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

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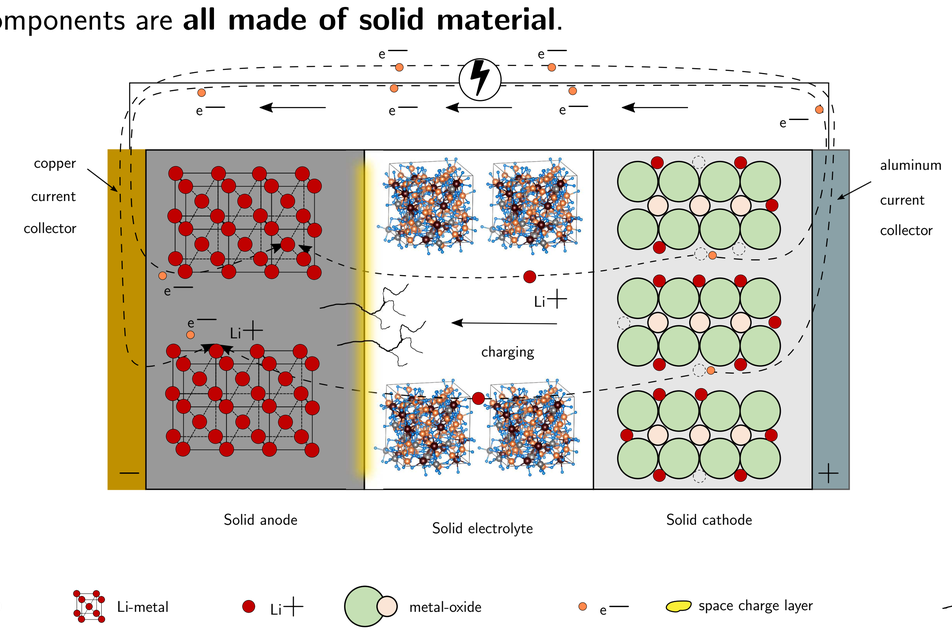
Next-generation All-solid-state battery (ASSB)

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.

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

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: 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.

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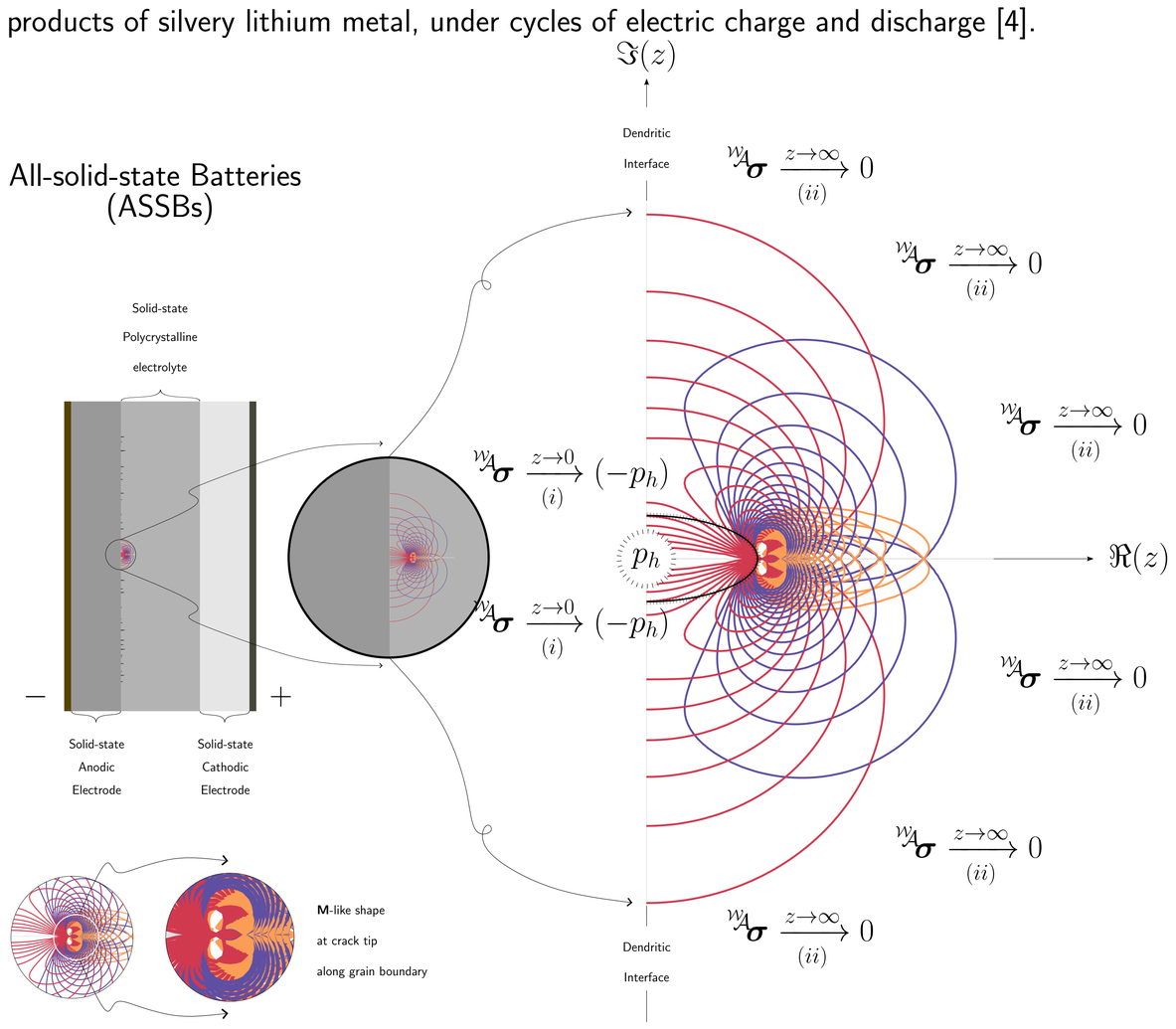
Mathematical model

Interface between solid electrode and solid-state electrolyte (SE|SSE) taking place at space charge layer (SCL) [2] found in all-solid-state lithium-ion batteries (ASSLiBs) critically exhibits mechanical and electrochemical instability [3]. This evidence points directly to the fact that the soft metallic lithium negative electrode is erroneously prone to triggering dendritic by-products of silvery lithium metal, under cycles of electric charge and discharge [4].



Besides, polycrystalline garnet-typed solid-state electrolyte such as LLZO exhibit grain boundaries and various sizes and shapes of grains under microscopic observation. Therefore, this type of microstructure distinctively leads to nuance destruction of ceramic-like materials. Consequentially, dendritic by-products contribute to degradation of ionic conductivity and trace along grain boundaries in SSE. This phenomenon, notwithstanding, is predicted, quantified, and controlled based on analysing the multi-scale coupled problem subjected to conditions of Griffith criterion.

References

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