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

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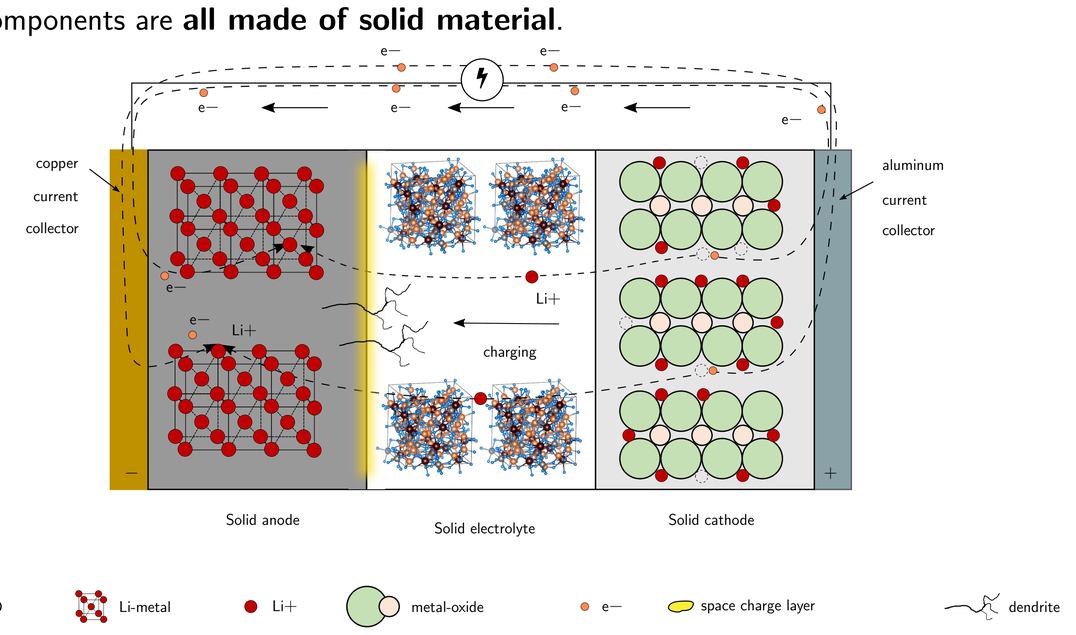
Next-generation All-solid-state battery

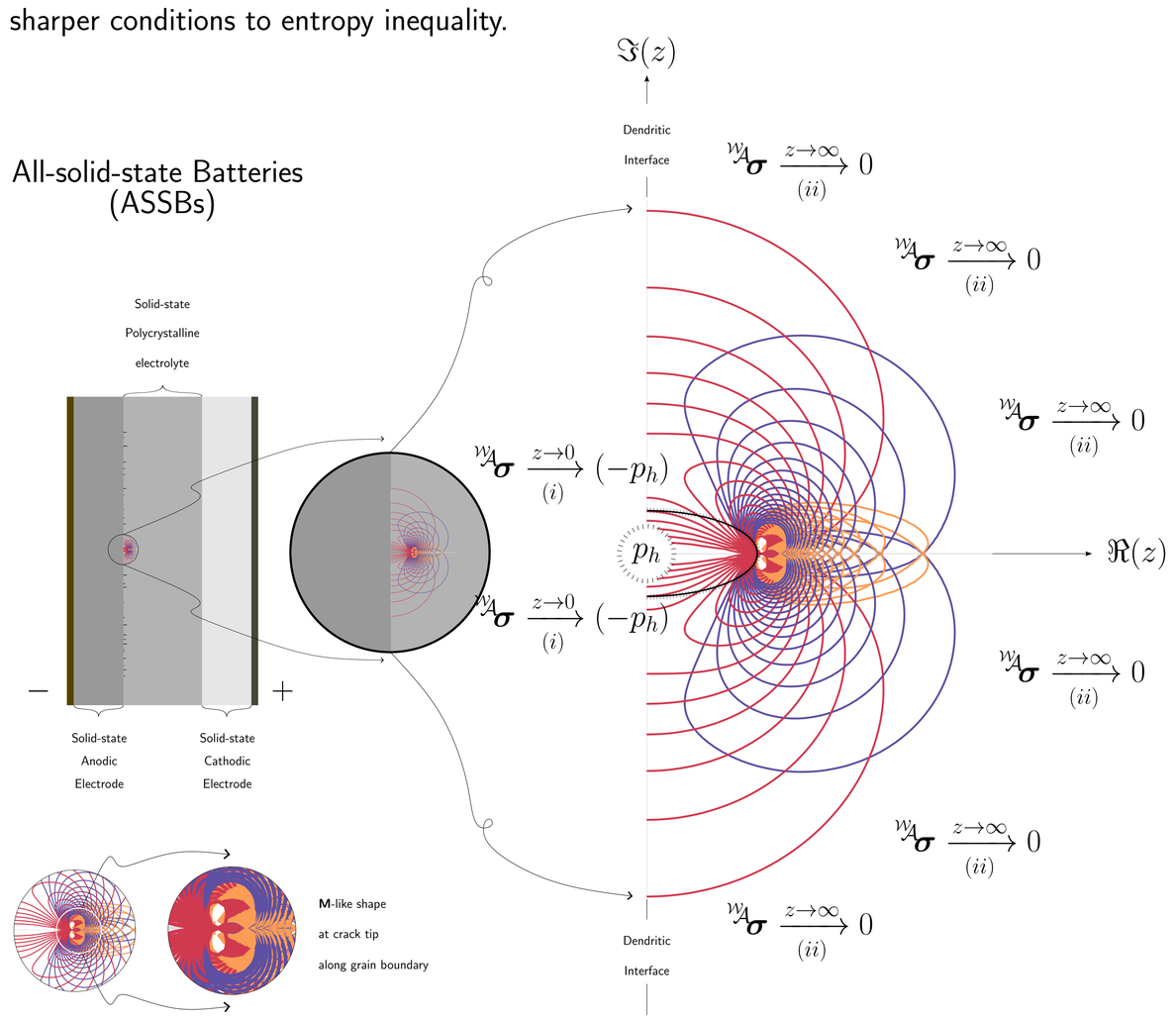
Rechargeable Lithium-ion battery (LIB) stays at the heart of every energy storage system and electric vehicle. Undoubtedly, LIB benefits human life efficiently as well as friendly-environment. Besides, a more advanced LIB, so-called **all-solid-state battery** (ASSB), is introduced recently as ASSB is 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**.



Mathematical model

Constitutive equation is first derived from considering local balance laws and enforcing sharper conditions to entropy inequality.



Modelling goal: Interface analysis + Numerical modelling

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.

$$a_{\text{Griffith}} := a^* = \arg\min_{a\in\mathbb{R}} \iiint_\Omega f(a, \boldsymbol{u}; \lambda, \mu, \boldsymbol{d}\otimes\boldsymbol{d})\, d\Omega - \iint_\Gamma f(a;\gamma)\, d\Gamma \Big|_{\boldsymbol{u}^{(s)}}$$

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