# Multiphysics modeling of solid polymer electrolytes: A finite element method investigation

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## ABSTRACT

Structural batteries and 3-D architecture micro-batteries have largely been investigated in response to the need for higher energy density lithium-ion batteries and micro-scaled power sources required in automotive and microelectronic industries. Solid polymer electrolytes (SPEs) have been subject to intense research studies for their possible application in these families of devices. They can be cast into complex 3-D geometries without leakage and can be employed as multifunctional materials that serve both as the structural matrix of a fiber-reinforced composite and the electrolyte of a battery [1].
The ionic conductivity that can be attained with solid polymers is however low compared to currently used liquid electrolytes. Moreover, experimental studies show that the conductivity further reduces when SPEs are processed in order to achieve improved mechanical performances (e.g. crosslinking). This constitutes the major drawback when developing structural batteries. Molecular dynamics simulations have been recently used to link the macroscopic multifunctional response to microstructural aspects [2], yet multiphysics modeling of SPEs from a continuum level perspective is still missing [1].

The current contribution aims at filling this gap. By following the approach detailed in Ref. [3] a model is presented for the coupled electro-chemo-mechanical response of a SPE.
The system under study is a polymer in which an inorganic salt dissolves and dissociates in two ions. The latter is modeled as a solid through which the transport of multiple charged species occurs and is described in terms of molar concentration of ions, electric potential and displacement field. The Nernst-Plank equation has been modified to account for the effect of a pressure gradient on the ionic fluxes. Use of the electroneutrality approximation was made [4]. A finite element formulation has been derived and the results of the simulations of 3-D structured batteries are presented. The impact of deformations and stresses on the electrochemical battery response has been analyzed in terms of modification of the electric potential and ionic concentration distributions that follow from different mechanical solicitations. Comparison of the numerical results against results of previous simulations [4] highlights the impact of the mechanical contribution on the battery performance.

## REFERENCES

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