Site-Specific Atomic Resolution Probing of Structure-Property Relationship under Dynamic and/or *Operando* Conditions

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Purpose

Develop capabilities that drive the atomic-level imaging and spectroscopic analysis of materials under *in situ/operando* conditions

Probe the electronic structure of energy materials

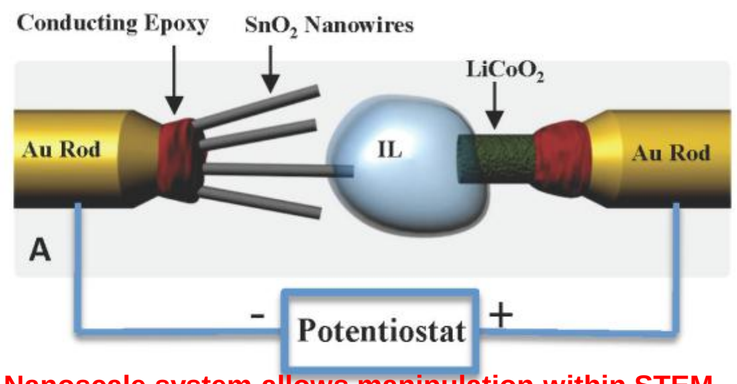
Search the guiding principles for accelerated discovery of much-needed materials for next-generation energy and environment-related applications

Expected Outcomes

Fundamental insights relating properties of energy materials under dynamic conditions with the atomic and electronic structure

Correlate the experimental data with multiscale computational modeling

Scientific understanding of the mechanisms responsible for capacity fading and power – new energy storage materials development



Nanoscale system allows manipulation within STEM column, enabling *in situ* study

Accomplishments to Date

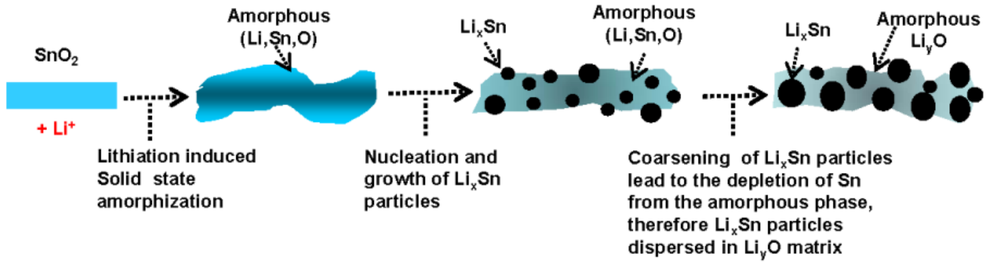
- Developed aberration-corrected S/TEM with proven Angstrom resolution for STEM imaging and sub-Angstrom information limit for HRTEM imaging
- Built nanoscale manipulation system
- Canadian Light Source members on team
- Based on *in situ* experiments, proposed model of structural evolution in SnO_2 anode upon initial charging
- Scientific outreach
  - CM Wang et al., *Nano Letters*, online April 2011
  - LQ Zhang et al., *ACS Nano*, online May 2011
  - Gave 4 invited and 2 contributed presentations
  - Co-organizer for a symposium, M&M 2011
  - Proposal to organize symposium, MRS 2012 Fall

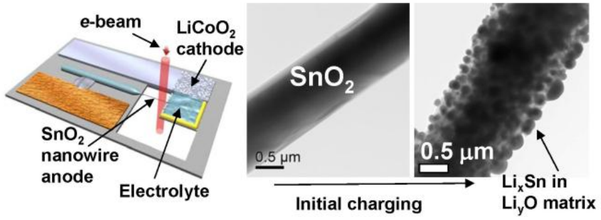
Path Forward

- *In situ* TEM investigation of anode and cathode materials to establish battery failure mechanism
- Integrate *in situ* TEM and STEM with STXM
- Integrate TEM and APT imaging for energy materials
- Integrate *in situ* observation with multiscale predictive modeling to accelerate new energy materials discovery

Path to Programmatic Funding

- Full proposal for NA-22, requested $2M for 3 years
- White paper to ARPA-E for energy materials





A new model for structural evolution of SnO_2 upon charging

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