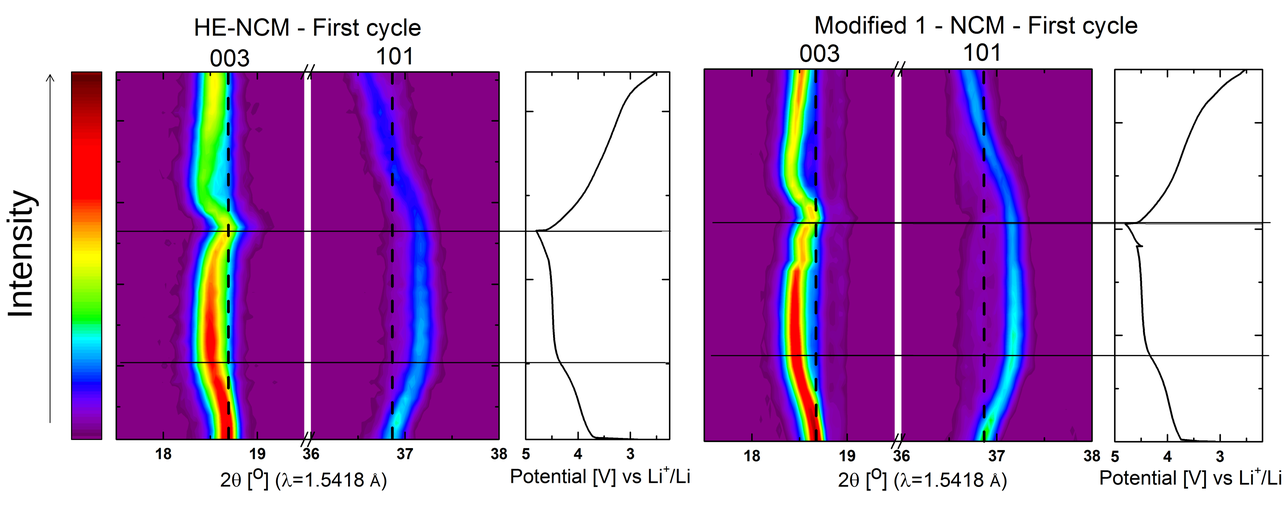


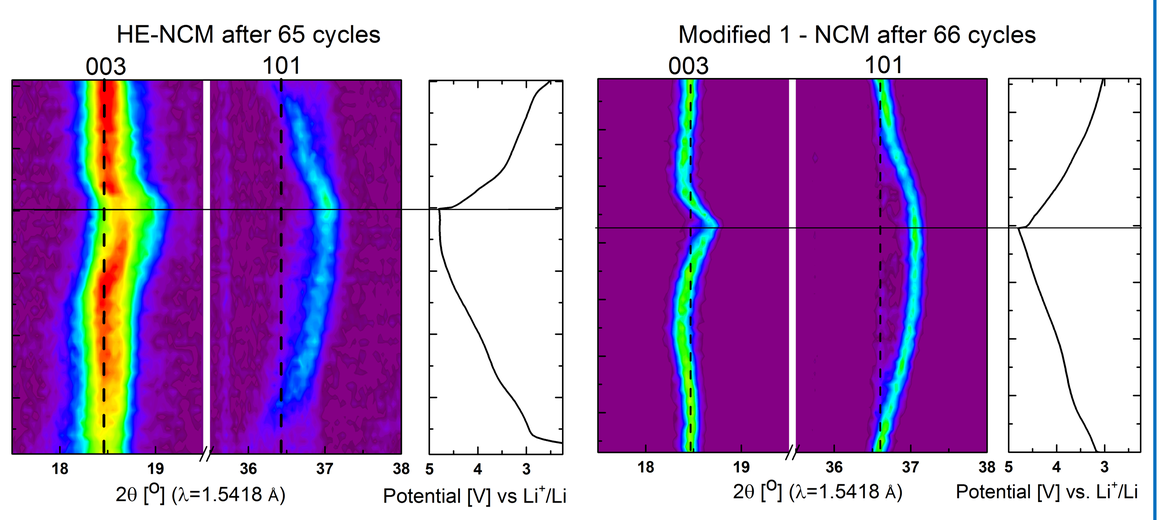


Structural changes more pronounced for HE-NCM

- Spinel observed for HE-NCM only
- More electrochemical activity at potentials > 3.5 V for modified -NCM

Operando XRD characterisations - *HE-NCM and modified 1 - NCM*





First cycle:

Same trends observed: Li_2MnO_3 activation on the 1st charge

Less shift of the (003) peak for modified 1 - NCM at the end of charge

Less structural changes on the first cycles for modified 1 - NCM

After 65 cycles:

(003) peak less broad, less shifting at the end of charge for modified 1 - NCM

Less changes in lattice parameter along the *c*-axis on charge

Conclusions and outlook

- **Cycling stability** improved for modified 1 - NCM and **specific charge** maintained > 200 mAh/g after 100 cycles
- Voltage drop mitigated
- Fewer structural changes observed