Computational Analysis of the Mechanical and Thermal Stresses in a Thin Film PProDOT-Based Redox Capacitor

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Introduction

Among the several types of capacitors, the double-layer and redox types have gathered increasing attention to address some of the heavy power demands of modern technology. In the double-layer kind, the stored electrical energy is based on the separation of charged species in the electrical double layer between an electrolyte and an electron conductor typically constituted by a carbonaceous material. In redox capacitors, charge is stored chemically via oxidation/reduction processes in the active materials like electroactive polymers (EAPs) or metal oxides. However, advantages of EAPs such as reduced cost and the ability to tailor properties like conductivity, voltage window, and storage capacity through chemical modification underscore the attractiveness of organic supercapacitor devices over the metal oxide counterparts. This work investigates the stresses and heat flux of the electrode – separator membrane interaction in a thin film redox capacitor at scales under a micrometer. The Type I redox capacitor being studied contains as electrode couples films in different doped states of the EAP Poly(3,4-propylenedioxythiophene) (PProDOT) that was electrochemically deposited on platinum electrodes . The separator is a polypropylene porous membrane impregnated with an electrolyte composed of the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide (EMIBTI) in propylene carbonate. Experimental devices of this type show abrasion of the electrode surface after N charge-discharge cycles. Understanding the causes of this phenomenon is important since these defects may lead to significant degradation in the performance of the device.

Use of COMSOL Multiphysics

Computational analysis of stresses occurring in supercapacitors which model a complete device often use an homogeneous model of the separator membrane, electrodes with thicknesses similar to that of the membrane, or modeling thin electrodes with a domain one dimension smaller than the rest of the device (eg. a 2D domain in a 3D model). These types of simulations do not account for the type of damage described above. For instance, when using thin film electrodes, the pores of the separator membrane are, in average, wider that the thickness of the film. This is an important feature that is not accounted for in a homogeneous model of the separator neither in a model of the electrode with reduced dimensions.

COMSOL Multiphysics was used to model the electrode – separator membrane interaction using stress, conductive heat flux and convective heat flux model combinations. Results show significant stresses and deformations occurring in the PProDOT-based electrodes as well as temperature variations that provide a plausible explanation for the abrasion phenomena.