Pore-Scale Transport Resolved Model Incorporating Cathode Microstructure and Peroxide Growth in Lithium-Air Batteries

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**Motivation**

Li-ion technology in electric vehicles is limited to ~100 miles. Li-air battery is an attractive high energy density alternative.

**Methodology**

- **Pore-scale modeling**
  - Li\(_2\)O\(_2\) Deposits
  - Continous BC
  - Simulation Domain:
    - Homogeneous continuum
    - Multiphase
  - Microstructures:
    - Volume-averaged
    - Fully resolved
  - Li\(_2\)O\(_2\) formation:
    - Porosity change
    - Explicitly modeled

- **Thickness dependent conductivity**
  - High conductivity for ultra-thin Li\(_2\)O\(_2\) layer due to electron tunneling

- **Peroxide growth modeling**
  - As reactions occur at the electrolyte/electrode interface Li\(_2\)O\(_2\) “fills up” each voxel during discharge

  - Li\(_2\)O\(_2\) grows when it reaches saturation concentration

**Results**

- **Effect of Li\(_2\)O\(_2\) Conductivity**
  - Porosity: 85%
  - Specific Surface Area: 100 m\(^2\)/g
  - Local current density: 2.5 mA/m\(^2\)
  - Constant conductivity doesn’t capture flat initial voltage and sudden voltage drop.

- **Effect of Applied Current**
  - Lower current density yields higher voltage and longer discharge time
  - A higher reaction rate constant improves the cell voltage.

- **Effect of Nanostructure Spacing**
  - Specific discharge capacity increases with nanostructure spacing.
  - Larger spacing prevents pore-blocking and loss of active area.

- **Effect of Nanostructure Height**
  - Larger nanostructure height yields higher voltage and larger specific capacity due to increased active surface area.

**References**

