

Coal as Value-Added for Lithium Battery Anodes

Annual Project Review
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Presenter: Kyle Marcus

kmarcus@semplastics.com

Agenda

- Project Description and Objectives
- Project Update
- Preparing Project for Next Steps
- Concluding Remarks

Project Description and Objectives

Purpose, Strategic Alignment, Initial Status

Purpose of Project

To utilize coal in polymer-derived ceramics to produce a commercially viable anode

Strategic Alignment with Fossil Energy Objectives

Within Advanced Energy Systems, the Coal Beneficiation program seeks to increase the value of the Nation's domestic coal resource by funding technologies that improve the quality of coal feedstocks and convert coal to other valuable byproducts. By using coal combined with our proprietary resin, Semplastics will be able to create a new type of anode made with up to 70wt% coal

Status at Beginning of Project:

Can coal be used to produce an anode that can rival the performance of graphite in lithium-ion batteries?

Technology Benchmarking

Anode Material	Specific Capacity (mAh/g)	Volume Expansion	Lifetime
Lithium (Li)	3,862	High	Low
Silicon (Si)	4,200	High	Low
Aluminum (Al)	2,235	High	Low
Tin (Tn)	990	Medium / High	Medium
Li / Silicon	4,200	High	Low
$\text{Li}_4\text{Ti}_5\text{O}_{12}$	175	High	High
Graphite	372	Low	Medium
Semplastics Coal Core Composite	600	Low	High

Current Status of Project

- Results compared to Benchmark: To be discussed later in presentation
- Project Goals/objectives have not changed.
- Battery Innovation Center visit in December 2020:
 - Evaluation and validation of materials fabricated at Semplastics facilities by an industry expert
 - We received confirmation and positive feedback that our mixing, coating, and assembly processes met expectations based on equipment and facility constraints

Project Update

Overview and Milestone Status Report

- Fabricated and tested approximately 240 coin cells in-house
- Successfully determined the best coal material to move forward with the project
- On track to begin full coin cell testing

Task / Subtask	Milestone Title / Description	Planned Completion Date	Actual Completion Date	Verification Method
2.3	Capability to test powders established	15 Jul 2020	20 Jul 2020	Results obtained for first slurry-bonded powder
4.1	Best coal material identified	30 Dec 2020	28 Dec 2020	Acceptable data from short-term half-cell testing of multiple resin formulations
4.2	Best overall composition identified	11 Aug 2021	n/a	Favorable results from Battery Innovation Center testing
2.4	Production and testing capability for pouch cells established	29 Jul 2022	n/a	Results obtained from testing of initial pouch cells
6.0	Initial set of industry-standard batteries produced	30 Dec 2022	n/a	Favorable initial test results from Battery Innovation Center testing
5.0	Pilot line for scaled-up material production established	28 Apr 2023	n/a	Demonstrated vendor production of 50 kg of material per week

Battery Innovation Center (BIC)

- Located in Newberry, Indiana
- Specialize in battery materials and systems development
- 36,000 square foot facility with all equipment and expertise required for materials development, assembly and testing of coin cells, pouch cells and 18650 industrial standard cylindrical cells
- December 15-17, 2020
- Evaluation and validation of materials fabricated at Semplastics facilities
- We received confirmation and positive feedback that our mixing, coating, and assembly processes met expectations based on equipment and facility constraints



Improvements to Slurry Formation

- Centrifugal Mixing results in better dispersion of conductive carbon and active material
- Utilization of Premixes minimizes variability in the process and decreases the amount of time needed for mixing
- Measuring dispersion using a Hegman Gauge results in a measurable and trackable process

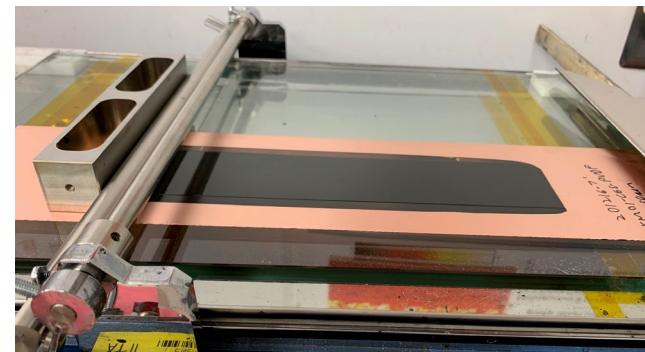
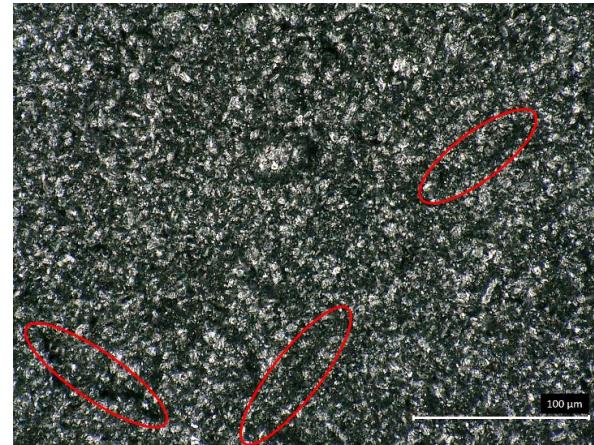


Thinky AR-100



Improvements to Electrode Coatings

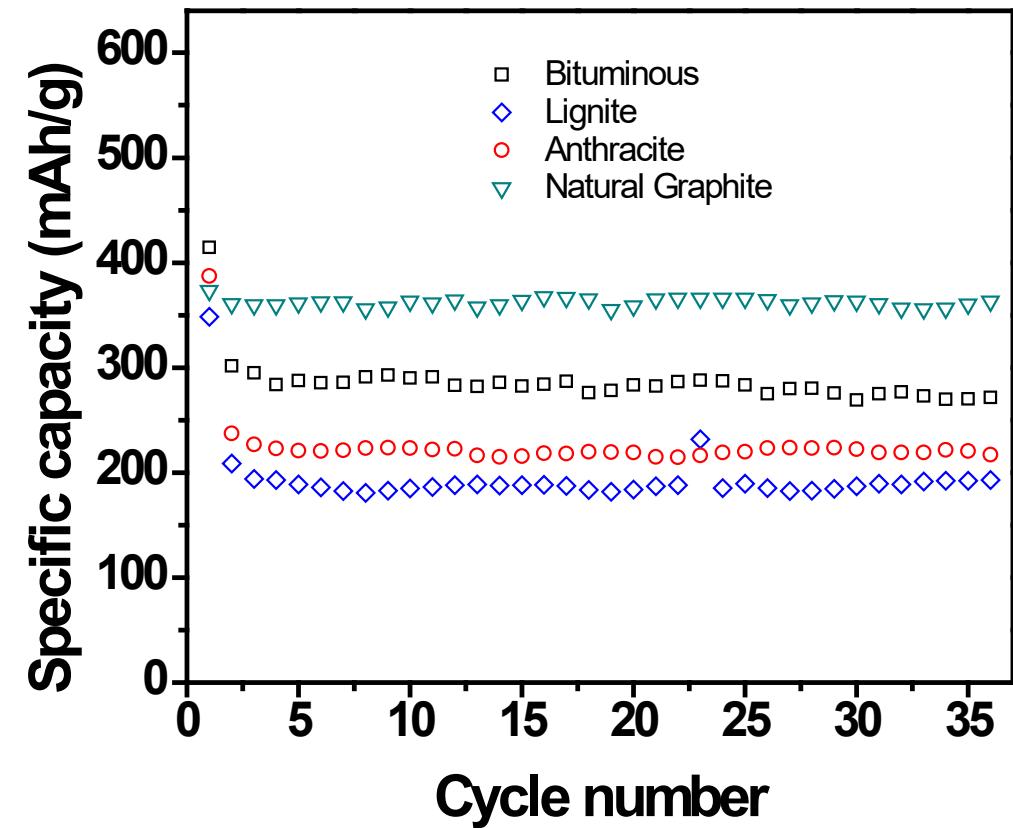
- A fixed blade-height applicator allows for a controlled wet coating height vs. a variable or adjustable gate
- A slower drying process could also be an improvement and result in fewer cracks on the electrode surface.
- Utilizing a press to achieve ~20% compression could help create a more uniform and denser electrode (Future Work)





Selective Coal as Standalone Anode Comparison

	1 st Lithiation (mAh/g)	1 st Delithiation (mAh/g)	Irreversible Capacity (mAh/g)	First Cycle Efficiency (%)	10 th Lithiation (mAh/g)
Bituminous	414.6	296.0	118.6	71.4	290
Lignite	348.6	196.5	152.1	56.4	184.8
Anthracite	387.3	231.3	156	59.7	223.2
Natural Graphite	373.3	347.0	26.3	92.9	363.2



PDC Coal Core Composite Anodes Comparison

Specific discharge capacity (mAh/g) comparing experimental Half-Cells to a Natural Graphite Control Half-Cell.

Active Material: 25wt% coals mixed with a proprietary X-MAT® Polymer Derived Ceramic (PDC) forming resin.

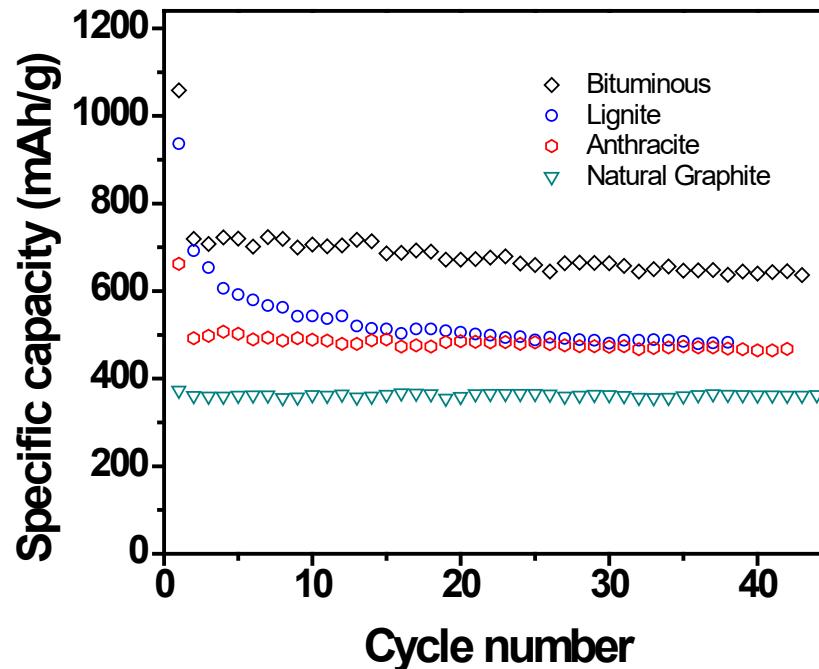
Half 2032-coin cells assembled and tested In-House

Electrode ratios are 85:10:5

- Active Material:PVDF Binder:C65 Conductive Carbon

Low Cycling Rate

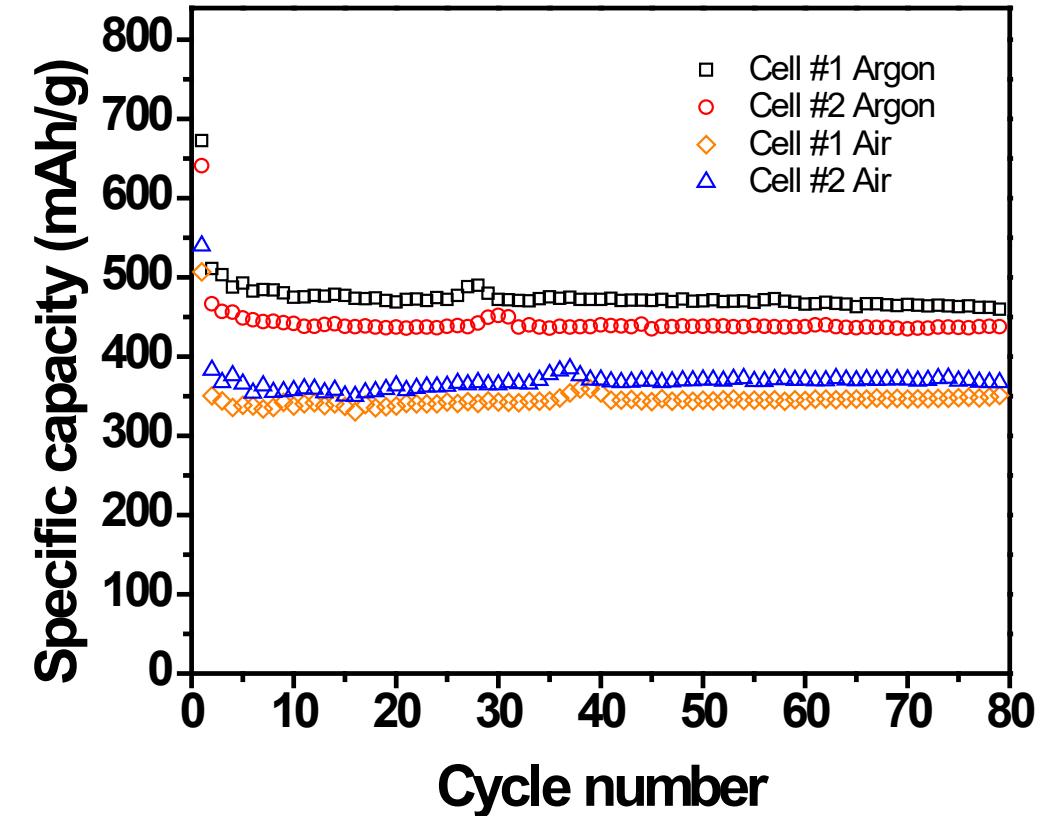
AM Mass Loading: ~2.3-2.6 mg/cm²



	1 st Lithiation (mAh/g)	1 st Delithiation (mAh/g)	Irreversible Capacity (mAh/g)	First Cycle Efficiency (%)	10 th Lithiation (mAh/g)
Bituminous	1058.4	735.2	323.2	69.4	706.3
Lignite	936.3	691.2	245.1	73.8	543.1
Anthracite	662.3	480.8	181.5	72.6	489.2
Natural Graphite	373.3	347.0	26.3	92.9	363.2

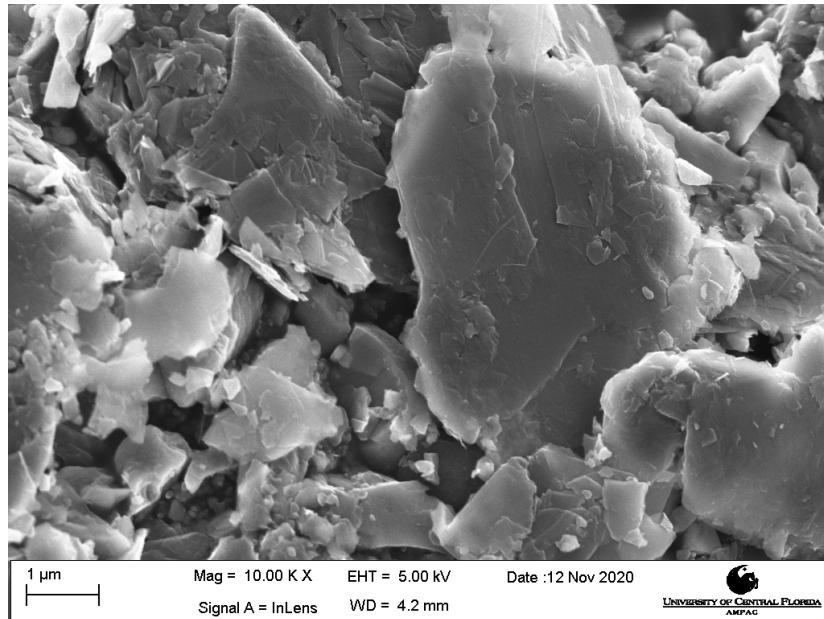
Processing Conditions Vs Performance

- Half coin cell discharge cycling performance for Batch 60 combined with 85wt% bituminous coal samples cured in argon gas (black / red) or in air (blue / orange).
- Cells cured in argon have superior performance in terms of capacity
- The average FCE for the argon cells is 75.35%, where the air cells have an average FCE of 69.3%

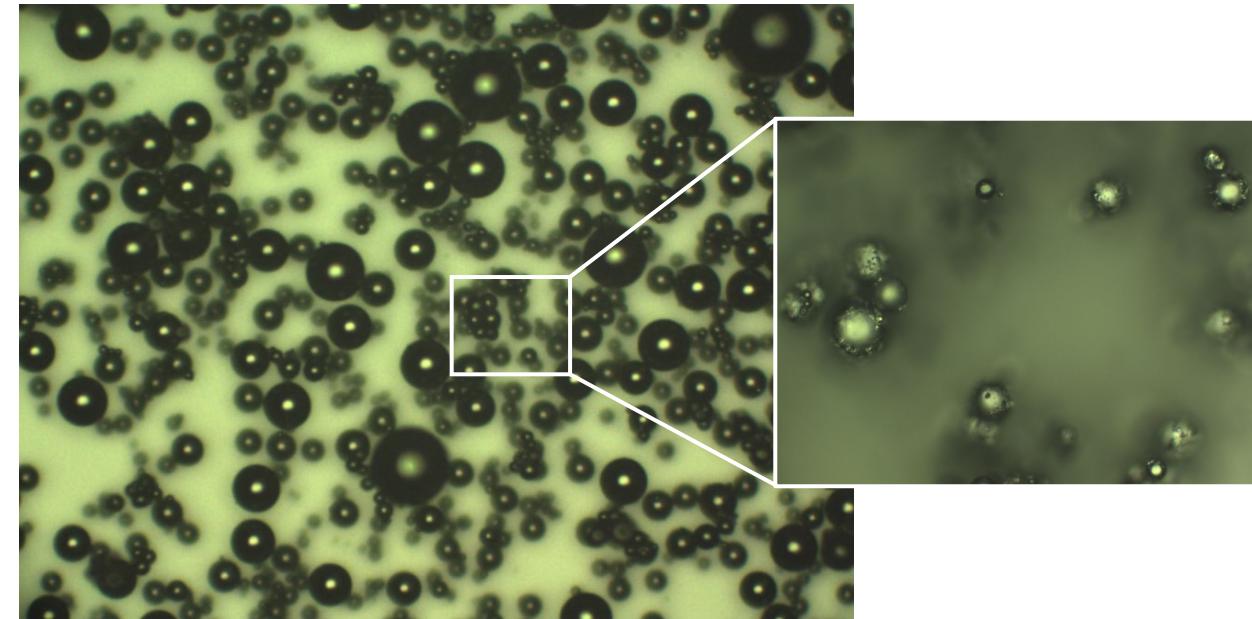


New PDC Anode Powder Technology

Milled PDC Material



Spherical PDC Material



Preliminary Data – Spherical PDC Technology

Specific discharge capacity (mAh/g) comparing experimental Half-Cells #1 #2 and #3 to a Natural Graphite Control Half-Cell.

Half-Coin Cells #1, #2, and #3 are replicates

Active Material: 25wt% Coal mixed with a proprietary X-MAT® Polymer Derived Ceramic (PDC) forming resin.

Half 2032-coin cells assembled and tested In-House

Electrode ratios are 85:10:5

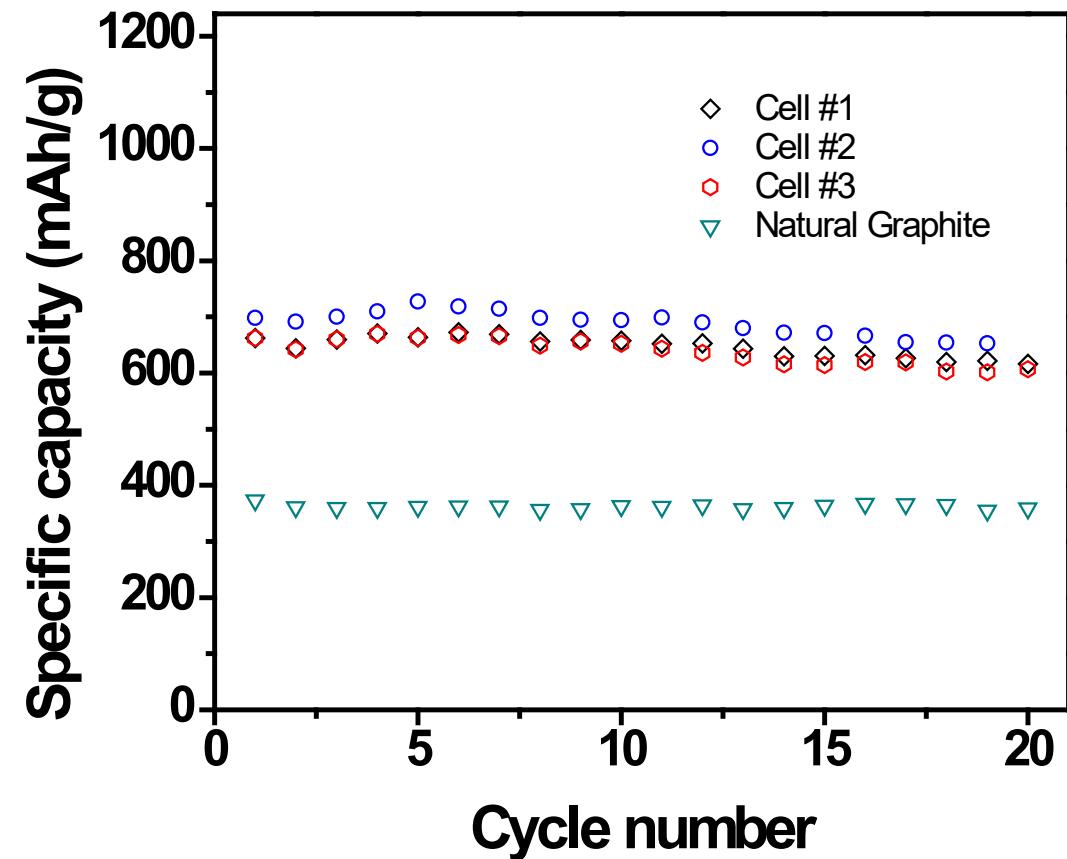
- Active Material:PVDF Binder:C65 Conductive Carbon

Low Cycling Rate

AM Mass Loading: ~3.74-4.12 mg/cm²

First Cycle Efficiency (FCE):

- Cell #1: 69.93%
- Cell #2: 69.89%
- Cell #3: 70.14%
- Control Natural Graphite: 93.95%



Technical Challenges

- Improving first cycle efficiency (FCE)
 - The current FCE is much too low for a viable, full cell LIB technologies
 - Potential solutions:
 - Prelithiate the PDC resin prior to curing or pyrolysis
 - Use electrochemical prelithiation methods or other additives such as Lithium foil or Stabilized Lithium Metal Particles (SLMP)
 - Identify what chemical species is contributing to irreversible capacity loss
- Controlling PDC Coal Core Composite powder morphology
 - Current processing methods are too erratic and powder morphology is difficult to control
 - Potential Solutions:
 - Pursue and characterize a newly developed process to fabricate spherical PDC particles

Preparing Project for Next Steps

Materials



- Continue development of the PDC Coal Core Composite raw powder and electrodes
 - Improvements in processing parameters, slurry formation, and coating methods
- Improve FCE by prelithiation methods
- Begin working with commercially available cathode materials for matching in full cells
- Determine the best performing materials and processes for implementation into full coin and larger format cells

Testing



- Anodes consisting of PDC and PDC Coal Core Composites
- Electrochemical Testing
 - In-House and at the BIC
 - Cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic charge/discharge (GCD) cycling performance
- Further characterization of physical and chemical compositions of PDCs and PDC coal core composite powders and spheres
 - Intertek – N2 Sorption and Activation, Helium Pycnometry, Horiba Laser Diffraction
 - Surface Area, Pore Distribution, Particle Size Distribution
 - UCF – X-ray Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy(SEM) and Energy Dispersive Spectroscopy (EDS)
- Prepare for Full Cell testing in coin cells and larger format

Value Proposition

- The battery application for the coal core composites enables NETL to realign coal with the green energy movement that is currently underway globally.
- Since Coal Core electrode products could use up to 70 wt% coal, they can provide a substantial source for coal and CO₂ sequestration (~60,000 metric tons up to 2028 post commercial launch).
- Can be applied as a performance enhancing coating on graphite for existing battery systems

Concluding Remarks

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- Alignment to Strategic Goals:
 - By using coal combined with our proprietary resin, Semplastics will be able to create a new type of anode made with up to 70wt% coal.
- Next Steps:
 - Continue development of the PDC Coal Core Composite raw powder and electrodes
 - Continue testing anodes
- Technical Challenges:
 - Improve First Cycle Efficiency,
 - Control PDC Coal Core Composite powder morphology