# Numerical Analysis of the Mechanical-Electrochemical Coupling in Structural Supercapacitors

The effect of mechanical loads on the electrochemical performance of structural supercapacitors is investigated through a coupled multiphysics analysis on a structural electrolyte.

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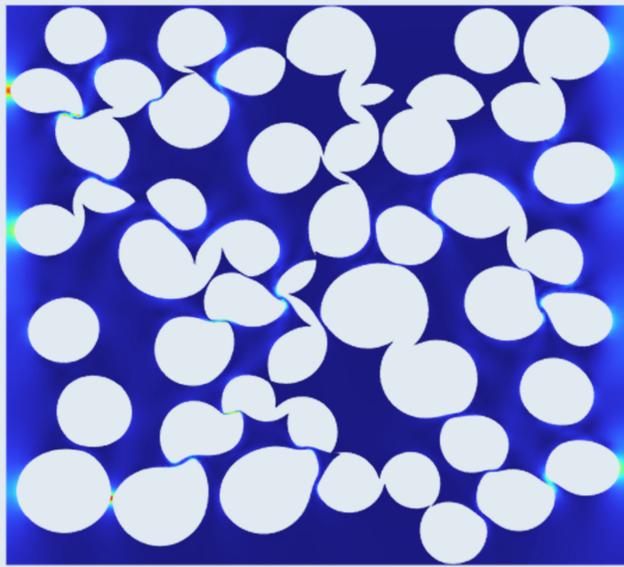
Abstract

Structural Supercapacitors (SSC), as Multifunctional Energy Storage Composites (MESC), can have huge aerospace and automotive applications. As integrated structural parts, an SSC must retain its electrochemical performance under mechanical loads. In addition to fiber electrodes, a key ingredient of SSCs are the structural electrolytes. A promising type of structural electrolytes are bicontinuous materials which comprise a non-conducting high performance epoxy resin skeleton/structure that provides the required mechanical strength; and an ionic liquid (IL) component which is responsible for the SSC electrochemical function. (Ref. 1) Capacitance depends on the diffusion of the ionic species, which move exclusively through the diffusion paths, i.e. electrolyte porosities. In addition, the effective diffusion coefficient of a bicontinuous electrolyte relies on the bulk diffusion coefficient as well as the morphological factors of the structure. (Ref. 2) The current study aims to model and numerically simulate the mechanical-electrochemical coupling in a bicontinuous electrolyte.
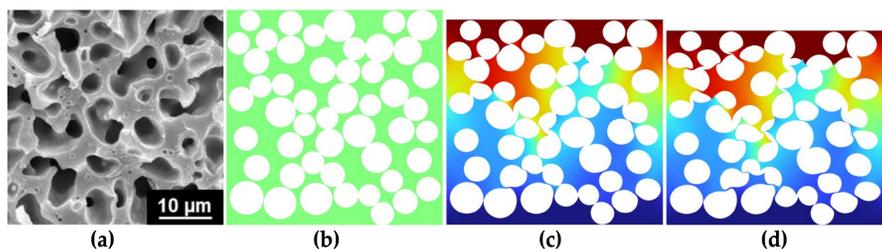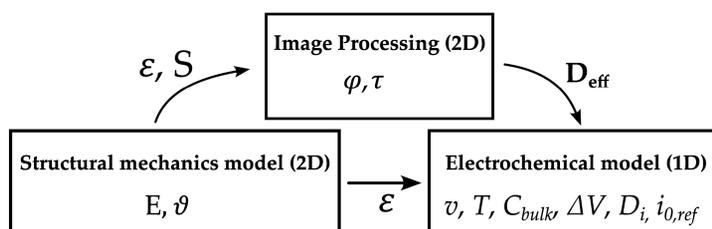
FIGURE 1. (a) electrolyte SEM (Ref. 1), (b) the corresponding simplified RVE, and deformation plots at (c) ε=5%, and (d) ε=10%

Methodology

A representative volume element (RVE) of the bicontinuous electrolyte was selected using SEM images. A simplified 2D bead model of the porous structure was then generated. Various compressive strains were applied on the RVE. The emerging porosity (φ) and tortuosity (τ) of the structure were measured using an image processing tool. The values were then used to calculate the effective diffusion coefficient at every strain value employing the following expression: (Ref. 2)

$$D_{\text{eff}} = \frac{\varphi}{\tau} D_{\text{bulk}}$$

The cyclic voltammetry testing of the electrolyte was then simulated at different strain steps using the calculated D_{eff}.

Results

According to Figure 2, increased compressive strain in the structural bicontinuous electrolyte resulted in noticeable decrease in the SSC's energy density. This can be explained by the fact that the compressive stress deforms the polymer skeleton which results in a change in its morphology, i.e. porosity and tortuosity. As an outcome, the available ion conductive pathways evolve leading to a change in the effective diffusion coefficient of the electrolyte. In this particular case, deformations led to a decreased diffusion coefficient, which resulted in lower specific capacitance values (the internal surface area of CV graphs). This translates into a lower energy density for the SSC.
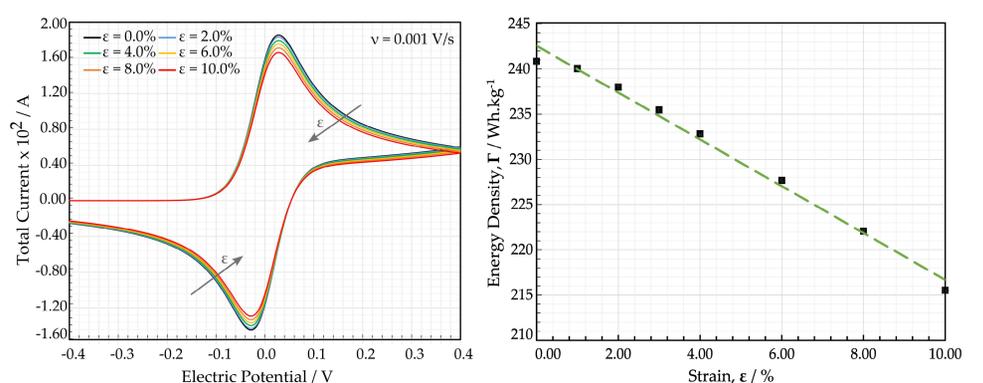

FIGURE 2. (left) simulated cyclic voltammetry graphs of SSC at different strains; (right) SSC energy density at different strains.

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