

EMERGENCE OF ELASTOSTATIC STRAIN-GRADIENT EFFECTS FROM TOPOLOGICAL OPTIMIZATION

V. CALISTI, A. LEBÉE, A.A. NOVOTNY, AND J. SOKOLOWSKI

ABSTRACT. There are very few examples of architected materials producing significant strain-gradient effects in elastostatics. In the present paper, we generate for the first time new microstructures featuring these effects from topological optimization of two-dimensional periodic media. The optimized shape functionals depend on the first and second-order homogenized tensors, obtained from a two-scale asymptotic expansion homogenization scheme. The optimization method applied here relies on the recently rigorously derived topological derivative of the second-order homogenized tensor, measuring the strain-gradient sensitivity with respect to a small circular inclusion at the microscopic level endowed with different material property from the background. This previous theoretical work allows an accurate numerical implementation.

1. INTRODUCTION

Additive manufacturing and topological optimization sparked a renewed interest in the study of *architected materials* over the past two decades, partly due to the emergence of 3D printers and the improvement of the computational methods and power. In the present study, we are interested in two-dimensional continuous periodic materials, designed in such a way that the required macroscopic properties are obtained after organizing their inner microstructure. The framework describing macroscopic properties of a material from the analysis of its microstructure, called *homogenization*, usually allows to describe an architected material by an approximated first-gradient macroscopic model. Namely, the sole first gradient of the macroscopic displacement field is used for measuring the elastic energy. Such models have been extensively studied and optimized (see [9, 11, 43], among others), but they are valid under a hypothesis of scale separation and finite geometric contrast within the cell.

However, this hypothesis may not be satisfied in practice. In this case, other macroscopic models also called *generalized continua* are needed, such as higher order models, having additional degrees of freedom (for instance *Cosserat materials*), or higher gradient models for which higher-order gradients of the macroscopic displacement field are used for measuring the elastic energy (see e.g., [21]). Thus, we explore how to produce new microstructures yielding non-classical and interesting behavior, and how to optimize these effects. In particular, we study the numerical synthesis of novel periodic continuous microstructures featuring higher gradient macroscopic effects, and more precisely strain-gradient effects.

In dynamics, strain-gradient elasticity is relevant when the wavelength is of the same order as the size of the heterogeneities of a material, leading for example to new dispersive properties (see e.g., [34]). In an effort to improve these effects, the shape and topological optimization have been investigated for wave equations in periodic structures, some based on the shape sensitivity [4], others on the topological sensitivity [13, 18].

In elastostatics, the macroscopic length scale is typically the size of the domain and strain-gradient effects may be understood as small corrections of classical elasticity. Hence, contrary to dynamics, they are difficult to observe unless some specific stiffness contrast assumptions are made. Indeed, it was shown theoretically in [17] that many different models of generalized continua can be obtained from the homogenization of a mixture of materials with large contrast

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and some microstructures were investigated in this framework (see [2, 1], among others). Nevertheless, in practice, there are not so many microstructures that result in a generalized continuum for the elastostatic case. For this reason, we generate such microstructures in the present work. Instead of making assumptions on the contrast of the materials, we use topological optimization to produce non-classical effects arising from geometrical contrasts. In particular, we focus on the optimization of strain-gradient effects in elastostatics.

For this, we rely on the classical two-scale asymptotic expansion method, which brings out higher-gradient terms as corrections of the first-gradient elasticity, and allows to identify the higher-order homogenized tensors by computing the macroscopic elastic energy. In [39], a higher order convergence result is given for an infinite periodic media with a finite material contrast. Although the assumptions are restrictive, this result gives an interesting heuristic, and has been used in [19] to detect strain-gradient effects in a material with voids inclusions by a numerical investigation. To achieve this result, the first-gradient homogenized tensor should be degenerated to create zero-energy modes, so that the strain-gradient terms, which are usually small correction terms, become predominant. Thus, we follow such an approach in order to maximize strain-gradient effects in periodic media, for which the unit cell is a mixture of two elastic materials with a property contrast.

In order to produce some new microstructures, a possible strategy is to use shape or topological optimization methods, which have been widely applied to structural optimization problems (see e.g., [41, 35] for reviews, and [3, 38] for detailed introductions), as well as to many other fields, such as imaging, fluid mechanics, heat conduction problems, acoustic, electromagnetic, inverse problems, and piezoelectric. Among the main ones, we can mention the *evolutionary approaches* (see e.g., [5]), *phase-field approaches* (see e.g., [42]), the *density methods* (such as the homogenization approach [3], or the SIMP method [12, 44]), and the *level-set methods* (introduced in [33], see e.g. [41] for a review).

In this paper the topological derivative method is adopted, applying and adapting the theoretical results from [15] and the algorithm introduced in [8]. In contrast to the above mentioned methods, the topological derivative has been specifically conceived to provide a precise information on the sensitivity of a given shape functional with respect to topological domain perturbations. The origin of the topological derivative method in optimal design can be dated to the work by Schumacher et al. [20, 36] on the optimal location of holes within elastic structures. The first mathematical justifications for topological derivatives in the framework of partial differential equations are due to [40] and [22], in the context of the Poisson equation and the Navier system for Neumann and Dirichlet holes. Therefore, this relatively new concept in shape optimization has applications in many different fields such as shape and topology optimization, geometrical inverse problems, image processing, multi-scale material design and mechanical modelling, including damage and fracture evolution phenomena. See, for instance, the book [32] and the special issue on the topological derivative method and its applications in computational engineering [29], covering various topics ranging from new theoretical developments up to industrial applications.

Concerning architected materials, this method has already been used in [9] for periodic media made of the mixture of two materials, whose macroscopic behaviours are described by first-gradient models. In the present paper, we are interested in the synthesis of periodic media, which feature significant strain-gradient effects.

Thus, we use the topological derivatives of the related higher-order homogenized tensors which were derived in [15], in order to tackle numerically the problem. The synthesis of periodic media is made by optimizing the distribution of the two materials, in Ω and $\mathcal{Y} \setminus \bar{\Omega}$, composing the unit cell \mathcal{Y} . For this, we optimize the homogenized tensors $C^h(\Omega)$ and $D^h(\Omega)$, carrying respectively the strain and the strain gradient terms in the macroscopic elastic energy, and depending on the

distribution of material. Hence, we numerically investigate the following problem:

$$\min_{\Omega} \left\{ \mathcal{J}(C^h(\Omega), D^h(\Omega)) \right\}, \quad (1.1)$$

where \mathcal{J} is a shape functional depending on Ω through the homogenized tensors. The effective mechanical properties contained in the fourth order tensor $C^h(\Omega)$ are known. However it is not trivial to derive from the higher-order tensor $D^h(\Omega)$ some coefficients being meaningful from a mechanical point of view. The approach we follow in this study is based on some natural characteristic intrinsic lengths defined as square roots of ratios between the components of the homogenized tensors: $(D_{ijklmn}^h(\Omega)/C_{ijlm}^h(\Omega))^{1/2}$. From the point of view of shape and topology optimization the shape functional actually depends on the characteristic function of $\Omega \subset \mathcal{Y}$.

The paper is organized as follows. In Section 2, we start by introducing the framework of microstructure optimization. We present the homogenization scheme, based on the *asymptotic expansion method*, allowing us to define the so-called higher homogenized tensors, which encapsulate information about the macroscopic properties of this material. Then, the topological derivative is presented in Section 3. We describe the topological perturbation of the problem, and recall the topological derivatives of higher-order homogenized tensors which were derived in [23] and [15]. The latter measure how the homogenized tensors change when a small circular inclusion is introduced at the microscale level. In Section 4, we present the gradient type algorithm based on these topological derivatives, that we use in Section 5 in order to investigate the maximization of characteristic lengths, and generate new microstructures featuring strain-gradient effects.

2. HIGHER-ORDER HOMOGENIZED TENSORS FROM THE TWO-SCALE ASYMPTOTIC EXPANSION

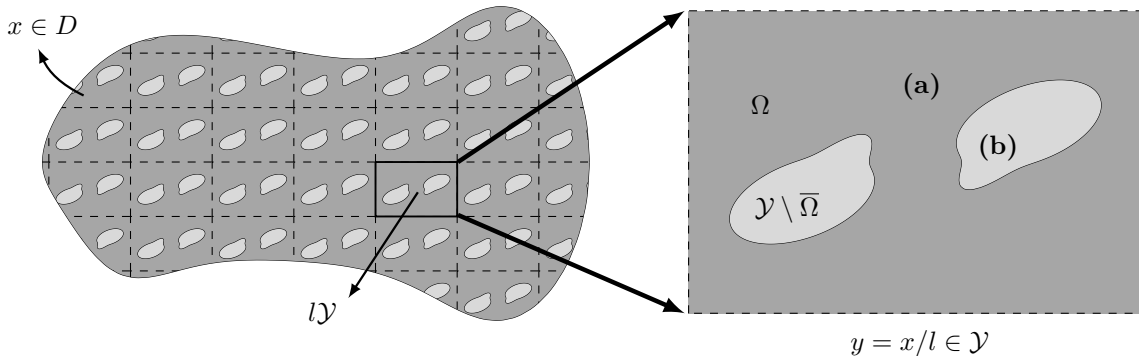


FIGURE 1. The domain D is paved with the unit cell domain \mathcal{Y} , weighted by the length parameter l . The unit cell is composed of two different materials, a stiff material **(a)** and a soft material **(b)**, represented respectively by the domains Ω and $\mathcal{Y} \setminus \bar{\Omega}$.

Let D be a connected bounded regular open subset of \mathbb{R}^2 representing an elastic body having a periodic micro-structure (see Figure 1). We assume that this material is a *first-gradient material*, completely characterized by its *elasticity tensor*.

2.1. The unit cell \mathcal{Y} . Let $\{e_1, e_2\}$ be an orthonormal basis of \mathbb{R}^2 , and

$$\mathcal{Y} = (0, l_1) \times (0, l_2) \quad (2.1)$$

be an open rectangle of \mathbb{R}^2 , for $0 < l_1, l_2$. The open set \mathcal{Y} stands for the *unit cell* of the periodic material. We assume that this unit cell \mathcal{Y} is composed of two different homogeneous and isotropic elastic materials: a stiff material **(a)**, and a soft material **(b)**. The stiff material

occupies an open subset Ω of \mathcal{Y} , and the soft material occupies the complementary domain $\mathcal{Y} \setminus \bar{\Omega}$ in the unit cell (see Figure 1). These two elastic materials are characterized by the same *Poisson's coefficient* ν , and by *Young's moduli* differing from a ratio $0 < \gamma_0 < +\infty$, where γ_0 is called the *contrast* of elastic properties between the two materials. Let C_0 be the constant elasticity tensor describing the stiff elastic material (\mathbf{a}), defined by

$$C_0 = \frac{E}{1 - \nu^2} ((1 - \nu)\mathbb{I} + \nu\mathbf{I} \otimes \mathbf{I}), \quad (2.2)$$

where E is the Young's modulus of the stiff elastic material. The tensor $\mathbf{I} = e_i \otimes e_i$ is the identity second order tensor, and \mathbb{I} the fourth order symmetric identity tensor. They are defined by

$$\mathbf{I}_{ij} = \delta_{ij}, \quad (2.3)$$

$$\mathbb{I}_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \quad (2.4)$$

δ_{ij} being the Kronecker symbol. Then we can write the elasticity tensor characterizing the unit cell \mathcal{Y} . The two phases of material result in a piecewise constant fourth order tensor $C = (C_{ijkl})_{1 \leq i,j,k,l \leq 2}$, which is defined as follows:

$$C(y) := \begin{cases} C_0, & y \in \Omega, \\ \gamma_0 C_0, & y \in \mathcal{Y} \setminus \bar{\Omega}. \end{cases} \quad (2.5)$$

Before going further in the description of the model, we write the convention we use for tensor calculus. Let u and v be two vectors of \mathbb{R}^2 , A and B be two second order tensors of \mathbb{R}^2 , C and D be two third order tensors, E be a fourth order tensor, and F be a sixth order tensor, we write:

$$FC = F_{ijklmn} C_{lmn} e_i \otimes e_j \otimes e_k, \quad EA = E_{ijkl} A_{kl} e_i \otimes e_j, \quad (2.6)$$

$$AB = A_{ik} B_{kj} e_i \otimes e_j, \quad Au = A_{ij} u_j e_i, \quad (2.7)$$

$$C \cdot D = C_{ijk} D_{ijk}, \quad A \cdot B = A_{ij} B_{ij}, \quad (2.8)$$

$$u \cdot v = u_i v_i, \quad (2.9)$$

by using the Einstein summation convention, and where $e_i \otimes e_j$ is a matrix such that $(e_i \otimes e_j)_{kl} = \delta_{ik}\delta_{jl}$. We finally define

$$u \otimes_s v := \frac{u \otimes v + v \otimes u}{2}. \quad (2.10)$$

2.2. The periodic body. We define the elasticity tensor characterizing the elastic body D . Let $0 < l$ be a microscopic length parameter describing the length-scale of the microscopic variations of the elasticity tensor, and let $0 < L$ be a macroscopic length parameter which can be for example defined by $L = \text{diam}(D)$, such that $l \ll L$. We denote by ϵ the scale ratio

$$\epsilon = l/L. \quad (2.11)$$

For convenience, we assume that $L = 1$, and thus $\epsilon = l \ll 1$. Actually, the periodic medium we are interested in, consists of the domain D , which is paved with the *microscopic periodic cell* $\epsilon\mathcal{Y}$ (see Figure 1). Thus we define the elasticity tensor of the periodic material D , depending on the parameter ϵ , as follows:

$$C^\epsilon(x) := C(x/\epsilon), \quad (2.12)$$

where C is defined in (2.5). We notice that the tensor C^ϵ of microscopic moduli does not depend on the macroscale position $Y := x$, but only on the microscale variable $y := x/\epsilon$.

This material is subjected to *body forces* $f \in L^2(D)$, and the *displacement field* $u^\epsilon : D \rightarrow \mathbb{R}^2$, which is the unknown of the problem, is fixed on the boundary ∂D . The displacement vector

field u^ϵ is then given by the solution of the following boundary value problem of linearized elasticity

$$\begin{cases} -\operatorname{div}_x(\sigma_x^\epsilon(u^\epsilon)) = f & \text{in } D, \\ u^\epsilon = 0 & \text{on } \partial D, \end{cases} \quad (2.13)$$

where the second order tensor field $\sigma_x^\epsilon(u^\epsilon)$ is the *stress tensor*, defined throughout the following constitutive stress-strain relation in the linear elastic regime:

$$\sigma_x^\epsilon(u^\epsilon) := \mathbf{C}^\epsilon \varepsilon_x(u^\epsilon), \quad (2.14)$$

$$\varepsilon_x(u^\epsilon) := \nabla_x^s u^\epsilon := \frac{1}{2} \left(\nabla_x(u^\epsilon) + \nabla_x(u^\epsilon)^\top \right), \quad (2.15)$$

where the right lower index of a differential operator denotes the differentiation variable, and where $\varepsilon_x(u^\epsilon)$ is the *linearized strain tensor*.

2.3. The homogenized material and homogenized tensors. The two-scale asymptotic expansion method is used to define the higher-order homogenized tensors. The interested reader can refer to [15] for more details and references.

2.3.1. Second-order truncation, definition of the homogenized tensors. We define

$$y = x/\epsilon \quad \text{and} \quad Y = x, \quad (2.16)$$

respectively the microscopic and macroscopic variables, for all $x \in D$ (see Figure 1). The method relies on an asymptotic expansion of the displacement field with respect to the scale ratio ϵ , by using corrector fields depending on both the macroscopic variable and the microscopic variable. From this, the displacement field is approximated by a truncation of this expansion. In the present case, we consider the following truncation up to the second order of the parameter ϵ :

$$\bar{u}^\epsilon(Y, y) = U(Y) + \epsilon h_{ij}^1(y) E_{ij}(Y) + \epsilon^2 h_{ijk}^2(y) K_{ijk}(Y), \quad (2.17)$$

where $E(Y) = \nabla^s U(Y)$ is the macroscopic strain, and $K(Y) = \nabla E(Y)$ is the corresponding strain-gradient. The displacement corrector fields h_{ij}^1 and h_{ijk}^2 are respectively solutions of the following canonical set of variational problems (see [15]):

$$h_{ij}^1 \in \mathcal{V} : \int_{\mathcal{Y}} \sigma_y(h_{ij}^1) \cdot \varepsilon_y(\eta) + \int_{\mathcal{Y}} \mathbf{C}(e_i \otimes_s e_j) \cdot \varepsilon_y(\eta) = 0, \quad \forall \eta \in \mathcal{W}, \quad (2.18)$$

and

$$h_{ijk}^2 \in \mathcal{V} : \int_{\mathcal{Y}} \sigma_y(h_{ijk}^2) \cdot \varepsilon_y(\eta) + \int_{\mathcal{Y}} \mathbf{C}(h_{ij}^1 \otimes_s e_k) \cdot \varepsilon_y(\eta) = \int_{\mathcal{Y}} (\sigma_y(u_{ij}) - \mathbf{C}^h(e_i \otimes_s e_j)) e_k \cdot \eta, \quad \forall \eta \in \mathcal{W}, \quad (2.19)$$

where u_{ij} and \mathbf{C}^h are respectively given in (2.26) and (2.29) below, $\sigma_y(h_{ij}^1) = \mathbf{C} \varepsilon_y(h_{ij}^1)$, and the spaces \mathcal{W} and \mathcal{V} are defined as follows:

$$\mathcal{W} := H_{\text{per}}^1(\mathcal{Y}; \mathbb{R}^2) / \mathbb{R}, \quad (2.20)$$

$$\mathcal{V} := \left\{ \eta \in H_{\text{per}}^1(\mathcal{Y}; \mathbb{R}^2) : \langle \eta \rangle = 0 \right\}. \quad (2.21)$$

Here for all tensor fields A , we define the *volume averaging* of A

$$\langle A \rangle := \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} A(y) dy, \quad (2.22)$$

where $|\mathcal{Y}|$ denotes the area of the unit cell.

From this, we define the approximated macroscopic energy $\mathcal{E}^h(\bar{u}^\epsilon)$ as being the average of the microscopic elastic energy $\mathcal{E}_\mu(\bar{u}^\epsilon)$ on the unit cell domain \mathcal{Y} defined by

$$\mathcal{E}_\mu(\bar{u}^\epsilon) = \frac{1}{2} \sigma_x(\bar{u}^\epsilon) \cdot \varepsilon_x(\bar{u}^\epsilon), \quad (2.23)$$

so that

$$\mathcal{E}^h(\bar{u}^\epsilon) = \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \frac{1}{2} \sigma_x(\bar{u}^\epsilon) \cdot \varepsilon_x(\bar{u}^\epsilon) dy = \left\langle \frac{1}{2} \sigma_x \cdot \varepsilon_x \right\rangle. \quad (2.24)$$

By calculating the strain tensor induced by \bar{u}^ϵ , we find

$$\varepsilon_x(\bar{u}^\epsilon) = \varepsilon_y(u_{ij}) E_{ij} + \epsilon(h_{ij}^1 \otimes_s e_k + \varepsilon_y(h_{ijk}^2)) K_{ijk} + \epsilon^2(h_{ijk}^2 \otimes_s e_l) \partial_{Y_l} K_{ijk}, \quad (2.25)$$

where u_{ij} is given by

$$u_{ij}(y) := (e_i \otimes_s e_j) y + h_{ij}^1(y). \quad (2.26)$$

Then we can compute $\frac{1}{2} \sigma_x(\bar{u}^\epsilon) \cdot \varepsilon_x(\bar{u}^\epsilon)$, and evaluate the truncated homogenized energy $\mathcal{E}^h(\bar{u}^\epsilon)$ defined by (2.24). The expression of $\mathcal{E}^h(\bar{u}^\epsilon)$ allows to identify the homogenized tensors, which are thus defined as integrals over the cell \mathcal{Y} of products of the y -depending fields from expression (2.25). This gives the following expression

$$2\mathcal{E}^h = E_{ij} C_{ijkl}^h E_{kl} + \epsilon E_{ij} E_{ijpq}^h K_{pqr} + \epsilon^2 (K_{ijk} F_{ijkpqr}^h K_{pqr} + 2E_{ij} G_{ijkpqr}^h \partial_{Y_k} K_{pqr}) + o(\epsilon^2), \quad (2.27)$$

in which C^h , E^h , F^h and G^h are so-called homogenized tensors. The energy depends on the gradient of the strain-gradient ∇K at order ϵ^2 . In order to only deal with strain-gradient coupling effects, it is necessary to perform a macroscopic integration by part to transform the coupled terms $E_{ij} \partial_{y_k} K_{pqr}$ into $K_{ijk} K_{pqr}$. By doing this, we only consider the bulk of the material D , and we do not take into account the boundary terms (see [19]). As a result, the truncated homogenized energy can be written as

$$\mathcal{E}^h = \frac{1}{2} E_{ij} C_{ijkl}^h E_{kl} + \epsilon E_{ij} E_{ijpq}^h K_{pqr} + \epsilon^2 \frac{1}{2} K_{ijk} D_{ijkpqr}^h K_{pqr} + o(\epsilon^2), \quad (2.28)$$

where $D^h = F^h - 2G^h$. In particular, we focus on the optimization of functionals depending only on the fourth order tensor $C^h = (C_{ijkl}^h)_{1 \leq i,j,k,l \leq 2}$, and the sixth order tensor $D^h = (D_{ijkpqr}^h)_{1 \leq i,j,k,p,q,r \leq 2}$, which are defined from (2.25), (2.24) and (2.28), and respectively given in index format by

$$C_{ijkl}^h := \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \sigma_y(u_{ij}) \cdot \varepsilon_y(u_{kl}) = \langle \sigma_y(u_{ij}) \cdot \varepsilon_y(u_{kl}) \rangle, \quad (2.29)$$

and

$$\begin{aligned} D_{ijkpqr}^h &:= \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} C(h_{ij}^1 \otimes_s e_k + \varepsilon_y(h_{ijk}^2)) \cdot (h_{pq}^1 \otimes_s e_r + \varepsilon_y(h_{pqr}^2)) \\ &\quad - \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \left(\sigma_y(u_{ij}) \cdot (h_{pqr}^2 \otimes_s e_k) + \sigma_y(u_{pq}) \cdot (h_{ijk}^2 \otimes_s e_r) \right) \\ &:= \left\langle C(h_{ij}^1 \otimes_s e_k + \varepsilon_y(h_{ijk}^2)) \cdot (h_{pq}^1 \otimes_s e_r + \varepsilon_y(h_{pqr}^2)) \right\rangle \\ &\quad - \left\langle \left(\sigma_y(u_{ij}) \cdot (h_{pqr}^2 \otimes_s e_k) + \sigma_y(u_{pq}) \cdot (h_{ijk}^2 \otimes_s e_r) \right) \right\rangle. \end{aligned} \quad (2.30)$$

3. TOPOLOGICAL SENSITIVITY

So far, we have defined the homogenized tensors C^h , and D^h . We are now interested in the optimization of the topology of the unit cell composing a periodic body, in order to improve some of its macroscopic properties by using the topological derivative method. We refer to the books [31], and [30] for a comprehensive introduction on the subject. For practical use and future investigations, we mention that the topological sensitivities of the homogenized tensors E^h , F^h and G^h were also computed in [16].

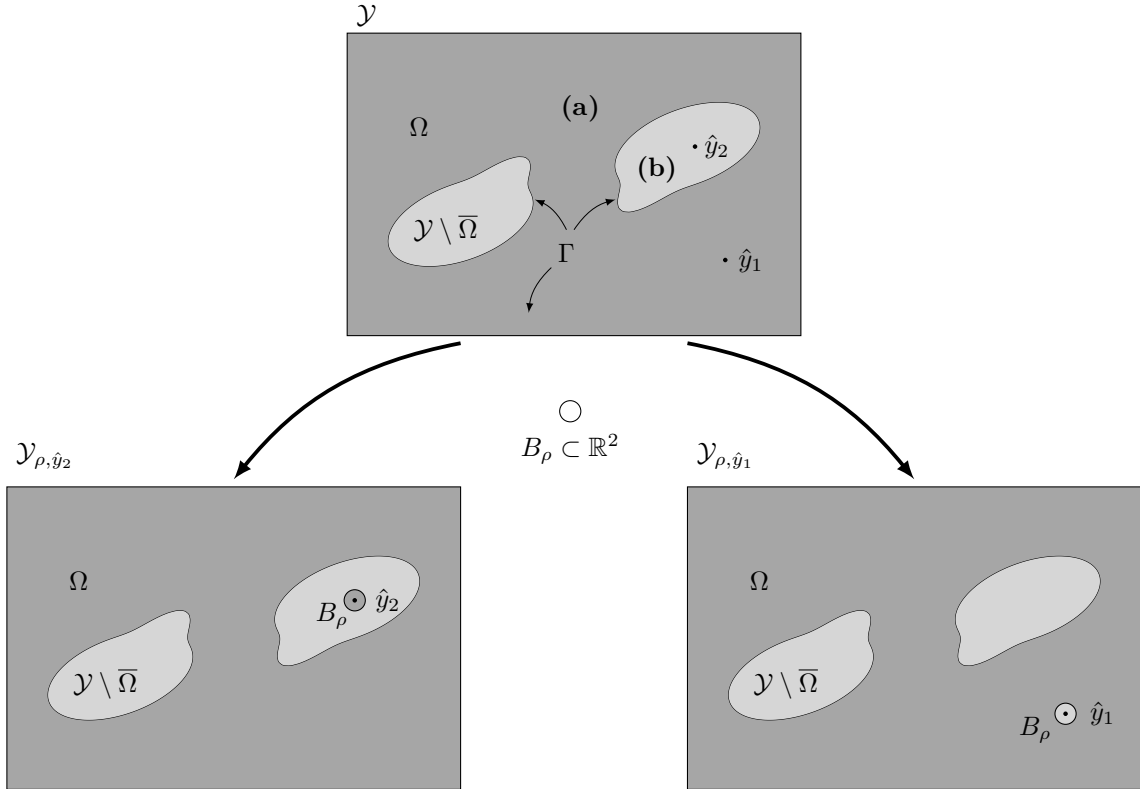


FIGURE 2. Introduction of an inclusion centered at \hat{y}_1 or \hat{y}_2 into the domains Ω or $\mathcal{Y} \setminus \bar{\Omega}$ respectively. The resulting domains are denoted by $\mathcal{Y}_{\rho, \hat{y}_1}$ and $\mathcal{Y}_{\rho, \hat{y}_2}$.

3.1. Perturbation of the unit cell. We consider the unit cell of a periodic material \mathcal{Y} , which is made of a mixture of two materials, defined in Section 2.1. From there, \mathcal{Y} is subjected to a perturbation confined in a small circular open set $B_\rho(\hat{y})$ of radius ρ and centered at an arbitrary point \hat{y} of \mathcal{Y} , such that its closure is included in \mathcal{Y} , and which does not touch the interface Γ (see Figure 2). Then, the region occupied by $B_\rho(\hat{y})$ is filled by an inclusion with different material property from the background. The material properties of the perturbed domain are characterized by the piecewise constant function γ_ρ of the form

$$\gamma_\rho(x) := \begin{cases} 1 & \text{if } x \in \mathcal{Y} \setminus \bar{B}_\rho, \\ \gamma(x) & \text{if } x \in B_\rho, \end{cases} \quad (3.1)$$

where

$$\gamma(x) := \begin{cases} \gamma_0 & \text{if } x \in \Omega, \\ \gamma_0^{-1} & \text{if } x \in \mathcal{Y} \setminus \bar{\Omega}. \end{cases} \quad (3.2)$$

Namely we introduce either a small ball of soft material into the stiff one, or a small ball of stiff material into the soft one. Finally the elasticity tensor is given by $\gamma_\rho \mathbf{C}$ in the perturbed domain.

The topologically perturbed counterparts of problems (2.18) and (2.19) are respectively given by

$$h_{ij}^{1,\rho} \in \mathcal{V} : \int_{\mathcal{Y}} \gamma_\rho \sigma(h_{ij}^{1,\rho}) \cdot \varepsilon(\eta) = - \int_{\mathcal{Y}} \gamma_\rho \mathbf{C}(\mathbf{e}_i \otimes_s \mathbf{e}_j) \cdot \varepsilon(\eta), \quad \forall \eta \in \mathcal{W}, \quad (3.3)$$

and

$$h_{ijk}^2 \in \mathcal{V} : \int_{\mathcal{Y}} \gamma_\rho \sigma(h_{ijk}^2) \cdot \varepsilon(\eta) = - \int_{\mathcal{Y}} \gamma_\rho \mathbf{C}(h_{ij}^1 \otimes_s \mathbf{e}_k) \cdot \varepsilon(\eta) + \int_{\mathcal{Y}} (\gamma_\rho \sigma(u_{ij}^\rho) - \mathbf{C}_\rho^h(\mathbf{e}_i \otimes_s \mathbf{e}_j)) \mathbf{e}_k \cdot \eta \quad \forall \eta \in \mathcal{W}, \quad (3.4)$$

where from now on we leave the lower indices of differential operators behind. As we did in Section 2, we can define the topologically perturbed counterparts of the homogenized tensors, denoted as \mathbf{C}_ρ^h , and \mathbf{D}_ρ^h . By setting

$$u_{ij}^\rho := (\mathbf{e}_i \otimes_s \mathbf{e}_j)y + h_{ij}^1 \rho, \quad (3.5)$$

we have

$$(\mathbf{C}_\rho^h)_{ijkl} = \left\langle \gamma_\rho \sigma(u_{ij}^\rho) \cdot \varepsilon(u_{kl}^\rho) \right\rangle, \quad (3.6)$$

$$\begin{aligned} (\mathbf{D}_\rho^h)_{ijkpqr} &= \left\langle \gamma_\rho \mathbf{C}(h_{ij}^1 \otimes_s \mathbf{e}_k + \varepsilon(h_{ijk}^2)) \cdot (h_{pq}^1 \otimes_s \mathbf{e}_r) \right\rangle \\ &\quad - \left\langle (\mathbf{C}_\rho^h(\mathbf{e}_i \otimes_s \mathbf{e}_j) \cdot (h_{pqr}^2 \otimes_s \mathbf{e}_k) + \gamma_\rho \sigma(u_{pq}^\rho) \cdot (h_{ijk}^2 \otimes_s \mathbf{e}_r)) \right\rangle. \end{aligned} \quad (3.7)$$

From there, we denote by \mathcal{H} any homogenized tensor we are interested in, namely \mathbf{C}^h or \mathbf{D}^h . We assume that the following topological asymptotic expansion holds true

$$\mathcal{H}_\rho = \mathcal{H} + g(\rho) D_T \mathcal{H}(\hat{y}) + o(g(\rho)), \quad (3.8)$$

where g is a positive function, such that $g(\rho) \rightarrow 0$ with $\rho \rightarrow 0$. Then the function

$$\hat{y} \in \mathcal{O} \longmapsto D_T \mathcal{H}(\hat{y}) \quad (3.9)$$

is called the *topological derivative* of \mathcal{H} at \hat{y} .

3.2. Topological derivatives of the homogenized tensors. In this section, we give the rigorous formulas of the topological derivatives of the homogenized elasticity tensors \mathbf{C}^h (see [23]) and \mathbf{D}^h . Unlike for \mathbf{C}^h , the computation of topological derivative of \mathbf{D}^h , requires the introduction of so-called *adjoint states* $p_{ijk}^r \in \mathcal{V}$ for $i, j, k, r \in \{1, 2\}$ (see [15]). For \mathbf{C}^h , the associated problem is self-adjoint, and then no Lagrangian needs to be introduced. But the correctors h^1 and h^2 both involved in the definition of \mathbf{D}^h are solutions of a coupling problem, which leads to the emergence of a Lagrangian and its associated adjoint states.

The topological derivatives of the components of tensors \mathbf{C}^h and \mathbf{D}^h are given by

$$(D_T \mathbf{C}^h)_{ijkl}(\hat{y}) = \mathbb{P} \sigma(u_{ij})(\hat{y}) \cdot \varepsilon(u_{kl})(\hat{y}), \quad (3.10)$$

and

$$\begin{aligned} (D_T \mathbf{D}^h)_{ijkpqr}(\hat{y}) &= \mathbb{P}(\sigma(h_{ijk}^2)(\hat{y}) + \mathbf{C}(h_{ij}^1(\hat{y}) \otimes_s \mathbf{e}_k)) \cdot (\varepsilon(h_{pqr}^2)(\hat{y}) + (h_{pq}^1(\hat{y}) \otimes_s \mathbf{e}_r)) \\ &\quad - \mathbb{P} \sigma(u_{ij})(\hat{y}) \cdot (\varepsilon(p_{pqr}^k)(\hat{y}) + (h_{pqr}^2(\hat{y}) \otimes_s \mathbf{e}_k)) \\ &\quad - \mathbb{P} \sigma(u_{pq})(\hat{y}) \cdot (\varepsilon(p_{ijk}^r)(\hat{y}) + (h_{ijk}^2(\hat{y}) \otimes_s \mathbf{e}_r)), \end{aligned} \quad (3.11)$$

where \hat{y} is the location of the perturbation, u_{ij} is given by (2.26), h_{ij}^1 and h_{ijk}^2 are solutions to the set of canonical variational problems (2.18) and (2.19), p_{ijk}^r are the associated adjoint states, solutions of the following set of variational problems:

$$\begin{aligned} p_{pqr}^k \in \mathcal{V} : \int_{\mathcal{Y}} \sigma(p_{pqr}^k) \cdot \varepsilon(\eta) &= \int_{\mathcal{Y}} (\sigma(\tilde{u}_{pqr}) + \mathbf{C}(\tilde{u}_{pq} \otimes_s \mathbf{e}_r)) \cdot (\eta \otimes_s \mathbf{e}_k) - \int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{pqr} \otimes_s \mathbf{e}_k) \cdot \varepsilon(\eta) \\ &\quad - \int_{\mathcal{Y}} \langle \sigma(\tilde{u}_{pqr}) + \mathbf{C}(\tilde{u}_{pq} \otimes_s \mathbf{e}_r) \rangle \cdot (\eta \otimes_s \mathbf{e}_k), \quad \forall \eta \in \mathcal{W}. \end{aligned} \quad (3.12)$$

Here, \mathbb{P} is the polarization tensor defined as

$$\mathbb{P} = -\frac{1-\gamma}{1+\gamma\beta} \left((1+\beta)\mathbb{I} + \frac{1}{2}(\alpha-\beta) \frac{1-\gamma}{1+\gamma\alpha} \mathbf{I} \otimes \mathbf{I} \right), \quad (3.13)$$

where \mathbb{I} and \mathbb{II} are defined in (2.3) and (2.4), and the parameters α and β given by

$$\alpha = \frac{\lambda + \mu}{\mu} \quad \text{and} \quad \beta = \frac{\lambda + 3\mu}{\lambda + \mu}. \quad (3.14)$$

With the topological derivatives of the homogenized tensors C^h and D^h , an optimization procedure can now be set up.

4. GRADIENT TYPE METHOD FOR TOPOLOGICAL OPTIMIZATION

In a general manner, we consider the following minimization problem:

$$\inf_{\Omega} \left\{ \mathcal{J}(\Omega) := j(C^h(\Omega), D^h(\Omega)) \right\}, \quad (4.1)$$

where Ω is the stiff part of the unit cell \mathcal{Y} defined in Section 2, and the shape functional \mathcal{J} is defined from a smooth real-valued map j depending on the homogenized tensors.

4.1. The algorithm. To solve problem (4.1), we use a gradient-type method based on the topological derivative, which was introduced in [8], and used in [9] to tackle optimization problems of functionals depending only on C^h .

4.1.1. Outline of the algorithm. For a complete description of the algorithm, we refer to the pioneering papers [8, 7]. The basic idea is to make use of the topological derivative as a steepest-descent direction, analogously to the methods using the gradient of the cost function in classical optimization. Here we consider, as in Section 3.1, the case where the perturbation of the domain is performed by either the inclusion of a small circular set of material **(a)** into the material **(b)**, or the inclusion of a small circular set of material **(b)** into the material **(a)**. Thus we want to use the following topological asymptotic expansion to implement an optimization procedure:

$$\mathcal{J}(\Omega_{\rho, \hat{y}}) = \mathcal{J}(\Omega) + g(\rho) D_T \mathcal{J}(\Omega)(\hat{y}) + o(g(\rho)). \quad (4.2)$$

This expansion delivers the following necessary local optimality condition for the problem (4.1) under the class of domain perturbations depicted above, which is

$$D_T \mathcal{J}(\Omega)(\hat{y}) \geq 0, \quad \forall \hat{y} \in \Omega \cup (\mathcal{Y} \setminus \bar{\Omega}). \quad (4.3)$$

To take advantage of the optimality condition (4.3), we start representing the distribution of material composing the cell with a level-set function ψ . Namely we have

$$\Omega = \{x \in \mathcal{Y} \mid \psi(x) < 0\}, \quad (4.4)$$

$$\mathcal{Y} \setminus \bar{\Omega} = \{x \in \mathcal{Y} \mid \psi(x) > 0\}, \quad (4.5)$$

$$\Gamma = \{x \in \mathcal{Y} \mid \psi(x) = 0\}. \quad (4.6)$$

Now the idea is somehow to let the topological derivative $D_T \mathcal{J}(\Omega)$ plays the role of a “target level-set”. Indeed, by defining a new signed topological derivative g_{Ω}^T as follows:

$$g_{\Omega}^T(\hat{y}) = \begin{cases} -D_T \mathcal{J}(\Omega)(\hat{y}) & \text{if } \hat{y} \in \Omega, \\ +D_T \mathcal{J}(\Omega)(\hat{y}) & \text{if } \hat{y} \in \mathcal{Y} \setminus \bar{\Omega}, \end{cases} \quad (4.7)$$

we can rewrite the optimality condition (4.3) as being equivalent to the collinearity between the level-set ψ and the signed topological derivative g_{Ω}^T . Thus the optimality condition becomes

$$\exists c > 0, \quad \psi = c g_{\Omega}^T. \quad (4.8)$$

The distribution defined by the level-set ψ remains unchanged when we multiply it by a positive scalar. We can therefore normalize in L^2 norm both ψ and g_{Ω}^T without changing the procedure. From now we consider that $\|\psi\|_{L^2(\mathcal{Y})} = 1$ and $\|g_{\Omega}^T\|_{L^2(\mathcal{Y})} = 1$. In order to control and drive the collinearity between this two fields, we choose to use θ the non orienting angle between them

$$\theta = \arccos(\langle g_{\Omega}^T, \psi \rangle_{L^2(\mathcal{Y})}). \quad (4.9)$$

For achieving the optimality condition, we make the level-set evolve “in the direction” of the topological derivative by rotating it of an angle $\kappa\theta$ in the plane $\text{span}\{\psi, g_{\Omega}^T\}$, where $\kappa \in [0, 1]$

plays the role of a step size. We denote by $C_{\kappa,\theta}(\psi)$ the result of this rotation, which is a linear combination of ψ and g_Ω^T given by (see [8])

$$C_{\kappa,\theta}(\psi) = \frac{1}{\sin \theta} \left(\sin((1 - \kappa)\theta)\psi + \sin(\kappa\theta)g_\Omega^T \right). \quad (4.10)$$

Thus the evolution of the level-set will follow the fixed point procedure $\psi = C_{\kappa,\theta}(\psi)$. The procedure is summarized in the following steps (see [7] for more details).

- Choose an initial level-set ψ_0 and an initial step size κ_0 .
- While the optimality condition (4.8) is not satisfied: iterate on $n \geq 0$
 - calculate the associated topological derivative g_n^T
 - update the level-set function within a line search

$$\psi_{n+1} = C_{\kappa_n,\theta_n}(\psi_n). \quad (4.11)$$

The step size κ_n is adapted in order to make sure that the level-set follows a descent direction: $\mathcal{J}(\Omega_{n+1}) < \mathcal{J}(\Omega_n)$, where $\Omega_{n+1} := \{\psi_{n+1} < 0\}$. Thus, the step size is decreased if the criterion is not improved.

We recall that our topological optimization problem depends on the homogenized tensors, for which we gave explicit formulas of the topological derivatives, and we made in the previous section the assumption that j in (4.1) is smooth. Thus we directly have the exact topological derivative of the shape functional \mathcal{J} given by the chain rule

$$D_T \mathcal{J}(\Omega) = \left\langle D_1 j, D_T C_\Omega^h \right\rangle + \left\langle D_2 j, D_T D_\Omega^h \right\rangle. \quad (4.12)$$

4.1.2. Numerical computation of the topological derivatives. As we saw in the previous sections, in order to calculate the homogenized tensors and the topological derivatives of the homogenized tensors, we need to solve auxiliary boundary value problems defined on the cell, giving the first and second order correctors and the adjoint states.

We solve these problems and implement the optimization procedure in a *Matlab* code, for a computation of the fields by a Finite Element (FE) discretization. This code was implemented for the first-order homogenization and optimization of C^h in [9]. For the present article, we have added the higher-order homogenization scheme, in order to compute the higher-order homogenization tensor, together with its topological derivative.

The design variable is the level-set ψ . For the discretization, we select a mesh \mathcal{M}_h , and we use P_1 elements. The numerical level-set ψ is defined by its nodal values. From this we define the field γ characterizing the distribution setting $\gamma = 1$ on the nodes for which the level-set $\psi < 0$, and $\gamma = \gamma_0$ on the nodes where $\psi \geq 0$. At this stage, the contrast field γ is defined by its nodal values. Then by linear interpolation from the nodes to the centers of the triangles, we calculate a contrast field which is constant on each triangle. The periodic boundary conditions imposed for the vector fields is ensured by a procedure described in [24]. The solutions of approximated auxiliary problems (i.e. correctors and adjoint states) are computed and take their values on the nodes, while their gradients are constant on each triangular element. The homogenized tensors and their topological derivatives depend on the contrast field, and on the correctors, the adjoint states and their gradients. Thus we also interpolate the correctors and adjoint states from the nodes to the centers of the triangular elements.

4.2. Settings of the numerical study. The sequence of domains $(\Omega_n)_{n \geq 0}$ produced by the optimization process are defined by $\Omega_n = \{\psi_n < 0\}$ and $\mathcal{Y} \setminus \overline{\Omega_n} = \{\psi_n > 0\}$, where ψ_n is the level-set at the step n , and where the cell is the unit square

$$\mathcal{Y} := (0, 1) \times (0, 1). \quad (4.13)$$

Both domains are characterized by the same Poisson coefficient

$$\nu := 0.3 \quad (4.14)$$

and by Young's moduli which differ from a contrast $\gamma_0 = 0.01$, that is

$$E_{\{\psi < 0\}} = 1, \quad (4.15)$$

$$E_{\{\psi > 0\}} = 0.01. \quad (4.16)$$

Except when specified, the initial step size κ_0 is taken equal to 1, and the initial distribution $\Gamma_0 = \{x \in \mathcal{Y} \mid \psi_0(x) = 0\}$ that we consider is a disk (see Figure 3).

The procedure is sensitive to the initialization. It depends both on the size of the mesh and on the initial shape Γ_0 , and can converge to different local solutions. Indeed the minimization problems we tackle numerically are not well-posed. They can have several local minima, and may not even have global minimum. However we will see in Section 5.2.1 that algorithm encounters a form of stability with respect to the initial data. We start with a rather coarse mesh, so that we can reach rapidly but not precisely a local minimum, and then we refine the mesh. The mesh we choose is made with structured triangles (see Figure 3). We divide the cell \mathcal{Y} with n_i^2 squares crossed by their diagonals, giving $4n_i^2$ triangles elements. When a *homogeneous refinement* is performed, each triangle element is subdivided into four triangle elements of the same area. When a *local refinement* is performed, only the elements on which the topological derivative is high are subdivided, and the threshold is empirically set at 75% of the maximum value of the topological derivative. Now we present in the following and last section the optimization problems we have investigated.

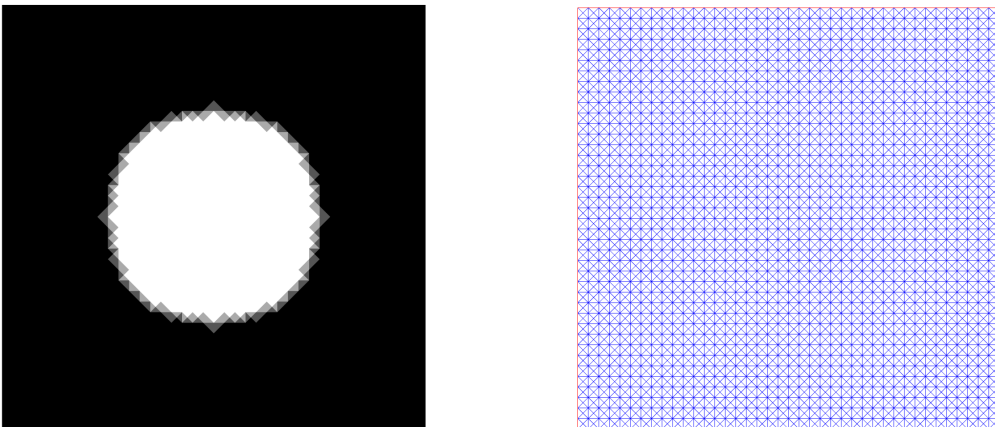


FIGURE 3. Initial black (stiff material) and white (soft material) distribution on the left, and initial mesh on the right, both given for a number of squares $n_i = 40$ along one side of \mathcal{Y} .

5. OPTIMIZED MICROSTRUCTURES

After having made a state of the art of the results we need, we now present their application to the synthesis of microstructures featuring strain-gradient effects. We start by defining in Section 5.1 the characteristic lengths on which relies the optimization procedure. Then different shape functionals are investigated in Sections 5.2 to 5.4, as well as a study of the convergence and the sensitivity to the initialization of the optimization procedure. Finally, the optimized microstructures are evaluated for a large material property contrast in Section 5.5.

5.1. Strain-gradient characteristic lengths. A second-gradient model having a macroscopic strain energy given by (2.28) contains some intrinsic characteristic lengths. Indeed, by considering a strain tensor E , and a vector $e \in \mathbb{R}^2$, we can define an intrinsic characteristic length as

follows:

$$l_{E,e} = \sqrt{\frac{(E \otimes e) \cdot D^h(E \otimes e)}{E \cdot C^h E}}, \quad (5.1)$$

which can be interpreted as a measure of the sensitivity of the material to a variation of the strain E in the direction e : $K = E \otimes e$. If a microstructure leads to a strain-gradient homogenized model, then the characteristic length measures the relative weight of C^h and D^h in the energy.

From now on, we fix a coordinate frame $\{e_1, e_2\}$ of \mathbb{R}^2 , and we consider that the optimization problems of strain-gradient effects are done relatively to this frame. From there, we consider the unit strains of uniaxial extension $E^{11} = e_1 \otimes e_1$, and $E^{22} = e_2 \otimes e_2$, and of pure shear $E^{12} = e_1 \otimes_s e_2$, and their variations in the directions e_1 and e_2 . This gives the following definition of the six different arising characteristic lengths:

$$\begin{aligned} l_{111} &= \sqrt{\frac{D_{111111}^h}{C_{1111}^h}}, & l_{221} &= \sqrt{\frac{D_{221221}^h}{C_{2222}^h}}, & l_{121} &= \sqrt{\frac{D_{121121}^h}{C_{1212}^h}}, \\ l_{112} &= \sqrt{\frac{D_{112112}^h}{C_{1111}^h}}, & l_{222} &= \sqrt{\frac{D_{222222}^h}{C_{2222}^h}}, & l_{122} &= \sqrt{\frac{D_{122122}^h}{C_{1212}^h}}. \end{aligned} \quad (5.2)$$

From this, we intend to maximize these characteristic lengths. Indeed, by maximizing these ratios, we force some components of the tensor C^h to be small, and even close to zero. In this case we obtain some zero strain energy modes, also called *floppy modes* [19], corresponding to this apparition of a kernel for C^h . Then, for strains belonging to this kernel, the strain-gradient elastic energy weighted by ϵ^2 and depending on D^h becomes more significant than the classical first-gradient energy depending on C^h in the energy (2.28). Namely, we numerically maximize the strain-gradient energy while minimizing the first-gradient energy relatively to some strain modes.

It is worth to note that in the case of a centrosymmetric unit cell, the odd order coupling tensor E^h between E and K vanishes (see [39]). As we choose centrosymmetric initial unit cells, it turns out that the optimized unit cells we obtain are also centrosymmetric, even if nothing enforces this symmetry. This very interesting conservation could indicate that a break in the centrosymmetry of the microstructure does not improve the considered functionals.

In addition, we want to observe the effects of a gradient of deformation throughout several cells. It means that the characteristic lengths need to be of order of several cells, or at least one cell. Indeed, in the expression of the energy, D^h is multiplied by ϵ^2 , and then the characteristic lengths deriving from the energy are given by ϵl_{ijk} . In view of the definition of the cell in (4.13), we wish to have l_{ijk} greater than 1.

In view of the isotropic initial distribution and the square shape of the unit cell (see Figure 3), we first only consider the maximization of l_{111} , l_{112} , and l_{121} , because from a square unit cell, we obtain the same results rotated with a $\pi/2$ angle by respectively maximizing l_{222} , l_{221} , and l_{122} .

Before numerical investigation, we give the values of these characteristic lengths for the initial cell defined in Figure 3, and for a mesh $n_i = 100$:

$$l_{111} \simeq i 0.3655, \quad (5.3)$$

$$l_{112} \simeq i 0.0926, \quad (5.4)$$

$$l_{121} \simeq i 0.0933, \quad (5.5)$$

noting that in each case the lengths are imaginary, because the coefficients D_{111111}^h , D_{121121}^h , and D_{121121}^h are negative. In the following, we are going to maximize the square of these lengths, and we will observe that for each optimized shape that we obtain, the components of D^h will be positive, and thus the optimized lengths will be real lengths. Indeed, it is observed in [19] that for a zero strain energy mode – which we are creating by maximizing the associated characteristic length –, the corresponding part of D^h turns to be positive.

5.2. The horizontal elongation. In [2, 37], the authors study a pantographic beam made of crossed rods connected via perfect junctions. This structure features an extensional floppy mode for a deformation E^{11} and a non zero energy for a gradient in the horizontal deformation K^{111} . This can be seen as $C_{1111}^h = 0$ and $D_{111111}^h > 0$ for the homogenized tensors of the structure. We would like to retrieve this strain-gradient behavior in the framework of continuous materials. Thus, we minimize the functional:

$$j(C^h, D^h) = -\frac{D_{111111}^h}{C_{1111}^h}. \quad (5.6)$$

The mesh is initialized with $n_i = 100$. We have made two local refinements of the mesh at the iterations 20 and 26, before the level-set finally reached an optimum for a total of 29 iterations, with an angle $\theta \simeq 9.30^\circ$. Here are the values of the components of interest for the final distribution:

$$C_{1111}^h \simeq 0.1079, \quad (5.7)$$

$$D_{111111}^h \simeq 0.0183, \quad (5.8)$$

that is

$$l_{111} \simeq 0.4114. \quad (5.9)$$

Surprisingly, despite the simplicity of the functional involved, we obtain in Figure 4 a pantographic like cell (see e.g., [37, 28, 27]). We can see the appearance of junctions that allow a small relative rotation of the stiff parts. For homogeneous deformation E^{11} , the rotations of all the stiff parts are compatible, and we can see on Figure 4 that the structure can extend because of these rotations (the South and North inner junctions are moving away while the East and West junctions are moving closer together). But for a gradient of deformation $K^{111} = e_1 \otimes e_1 \otimes e_1$, the rotations are incompatible, so that this macroscopic deformation mode costs in energy.

It is interesting to note that the junctions of the obtained microstructures play the role of *quasi-mechanism* (see e.g. [27]), meaning that some deformation modes are favored and cost few energy. This can be compared to *mechanisms*, which are perfect deformation modes with zero energy. The appearance of these junctions is common in topological optimization (see e.g., [25] on the amplification of the displacements in a given direction generated by thermal effects). This sometimes reflects the ill-posedness of an optimization problem (for instance the compliance minimization without regularization [5, Section 6.2.1]), and numerically, fractal phenomena appear in the vicinity of these junctions when the mesh is refined. We will see that this is not the case in our finite contrast problem in Section 5.2.3. In addition to these theoretical difficulties, these junctions can give rise to materials that are not manufacturable in practice, but this allows, from a continuous medium model, to bring out a need for mechanism or quasi-mechanism to feature certain mechanical behaviors.

In Figure 4, we also present three total displacement fields of the unit cell, when this latter is subjected either to an homogeneous strain deformation E^{11} , or to a homogeneous strain-gradient deformations K^{111} , or $K^{112} = e_1 \otimes_s e_1 \otimes e_2$. These deformation modes are derived from the expansion (2.17) by choosing suitable fields U , so that respectively $\nabla^s U(y) = e_1 \otimes_s e_1$, $\nabla \nabla^s U(y) = e_1 \otimes_s e_1 \otimes e_1$, and $\nabla \nabla^s U(y) = e_1 \otimes_s e_1 \otimes e_2$. Thus, the corresponding total displacement fields obtained can be respectively given by

$$u^{11}(y) = y_1 e_1 + h_{11}^1(y), \quad (5.10)$$

$$u^{111}(y) = \frac{1}{2} y_1^2 e_1 + h_{11}^1(y) y_1 + h_{111}^2(y), \quad (5.11)$$

$$u^{112}(y) = y_1 y_2 e_1 - \frac{1}{2} y_1^2 e_2 + h_{11}^1(y) y_2 + h_{112}^2(y). \quad (5.12)$$

For each of these deformation modes, the local norm of the corresponding stress fields $\|\sigma\| := (\sum_{i,j=1}^2 \sigma_{ij}^2)^{1/2}$ is represented in logarithmic scale only in the stiff material, and the deformed geometry is displayed with a scale factor for readability.

Remark 1. We emphasize that the functionals considered in this study do not take into account any soft phase volume constraint. Such a constraint was not needed because in the functionals, we impose a competition between the first-gradient and strain-gradient tensors, which avoids a saturation of the cell with only stiff or soft phase. For example, there is a 16.4% decrease in stiff phase volume compared to the initial stiff phase volume for the microstructure obtained in Figure 4, and 7.5% for the microstructure obtained in Figure 9.

Before exploring more functionals, we present the behavior of the optimization procedure with respect to the initialization, the choice of the cell and the mesh convergence.

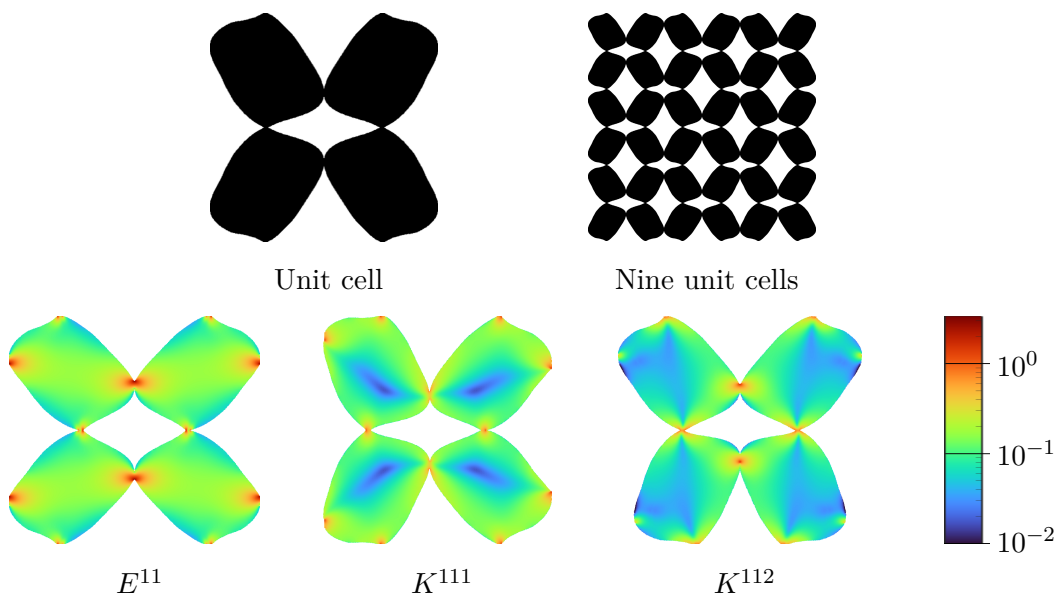


FIGURE 4. Results for the minimization of the cost function (5.6): maximization of the characteristic length l_{111} . From left to right: optimum unit cell; periodic microstructure; deformed geometry for the deformation modes E^{11} , K^{111} , and K^{112} , together with the corresponding local stress norm in logarithmic scale.

5.2.1. *Sensitivity to the initial guess and mesh.* First we investigate the effect of the initial level-set and of the initial mesh on the convergence of the algorithm. For this we consider the problem of minimization of the functional defined in (5.6), for several perturbations of the initial level-set in Figure 3. For all j in $\{-4, -3, \dots, 3, 4\}$ we consider the new initial level-set functions

$$\psi_{0,j} := \psi_0 + 0.05j. \quad (5.13)$$

At the same time we also consider, for each of these initial level-set functions, different initial meshes. Namely n_i varies in $\{40, 60, 80, 100, 120, 140\}$. The final resulting distributions are gathered in Figure 5.

As expected, the optimization procedure is sensitive to initial data, and both the initial level-set and the initial mesh influence the final result. Nevertheless, Figure 5 shows some characteristic patterns in the optimized results. In fact we observe that several optimized distributions do look like *pantographic* materials (see Figure 4) such as results (15 – 18), (21 – 24), (27, 28), (42). The result (1) has got also a lot of similar results (sometimes translated half a unit-cell): (3 – 11), (13 – 14), (19), (25), (29, 30), (33, 34), (38), (40, 41), (45 – 47), and (52 – 54). This

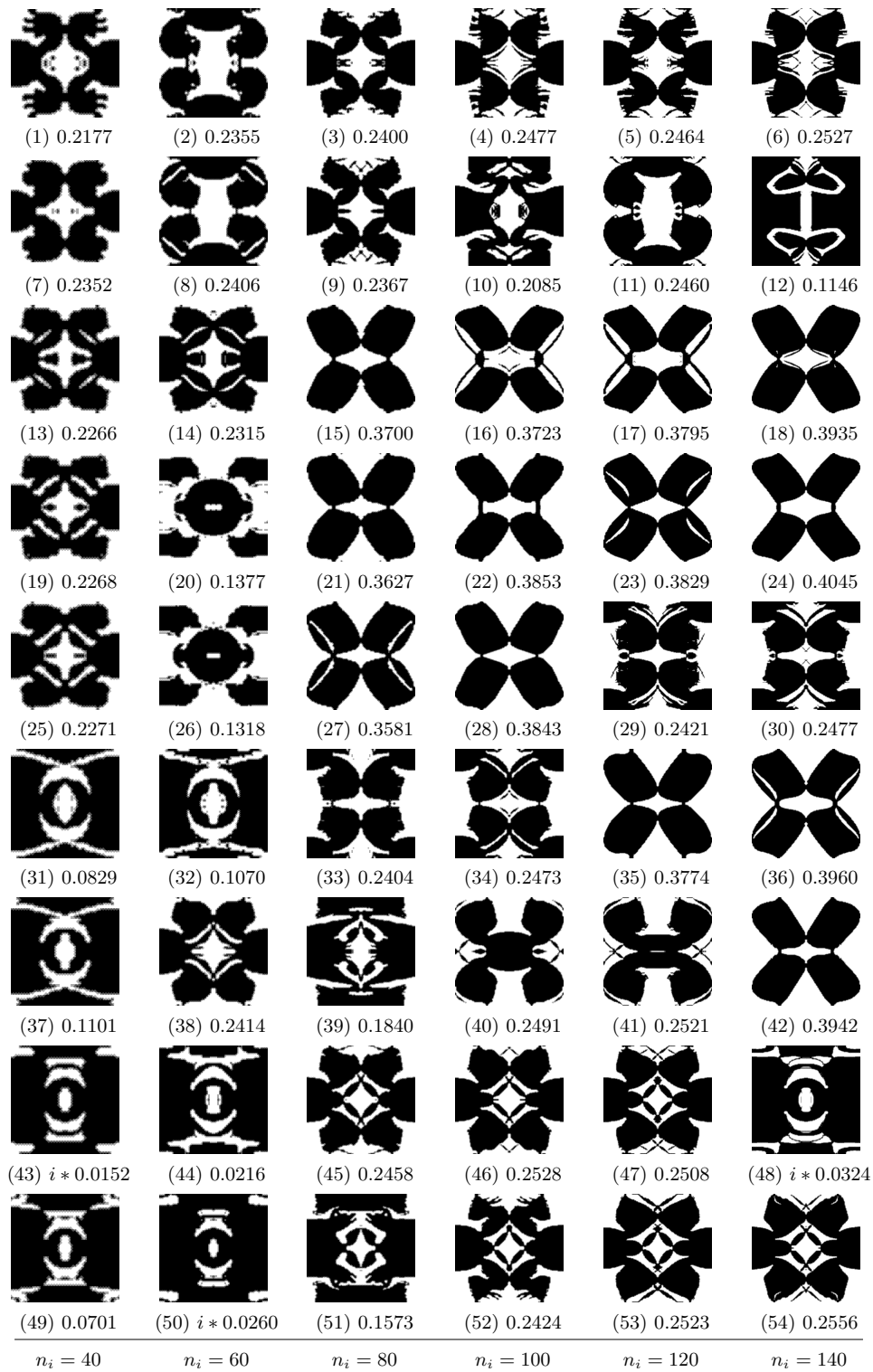


FIGURE 5. Different final level-sets and their corresponding characteristic lengths l_{111} obtained when the initial level-set and the size of the initial mesh vary. Each line from the top to the bottom is obtained for the level-sets from $\psi_{0,-4}$ to $\psi_{0,4}$ defined in (5.13). Each column corresponds to different mesh sizes.

indicates a kind of stability of the topological optimization procedure for the present functional.

Furthermore, even by changing the initial shape of the distribution (but with the same initial topology) the algorithm produces similar results. For example, still within the maximization of l_{111} , we consider an initial rectangular inclusion of material (see Figure 6 (d)). The final level-set obtained Figure 6 is quite similar to the result (1) from Figure 5. Finally, the microstructures having the best characteristic length l_{111} are actually the pantographic cells, such as the one we obtained in Figure 4.

5.2.2. Position and number of unit cells. It is known that the periodic solutions to the variational problems (2.18) and (2.19) remain unchanged up to a translation when the distribution of material is translated in the unit cell, or when the cell is redefined as the union of several unit cells. Then, from definitions (2.29) and (2.30), the homogenized tensors remain unchanged under such transformations. To observe this property, we consider the unit cells (a), (b) and (c) from Figure 6, with meshes defined by $n_i = 50$ for (a) and (c), and $n_i = 100$ for (b). From this we maximize the length l_{111} . For all the cases (a), (b), and (c), we perform a homogeneous refinement of the mesh at iteration 27, and the final topologies are obtained after a total of 37 iterations, for an final angle $\theta \simeq 5.88^\circ$ every time. The results are presented Figure 6, and show that the topological optimization procedure does not depend on the choice of the cell.

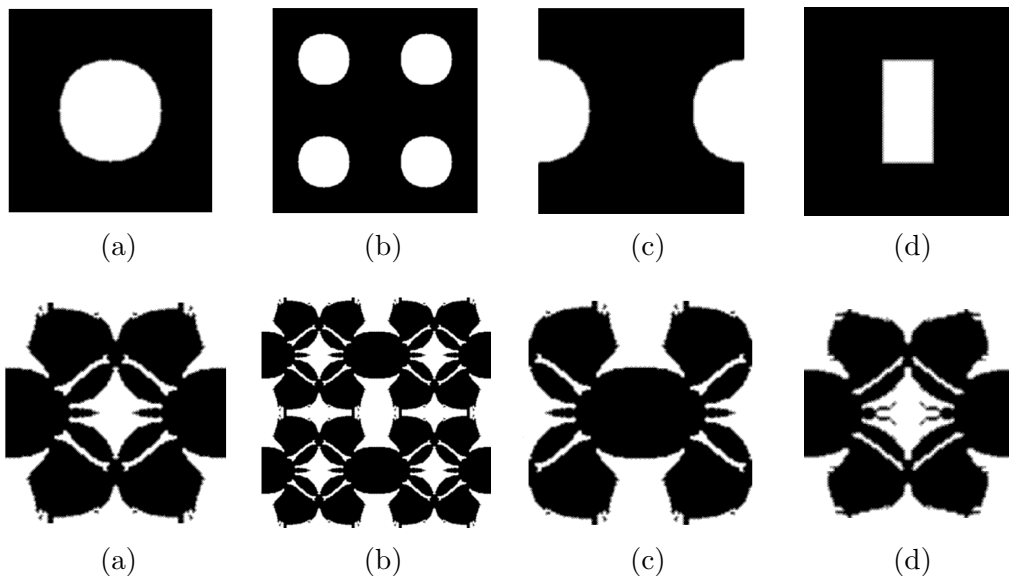


FIGURE 6. Maximization of the characteristic length l_{111} . From left to right: initial distribution; optimized distribution. From left to right: (a) $n_i = 100$, $\mathcal{Y}_a = (0, 1) \times (0, 1)$. (b) $n_i = 200$, $\mathcal{Y}_b = (0, 2) \times (0, 2)$. (c) $n_i = 100$, $\mathcal{Y}_c = (0.5, 1.5) \times (0, 1)$. (d) $n_i = 100$, $\mathcal{Y}_d = (0, 1) \times (0, 1)$.

5.2.3. Mesh convergence. Finally we investigate the algorithm convergence with respect to the mesh. We have seen in the previous paragraphs that the size of the initial mesh can affect the final result, and leads the algorithm to reach a local optimum rather than another. In order to analyse it, we go back to the initial circular level-set, and for an initial mesh characterized by $n_i = 100$. The algorithm converges to the solution that we display once again in Figure 7 (i), for a final angle $\theta \simeq 18.54^\circ$. After the algorithm reached the state (i), we perform a homogeneous refinement of the mesh leading to Figure 7 (ii) for a final angle $\theta \simeq 10.18^\circ$. We repeat the refinements one more time resulting in (iii) for an angle $\theta \simeq 9.08^\circ$.

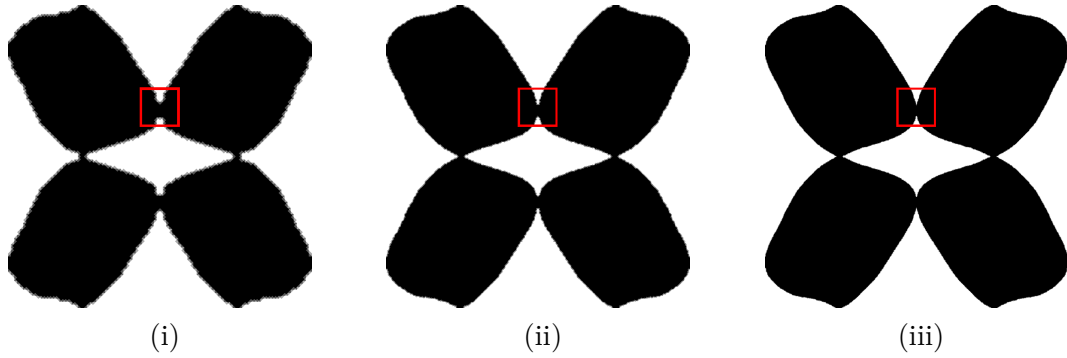


FIGURE 7. Final optimum topologies for the maximization of l_{111} , initial circular level-set, $n_i = 100$. (i) no refinement of the mesh. (ii) one refinement of the mesh. (iii) two refinements of the mesh.

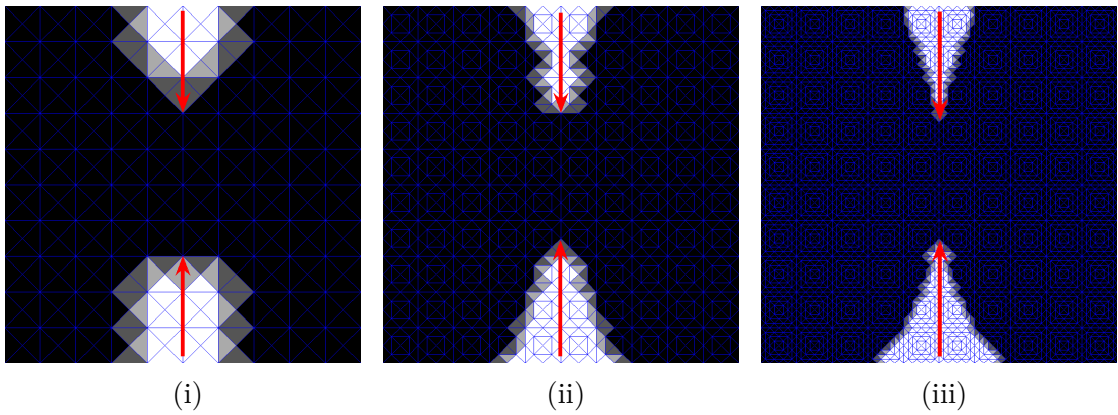


FIGURE 8. Zoom on the junctions surrounded by red rectangles from Figure 7. The new frame is $(0.45, 0.55) \times (0.6, 0.7)$.

Junction regions surrounded by the red rectangles in Figure 7, are displayed with a zoom in Figure 8. We measure the thinnest width between two nodes of black elements in the horizontal junction. The width is $\simeq 0.04$ for (i), $\simeq 0.035$ for (ii), and $\simeq 0.0325$ for (iii). Hence, it seems that the width of this junction is stable when the mesh size goes to zero. Indeed, the small decrease between (i) and (iii) is specific to the resolution: the fineness of the mesh making the measure more accurate.

Let us recall that, this kind of optimization procedure does not always converge with the mesh without a regularization of the optimization problem, such as perimeter or Von-Mises stress constraints. Such regularizations are often used in numerical procedures, and are generally necessary to show the theoretical existence of an optimum. In order to ensure the existence of an optimal domain to (1.1) e.g., the regularization by perimeter of Ω could be used in a proper way [6]. Nevertheless, we emphasize that in the present study we did not use any regularization. As explained in Remark 1, this could be due to the competition we require between the first-gradient and strain-gradient tensors.

5.2.4. *Length: l_{112} .* We are now interested in the effects of the gradient of the horizontal elongation in direction e_2 : K^{112} . In this case, we minimize the following functional:

$$j(C^h, D^h) := -\frac{D_{112112}^h}{C_{1111}^h}. \quad (5.14)$$

The mesh is initialized with $n_i = 100$. After 18 iterations, the level-set reaches almost its final shape, for an angle $\theta \simeq 8.15^\circ$. Then we perform a local refinement of the mesh, and we obtain the final distribution for a total number of iterations of 27, and a final angle $\theta \simeq 5.33^\circ$. Here are the values of the components of interest for the final distribution which is presented in Figure 9:

$$C_{1111}^h \simeq 0.0753, \quad (5.15)$$

$$D_{112112}^h \simeq 0.0034, \quad (5.16)$$

which corresponds to

$$l_{112} \simeq 0.2139. \quad (5.17)$$

The final distribution is made of stiff parts connected by rods. We notice that the deformation mode K^{112} results in high stress levels in comparison to K^{111} . This latter deformation mode can be seen as a bending of the unit cell, which is restrained by the incompatible relative rotations of the stiff parts.

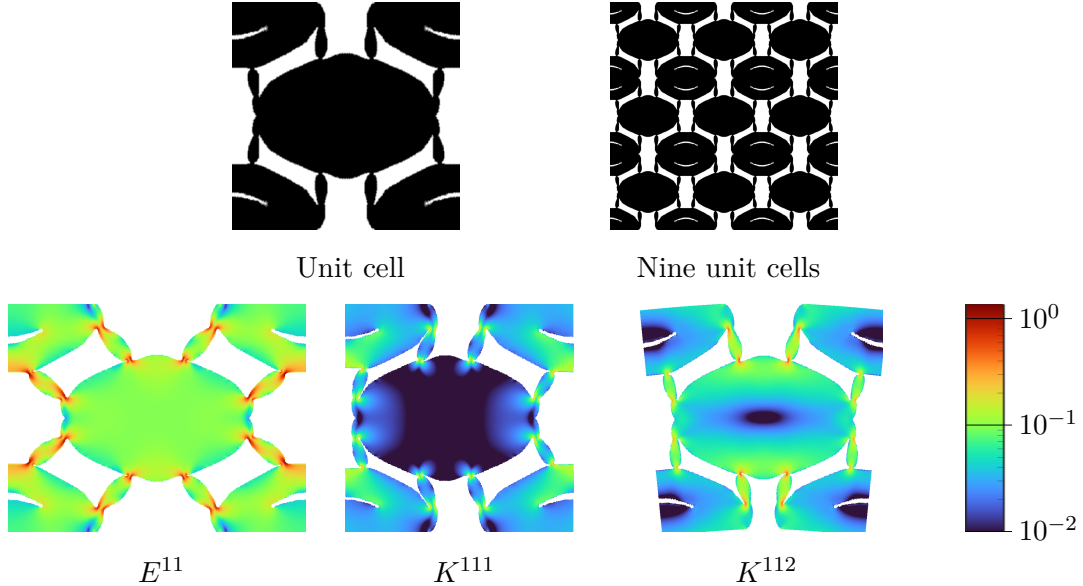


FIGURE 9. Results for the minimization of the cost function (5.14): maximization of the characteristic length l_{112} . From left to right: optimum unit cell; periodic microstructure; deformed geometry for the deformation modes E^{11} , K^{111} , and K^{112} , together with the corresponding local stress norm in logarithmic scale.

5.3. The shear deformation. Now we consider the pure shear deformation E^{12} , and maximize the gradient of pure shear deformation in the horizontal direction e_1 , by means of the following functional:

$$j(C^h, D^h) := -\frac{D_{121121}^h}{C_{1212}^h}. \quad (5.18)$$

The mesh is initialized with $n_i = 100$. The optimum distribution is reached after 17 iterations for an angle $\theta \simeq 0.01^\circ$ (see Figure 10). Here are the values of the component of interest for the final distribution:

$$C_{1212}^h \simeq 0.0250, \quad (5.19)$$

$$D_{121121}^h \simeq 0.0522, \quad (5.20)$$

that is

$$l_{121} \simeq 1.4442. \quad (5.21)$$

It is interesting to observe that we obtain a laminated cell. Indeed, it was shown in [14] that under certain conditions on the asymptotic behavior of material contrast and the volume fraction, a second gradient term – the gradient of the rotation – is appearing in the limit energy of a periodic laminated elastic material, resulting in a Koiter model. The result we obtain seems quite stable: for a change in the initial parameters such as the fineness of the mesh, or for a change in the initial distribution of material, the optimization scheme still leads to a laminated cell. We can observe that the horizontal strip of soft material allows a shear deformation without costing much elastic energy. But the presence of the horizontal beams of stiff material withstands to a horizontal gradient of the shear deformation.

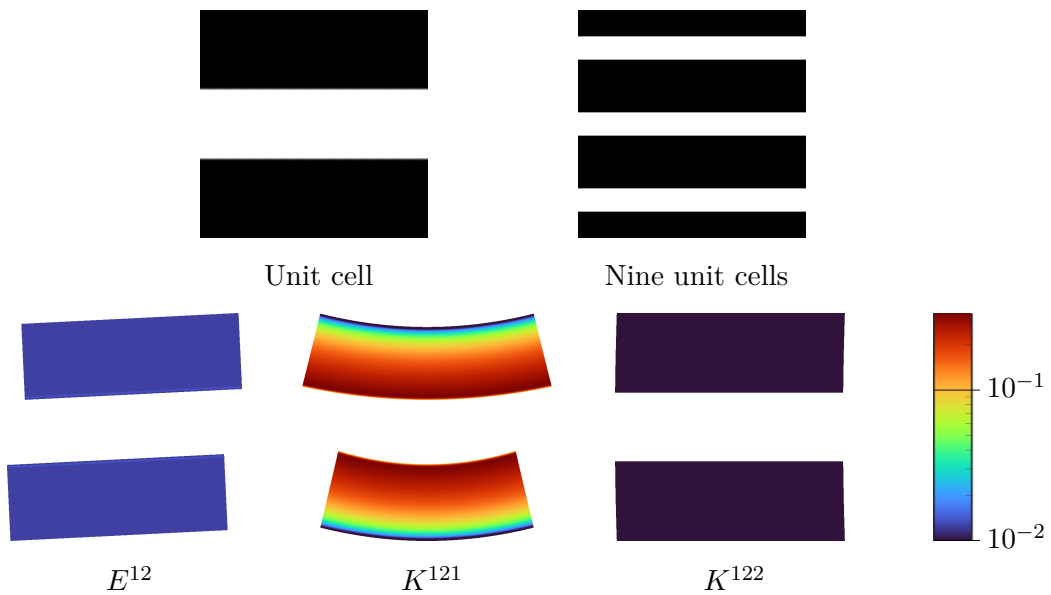


FIGURE 10. Results for the minimization of the cost function (5.18): maximization of the characteristic length l_{121} . From left to right: optimum unit cell; periodic microstructure; deformed geometry for deformation modes E^{12} , K^{121} , and K^{122} , together with the corresponding local stress norm in logarithmic scale.

Now we consider the maximization of both characteristic lengths l_{121} and l_{122} , namely we minimize the following functional:

$$j(C^h, D^h) := -\frac{D_{121121}^h + D_{122122}^h}{C_{1212}^h}. \quad (5.22)$$

The mesh is initialized with $n_i = 60$, and we take an initial step size $\kappa_0 = 0.75$. After a local refinement of the mesh, we obtain the final distribution after 19 iterations, and the final angle is $\theta \simeq 13.16^\circ$. As a result, the microstructure displayed in Figure 11 is composed with stiff parts in the form of discs connected to each other by two rods, and we obtain the following lengths:

$$\sqrt{l_{121}^2 + l_{122}^2} \simeq 0.7285, \quad \text{and} \quad l_{121} = l_{122} \simeq 0.5151. \quad (5.23)$$

We observe that shear deformations are facilitated by the presence of the connected rods which then start to rotate, and allow the stiff parts to move. In this case the stress is concentrated in the junction areas between the connecting rods and the stiff parts. But for a vertical or horizontal gradient of shear deformation, the connected rods are either stretched or compressed, and the stress propagate also in the stiff parts. In addition, we notice that the layout between the stiff parts and the connecting rods allows a small free rotation of the stiff parts.

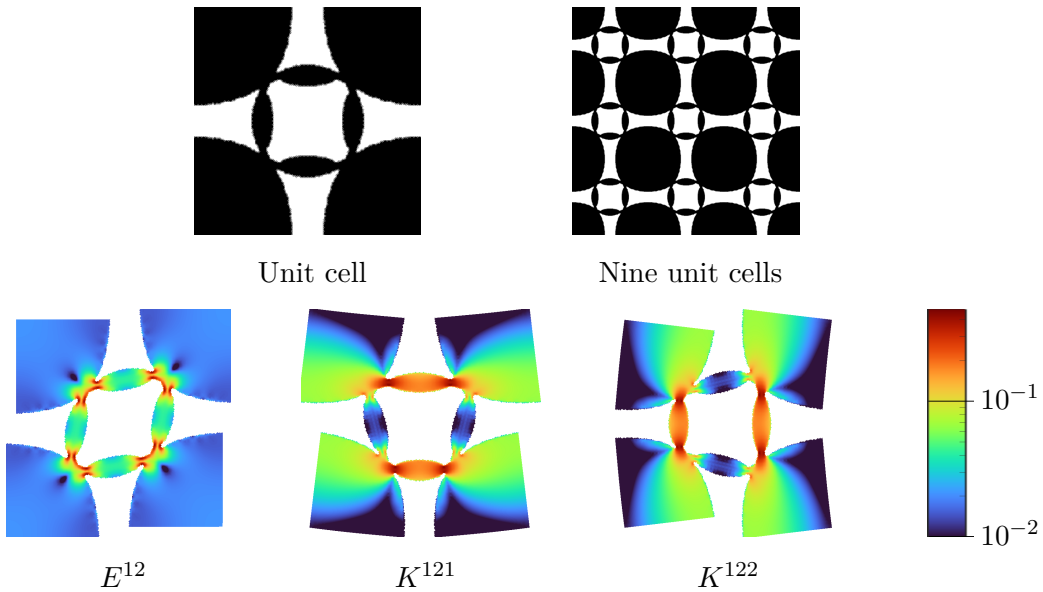


FIGURE 11. Results for the maximization of the cost function (5.22): maximization of the characteristic lengths l_{121} and l_{122} . From left to right: optimum unit cell; periodic microstructure; deformed geometry for the deformation modes E^{12} , K^{121} , and K^{122} , together with the corresponding local stress norm in logarithmic scale.

5.4. Pantographic-like microstructure. A *pantographic continuous material* has been introduced and studied in [19]. It corresponds to a 2-dimensional periodic material constituted with triangles and rhombuses being connected together via thin junctions (Figure 12). Their layout produces the behaviour of a pantographic-like material, which has floppy modes. One in extension E^{11} , and another one in shear E^{12} . Its macroscopic behaviour is described by a strain-gradient model. Surprisingly, we retrieve it through the topological optimization procedure.

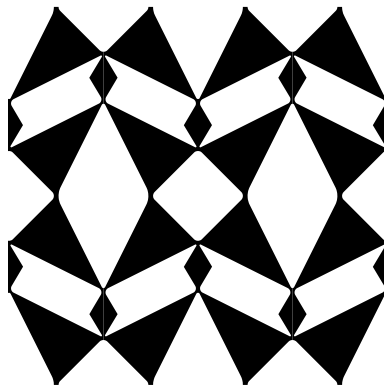


FIGURE 12. Pantograph (Figure from [19]).

For this we consider the rectangular unit cell

$$\mathcal{Y} = (0, 1) \times (0, 2). \quad (5.24)$$

In [19], the characteristic lengths of the pantograph for the unit cell \mathcal{Y} have been evaluated, and l_{111} and l_{112} turn to have significant values. We consider the following functional to be

minimized

$$j(C^h, D^h) = -\frac{D_{111111}^h + D_{112112}^h}{C_{1111}^h}. \quad (5.25)$$

We choose an initial mesh for which the vertical direction of the rectangle is subdivided into $n_i = 120$ crossed squares, and the horizontal direction is subdivided into $n_i = 60$ crossed squares. The initial step size is $\kappa_i = 0.75$. Finally we choose an initial level-set function which results into shifted strips of holes (see Figure 13). After 29 iterations, we perform a homogeneous refinement of the mesh, followed by a local refinement of the mesh after 9 iterations. For a total of 45 iterations, the final angle is $\theta \simeq 5.35^\circ$, and the optimized distribution is shown Figure 13. We finally get

$$l_{111} \simeq 0.2548, \quad l_{112} \simeq 0.4578. \quad (5.26)$$

We can notice that the shape we get in Figure 13 looks very much like the pantograph from Figure 12, for which the triangles are smoothed, the rhombuses are replaced by more elliptic shapes, and some extra connecting rods are present.

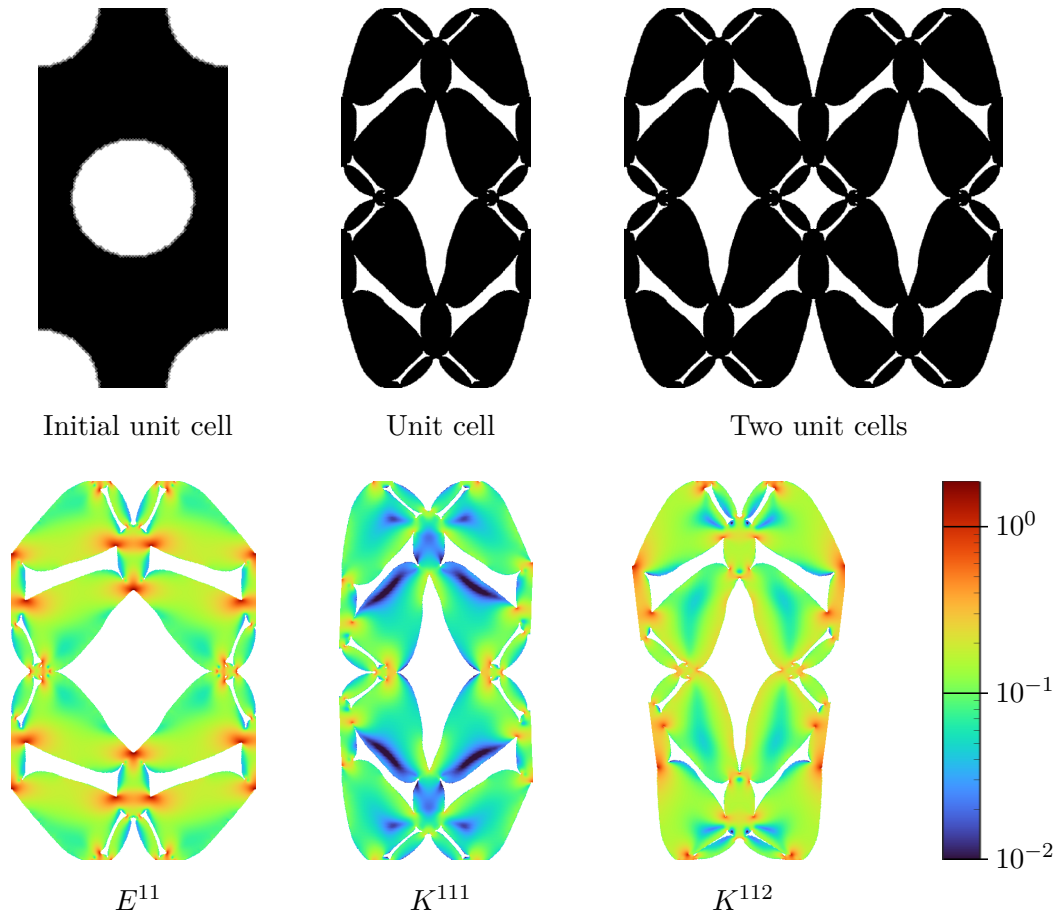


FIGURE 13. Results for the minimization of the cost function (5.25): maximization of the sum $l_{111} + l_{112}$. From left to right: initial unit cell; optimum unit cell; periodic microstructure; deformed geometry for the deformation modes E^{11} , K^{111} , and K^{112} , together with the corresponding local stress norm in logarithmic scale.

5.5. Very large contrast. In the previous sections, we have obtained new interesting microstructures by optimizing different strain-gradient effects. But the strain-gradient behaviour, which is quantified by the characteristic lengths we have introduced, is not very significant.

Except in the case of the laminated cell, we have obtained characteristic lengths between 0.2 and 0.5 times the size of the unit cell. In comparison, the strain-gradient effects observed in [19] are more pronounced. This difference has two possible explanations. First, the computations led in [19] are made in the case where the cell is made up of a stiff material and voids, whereas in the present case, the cell is a mixture of a stiff and soft materials. Secondly, the junction regions of the pantograph in [19] are chosen arbitrarily thin, which brings on the strain-gradient behaviour.

Therefore, we investigate the characteristic lengths of the microstructures we have obtained, assuming the soft material is replaced by voids. We consider the level-set functions ψ obtained after the topological optimization for a contrast $\gamma_0 = 10^{-2}$, and for each of these geometries, we compute for a contrast $\gamma_0 = 10^{-8}$ the homogenized tensors C^h and D^h . For this, we need to change slightly the model for the higher order correctors h_{ijk}^2 . Indeed we can see on equation (2.19) the presence of a body force depending on C^h which is applied homogeneously on the unit cell \mathcal{Y} . When the contrast γ_0 goes to zero, it means that a load is applied on the very weak material. We adopt the approach followed in [19]. Let φ be the normalized characteristic function defined by

$$\varphi(y) := \frac{1}{\int_{\mathcal{Y}} \chi} |\mathcal{Y}| \chi(y), \quad (5.27)$$

where χ is the characteristic function of the stiff material, defined directly from the level-set ψ . The first auxiliary problem (3.3) remains unchanged, because it does not involve any body force, while the second auxiliary problem (3.4) is replaced by

$$h_{ijk}^2 \in \mathcal{V} : \int_{\mathcal{Y}} \sigma(h_{ijk}^2) \cdot \varepsilon(\eta) + \int_{\mathcal{Y}} C(h_{ij}^1 \otimes_s e_k) \cdot \varepsilon(\eta) = \int_{\mathcal{Y}} (\sigma(u_{ij}^p) - \varphi C_{\rho}^h(e_i \otimes_s e_j)) \cdot (\eta \otimes_s e_k) \quad \forall \eta \in \mathcal{W}. \quad (5.28)$$




| | | | | |
|----------------------|--------------------|---|---|---|
| | |  |  |  |
| $\gamma_0 = 10^{-2}$ | l_{111} | 0.4114 | 0.1295 | 0.2548 |
| | l_{112} | 0.3166 | 0.2139 | 0.4578 |
| | C^h eigenvectors | $\begin{bmatrix} -0.19 \\ -0.98 \\ 0.00 \end{bmatrix} \begin{bmatrix} -0.98 \\ 0.19 \\ 0.00 \end{bmatrix} \begin{bmatrix} 0.00 \\ 0.00 \\ 1.00 \end{bmatrix}$ | $\begin{bmatrix} -0.18 \\ -0.98 \\ 0.00 \end{bmatrix} \begin{bmatrix} -0.98 \\ 0.18 \\ 0.00 \end{bmatrix} \begin{bmatrix} 0.00 \\ 0.00 \\ 1.00 \end{bmatrix}$ | $\begin{bmatrix} -0.19 \\ -0.98 \\ 0.00 \end{bmatrix} \begin{bmatrix} -0.98 \\ 0.19 \\ 0.00 \end{bmatrix} \begin{bmatrix} 0.00 \\ 0.00 \\ 1.00 \end{bmatrix}$ |
| | C^h eigenvalues | (0.2615, 0.1022, 0.0800) | (0.2596, 0.0694, 0.0433) | (0.3203, 0.0922, 0.1067) |
| $\gamma_0 = 10^{-8}$ | l_{111} | 1.2607 | 0.1714 | 0.6415 |
| | l_{112} | 1.1039 | 0.5554 | 1.2656 |
| | C^h eigenvectors | $\begin{bmatrix} 1.00 \\ -0.03 \\ 0.00 \end{bmatrix} \begin{bmatrix} -0.03 \\ -1.00 \\ 0.00 \end{bmatrix} \begin{bmatrix} 0.00 \\ 0.00 \\ 1.00 \end{bmatrix}$ | $\begin{bmatrix} -0.06 \\ -1.00 \\ 0.00 \end{bmatrix} \begin{bmatrix} -1.00 \\ 0.06 \\ 0.00 \end{bmatrix} \begin{bmatrix} 0.00 \\ 0.00 \\ 1.00 \end{bmatrix}$ | $\begin{bmatrix} 1.00 \\ -0.06 \\ 0.00 \end{bmatrix} \begin{bmatrix} -0.06 \\ -1.00 \\ 0.00 \end{bmatrix} \begin{bmatrix} 0.00 \\ 0.00 \\ 1.00 \end{bmatrix}$ |
| | C^h eigenvalues | (0.0177, 0.2188, 0.0705) | (0.2032, 0.0103, 0.0099) | (0.0209, 0.2528, 0.0813) |

FIGURE 14. Homogenization results of the previously obtained microstructures with a property contrast $\gamma_0 = 10^{-2}$, and homogenization results for the same microstructures with a new property contrast $\gamma_0 = 10^{-8}$. (I)

Figures 14 and 15 present the values of the characteristic lengths, for each of the microstructures we have obtained, for both the finite contrast $\gamma_0 = 10^{-2}$ of the previous sections and the new very small contrast $\gamma_0 = 10^{-8}$. We observe that for each microstructure, considering



| | | | |
|----------------------|--------------------|---|--|
| | |  |  |
| $\gamma_0 = 10^{-2}$ | l_{121} | 1.4442 | 0.5151 |
| | l_{122} | 0.0099 | 0.5151 |
| | C^h eigenvectors | $\begin{bmatrix} -1.00 \\ -0.02 \\ 0.00 \end{bmatrix} \begin{bmatrix} -0.02 \\ 1.00 \\ 0.00 \end{bmatrix} \begin{bmatrix} 0.00 \\ 0.00 \\ 1.00 \end{bmatrix}$ | $\begin{bmatrix} -0.71 \\ -0.71 \\ 0.00 \end{bmatrix} \begin{bmatrix} -0.71 \\ 0.071 \\ 0.00 \end{bmatrix} \begin{bmatrix} 0.00 \\ 0.00 \\ 1.00 \end{bmatrix}$ |
| | C^h eigenvalues | (0.6998, 0.0356, 0.0125) | (0.2843, 0.2348, 0.0176) |
| $\gamma_0 = 10^{-8}$ | l_{121} | 1472 | 1.3979 |
| | l_{122} | 9.2409 | 1.3979 |
| | C^h eigenvectors | $\begin{bmatrix} -1.00 \\ 0.00 \\ 0.00 \end{bmatrix} \begin{bmatrix} 0.00 \\ 1.00 \\ 0.00 \end{bmatrix} \begin{bmatrix} 0.00 \\ 0.00 \\ 1.00 \end{bmatrix}$ | $\begin{bmatrix} -0.71 \\ -0.71 \\ 0.00 \end{bmatrix} \begin{bmatrix} -0.71 \\ 0.071 \\ 0.00 \end{bmatrix} \begin{bmatrix} 0.00 \\ 0.00 \\ 1.00 \end{bmatrix}$ |
| | C^h eigenvalues | (0.6933, 4.10^{-8} , 1.10^{-8}) | (0.2353, 0.2055, 0.0024) |

FIGURE 15. Homogenization results of the previously obtained microstructures with a property contrast $\gamma_0 = 10^{-2}$, and homogenization results for the same microstructures with a new property contrast $\gamma_0 = 10^{-8}$. (II)

this very small contrast improves significantly the characteristic lengths. For example for the two pantographic structures in Figure 14, the characteristic lengths are multiplied by a factor between 2.5 and 3.5.

Whereas, for a finite contrast $\gamma_0 = 10^{-2}$, C^h eigenvalues remain quite comparable, when the contrast is set to $\gamma_0 = 10^{-8}$ the expected floppy modes clearly emerge. For instance, in Figure 15 column 1, the eigenvalue related to E^{11} significantly drops from $\gamma_0 = 10^{-2}$ to $\gamma_0 = 10^{-8}$ whereas the other eigenvalues are not quite affected. This can be clearly observed in Figure 16, where we can see that E^{11} corresponds to a floppy mode in comparison to the other deformation modes E^{22} and E^{12} . We also observe in this figure that while the stress associated to the deformation mode E^{11} is not significant (and is obviously localized in the thin junctions), stress associated to the deformations modes K^{111} and K^{112} is more significant. Thus the obtained pantographic structure effectively displays strain gradient effects for deformations in the the direction e_1 .

6. CONCLUSION

In the present article, we have numerically optimized strain-gradient effects for two-dimensional periodic material in elastostatics. For this purpose, criteria depending on the homogenized tensors C^h and D^h are optimized, via an optimization method based on the topological derivatives of these homogenized tensors.

We have obtained non trivial microstructures for functionals based on intrinsic characteristic lengths. The latter are defined as a ratio of the components of C^h and D^h . It is worth to notice that these microstructures are obtained by opening the kernel of C^h , so that the strain-gradient terms depending on D^h become predominant in the macroscopic elastic energy. In particular, we have strikingly obtained well known microstructures featuring strain-gradient effects, such as a pantographic unit cell, similar to the one studied in [19]. The convergence with respect to the mesh has been illustrated. Finally, the obtained microstructures has also been homogenized in the case of a large contrast between the stiff and the soft materials and strain-gradient effects were enhanced.

Note that, the homogenization scheme we used may also correctly predict second gradient effects in some situations where the material contrast is infinite (see [19]). Nevertheless, no general result of higher-order homogenization is known in this case (see [14, 26]). Hence, the

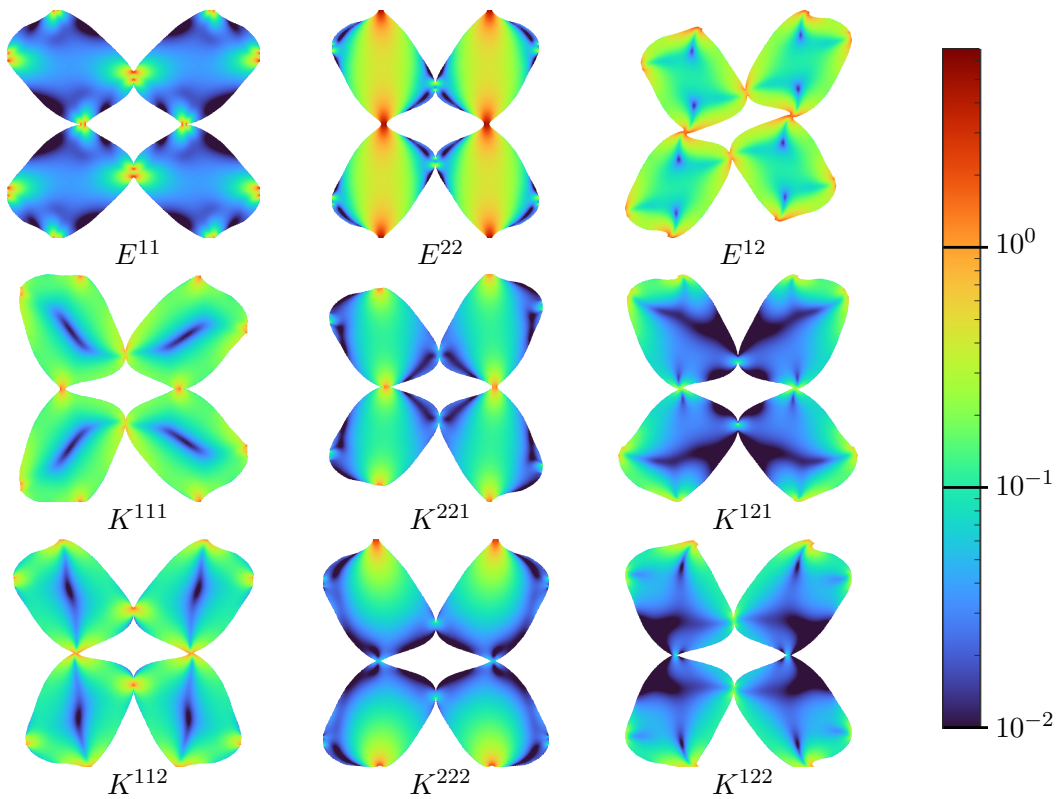


FIGURE 16. Deformed geometry of the pantographic cell obtained in Figure 4, for the deformation modes E^{ij} and K^{ijk} for $i, j, k = 1, 2$. The corresponding total displacement fields are computed in the case where the material contrast is $\gamma_0 = 10^{-8}$, and then the corresponding local stress norms are represented in logarithmic scale.

theoretical study of infinite contrast optimization of higher-order homogenization is also an open problem. As a consequence, it is not surprising that by optimizing second gradient effects defined by this finite contrast homogenization scheme, we could obtain microstructures corresponding to other homogenized models when the contrast is large. For example, the microstructure obtained in Figure 11 can be compared with the square grid with isolated diagonals from [26], case 3. In the referred article, it is numerically shown that a Cosserat model is the most accurate to describe this microstructure, in comparison to the first-gradient model and the second-gradient model, when the material contrast behaves as ϵ^3 , with the size of the cell ϵ going to zero.

To go further in the optimization of strain-gradient effects, two different approaches that we will follow in future works are possible. The first one is to study functionals depending on the invariants of the homogenized tensors. For C^h , these invariants are well-known. For D^h , there exists a very large number of invariants which were computed in [10], and their mechanical understanding is still a subject of study. The second one is to consider functionals depending of the fifth-order tensor E^h of coupling moduli between first and second gradient effects. In the present study, we were not interested in this tensor because it cancels in the case of a centrosymmetric unit cell. But new microstructures could be explored by taking it into account.

Finally, we would like to point out that the case of dimension 3 could be treated in a similar way from a theoretical point of view, although the practical implementation of the optimization procedure as well as the large number of strain-gradient elastic moduli make this task much more complex.

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