Ultra-Low Volume Change Silicon-Dominant Nanocomposite Anodes for Long Calendar Life and Cycle Life

2024-03-30

Final Technical Report for EE0009186

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Abstract:

Sila's ultra-low volume change silicon anode material was utilized to achieve high cycle life and calendar life with improved electrolyte formulations, simultaneously achieving the required 1000 cycles and 10 year calendar life required in an electric vehicle battery, while also enabling >900 Wh/L and >350 Wh/kg cell level energy density.

Funding Office: Office of Energy Efficiency & Renewable Energy, Vehicle Technologies Office

Performing Organization: Sila Nanotechnologies, Inc.

Reporting Period: October 2020 - December 2023

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Introduction

Beginning of Life Characteristics at 25°C	Cell Level
Usable Specific Energy @ C/3	>350Wh/kg
Usable Energy Density @ C/3	>750Wh/L
Calendar Life @ C/3	>10 Years
Cycle Life (C/3 deep discharge to 350Wh/kg, <20% energy fade)	>1,000

Table 1. Project goals

The objective of this grant was to research, fabricate, and test lithium battery cells that implement ≥ 30% silicon content electrodes with commercially available cathode technology and achieve cell performance identified in the Table 1.

Sila's nano-engineered particles enable ultra-low volume change silicon-dominant anodes and are the most promising candidate for silicon-based electric vehicle Li-ion batteries. This project utilizes Sila's proprietary particles and know-how for its application in standard Li-ion battery manufacturing processes. Both the bulk and surface properties of the particle are engineered for improved performance, and the electrode construction process is optimized around the adjustments made to the particle, as are electrolyte formulations. Sila's state of the art analysis techniques are also employed, and new methods are developed to understand how material and process changes impact cell performance.

In addition, Sila partnered with ARL to simulate electrolyte reaction mechanisms and reveal the causes of cell performance differences between formulations with different electrolyte components. Sila also partnered with PNNL to develop Localized High Concentration Electrolytes for higher automotive commercial readiness and achieve even better performance with Sila's anode material.

Conclusions

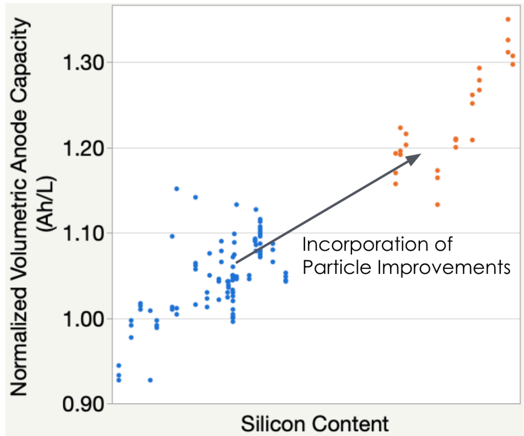

Figure 1. Silicon content of particles was improved to increase the volumetric capacity of the anodes.

To achieve high energy density, Sila increased the silicon content of its particles by modifying processes that affect bulk and surface properties. This increased the volumetric capacity of the anode (Figure 1) as well as the gravimetric capacity, ultimately resulting in higher cell energy density. Slurry recipes and electrode construction protocols were optimized to enable high energy, high cycle life, and high calendar life. Cell teardowns were performed to study the modes of degradation to assist in the development process.

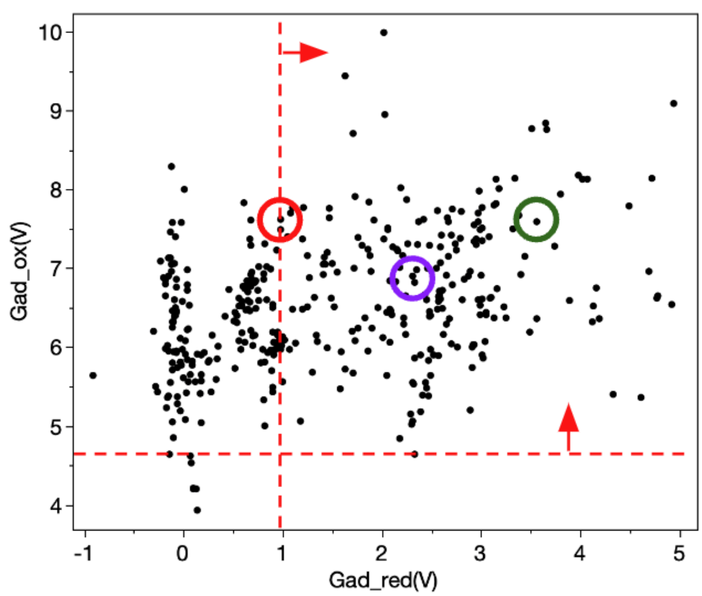

Figure 2. Reduction and oxidation potentials of various molecules were calculated to identify promising compounds for SEI formers. The red circle indicates FEC, and the purple and green circles represent Sila proprietary additives.

One portion of the development process involved electrolyte development. To explore novel additives, DFT simulations were performed at the Army Research Laboratory (ARL) by Oleg Borodin to calculate the relevant reduction and oxidation potentials. To improve the accuracy of the simulations, the reaction potentials were calculated for when the solvated molecules are in a contact pair with Li+. The red circle indicates FEC. By seeking molecules with high oxidation potential and high reduction potential, potential SEI formers were found. Indeed, SEI formers previously identified by Sila (purple and green) fell into this quadrant, validating this approach.

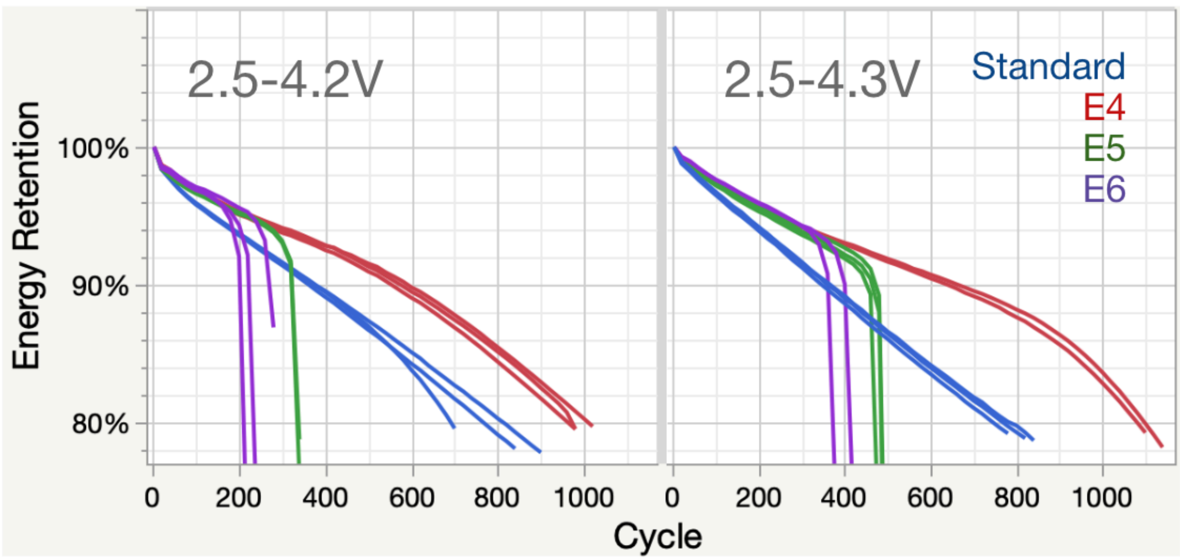

Figure 3. Cycle life of three Localized High Concentration Electrolytes tested with Sila anode, compared against a standard electrolyte.

Localized High Concentration Electrolytes (L-HCE) were also explored in collaboration with Jiguang Zhang at Pacific Northwest National Laboratory (PNNL). Figure 3 shows the comparison of three candidate L-HCEs, compared against a standard electrolyte. While not all electrolytes improved cycle performance, E4 (in red) improved cycle life both for the standard 2.5-4.2V cycling as well as the elevated 2.5-4.3V cycling, which enables higher cell energy density.

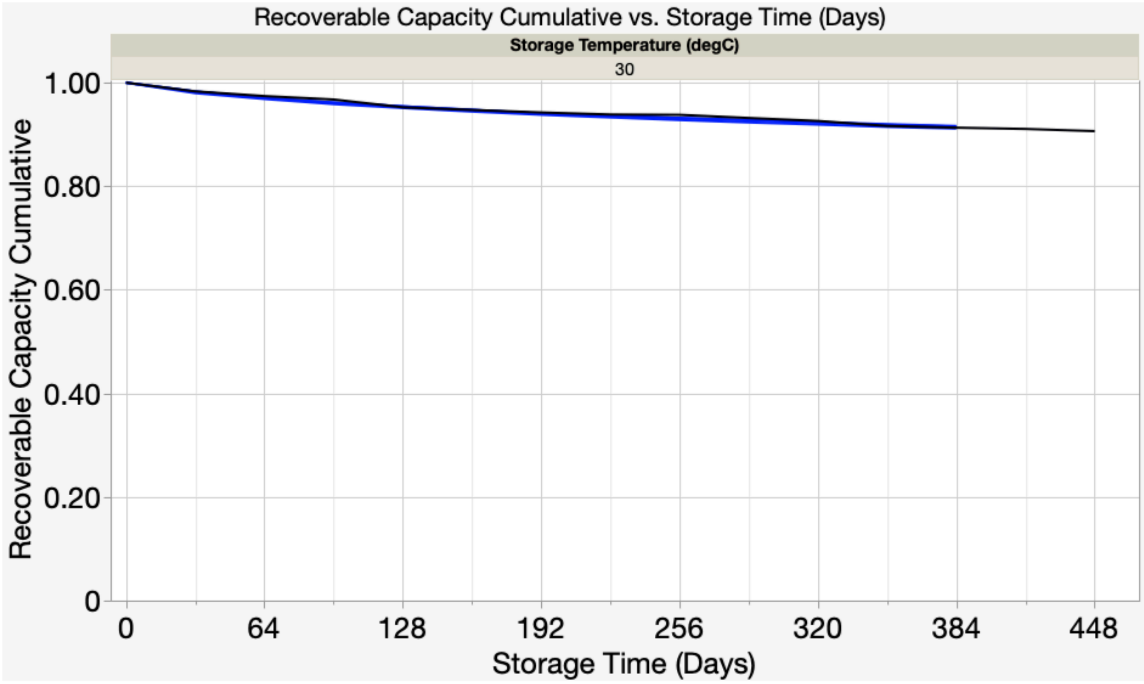

Figure 4. 30°C 100% SOC Calendar life of 1Ah interim cells tested at (blue) a prototyping partner and (black) Argonne National Laboratory using standard electrolyte.

In terms of performance, calendar life has generally been identified as a performance gap in most silicon anodes in existence. Sila's anode however, shows superior calendar life performance even using standard electrolyte, same as that used in Figure 3. Figure 4 shows the calendar life of 1Ah prototype cells delivered for the interim cell deliverable, tested at 2 different sites. The results were highly reproducible, and are projected to last 9 years to 80% of the target energy density. By improving the anode formulation, electrolyte formulation, cathode material, cell design, and formation protocol, further improvements have been achieved in other form factors.

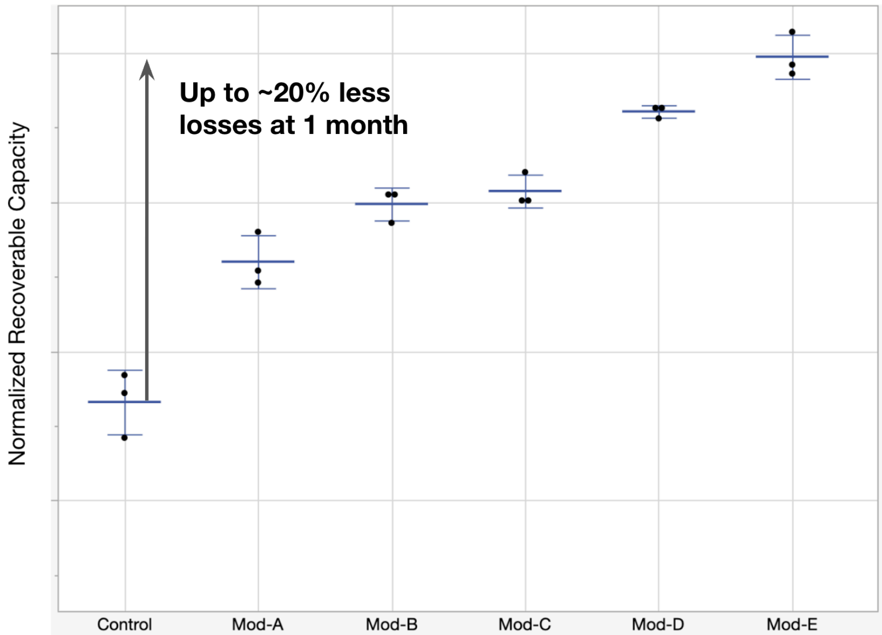

Figure 5. Modified electrolyte additive packages improving the recoverable capacity measured at 1 month.

One such achievement in the grant was the improvement of the electrolyte additive package. Figure 5 shows the improved recoverable capacity of cells utilizing improved additive mixtures, both by changing the selection of molecules and the concentration of the additives. The degradation rate could be reduced by up to 20% using only currently commercially deployed compounds readily available from all major electrolyte manufacturers.

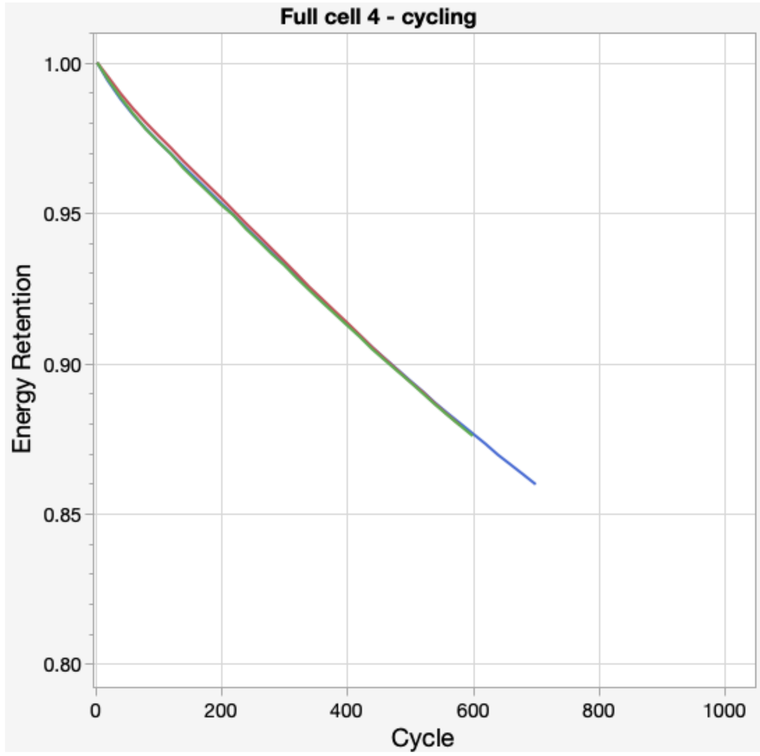

Figure 6. Preliminary cycling performance of final cells, tested in single layer pouch cells utilizing electrolyte improvements identified in Figure 5.

Oftentimes however, improvements to calendar life result in reductions in cycle life due to differing fundamental degradation mechanisms. Figure 6 shows confirmation that the 20% reduction in calendar life degradation could still be achieved while maintaining >1000 cycles to 80% energy retention. In a state of the art commercial form factor cell, Sila's ultra-low volume change silicon anode material, coupled with the improved electrolyte, can deliver >900 Wh/L and >350 Wh/kg while achieving >10 years calendar life and >1000 cycles to 80% energy retention, fulfilling the final goal of this grant.