Next-generation all-solid-state battery

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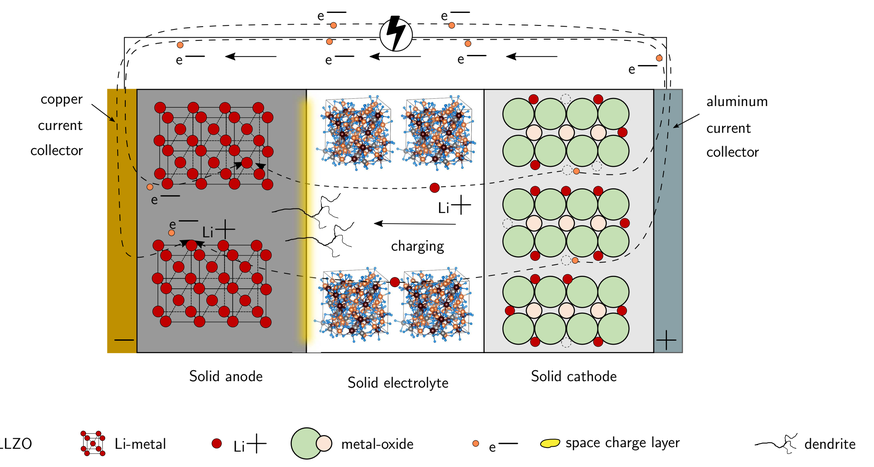
Mathematical modelling for the next-generation All-solid-state batteries: Nucleation (SE|SSE)$^{(*)}$-interface

Rechargeable Lithium-ion battery (LIB) stays at the heart of electric vehicles, portable electric devices, and energy storage systems [1]. Nowadays, LIBs help human life become more efficient as well as to cope with global environment issues thanks to its zero emission. However, conventional LIB (cLIB) is sensible to temperature and pressure, easily prone to flammable and explosive. This is mainly due to liquid-based electrolyte found in cLIBs. **All-solid-state battery** (ASSB) is, therefore, one of promising candidates to overcome bottlenecks of conventional LIBs. It is because the solid-state electrolyte (SSE) in ASSB, e.g. SSE made of the highly ionic-conductive polycrystalline LLZO, is highly stable towards temperature and pressure. Nevertheless, metallic Lithium dendrite triggered at (SE|SSE)-interface is the main drawback as these dendritic threads extrapolate into grain boundary network of SSE, causing degradation of ionic conductivity and the likelihood of short-circuit.

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

Next-generation All-solid-state battery (ng-ASSB) should, consequentially, be able to cope with micro-dendritic threads at the (SE|SSE)-interface, and hence, to foresee nucleation points caused by propagations



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

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Comparison: Analytical vs. Numerical solution

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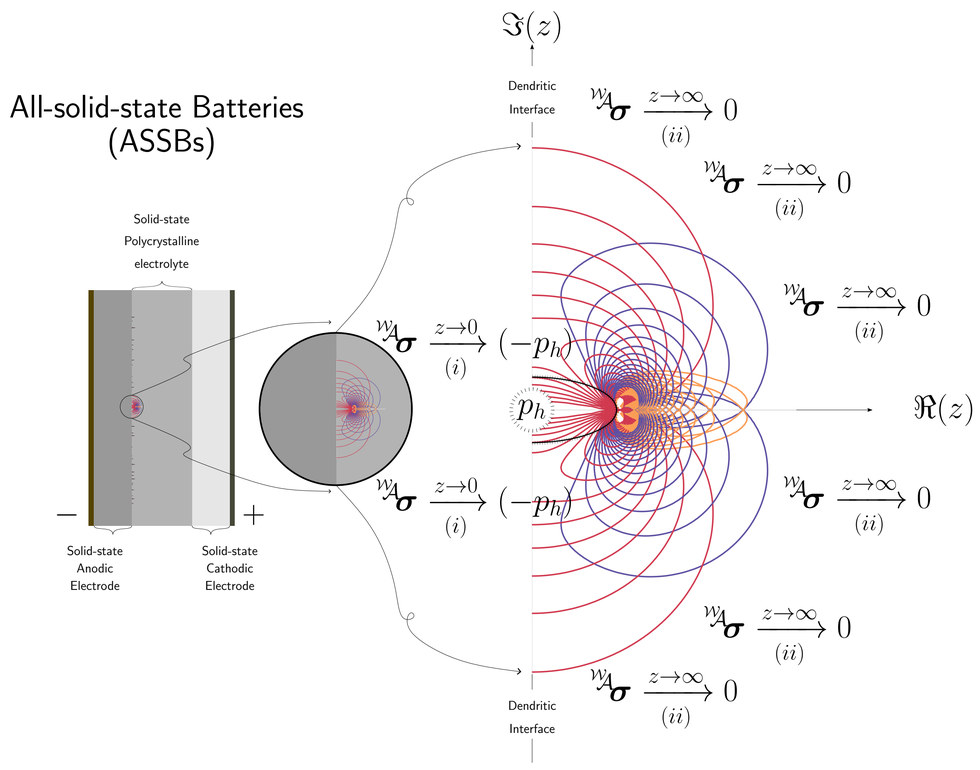
Nucleation interface

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].



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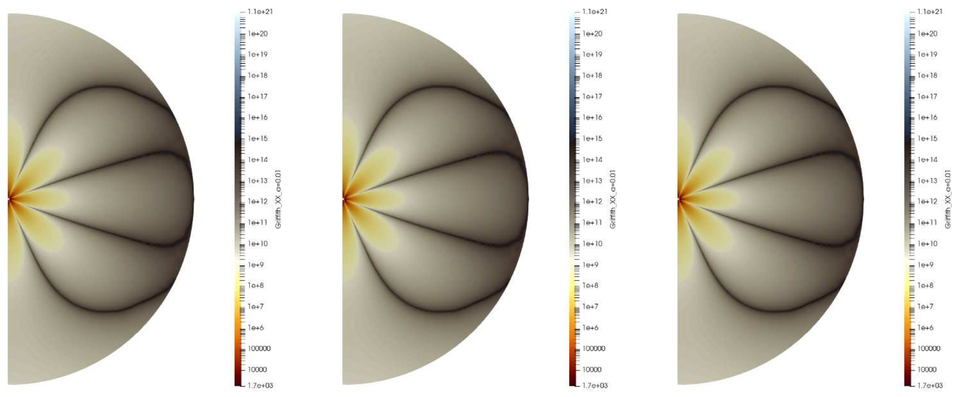

Besides, polycrystalline garnet-typed solid-state electrolyte such as LLZO exhibit grain boundaries and various sizes and shapes of grains under microscopic observation. Therefore, this type of microstructure distinctively leads to nuance destruction of ceramic-like materials. Consequentially, dendritic 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.

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