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Optimal design of periodic linear elastic microstructures

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Abstract

This paper presents two computational models to design the periodic microstructure of cellular materials for optimal elastic properties. The material equivalent mechanical properties are obtained through a homogenization model. The two formulations address the problem of finding the optimal representative microstructural element for periodic media that maximizes either the weighted sum of the equivalent strain energy density for specified multiple macroscopic strain fields, or a linear combination of the equivalent mechanical properties. Constraints on material volume fraction and material symmetries are considered. The computational models are established using finite elements and mathematical programming techniques and tested in several numerical examples. © 2000 Elsevier Science Ltd. All rights reserved.

Keywords: Optimal microstructures; Topology optimization; Cellular materials; Homogenization; Finite elements

1. Introduction

This paper considers the optimal design of periodic linear elastic microstructures, presenting two computational models to predict the topology of the microstructure for optimal equivalent material properties. The characterization of the equivalent material properties in this setting is made through the use of the mathematical theory of homogenization (see e.g. [13,16,20]) using only a representative microstructural element (representative unit cell). However, other methods for composite and cellular materials are known (see e.g. [7–9,14] and references therein).

The first computational model considers the problem of finding the topology of the representative microstructural element that maximizes a weighted sum of the equivalent strain energy densities, for given average strain fields, amount of material and material symmetry requirements. The second formulation, a generalization of the first, considers the case of finding the topology of the representative microstructural element that maximizes a linear combinations of the equivalent material properties under the same set of restrictions (amount of material and material symmetries).

The problem of finding the topologies of microstructures was first addressed by Sigmund [21,22] but in a different setting. There, the goal was to find the topology of the representative microstructural element that would minimize the volume fraction, satisfying a given set of equivalent material properties. Similar approach was used in Ref. [5]. More recently, for linearized thermoelasticity, the problem of finding the microstructure topology for extreme thermal expansion coefficients was addressed in Refs. [23,24].

The existence of optimal bounds for the elastic properties of two-phase composite materials is well known (see, e.g. [3,6,9] and references therein); however, the microstructures associated with these bounds are ranked material which is impractical for engineering

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applications. Simpler microstructure geometries can be found for linearized bounds on low volume fraction cellular materials [4]. The computational model described below tries to overcome this problem restricting the design to only one level of microstructure.

The following sections present the homogenization results, the material symmetry characterization, the material optimization models, the computational models, the application examples, and final remarks.

2. Homogenization model

Within the scope of linearized elasticity, the equivalent mechanical properties of materials with periodic microstructure can be computed using the homogenization method. This method is based on the fact that the representative size of the microstructure d, is much smaller that the representative size of a global structure D. The fundamentals of this method can be found, for example, in Refs. [13,16,20]. The homogenized (equivalent) material properties, established for the limiting case of $\varepsilon = d/D \rightarrow 0$, are given by:

$$E^{H}_{ijkm} = \frac{1}{|Y|}\int_{\Psi}\left(E_{ijkm} - E_{ijpq}\frac{\partial \chi_p^{km}}{\partial y_q}\right)\mathrm{d}Y \tag{1}$$

where Ψ identifies the solid part of the microstructure as shown in Fig. 1, and the set of functions χ^{km} is the solution of:

Find χ^{km} Y-periodic such that:

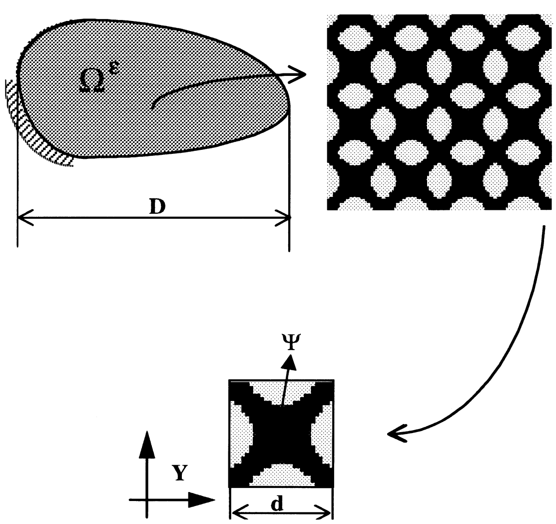


Fig. 1. Body, composite microstructure, representative microstructural element.

$$\int_{\Psi} E_{ijpq}\frac{\partial \chi_p^{km}}{\partial y_q}\frac{\partial v_i}{\partial y_j}\,\mathrm{d}Y = \int_{\Psi} E_{ijkm}\frac{\partial v_i}{\partial y_j}\,\mathrm{d}Y, \tag{2}$$

$\forall \boldsymbol{v}$ admissible, Y-periodic.

The homogenized material properties (1) can be written in equivalent form as:

$$E^{H}_{ijkm} = \frac{1}{|Y|}\int_{\Psi} E_{pqrs}\left(\delta_{ri}\delta_{sj} - \frac{\partial \chi_r^{ij}}{\partial y_s}\right)\left(\delta_{pk}\delta_{qm} - \frac{\partial \chi_p^{km}}{\partial y_q}\right)\mathrm{d}Y \tag{3}$$

3. Material symmetry in two-dimensional case

For linearized elasticity, the relation between the Cauchy stress tensor, σ_{ij}, and the infinitesimal strain tensor, ε_{km}, (constitutive equation, or generalized Hook's law) is

$$\sigma_{ij} = E_{ijkm}\varepsilon_{km} \tag{4}$$

where E_{ijkm} is the constitutive tensor, a fourth-order symmetric tensor ($E_{ijkm} = E_{jikm} = E_{ijmk} = E_{kmij}$), characterizing the elastic properties of the material.

The general case can be reduced to two-dimensional for plain strain or plane stress assumptions.

In the two-dimensional case, the constitutive tensor can be represented in the following compact matrix form.

$$\mathbf{E} = \begin{bmatrix} E_{1111} & E_{1122} & E_{1112} \\ & E_{2222} & E_{2212} \\ \text{sym.} & & E_{1212} \end{bmatrix} \tag{5}$$

For a general anisotropic material there are six independent components of the constitutive tensor. If material symmetries exist such as orthotropy, square symmetry, etc., the number of independent constants reduces, being only two for the isotropic case.

Particular material symmetry cases can be identified through the following parameters [11,18]:

$$C_2 = \frac{1}{2}(E_{1111} - E_{2222}) \tag{6}$$

$$C_3 = \frac{1}{8}\left[(E_{1111} + E_{2222}) - 2(E_{1122} + 2E_{1212})\right] \tag{7}$$

$$C_6 = \frac{1}{2}(E_{1112} + E_{2212}) \tag{8}$$

$$C_7 = \frac{1}{2}(E_{1112} - E_{2212}) \tag{9}$$

For orthotropic materials,

$$C_7C_2^2 - 4C_7C_6^2 - 4C_6C_3C_2 = 0. \tag{10}$$

For square symmetry, Eq. (10) plus

$$C_2 = 0, \tag{11}$$

and for isotropy, Eqs. (10) and (11) plus

$$C_3 = 0. \tag{12}$$

For isotropic materials, only two independent constants are necessary to characterize the constitutive tensor. Different constants can be used, and the most usual ones are the Young modulus E, the Poisson coefficient v, the shear modulus G, the volumetric (bulk) modulus K, and Lamé coefficient λ. Table 1 summarizes the relation between these constants for the plane strain and plane stress case. Note that the bulk modulus K for these cases refers to the relation between the two-dimensional hydrostatic pressure and the change of area, and that the two-dimensional components of the constitutive tensor are used.

When considering the material symmetries for the homogenized material constants for a given microstructure with an isotropic base material, geometric symmetries produce material symmetries [12]. Thus, a representative microstructural element with two symmetry planes will produce an orthotropic material, a square unit cell with 45° geometric symmetry ("diagonal symmetry") will produce square material symmetry, and a unit cell with 60° geometry symmetry will produce isotropic materials. This fact will be used with advantage in the optimization algorithm.

4. Material models for optimal design of periodic linear elastic microstructures

4.1. Optimal microstructure for given average strain fields

This model addresses the problem of identifying the topology of the microstructure, for a given amount of available material (volume fraction) such that a weighted sum of average strain energy densities is maximized. Also, symmetry conditions associated with the microstructure can be taken into account. Another way of considering it is to find the stiffest microstructure for a multi-load situation, with a prescribed amount of available material and symmetry conditions.

Optimal microstructures for average energy density are known to be higher-order ranking laminates [6]; however, here only one level of microstructure is assumed.

The problem can then be stated as:

$$\underset{\mu_{\min} \le \mu \le \mu_{\max}}{\text{Minimize}} \quad -\sum_{r=1}^{nc}\left[w^r E^H_{ijkm}(\mu) e^r_{ij} e^r_{km}\right] \tag{13}$$

subject to:

$$\int_Y \mu \, \mathrm{d}Y = V_0 \tag{14}$$

$$\int_Y E_{ijpq}(\mu) \frac{\partial \chi_p^{km}}{\partial y_q} \frac{\partial v_i}{\partial y_j} \, \mathrm{d}Y = \int_Y E_{ijkm}(\mu) \frac{\partial v_i}{\partial y_j} \, \mathrm{d}Y, \quad \forall \boldsymbol{v} \text{ admissible, } Y-\text{periodic} \tag{15}$$

$$\text{Material symmetry constraints (10)–(12)} \tag{16}$$

where nc is the number of imposed e^r_{ij} average strain fields, μ is the pointwise material volume fraction distribution, $V_0 < |Y|$ is the available resource, the homogenized material constants are computed by,

$$E^H_{ijkm} = \frac{1}{|Y|} \int_Y E_{pqrs}(\mu) \left(\delta_{ri}\delta_{sj} - \frac{\partial \chi_r^{ij}}{\partial y_s}\right) \times \left(\delta_{pk}\delta_{qm} - \frac{\partial \chi_p^{km}}{\partial y_q}\right) \mathrm{d}Y$$

and the material symmetry constraints can be used to

Table 1
Relations between elastic properties

		E	v	K	G	λ'
Plane stress	E, v	E	v	$\frac{E}{2(1-2v)}$	$\frac{E}{2(1+2v)}$	$\frac{Ev}{(1-v^2)}$
	E_{ijkm}	$E_{1111} - \frac{E_{1122}^2}{E_{1111}}$	$\frac{E_{1122}}{E_{1111}}$	$\frac{E_{1111}+E_{1122}}{2}$	E_{1212}	E_{1122}
Plane strain	E, v	E	v	$\frac{E}{2(1-2v)(1+v)}$	$\frac{E}{2(1+v)}$	$\frac{Ev}{(1+v)(1-2v)}$
	E_{ijkm}	$\frac{(E_{1111}-E_{1122})(E_{1111}+2E_{1122})}{(E_{1111}+E_{1122})}$	$\frac{E_{1122}}{E_{1111}+E_{1122}}$	$\frac{E_{1111}+E_{1122}}{2}$	E_{1212}	E_{1122}

impose orthotropy, square symmetry or isotropy on the homogenized material constants E^H_{ijkm} as described in Section 3. The dependence of the constitutive tensor $E_{ijkm}(\mu)$ on the volume fraction distribution can be assumed to be relaxed through the use of the homogenization theory one step further, as in the usual topology optimization procedures [1,2], or to be an artificial function as in Ref. [15].

4.2. Optimal microstructure for a linear combination of elastic properties

The previous formulation, when implemented computationally, depending on the $E_{ijkm}(\mu)$ function, may predict that portions of the microstructure will have intermediate volume fraction values, indicating the presence of porous material. Since it would be desirable, for practical purposes, that the microstructure would only have material zones ($\mu = 1$) or void zones ($\mu = 0$), the previous formulation can be modified and generalized as:

$$\underset{\mu_{\min} \leq \mu \leq \mu_{\max}}{\text{Minimize}} - \beta_{ijkm} E^H_{ijkm}(\mu) + \frac{1}{|Y|} \int_Y \mu(1-\mu)\, \mathrm{d}Y \tag{18}$$

subject to:

$$\int_Y \mu\, \mathrm{d}Y = V_0 \tag{19}$$

$$\int_Y E_{ijpq}(\mu) \frac{\partial \chi_p^{km}}{\partial y_q} \frac{\partial v_i}{\partial y_j}\, \mathrm{d}Y = \int_Y E_{ijkm}(\mu) \frac{\partial v_i}{\partial y_j}\, \mathrm{d}Y, \quad \forall \boldsymbol{v} \text{ admissible}, \ Y-\text{periodic} \tag{20}$$

$$\text{Material symmetry constraints (10)–(12)} \tag{21}$$

where β_{ijkm} is a given fourth-order tensor and the term $\alpha/|Y| \int_Y \mu(1-\mu)\, \mathrm{d}Y$ corresponds to a penalization on intermediate volume fraction values [10] with given penalty factor α. This penalty term is intended to reduce the intermediate values of μ on the final solution.

If the components of the fourth-order tensor β_{ijkm} are chosen such that $\beta_{ijkm} = \sum_{r=1}^{nc} w^r e^r_{ij} e^r_{km}$, the previous formulation is recovered when $\alpha = 0$.

5. Computational model

To solve numerically the problem described in the previous section, a computational model is introduced using the mathematical programming method of moving asymptotes, MMA (see [25]). State equation (20) is solved using a finite element discretization, and the volume fraction distribution μ is assumed constant within each finite element. Also, to stabilize the numerical model with respect to mesh refinements and control numerical instabilities (development of checkerboard patterns) mesh independence techniques (see [21]) are implemented.

The gradient information required by MMA is computed using the analytical sensitivity results (see Refs. [17,21] for details)

$$\frac{\partial E^H_{ijkm}}{\partial \mu_\mathrm{e}} = \frac{1}{|Y|} \int_{Y_\mathrm{e}} \frac{\partial E_{pqrs}(\mu_\mathrm{e})}{\partial \mu} \left(\delta_{pk}\delta_{qm} - \frac{\partial \chi_p^{km^h}}{\partial y_q} \right) \times \left(\delta_{ri}\delta_{sj} - \frac{\partial \chi_r^{ij^h}}{\partial y_s} \right) \mathrm{d}Y \tag{22}$$

where Y_e is the finite element area, χ^{ij^h} the finite element solution of problem (2), and $(\partial E_{pqrs}(\mu_\mathrm{e}))/(\partial \mu)$ is computed using homogenization results (see [19]).

To control design changes between iterations, the design variable changes are bounded by

$$\mu_{k+1}^{\min} = \max\left[(1-\zeta)\mu_k, \mu_{\min}\right]$$

$$\mu_{k+1}^{\max} = \min\left[(1+\zeta)\mu_k, \mu_{\max}\right] \tag{23}$$

where ζ is a user defined control parameter.

6. Examples

In the examples, the finite element method for two-dimensional continuum models is used, and the design variables (the local volume fraction) are constant within each finite element. A square design domain, associated with the representative microstructural element, is used for all the examples. The symmetry constraints for orthotropy and symmetry can be imposed through the microstructural geometrical symmetry properties (see [12]), thus reducing the number of constraint conditions on the optimization algorithm. In particular, for orthotropy requirements, only one quarter of the representative microstructural element is sufficient, and for square symmetry it also sufficient to impose that the design elements are symmetric with respect to the diagonals.

The dependence of the base material properties on the volume fraction, $E_{ijkm}(\mu)$, is characterized through the homogenization of a sub-microstructure with square holes as in Ref. [19] assuming, $E = 1$ MPa, $\nu = 0.3$, and plane strain.

For the figures, the optimal volume distribution is represented using a gray scale from white, very week material ("hole", $\mu = \mu_{\min}$), to black, full material ($\mu = 1$).

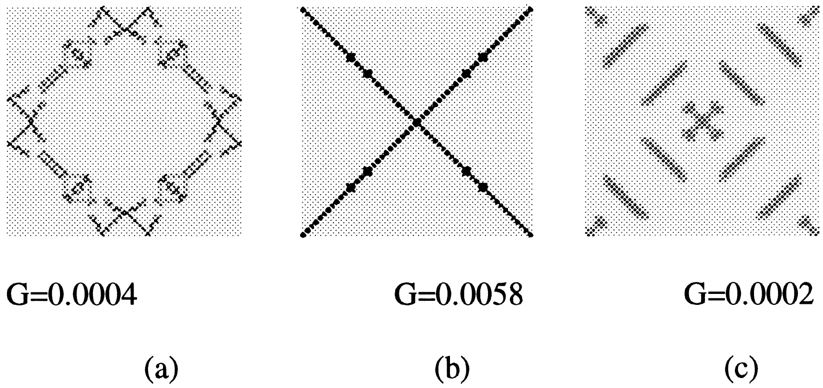


Fig. 2. Volume constraint $V_0 = 0.04|Y|$.

6.1. Example 1

The objective is to find the representative microstructural topology that maximizes the shear modulus G ($\beta_{1212} = 1$ and all others null) for given volume constraint, and material symmetry requirements.

Orthotropy material symmetry is imposed, using a quarter of the representative microstructural element together with appropriate boundary conditions (see [12]). This domain is then discretized by 28×28 square nine-node isoparametric finite elements ($Q9$). In the first application only orthotropy is considered for different volume constraints. Figs. 2–5 show the results for three different implementations using the MMA algorithm:

(a) With no control parameter (see Eq. (23))
(b) With control parameter
(c) With control parameter and mesh independence techniques

These results show that for very low volumes, the control parameter helped improving the solution, but mesh independence had some difficulties (see Fig. 2(c)). Also different topologies may be obtained for the different implementations. It is interesting to note that in the (c) implementation and higher volume constraints, the optimal G value improved. This is somewhat unexpected since using the mesh independence restricts the design space. However, note that there is no uniqueness and there are many local minima.

The second application verifies the influence of the mesh refinement for situation (a) for 14×14, 28×28, and 56×56 mesh sizes, and only orthotropy requirements. The final topologies are shown in Figs. 6 and 7.

These results show that mesh refinement may alter significantly the final topology as shown in Fig. 7. The obtained values for G improve with the refinement, although with more complex geometry. A typical number of iterations for this example was 70 iterations.

6.2. Example 2

The objective is to find the representative microstructural topology that maximizes the bulk modulus

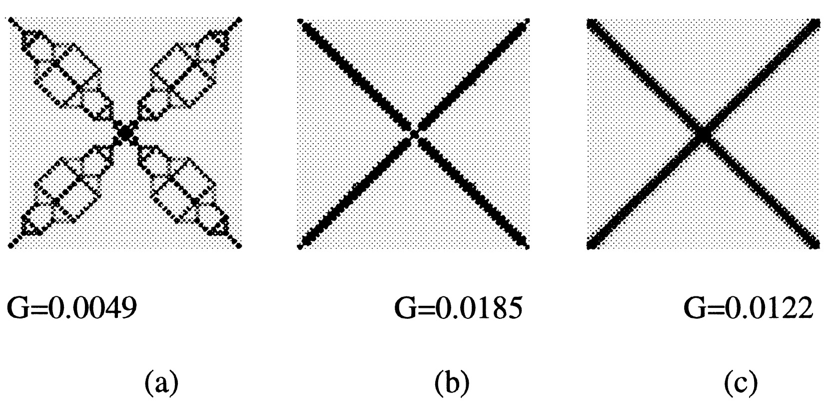


Fig. 3. Volume constraint $V_0 = 0.1|Y|$.

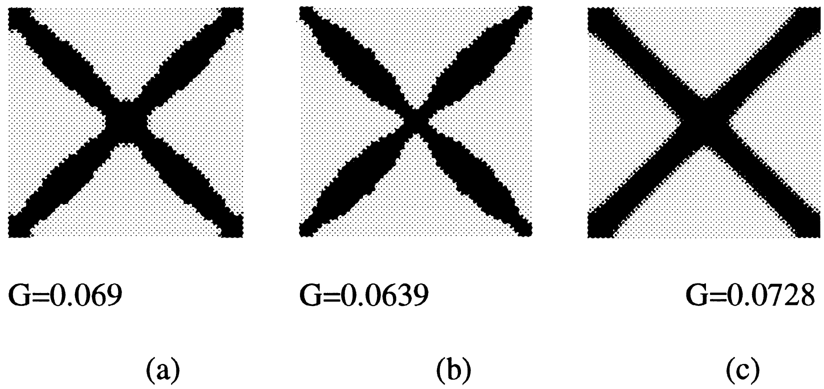


Fig. 4. Volume constraint $V_0 = 0.3|Y|$.

K ($\beta_{1111} = 0.5$, $\beta_{1122} = 0.5$ and all others null) for given volume constraint, and isotropy requirements. Orthotropy and square material symmetry is imposed, using a quarter of the representative microstructural element together with appropriate boundary conditions, and with design symmetry for 45° (see [12]). The results are shown in Fig. 8, for a mesh discretization of 28×28 $Q9$ finite elements, obtained with mesh independence and control parameter (Eq. (23)).

In Fig. 9, values of obtained bulk modulus are compared with predicted values for Hashin–Strickman bounds (Kup). The predicted values, K, are always under the Kup curve, and sometime present significant differences. It should be noted, however, that the isotropy requirement is more difficult to meet. Also from the results, it is clear that the model tries to generate sub-microstructure. Improvement can still be expected by adjusting the algorithm parameters, and choosing finer meshes. A typical number of iterations for this example was 150 iterations.

7. Final remarks

A formulation was presented for the optimal design of periodic microstructures. This formulation was generalized and a computational model was introduced using the method of moving asymptotes. To stabilize the numerical model with respect to mesh refinements and control numerical instabilities (development of checkerboard patterns) mesh independence techniques were implemented. This reduced the problem of multiple local minima, and eliminated the checkerboard instability. The introduction of isotropy requirements was a more difficult issue to handle. It was solved by a proper choice of geometry and design symmetries. In general, the method of moving asymptotes algorithm showed to be an efficient optimization tool for this type of problems.

For very low quantity of available material, the continuum approach described showed difficulties in converging to well characterized final topologies unless very refined meshes are used. In this case it could be

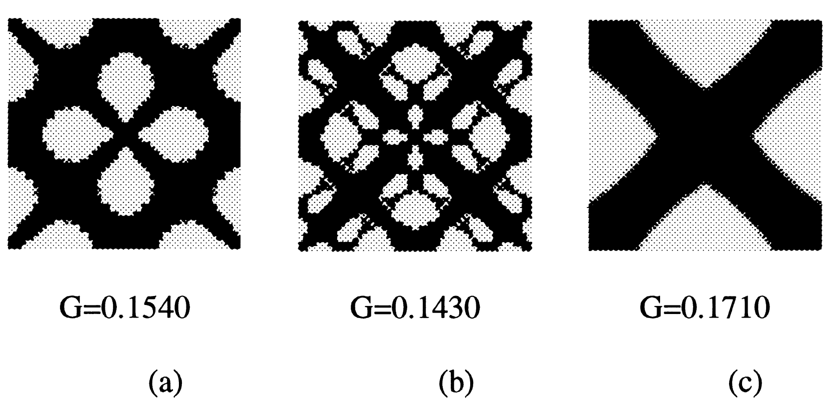
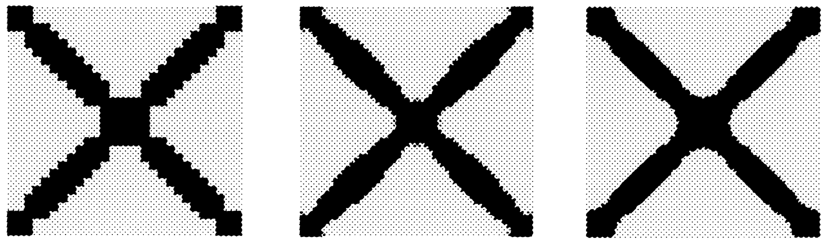


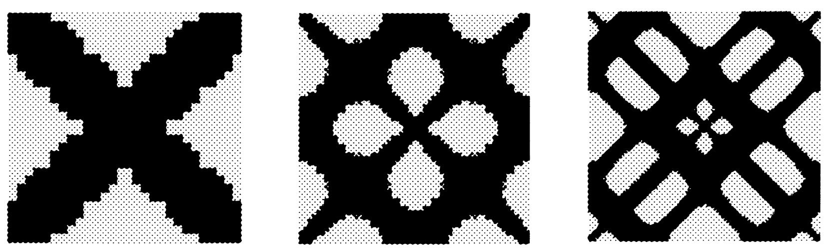
Fig. 5. Volume constraint $V_0 = 0.6|Y|$.



G=0.0631 G=0.069 G=0.0745

14x14 28x28 56x56

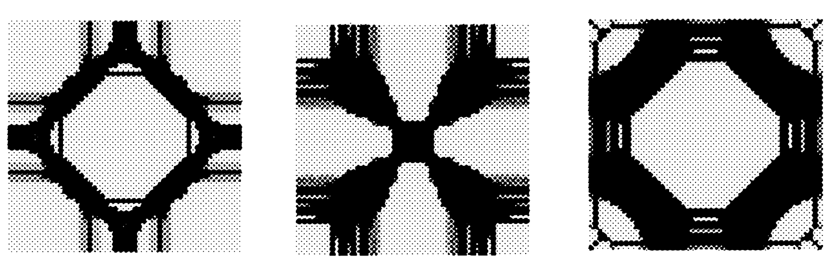
Fig. 6. Volume constraint $V_0 = 0.3|Y|$.



G=0.151 G=0.154 G=0. 160

14x14 28x28 56x56

Fig. 7. Volume constraint $V_0 = 0.6|Y|$.



K=0.0915 K=0.124 K=0. 228

$V_0 = 0.3|Y|$ $V_0 = 0.45|Y|$ $V_0 = 0.55|Y|$

Fig. 8. Bulk modulus (28 × 28).

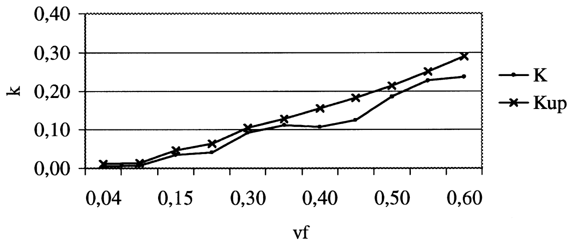


Fig. 9. Bulk modulus versus volume fraction.

advantageous to reformulate the problem in a dimensionally reduced linear elastic formulation (e.g. bars or beams) instead of a two-dimensional linear elasticity continuum model.

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