In-silico Design and Computational Modelling of Electroactive Polymer based Soft Robotics ⋆

A.J. Gil[1][0000−0001−7753−1414], R. Ortigosa[2][0000−0003−4152−6108], J. Martínez-Frutos[2][0000−0002−7112−3345], and N. Ellmer[1][0000−0003−0926−0485]

[1] Zienkiewicz Centre for Computational Engineering,
Bay Campus, Swansea University, Swansea, United Kingdom
A.J.Gil@swansea.ac.uk n.s.ellmer@swansea.ac.uk
[2] Technical University of Cartagena, Murcia, Spain
rogelio.ortigosa@upct.es jesus.martinez@upct.es

Abstract. The use of Electro-Active Polymers (EAPs) for the fabrication of evermore sophisticated miniaturised soft robotic actuators has seen an impressive development in recent years. This paper unveils the latest computational developments of the group related to three significant challenges presented in the *in-silico* modelling of EAPs, that are being explored with our in-house computational platform. These challenges, unique to the simulation of EAPs, include (i) robustly resolving the onset of potentially massive strains as a result of the significant flexibility of EAP components for soft robotics; (ii) accurately capturing the properties of multi-phased composites at a micro-scale within the macroscopic fields used in well-established computational modelling approaches (i.e. Finite Element Method); and (iii) optimising the electrode meso-architecture to enable device customisation for specific application required deformations. This paper also aims to demonstrate the in-silico design tools capability, robustness and flexibility, provided through a comprehensive set of numerical examples, including some novel results in eletrode and EAP multi-material optimisation. With the upcoming addition of a 3D Direct-Ink-Writer (DIW) printer, the authors aim to close the loop allowing for in-house device design and optimisation, simulation and analysis as well as fabrication and testing.

Keywords: Electroactive Polymers · In-silico design · Topology Optimisation · Rank-one Laminates · Soft Robotics

1 Introduction

Electroactive Polymers (EAPs) have emerged as a subclass of soft smart materials which are activated through the application of an electric stimulus. In recent years, research in these materials has significantly increased due to their incredible potential capabilities. Their low stiffness enables unprecedented strains,

⋆ The first and fourth authors acknowledge the financial support received from the UK Defence Science and Technology Laboratory.

with extreme values of 1980%, as demonstrated experimentally [8]. The capabilities of EAP actuators have been demonstrated experimentally and research also shows that EAPs can be used as sensors and flexible energy harvesters [18]. Whilst applying an electric field triggers deformation as a result of electrostriction, physically deforming an EAP can produce an electric signal, due to the piezoelectric effect, which when received can be used for sensing capabilities or stored for energy harvesting purposes.

EAPs have often been referred to as artificial muscles given their actuation capabilities, fast response and high energy efficiencies [2]. This makes them perfect candidates for a wide range of soft robotic applications. In the field of humanoid robotics, EAPs can be used in stacks to form artificial muscles enabling human-like smooth control as opposed to traditional hard robotic mechanisms. This has been demonstrated by Duduta et al. [2] where EAP stacks were used to replicate a bicep, and extended by Guo et al. [4] to demonstrate muscles in the jaw and muscles enabling eye rotation. This ability to decrease robotic nature has the potential to vastly improve the development of prosthesis since the prosthetic could more closely mimic human limbs. An advantage of EAPs over other materials is that they have the ability to act as sensors as well as actuators, resulting in a self sensing capability. Once again this could accelerate the rate of improvement of prosthetics enabling functionality such as thermal and pressure sensing. Beyond the field of humanoid robotics, EAPs have multiple other applications in soft robotics. Figure 1 provides examples of crawling, swimming and flying robots which utilise EAP actuators. Other uses include grippers, tunable lenses and adaptive Braille displays.

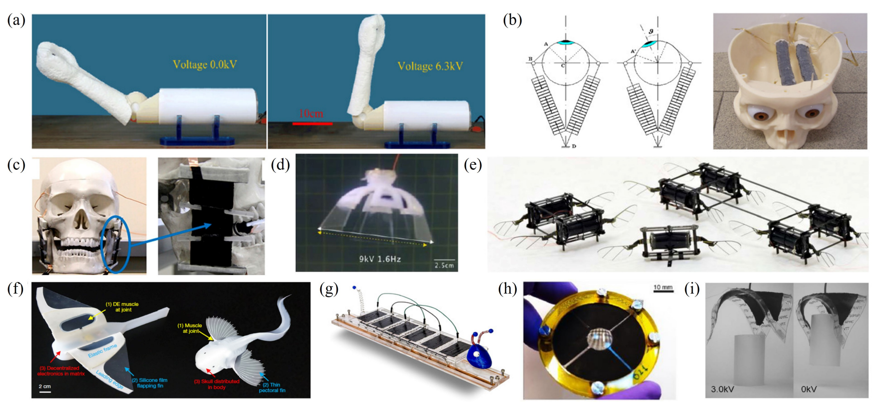


Fig. 1: Demonstration of the vast range of applications for EAPs in the field of soft robotics. [4] (a) EAP biomimetic bicep muscle; (b) Stacked DE configuration to rotate eyeball; (c) Stacked DE configuration to drive jaw; (d) Soft robotic jellyfish; (e) Flying robot; (f) Deep-sea soft robot; (g) Crawling caterpillar inspired robot; (h) EAP driven tunable lens; (i) Tulip inspired EAP gripper.

Amongst others, there are three significant challenges associated with modelling EAPs which are currently being addressed by the authors. The first one relates to modelling soft materials producing large strains (potentially massive), not previously an issue in hard robotics due to the use of mechanisms. Soft materials produce a highly non-linear and complex response which often requires an iterative solution approach, as implemented in the in-house in-silico computational tool, to solving for electric potential and displacement within the Finite Element Method (FEM). The next challenge relates to modelling a composite comprised of two or more materials. At a micro-scale, each Finite Element could be comprised of multiple materials. This creates a challenge when selecting or developing a constitutive model to use, since the properties of that material combination may not be accurately represented. The final challenge relates to designing a device that can produce the output required for a specific application. A large factor effecting the final deformation mode is the arrangement of electrodes and thus topology optimisation can be used to compute the optimal electrode meso-architecture.

Whilst the in-house in-silico design tool is continually being developed, the authors are about to explore the fabrication and testing of EAPs. 3D printing is a key progressive method of fabrication and with a Direct-Ink-Writing (DIW) 3D printer, the authors will have the ability to design and optimise EAPs using the developed framework, fabricate the configurations and test them, thus validating the simulation results. Having this capability closes the loop and potentially leads to real change in the way these materials are currently being designed. However, this goes beyond the scope of the current contribution.

This paper is organised as follows; Section 2 addresses all presented problems with the following subsection breakdown. Section 2.1 introduces a typical EAP and the problem definition before proceeding to address the challenges of solving highly non-linear problems using the concept of multi-variable convexity. Section 2.2 presents rank-one laminates and the challenges surrounding obtaining material properties for a combination of material phases represented by a single energy function. Section 2.3 details the use of topology optimisation to optimise the arrangement and design of electrodes to conform to a set of design criteria. Section 3.3 provides a comprehensive set of numerical examples to demonstrate the need to address the discussed challenges whilst showcasing the capability, robustness and flexibility of the in-house in-silico design and simulation tool. Finally, some concluding remarks are presented in Section 4.

2 In-silico design modelling approach

2.1 Nonlinear Solid Electromechanics: a new modelling paradigm

The set of equations governing the physics of EAPs, namely the conservation of linear momentum and Gauss's law [9], can be mathematically stated as,

$$\mathrm{DIV}\boldsymbol{P} + \boldsymbol{f}_0 = \boldsymbol{0}; \qquad \mathrm{DIV}\boldsymbol{D}_0 - \rho_0 = 0, \tag{1}$$

where $\boldsymbol{P}$ is the first Piola-Kirchhoff stress tensor, $\boldsymbol{f}_0$ denotes a Lagrangian body force, $\boldsymbol{D}_0$ is the Lagrangian electric displacement field and ρ_0 represents the electric charge per unit volume. Rotational equilibrium dictates that $\boldsymbol{F}^T\boldsymbol{P} = \boldsymbol{P}\boldsymbol{F}^T$, where $\boldsymbol{F}$ represents the deformation gradient tensor. Faraday's law can be written as $\boldsymbol{E}_0 = -\boldsymbol{\nabla}_0\phi$, with $\boldsymbol{E}_0$ the Lagrangian electric field and ϕ the electric potential. The internal energy density e that encapsulates the necessary constitutive information to close the system of governing equations in (1) is introduced as $e = e(\boldsymbol{F}, \boldsymbol{D}_0)$.

The actuation (and strain) capability of EAPs is massive and this poses real challenges when modelling the materials electromechanical response, since the simulation must remain robust and reliable beyond the potential limited experimental information for moderate actuation. Fundamentally, the constitutive model must be sufficiently robust such that when simulations go beyond that of the laboratory experiments from which the constitutive model was developed, the reliability and accuracy of the model does not breakdown [3]. Figure 2(a) demonstrates a common prototypical example where an isotropic EAP film is undergoing material characterisation through classical experimentation [15]. Figure 2(b) presents the response of the constitutive model and careful analysis (i.e. computation of acoustic wave speeds) has shown that the constitutive model becomes ill-posed for any combination of $\boldsymbol{E}_0$ and stretch λ within the red region, hence either limiting the simulation capability to smaller strains or providing unphysical results, the latter demonstrated by Figure 2(c) with the appearance of a zero thickness shear band.

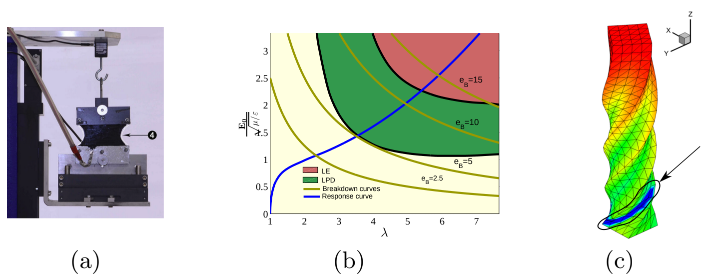


Fig. 2: (a) Material characterisation of EAP VHB4910; (b) Response curve (in blue) and stability analysis of widely used constitutive model for the standard experimental set up described here; (c) Development of localised deformations in unrealistic zero thickness shear bands in the simulation of a piezoelectric EAP.

Recently, the concept of multi-variable convexity has been introduced by the authors [3, 6, 12, 13] allowing for the internal energy function to be given as,

$$e\left(\boldsymbol{\nabla}_0\boldsymbol{x}, \boldsymbol{D}_0\right) = W\left(\boldsymbol{F}, \boldsymbol{H}, J, \boldsymbol{D}_0, \boldsymbol{d}\right); \quad \boldsymbol{d} = \boldsymbol{F}\boldsymbol{D}_0, \tag{2}$$

where W represents a convex multi-variable functional in terms of its extended set of arguments $\mathcal{V} = \{\boldsymbol{F}, \boldsymbol{H}, J, \boldsymbol{D}_0, \boldsymbol{d}\}$, with $\{\boldsymbol{H}, J\}$ the co-factor and the Jacobian of $\boldsymbol{F}$, respectively. The concept of multi-variable convexity is paramount in ensuring a well-posed computer model, such that the problem guarantees the existence of real wave speeds and hence continues to produce physical results for the constitutive model regardless of the level of actuation, opening the possibility to explore unthinkable actuation possibilities.

2.2 Electroactive Polymer Design: Microstructure

Material properties are fundamental with respect to EAP performance. It is desirable to select a material with high electric permittivity in order to maximise the actuation range. However, materials with higher electric permittivity also exhibit higher stiffness which in itself can hinder the final actuation response [5]. This in turn counteracts the advantage gained. Since using one single material has its limitations in gains through material properties, focus has turned towards the design of tailor-made composite arrangements of multiple materials with varying properties to complement one another.

This brings with it significant challenges with regards to the constitutive model. When using a single material phase, the corresponding material constitutive model can be obtained through classical experiments in conjunction with a phenomenological based model [7]. Likewise, when using multiple material phases at a macro-scale, multiple constitutive models can be implemented and interchanged as the material definition changes. However, a significant challenge arises when modelling an EAP device, with multiple material phases at a micro-scale, requiring thus the development of multi-scale constitutive models. The authors presented in [9] a novel computational framework for the accurate simulation of rank-one EAP laminates and applied the principles of a rank-n homogenisation of convex multi variable phases in the context of highly deformable EAPs for soft robotics applications. The structure for a biphasic DE device can be seen below in Figure 3.

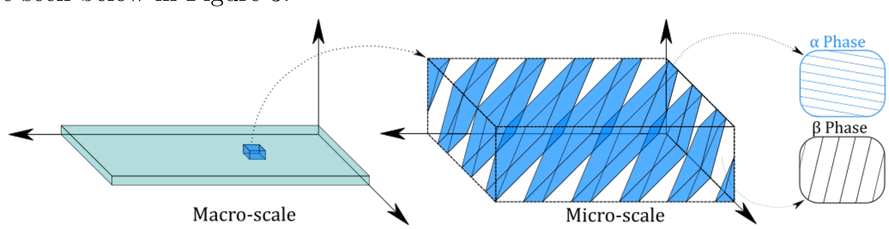


Fig. 3: Schematics of EAP device fabricated such that it is laminated with multiple material phases (α and β in this case) at a micro-scale level. The micro-scale image demonstrates that the lamination of a rank-one laminate does not need to be in an orthogonal direction. On the far right, the Figure presents the possibility of a rank-two laminate such that the various phases can also be formed of a laminate. This details a further challenge; can such a material be printed?

Section 2.1 presented the definition of the problem through the governing equations (1). This identified two quantities which are vital for the constitutive model, namely the deformation gradient tensor, $\boldsymbol{F}$, and the electric displacement field, $\boldsymbol{D}_0$. Since Figure 3 presents two phases used at a micro-scale, the macro-scale quantities $\boldsymbol{F}$ and $\boldsymbol{D}_0$ need to be obtained such that they represent both material phases. Under the assumption of a homogeneous response in each phase, these quantities are defined as the weighted sum of those in each phase, namely

$$\boldsymbol{F} = c^a \boldsymbol{F}^a + (1 - c^a)\, \boldsymbol{F}^b; \qquad \boldsymbol{D}_0 = c^a \boldsymbol{D}_0^a + (1 - c^a)\, \boldsymbol{D}_0^b, \tag{3}$$

where c^a is the volume fraction of phase a ($1 - c^a$ for phase b). Whilst $\boldsymbol{F}$ and $\boldsymbol{D}_0$ can be decomposed to combine multiple materials, the internal energy functional also needs to represent the combination of material phases. This can be done through the introduction of an effective internal energy functional, $\hat{e}(\boldsymbol{F}, \boldsymbol{D}_0, \boldsymbol{\alpha}, \boldsymbol{\beta})$, which similarly can be decomposed such that

$$\begin{aligned} \hat{e}(\boldsymbol{F}, \boldsymbol{D}_0, \boldsymbol{\alpha}, \boldsymbol{\beta}) = c^a e^a \left(\boldsymbol{F}^a (\boldsymbol{F}, \boldsymbol{\alpha}), \boldsymbol{D}_0^a (\boldsymbol{D}_0, \boldsymbol{\beta})\right) \\ + (1 - c^a)\, e^b \left(\boldsymbol{F}^b (\boldsymbol{F}, \boldsymbol{\alpha}), \boldsymbol{D}_0^b (\boldsymbol{D}_0, \boldsymbol{\beta})\right) \end{aligned} \tag{4}$$

where e^a and e^b are the respective materials internal energy functionals written in terms of the micro-scale fluctuations $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$. As a result of these decompositions, the various macroscopic quantities can be expressed as weighted averages of multiple materials, enabling the use of the same computational framework with the fields and models described by (3) and (4).

Another solution currently explored by the authors is that of developing a single internal energy functional which can closely model the response of a rank-one laminate without attempting to represent the different materials individually, with the potential to drastically simplify the modelling of multiple materials. It is also worth noting that in the future this raises the potential for a new design challenge, the optimisation of the volume fractions of materials to maximise the deformation.

2.3 Electrode Design: Meso-architecture

The design and arrangement of electrodes is another important factor when optimising EAP performance. Stacked configurations enable the designer to strategically place different designs of electrodes in specific locations to produce complex and novel deformations. Designing the electrode to form only a region of the layer results in the elastomer sandwiched within this region to experience an electric stimulus resulting in actuation whilst the remaining material does not experience an electric stimulus thus remaining passive and thereby enabling complex actuation. Figure 4 demonstrates the customisability of the design and placement of electrodes to produce a novel and complex mode of deformation.

When considering the use of EAPs for applications such as soft robotics, it is clear that the designer will have an end goal in the form of a desired actuation. It is therefore necessary that there be an approach in place to optimise the design for a given set of criteria. There is a wide spectrum of robust approaches available for topology optimisation of the meso-architecture, ranging from density-based methods, with the Solid Isotropic Material with Penalisation (SIMP) method as their maximum representative, level-set methods, phase-field methods, topological derivative methods and evolutionary methods [1,11,16,17].

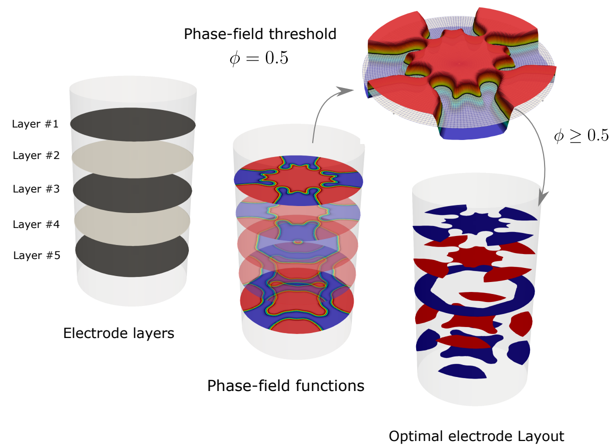
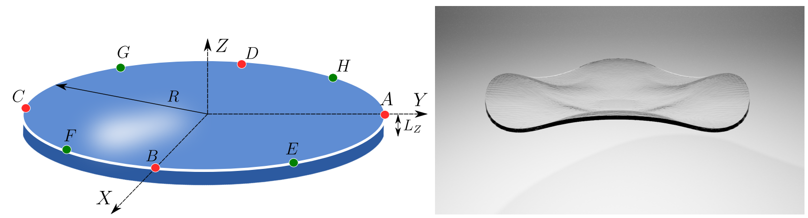


Fig. 4: Layer-by-layer extruded layout clearly displaying the intercalated electrodes. **Left**: DE device comprising of six elastomer layers and five intercalated surface regions. **Centre**: final distribution of the phase-field functions with the electrode regions in red and the voids in blue. **Right**: representation of the five electrodes by selecting the phase-field threshold equal to 0.5 [10].

The authors have explored the use of the phase-field method [10], where a continuous phase-field is used to describe the presence of an electrode region within the interface layer, being $\Psi_\varepsilon = \{\Psi_{\varepsilon^1} \ldots \Psi_{\varepsilon^N}\}$ the set of N phase field functions. This electrode phase field functions are extended to the volume via a suitable Laplacian extension, where the overall volume phase field function in the range $[0, 1]$, where 0 represents a purely EAP region and 1 represents an electrode region. Intermediate values represent electrode boundaries. As a final ingredient of the phase field method, it remains to define a spatially varying free (enthalpy-type) energy density $\Psi(\Psi_\varepsilon, \boldsymbol{F}, \boldsymbol{E}_0)$ comprised of purely mechanical and electro-mechanical contributions.

To summarise the optimisation process, first consider the elastomeric configuration described in Figure 5. The underlying objective of this particular layout is not to perfectly fit the electrically deformed EAP to a given target shape, but to ensure that its deformed configuration is endowed with certain desired morphological features. This can be achieved by focusing on the displacement, $\boldsymbol{u} = \boldsymbol{\phi}(\boldsymbol{X}) - \boldsymbol{X}$ (where $\boldsymbol{X}$ is the initial material coordinate and $\boldsymbol{\phi}(\boldsymbol{X})$ represents the mapping of $\boldsymbol{X}$ to its current spatial position), of specific critical points which can ultimately induce the desired morphological peculiarities. Considering the displacement of critical points allows for the formulation of an objective function which the topology optimisation process aims to minimise, subject to the satisfaction of a series constraints defined by the set of governing equations defining the problem (see Section 2.1). An initial electrode arrangement seed can then be used as an input and a Newton-Raphson nonlinear iterative algorithm is exploited until convergence. This topology optimisation technique has recently been extended to the possibility of considering a multi-material EAP, providing thus the capacity to optimise the design of both the electrode and the EAP polymer itself.



(a) (b)

Fig. 5: (a) Points selected for optimisation. (b) Topology optimisation aided electrode design: the Z displacement of the red and green target points must be maximised along the positive and negative Z direction, respectively [10].

3 Examples

3.1 Example 1: Demonstration of In-silico Design Tool Capability

The objective of this first example is to demonstrate the large strain and complex deformation capability of the in-silico design tool. The configuration is displayed in Figure 6 and it presents a DE device which clearly provides a blueprint which could be used as a concept for a soft robotics gripper. Bending is obtained by positioning electrodes across the full span of each 'finger' and fixing it to a central square of material which remains passive hence providing a fixed plane enabling span-wise actuation.

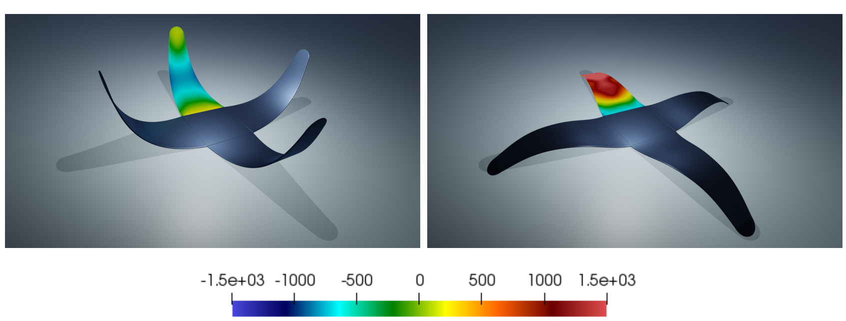


Fig. 6: Presents the rendering of a deformed configuration, demonstrating a large strain, and contour plot of the distribution of hydrostatic pressure p. These results have been obtained with the in-house in-silico design tool [14].

3.2 Example 2: Effects of Fibre Orientation

The objective of this example is to demonstrate the influence of microstructure fibre orientation on the deformation produced. A basic rectangular EAP device was used in this example which similarly to Example 3.1 has two full aerial electrodes, arranged at half thickness and at the bottom of the device. As the elastomer bends due to the applied electric field, the fibre orientation induces an additional torsional mode. Figure 7 clearly displays that with the fibres orientated at 0°, or parallel to the length, does not induce torsion but does reduce bending capability. With the fibres orientated at 45°, torsion and bending are induced and can thus be customised.

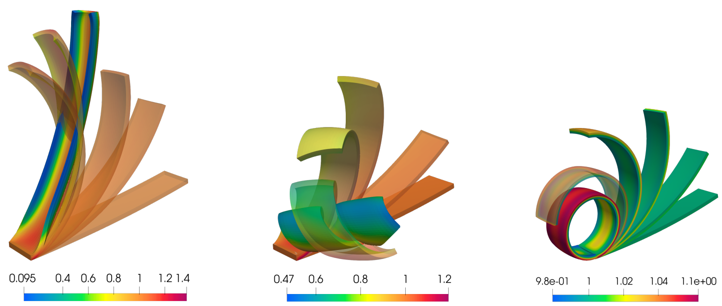


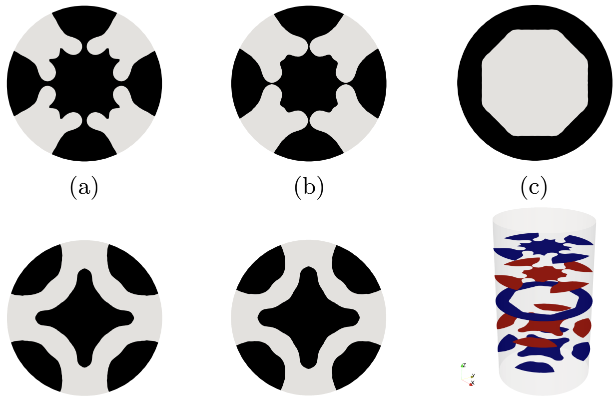
Fig. 7: Presents the deformations of an EAP with different fibre alignment, from left to right corresponding to orientations of $0°, 45°$ and $90°$. The various snapshots corresponds to the actuation increments and the contour plots represent the deformation gradient tensors F_{22} component [6].

3.3 Example 3: Effects of Electrode Design Meso-architecture

This final example is being presented to demonstrate the use of topology optimisation as discussed in Section 2.3. The objective for this specific configuration is to maximise the displacement at locations $\{A, B, C, D\}$ and minimise at locations $\{E, F, G, H\}$. The success of the optimisation is calculated through the objective function given by

$$\mathcal{J}(\boldsymbol{\phi}) = -\left(\boldsymbol{u}_A + \boldsymbol{u}_B + \boldsymbol{u}_C + \boldsymbol{u}_D\right) + \left(\boldsymbol{u}_E + \boldsymbol{u}_F + \boldsymbol{u}_G + \boldsymbol{u}_H\right) \tag{5}$$

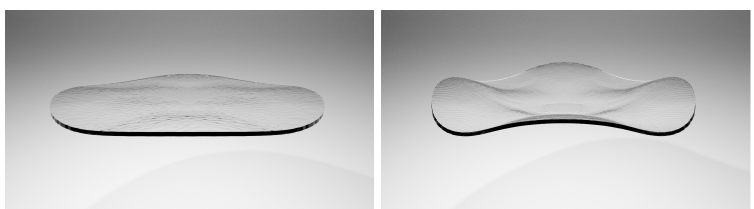
where $\boldsymbol{u}_Y$ is the vertical displacement of the specified point Y. The outcome of the optimisation process for the actuation mode is presented in Figure 9. To summarise, Figure 8 shows the five electrode layer extrusions demonstrating the optimised design of electrodes to obtain the deformation presented in Figure 9. It is worth noting that even a slight change in objective can result in a significantly altered optimised configuration. This also demonstrates the usefulness of topology optimisation given that the optimised solution may not be trivial or easily conceived by an inexperienced designer.



(a) (b) (c)

(d) (e) (f)

Fig. 8: (a)-(e) Final distribution of the phase-field functions at final TO iteration. Black colour is associated with electrodes and grey colour, with voids. (f) Displays a layer-by-layer layout with intercalated optimal electrode distribution (a phase-field threshold value of 0.5 has been used) where the Z dimension of the DE device has been enlarged for visualisation purposes [10].



(a) (b)

Fig. 9: Presents the evolution of the deformed configuration of the optimised layer-by-layer DE device for increasing values of the voltage gradient, $\Delta\varphi$, between alternating electrodes [10].

4 Concluding Remarks

This paper has presented some recent computational results regarding the in-silico design and analysis of Electro-Active Polymers (EAPs) subjected to potentially extreme actuation. First, the use of polyconvex strain energy functions is shown as a very beneficial mathematical requirement in order to ensure robust and accurate simulations. Subsequently, the consideration of rank-laminates for the EAP micro-architecture is shown as a useful tool in order to attain a variety of actuation modes. Finally, the use of topology optimisation in the design of the electrode meso-architecture demonstrates the unparalleled design opportunities offered by EAPs. Having a computational framework coupled with the ability to fabricate and test EAPs will enable future in-house experimental validation, further offering physical proof of concept alongside simulation results.

References

1. Aage, N., Andreassen, E., Lazarov, B., Sigmund, O.: Giga-voxel computational morphogenesis for structural design. Nature **550**, 84–86 (2017)
2. Duduta, M., Hajiesmaili, E., Zhao, H., Wood, R., Clarke, D.: Realizing the potential of dielectric elastomer artificial muscles. PNAS **116**, 2476–2481 (2019)
3. Gil, A.J., Ortigosa, R.: A new framework for large strain electromechanics based on convex multi-variable strain energies: Variational formulation and material characterisation. CMAME **302**, 293–328 (2016)
4. Guo, Y., Liu, L., Liu, Y., Leng, J.: Review of dielectric elastomer actuators and their applications in soft robots. Advanced Intelligent Systems **3** (2021)
5. Hajiesmaili, E., Clarke, D.: Reconfigurable shape-morphing dielectric elastomers using spatially varying electric fields. Nature Communicationes **10**(183), 1–7 (2019)
6. Horák, M., Gil, A., Ortigosa, R., Kruzik, M.: A polyconvex transversely-isotropic invariant-based formulation for electro-mechanics: stability, minimisers and computational implementation. Under review (2022)
7. Hossain, M., Navaratne, R., Peric, D.: 3d printed elastomeric polyurethane: Viscoelastic experimental characterizations and constitutive modelling with nonlinear viscosity functions. IJNLM **126**, 293–328 (2020)
8. Li, T., Keplinger, C., Baumgartner, R., Bauer, S., Yang, W., Suo, Z.: Giant voltage-induced deformation in dielectric elastomers near the verge of snap-through instability. JMPS **61**(2), 611–628 (2013)
9. Marín, F., Martínez-Frutos, J., Ortigosa, R., Gil, A.: A convex multi-variable based computational framework for multilayered electro-active polymers. CMAME **374** (2021)
10. Martínez-Frutos, J., Ortigosa, R., Gil, A.J.: Computational design and optimization of electrode meso-arquitecture for shape morphing dielectric elastomers. JMPS **157** (2021)
11. Munk, D.J., Steven, G.P.: Topology and shape optimization methods using evolutionary algorithms: a review. Structural and Multidisciplinary Optimization **52**, 613–631 (2015)
12. Ortigosa, R., Gil, A.J.: A new framework for large strain electromechanics based on convex multi-variable strain energies: Conservation laws, hyperbolicity and extension to electro-magneto-mechanics. CMAME **309**, 202–242 (2016)
13. Ortigosa, R., Gil, A.J.: A new framework for large strain electromechanics based on convex multi-variable strain energies: Finite element discretisation and computational implementation. CMAME **302**, 329–360 (2016)
14. Ortigosa, R., Gil, A.J., Martínez-Frutos, J., Franke, M., Bonet, J.: A new energy-momentum time integration scheme for non-linear thermo-mechanics. CMAME **372** (2020)
15. Siboni, M.H., Castañeda, P.P.: Fiber-constrained, dielectric-elastomer composites: Finite-strain response and stability analysis. Journal of the Mechanics and Physics of Solids **68**(0), 211–238 (2014)
16. Takezawa, A., Nishiwaki, S., Kitamura, M.: Shape and topology optimization based on the phase field method and sensitivity analysis. Journal of Computational Physics **229**(7), 2697 – 2718 (2010)
17. Wang, M., Wang, X., Guo, D.: A level-set method for structural topology optimization. CMAME **192**, 227–246 (2003)
18. Zhao, Y., Yin, L.J., Zhong, S.L., Zha, J.W., Dang, Z.M.: Review of dielectric elastomers for actuators, generators and sensors. IET Nanodielectrics **3** (2020)