Coal as Value-Added for Lithium Battery Anodes

Project Review

Award No. DE-FE0031879

November 6th 2020

Project Summary

- Semplastics has begun development of a novel material based on our X-MAT® polymer-derived ceramic (PDC) technology for use as an anode material in lithium-ion batteries
- The X-MAT anode material is a composite of chemically tailored silicon oxycarbide (SiOC) and domestically sourced coal powder, designed to be a drop-in replacement for graphite within lithium-ion batteries
- Preliminary tests of this material have shown more than twice the reversible capacity of graphite anodes
- Through this project, Semplastics proposes to complete development and begin commercialization of this material

Project Description and Objectives

What are X-MAT Coal-Core Composite Powders?

- Raw coal powder mixed with our proprietary polymer derived ceramic (PDC)-forming resin to produce coal-core composite powder materials
  - Electrically conductive
  - Low cost – Coal is 1-5¢/lb
  - The raw coal will not be burned during materials processing, and the resulting powder composite will not burn
  - Easily manufactured compared to typical ceramics – no sintering needed
  - Capable of using a variety of coals including lignite, bituminous, and anthracite particles in an “as-is” state with our proprietary PDC technology

How is this different from other approaches?

- Our PDCs can be tuned at the Atomic Level to contain varying amounts of silicon, oxygen and carbon
- Uses a “green” low-energy method – does not involve high-energy processes including high-temperature calcination / graphitization or deposition techniques
  - No chemical vapor deposition (CVD)
  - No physical vapor deposition (PVD)
  - No atomic layer deposition (ALD)
- Does not involve multiple product streams such as char, mixed gas, or light liquids

Coal-Based Anode Material Evaluation

- Primary goal is to determine the best formulation for technical performance and economic viability
- Determine the optimum percentage and type of raw coal to be used in combination with Semplastics PDC resin system as anode material for LIB
  - Lignite, Bituminous, Anthracite are candidates
- Determine the best-performing PDC resin system to be integrated with raw coal

Primary Objectives

- Produce new battery anode materials targeting specific capacity 3x that of current graphite anodes or better
- Identify an industrial LIB prototype developer and provide best formulations to them
- Identify LIB developer to assemble industrial 18650 cylindrical batteries and perform testing to verify performance meeting project goals

Supporting Objectives

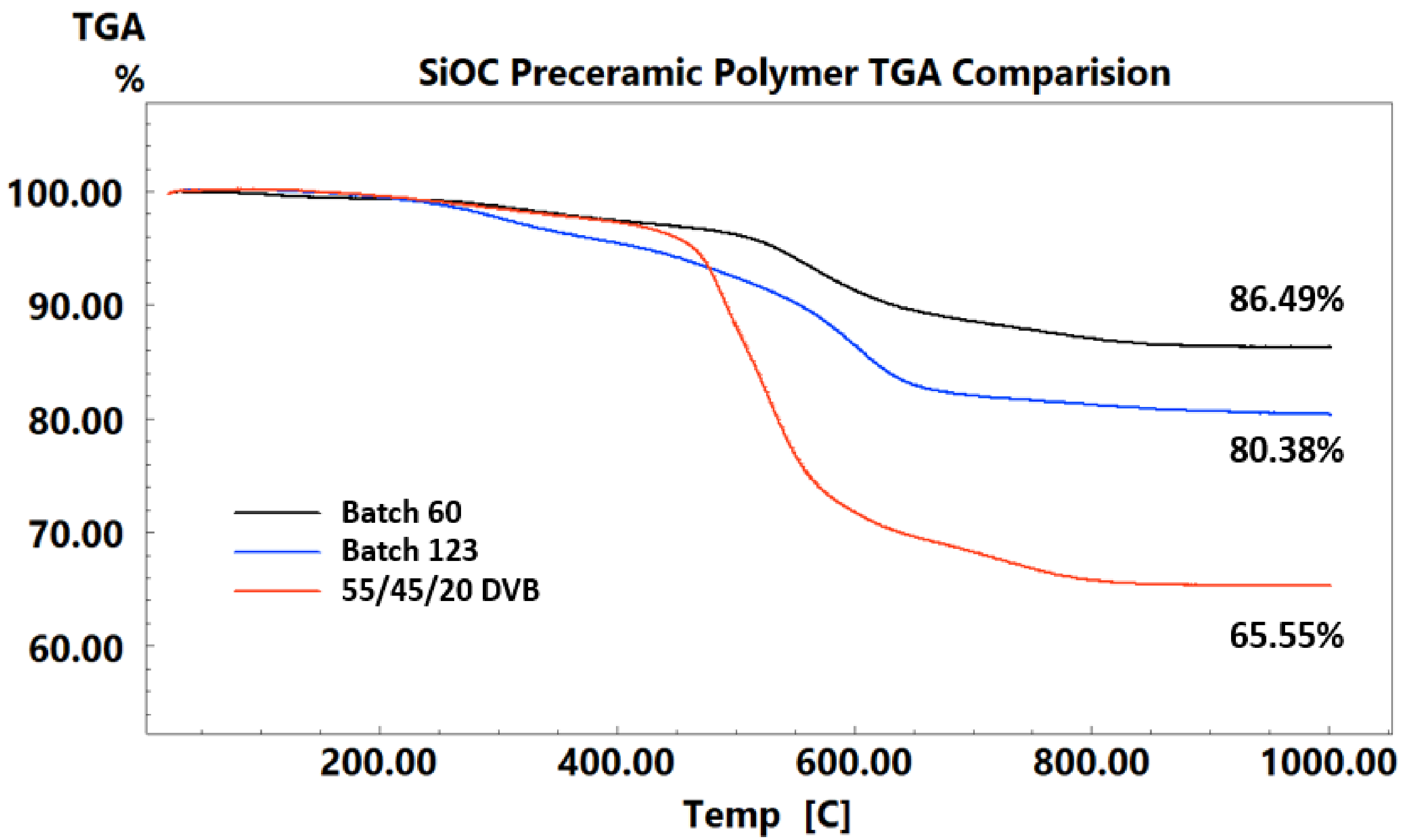
- Develop novel materials based on SiOC ceramics suitable for use in LIB anodes
- Increase specific capacity capability of anode material in half-cells
  - Goal: 1,100 mAh/g after 100 charge/discharge cycles
  - Stretch Goal: 2,000 mAh/g
- Produce half- and full-cell batteries in-house
- Perform extensive testing and analysis in-house and through the Battery Innovation Center (BIC)

Success Criteria

- Year 1: Demonstration of anode performance in half coin cell of 600 (threshold) to 900 (objective) mAh/g for 100 charge / discharge cycles
- Year 2: Demonstration of performance of full coin cell of 160 (threshold) to 220 (objective) mAh/g for 100 charge / discharge cycles
- Year 3: Demonstration of prototype industrial-grade 18650 cylindrical cell battery performance of 3,000 (threshold) to 5,000 (objective) mAh

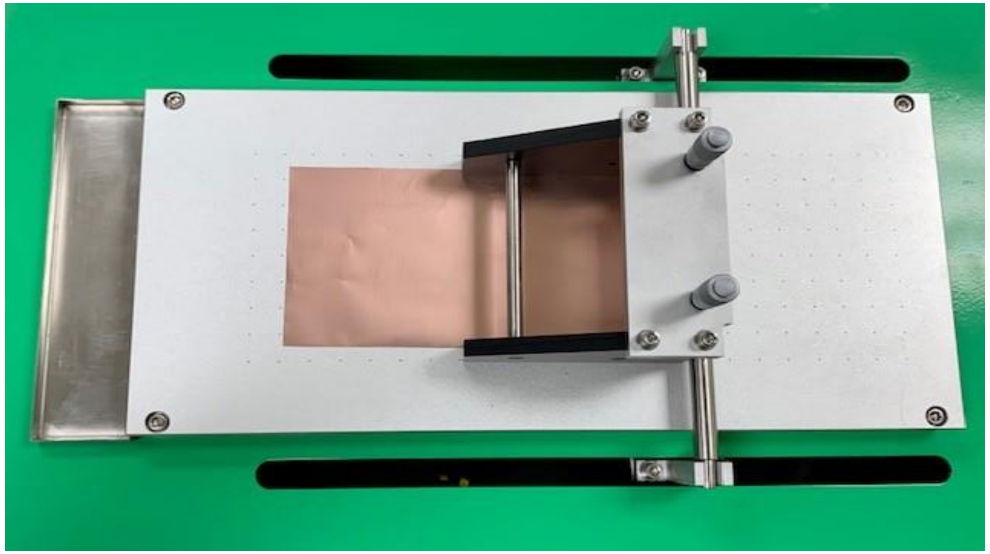
Project Update

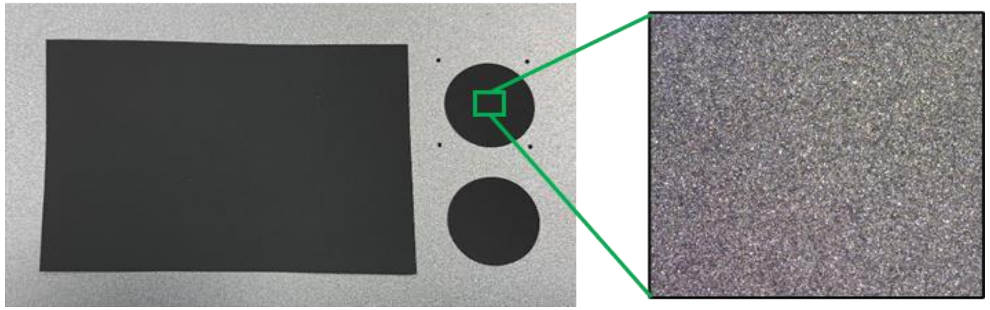
Ceramic Yields of Different SiOC PDCs



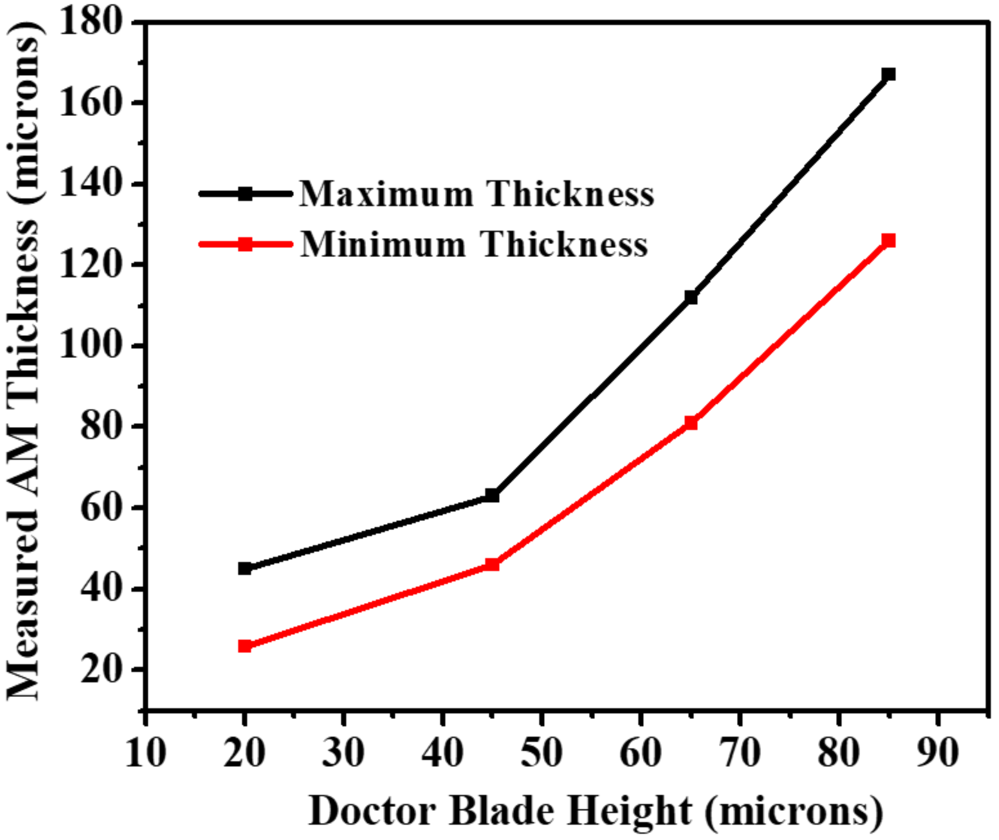
Tabletop Coating Applicator Trials

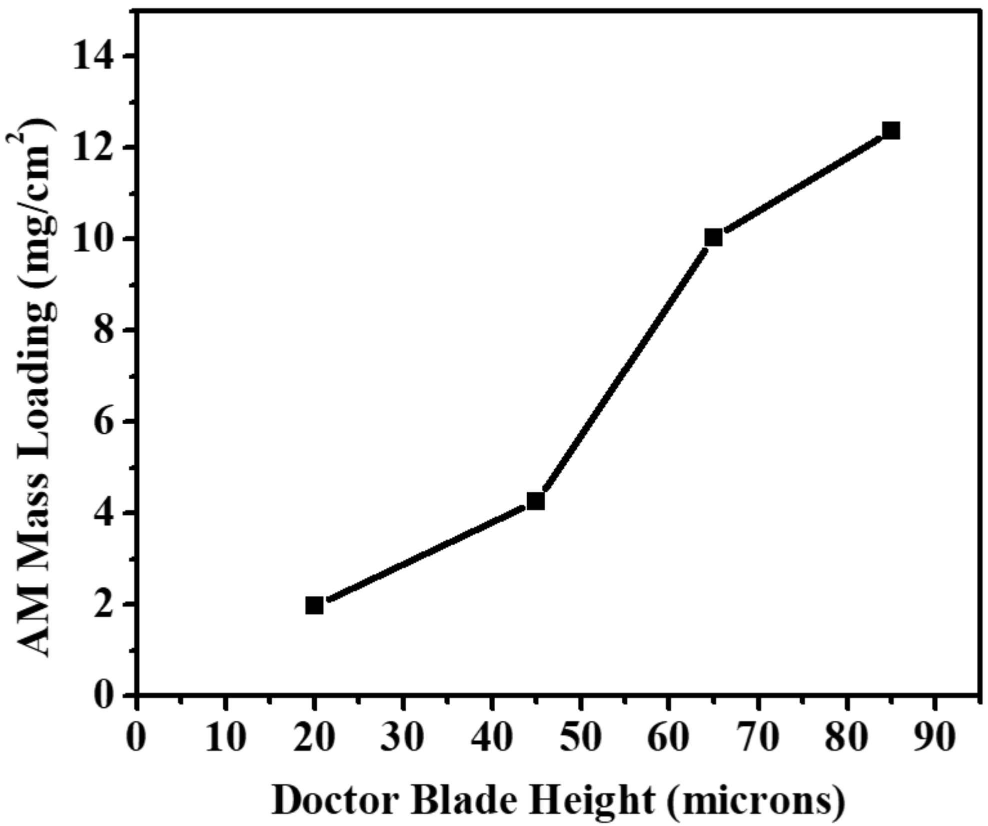
- Experimentation was needed to build a proper correlation between doctor blade height and coating thickness.
- A graphite slurry was formulated, and four different coating heights were selected:
    - 20 microns
    - 45 microns
    - 65 microns
    - 85 microns





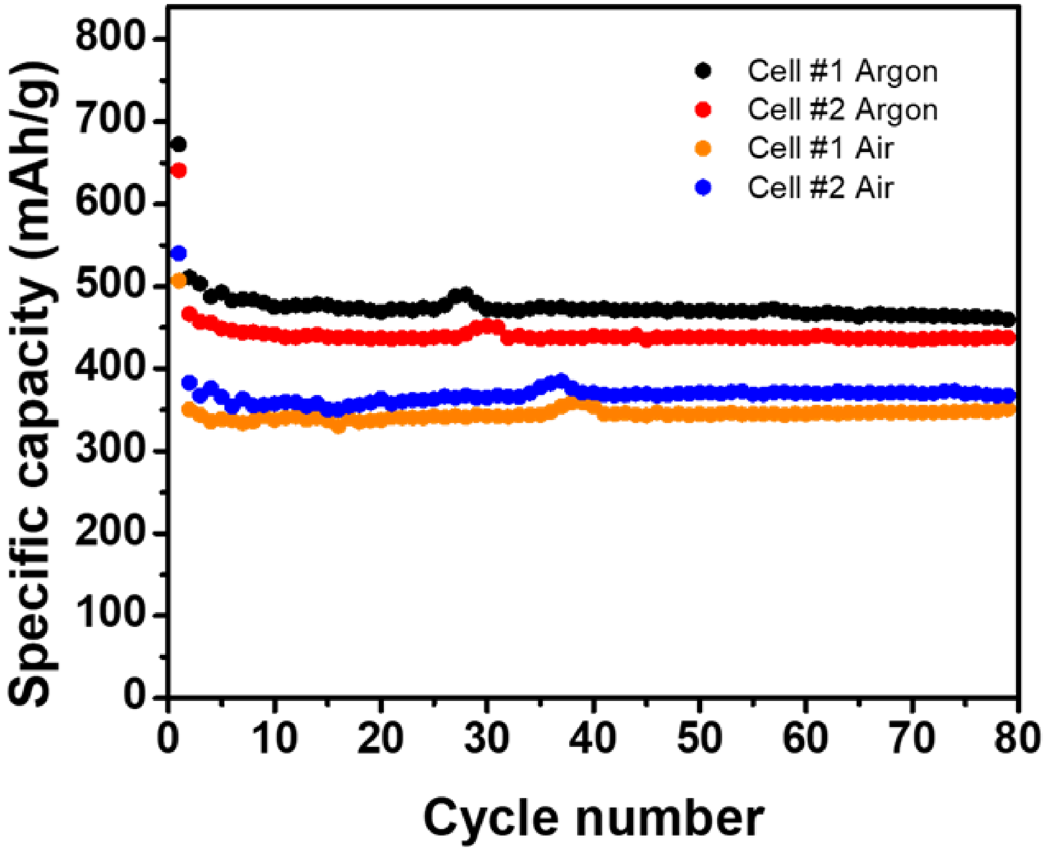
Correlation of Mass Loading to Coating Thickness





Cycling 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%



Technical Challenges

- Improving first cycle efficiency (FCE)
  - The current FCE is much to low for a viable LIBs
- Potential solutions
  - Prelithiate the binder, such as Li-Polyacrylic acid (PAA)
  - Prelithiate the electrode using Li foil or stabilized lithium metal powder (SLMP)
  - Prelithiate the PDC resin prior to curing or pyrolysis

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 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

The Case for Graphite Replacement

- Graphite is the key anodic electrode material of the lithium ion battery- one of the key technologies that is currently fueling the green economy (>90% of the market share for anodic materials in Li ion batteries)
- There is no current natural graphite production source in the USA*
- The gap in supply and demand forces the USA to be a net importer of BOTH natural and synthetic graphite
- The USA imports the majority of its graphite from China (which could pose a national security concern)
- Given 100% replace rate of graphitic anodes in Li ion batteries by 2024, the amount of sequestered coal in the batteries would reach 27,300 tons.

Next Steps

- We will continue to investigate different mixtures of coal types and PDC resins by processing them to form coal-core composite powders for evaluation in a lithium-ion battery environment using half-2032 coin cells.
- Electrode slurry trials will continue with control and experimental groups consisting of aqueous and non-aqueous binder combinations, including carboxymethyl cellulose (CMC), polyacrylic acid (PAA) and polyvinylidene fluoride (PVDF).
- Various in-house battery testing methods will be used to evaluate the half-coin cells including cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic charge/discharge (GCD) cycling performance.