Numerical simulation of electronic electro-active polymers

Duc Khoi Vu and Paul Steinmann
Chair of Applied Mechanics, University of Erlangen-Nuremberg
Egerlandstrasse 5, 91058 Erlangen, Germany

1. Introduction

This work is part of a project on experiment, modeling and simulation of electronic electro-active polymers (EEAPs), which arise nowadays as novel materials with promising applications [1]. For many years, EEAPs have been known to be capable of changing shape and size under the application of electric loading, but the applications of EEAPs only caught attention recently with the discovery of new materials, which can produce giant deformation. EEAPs offer the possibility to make actuators that can be used in the development of lightweight, inexpensive, resilient, damage tolerant, noiseless and agile robotic systems. These materials have been considered as a potential alternative to materials that are commonly used for actuators in adaptive structures like piezoelectric ceramics, piezoelectric composites, shape memory metals and alloys, magneto- and electro-rheological fluids. However, the application of EEAPs is not limited to the development of actuators. Because of their capability to produce large deformation and to change their electrical properties when undergoing large deformation, EEAPs can also be used as sensors to measure large strains. Note that in actuation mode EEAPs are subjected to electric loading and in sensing mode, by measuring the capacitance of the materials, the amount of deformation can be determined [4].

EEAPs can be classified as a sub class of the so-called electro-active polymers (EAPs). Another sub class of EAPs is called ionic electro-active polymers (IEAPs). The main difference between EEAPs and IEAPs is that EEAPs are driven by Maxwell forces while IEAPs are driven by the diffusion of ions inside the materials. The advantage of IEAPs is the requirement for low drive voltages but they have slow response and there is the need to maintain their wetness. In addition, it is difficult to sustain direct-current-induced displacements. The major disadvantage of EEAPs is that they require high voltages. However, the advantages of using EEAPs in developing actuators include rapid response, the ability to operate in room conditions for a long period of time and very importantly the ability to hold the induced displacement under activation by a direct-current voltage. These properties make EEAPs very suitable for actuators and sensors.

As EEAPs have a great potential in the development of actuators and sensors, understanding the response of EEAPs under both electric and mechanical loading is a key problem. Despite this, there exist until now only a few experimental works that can actually serve to characterize the electro-mechanical properties of these materials. Besides, despite the fact that there exists a coupling phenomenon between the mechanical and the electrical response of the materials, and despite the fact that there exist discrepancies between measurement, modeling and simulation, until now only simple models are used to explain experimental data. In modeling and simulation of EEAPs, large deformation, nonlinear polarization and viscosity should be taken into account together with the consideration of the electric field in the free space surrounding the body of interest [2,3,5-8]. Therefore, from the modeling side, in order to understand and correctly describe the behavior of EEAPs, there is the need for a more comprehensive approach that uses extended versions of conventional models in electricity and elasticity and takes both the fully coupled nonlinear electroelastic and viscoelastic effects into account. From the simulation side, the numerical simulation of EEAPs requires the use of the finite element method in combination with, for example, the boundary element method in the case no simple formula can be used to take into account the effect of the electric field in the free space surrounding the body of interest.

In this paper, we present the simulation of EEAPs by taking into account large deformation, nonlinear electric polarization and the contribution of the free space surrounding the body of interest using the coupling between the boundary element method and the finite element method. In what follows, the formulation of the problem is described and a numerical example is presented to demonstrate the importance of the contribution of the free space.

2. Formulation

Let us denote the undeformed configuration of the body under consideration by B_0 with the coordinate of each point denoted by $\boldsymbol{X}$ and the deformed configuration by B_t with the coordinate of each point denoted by $\boldsymbol{x} = \boldsymbol{\varphi}(\boldsymbol{X})$. Corresponding to these two configurations we denote the electric field, the electric displacement and the electric polarization by $\boldsymbol{E}$, $\boldsymbol{D}$, $\boldsymbol{P}$ and $\boldsymbol{e}$, $\boldsymbol{d}$, $\boldsymbol{p}$ in B_0 and B_t respectively. In the case considered here, we assume that the electric loading is static, there is no magnetic field and when viscous elastic effects can be neglected, the behavior of EEAPs can be modeled by using the theory of nonlinear electro-elasticity, in which with the help of a free energy density function $\hat{W}$ that depends on the current state of deformation represented by the deformation gradient $\boldsymbol{F} = \partial\boldsymbol{x}/\partial\boldsymbol{X}$ and on the electric field $\boldsymbol{E}$, a virtual work formulation of the problem can be constructed. This virtual work formulation can then be used to solve the problem of nonlinear electro-elasticity numerically by using, for example, the finite element method. An EEAP material considered here is said to be isotropic if $\hat{W}$ is an isotropic function of the Cauchy-Green tensor $\boldsymbol{C} = \boldsymbol{F}^t \cdot \boldsymbol{F}$ and the tensor $\boldsymbol{E}\otimes\boldsymbol{E}$. In this case the free energy density function is an isotropic function of six invariants I_1 to I_6 defined as: $I_1 = \boldsymbol{C}:\boldsymbol{I}$, $I_2 = \boldsymbol{C}:\boldsymbol{C}$, $I_3 = det\ \boldsymbol{C}$; $I_4 = \boldsymbol{I}:[\boldsymbol{E}\otimes\boldsymbol{E}]$, $I_5 = \boldsymbol{C}:[\boldsymbol{E}\otimes\boldsymbol{E}]$, $I_6 = \boldsymbol{C}^2:[\boldsymbol{E}\otimes\boldsymbol{E}]$, where $\boldsymbol{I}$ is the rank two unit tensor. The function $\hat{W}$ can be constructed so that, in the absence of electric stimulations, the material behaves exactly as a nonlinear material in nonlinear elasticity. The purely elastic behavior of the material is controlled by the three invariants I_1 to I_3. When the material is subjected to an electric field, the effect of the electric field is accounted for by the three invariants I_4, I_5 and I_6. The dependency of the free energy density function $\hat{W}$ on the two invariants I_5 and I_6 means that the material will exhibit a nonlinear electro-mechanical coupling behavior through these two terms. In order to determine the format and parameters of the free energy density function $\hat{W}$, a model is chosen and experimental tests are performed. The model's parameters are then determined from experimental data.

The above mentioned energy function can be constructed by assuming that there exists a function $W_{0\boldsymbol{e}}$ such that the Cauchy stress tensor $\boldsymbol{\sigma}$ and the electric polarization $\boldsymbol{p}$ in B_t can be computed by

$$\boldsymbol{\sigma} = J^{-1}\left[\partial_{\boldsymbol{F}} W_{0\boldsymbol{e}}\right]\cdot \boldsymbol{F}^t \tag{1}$$

and:

$$\boldsymbol{p} = -J^{-1}\partial_{\boldsymbol{e}} W_{0\boldsymbol{e}} \tag{2}$$

where $J = det\,\boldsymbol{F}$.

In addition we define the total stress tensor $\hat{\boldsymbol{\sigma}}$ as the combination of the Cauchy stress tensor $\boldsymbol{\sigma}$ and the stress induced by the electric body force

$$\hat{\boldsymbol{\sigma}} = \boldsymbol{\sigma} + \boldsymbol{e}\otimes\boldsymbol{d} - \frac{1}{2}\varepsilon_0\left[\boldsymbol{e}\cdot\boldsymbol{e}\right]\boldsymbol{I} \tag{3}$$

where ε_0 is the electric permittivity of vacuum. By using this assumption, the electric displacement in reference to the deformed configuration B_t and the total stress tensor can be computed as

$$\boldsymbol{d} = -J^{-1}\boldsymbol{F}\cdot\partial_{\boldsymbol{E}}\hat{W}_{0\boldsymbol{F}} \tag{4}$$

and

$$\hat{\boldsymbol{\sigma}} = J^{-1}\left[\partial_{\boldsymbol{F}}\hat{W}_{0\boldsymbol{F}}\right]\cdot\boldsymbol{F}^t \tag{5}$$

where

$$\hat{W}_{0\boldsymbol{F}} = W_{0\boldsymbol{E}}\left(\boldsymbol{F},\boldsymbol{E}\right) - \frac{1}{2}\varepsilon_0 J\boldsymbol{C}^{-1} : \left[\boldsymbol{E}\otimes\boldsymbol{E}\right] \tag{6}$$

in which $W_{0\boldsymbol{E}}\left(\boldsymbol{F},\boldsymbol{E}\right)$ is an energy function such that: $W_{0\boldsymbol{e}}\big|_{\boldsymbol{F},\boldsymbol{e}} = W_{0\boldsymbol{E}}\big|_{\boldsymbol{F},\boldsymbol{E}}$.

In addition, in reference to the undeformed configuration B_0 we have

$$\boldsymbol{P} = -\partial_{\boldsymbol{E}} W_{0\boldsymbol{E}} \tag{7}$$

and

$$\boldsymbol{D} = -\partial_{\boldsymbol{E}} \hat{W}_{0\boldsymbol{F}} \tag{8}$$

With the above assumption and definitions, the coupled electro-mechanical problem can be formulated as the following virtual work equation

$$\delta \int_{B_t} \hat{W}_{t\boldsymbol{F}} dv - \int_{B_t} \boldsymbol{b}_t \cdot \delta\boldsymbol{\varphi} dv - \int_{\partial B_t} \bar{\boldsymbol{t}}_t \cdot \delta\boldsymbol{\varphi} ds + \int_{\partial B_t} \delta\psi \cdot \bar{q}_t ds = 0 \tag{9}$$

where $\boldsymbol{b}_t$ is the mechanical body force, $\bar{\boldsymbol{t}}_t$ is the surface traction, $\bar{q}_t$ is the surface charge, $\hat{W}_{t\boldsymbol{F}} = J^{-1}\hat{W}_{0\boldsymbol{F}}$ and ψ is the electric potential defined such that

$$\boldsymbol{e} = -\nabla_{\boldsymbol{x}} \psi \tag{10}$$

Note that the equation (9) is used to describe only the finite domain B_t. In the case the infinite domain V_t^f of the free space surrounding B_t should be taken into account, the electric field in V_t^f can be computed using the following system of equations

$$\begin{cases} \nabla_{\boldsymbol{x}}^2 \psi = 0 & in\ V_t^f \\ \psi = \psi_t & on\ \partial V_t^{f\psi} \\ \boldsymbol{d} \cdot \boldsymbol{n} = \bar{q}_t & on\ \partial V_t^{fq} \end{cases} \tag{11}$$

which can be transformed into a boundary integral equation in the format

$$\varepsilon_0 \psi(\boldsymbol{\xi}) - \varepsilon_0 \psi_\infty - \varepsilon_0 \int_{\partial V_t^f} [\psi(\boldsymbol{x}) - \psi(\boldsymbol{\xi})] \frac{\partial G(\boldsymbol{\xi}, \boldsymbol{x})}{\partial n} ds + \int_{\partial V_t^f} qG(\boldsymbol{\xi}, \boldsymbol{x}) ds = 0 \tag{12}$$

where $\boldsymbol{\xi}$ is the source point, $\boldsymbol{x}$ is the field point, G is the fundamental solution of the Laplace's equation in (11) and $\frac{\partial G(\boldsymbol{\xi}, \boldsymbol{x})}{\partial n}$ is the derivative of G along the unit normal vector $\boldsymbol{n}$ of the boundary ∂V_t^f, q is the flux defined as

$$q = \varepsilon_0 \frac{\partial \psi(\boldsymbol{x})}{\partial n} \tag{13}$$

In addition to equation (12), we assume that the total charge of the system is zero, therefore

$$\int_{\partial V_t^f} q ds = 0 \tag{14}$$

The three equations (9), (12) and (14) form a coupled system of equations that can be used to describe the coupled electro-mechanical problem under consideration. Here we use the finite element method to discretize equation (9) and the boundary element method to discretize equations (13) and (14). In order to solve the resulting system of equations, the Newton-Raphson method is used and we have a coupled BEM-FEM procedure. For further details, see [6,7].

3. Numerical example

In order to demonstrate the coupled BEM-FEM mentioned above, we consider here the 2-D simulation of a C-shaped actuator as depicted in Figure 1. The thickness of the actuator is 15 μm, the height is 45 μm and the length is 60 μm. Between the bottom and the top of the actuator we put an electric potential of 1 KV. The simulation is carried out by using two approaches: by using only the finite element method and by using the coupled BEM-FEM presented above. In the first approach, the mesh used in the FEM simulation is presented in Figure 1 with 200 4-node quadrangular elements. In the second approach, the same FEM mesh is used but on the boundary of the FEM mesh, 90 linear 2-node boundary elements are used to simulate the contribution of the space surrounding the actuator. As numerical example, the material properties are given using the following energy function:

$$\hat{W}_{0\boldsymbol{F}} = \frac{\mu}{2}[\boldsymbol{C} : \boldsymbol{I} - 3] - \mu \ln J + \frac{\lambda}{2}[\ln J]^2 + \alpha \boldsymbol{I} : [\boldsymbol{E} \otimes \boldsymbol{E}] + \beta \boldsymbol{C} : [\boldsymbol{E} \otimes \boldsymbol{E}] - \frac{1}{2}\varepsilon_1 J \boldsymbol{C}^{-1} : [\boldsymbol{E} \otimes \boldsymbol{E}] \tag{15}$$

in which the following parameters are chosen:

$$\mu = 0.05 MPa, \quad \lambda = 0.06 MPa, \quad \alpha = 0.2\varepsilon_0, \quad \beta = \varepsilon_0. \quad \varepsilon_1 = 5\varepsilon_0 \tag{16}$$

The numerical results are plotted in Figures 2 and 3. In Figure 2, the simulated deformed shapes of the actuator are presented, on the left by using only the finite element method (the first approach) and on the right by using both the finite element method and the boundary element method (the second approach). For convenience, the undeformed configuration is also presented. It can be seen that not only the

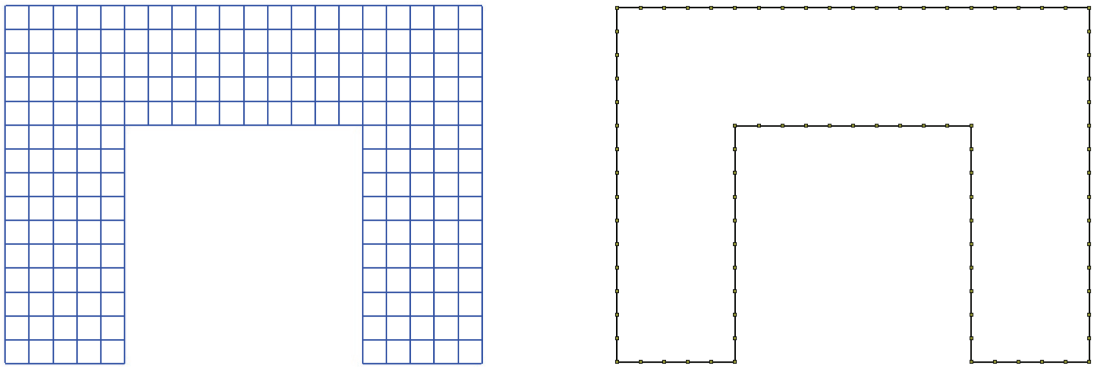

Figure 1: C-shaped actuator: FEM and BEM mesh

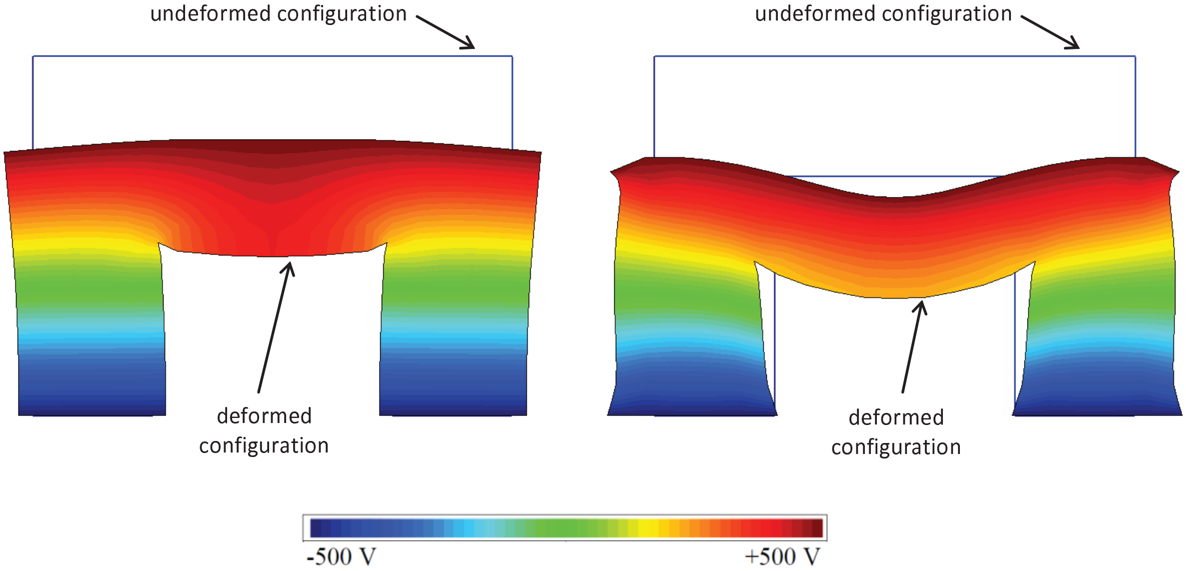

Figure 2: Electric potential under deformed configuration: FEM (left) and BEM-FEM (right)

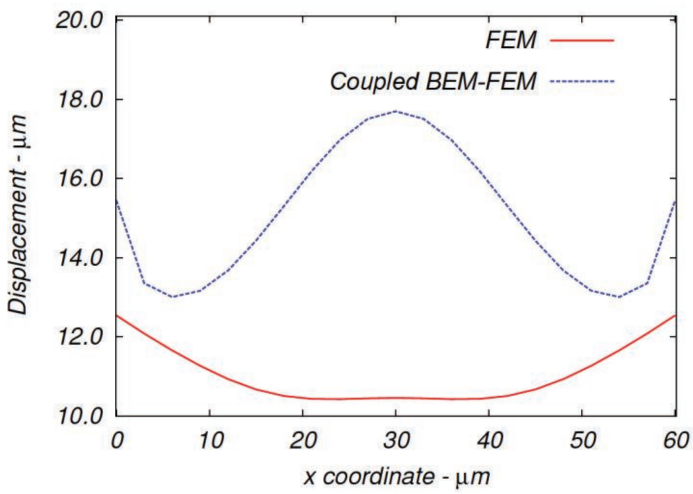

Figure 3: Total displacement of the top line

distributions of the electric potential but also the deformations are different in the two cases. In order to emphasize further these differences, in Figure 3 the simulated displacements of the top line of the actuator are plotted.

4. Conclusion

Numerical simulations show that in simulating EEAPs, the contribution of the free space surrounding the body of interest should be taken into account. The difficulty in doing so lies in the fact that in using the finite element method, not only a large mesh is required but, because of large deformation, the mesh itself should be updated frequently. A combination of boundary element method and finite element method is particularly suitable here since, on the one hand the boundary element method is very suitable for linear problems in infinite domains, on the other hand, the finite element method is convenient in dealing with nonlinear problems but cumbersome when the domain of interest is large and a remesh of the domain is required after every few iterations.

Acknowledgments

The authors greatly acknowledge financial support of the German Research Foundation (DFG) under the project ”Electronic electroactive polymers under electric loading: Experiment, Modelling and Simulation”, Grant Number: STE 544/36-1.

References

[1] Bar-Cohen Y. Electro-active polymers: current capabilities and challenges. Proc. SPIE- Smart Structures and Materials: Electroactive Polymer Actuators and Devices, 2002; 4695: 1-7.

[2] Dorfmann A and Ogden RW. Nonlinear electroelasticity. Acta Mech., 2005; 174(12):167-183.

[3] Goulbourne N, Frecker M, Mockensturm E and Snyder A. Modeling of a dielectric elastomer diaphragm for a prosthetic blood pump. Proc. SPIE - mart Structures and Materials: Electroactive Polymer Actuators and Devices, 2003; 5051: 319-331.

[4] Fox J W. Electromechanical Characterization of the Static and Dynamic Response of Dielectric Elastomer Membranes, 2007. Master Thesis. Virginia Polytechnic Institute.

[5] Kofod G. Dielectric elastomer actuators, 2001. PhD Thesis. Riso-R-1286 (EN), Denmark.

[6] Vu D K and Steinmann P. A 2-D coupled BEM-FEM simulation of electro-elastostatics at large strain. Computer Methods in Applied Mechanics and Engineering, 2010; 199(17-20), 1124-1133.

[7] Vu D K, Steinmann P and Possart G. Numerical modeling of nonlinear electroelasticity. International Journal for Numerical Methods in Engineering, 2007; 70(6), 685 - 704.

[8] Wissler M and Mazza E. Modeling and simulation of dielectric elastomer actuators. Smart Mater. Struct., 2005; 14: 1396-1402.