Orientation control in NMC 811 thin films for interface analysis

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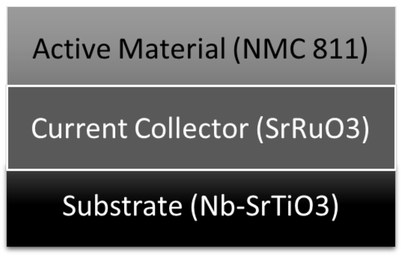
Motivation

$LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811)
- ✓ High energy density (~ 800 Wh/kg)
- ✓ Less cobalt usage
- X Reduced stability
- X Capacity fading over cycling

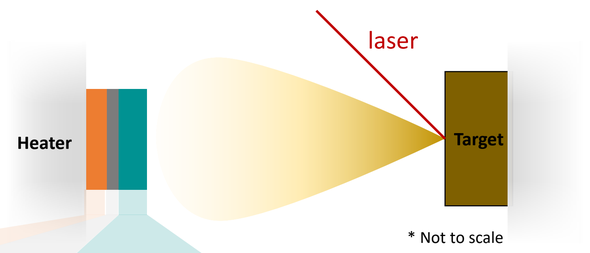
Thin film battery model
- ✓ Without conductive materials or binder
- ✓ Tunable crystal orientation
- ✓ Surface-enhanced electrode
- ✓ Enabling analysis of cathode - electrolyte interface

Scientific Challenge
- The impact of crystal facet on performance at the interface
- Study the parasitic reactions occurring at the electrolyte/cathode interface



Thin Film Model

Thin Film Synthesis
Pulsed Laser Deposition



$Nb:SrTiO_3$ (100), (110),(111)	$SrRuO_3$	NMC811
Nb: 0.5 wt%	T: 600 °C	T: 700 °C
Annealed:	v: 2 Hz	v: 10Hz
950 °C, 90 min	P: 0.13 mbar	P: 0.23 mbar
	#: 5400	#: 7200
	60 nm	70 nm

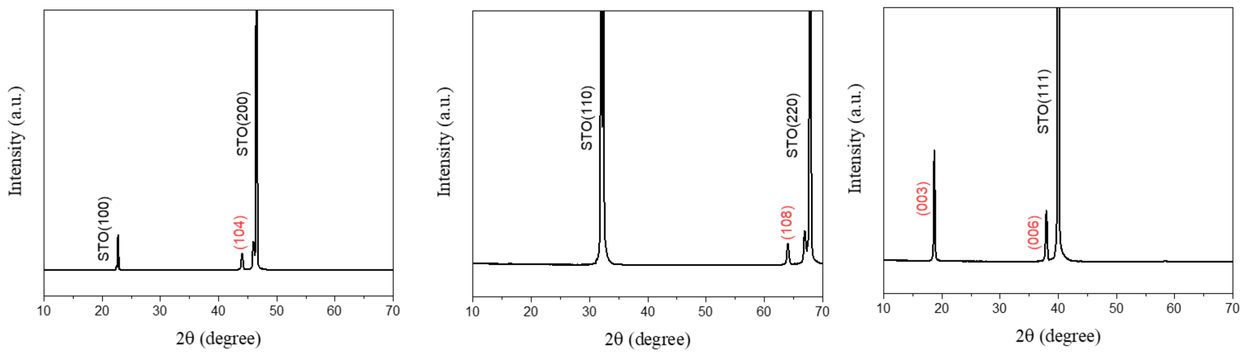
Characterization

- **Inductively coupled plasma mass spectrometry**

  The stoichiometry of thin film is $Li_{1.092}Ni_{0.803}Mn_{0.097}Co_{0.099}$

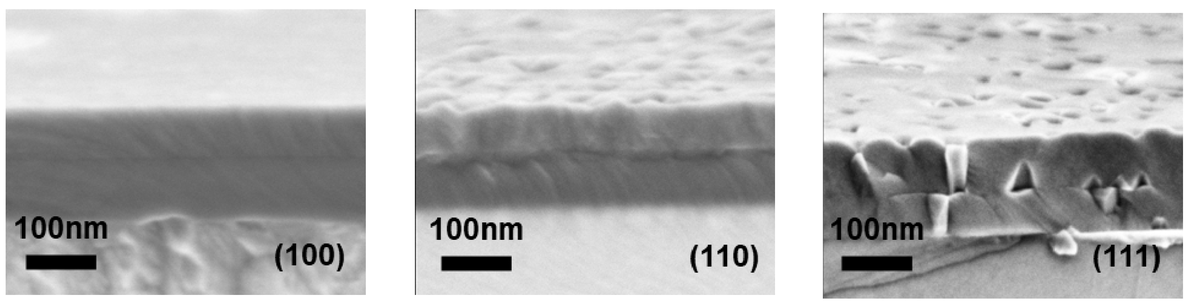
- **X-ray Diffraction**

  Variation of the crystal orientation of the underlying substrate template leads to different types of NMC811 thin films each exhibiting a single crystal orientation, i.e. (104), (018) or (003).



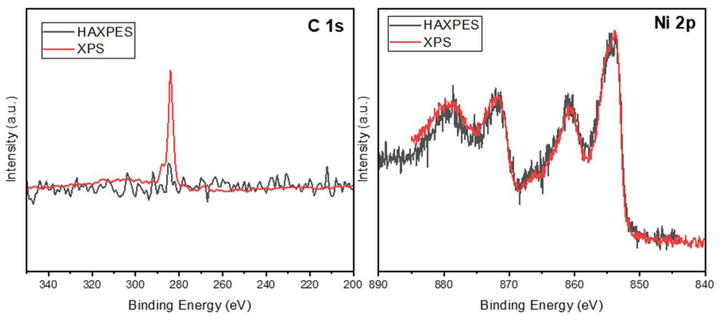
- **Scanning Electron Microscopy**

  Cross-sectional morphology of the NMC811 thin film indicates dense structures with flat surfaces, exhibiting a roughness of approximately 5 nm.

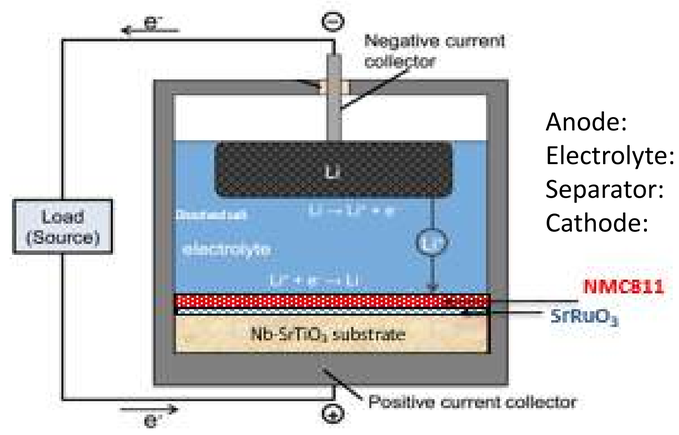


- **X-ray Photoelectron Spectroscopy**

  XPS and HAXPES spectra exhibit the same shape for the Ni 2p peak, indicating similarity between the surface and bulk composition of the thin film**.**



Cell Assembly

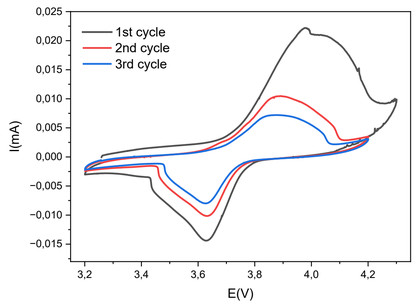


Anode: Li metal
Electrolyte: 1M $LiPF_6$ in 1:1 EC:DMC
Separator: Glass fiber
Cathode: NMC 811 thin film

Electrochemical Property

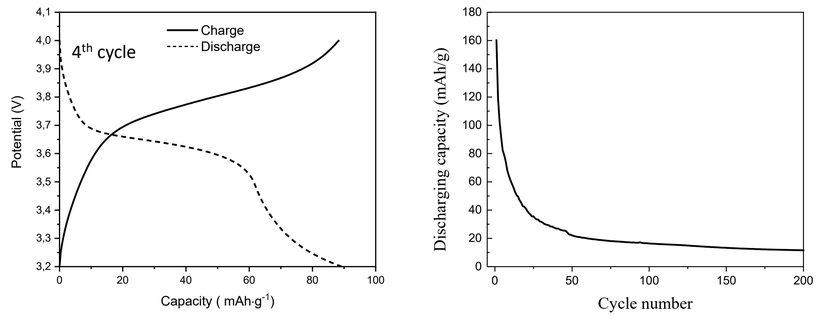
- **Cyclic Voltammetry**

* On Nb-STO (111)

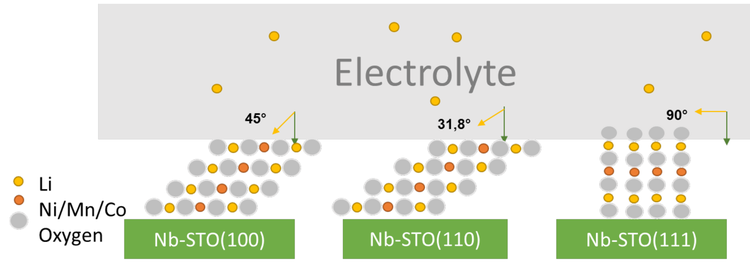


CV was measured within a potential range of 3.2 V to 4.3 V at a sweep rate of 1 mV/s and shows redox peaks at approximately 3.9 V, corresponding to changes in the valence state of nickel. The peak observed in the first cycle is believed to result from a side reaction occurring in the active nano-material during the initial stage of the reaction.

- **Galvanostatic charge and discharge**



- **Illustration of lithiation dependence on structure**



Conclusion

- The similarity between the thin film model systems and conventional powder-based composite electrodes was demonstrated through X-ray diffraction (XRD), Inductively Coupled plasma Spectroscopy (ICP), and Cyclic Voltammetry (CV).
- These results indicate the potential of these NMC811 thin films to serve as a highly controlled model system for analyzing the interface towards the adjacent liquid (or solid state) electrolyte.

Perspectives

Understanding the impact of crystal orientation on battery performance
- Scanning transmission electron microscopy (STEM)
- Neutron depth profiling (NDP)
- X-ray absorption spectroscopy (XAS)

Acknowledgements

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