Mathematical modelling for all-solid-state battery: (SE|SSE)-Interface

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

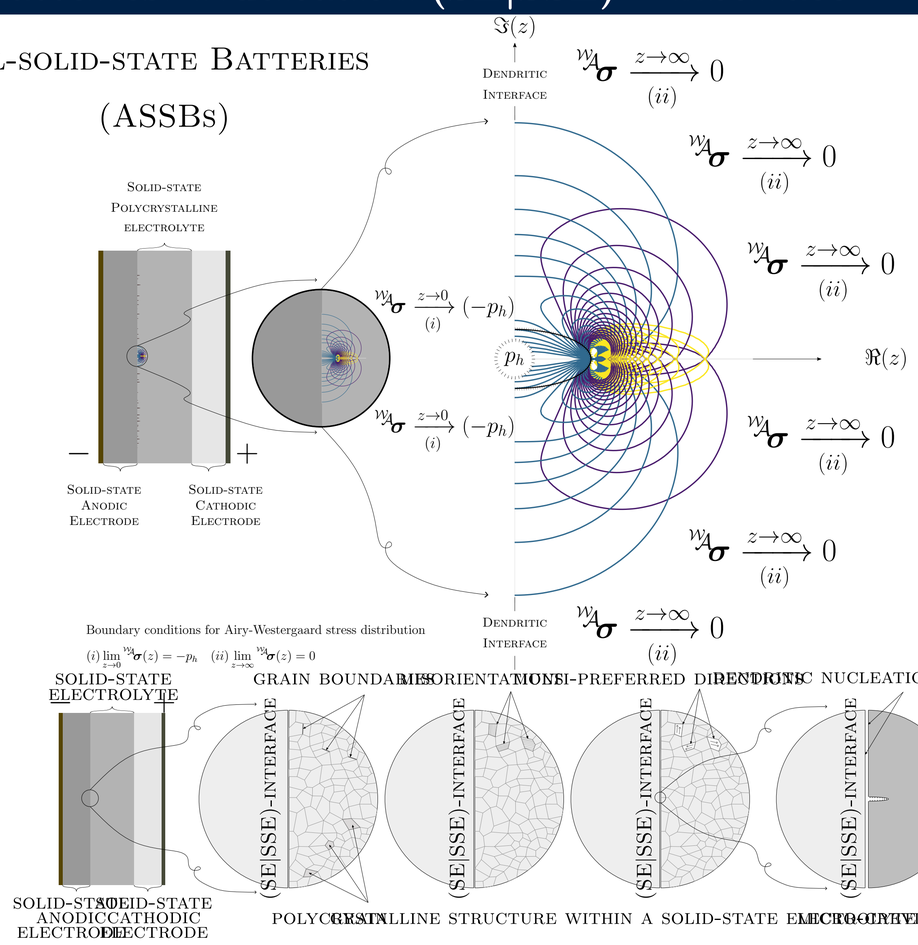
Rechargeable Lithium-ion battery (LIB) is at the heart of every electric vehicle (EV), portable electronic device, and energy storage system [1]. Nowadays, LIBs enable human life more efficient and help to solve global environment issues thanks to EVs' zero emission. However, conventional LIB (c-LIB) is sensible to temperature and pressure, hence, flammable and explosive, which is undesirable. This bottleneck is mainly due to liquid-based electrolyte found in c-LIBs.

All-solid-state battery (ASSB) is one of promising candidates to overcome bottlenecks of c-LIBs. Thanks to solid-state electrolyte (SSE), ASSB is highly stable towards temperature and pressure. Nevertheless, Li-metal dendrite triggered at (SE|SSE)-interface [5] is the main drawback of ASSB since these dendritic threads extrapolate into SSE grain boundary network, causing crevice, degradation of ionic conductivity, and the probability of short-circuit, which is unfavorable.

Next-generation All-solid-state battery (ng-ASSB) with a consideration of nucleation criterion defined by

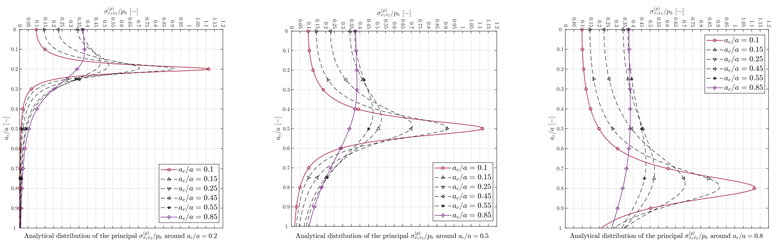
$$a_{\text{Griffith}} := a^* = \arg\min_{a\in\mathbb{R}} \iiint_{\Omega} f(a, \boldsymbol{u}, \theta; \lambda, \mu, \boldsymbol{d}^{(\star)} \otimes \boldsymbol{d}^{(\star)})\, d\Omega - \iint_{\Gamma} f(a; \gamma)\, d\Gamma \Big|_{\bar{\boldsymbol{u}}}$$

where $\boldsymbol{u}$ displacement field, θ temperature field, a crevice length, λ, μ Lamé constants, $\boldsymbol{d}^{(\star)} \otimes \boldsymbol{d}^{(\star)}$ embedded misorientation structural tensor, and γ cracking-surface energy density, can help to improve ASSB performance.

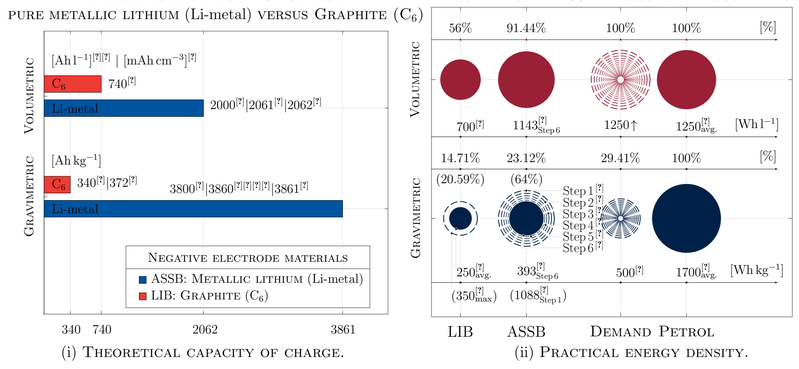


(SE|SSE)-Interface Analysis

Interface between solid electrode and solid-state electrolyte (SE|SSE) taking place at space charge layer (SCL) [2] found in ASSBs critically exhibits mechanical and electrochemical instability [3]. This evidence points directly to the fact that the soft metallic li anode is erroneously prone to triggering dendrites, under cycles of electric charge & discharge [5].

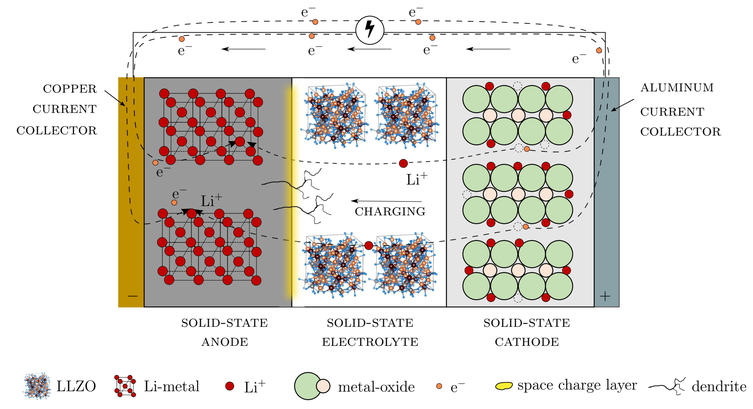


Distribution: ana. max. shear stress ${}^{\mathcal{A}}\sigma^{\Pi}_{x_1x_2}$ around crack tip a_c.



Next-generation All-solid-state battery

Nucleation criterion governs the instable (SE|SSE)-interface [3]



✓ **Thermodynamic consistency** is satisfied, followed by [2].
✓ **Closure** $\bar{\Omega}$ is fulfilled by 15 moments, followed by [4].

Embedded structural-tensor in SSE

Polycrystalline garnet-type SSE [5] such as LLZO exhibit grain boundary network, and grains with variation of {size, shape} under microscopic observation. Hence, this microstructure is potentially prone to nuances of destruction.

$$\boldsymbol{M} = \boldsymbol{d}^{(\star)}_{G_1} \otimes \boldsymbol{d}^{(\star)}_{G_2} \quad \text{given by} \quad \mathbb{G} := \{\boldsymbol{Q}_{||_d}, \boldsymbol{Q}_{\perp_d}\} \subset \mathcal{O}(3).$$