

MODELING AND ANALYSIS FOR RECYCLING

Project ID: bat382



Q. DAI

Argonne National Laboratory

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2019 DOE Vehicle Technologies Office
Annual Merit Review

OVERVIEW

Timeline

- Project start: October 2018
- Project end: September 2021
- Percent complete: ~15%

Barriers

- Recycling and Sustainability
 - Cost to recycle is currently 5-15% of battery cost
 - Material shortage (Li, Co, and Ni)
 - Varying chemistries result in variable backend value

Budget

Year 1	\$4,615k
<i>Argonne</i>	<i>\$2650k</i>
<i>NREL</i>	<i>\$965k</i>
<i>ORNL</i>	<i>\$550k</i>
<i>UCSD</i>	<i>\$150k</i>
<i>WPI</i>	<i>\$150k</i>
<i>MTU</i>	<i>\$150k</i>

Partners

- Argonne National Laboratory
- National Renewable Energy Laboratory
- Oak Ridge National Laboratory
- University of California, San Diego
- Worcester Polytechnic Institute
- Michigan Technological University

RELEVANCE - RECELL CENTER

Objective:

Foster the development of cost-effective and environmentally sound processes to recycle lithium-ion batteries

Bring together battery recycling experts to bridge technical and economic gaps to enable industry adoption

Impact:

Reduced cost of ownership and helping to drive battery costs to DOE's \$80/kWh goal

Reduce primary material production to avoid material shortages and reliance upon foreign sources, increasing our nation's energy security

Minimize environmental impacts of the battery life cycle

MILESTONES

Q1 (Center) Establish the battery recycling center's mission and include its targets and goals

✓ COMPLETED 12/21/18:

“Decrease the cost of recycling lithium ion batteries to ensure future supply of critical materials and decrease energy usage compared to raw material production”

Q2 (NREL) Provide an initial progress report on roll-to-roll relithiation

✓ COMPLETED 3/29/19: Roll-to-roll relithiation work is progressing and the concept is currently being tested using coin cells

Q3 (ORNL) Provide an initial progress report on design for recycle initiative

In progress

Q4 (ANL) Establish the ReCell Center's Battery Recycling Laboratory and Scale-up Facility

In progress

APPROACH – MODELING AND ANALYSIS

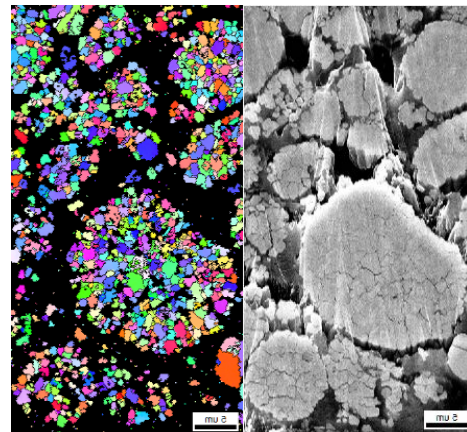
There are many potential recycling pathways for batteries that no longer meet their performance criteria. It would be expensive and time-consuming to explore all possible process options; researchers need tools to direct them to the most efficient and economic processes.

- Diagnostics on Aged Materials, S.Santhanagopalan (NREL)
- Thermal Analysis, M. Keyser (NREL)
- TEA/LCA Modeling (EverBatt), Q. Dai (Argonne)
- Supply Chain Analysis (LIBRA), M. Mann (NREL)

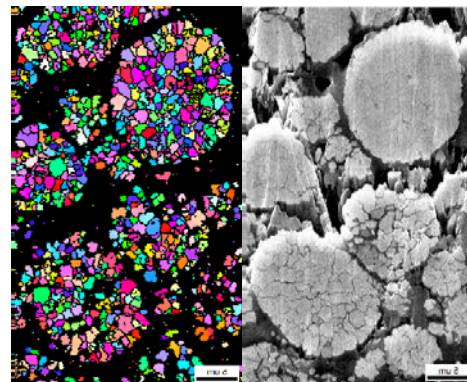


DIAGNOSTICS ON AGED MATERIALS

- Methodology to obtain grain orientation from cathode samples via electron back-scattering diffraction (EBSD) in place. Initial scanning transmission electron microscope (STEM) studies underway.
- Dry samples as well as first batch of cycled off-the-shelf $\text{LiNi}_{0.5}\text{Mn}_{0.3}\text{Co}_{0.2}\text{O}_2$ (NMC532) were characterized. Initial results for $\text{LiNi}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3}\text{O}_2$ (NMC111) from Argonne being processed.
- EBSD patterns observed after 20% loss of capacity indicate no significant changes to particle size, grain orientation, etc. except for some hairline cracks. Some orientations show attrition; but nothing statistically significant yet.



Uncycled NMC532



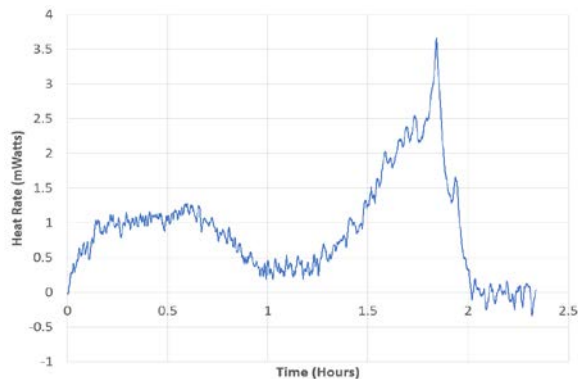
Cycled to 20% capacity loss

THERMAL ANALYSIS

- Thermally characterize existing lithium nickel manganese cobalt oxide (NMC) cathode compositions to understand how the thermal signature of a battery changes from the beginning of life to the end of life.
- Thermally characterize NMC/graphite cells with a known contaminant in both anode and cathode.
- Match the extent and type of thermal degradation to target recycling methods, based on load profiles, cycling windows, and cost metrics.



NREL's microcalorimeter.
Figure Credits, Josh Major, NREL

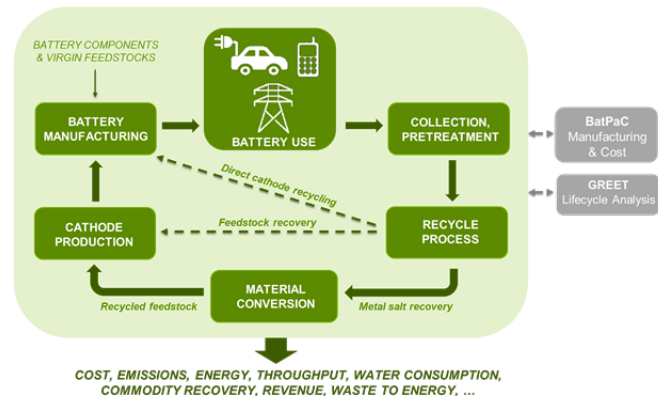


Heat generation of an NMC532/graphite cell
under a C/2 constant current discharge.

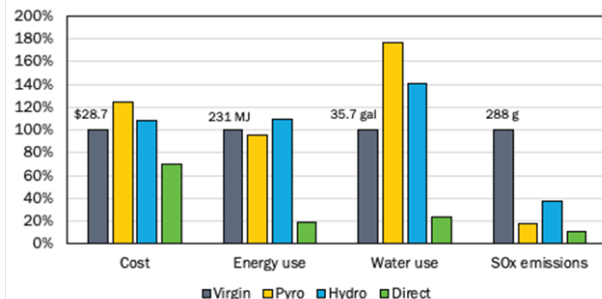
Figure Credits: Matt Keyser, NREL

TEA/LCA MODELING (EVERBATT)

- Incorporated most recent BatPaC and GREET background data, and new industry information for recycling and cathode production processes.
- Model released in May 2019, available at: <https://www.anl.gov/egs/everbatt>
- Identified direct cathode recycling as a promising opportunity to reduce the cost and environmental burden of cathode materials.
- Expansion of model underway to enable modeling of new direct cathode recycling technologies, processes that recover anodes and electrolyte components, and design-for-recycle strategies.



EverBatt Model Schematic

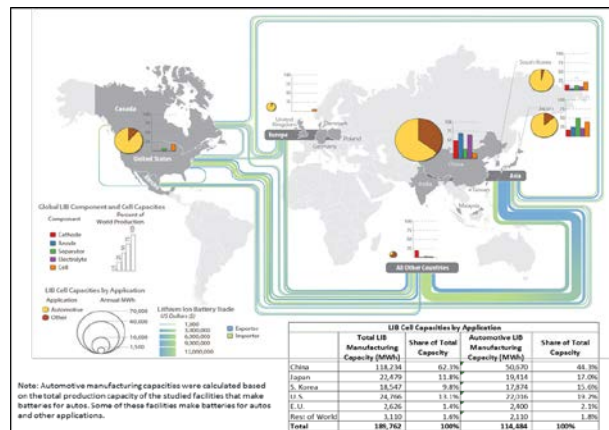
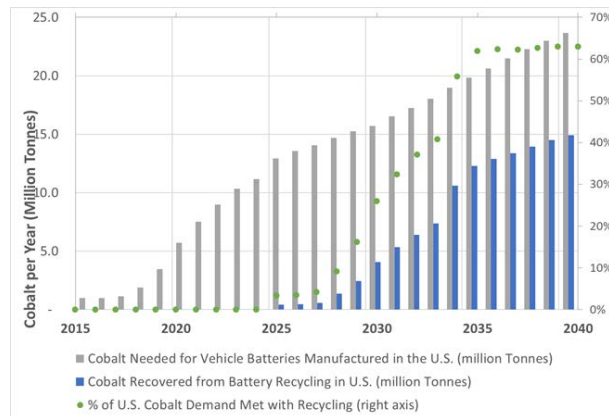


Cost and Environmental Impacts Comparison for 1kg Produced NMC111 Powder

SUPPLY CHAIN ANALYSIS (LIBRA)

- Updated 2014 analysis of supply chain of lithium-ion battery cells.
- Evaluated share of country-specific manufacturing for LIB for automotive, consumer electronic, and stationary energy storage markets.
- Determined fraction of the cobalt needed for vehicle manufacturing in the U.S. can be met with Li-ion battery recycling.
- Began development of Lithium Ion Battery Recycling Analysis (LIBRA) model – system dynamics model to study supply and demand of critical materials for batteries.

Sources of data: Trade Map 2017; BNEF 2017; Avicenne 2017; NREL analysis 2018



RESPONSE TO REVIEWERS

- **New Project FY19**

REMAINING CHALLENGES AND BARRIERS

- No correlations can be drawn between crystal structure and degradation mechanisms and recyclability.
- Typical contaminant levels may not be detectable during cycling in the thermal analysis effort.
- The availability of industrial data to populate the EverBatt model may be incomplete and/or difficult to obtain.
- The impact of policies and market dynamics on future battery material supply and demand may be hard to quantify.
- The assumptions that will be used to provide data based upon scaled-up ReCell process projects may be insufficient.

FUTURE WORK

- **Diagnostics on Aged Materials:** Build EBSD maps for cathode materials that are recovered/treated by different processes; Evaluate relationship between performance and grain size/orientation.
- **Thermal Analysis:** Measure the heat generation at the beginning and end of life and use the data as a baseline to assess the performance of future recycled material and processes; Use calorimetry to determine how contaminants on cathode and anode affect the performance of the cells.
- **TEALCA Modeling (EverBatt):** Refine methodologies for techno-economic analysis and life cycle analysis; Continue to update model as new data/information become available; Continue to improve model usability.
- **Supply Chain Analysis (LIBRA):** Evaluate investment decisions for recycling based on price of cobalt, policies, cost of recycling technology, and purity requirements; analyze material supply risk.
- **Focus Area:** Incorporate material characterization parameters into EverBatt.

Any proposed future work is subject to change based on funding levels

SUMMARY

- **Overarching goal:** Identify the optimal recycling processes for batteries, and inform and direct the R&D efforts under the ReCell Center.
- **Diagnostics on Aged Materials:** Identify chemical signatures of a battery corresponding to its efficiency losses; inform electrochemical relithiation conditions; match the extent and type of degradation to target recycling methods.
- **Thermal Analysis:** Understand how the thermal signature of a battery changes from the beginning of life to the end of life; thermally characterize cells with a known contaminant; match the extent and type of thermal degradation to target recycling methods .
- **TEA/LCA Modeling (EverBatt):** Estimate the cost and environmental impacts of recycling processes and design-for-recycle strategies; identify hotspots and opportunities of improvement; identify possible barriers to process/design commercialization.
- **Supply Chain Analysis (LIBRA):** Evaluate critical supply chain questions for battery recycling, including insights into material availability, the impact of demand from EV and stationary energy storage markets, and global economic competitiveness of battery manufacturing.

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