Solid-state Architecture Batteries for Enhanced Rechargeability and Safety (SABERS)

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The Problem

Current SOA batteries are not designed to meet the unique performance & safety requirements of electric aircraft.

**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**

![Diagram showing performance and safety requirements for electric vehicles.](image-url)
Current performance targets for the automotive sector are a battery pack with 250 – 300 Wh/kg.
Aeronautics Challenges

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

![Diagram showing Electric Aircraft, Energy, Power, Safety, Packaging, and Scalability, with overlapping areas indicating different battery technologies for automotive and electric aircraft sectors.](image-url)
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
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

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
A 0.4C Discharge Rate Exceeds 1100 Wh/kg for thicker electrode (2.8mAhcm$^{-2}$)

- 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
Multiscale Modeling Approach

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

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

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

*C** **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)
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
- Compress the powder composite

Cathode Representative Volume Element (RVE)
Multiscale Modeling Approach

- Continuum Scale
- Physics based modeling
- Experimental benchmarking

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

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

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

- 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 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 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
SABERS Team/Acknowledgements

Aerospace Industry

- Electrified aircraft is a core NASA thrust

Battery Industry

Excitement to partner with world leader in aeronautics technology

Department of Energy

- NASA is a “thought leader” in aeronautics
- Industry peers state NASA should lead feasibility assessment of 500 Wh/kg battery