Mitigating Cathode Degradation in Li-ion Batteries

Beamline: ISS and XPD

Scientific Achievement

Scientists reveal and visualize chemical outliers, which cause capacity fading upon high voltage charging, in Nickel-rich-layered cathodes using machine-learning techniques.

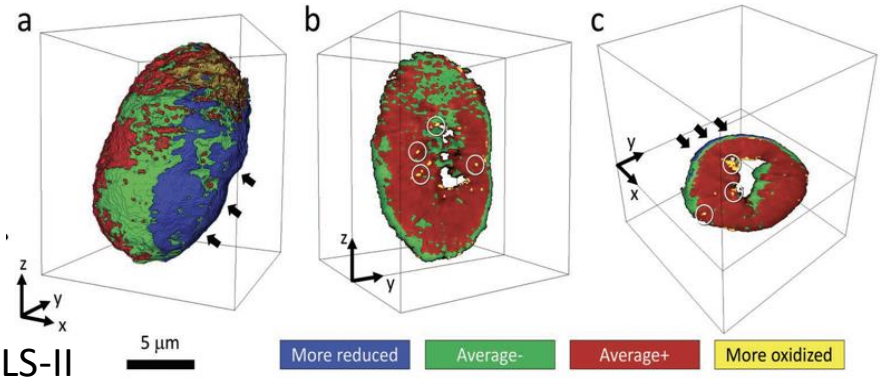
Significance and Impact

Nickel-rich layered materials are promising candidates for high-energy-density lithium-ion battery cathodes. This study offers a pathway to overcome the capacity fading problem.

Research Details

- Synchrotron bulk diffraction and spectroscopy at NSLS-II suggest that the majority of the material is rather robust with some local disordering
- Assisted by machine learning methodology, x-ray nanotomography at SSRL reveals undesired chemical outliers within the particles that lead to degradation
- Finite element modeling suggests morphological engineering as a potential remedy to suppress damage in the particles

3D distributions of different chemical phases with different Ni oxidation states within a Ni-rich secondary particle that was aggressively cycled. State-of-charge heterogeneity that leads to performance degradation is observed and reconstructed by a hybrid supervised-and-unsupervised machine learning algorithm, which facilitates the extraction of the information that is otherwise unavailable.



Y. Mao, X. Wang, S. Xia, K. Zhang, C. Wei, S. Bak, Z. Shadike, X. Liu, Y. Yang, R. Xu, P. Pianetta, S. Ermon, E. Stavitski, K. Zhao, Z. Xu, F. Lin, X.-Q. Yang, E. Hu, Y. Liu, *Adv. Funct. Mater.* 1900247 (2019).

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