Title
Mesoscale Chemomechanical Interplay of the NCA Cathode in Solid-State Polymer Batteries

Author
Doeff, Marca

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CRADA Final Report Form

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PI Marca Doeff

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OSTI Number_____

1. Parties: California Clean Energy Fund (Prime Sponsor: Robert Bosch LLC Research and
   Technology Center)

2. Title of the Project: Understanding and Quantifying Aging Mechanisms in Nickelate Cathode Materials

3. Summary of the specific research and project accomplishments:
   (Were key major goals of the CRADA achieved?)
   Note: Final Reports and Forms containing Protected CRADA Information are to be emailed directly to the SPO close out requestor, along with a confirmation of the public release date. Do not submit via eSRA. Also, please do not include any Proprietary Information (defined below) in CRADA Final Reports and Forms.*

4. Deliverables:

Deliverables met	Party (LBNL, Participant, Both)	Delivered to Other Party?
Final Report (this document)	LBNL	

5. Identify publications or presentations at conferences directly related to the CRADA?

   Thermally Driven Mesopore Formation and Oxygen Release in Delithiated NCA Cathode Particles" M. Besli, A. Shukla, C. Wei, M. Metzger, J. Alvarado, J. Boell, D. Nordlund, G. Schneider, S. Hellstrom, C. Johnston, J. Christensen, M. Doeff, Y. Liu, and S. Kuppan, **J. Mater. Chem. A**, submitted (2019).

   "Mesoscale Chemomechanical Interplay of the NCA Cathode in Solid-State Polymer Batteries" M. Besli, S. Xia, S. Kuppan, Y. Huang, M. Metzger, A. Shukla, G. Schneider, S. Hellstrom, J. Christensen, M. Doeff, and Y. Liu, **Chem. Mater.**, 31, 491 (2019).

6. List of Subject Inventions and software developed under the CRADA: (Please provide identifying numbers or other information.) N/A

7. A final abstract suitable for public release:
   (Very brief description of the project and accomplishments without inclusion of any proprietary information or protected CRADA information.)
   The behavior of NCA cathodes in solid-state polymer electrolyte cells was studied. X-ray tomography and transmission electron microscopy showed that cracking of NCA particles, which also occurs in Li-ion cells with liquid electrolytes, leads to rapid failure in polymer cells because of loss of contact between the electrolyte and cathode particles. While liquid electrolytic solutions can flow into the cracks and maintain the ionic pathways, polymer electrolytes do not, leading to disruption of ionic transport. In addition, oxidation of electrolyte occurs at particle/polymer interfaces. The chemomechanical and thermal properties of delithiated NCA materials were also studied using an array of X-ray techniques and microscopy. Upon heating, phase changes to reduced metal oxide phases such as spinels and rock salt occur. Oxygen loss occurs and is associated with intergranular and intragranular cracking as well as micropore formation.
8. Benefits to DOE, LBNL, Participant and/or the U.S. economy.
   Batteries for electric vehicles are potentially a multi-billion dollar industry for the US, so understanding failure mechanisms for battery materials is critical. This project with Bosch meshed well with the LBNL PI's own interests in cathode materials for Li-ion batteries. Because of concerns about cost and the ethics of mining cobalt, the U.S. Department of Energy is encouraging a transition to high Ni-content, low Co-content cathode materials for vehicle applications, but these materials have poor thermal stability and cycle life. Understanding the mechanisms of failure and thermal degradation are first steps to improving the materials for battery applications.

9. Financial Contributions to the CRADA:

DOE Funding to LBNL	$ 0.00
Participant Funding to LBNL	$ 14,306.00
Participant In-Kind Contribution Value	$ 0.00
Total of all Contributions	$ 14,306.00

** "Proprietary Information" means information, including data, which is developed at private expense outside of this CRADA, is marked as Proprietary Information, and embodies (i) trade secrets or (ii) commercial or financial information which is privileged or confidential under the Freedom of Information Act (5 U.S.C. 552 (b)(4)).*