ENGINEERING TRANSACTIONS • *Engng. Trans.* • **65**, 1, 31–38, 2017
Polish Academy of Sciences • Institute of Fundamental Technological Research (IPPT PAN)
National Engineering School of Metz (ENIM) • Poznan University of Technology

Two-Phase Isotropic Composites of Extremal Moduli – the Inverse Homogenization Problem

Tomasz ŁUKASIAK

Department of Structural Mechanics and Computer Aided Engineering
Faculty of Civil Engineering
Warsaw University of Technology
Aleja Armii Krajowej 16, 00-637 Warsaw, Poland
e-mail: T.Lukasiak@il.pw.edu.pl

This work deals with the inverse homogenization problem: for given two well-ordered elastic and isotropic materials characterized by the bulk and shear moduli (κ_1, μ_1), (κ_{12}, μ_2) and the volume fraction ρ of the second material reconstructing the layout of the most second-rank orthogonal laminates within a hexagonal 2D periodicity cell Y corresponding to the predefined values of moduli (κ^*, μ^*) of the effective isotropic composite. The used algorithm follows from imposing the finite element (FE) approximation on the solution to the basic cell problems of the homogenization theory [7] along with periodicity assumptions. The material properties of each element are described by three independent parameters. Thus, the formulated inverse problem is solved numerically by the gradient method. The adopted cell structure, i.e., the hexagonal cell with the rotational symmetry of 120° angle guarantees the isotropic effective properties of the composite, and thus the optimization problem is greatly simplified. Isotropic constraints do not appear in the formulated optimization problem.

Key words: laminates, isotropic composites, inverse-homogenization.

1. Introduction

The aim of this paper is to show the microstructures of isotropic composites, corresponding to points in the plane: effective bulk modulus κ versus effective shear modulus μ, of extremal properties characterized by the contour of the Cherkaev-Gibiansky (CG) domain [3]. The CG domain has a form of curvilinear polygon, see Fig. 1.

The microstructures corresponding to the interior of the CG polygon can be of an arbitrary rank in the meaning of the hierarchical homogenization. Moreover, it is well-known that the rank-1 microstructures cannot reach the regions close to the vertices and boundary lines of the CG. These bounds are attainable

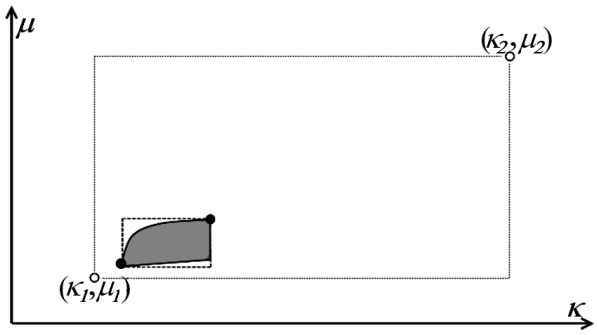

FIG. 1. The juxtaposition of the given $(\kappa_\alpha,\ \mu_\alpha)$ points $\bullet$ and $G\rho$-closure of isotropic materials (shaded area) for $\rho = 0.5$ bounded by the CG (black).

by the second-rank microstructures [11]. The specific challenge is to build such "extremal" composites that reach the points lying on the boundaries of the CG area.

A new inverse homogenization technique is developed to construct these extremal microstructures of isotropic effective moduli. The constructed layouts correspond to the points lying very close to the contour of the CG domain.

On the other hand, the present paper delivers a method of enhancing the isotropic material designs (cf. [4]) with microstructures reflecting the optimal isotropic properties.

2. Homogenization of periodic media

We consider the periodic composites the RVE's of which are identified with the periodicity cells Y. Tessellation of Y gives a structure of the material at the *macro* level. The effective properties of periodic composites are determined by the solutions to the basic cell problems of the homogenization theory. To sufficiently obtain accurate results, the mesh of Y must be properly constructed [1] and the conditions of periodicity must be properly modeled. The basic cell problems are solved by assuming the FE approximation of displacements $\mathbf{u} = \mathbf{Nq}$ and strains $\boldsymbol{\varepsilon} = \mathbf{Bq}$ by nodal displacements $\mathbf{q}$ and the appropriate shape functions $\mathbf{N}$ within each element Ω_k. Here $\mathbf{B} = \mathbf{DN}$, where $\mathbf{D}$ is the matrix of the differential operators of the considered problem. Let $|\bullet|$ be the volume of $\bullet$. The effective constitutive matrix is expressed by

$$\mathbf{E}^{\mathrm{H}} = \langle \mathbf{E} \rangle - \left(\mathbf{H}\mathbf{K}^{-1}\mathbf{H}^{\mathrm{T}}\right) |Y|^{-1}, \tag{2.1}$$

with $\mathbf{K}$ being the FE stiffness matrix, $\mathbf{H}$ – matrix of the vectors, i.e., self-equilibrated load cases, both obtained by the FE aggregation of an element

matrices $\mathbf{K}_k$, $\mathbf{H}_k$, and $\langle \mathbf{E} \rangle$ – averaged constitutive matrix. These are calculated by the following formulas:

$$\langle \mathbf{E} \rangle = |Y|^{-1} \int_Y \mathbf{E} dY = |Y|^{-1} \sum_k \mathbf{E}_k \, |\Omega_k|,$$

$$\mathbf{K}_e \left(\mathbf{E}_k \right) = \mathbf{K}_k = \int_{\Omega_k} \mathbf{B}_k^{\mathrm{T}} \mathbf{E}_k \mathbf{B}_k d\Omega_k, \qquad \mathbf{H}_e \left(\mathbf{E}_k \right) = \mathbf{H}_k = \int_{\Omega_k} \mathbf{E}_k \mathbf{B}_k d\Omega_k.$$

Note that a three-column (for 2D) matrix $\mathbf{H}^{\mathrm{T}}$ is uniquely defined by the distribution of the material in Y. Periodicity condition can be met by using a simple trick of FE. The opposite edges must be identically meshed. For such mesh, the same degrees of freedom should be assigned for the nodes on corresponding opposite edges.

3. Inverse homogenization

The inverse homogenization problems state the questions on the *optimal* layout of several materials in given proportions within domain Y. Here, *optimal* means such a layout that gives assumed homogenized properties $\mathbf{E}^*$ of the periodic composite. As such, the problem can be treated as a topology optimization problem: to minimize the gap between the given $\mathbf{E}^*$ and the calculated $\mathbf{E}^{\mathrm{H}}$. The conventional process of the optimization is carried out usually on the rectangle Y. The cell is meshed uniformly into n finite-elements Ω_k $(k = 1, ..., n)$. In the case of the two materials of moduli $\mathbf{E}_1$ and $\mathbf{E}_2$ and their volume fractions expressed by $1-\rho$, $0 < \rho < 1$, for each element a variable ρ_k is assigned a number such that:

$$\rho_k = \begin{cases} 0, & \Omega_k \in \mathbf{E}_1 \\ 1, & \Omega_k \in \mathbf{E}_2 \end{cases} \quad \text{and} \quad \sum_{k=1}^{n} \rho_k = n\rho. \tag{3.1}$$

By creating a few configurations of $\boldsymbol{\rho} = \{\rho_k\}$, i.e., layouts of materials, one can try to get the expected result described by the assumed $\mathbf{E}^*$. The problem defined in this way is a difficult, binary programming problem with a large number of variables $\boldsymbol{\rho}$. An accurate representation of the structure requires a large number n of elements, and produces at most $n!/(m!(n-m)!)$ possible configurations to check, where $m = \rho n$. Such a pure 0-1-element-wise optimization problem can be solved by using the so-called 'hard-kill' methods such as evolutionary structural optimization (ESO) or bidirectional ESO (BESO). However, the above-mentioned methods do not guarantee achieving the global or local optimum.

For large n ($\approx 10\,000$), the optimization problem must be relaxed to be effectively solved. The relaxation allows variation $\rho_k \in \langle 0, 1\rangle$ and makes the material characteristics dependent on "pseudo-density" variables ρ_k. The final proper solution must be characterized only by $\rho_k = \{0, 1\}$. Here, the parameters ρ_k are the only decision variables in each finite element. The introduction of a continuous variable ρ_k allows determining the gradient of the objective function and using the efficient gradient methods to search for the minimum. The relaxed formulation admits mixing the given materials in some proportion (infinitely fine mixtures). This requires proper calculating of effective properties $\mathbf{E}(\rho_k)$ for intermediate values ρ_k usually by adopting the so-called material interpolation scheme, e.g., SIMP [2], RAMP [12], GRAMP [5] or the proposed by the author: HSρ [10], all for an artificial isotropic material (in fact these models are not exactly single-parameter and they depend on an additional coefficient p). This interpolation is crucial for relaxed topology optimization problems. For a wrong approximation $\mathbf{E}(\rho_k)$ the obtained result may lie very far from the global optimum.

Instead of artificial isotropic one-parameter models, the more complicated multi-parameter ($\bullet$) microstructures (MpM) can be adopted as underlying structures. Calculating $\mathbf{E}_k(\bullet)$ for some of them can be done exactly (leading to laminates) or by the homogenization approach. On the other hand, one can prepare a multi-parameter interpolation scheme. The MpM approach causes great limitations – the resulting solution by definition is limited to a narrow class of the assumed microstructures. Main complications caused by MpM are the additional design variables required to describe the structure of composites, i.e., the number and the angles of orientation of layers, the diameters and orientations of inclusions, etc. Moreover, the number of parameters depends on the selected type of the underlying structure.

One of many periodic composites are materials known as laminates, in fact: in-plane laminates. The first- rank laminate is a heterogeneous material that is composed of periodically repeating layers of materials of any constitutive properties. For such a constructed laminate the constitutive matrix $\mathbf{E}^{\mathrm{I}}$ is given by Lurie-Cherkaev-Fiodorov formula, see [8]

$$\mathbf{H}^{\mathrm{I}} = \langle \mathbf{H} \rangle - (1-\rho)\,\rho \Delta \mathbf{H} \mathbf{Q} \left[\mathbf{Q}^{\mathrm{T}} \mathbf{H}^{\mathrm{sa}} \mathbf{Q}\right]^{-1} \mathbf{Q}^{\mathrm{T}} \Delta \mathbf{H}, \tag{3.2}$$

where $\mathbf{H} = \mathbf{H}_{\alpha\beta} E_\alpha \otimes E_\beta$ is the matrix representation of Hooke's tensor ($\alpha, \beta = 1, 2, 3$), $\mathbf{H}^{\mathrm{sa}} = (1-\rho)\mathbf{H}_2 + \rho \mathbf{H}_1$, $\Delta \mathbf{H} = (\mathbf{H}_2 - \mathbf{H}_1)$, and (for the orthogonal versors e_1, e_2, and the basis $\mathbf{E}_\alpha = e_\alpha \otimes e_\alpha$, $\mathbf{E}_3 = \sqrt{2}(e_1 \otimes e_2 + e_2 \otimes e_1)/2$)

$$\mathbf{H} = \begin{bmatrix} E_{11} & E_{12} & \sqrt{2}E_{13} \\ & E_{22} & \sqrt{2}E_{23} \\ \text{sym.} & & 2E_{33} \end{bmatrix},$$

$$\mathbf{Q} = \frac{\sqrt{2}}{2}\begin{bmatrix} \sqrt{2}\cos^2(\alpha) & -\sin(2\alpha) \\ \sqrt{2}\sin^2(\alpha) & \sin(2\alpha) \\ \sin(2\alpha) & \sqrt{2}\cos(2\alpha) \end{bmatrix}.$$

Here α is the angle of the direction of lamination (for details see [6]).

The material thus obtained – the first rank laminate $\mathbf{E}^{\mathrm{I}}$, can be used for the construction of the laminate of the second rank of moduli $\mathbf{E}^{\mathrm{II}}$, calculated again by formula (3.2).

This study assumed the laminate of two components with orthogonal layers of lamination, i.e., $\alpha = \{90^\circ, 0^\circ\}$. Such a laminate of the second rank can be described by three parameters (ρ, η, φ) as shown in Fig. 2, (ρ, $\eta \in \langle 0, 1\rangle$). The effective properties $\mathbf{E}^{\mathrm{II}}$ of the defined laminate are calculated by repetitive application of Eq. (3.2). The first lamination, for $\alpha = 90^\circ$, determines the properties of the first rank laminate $\mathbf{E}^{\mathrm{I}}$ consisting of $(1-\rho)/\rho^{\mathrm{I}}$ and $(1-\eta)\rho/\rho^{\mathrm{I}}$ fractions of materials of moduli $\mathbf{E}_1(\kappa_1, \mu_1)$ and $\mathbf{E}_2(\kappa_2, \mu_2)$, respectively, where $\rho^{\mathrm{I}} = 1 - \eta\rho$. The next one (for $\alpha = 0^\circ$) contains $1 - \eta\rho$ fraction of $\mathbf{E}^{\mathrm{I}}$ and $\eta\rho$ fraction of $\mathbf{E}_2$. Then, the resulting constitutive matrix $\mathbf{E}^{\mathrm{II}}$ is rotated by the angle φ that defines the orientation of the material in the global coordination system of the analyzed cell Y. Such model of the pre-homogenized orthotropic material allows for the description of the isotropic material (for $\rho = 0$ is $\mathbf{E}^{\mathrm{II}} \equiv \mathbf{E}_1$, while for $\rho = 1$ is $\mathbf{E}^{\mathrm{II}} \equiv \mathbf{E}_2$), a first rank laminate (for $\eta = 1$ or for $\eta = 0$ and $\rho > 0$) and a second-rank laminate.

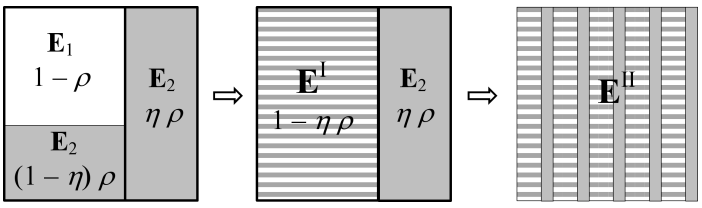

FIG. 2. Scheme of the second order orthogonal laminate.

4. RESULTS

In the present work, in order to achieve the boundary of the CG domain, a variety of isotropic composites are constructed based on $\mathbf{E}^{\mathrm{II}}$ underlying laminates. Equation (3.2) is used to determine the homogenized constitutive values described by (ρ_k, η_k, φ_k) for each element within the hexagonal cell Y. The minimized objective function $P(\rho_k,\ \eta_k,\ \varphi_k)$ for the studied inverse problem is chosen (due to a special choice of the isotropic hexagonal cell) as below:

$$P(\rho_k, \eta_k, \varphi_k) = \left(\frac{\kappa^* - \kappa}{\kappa^*}\right)^2 + \left(\frac{\mu^* - \mu}{\mu^*}\right)^2. \tag{4.1}$$

The formulated optimization problem, although strongly nonlinear, is solved numerically by the gradient method. At the starting point, the triplets $(\rho_k,\ \eta_k,\ \varphi_k)$ are randomly selected (here, for all the presented cases – they are the same), yet satisfying the isoperimetric condition corresponding to a given $\rho = 0.5$. The effective isotropic moduli for the analyzed microstructure and the gradient are computed according to the homogenization algorithm (2.1) using the FE techniques along with periodicity assumptions. The material data $(\kappa,\ \mu)$ adopted are (0.0357, 0.0192) and (0.7143, 0.3846), respectively. The obtained results are presented below. In Fig. 3, grey lines show the bounds of the "extreme" first rank microstructures, which were created in a similar manner but for 3200 decision variables each (single-parameter elements) by using the HSρ-isotropic interpolation scheme [9]. The results, shown by black dots, were recently obtained by using $\mathbf{E}^{\mathrm{II}}$ microstructures. The topology of the cell Y for some points with the values of the objective function (4.1), is presented in Fig. 4.

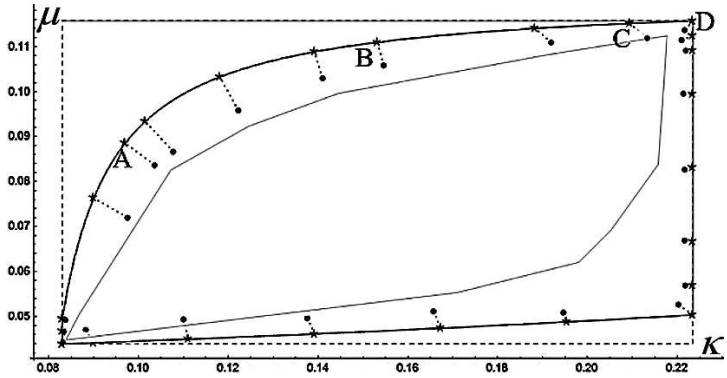

FIG. 3. CG bounds and • – obtained $(\kappa^{\mathrm{H}},\ \mu^{\mathrm{H}})$ for the proposed $\mathbf{E}^{\mathrm{II}}$ microstructures with ★ – assumed $(\kappa^*,\ \mu^*)$ (connected by dotted lines respectively).

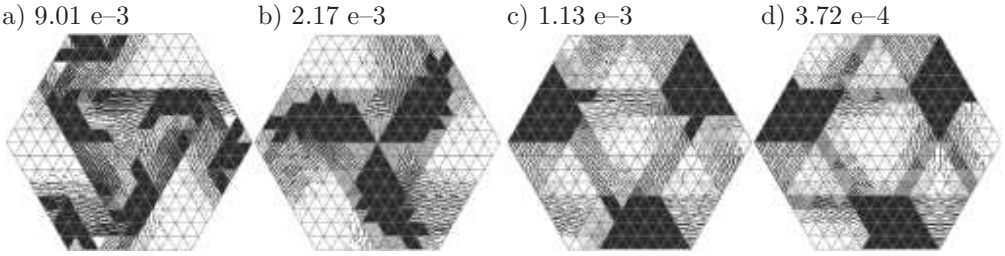

FIG. 4. Examples of the obtained Y cells for $\mathbf{E}^{\mathrm{II}}$ underlying microstructures in each element.

5. Final remarks

This paper is aimed at finding (at most) the rank-3 subclass of the isotropic composites of effective moduli achieving the CG bounds. The structures built on

one-parameter model of an isotropic material do not reach these limits. Using a simple tri-parameter model of orthogonal laminates gives much better results that lie much closer to the boundaries. Moreover, this results in a significant reduction in the number of the decision variables involved in the process. The number of the decision variables for the proposed model is nearly 10 times smaller than for first rank microstructures, which significantly reduces the time of computation. Exact isotropic result is ensured by the use of hexagonal cells of periodicity with rotational symmetry of an angle of 120 degree.

Acknowledgment

This paper was prepared within the Research Grant no 2013/11/B/ST8/04436 financed by the National Science Centre (Poland), entitled: Topology optimization of engineering structures. An approach synthesizing the methods of: free material design, composite design and Michell-like trusses.

References

1. Bendsøe M.P., Kikuchi N., *Generating optimal topologies in optimal design using a homogenization method*, Computer Methods in Applied Mechanics and Engineering, **71**(2): 197–224, 1988, doi: 10.1016/0045-7825(88)90086-2.

2. Bendsøe M.P., Sigmund O., *Material interpolation schemes in topology optimization*, Archive of Applied Mechanics, **69**(9): 635–654, 1999, doi: 10.1007/s004190050248.

3. Cherkaev A.V., Gibiansky L.V., *Coupled estimates for the bulk and shear moduli of a two-dimensional isotropic elastic composite*, Journal of the Mechanics and Physics of Solids, **41**(5): 937–980, 1993, doi: 10.1016/0022-5096(93)90006-2.

4. Czarnecki S., *Isotropic material design*, Computational Methods in Science and Technology, **21**(2): 49–64, 2015, doi: 10.12921/cmst.2015.21.02.001.

5. Dzierżanowski G., *On the comparison of material interpolation schemes and optimal composite properties in plane shape optimization*, Structural and Multidisciplinary Optimization, **46**(5): 693–710, 2012, doi: 10.1007/s00158-012-0788-2.

6. Dierżanowski G., *Optimization of material layout in thin elastic plates* [in Polish], Oficyna Wydawnicza Politechniki Warszawskiej, Warszawa, 2010.

7. Hassani B., Hinton E., *Homogenization and structural topology optimization: theory, practice and software*, Springer, New York, 1998.

8. Lewiński T., Telega J.J., *Plates, laminates, and shells: asymptotic analysis and homogenization*, World Scientific, Singapore, 2000.

9. Łukasiak T., *Two-phase isotropic composites with prescribed bulk and shear moduli*, [in:] *Recent Advances in Computational Mechanics*, Łodygowski T., Rakowski J., Litewka P. [Eds.], pp. 213–222, CRC Press, London, 2014, doi: 10.1201/b16513-29.

10. Łukasiak T., *HSρ – an isotropic interpolation scheme based on Hashin-Shtrikman variational bounds*, [in:] *Advances in Mechanics: Theoretical, Computational and Interdisciplinary Issues*, Proceedings of the 3rd Polish Congress of Mechanics (PCM) and 21st International Conference on Computer Methods in Mechanics (CMM), Gdansk, Poland, 8–11 September 2015, Kleiber M., Burczyński T., Wilde K., Górski J., Winkelmann K., Smakosz Ł. [Eds.], pp. 355–360, CRC Press, London 2016, doi: 10.1201/b20057-77.

11. Sigmund O., *A new class of extremal composites*, Journal of the Mechanics and Physics of Solids, **48**(2): 397–428, 2000, doi: 10.1016/S0022-5096(99)00034-4.

12. Stolpe M., Svanberg K., *An alternative interpolation scheme for minimum compliance optimization*, Structural and Multidisciplinary Optimization, **22**(2): 116–124, 2001, doi: 10.1007/s001580100129.

Received November 10, 2016; accepted version November 14, 2016.