Design of functionally graded piezocomposites using topology optimization and homogenization – Toward effective energy harvesting materials

S.L. Vatanabe a, G.H. Paulino b, E.C.N. Silva a,*

a Department of Mechatronics and Mechanical Systems Engineering, Polytechnic School of University of São Paulo, SP, Brazil
b Newmark Laboratory, Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, IL, USA

A B S T R A C T

In the optimization of a piezocomposite the objective is to obtain an improvement in its performance characteristics, usually by changing the volume fractions of constituent materials, its properties, shape of inclusions, and the mechanical properties of the polymer matrix in the composite unit cell. Thus, this work proposes a methodology based on topology optimization and homogenization to design functionally graded piezocomposite materials that considers important aspects in the design process aiming at energy harvesting applications, such as the influence of piezoelectric polarization directions and the influence of material gradation between the constituent materials in the unit cell. The influence of the piezoelectric polarization direction is quantitatively verified using the Discrete Material Optimization (DMO) method, which combines gradients with mathematical programming to solve a discrete optimization problem. The homogenization method is implemented using the graded finite element concept which takes into account the continuous gradation inside the finite elements. One of the main questions answered in this work is, quantitatively, how the microscopic stresses can be reduced by combining the functionally graded material (FGM) concept with optimization. In addition, the influence of polygonal elements is investigated, quantitatively, when compared to quadrilateral 4 node finite element meshes which are usually adopted in material design. However, quads exhibit one-node connections and are susceptible to checkerboard patterns in topology optimization applications. To circumvent these problems, Voronoi diagrams are used as an effective means of generating irregular polygonal meshes for piezocomposite design. The present results consist of bi-dimensional unit cells that illustrate the methodology proposed in this work.

© 2013 Elsevier B.V. All rights reserved.

1. Introduction

This work proposes a methodology, based on topology optimization and homogenization, to design functionally graded piezocomposite materials that considers important aspects in the material design process aiming at energy harvesting applications, such as the influence of piezoelectric polarization directions and the influence of material gradation between the constituent materials in the unit cell. Usually some gradient is obtained in the manufacturing process of piezocomposites – the proposed methodology can take this feature into account in the design. The homogenization method is implemented using the graded finite element concept, which takes into account the continuous gradation inside the finite elements. Macroscopic and microscopic stress values are compared using the homogenization method when the optimized piezocomposites are subjected to an external load. The variation of the polarization direction is implemented by means of a discrete material optimization approach. Quadrilateral 4 node finite element meshes are usually adopted in material design; however, they exhibit one-node connections and are susceptible to checkerboard patterns in topology optimization applications and polygonal elements can be very useful in this aspect.

Thus, in this work, Voronoi diagrams are also used as a natural and effective means for generating irregular polygonal meshes for piezocomposite design. The results obtained consist of bi-dimensional unit cells that illustrate the methodology proposed in this work.

1.1. Piezoelectric materials

Piezoelectric materials have a crystalline structure that provides them with the ability to transform mechanical strain
energy into electrical charge and, vice versa, by converting an applied electrical potential into mechanical strain. The term piezocomposite applies to any composite resulting from the combination of any piezoelectric material (ceramic or polymer) with other non-piezoelectric materials, including air-filled voids [1]. Piezocomposite materials provide effective properties (elastic, piezoelectric, and dielectric) leading, in general, to better performance than pure piezoelectric materials. The performance characteristics depend on the volume fractions of constituent materials, its properties, shape of inclusions, and the mechanical properties of the polymer matrix in the composite unit cell. In the piezocomposite applications considered in this work, we assume that the excitation wavelengths are so large that the detailed structure of the unit cell is not relevant, and the material may be considered as a new homogeneous medium with “effective” properties. Then, the excitation (vibrational forces, for example) will average out over the fine scale variations of the composite medium, in the same way as averaging occurs in the micron-sized grain structure in a conventional ceramic.

1.2. Energy harvesting

An interesting application for piezoelectric materials is energy harvesting devices. Energy harvesting is a process in which energy that would otherwise be wasted is processed and stored for future use by an application. The use of harvested energy could extend the operational life of devices traditionally powered by batteries. This is particularly advantageous in systems with limited accessibility such as biomedical implants and structures with embedded micro and wireless sensors. It is feasible that such devices would have the ability to generate their own power from the environment. This can either prolong the life of an existing battery or even eliminate it. With advances in design and manufacturing as well as reduced power requirements, the use of energy harvesting methods have become practical and have gained significant popularity [2,3]. Piezoelectric property allows the material to capture mechanical energy from its surroundings, usually ambient vibration, and transform it into electrical energy that can power other devices. The use of piezoelectric materials to capitalize on the surrounding ambient vibrations has seen a dramatic rise due to the direct conversion of energy between the mechanical and electrical domain. The interest in piezoelectric energy harvesting is reflected in a number of reviews that have been written in recent years [4,5]. Thus, designing improved piezocomposites for energy harvesting applications is always a goal to be achieved.

1.3. Functionally graded materials

Functionally Graded Materials (FGM) are composite materials whose properties vary gradually and continuously along a specific direction within the domain of the material. The property variation is generally achieved through continuous change of the material microstructure [6]; in other words, FGMs are characterized by spatially-varying microstructures created by non-uniform distributions of the constituent phases. This variation can be accomplished by using reinforcements with different properties, sizes, and shapes, as well as by interchanging the role of reinforcement and matrix (base) material in a continuous manner. Several authors have highlighted the advantages of the FGM concept applied to piezoelectric structures [7,8], which involve local reduction of thermal and mechanical stress concentration [7,9], improved stress redistribution [7], maximization of output displacement, and increased bonding strength [10]. Among many available techniques, FGMs can be manufactured by using Spark Plasma Sintering (SPS), which has certain features such as high heating efficiency, quick temperature rising, self-cleaning of the surface of the materials and improvement of sintering activation, resulting in fast sintering at a lower temperature [11].

1.4. Homogenization

The homogenization method replaces the piezocomposite as a homogeneous medium and it allows the calculation of its effective properties by considering the topology of the composite microstructure and the properties of its constituents [12]. The homogenization theory for piezoelectricity considering static case (where the operational wavelength is much larger than the unit cell dimensions) was developed by Teleaga [13] using the variational method of C-convergence. Silva et al. [14–16] presented a method for designing piezoelectric microstructures with high performance characteristics using topology optimization techniques and the homogenization method, such as hydrostatic coupling coefficient, figure of merit, and electromechanical coupling factor. Sigmund et al. [17] used topology optimization method to design 1–3 piezocomposites with optimal performance characteristics for hydrophone applications. Buehler et al. [18] applied the homogenization technique to calculate the effective properties of an unit cell incorporating piezoelectric and conventional material. This unit cell was used in a topology optimization problem that maximizes the displacement of an arbitrary point due to an applied electric field, while specifying the structure stiffness. Jayachandran et al. [19–21] used a stochastic global optimization combined with homogenization method to obtain the optimal granular configuration of the ferroelectric ceramic microstructure for application in piezoelectric actuators.

In the case of energy harvesting applications, where piezocomposites are used as high quality structural materials that have to satisfy strict engineering requirements, it is necessary to evaluate the stress and strain values in the unit cell when the piezocomposite is subjected to external loads. However, stresses determined by taking the composite as (macro) homogeneous material, denoted by effective stresses, can only reflect the response of the composite to external (macro) environments, ignoring the effects of micro-heterogeneity. Thus, detailed information of stress distribution is necessary for structural design and optimization. The information is particularly useful in determining material strength and micro cracks/defects in the material. Guedes and Kikuchi [12] used homogenization to compute stress and strain distributions within composite structures. Ni et al. [22] investigated the microscopic stresses in sphere-reinforced composite and unidirectional fiber-reinforced composite and calculated the effective stress level determined based on a macro-dimensional scale. They concluded that the effective stresses might be much lower than the actual maximum values occurring in the microstructure. In this method, specific loads are applied to the unit cell and finite element analysis is used to determine the stress distribution and to give the information of stress concentration at interfaces.

1.5. Topology optimization

Topology optimization is a method which allows finding the layout, or topology, of a structure or material such that a prescribed objective is maximized or minimized subjected to design constraints. Topology optimization can be combined with the homogenization method to design unit cells with complicated shape. Therefore, a richer class of material properties can be achieved, and new kinds of composite materials can be generated rather than the usual fiber-reinforced or laminate types. Moreover, these new materials may be designed to achieve unusual properties [23–25].
The polarization direction of piezoelectric materials can be defined as design variables in the topology optimization method [26]. In a finite element structure, the direction of local polarization at each element is defined by the angle \( \theta \) on a fixed reference. Thus, the design variables can assume continuous values within a certain pre-defined range. However, a disadvantage of this approach is that the global solution space becomes non-convex, and hence, the problem of multiple local minima needs to be dealt with [27]. The Discrete Material Optimization (DMO) method combines gradients with mathematical programming to solve a discrete optimization problem. This approach has been introduced by Stegmann and Lund [27], who applied it to solve the orientation problem of orthotropic materials and the material selection problem formulation. In Section 6, numerical examples demonstrating the concept, and the sensitivity analysis, as well as the discrete problem formulation. In Section 4, the topology optimization concept is described. In Section 3, the homogenization method is presented. In Section 2, the constitutive equations are presented. In Section 5, the numerical implementation is described, including the implementation of polygonal finite element mesh applied to piezocomposite material design, the DMO concept, and the sensitivity analysis, as well as the discrete problem formulation. In Section 6, numerical examples demonstrating the influence of either quadrilateral or polygonal mesh are shown, as well as the influence of material gradation and piezoelectric polarization direction in the piezocomposite design for high performance. Finally, in Section 7, some conclusions are inferred.

1.6. Paper organization

This paper is organized as follows: in Section 2, piezoelectric constitutive equations are presented. In Section 3, the homogenization method applied to piezoelectric materials considering the FGM concept is described. In Section 4, the topology optimization formulation is presented. In Section 5, the numerical implementation is described, including the implementation of polygonal finite element mesh applied to piezocomposite material design, the DMO concept, and the sensitivity analysis, as well as the discrete problem formulation. In Section 6, numerical examples demonstrating the influence of either quadrilateral or polygonal mesh are shown, as well as the influence of material gradation and piezoelectric polarization direction in the piezocomposite design for high performance. Finally, in Section 7, some conclusions are inferred.

2. Piezoelectric constitutive equations

The stress-charge form of the constitutive relation for piezoelectric media are given by:

\[
T = e^s \varepsilon - dE, \quad D = e^c \varepsilon + e^p \varepsilon,
\]

where \( T, e, D, \) and \( E \) are respectively the mechanical stress tensor, the mechanical strain tensor, the electric charge vector, and the electric field vector. The term \( e^s \) represents the elastic stiffness tensor, which is evaluated at constant electric field. Terms \( e^c \) and \( e^p \) are respectively the piezoelectric tensor, and the dielectric tensor evaluated at constant strain.

In this work, a bi-dimensional model is considered. As a convention, the polarization axis of the piezoelectric material is considered in the \( z \) (or \( 3 \)) direction. Besides, a plane-strain assumption is considered for modeling the two-dimensional microstructures. Therefore, assuming the model is in the plane \( 1-3 \) (or \( x-z \)) \( (y \) is the normal direction) and that the piezoelectric material employed to build the piezocomposite belongs to the hexagonal \( 6 \text{mm} \) class, the correspondent plane-strain properties can be obtained by considering \( e_y = 0 \) and \( E_y = 0 \) in Eq. (1), and rewriting them using only the terms \( e_2, T_2, D_2, \) and \( E_2 \) for \( i = 1 \) or \( 3 \). A plane-strain model could also be considered; however, it is less realistic than the plane-strain model for representing the composite behavior which is assumed to have an infinite length in the \( y \)-direction for the two-dimensional case.

These constitutive equations can also be represented by an alternative form [28]:

\[
\varepsilon = S^T \varepsilon - 2dE, \quad D = e^c \varepsilon + e^p \varepsilon,
\]

where \( S^T \) is the compliance tensor under short-circuit conditions, \( e^p \) is the clamped body dielectric tensor, and \( d \) is the piezoelectric stress tensor. The relations among the properties in Eqs. (1) and (2) are [28]:

\[
s^T = (e^c)^{-1}, \quad e^c = e^s + d^T (s^T)^{-1} d, \quad d = (s^T) \varepsilon.
\]

3. Homogenization method applied to FGM piezoelectric materials

In this section, it is briefly discussed the application of the homogenization theory to piezoelectricity considering FGM concept. Considering the standard homogenization procedure, the two-dimensional unit cell is defined as \( Y = [0, Y_1] \times [0, Y_2] \) and the material functions \( e^p_{ij}, e^c_{ij} \) and \( e^p \) are considered to be \( Y \)-periodic functions:

\[
c^{p,ij}(x) = c^{p,ij}(x, Y), \quad e^{c,ij}(x) = e^{c,ij}(x, y), \quad e^c(x) = e^c(x, y), \quad e^p(x) = e^p(x, y), (4)
\]

and where \( y = x/\varepsilon \) where \( \varepsilon > 0 \) is a parameter with small value which represents the microscale in which the properties are changing (composite microstructure scale), and \( x \) and \( y \) are coordinates associated with macro- and micro-dimensions of the composite material, respectively.

Expanding the piezocomposite displacement \( u \) and electric potential \( \phi \) asymptotically [13], one obtains:

\[
u^p(x, y) = u_0(x) + \varepsilon u_1(x, y), \quad \phi^p(x, y) = \phi_0(x) + \varepsilon \phi_1(x, y), (5)
\]

where only the first-order variation terms are considered since it is supposed the operational wavelength to be much larger than the unit cell dimensions, and \( u_1 \) and \( \phi_1 \) are \( Y \)-periodic. The strains and electrical potential gradients are written as:

\[
u^p(x, y) = \partial_x u_0(x) + \varepsilon [\partial_x u_1(x, y) + \partial_y u_1(x, y)], \quad V_x \phi^p(x, y) = V_x \phi_0(x) + \varepsilon [V_x \phi_1(x, y) + V_y \phi_1(x, y)], (6)
\]

where \( \varepsilon \) is the mechanical strain and:

\[
(\partial_\nu)_{ij} = \frac{1}{2} \left( \frac{\partial(\cdot)}{\partial x} + \frac{\partial(\cdot)}{\partial y} \right)_i (\partial_j(\cdot)), \quad (\partial\phi)_{ij} = \frac{1}{2} \left( \frac{\partial(\cdot)}{\partial x} + \frac{\partial(\cdot)}{\partial y} \right)_i (\partial_j(\cdot)). (7)
\]

After some algebraic manipulations (see [15]), it is possible to get the following equations of the effective (or homogenized) properties:

\[
c^p_{ij}(x, y) = \frac{1}{|V|} \int_Y \left\{ \left( 1 + \partial_y \chi(x, y) \right) V_x \varepsilon^p_{ij}(x, y) \right\} dY \] (8)

\[
e_{ij}(x, y) = \frac{1}{|V|} \int_Y \left\{ \left( 1 + \partial_y \chi(x, y) \right) V_x \varepsilon_{ij}(x, y) \right\} dY \quad \text{(9)}
\]

\[
c_{ij}(x, y) = \frac{1}{|V|} \int_Y \left\{ \left( 1 + \partial_y \chi(x, y) \right) \varepsilon^c_{ij}(x, y) \right\} dY \] (10)

where \( \chi(x, y) \) is the characteristic displacement of the unit cell, \( R(x, y) \) is the characteristic electrical potential of the unit cell, and \( \chi(x, y) \) and \( \Phi(x, y) \) are the characteristic “coupled” functions of...
the unit cell. All these functions are \( Y \)-periodic. The relationships between \( \mathbf{u}_i \) and \( \phi_i \), and the characteristic functions are given by

\[
\mathbf{u}_i = \chi(\mathbf{x}, \mathbf{y})\mathbf{u}_i(\mathbf{x}) + \Phi(\mathbf{x}, \mathbf{y})V_x \phi_i(\mathbf{x}),
\]

\[
\phi_i = \psi(\mathbf{x}, \mathbf{y})\mathbf{u}_i(\mathbf{x}) + R(\mathbf{x}, \mathbf{y})V_x \phi_i(\mathbf{x}),
\]

(11)

Thus, it is possible to evaluate the stress distributed in the unit cell by using Eq. (14) [12,22].

\[
\sigma(\mathbf{x}, \mathbf{y}) = \left[ c^e(\mathbf{x}, \mathbf{y}) : (I + \partial_y \chi(\mathbf{x}, \mathbf{y}) + \mathbf{e}(\mathbf{x}, \mathbf{y})V_y \psi(\mathbf{x}, \mathbf{y})) \partial_x \mathbf{u}_i(\mathbf{x}) - \left[ c^e(\mathbf{x}, \mathbf{y}) : \partial_y \Phi(\mathbf{x}, \mathbf{y}) + \mathbf{e}(\mathbf{x}, \mathbf{y})(I + V_y R(\mathbf{x}, \mathbf{y})) \right] V_x \phi_i(\mathbf{x}) \right].
\]

(14)

The formulation of the homogenization method is the same for the case with or without material gradation. However, in the FGM case, the properties vary at each position in the unit cell, according to the material gradation control law further described in Section 5.3.

4. Topology optimization method

A major concept in topology optimization is the extended design domain, which is a large fixed domain that must contain the whole structure to be determined by the optimization procedure. The objective is to determine the holes and connectivities of the structure by adding and removing material in this domain. Because the extended domain is fixed, the finite element model is not changed during the optimization process, which simplifies the calculation of derivatives of functions defined over the extended domain [29,30]. In the case of material design, the extended design domain is the unit cell domain.

In Fig. 1, the scheme of a topology optimization procedure for piezocomposite material design is presented. Within the initial domain the mesh is generated and the optimization procedure is performed, providing a topology that can be post-processed, verified, and manufactured.

The discrete problem, where the amount of material at each element can assume only values equal to either zero or one (i.e. void or solid material, respectively), is an ill-posed problem. A typical way to seek a solution for topology optimization problems is to relax the problem by allowing the material to assume intermediate property values during the optimization procedure, which can be achieved by defining a special material model [30,31]. Essentially, the material model approximates the material distribution by defining a function of a continuous parameter (design variable) that determines the mixture of basic materials throughout the domain. In this sense, the relaxation yields a continuous material design problem that no longer involves a discernible connectivity.

A topology solution can be obtained by applying penalization coefficients to the material model to recover the 0–1 design (and thus, a discernible connectivity), and some gradient control on material distribution, such as a filter or projection [32]. It turns out that this relaxed problem is strongly related to the FGM design problem, which essentially seeks a continuous transition of material properties [33]. Thus, while the 0–1 design problem (needs complexity control, such as filter) does not admit intermediate values of design variables, the FGM design problem admit solutions with intermediate values of the material field.

Thus, the objective of the present work is to design FGM piezocomposites using the concept of the relaxed problem in continuum topology optimization. The problem consists of maximizing the electromechanical coupling coefficient defined in Section 4.2.

4.1. Material model

In this work, the topology optimization formulation employs a material model based on the SIMP (Solid Isotropic Material With Penalization) model [32], which states that at each point of the domain, the local effective property of the mixture is

\[
\mathbf{c}^e = \rho^p \mathbf{c}_{mat_1} + (1 - \rho^p) \mathbf{c}_{mat_2},
\]

\[
\mathbf{e}^0 = \rho^p \mathbf{e}_{mat_1} + (1 - \rho^p) \mathbf{e}_{mat_2},
\]

\[
\mathbf{e}^h = \rho^p \mathbf{e}_{mat_1} + (1 - \rho^p) \mathbf{e}_{mat_2},
\]

(15)

where \( \mathbf{c}_{mat_1} \), \( \mathbf{c}_{mat_2} \), and \( \mathbf{e}_{mat_2} \) correspond to the elastic, piezoelectric, and dielectric tensors of Eq. (1), respectively, for materials 1 and 2. The variable \( \rho \) is a pseudo-density describing the amount of material at each point of the domain, which can assume values between 0 and 1. A topology solution can be obtained by applying penalization coefficients \( p_1 \), \( p_2 \), and \( p_3 \) to the material model to recover the 0–1 design, and some gradient control on material distribution, such as a filter or projection [32]. These penalization coefficients are chosen according to two conditions that the three penalty exponents must satisfy for stable convergence developed by Kim et al. [34]. The first condition is an intrinsic condition ensuring better energy conversion efficiency between mechanical and electric energy for more piezoelectric material usage and the second one is an objective-dependent condition favoring a distinct material distribution over an intermediate material distribution for the same amount of piezoelectric material used.

In order to vary the polarization directions in the unit cell, it is necessary to add more design variables at each point of the design domain, called orientation variable \( \gamma_n \), which are continuum variables, ranging from 0 to 1, representing each candidate angle of polarization for the piezoelectric material. These variables are further described in Section 5.4.

4.2. Design problem formulation

The optimization problem aiming at energy harvesting applications consists of finding a distribution of material that maximizes the electromechanical coupling coefficient \( k \), which represents the coupling between the directions of stress and electrical fields. It is related to energy in the sense that it is the ratio of the peak
energy stored in the “capacitor” of the piezoelectric material to the peak strain energy with electrodes open, and its square is equal to the ratio of the converted electrical energy and the input mechanical energy. Therefore, the electromechanical coupling coefficient is an important parameter for describing the energy conversion capability of the piezoelectric material, and the optimization problem aiming at energy harvesting applications in quasi-static operation must find the material distribution that maximizes the electromechanical coupling coefficient $k$, which is given by (15):

$$k = \sqrt{\frac{(dh)^2}{S_p E_{13}}}$$  \hspace{1cm} (16)

Thus, the objective optimization problem studied can be stated as:

Maximize : $F(\rho(x), \theta(x)) = k$

subject to:

- $0 \leq \rho(x) \leq 1$
- $-90^\circ \leq \theta(x) \leq 90^\circ$
- symmetry conditions
- gradation control

where $F$ is the function to be maximized, and $\rho(x)$ and $\theta(x)$ are the design variables at each position $x$ of the design domain. The values of $\rho$ vary from 0 to 1, representing the presence of material 1 or 2, and values of $\theta$ vary from $-90^\circ$ to $90^\circ$, representing the polarization direction of the piezoelectric material at each point.

5. Numerical implementation

A continuum distribution of the design variable inside the finite element domain is considered allowing representation of a continuous material variation during the design process. The interest here is to obtain solutions with a continuous distribution of material, intermediate materials (no penalization) are allowed. A material model based on the SIMP model together with the DMO concept [27] is applied to verify the influence of the piezoelectric polarization direction in the objective function. A gradient control constraint in the unit cell domain is implemented based on projection techniques [35,36]. This gradient control capability allows the address of the influence of FGM gradation in the design of graded materials. It also avoids the problem of mesh dependency in the topology optimization implementation [32]. The actual optimization problem is solved by the MMA (“Method of Moving Asymptotes”) [37].

In this section, the finite element scheme for convex $n$-gons outlined in [38] is reviewed and extended to piezoelectric materials. Then, the homogenization method is applied to piezoelectric materials using polygonal elements and material gradation control. After that, the implementation of the DMO concept applied to piezoelectric polarization direction is explained, considering that the design variables are located at nodes. The sensitivity analysis is presented and, finally, the discrete problem formulation is defined.

5.1. Piezoelectric polygonal element

Most published articles that work with topology optimization method uses the quadrilateral 4 node finite element, also known as Q4. However, such meshes exhibit one-node connections and are susceptible to checkerboard patterns in topology optimization applications, which have been the subject of extensive research [39]. Polygonal elements can be very useful in this respect since they naturally exclude checkerboard layouts [40]. In this work, Voronoi diagrams are used as a natural and effective means for generating irregular polygonal meshes. An attractive feature of the method is that randomness and subsequently higher levels of geometric isotropy are obtained as a byproduct of arbitrary seed placement. Furthermore, the use of Lloyd’s algorithm [41] can remove excessive element distortion, and allows for construction of meshes that are uniform in size. In this work, the formulation described by Talischi et al. [42–44] is extended to piezoelectric materials. Eqs. (8)–(10) are solved by using the Finite Element Method (FEM). It is assumed that the unit cell is discretized by $N$ finite elements, that is:

$$Y = \bigcup_{n=1}^{N} \Omega^n,$$  \hspace{1cm} (17)

where $N$ is the number of finite elements and $\Omega^n$ is the domain of each element.

The approach presented by Sukumar and Tabarraei [38] constructs a conforming approximation space on polygonal meshes using natural neighbor bilinear interpolation functions and isoparametric transformations. For $n = 3$ and $n = 4$, the resulting finite element is identical to the constant strain triangle and bilinear quadrilateral, respectively.

Now, consider a set of nodes $\{q_i\}$ and point $p$ located where nodal data should be interpolated. Points $p$ and $\{q_i\}$ are “natural neighbors” if their Voronoi cells have a common edge [38]. The set of natural neighbors of $p$ are defined as follows:

$$\mathcal{I}(p) = \{i | V_i \cap V_p \neq \emptyset\},$$  \hspace{1cm} (18)

where $V_i$ and $V_p$ denote the Voronoi cells of $q_i$ and $p$, respectively. The Laplace interpolant corresponding to $q_i$ is given by:

$$N_i(x) = \frac{w_i(x)}{\sum_{j=1}^{n} w_j(x)} \text{ where } w_i(x) = \frac{s_i(x)}{h_i(x)}.$$  \hspace{1cm} (19)

Here $x$ is the location of $p$, $s_i$ is the length of the Voronoi edge common to $V_i$ and $V_p$, and $h_i$ denotes the distance between $p$ and $q_i$, as illustrated in Fig. 2. By construction, the Laplace functions are non-negative, bounded and satisfy partition of unity:

$$0 \leq N_i(x) \leq 1, \hspace{1cm} \sum_{i=1}^{n} N_i(x) = 1.$$  \hspace{1cm} (20)

Furthermore, it can be shown that these functions are linearly precise:

$$\sum_{i=1}^{n} x_i N_i(x) = x.$$  \hspace{1cm} (21)

where $x_i$ represents the location of node $q_i$. This property along with constant precision (partition of unity) ensures the convergence of the Galerkin method for second-order partial differential equations. Moreover, Laplace functions are linear on the boundary of the convex hull of $\{q_i, i \in \mathcal{I}\}$ [45], and satisfy the Kronecker-delta property, meaning that the interpolated value at a node is equal
to the nodal value. If the nodes are located at the vertices of a convex polygon, any interior point of this polygon has \( q \), as its natural neighbors. Therefore, Laplace shape functions corresponding to \( q \), lead to a finite element for that polygon. Furthermore, an isoparametric mapping from regular \( n \)-gons to any convex polygon can be constructed using these shape functions. Since the interpolated field varies linearly on the boundary, the resulting approximation is conforming. Following the usual approach in the finite element community, the shape functions are defined on the parent domain, where the weak form integrals are evaluated numerically. The reference \( n \)-gon is divided into \( n \) triangles (by connecting the centroid to the vertices) and well-known quadrature rules are used on each triangle.

Considering that the topology optimization results in a smoothly graded material, a more natural way of representing the material distribution emerges by considering a continuous representation of material properties [46,47], which is achieved by interpolating the properties inside the finite element using shape functions [35,46,48]. Thus, nodal design variables are defined rather than the usual element based design variables. Thus, the design variable inside each finite element is given by

\[
\rho_i(\mathbf{x}) = \sum_{i=1}^{m} \rho_i N_i(\mathbf{x}),
\]

where \( \rho_i \) is the nodal design variable, \( N_i \) is the Laplace shape function described above, and \( m \) is the number of nodes at each element. This formulation allows a continuous distribution of material along the design domain instead of the traditional piecewise. This formulation allows a continuous distribution of material along the design domain instead of the traditional piecewise constant material distribution applied by previous formulations of topology optimization [32].

5.2. Homogenization method using polygonal elements applied to piezoelectric materials

Bilinear interpolation functions are considered for displacements and electrical potentials. Therefore, the characteristic functions previously defined are expressed in each element as a function of the shape functions \( N_i \):

\[
\begin{align*}
\phi_i^{(mm)} &\equiv N_i q_i^{(mm)}, \\
\psi_i^{(mm)} &\equiv N_i q_i^{(mmm)}, \\
\Phi_i^{(m)} &\equiv N_i \Phi_i^{(m)}, \\
\Phi_i^{(mm)} &\equiv N_i \Phi_i^{(mm)},
\end{align*}
\]

where \( NN \) is the number of nodes per finite element (in the case of polygonal elements, it usually varies from 3 to 7). Assembling the individual matrices for each element, the following global matrix system for each load case \( mn \) or \( m \) [15,49,50] is obtained:

\[
\begin{bmatrix}
K_{uu} & K_{up} \\
K_{pu} & K_{pp}
\end{bmatrix}
\begin{bmatrix}
\mathbf{\phi}^{(m)} \\
\mathbf{\psi}^{(m)}
\end{bmatrix}
= 
\begin{bmatrix}
\mathbf{F}^{(m)} \\
\mathbf{Q}^{(m)}
\end{bmatrix} \Rightarrow \mathbf{KX} = \mathbf{Y}.
\]

(24)

The stiffness, piezoelectric, and dielectric global matrices (\( K_{uu}, K_{up}, \) and \( K_{pp} \), respectively) are obtained by assembling each element’s individual matrix, and the global force and electrical charge vectors (\( \mathbf{F} \) and \( \mathbf{Q} \)) are the assembly of the element force and electrical charge vectors (\( \mathbf{F}^{(m)} \) and \( \mathbf{Q}^{(m)} \), respectively) for all finite elements:

\[
\begin{align*}
K_{uu} &= \sum_{i=1}^{N} K_{uu}^{(m)}, & K_{up} &= \sum_{i=1}^{N} K_{up}^{(m)}, & K_{pp} &= \sum_{i=1}^{N} K_{pp}^{(m)}, & \mathbf{F} &= \sum_{i=1}^{N} \mathbf{F}^{(m)}, \\
Q &= \sum_{i=1}^{N} \mathbf{Q}^{(m)}.
\end{align*}
\]

(25)

The element matrices and vectors \( K_{uu}^{(m)}, K_{up}^{(m)}, K_{pp}^{(m)}, \mathbf{F}^{(m)}, \) and \( \mathbf{Q}^{(m)} \) are calculated by the following equations [15].

5.3. Material gradation control

In this work, a gradient control constraint in the unit cell domain is implemented based on the same approach developed by Carbonari et al. [36], which used nodal design variables and projection functions [51]. This gradient control capability allows the address of the influence of FGM gradation in the design of extreme materials. It also avoids the problem of mesh dependency in the topology optimization implementation when aiming at a discrete solution [32]. This technique adds a new layer of pseudo-nodal material densities \( (d_i) \) superimposed on the current layer of nodal design variables \( (\rho_i) \). For each design variable \( \rho_i \), a circular area \( \Omega_i \) of radius \( r_{grad} \) is defined, whose center is located in the same coordinates of the node \( i \), as shown in Fig. 3. The values of \( \rho_i \) become a function of the \( n \) pseudo-densities values belonging to the circular area \( \Omega_i \) and the distances between each pseudo-density and the center of the area. Thus:

\[
\rho_i = f(d_i),
\]

(27)

where

\[
\rho_i = \frac{1}{\sum_{j\in S_i} d_j(\mathbf{r}_j)} \sum_{j\in S_i} \mathbf{Z}(\mathbf{r}_j)
\]

(28)

in which \( \mathbf{r}_j \) is the distance between nodes \( i \) and \( j \)

\[
\mathbf{r}_ij = ||\mathbf{x}_j - \mathbf{x}_i||
\]

(29)

and \( S_i \) is the subset of the interior nodes in the circular area. The weight factor \( \mathbf{Z} \) is defined by:

\[
\mathbf{Z}(\mathbf{r}_j) = \begin{cases} 
\frac{r_{grad}^2 - \mathbf{r}_ij^2}{r_{grad}^2}, & \text{if } \mathbf{x}_j \in S_i, \\
0, & \text{otherwise}.
\end{cases}
\]

(30)

Fig. 3. Projection technique.
5.4. Discrete material optimization (DMO)

The formulation brought by Stegmann and Lund [27], called Discrete Material Optimization (DMO), uses the mixed material strategy suggested by Sigmund et al. [25,52] for multi-phase topology optimization, where the total material stiffness is computed as a weighted sum of candidate materials. In this present work, this method has been applied to optimize polarization direction of piezoelectric materials. This methodology can be defined as: for every element in the design domain, it finds a distinct material from a set of candidate materials, such that the objective function is maximized. In the case of polarization direction of piezoelectric materials, each candidate has the piezoelectric properties calculated at a specific polarization angle. Thus, a predetermined number of polarization angles are chosen and the optimization process indicates which is the best candidate material (see Fig. 4).

As the classical approach of the topology optimization method, the parametrization of the DMO is performed at the finite element level. The piezoelectric tensor of the element, $\mathbf{e}^j$, is expressed as a weighted sum of the piezoelectric tensors of the candidate materials, $\mathbf{e}$, as shown in Eq. (31):

$$
\mathbf{e}_{\text{mat}}^j = \sum_{i=1}^{n'} w_i \mathbf{e}_i = w_1 \mathbf{e}_1 + w_2 \mathbf{e}_2 + \cdots + w_{n'} \mathbf{e}_{n'}, \quad 0 \leq w_i \leq 1,
$$

where $w_i$ are weighting factors, $n'$ is the number of finite elements in the design domain, $\mathbf{e}_{\text{mat}}^j$ is the resultant piezoelectric tensor of the element $e$ for material $j$, and $\mathbf{e}_i$ is the piezoelectric tensor of the candidate material $i$. Each constitutive matrix $\mathbf{e}$ can be calculated by the following expression:

$$
\mathbf{e}_i = \left( \mathbf{R}^1 \right)^j \mathbf{e}_{\text{mat}}^j \mathbf{R}^2
$$

and

$$
\mathbf{R}^1 = \begin{bmatrix}
  c^2 & s^2 & sc \\
  s^2 & c^2 & -sc \\
  -2sc & 2sc & c^2 - s^2
\end{bmatrix} \quad \text{and} \quad \mathbf{R}^2 = \begin{bmatrix}
  c & s \\
  -s & c
\end{bmatrix},
$$

where $\mathbf{e}_{\text{mat}}^j$ is the original piezoelectric matrix of material $j$ without rotation, $s = \sin(\theta_i)$, $c = \cos(\theta_i)$, and $\theta_i$ is the discrete angle adopted for each material phase. Index $i$ represents the number of candidate angles and index $j$ represents the number of materials that is distributed in the topology, according to the material model presented in Eq. (15). In the examples adopted in this work only two types of materials are considered (PZT-5A and epoxy), thus, $j = 1, 2$.

The weighting factors $w_i$ in Eq. (31) must have values between 0 and 1 as no piezoelectric tensor can contribute more than the piezoelectric material property and a negative contribution is physically meaningless.

In this way, as in classical topology optimization, the weights on the constitutive matrices become “switches” that turn on and off stiffness contributions such that the objective is minimized and a distinct choice of candidate material is made. At the beginning of the optimization, $\mathbf{e}_i$ consists of contributions from several candidate materials, however, at the end of the design optimization, the parameterization for the weighting functions has to fulfill the demand that one distinct candidate angle is chosen [27]. This underlines that the DMO method relies heavily on the ability of the optimizer to push all weights to the limit values. Any element having intermediate values of the weights must be regarded as undefined since the constitutive properties are non-physical. To achieve this objective, one more design variable need to be adopted, called orientation variable $\gamma_i$, which is a continuum variable (from 0 to 1) representing each candidate angle. This formulation leads to a high number of variables.

With respect to local optimized solutions, Stegmann and Lund [27] investigated this phenomena when the fiber direction in composites are directly handled as design variables. They illustrated this issue by solving a simple problem using a continuous formulation and the method of moving asymptotes (MMA) [37]. The results have shown that the global optimum solution is very dependent on the initial guess. This is not a new realization, of course, and several methods have already been proposed to circumvent the problem of local optimum solutions, such as analytical methods, improved mathematical programming techniques, or parameterization methods. The DMO parametrization is a novel method that aims to circumvent the local minima problem [27]. Thus, the weighting functions can be calculated by

$$
w_i = \frac{w_i}{\sum_{k=1}^{n'} w_k}, \quad \text{where} \quad w_i = (\gamma_i)^p \prod_{j=1 \neq i}^{n'} \left(1 - (\gamma_i)^p \right).
$$

To push the orientation variables $\gamma_i$ towards 0 or 1, a penalization technique has been adopted by introducing the power, $p$, to penalize intermediate values of $\gamma_i$. A low value of $p$ does not guarantee the prevalence of only one polarization direction, what does not make sense from a physical point of view. In addition to that, a high value of $p$ affects the choice of the polarization direction similar to what happens in the SIMP model, i.e., the relaxation of the problem is practically removed and the problem may become close to a discrete problem which is ill-posed. However, there is an heuristic in the choice of this value. In this work, different values of $p$ are previously tested and the best results are obtained for $p = 6$.

Moreover, the term $\left(1 - (\gamma_i)^p \right)$ is introduced such that an increase in $\gamma_i$ results in a decrease of all other weighting functions. Finally, the weights have been normalized to satisfy the constraint that the sum of the weighting functions is equal to 1. Note that the expression in Eq. (34) means that complicated additional constraints on the design variables $\gamma_i$ are avoided and only simple box constraints have to be dealt with.

5.5. Sensitivity analysis

In this section, the expressions for the sensitivities with respect to the design variables $\rho_j$ (which can be substituted by the design variables $d_j$) and $\gamma_i$ are presented. The sensitivity analysis provides the gradients of homogenized properties, allowing the optimization solver to set the directions to be taken for each design variable.

The sensitivity with respect to the design variables $d_i$ are obtained using the chain rule:

$$
\frac{\partial (\cdot)}{\partial d_i} = \sum_{j \in \Omega} \frac{\partial (\cdot)}{\partial p_j} \frac{\partial p_j}{\partial d_i}
$$

where $\Omega$ is the design domain and $\partial p_j / \partial d_i$ is not zero only at nodes $j$ belonging to $S_i$ with respect to node $i$. Furthermore,

$$
\frac{\partial p_j}{\partial d_i} = \frac{\alpha(r_j)}{\sum_{k \in S_i} \alpha(r_k)}.
$$
\( \partial (\cdot) / \partial \rho_{i} \) is calculated using traditional methods, such as adjoint method, as described ahead.

The differentiation of the objective function described in Eq. (16) is straightforward by using the chain rule. However, the partial derivatives depend on the differentiation of the terms written in Eq. (3), which depend on the differentiation of the homogenized properties of Eqs. (8)-(10). Therefore, the steps describe how to calculate the sensitivity of the homogenized properties \( e_{i}, e_{h}, \) and \( e_{d} \) as a function of the design variables.

By differentiating the equation system of Eq. (24), it is obtained:

\[
\frac{\partial \mathbf{K}}{\partial \rho_{i}} + \mathbf{K} \frac{\partial \mathbf{X}}{\partial \rho_{i}} = \frac{\partial \mathbf{Y}}{\partial \rho_{i}} \iff \frac{\partial \mathbf{X}}{\partial \rho_{i}} = \mathbf{K}^{-1} \mathbf{M},
\]

where \( \mathbf{M} = \frac{\partial \mathbf{Y}}{\partial \rho_{i}} - \frac{\partial \mathbf{K}}{\partial \rho_{i}} \mathbf{X} \).

For each finite element, we have that:

\[
\left\{ \frac{\partial \chi^{(m,m)}}{\partial \rho_{i}} \right\}_{e} = \mathbf{H}_{e} \mathbf{K}^{-1} \mathbf{M}_{e} \Rightarrow \left\{ \frac{\partial \chi^{(m,m)}}{\partial \rho_{i}} \right\}_{e} = \left( \mathbf{M}_{e} \right)^{t} \mathbf{K}^{-1} \mathbf{H}_{e}.
\]

(38)

\[
\left\{ \frac{\partial \chi^{(m,n)}}{\partial \rho_{i}} \right\}_{e} = \mathbf{H}_{e} \mathbf{K}^{-1} \mathbf{M}_{e} \Rightarrow \left\{ \frac{\partial \chi^{(m,m)}}{\partial \rho_{i}} \right\}_{e} = \left( \mathbf{M}_{e} \right)^{t} \mathbf{K}^{-1} \mathbf{H}_{e}.
\]

(39)

where \( \mathbf{H}_{e} \) is a matrix of \( N \times 5 \) filled by 1 at each electrical degree of freedom and 0 at all others, and \( \mathbf{K}_{e} \) is a matrix \( NE \times 5 \) filled by 1 at each electrical degree of freedom and 0 at all others. \( NM \) and \( NE \) are, respectively, the number of mechanical and electrical degrees of freedom in the entire domain.

By differentiating Eq. (8) with respect to the design variable \( \rho_{i} \), one obtains [15]:

\[
\frac{\partial \chi^{(m,m)}}{\partial \rho_{i}} \mathbf{K}_{e} = \left( \mathbf{M}_{e} \right)^{t} \mathbf{K}^{-1} \mathbf{H}_{e} \Rightarrow \frac{\partial \chi^{(m,m)}}{\partial \rho_{i}} = \left( \mathbf{M}_{e} \right)^{t} \mathbf{K}^{-1} \mathbf{H}_{e}.
\]

(40)

The explicit calculation of \( \partial \chi^{(m,m)} / \partial \rho_{i} \) and \( \partial \chi^{(m,n)} / \partial \rho_{i} \) presents a high computational cost due to the dependency of all design variables. Thus, the adjoint method is applied to avoid this problem. The third component of Eq. (40) can be rewritten by:

\[
\left\{ \frac{\partial \chi^{(m,m)}}{\partial \rho_{i}} \right\}_{e} \mathbf{K}_{e} = \left( \mathbf{M}_{e} \right)^{t} \mathbf{K}^{-1} \mathbf{H}_{e} \Rightarrow \frac{\partial \chi^{(m,m)}}{\partial \rho_{i}} = \left( \mathbf{M}_{e} \right)^{t} \mathbf{K}^{-1} \mathbf{H}_{e}.
\]

(41)

and

\[
\mathbf{K}_{e} = \mathbf{J}_{e}.
\]

(42)

where \( \mathbf{J}_{e} = \mathbf{H}_{e} \mathbf{K}_{e} \). By calculating \( \mathbf{J}_{e} \), it is possible to calculate Eq. (38). Similarly, it is possible to evaluate the fourth component of Eq. (40) by doing:

\[
\left\{ \frac{\partial \chi^{(m,n)}}{\partial \mathbf{X}} \right\}_{e} \mathbf{K}_{e} = \left( \mathbf{M}_{e} \right)^{t} \mathbf{K}^{-1} \mathbf{H}_{e} \Rightarrow \frac{\partial \chi^{(m,n)}}{\partial \mathbf{X}} = \left( \mathbf{M}_{e} \right)^{t} \mathbf{K}^{-1} \mathbf{H}_{e}.
\]

(43)

and

\[
\mathbf{K}_{e} = \mathbf{J}_{e}.
\]

(44)

where \( \mathbf{V}_{e} = \left( \mathbf{I} + \chi^{(m,m)} \right) \mathbf{K}_{e} \). Calculating \( \mathbf{P}_{e} \), it is possible to calculate Eq. (39). In an analogous way, it is possible to calculate the sensitivity of the piezoelectric and dielectric properties by using the adjoint method, reducing the computational cost.

With respect to the DMO formulation, by differentiating Eq. (31) it is obtained:

\[
\frac{\partial \mathbf{e}_{\text{hom}}}{\partial \rho_{i}} = \sum_{i=1}^{N} \frac{\partial W_{i}}{\partial \rho_{i}} \mathbf{e}_{i}, \text{ and } \frac{\partial W_{i}}{\partial \rho_{i}} = \frac{\delta W_{i}}{\delta \rho_{i}} = \sum_{k=1}^{N} W_{k}.
\]

(45)

where

\[
\frac{\partial W_{i}}{\partial \rho_{i}} = \begin{cases} p_{i} \left( \gamma_{i}^{P} \right)^{p_{i}-1} \prod_{j=1}^{n} \left( 1 - \left( \gamma_{j}^{P} \right)^{p_{j}} \right) & \text{if } n = i, \\ - \left( \gamma_{i}^{P} \right)^{p_{i}} p_{i} \prod_{j=1}^{n} \left( 1 - \left( \gamma_{j}^{P} \right)^{p_{j}} \right) & \text{if } n = j. \end{cases}
\]

(46)

5.6. Discrete problem formulation

The final optimization problem studied can be stated in the discrete form as:

\[
\text{Maximize: } F(d_{i}, \gamma_{i}) = k
\]

\[
0 \leq d_{i} \leq 1, \quad i = 1, \ldots, N
\]

\[
0 \leq \gamma_{i} \leq 1
\]

symmetry conditions

gradation control

where \( F \) is the function to be maximized, \( N \) is the number of nodes in the design domain, \( d_{i} \) and \( \gamma_{i} \) are the design variables at each position \( \chi_{i} \) of the design domain. The values of \( d_{i} \) vary from 0 to 1, representing the presence of material 1 or 2, and values of \( \gamma_{i} \) vary from 0 to 1, representing the influence of the polarization direction of the orientation candidate at each node.

A flowchart of the optimization algorithm describing the steps involved is shown in Fig. 5. The method is implemented in MATLAB.

6. Numerical results

In this section, numerical examples of optimized microstructures are provided. First, unit cells are obtained with no material gradation, in order to verify the influence of the finite element mesh and the polarization direction. Later, the same verification is performed again to evaluate the influence of gradation in material design.

---


---
is applied to the macroscopic periodic matrix formed by 3 unit cells, and (c) microscopic stress distribution in the unit cell.

The adopted design domain is a quarter of a square two-dimensional unit cell, in order to reduce the computational cost. Therefore, before the optimization iterative process starts, it is necessary to perform a mapping scheme of the nodal values along the unit cell, with respect to the design variables in the design domain. For the cases where the polarization direction is fixed in the vertical direction, the material distribution is symmetric with respect to both axes, $x$ and $y$. For the cases where the polarization direction is included in the optimization, the material distribution is also symmetric in $x$ and $y$ axes; however, the polarization direction is symmetric only with respect to the $y$-axis. In relation to the $x$-axis, the polarization direction of the nodal values is identical to the respective design variables. Fig. 6 illustrates this mapping scheme. The simulation is performed taking into account the entire unit cell, applying periodic constraints. The design domain is discretized with 81 elements, so the quadrilateral mesh consists of 9 × 9 elements and in the polygonal mesh the elements are generated according to the Voronoi diagrams and Lloyd’s algorithm (see Section 5.1). The material properties of PZT-5A and epoxy polymer are listed in Table 1. The adopted penalization coefficients of Eq. (15) are $p^e = 2$, $p^p = 2$, and $p^p = 4$, according to two conditions that they must satisfy for stable convergence [34].

In this case, the variation of polarization direction of PZT-5A is considered, three different angles are adopted, 0°, 45° and 90°, and therefore, Eq. (31) has three parts, one for each angle. The adopted value for penalization coefficient $p$ of Eq. (34) is equal to 5, to ensure that only one direction is chosen. Approximately 10 full optimization processes are performed for each case, each of them considering a random initial material distribution, in order to avoid the dependency on the initial guess. Then, the best performance obtained for each case is illustrated in this section.

After obtaining the optimized microstructures for each case, homogenized elastic, piezoelectric and dielectric properties are calculated. These homogenized properties are used in a homogeneous macroscopic model to evaluate the macroscopic stress distribution. A uniform pressure $\sigma_0$ is applied to the macroscopic model, as shown in Fig. 7a. The adopted two-dimensional macroscopic model consists of a rectangular block of $20 \times 5$ mm, made of an homogeneous material, whose properties are the effective properties of each microstructure obtained by the optimization method. This macroscopic model is analyzed by considering a plane strain analysis.

From the macroscopic model analysis, the macroscopic strain and the macroscopic electric field are obtained, which are uniform for the entire model. Then, the microscopic stress is calculated for corresponding unit cell using Eq. (14). The stress distributions inside the optimized unit cells are shown in the next figures.

The electromechanical coupling coefficient of a unit cell made of pure PZT-5A has a value of 0.145. Varying the volume fraction, the 2–2 piezocomposite (see Fig. 7b) with fixed vertical polarization direction, a maximum electromechanical coupling coefficient equal to 0.145 is also obtained [15]. The performance of the optimized results presented in Sections 6.1 and 6.2 are compared with the performance of pure PZT-5A and also with the 2–2 piezocomposite. These values are considered as references for the optimized results.
6.1. Optimized non-FGM cell design

Material design examples, using the implemented software, are presented. The first approach is to verify the influence of the type of finite element mesh and the polarization direction in the objective function, considering no gradation in the unit cell. Fig. 8 shows the optimized unit cell for a quadrilateral mesh keeping the polarization in the vertical direction, the periodic matrix formed by $3 \times 3$ unit cells, and the microscopic stress distribution in the unit cell. Fig. 9 shows results for a polygonal mesh keeping the polarization in the vertical direction. Figs. 10 and 11 show the optimized results for the quadrilateral and polygonal mesh, respectively.

![Figures 8 to 11 showing optimized microstructures with different meshes and polarization directions.]

<table>
<thead>
<tr>
<th>Figure</th>
<th>Pol.</th>
<th>Mesh</th>
<th>$E_H$ (MPa)</th>
<th>$\varepsilon_H$ (C/m²)</th>
<th>$\varepsilon_H'/\varepsilon_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>Fixed</td>
<td>Quad.</td>
<td>38.36 16.70</td>
<td>0 0.95</td>
<td>906 0</td>
</tr>
<tr>
<td>9</td>
<td>Fixed</td>
<td>Poly.</td>
<td>31.37 15.30</td>
<td>0 1.49</td>
<td>764 0</td>
</tr>
<tr>
<td>10</td>
<td>Free</td>
<td>Quad.</td>
<td>49.55 13.05</td>
<td>0 -0.05</td>
<td>1038 0</td>
</tr>
<tr>
<td>11</td>
<td>Free</td>
<td>Poly.</td>
<td>59.43 17.08</td>
<td>0 -0.31</td>
<td>1249 0</td>
</tr>
</tbody>
</table>

Table 2: Homogenized properties of the optimized structures with no material gradation.
respectively, using the DMO concept, for 0°, 45°, and 90°. The homogenized properties for each case are listed in Table 2.

In Table 3, it can be seen the values of $k$ for the four optimized microstructures, their relative gains with respect to the pure PZT-5A or 2–2 piezocomposite, whose values of $k$ are equal to 0.145, and the maximum microscopic relative stress values in the unit cell. The stress distributions presented in these figures are the maximum principal stresses divided by the macroscopic stress value $\sigma_0$. Comparing the optimized microstructures with fixed polarization direction, it is possible to notice that the polygonal mesh model, whose gain is of 105.5%, has a better performance than the quadrilateral mesh model, whose gain is of 100.7%. This effect is repeated for the cases with free polarization direction of Figs. 10 and 11. In this approach, the quadrilateral mesh model has a gain of 113.1% and the polygonal mesh, 120.0%. Moreover, comparing the influence of the polarization direction, it is noted that the performances of the microstructures of Figs. 10 and 11 are better than the performances obtained with fixed polarization direction, presented in Figs. 8 and 9. In the case of Fig. 8, note that the maximum microscopic relative stress values can reach 7.8 times higher than the macroscopic stress $\sigma_0$. For the cases of Figs. 9–11, the maximum microscopic stress relative values are 7.6, 7.9, and 7.5 times greater than $\sigma_0$, respectively. From these results, it is concluded that by using the same number of finite elements,
polygonal meshes guide the problem toward better local minima. In addition, the variable polarization direction in the unit cell is an important factor and allows microstructure designs with better performance, however with higher stresses.

In order to verify the mesh convergence, non-FGM cells are optimized using coarse and refined meshes for both types of elements, quadrilateral and polygonal. The results are shown in Figs. 12 and 13. Fig. 12 presents the convergence of the \( k \) value as a function of the quantity of elements in the unit cell, for both cases. It is clear that, although the value of \( k \) still increases as long as the mesh became more discretized, the gain is not significant (less than 0.4%). However, by refining the quadrilateral mesh a large variation of the \( k \) value is verified (approximately 2.7%). Thus, the conclusion obtained from these examples is that, by using polygonal meshes, it is possible to satisfy mesh convergence with less elements than quadrilateral meshes. This effect can be seen more clearly in Fig. 13, where three examples for each type of element are shown. By comparing these meshes with the same number of elements, it is noticed that the quadrilateral meshes have bias in the optimized topology, i.e., the contours of PZT-5A follow the structural meshes, presenting linear boundaries. Rounded contours appear only in more discretized quadrilateral meshes. Polygonal meshes, on the contrary, the contour of PZT-5A is smoother even with few elements. Thus, polygonal meshes converge more rapidly.

6.2. Optimized FGM cell design

It is known that materials designed to achieve better performances can only be obtained with solid-void (0–1) designs and steep material variation [53]. However, usually, some gradation is obtained in the manufacturing processes of such materials. Thus, this gradation must be taken into account in the design phase. The same investigation presented previously is performed, considering a gradation radius of 10% of the unit cell length. Figs. 14–17 show the optimized FGM microstructures obtained. The homogenized properties for each case are listed in Table 4.

In Table 5, the values of \( k \) for the four optimized microstructures considering material gradations, their relative gains with respect to the pure PZT-5A or 2–2 piezocomposite, and the maximum microscopic stress relative values in the unit cell are listed. By comparing the optimized microstructures with fixed or

---

**Fig. 14.** Optimized microstructure with material gradation, using quadrilateral mesh and fixed polarization direction: (a) material distribution in the unit cell, (b) periodic matrix formed by 3 \( \times \) 3 unit cells, and (c) microscopic stress distribution in the unit cell.

**Fig. 15.** Optimized microstructure with material gradation, using polygonal mesh and fixed polarization direction: (a) material distribution in the unit cell, (b) periodic matrix formed by 3 \( \times \) 3 unit cells, and (c) microscopic stress distribution in the unit cell.

**Fig. 16.** Optimized microstructure with material gradation, using quadrilateral mesh and free polarization direction: (a) material distribution in the unit cell, (b) periodic matrix formed by 3 \( \times \) 3 unit cells, and (c) microscopic stress distribution in the unit cell.
Fig. 17. Optimized microstructure with material gradation, using polygonal mesh and free polarization direction: (a) material distribution in the unit cell, (b) periodic matrix formed by 3 x 3 unit cells, and (c) microscopic stress distribution in the unit cell.

Table 4 Homogenized properties of the optimized structures with material gradation.

<table>
<thead>
<tr>
<th>Figure</th>
<th>Pol.</th>
<th>Mesh</th>
<th>$c_{ij}$ (MPa)</th>
<th>$e_i$ (C/m²)</th>
</tr>
</thead>
</table>
| 14     | Fixed| Quad.| [42.68, 13.32, 0]
         |      |      | [13.32, 22.92, 0]
         |      |      | [0, 0, 4.63]   |
| 15     | Fixed| Poly.| [28.25, 13.48, 0]
         |      |      | [13.48, 20.93, 0]
         |      |      | [0, 0, 5.85]   |
| 16     | Free | Quad.| [57.32, 17.55, 0]
         |      |      | [17.55, 32.09, 0]
         |      |      | [0, 0, 5.36]   |
| 17     | Free | Poly.| [57.66, 16.52, 0]
         |      |      | [16.52, 28.76, 0]
         |      |      | [0, 0, 5.86]   |

Table 5 Comparison of optimized FGM microstructures.

<table>
<thead>
<tr>
<th>Figure</th>
<th>Polarization direction</th>
<th>Mesh</th>
<th>$k$</th>
<th>Gain (%)$^a$</th>
<th>$\sigma/\sigma_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>Fixed</td>
<td>Quadrilateral</td>
<td>0.285</td>
<td>96.6</td>
<td>5.7</td>
</tr>
<tr>
<td>15</td>
<td>Fixed</td>
<td>Polygonal</td>
<td>0.294</td>
<td>102.8</td>
<td>5.1</td>
</tr>
<tr>
<td>16</td>
<td>Free</td>
<td>Quadrilateral</td>
<td>0.299</td>
<td>106.2</td>
<td>5.9</td>
</tr>
<tr>
<td>17</td>
<td>Free</td>
<td>Polygonal</td>
<td>0.305</td>
<td>110.3</td>
<td>6.0</td>
</tr>
</tbody>
</table>

$^a$ With respect to pure PZT-5A ($k = 0.145$).

variable polarization directions, it is possible to notice that the polygonal mesh models have better performances than the quadrilateral mesh models, similar to the cases with no material gradation presented before. By comparing the maximum relative stress values listed in Table 5, again, polygonal mesh models present smaller values in the microstructure than quadrilateral mesh models. By comparing the influence of material gradation in the maximum relative stress values, it can be noticed that the gain values of $k$ with respect to the pure PZT-5A are smaller than the values obtained with non-FGM microstructures. However, the FGM microstructures shown in Figs. 14–17, present smaller maximum relative stress values when compared to the non-FGM microstructures shown in Figs. 8–11. Thus, although the objective function values decrease considering material gradation in the unit cell, the maximum microscopic stress values also decrease, which means that the piezocomposite can be subjected to higher loads and thus, a higher amount of energy can be obtained.

7. Conclusions

This work proposes a methodology to design functionally graded piezocomposites materials that considers important aspects in the piezocomposite material design process aiming at energy harvesting applications, such as the influence of piezoelectric polarization directions, the influence of material gradation between the constituent materials in the unit cell, and the influence of quadrilateral or polygonal finite element mesh in the obtained designs. The variation of the polarization direction is implemented using the DMO concept. From the examples of microstructure designs presented in this work, we conclude that the variable polarization directions in the unit cell is an important factor and allows microstructure designs with better performance. The results presented show that the FGM concept can be applied to design piezocomposite materials with greater performance than pure materials, such as PZT-5A, or 2–2 piezocomposites, for example. As expected, material gradation generates unit cell designs with electromechanical coupling coefficient $k$ values smaller than $k$ values obtained with discrete material distribution. By using the same number of finite elements, polygonal meshes guide the problem toward better local minima than using traditional quadrilateral elements. In addition, by using polygonal meshes, it is possible to satisfy mesh convergence with about 40% less number of elements than quadrilateral meshes. One of the main questions answered in this work is, quantitatively, how the microscopic stresses can be reduced by combining the functionally graded material (FGM) concept with optimization, notice that stress concentration is redistributed due to the material gradation in the unit cell. Thus, the main conclusion is that although 0–1 structures present higher values of $k$, they also present higher microscopic stress values, then supporting lower external loads to avoid failure and, consequently, less electrical energy can be harvested. On the contrary, although FGM structures present lower values of $k$, they present lower microscopic stress values, then supporting higher external loads and, consequently, more electrical energy can be harvested.

Acknowledgments

The first author is thankful for the financial support received from CNPq (National Council for Research and Development, Brazil) and FAPESP (São Paulo State Foundation Research Agency) by supporting him in his graduate studies through the fellowship.
REFERENCES


