



Applied and
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Mathematics

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Mathematical modelling for the next-generation all-solid-state battery: Nucleation interface

Tuan Vo

ACoM, Applied and Computational Mathematics, RWTH Aachen University

Next-generation All-solid-state battery

Rechargeable Lithium-ion battery (LIB) stays at the heart of every energy storage system and electric vehicle. Undoubtedly, LIB benefits human life efficiently as well as friendly-environment. Besides, a more advanced LIB, so-called **all-solid-state battery** (ASSB), is introduced recently as ASSB is expected with non-inflammation and non-explosion as seen in common LIBs. Yet, defect due to polarization is one natural phenomenon of **solid electrolyte** (SE) to be tackled.

This poster is aimed to model the polarized SE with the use of **structural tensor**. A typical LIB includes three main components: cathode, anode and electrolyte. Different types of LIB have a variation of constitutive material composed of battery. An ASSB means that the three main components are **all made of solid material**.

Modelling goal

Two main goals to model the solid electrolyte part of the all-solid-state battery is as follows:

1. To capture the **preferred direction** behaviour of the solid electrolyte due to electric potential.
2. To satisfy **thermodynamic consistency**:
 - Conservation of mass, linear & angular momentum and energy for the solid electrolyte.
 - Entropy inequality is guaranteed with sharper conditions, which lead to constitutive equation.

Continuum physics kinematic

Green-Lagrange strain tensor \mathbf{E} with respect to **small** displacement $\partial \mathbf{u} / \partial \boldsymbol{\xi} = \mathcal{O}(\epsilon)$, $\epsilon \ll 1$:

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^\top \mathbf{F} - \mathbf{I}) = \frac{1}{2} \left(\frac{\partial \mathbf{u}}{\partial \boldsymbol{\xi}} + \left(\frac{\partial \mathbf{u}}{\partial \boldsymbol{\xi}} \right)^\top + \underbrace{\left(\frac{\partial \mathbf{u}}{\partial \boldsymbol{\xi}} \right)^\top \left(\frac{\partial \mathbf{u}}{\partial \boldsymbol{\xi}} \right)}_{\text{Neglected}} \right) \rightarrow \boldsymbol{\epsilon} := \frac{1}{2} \left(\frac{\partial \mathbf{u}}{\partial \boldsymbol{\xi}} + \left(\frac{\partial \mathbf{u}}{\partial \boldsymbol{\xi}} \right)^\top \right)$$

Polarization phenomenon

Due to a source of electric potential pointing from cathode (+) to anode (−) pole, a uniform electric field created has suppressed on the SE occupied between these two poles. Consequently, SE yields to a **preferred direction** under external deformations such as mechanical loading forces.

Contact

Tuan Vo · RWTH Aachen University · Email: vo@acom.rwth-aachen.de