Next-generation all-solid-state battery

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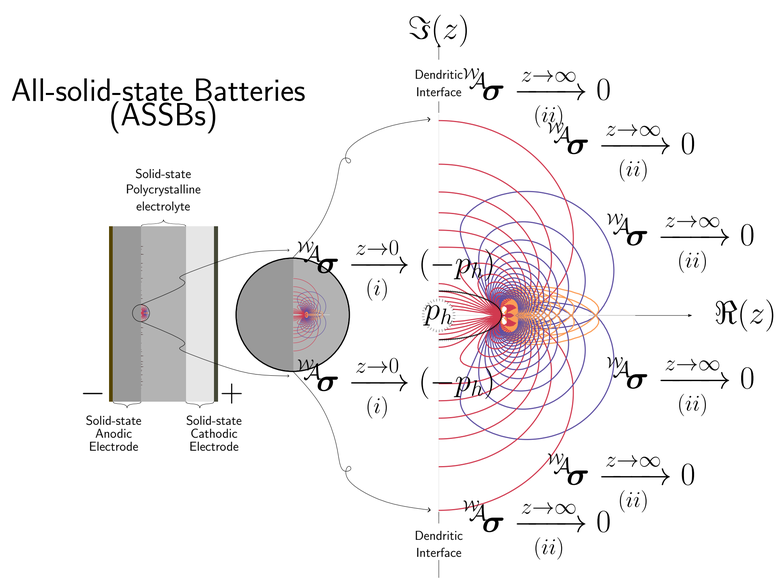
Mathematical modelling for the next-generation All-solid-state batteries: Nucleation (SE|SSE)$^{(*)}$-interface

Rechargeable Lithium-ion battery (LIB) 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. This bottleneck is mainly due to liquid-based electrolyte 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, metallic Li-dendrite triggered at (SE|SSE)-interface is the main drawback as these dendritic threads extrapolate into grain boundary network of SSE, causing crevice, degradation of ionic conductivity, and the probability of short-circuit. **Next-generation All-solid-state battery** (ng-ASSB) with a consideration of nucleation criterion defined by

$$\rho\,\partial_{t^2}^2\boldsymbol{u}^{(s)} + \nabla\cdot\left(\overset{4}{\mathbb{C}}{}^{\mathbb{D}(\Omega)}_{(\lambda,\mu)} : \nabla\boldsymbol{u}^{(s)}\right) + \rho\nabla V_e = \mathbf{0},$$

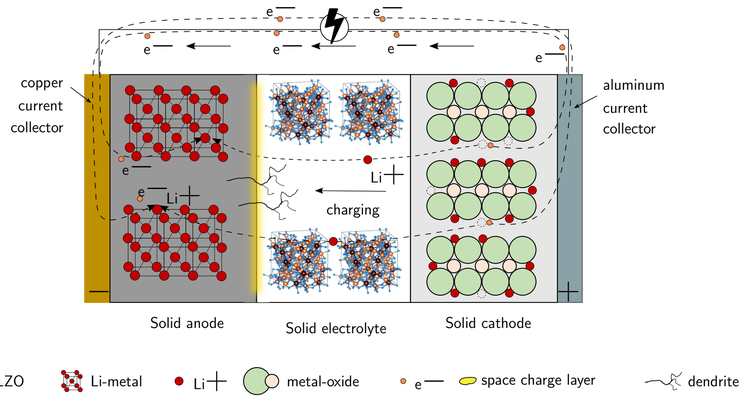
$$\text{s.t. } a_{\text{Griffith}} := a^* = \arg\min_{a\in\mathbb{R}} \iiint_{\Omega} f(a,\boldsymbol{u};\lambda,\mu,\boldsymbol{d}\otimes\boldsymbol{d})\,d\Omega - \iint_{\Gamma} f(a;\gamma)\,d\Gamma\Big|_{\boldsymbol{u}^{(s)}}$$

where,
can help to improve ASSB performance.



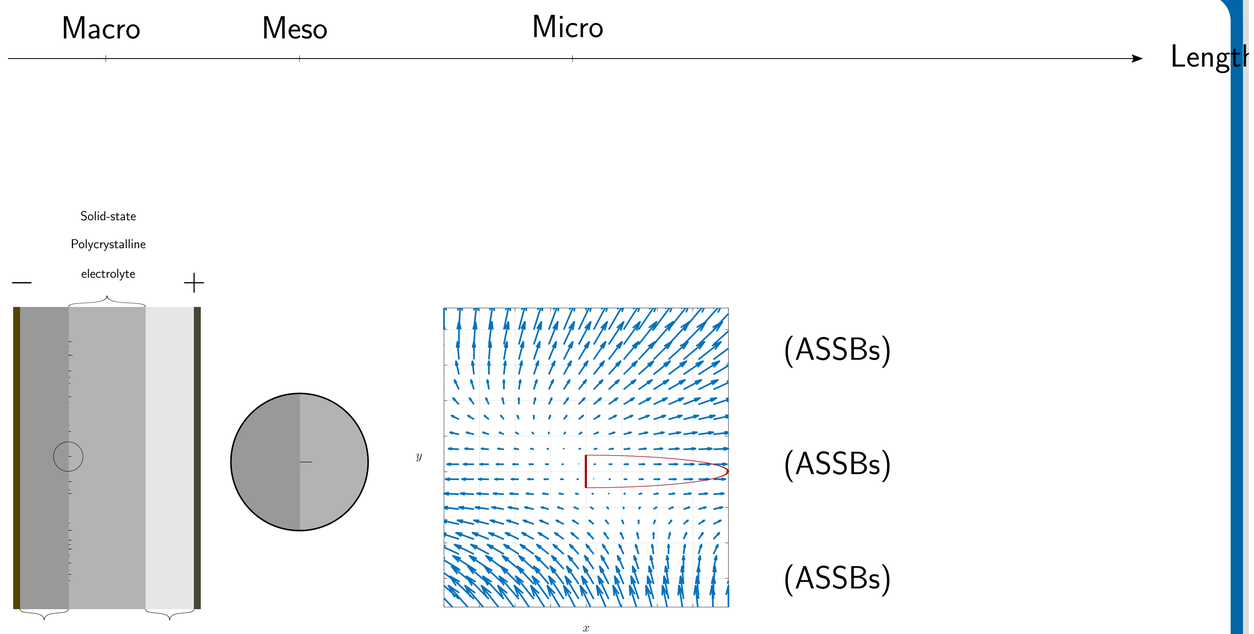
Next-generation All-solid-state battery

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 & 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.

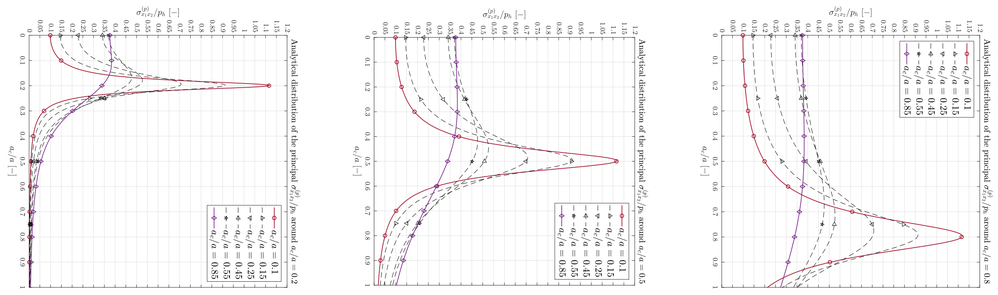
abc



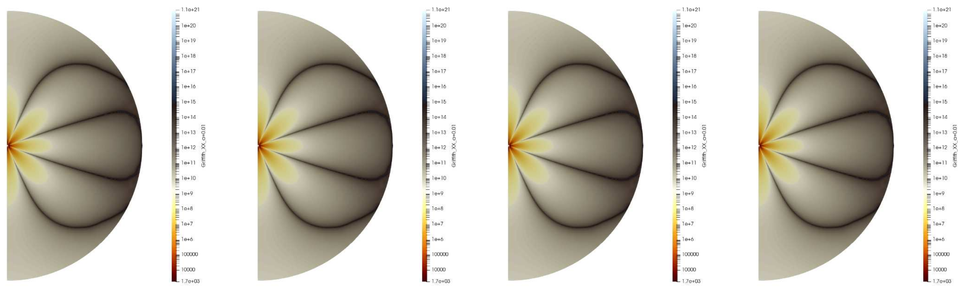
Nucleation interface: Taking place at the critical dendritic interface

Nucleation interface: Taking place at the critical dendritic interface (SE|SSE)

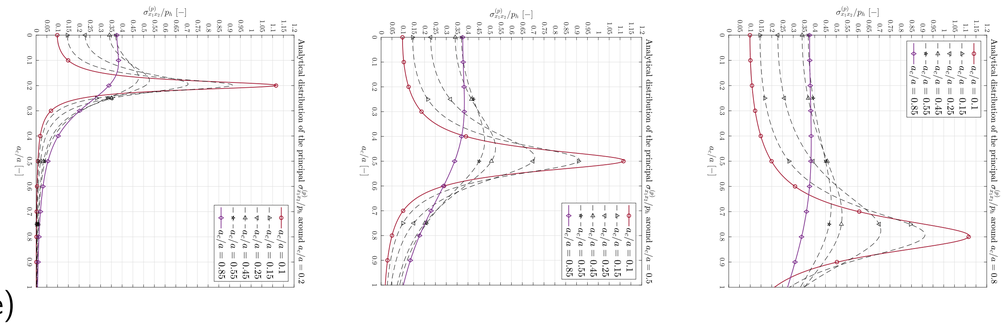
Distribution of the analytical maximal shear stress component ${}^{\mathcal{W}_A}\sigma^{\Pi}_{x_1x_2}$, around the crack tip a_c.



The set of boundary conditions is likewise the path of the pressure-centric dendritic crack.



Comparison



Nucleation interface: Taking place at the critical dendritic interface (Solid electrode | Solid-state electrolyte)

Contact

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References

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[2] **S.Braun**, C.Yada and A.Latz, *Thermodynamically consistent model for Space-Charge-Layer formation in a solid electrolyte*. Jr. Phys. Chem., 119, 22281-22288, 2015.
[3] **C.Hüter**, S.Fu, M.Finsterbusch, E.Figgemeier, L.Wells, and R.Spatschek. *Electrode-electrolyte interface stability in solid state electrolyte system: influence of*