Modeling and simulations towards the design of high performance batteries.

M. Bastanfar, M. Berlato, L. Cabras, T. Dev, S. Esmizadeh,
M. Serpelloni, N. Valizadeh, E. Yildiz, A. Salvadori

University of Brescia, DIMI, m4lab, 25123-Brescia, Italy

The upcoming request of renewable energy requires high performance energy storage and power delivery systems. The conventional batteries rely on liquid electrolytes, which is still the state of art due to their high ionic conductivity. These systems, though, show safety concerns in view of the flammability of toxic organic solvents. Therefore, there is a great effort to introduce novel electrolyte materials with excellent transport properties, low interfacial resistance, good mechanical strength, and safer behavior. Solid-state electrolytes are promising candidates. Upon combining with Li or Na metal anodes they have the potential to deliver higher energy densities with enhanced safety compared to liquid electrolyte batteries. However, upon charging such cells at current densities greater than a critical value, "dendrites" nucleate and grow from the metal electrode and result in short-circuiting the cell. Furthermore, SSE present contact problem with the porous electrode interfaces.

For this reason, gel polymer electrolytes (GPE) can be seen as a valid alternative. It is composed by a polymer network with solvent filling the interstitial spaces, the confined liquid into the polymer matrix can boost the conductivity and can provide better adhesion at the electrode interfaces. It is well known that low ionic diffusivities cause high concentration and potential polarization across thick, porous cathodes at high current rates. Furthermore, the rapid depletion of Li+ ions at the reaction surface limits the rate capability of thick electrode-based Li-ion batteries.

In a series of different research endeavours, modelling and simulations have been carried out at the m4lab towards the design of the next generation of electrochemical storage systems. In this talk, a brief overview will be presented at first, concerning dendritic growth and a multiscale compatible approach in electrolytes. Eventually, a detailed investigation of gel polymer electrolytes, optimal electrode design, and the influence of ionic additives in the porous carbon-binder network will be presented and validated against experimental evidence.

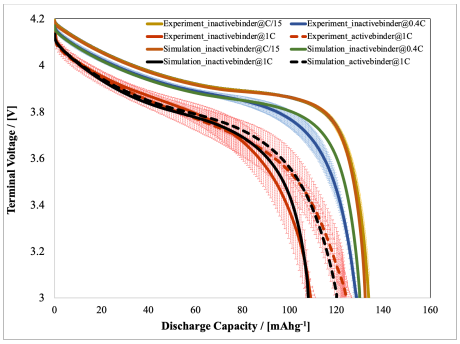

Figure 1: model validation

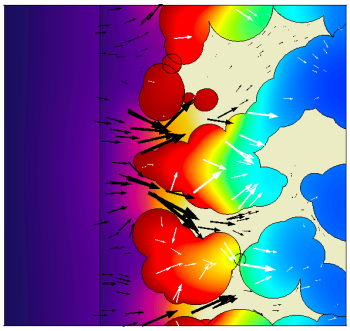

Figure 2: Li distribution and flux