Nanoscale mapping of crystallographic phases in battery reactions

Scientific Achievement

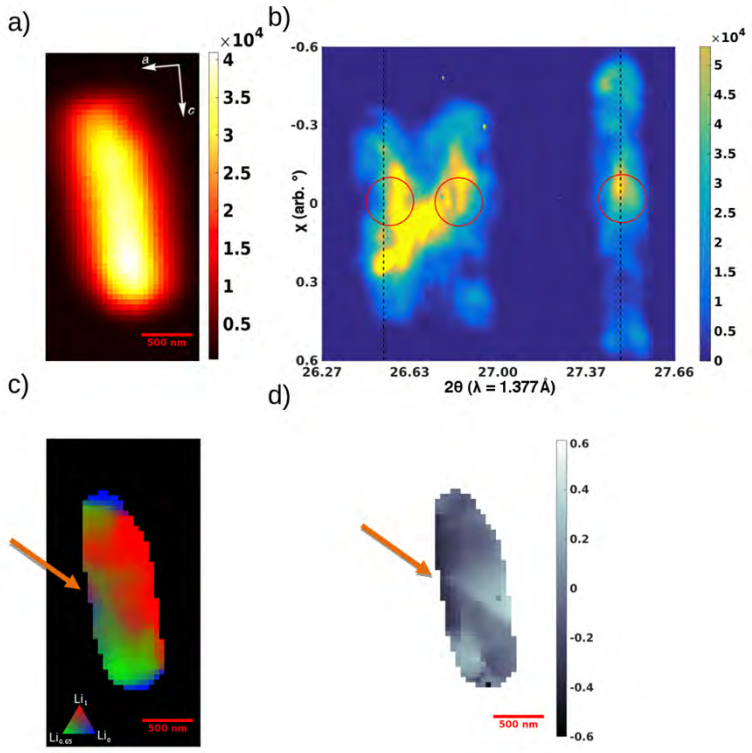
Scanning X-ray Diffraction Microscopy (SXDM) revealed intermediate compositions in single microcrystals of Li_xFePO_4, previously undetected by other methods.

Significance and Impact

The observations agree with predictions that the $LiFePO_4$ - $FePO_4$ phase diagram can be manipulated using coherency strain at interfaces. SXDM maps crystallographic phases in single particles to accurately define mechanisms of battery reactions and the associated chemo-mechanical coupling.

Research Details

- Single microplatelets of $LiFePO_4$ were chemically delithiated for nanoscale imaging.
- Novel method of nanoscale chemical imaging with unprecedented structural sensitivity developed with CNM / ANL using the Hard X-ray Nanoprobe
- Spectromicroscopy confirmed redox changes.



Findings: SXDM mapping in single particle $Li_{0.5}FePO_4$ showed miscibility in the diffraction pattern (top right) between the phases $LiFePO_4$ and $Li_{0.6}FePO_4$, 26.61°-26.85° 2θ, respectively. Composition (bottom left) and microstructure (bottom right) maps show correlation between chemical and mechanical effects from delithiation.

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Work performed at UIC, CNM / ANL, and Cambridge.