Solid-state Architecture Batteries for Enhanced Rechargeability and Safety for Electric Aircraft

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The Problem

Battery Performance Requirements
- NASA Battery Workshop 2017 and industry representatives state “The primary barrier to electric aviation is battery performance”
- SOA lithium ion batteries do not meet energy density requirements needed to enable electric aircraft designs
- Unique flight critical metrics (e.g. high power) required

Battery Safety Requirements
- Current batteries under development will always have fire safety challenges due to flammable electrolytes used
- Safety is required for aerospace applications
- SOA lithium ion batteries have caused a number of safety incidents on aircraft
- Parasitic weight from excess packaging and cooling is undesirable

Vehicle Performance & Efficiency

SOA lithium ion batteries have caused safety incidents on aircraft, such as the Boeing 787 Li-Ion Battery and the UPS Cargo Flight Grounded. These incidents highlight the need for improved battery safety and performance in electric aviation.
Current performance targets for the automotive sector are a battery pack with 250 – 300 Wh/kg.
Can a battery be designed for electric aircraft, following system level analyses, that provides the combination of required properties?

- Safety
- Energy density
- Discharge rate
- Packaging design for minimal weight
- Scalability

**SABERS Concept**: Design a battery using system level analyses to guide target properties, combine existing materials technologies, and a bi-polar stack design.
The Big Question

How do we meet **ALL** demanding battery needs of electric aircraft?

- State-of-the-art lithium-ion batteries
- Lithium sulfur batteries
- Solid state batteries
SABERS Transformative Technology

Combination of unique materials technologies to achieve performance goals
SSE-enabled bi-polar stack design minimizes safety containment in packaging

Lithium-Ion Battery (SOA) Packaging
- Contains flammable electrolytes
- Requires heavy housing and cooling system
- The added pack weight reduces energy density

Bi-Polar Stack Packaging Enabled by SSE
- Contains no flammable liquids
- Enables a shared current collector (bi-polar)
- Reduces safety containment weight
- Minimal/passive cooling system possible
- Potential for higher power density and C-rates
- 90% of cell specific energy can be retained in pack
**Thermal/Weight Systems Level Analysis**

- **SABERS operating temperature (150°C) versus for Li-Ion chemistries (50-60°C)**
- **Thermal heat load well within SABERS temperature limits (simple passive system)**
- **Advanced Li-Ion batteries require:**
  - *Active system:* adds 20-30% weight, 30-50% volume, 1-3% of power used
  - *Semi-passive:* system with phase change material: 10-20% weight and volume penalty

**SABERS Bi-Polar Stack**
- Effectively 10-30% less battery pack “overhead”
- Improved specific energy and power
- Critical enabling technology for all-electric, battery vehicles/missions
Holey Graphene Conductive Scaffold

Encapsulate S/Se with holey graphene hosts to maximize energy and power utilization

- Unique NASA-developed technology
  - High conductivity, ultralightweight electrode scaffold
  - Through-thickness ion transport enabling fast kinetics
  - Enables universal dry electrode processing
  - Scalable

Battery with Holey Graphene Scaffolding

Scale-Up to Production
Holey Graphene Fabrication and Performance

- Extremely facile: single-step, no mixing needed
- Widely applicable: S, Se, SeₓSᵧ, Li₂S
- Ultrahigh mass loading (>10 mg/cm²) cathodes from hG-enabled dry-press technique are advantageous toward cell- and pack-level performance.
- Addition of holey graphene significantly improves the initial discharge capacity of the cell

- High active material content (up to 90 wt%)
- High mass loading: high areal capacity
- Excellent current collector– cathode contact
- Extremely facile: single-step, no mixing needed
- Widely applicable: S, Se, SeₓSᵧ, Li₂S

Diagram:
- Composite Mixture
- Dry-Press
- Composite
- Layered Composite
- Sandwich

Graph:
- Cathode w/ and w/o Addition of Holey Graphene
- Addition of holey graphene
- No holey graphene

- Voltage (V)
- Time (S)
50 wt% Sulfur:Carbon with a liquid electrolyte able to achieve 1100 Wh/kg at 0.4C discharge rate
Traditional SSB Manufacturing Approach vs. SABERS Approach

**Traditional SSB Manufacturing Approach**
- Glass Electrolyte
- Lithium flow through electrolyte-cathode
- Sulfur-Carbon-Electrolyte Composite
- Cathode
- Electrolyte
- Anode

**SABERS Approach**
- Polypropylene
- Li-metal
- Li-Ni fibers
- Cathode
- Electrolyte
- Anode
Cathode Composition and Microstructure

Solid State Cathode constituents:

- Cathode active material (CAM) - S, Se, $Se_xS_y$, $Li_2S$
- Solid electrolyte (SE) with high $Li^+$ ionic conductivity - $Li_{10}GeP_2S_{12}$ (LGPS) (7-12 mS/cm); $Li_6PS_5Cl$ (Argyrodite) (2-4 mS/cm)
- Electronic conductive agent (ECA) with high electron conductivity – CB, hG

S + 2$Li^+$ + 2$e^-$ → $Li_2S$

Optimal Cathode should have:

- High amount of CAM, or cathode loading - 50-90 vol%
- Sufficient, but minimal amount of SE, with good CAM/SE contact to ensure sufficient $Li^+$ diffusion
- Sufficient, but minimal amount of ECA for $e^-$ transport

Critical parameters for optimal cathode performance:

- Grain size of the components – the smaller, the better
- Composition ratio between CAM : SE : ECA – depends on the grain size – network percolation problem
- $Li^+$ and $e^-$ conductivities of SE and ECA
- Mass weight of the components – affects the overall battery weight
Multiscale Modeling Approach

- Ab initio simulations
- Material and transport properties
- Doping strategies

- Particle dynamics methods: electro-mechanical model
- Grain structure properties
- SE/CAM ratios, cathode utilization

- Physics based continuum scale modeling: electrochemical and thermal models
- Experimental benchmarking

Length Scale

Computational simplicity

Cathode material

Crystal lattice

Battery

∼ 10−100 μm

∼ 1−2 nm
Particle Dynamics Method

Electro-mechanical model: Solid Electrolyte Sphere Approximation Model (SESAM)

(NTR: LAR-19842-1)

- Represents the cathode composite as a system of tightly packed spheres of different types and sizes with assigned specific Li$^+$ and e$^-$ conductivities.

- Calculates the total conductivities for Li$^+$ and e$^-$ of the mixed powder composite as dependent on the particle size, density and composition ratio.

*Solid Electrolyte Sphere Approximation Model (SESAM) is pending NASA Release*
**Particle Dynamics Method**

**Electro-mechanical model: Solid Electrolyte Sphere Approximation Model (SESAM)**

(NTR: LAR-19842-1)

**Model construction:**

- Generate particles of given type (SE, C, S) and given size distribution
- Fills the system box (or RVE) with particles of all types randomly

![Cathode Representative Volume Element (RVE)](image)
Model construction:

- Generate particles of given type (SE, C, S) and given size distribution
- Fills the system box (or RVE) with particles of all types randomly
- Compress the powder composite
**Multiscale Modeling Approach**

- Continuum Scale
- Physics based modeling
- Experimental benchmarking

Mass conservation
\[
\phi \frac{dC_{Li}}{dt} - \frac{\partial}{\partial x} \left( \phi D_{Li} \frac{dC_{Li}}{dx} + uC_{Li} F \frac{d\varphi_2}{dx} \right) = -\alpha j_n
\]

Electron charge conservation
\[
\frac{\partial}{\partial x} (i_1) = \frac{\partial}{\partial x} (\sigma \frac{\partial \varphi_1}{\partial x}) = \alpha j_n F
\]

Ion charge conservation
\[
\frac{\partial}{\partial x} (i_2) = \frac{\partial}{\partial x} (\kappa \frac{\partial \varphi_2}{\partial x}) = -\alpha j_n F
\]

- Computational simplicity
  - Particle dynamics level
  - Electromechanical and grain interaction model

- Length Scale
  - ∼ 1−2 nm
    - Ab initio simulations
    - Material and transport properties
    - Doping strategies

- Continuum Scale
  - Physics based modeling
  - Experimental benchmarking

- SESAM takes input from experimental data and ab-initio QM simulations on material properties
- SESAM predicts cathode ion and electron conductivities as input to mesoscale battery models
Conclusions

- Elevated temperature operation is a design parameter that can be modified.
  - If you increase operating temperature from 40 to 50 °C, energy is increased by 10%.
  - SABERS is a solid-state battery which enables high temperature operation (150 °C).

- Addition of holey graphene improves cathode performance.
  - Holey graphene provides high electrical conductivity and binderless dry compressibility.
  - It increases cathode electrical conductivity and initial voltage discharge profile.

- SABERS 1C-rate for lithium-sulfur (804 Wh/kg) is comparable to a 3C-rate for lithium-ion.
  - The standards for electric aircraft are given in terms of lithium-ion batteries.
  - Different chemistries require defining unique standards.

- Optimizing the composition ratio between SE, active material, and conductive agent can significantly improve battery performance.
  - Particle size has a significant effect on the ionic and electronic conductance.
  - The model suggests using large particles.
The SABERS Team would like to gratefully acknowledge funding for this project from Convergent Aeronautics Solutions (CAS).