NANOTECHNOLOGIES



Phase and Composition Mapping of Polycrystalline Li-ion NCM Cathodes

C. F. Almeida Alves¹, Qiang Xie², Arumugam Manthiram², P. J. Ferreira^{1,2,3}

¹INL - International Iberian Nanotechnology Laboratory, Av. Mestre José Veiga s/n, 4715-330 Braga, Portugal ²Materials Science and Engineering Program, University of Texas at Austin, Austin, Texas 78712, USA ³Mechanical Engineering Department and IDMEC,

Instituto Superior Técnico, University of Lisbon, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

Background

 $LiNi_{x}Co_{y}Mn_{z}O_{2}$ (NCM), one of the most common cathode battery materials, exhibits a specific capacity and operating voltage comparable to $LiCoO_2$, while being less toxic. However, single-phase NCM particles are susceptible to phase transformations during charge/discharge due to Li mobility, which deteriorates the cycling performance of Li-ion cathodes. These layered materials exhibit a large degree of cation disorder and thus Ni exchanges with Li in the Li₂MO₃ layer, which disrupts the Li⁺ pathways and creates a continuous MO₂ layer, which decreases the Li mobility and degrades the cycling performance.



Methodology

LiNi_{0.90}Co_{0.05}Mn_{0.05}O₂ particles were prepared by FIB using a Helios 450S (FEI) -Dual FIB with UHRSEM. Thereafter, , the chemical composition and structure were investigated by FIB-SEM, double-corrected TEM-STEM and EDS mapping.





Results

Cross section aberration-corrected TEM



Selected area electron diffraction of the cross section TEM image.



EDS spectrum images showing the elemental distribution for the $LiNi_{0.90}Co_{0.05}Mn_{0.05}O_2$ particle: a) Mn + Ni overlay; b) Mn; c) O; d) Ni; e) Co; f) HAADF image at particle center; and g) Mn + Ni overlay at particle center.



Conclusions

STEM-EDS analysis reveals variations in chemical composition across the particle, in particular Mn-segregation at the particle center grain boundaries.









