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Design of composite structures with extremal elastic properties in the presence of technological constraints

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ABSTRACT

In this paper, composites made of periodically repeating micro structures are investigated. The study aims at identifying the optimal spatial distribution of constituents within a composite material to obtain the material of desired/improved functional properties. To find the relationship between micro- and macro-structural properties of the composite material, the method of homogenization is used. The problem of finding optimal microstructures of various materials, with the aim of obtaining maximum rigidity, i.e., maximum volume and shear modules for the base cell of a composite that contains the original installation of technological holes and/or inclusions was first investigated. For illustration and validation of the proposed approach, numerical examples are provided.

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1. Introduction

It is well known that mechanical properties of composite materials can be improved by modifying the topology of the material microstructure. For instance, an approach based on the structural topology optimization can be employed to find the best space distribution of material phases constituting the composite microstructure. The main idea of designing a microstructure of a composite material having periodic patterns/cells is based on finding optimal distribution of periodic stress-strain fields already on a micro-scale, for a periodic elementary cell, called a base cell. A base cell can be studied with the help of the finite element method, and then a procedure of the topological optimization of this elementary, periodically repeated cell can be investigated instead of studying the whole composite structure. Usually, the method of homogenization is applied in order to average the complex micro structural behavior of an elastic medium to determine the macroscopic properties of a unit cell. The theory of homogenization has been recognized as a rigorous modeling methodology for characterizing the mechanical behavior of cellular materials and composites with periodic microstructures [1–3]. However, for complex microstructures of the elastic medium, analytical determination of the stress/strain fields is extremely difficult. Therefore, to find the most effective properties of the elastic medium, the homogenization procedure is employed by means of numerical approaches like the finite element method (FEM) [4,5].

The inverse problem is to design a new microstructure of the periodic unit cell so that the resulting material has desirable physical properties. The material design concept based on topology optimization and homogenization has been applied to design elastic [6–13] and thermo elastic [14,15] composite materials. A systematic and scientific means of microstructural design is formulated as an optimization problem for the parameters that represent the material properties and topology of the material microstructure.

Over the last two decades, various topology optimization algorithms and interpolation schemes, e.g. solid isotropic material with penalization (SIMP) [16–19], evolutionary structural optimization (ESO) [20], and level set technique [21,22] have been developed. These topology optimization techniques have been used extensively to solve design problems not only for macroscopic structures, but also for microstructures of materials/composites in recent years.

Some attempts have been also made to design new materials with extraordinary physical properties, e.g., extreme thermal conductivity [23] and maximum stiffness and thermal conductivity

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[24], designing a microstructure of functionally graded materials having their physical properties changing along with the gradient distribution of constituents [25].

In the above studies, the optimization was carried out for composites of one or two materials for a homogeneous base cell. In this work, maximization of static stiffness problem for a base cells composite materials, i.e. having maximum bulk modulus or shear modulus, has been considered. The problem of topological optimization for the base cell of the composite containing initially established technological holes and/or inclusions has been first solved. Topological optimization of reinforcing inclusions, embedded in a matrix with desired properties, is carried out only in the area of the base cell not connected with technological restrictions.

2. Definition of the effective elastic tensors of a base cell

The following assumptions are taken while carrying out the investigations: (i) an elastic composite is linear; (ii) the composite is microscopically (transversely) isotropic; (iii) there is a lack of initial stresses; (iv) the inclusions are homogenous, linear elastic, isotropic, and regularly packed; (v) the matrix material is homogenous, linear and isotropic.

Composites made from linear elastic materials are governed by linear equations of elasticity derived for a homogenized base cell.

In the elastic regime, the macroscopic behavior of a unit cell made from an anisotropic material can be characterized by the effective stress tensor $\bar{\sigma}_{ij}$ and the deformation tensor $\bar{\varepsilon}_{ij}$ of a homogenized medium, which are coupled by the so-called effective elasticity tensor C^{eff}_{ijkl} as follows:

$$\bar{\sigma}_{ij} = C^{eff}_{ijkl}\bar{\varepsilon}_{kl}, \tag{1}$$

where C^{eff}_{ijkl} depends on the filler volume fraction and properties of the base cell microstructure. In what follows, a local coordinate system (Y) is introduced with the use of the multiple scale method [1,2] in order to describe rapid changes in the material microstructure properties in the global coordinate system (X). In this method, the solution to the problem is searched in the form of a series of different powers of a small perturbation parameter ε with coefficients depending on variables x_i (called slow or macroscopic) and y_i (fast, microscopic variables). The mentioned series is substituted into the initial system of governing differential equations, and then the system is split into equations standing by the same powers of ε, which yield equations regarding the function u^i. Note that the function u^0 and the coefficients of equations with respect to u^0 are independent of fast variables. Here, a local coordinate y can be taken as a fast coordinate coupled with a slow coordinate x by the ratio $y = x/\varepsilon\,(\varepsilon << 1)$. Displacement of an arbitrary point of an elastic body can be approximated by a two-scale asymptotic expansion [1,2] of the form:

$$u^{\varepsilon}(x) = u^0(x,y) + \varepsilon u^1(x,y) + \varepsilon^2 u^2(x,y) + \ldots \tag{2}$$

Substitution of (2) into equilibrium equations yields the following effective tensor of elastic properties:

$$C^{eff}_{ijkl} = \frac{1}{|Y|}\int_Y \left(C_{ijkl} - C_{ijpq}\frac{\partial \chi^{kl}_p}{\partial y_q}\right)dy, \tag{3}$$

where $|Y|$ denotes the area of the base cell, χ^{kl}_p stands for $Y-$ periodic virtual displacements fields for the case of loading kl [1]. The index p (p = 1, 2) denotes the number of the coordinate of the virtual displacement (χ_1 and χ_2) while the index q (q = 1, 2) is the number of the local coordinate, i.e. either y_1 or y_2.

The following integral equation regarding the base cell with periodic boundary conditions holds:

$$\int_Y C_{ijpq}\frac{\partial \chi^{kl}_p}{\partial y_q}\frac{\partial v_i}{\partial y_j}dY = \int_Y C_{ijkl}\frac{\partial v_i}{\partial y_j}dY, \quad \forall \mathbf{v} \in Y, \tag{4}$$

where $\mathbf{v}$ stands for the (kinematically admissible) virtual displacement field.

The so far considered problem (4) is further solved for the base cell using the FEM. The corresponding compatibility conditions are formulated along the boundaries of different phases. In the plane stress state, there are three independent cases of load, i.e. $kl = 11,\ 22,\ 12$. Eq. (3) can be recast to the following form:

$$C^{eff}_{ijkl} = \frac{1}{|Y|}\int_Y \left(C_{ijkl} - C_{ijpq}\frac{\partial \chi^{kl}_p}{\partial y_q}\right)dY = \langle C_{ijkl}\rangle - \langle \sigma^{kl}_{ij}\rangle, \tag{5}$$

where $\langle C_{ijkl}\rangle$ denotes the average elastic tensor depending on the volume fraction of the used material. Its estimation is carried out according to the classical rule of material mixing, and $\langle \sigma^{kl}_{ij}\rangle$ denotes the average stress tensor associated with the base cell in the case of the load kl. Naturally, $\langle \sigma^{kl}_{ij}\rangle$ plays a role of the correction term reflecting the influence of the microstructure of the material elementary cell.

In a more understandable notation (5) may be written as [19,26]

$$C^{eff}_{ijkl} = \frac{1}{|Y|}\int_Y C_{pqrs}\left(\varepsilon^{0(ij)}_{pq} - \varepsilon^{*(ij)}_{pq}\right)\left(\varepsilon^{0(kl)}_{rs} - \varepsilon^{*(kl)}_{rs}\right)dy, \tag{6}$$

where $\varepsilon^{*(ij)}_{pq} = \frac{1}{2}\left(\frac{\partial \chi^{ij}_p}{\partial y_q} + \frac{\partial \chi^{ij}_q}{\partial y_p}\right)$ and $\varepsilon^{0(ij)}_{pq}$ are linearly independent unit test strains, which are applied to the base cell to determine the characteristic strain fields $\varepsilon^{*(ij)}_{pq}$. Three test strain fields are required for 2D problems. In 2D the test strain fields take the form of $\varepsilon^{0(11)}_{pq} = [1\,0\,0]$, $\varepsilon^{0(22)}_{pq} = [0\,1\,0]$ and $\varepsilon^{0(12)}_{pq} = [0\,0\,1]$ [7,27]. It is noted that due to symmetry, $\varepsilon^{0(12)}_{pq} = \varepsilon^{0(21)}_{pq}$ reducing the required test strains from four to three in 2D.

Note that, for an arbitrary microstructure, although C is isotropic, there is no reason for C^{eff} to be isotropic or orthotropic. However, many authors enforce the homogenized material to be isotropic or orthotropic. For microstructures having square symmetry (Fig. 1), the homogenized elastic tensor C^{eff} is orthotropic.

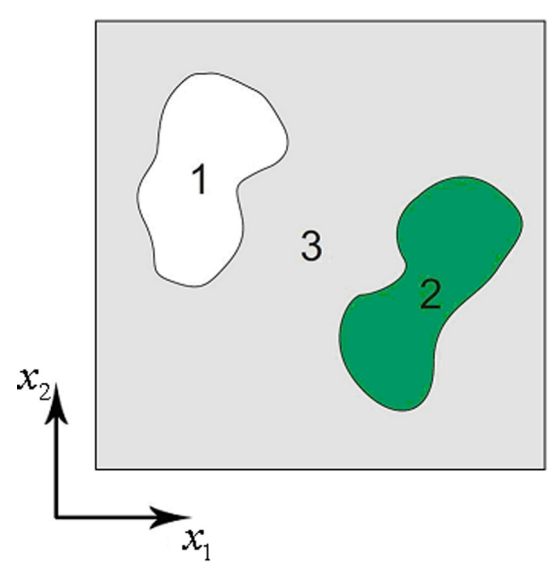


Fig. 1. Quarter base cell: 1 – technological hole; 2 – technological inclusion; 3 – domain of topological design.

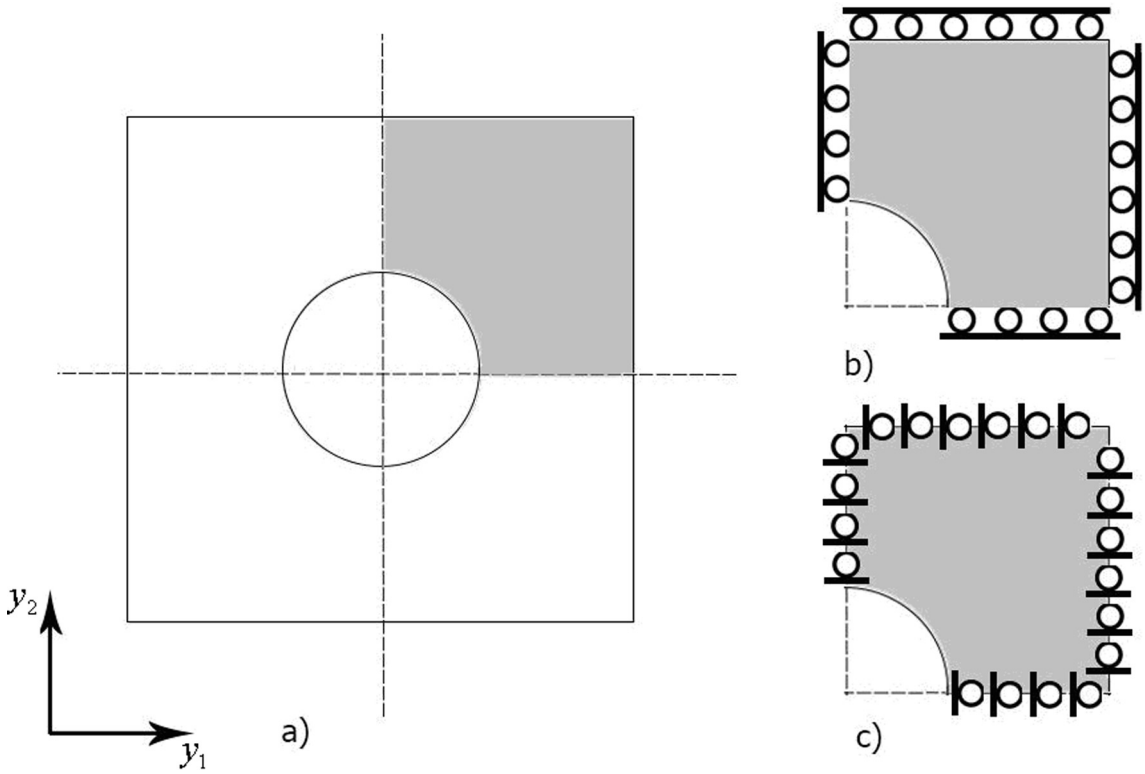


Fig. 2. Quarter base cell – a) and boundary conditions for cases b), c) on the quarter of the base cell.

For microstructures having hexagonal symmetry (Fig. 2), C^{eff} is isotropic. See [28] for more details.

Consider a 2-D symmetric base cell of an isotropic material. Its quarter is depicted in Fig. 1. For the plane stress, Eq. (1) can be rewritten as follows:

$$\begin{bmatrix} \bar{\sigma}_{11} \\ \bar{\sigma}_{22} \\ \bar{\sigma}_{12} \end{bmatrix} = \begin{bmatrix} C^{eff}_{1111} & C^{eff}_{1122} & 0 \\ C^{eff}_{1122} & C^{eff}_{1111} & 0 \\ 0 & 0 & C^{eff}_{1212} \end{bmatrix} \begin{bmatrix} \bar{\varepsilon}_{11} \\ \bar{\varepsilon}_{22} \\ 2\bar{\varepsilon}_{12} \end{bmatrix}. \tag{7}$$

For an isotropic material in two-dimensional problems the homogenized elasticity tensor C^{eff}_{ijkl} can be reduced to be $C^{eff}_{1111}, C^{eff}_{1122}, C^{eff}_{1212}$.

If loading is an initial strain ε^0 in x direction ($\varepsilon^0_{11} = 1, \varepsilon^0_{12} = 0, \varepsilon^0_{22} = 0$), then from Eq. (5) we have

$$C^{eff}_{1111} = \frac{1}{|Y|}\int_Y (C_{1111} - C_{1111}\varepsilon^{*(11)}_{11} - C_{1122}\varepsilon^{*(11)}_{22})\,dy. \tag{8}$$

Considering an initial strain ε^0 loading in y direction ($\varepsilon^0_{11} = 0, \varepsilon^0_{12} = 0, \varepsilon^0_{22} = 1$) we obtain C^{eff}_{1122}

$$C^{eff}_{1122} = \frac{1}{|Y|}\int_Y \left(C_{1122} - C_{1111}\varepsilon^{*(22)}_{11} - C_{1122}\varepsilon^{*(22)}_{22}\right)dy. \tag{9}$$

If we exert an unit initial shear strain ε^0 loading ($\varepsilon^0_{11} = 0, \varepsilon^0_{12} = 0, \varepsilon^0_{22} = 0.5$) from Eq. (5), we can get

$$C^{eff}_{1212} = \frac{1}{|Y|}\int_Y \left(C_{1212} - 2C_{1212}\varepsilon^{*(12)}_{12}\right)dy. \tag{10}$$

The calculation of effective properties can become computationally efficient by taking advantage of a symmetry of boundary conditions. The symmetry of an isotropic unit cell is relative to all axes. In this case, we can take advantage of these properties to reduce the computational cost and to conduct the optimization and homogenization in only one part of the domain. However, the appropriate periodic boundary conditions must be considered for the displacement characteristic function χ.

From the definition of periodicity for a 2D plane-strain case, we can get the boundary conditions that must be specified when only one fourth of the unit cell is considered [29] as described in Fig. 2.

These boundary conditions for the characteristic function χ may be written as:

a) for the case of load $i = j$ (1 or 2) at $y_1 = 0, y_1 = Y_1, \chi^{(ij)}_1 = 0$ and at $y_2 = 0, y_2 = Y_2, \chi^{(ij)}_2 = 0$ (Fig. 2b);
b) for the case of load $ij = 12$ (or 21) at $y_1 = 0, y_1 = Y_1, \chi^{(12)}_2 = 0$ and at $y_2 = 0, y_2 = Y_2, \chi^{(12)}_1 = 0$ (Fig. 2c).

Eq. (7) yields:

$$K^{eff} = C^{eff}_{1111} + C^{eff}_{1122}, \quad G^{eff} = C^{eff}_{1212}, \tag{11}$$

where K^{eff} stands for the bulk modulus, and G^{eff} for the shear bulk modulus.

3. Topology optimization

Finding materials with extreme stiffness in the form of either optimal bulk modulus or shear modulus belongs to examples of common problems while designing materials of desired technological properties. The material consisting of different phases and/or voids was modeled by microstructure within a periodical base cell which is discretized by N finite elements. Assume that each of them is characterized by a density variable ρ_e ($e = 1, N$). Following the SIMP [19], in which Young's modulus depends on the material density, the stress tensor is considered to be a function of Young's modulus E_{inc} of reinforcing inclusions, of Young's modulus E_m of the matrix and the artificially introduced density $\rho_e(\mathbf{x})$, which plays a

role of a control variable in the optimization problem. Thus, Young's modulus can be estimated in the following way:

$$E(\mathbf{x}) = E_m + \rho(\mathbf{x})^p (E_{inc} - E_m), \ \mathbf{x} \in \Omega. \tag{12}$$

The exponent of an order $p \geqslant 1$ is a penalty factor and an increase in p implies more articulated solution. Observe that for $\rho(x) = 1$ the whole volume is filled with the reinforcing material.

The homogenized or effective elastic tensor is expressed by Eq. (6). The sensitivities can be found directly from the strain fields already computed by the homogenization procedure.

The sensitivities of the effective stiffness tensor in (6) with respect to design variables ρ_e of element e can be found as follows [26]

$$\frac{\partial C^{eff}_{ijkl}}{\partial \rho_e} = -\frac{1}{|Y|}\int_{Y_e} \frac{\partial C^{e}_{pqrs}}{\partial \rho_e}\left(\varepsilon^{0(ij)}_{pq} - \varepsilon^{*(ij)}_{pq}\right)\left(\varepsilon^{0(kl)}_{rs} - \varepsilon^{*(kl)}_{rs}\right)dy. \tag{13}$$

The sensitivity of the local stiffness tensor (12) is

$$\frac{\partial C^{e}_{ijkl}}{\partial \rho_e} = \frac{p}{\rho_e}\left(C^{inc}_{pqrs} - C^{m}_{pqrs}\right). \tag{14}$$

By definition, the sensitivity of the bulk modulus stiffness K^{eff} and shear modulus G^{eff}, with respect to the element density variable ρ_e are expressed as

$$\frac{\partial K^{eff}}{\partial \rho_e} = \frac{\partial}{\partial \rho_e}\left(C^{eff}_{1111} + C^{eff}_{1122}\right), \quad \frac{\partial G^{eff}}{\partial \rho_e} = \frac{\partial C^{eff}_{1212}}{\partial \rho_e} \tag{15}$$

and easily calculated from (13) and (14).

The optimization of topology of the material microstructure is based on looking for the optimal microstructure of the elementary cell. Here, optimal microstructure is understood as the one having maximum stiffness regarding either bulk or shear modulus. For example, to increase K^{eff}, the following problem should be solved

$$\min_{\rho_e}\left\{\frac{(1-q)(-K^{eff})}{K_0} + q\frac{h_0 h_{\max}}{A}\int_{\Omega_3}|\nabla\rho_e(\mathbf{x})|^2 d\Omega\right\}, \tag{16}$$

with the following constraints:

$$\begin{aligned} &0 \leqslant \textstyle\int_{\Omega_3}\rho_e(\mathbf{x})d\Omega \leqslant \gamma A, \\ &0 \leqslant \rho_e(\mathbf{x}) \leqslant 1, \ e = 1, N \end{aligned} \tag{17}$$

where q – coefficient of balance between the target function (its first term) and the penalty function, h_0 – initial mesh size, $h_{\max}$ – current mesh size, K_0 – normalizing multiplier. Furthermore, γ denotes concentration of the inclusion material, Ω_3 is the domain of topological design on the elementary cell, and A stands for the area of domain Ω_3. The second term of the target function (16) is used as a penalty function and enables to avoid an unwanted and unrealistic phenomenon called the effect of the "chessboard" (i.e. the occurrence of area where solid and hollow elements are distributed in an alternating manner) in the optimal microstructure formation [19].

Similarly, to increase G^{eff}, the target formula (16) takes the following form:

$$\min_{\rho_e}\left\{\frac{(1-q)(-G^{eff})}{K_0} + q\frac{h_0 h_{\max}}{\mathrm{A}}\int_{\Omega_3}|\nabla\rho_e(\mathbf{x})|^2 d\Omega\right\} \tag{18}$$

with the constraints (17).

In order to account for the presence of holes Ω_1 and inclusions Ω_2 of the required shape at topological optimization for the problem shown in Fig. 1, we proceed as follows. The presence of holes is taken into account only through the assignment on their internal borders of the boundary conditions in the form

$$\sigma_{nn} = \sigma_{n\tau} = 0. \tag{19}$$

where $\sigma_{nn}, \sigma_{n\tau}$ – normal and shear stresses at the boundary of the hole.

Furthermore, the field of the control variables $\rho(x)$ and $E(\mathbf{x})$ in (12), should only be determined in the optimized region Ω_3, while in the field of fixed inclusions Ω_2, we introduce the value of the Young modulus, which correspond to the material of inclusion.

4. Numerical results

In the present section, several examples of optimizing periodic microstructures are presented. Void and inclusions are considered in a matrix of isotropic elastic material. In what follows, the optimal microstructure of a periodic composite made of steel with parameters $E_{inc} = 200 \cdot 10^9$ Pa, $\nu = 0.33$ (inclusion) and of the matrix with parameters $E_{inc} = 2.5 \cdot 10^4$ Pa, $\nu = 0.33$ is found by employing the homogenization method and the proposed scheme of the sensitivity analysis with the help of (13) and (15).

Example 1. Shapes of technological holes can be arbitrarily chosen depending on the needs, i.e. on the shape of the elements that are intended to be embedded in the plate. For instance, consider a periodic base cell of the composite with technological holes (in the shape of a square and an ellipse), as shown in Fig. 3.

The composite consists of a periodic system of squared holes of the side $c = 0.6$ as well as of the periodic system of elliptic holes with the half axes $a = 0.3$, $b = 0.1$. The centre of the ellipse is located in the first quadrant, at coordinates $(0.65; 0.65)$.

The first problem is aimed at optimizing the volume stiffness (bulk modulus) of the microstructure with the objective function (16), whereas the second problem focuses on maximizing the shear stiffness (shear modulus) by employing the objective function (18) with constraints (17) and volume fraction of inclusion $\gamma = 0.5$.

To study the effect of finite element discretization on the results of topology optimization, the problem governed by Eqs. (16), (17) and (18), (17) and illustrated in Fig. 3 is studied. The domain is discretized to different triangular meshing, ranging from 256 up to 4489 finite elements. The optimum microstructure for different finite element discretizations are shown in Table 1.

From the results above, we can see that the optimization problem how coarse meshes or fine meshes can converge quickly to the optimum layout. The final values K^{eff}_{opt} and G^{eff}_{opt} are also converge.

Since the maximum in such problem may be not global, we conducted a study of solutions for various initial conditions for ρ_{ini}. The results for $N = 1089$ are presented in Table 2.

From the results Table 2 it follows that all the resulting structures are similar and the best value for K^{eff}_{opt} and G^{eff}_{opt} is achieved if $\rho_{ini} = 0.6$. Fig. 4 reports the optimal microstructures (black areas correspond to inclusions, whereas grey – to the matrix material).

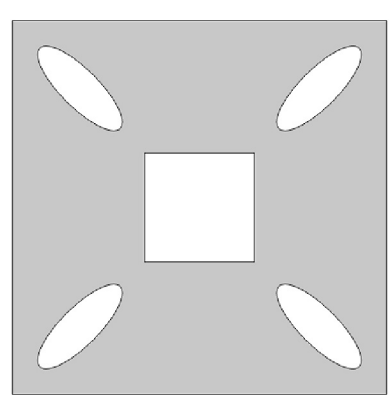


Fig. 3. Periodic composite cell with technological holes.

Table 1
Optimal microstructures for different finite element discretizations.

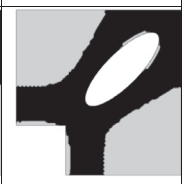
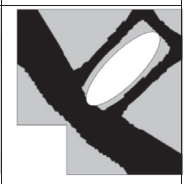
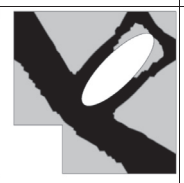
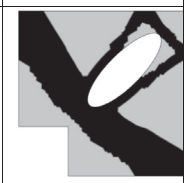
N	256	484	1089	4489
Optimal microstructures				
K_{opt}^{eff}, Pa	$4.7490 \cdot 10^{10}$	$4.9097 \cdot 10^{10}$	$5.0575 \cdot 10^{10}$	$5.2549 \cdot 10^{10}$
Optimal microstructures				
G_{opt}^{eff}, Pa	$1.6541 \cdot 10^{10}$	$1.7146 \cdot 10^{10}$	$1.8072 \cdot 10^{10}$	$1.9029 \cdot 10^{10}$

Table 2
The effect of initial conditions on the optimal microstructure.

ρ_{ini}	0.3	0.4	0.6	0.7
Optimal microstructures				
K_{opt}^{eff}, Pa	$5.0205 \cdot 10^{10}$	$5.0189 \cdot 10^{10}$	$5.0575 \cdot 10^{10}$	$4.9127 \cdot 10^{10}$
Optimal microstructures				
G_{opt}^{eff}, Pa	$1.8060 \cdot 10^{10}$	$1.8060 \cdot 10^{10}$	$1.8072 \cdot 10^{10}$	$1.8257 \cdot 10^{10}$

a) maximum bulk modulus

b) maximum shear modulus

Fig. 4. Optimal microstructures (example 1).

In the first case (Fig. 4a), when the optimization is aimed at achieving the maximum bulk modulus K^{eff}, the obtained optimal value is $K_{opt}^{eff} = 5.2549 \cdot 10^{10}$ Pa for the initial value $\rho_{ini} = 0.6$. In the second problem (Fig. 4b), when one conducts the optimization

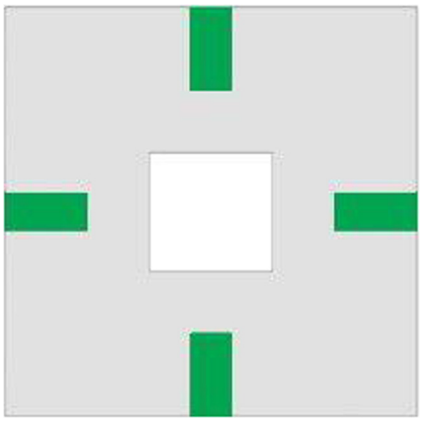


Fig. 5. Base cell of a composite with technological inclusions (green color) (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.).

Table 3
Values K_{opt}^{eff} and G_{opt}^{eff} for different finite element discretizations.

N	256	484	1089	4489
K_{opt}^{eff}, Pa	$7.2428 \cdot 10^{10}$	$7.4666 \cdot 10^{10}$	$7.6880 \cdot 10^{10}$	$7.9163 \cdot 10^{10}$
G_{opt}^{eff}, Pa	$2.1732 \cdot 10^{10}$	$2.3040 \cdot 10^{10}$	$2.4130 \cdot 10^{10}$	$2.4886 \cdot 10^{10}$

aimed at the shear modulus G^{eff}, the optimal value is $G_{opt}^{eff} = 1.9029 \cdot 10^{10}$Pa for the initial value $\rho_{ini} = 0.6$.

The results drawn in Fig. 4 indicate that under optimization the strengthening is observed in the vicinity of the holes along the edges of the square and ellipse.

Example 2. We consider a composite periodic structure made of repeating base cells containing holes as well as inclusions made from the material with given elastic properties (Fig. 5). Square holes have the size of 0.6×0.6, whereas rectangular inclusions have the size of 0.4×0.1, $E_{tech} = 100 \cdot 10^9$ Pa, and $\nu = 0.33$ (technological inclusion). Values of the remaining parameters are the same as in the previous example.

For this base cell the effect of the number of used finite elements on values K_{opt}^{eff} and G_{opt}^{eff} has been also investigated (Table 3).

Similarly to Example 1, it was found that the effect of initial conditions on the resulting optimal microstructure and the values K_{opt}^{eff} and G_{opt}^{eff} is insignificant.

The obtained optimal topology of the microstructure is shown in Fig. 6. The black color refers to the material with $E_{inc} = 200 \cdot 10^9$ Pa.

The maximum value of the bulk modulus obtained in the optimization process is $K_{opt}^{eff} = 7.9163 \cdot 10^{10}$Pa. In the second problem, the maximum value of the shear modulus is $G_{opt}^{eff} = 2.4886 \cdot 10^{10}$Pa (for the initial value $\rho_{ini} = 0.6$).

5. Conclusions

The problem of topological optimization for base cell of the composite containing initially established technological holes and/or inclusions was first investigated. The procedure of topology optimization has been described and implemented to find the optimal microstructure in the given composite structures. The results indicate that optimization aimed at obtaining the extreme bulk modulus and the extreme shear modulus has allowed finding a composite microstructure being significantly reinforcement. Thus, one can draw a conclusion that macro-scale elastic properties of a composite can be defined and designed by means of investigations conducted on a micro scale.

Acknowledgments

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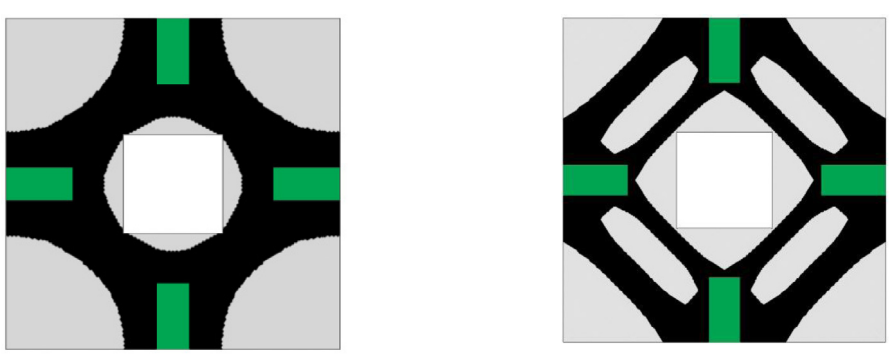

a) maximum bulk modulus b) maximum shear modulus

Fig. 6. Optimal microstructures to example 2.

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