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Tailoring materials with prescribed elastic properties

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Abstract

This paper describes a method to design the periodic microstructure of a material to obtain prescribed constitutive properties. The microstructure is modelled as a truss or thin frame structure in 2 and 3 dimensions. The problem of finding the simplest possible microstructure with the prescribed elastic properties can be called an inverse homogenization problem, and is formulated as an optimization problem of finding a microstructure with the lowest possible weight which fulfils the specified behavioral requirements. A full ground structure known from topology optimization of trusses is used as starting guess for the optimization algorithm. This implies that the optimal microstructure of a base cell is found from a truss or frame structure with 120 possible members in the 2-dimensional case and 2016 possible members in the 3-dimensional case. The material parameters are found by a numerical homogenization method, using Finite-Elements to model the representative base cell, and the optimization problem is solved by an optimality criteria method.

Numerical examples in two and three dimensions show that it is possible to design materials with many different properties using base cells modelled as truss or frame works. Hereunder is shown that it is possible to tailor extreme materials, such as isotropic materials with Poisson's ratio close to -1, 0 and 0.5, by the proposed method. Some of the proposed materials have been tested as macro models which demonstrate the expected behaviour.

Keywords: Material design; Homogenization; Inverse problems; Topology optimization; Negative Poisson's ratio; Extreme materials; Micromechanics

1. Introduction

The challenging desire of being able to tailor materials with any specified elastic properties has been expressed by several researchers in recent years.

In Bendsøe et al. (1994, 1995), weight optimal structures subject to simple and multiple loading cases are obtained by a free parametrization of the elasticity tensor at each point in the structure. It is concluded that a lower bound on compliance optimization can be reached, on the condition that one can make materials with arbitrary properties only restricted to be thermodynamically admissible.

Human bone structure is known to exhibit extreme elastic properties [including negative Poisson's ratio measured by Wiliams and Lewis (1982)], and Evans (1990) points out that it is important to mimic replaced tissue as closely as possible, in order to make the best artificial replacements of human bone structure in surgery.

Another example of the need for tailoring of materials is the interesting task of constructing an "artificial" Stradivarius. In Ashby and Jones (1986) a need is expressed of designing a synthetic material

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that reproduces the acoustic properties of wood as closely as possible, in order to construct great sounding violins.

Lately, researchers have been working on the problem of designing materials with negative Poisson's ratios (first reported by Almgren, 1985; Kolpakov, 1985; Gibson and Ashby 1988). Lakes (1987) (and several following papers by the same author) describes a foam material, and Evans (1990) describes an expanded polytetrafluoroethylene material, both of which have negative Poisson's ratios, and both authors point out several important features of such materials. The materials are expected to have better indentation resistance, shock absorption and fracture toughness, and they can, for example, be used as press-fit fasteners (see, e.g. Choi and Lakes, 1991) which are easily inserted, but their removal is resisted because the fasteners expand under tension.

Stiffness, strength and other material properties can be tailored to a certain extent by varying layer directions, layer thicknesses, types, etc., in fibre/matrix materials (see, e.g. Autio et al., 1993). Dvorak (1993) tailored conduction properties of a periodic 2-phase material by varying the shape of the inclusion phase. Both these papers produce solid materials which are more or less readily manufacturable, but the attainable material properties are limited by the choice of fibre/matrix material. If we want to tailor materials with extreme properties, as demanded in the above-mentioned papers, we must consider porous or near-porous materials.

In Milton and Cherkaev (1993) materials with elastic parameters ranging over the entire scale compatible with thermodynamics are constructed by a multi-scale layering of isotropic soft and strong material. From bounds obtained by Cherkaev and Gibiansky, (1993) we know that the stiffness ratio between the strong and the soft material should be very large (greater than 25 for a specific example) in order to be able to obtain isotropic materials with negative Poisson's ratios. A layered material with Poisson's ratio close to -1 was constructed from rigid and infinitely weak material by Milton (1992). These layered materials will be difficult if not impossible to produce in practice, and therefore this paper, in conjunction with Sigmund (1994), will propose a method to construct practically more realizable microstructures with extreme parameters.

In Sigmund (1994) a method was proposed to tailor the microstructures of 2-dimensional (2-d) materials with prescribed constitutive parameters. It was numerically shown that extreme materials including materials with Poisson's ratio close to -1 and 1, were attainable by modelling the microstructures as truss structures, and that a wide range of material properties could be obtained by modelling the microstructures as continuous disks of varying thicknesses. This paper will extend the above mentioned work to 3 dimensions (3-d), and the influence of modelling the microstructure by frame elements instead of truss elements will be tested and discussed.

The periodic materials considered in this paper are described by base cells, which are the smallest repetitive unit of the material, and the developments will be restricted to linear elasticity, both in the microscopic and the macroscopic scale. Calculation of the effective constitutive parameters (homogenization) can thus be performed by analyzing the base cell only. This procedure is described several times in literature. Some examples are Bensoussan et al. (1978), Sanchez-Palencia (1980), Bakhalov and Panasenko, (1989), Aboudi, (1991), Cioranescu and Saint Jean Paulin (1986) and Nemat-Nasser and Hori (1993). Considering more complicated microstructures, analytical determination of homogenized coefficients becomes an impossible task and numerically based methods must be used. Examples of numerically based homogenization methods are the finite-element-based numerical methods described in Bourgat (1977) and Guedes and Kikuchi (1990), Fourier-series approaches described in Walker et al. (1991) and Moulinec and Suquet (1994) and boundary integral methods described in Greenbaum et al. (1993). In this paper we use the finite-element-based approach describing the homogenization formulas in terms of element mutual energies.

The problem of tailoring materials with specified constitutive parameters is formulated as an inverse homogenization problem. The aim is to find the simplest possible microstructure (base cell) which gives us the specified elastic properties. The inverse problem is formulated as an optimization problem of minimizing the structural weight of the base cell, subject to equality constraints on the constitutive parameters. The optimization problem is solved by a modified version of an optimality criteria method proposed by Zhou and Rozvany (1993).

The paper is divided into five sections. In Section 2 we discuss the notation used for constitutive properties. Section 3 describes the homogenization method used to determine the constitutive properties. Section 4 is devoted to the optimization algorithm and section 5 shows numerical examples and working models of extreme materials in 2 and 3 dimensions.

2. Constitutive relations

Materials with properties governed by the general constitutive laws in 2-d and 3-d linear elasticity are the subject of this paper. Their constitutive laws are given by

$$\{\sigma\} = [E]\{\varepsilon\} \tag{1}$$

where $\{\sigma\}$ and $\{\varepsilon\}$ are the stress and strain vectors in the reference coordinate system, and $[E]$ is the positive semi-definite constitutive matrix relating strains to stresses.

For simplicity of examples, only orthotropic materials will be considered in this paper. Axes of orthotropy will be co-aligned with the coordinate system such that the constitutive matrix can be written in 2-d as

$$\left[E^{2\text{-d}}_{\text{ort}}\right] = \begin{bmatrix} E_{11} & E_{12} & 0 \\ E_{12} & E_{22} & 0 \\ 0 & 0 & E_{66} \end{bmatrix}. \tag{2}$$

and in 3-d as

$$\left[E^{3\text{-d}}_{\text{ort}}\right] = \begin{bmatrix} E_{11} & E_{12} & E_{13} & 0 & 0 & 0 \\ E_{12} & E_{22} & E_{23} & 0 & 0 & 0 \\ E_{13} & E_{23} & E_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{66} \end{bmatrix}. \tag{3}$$

Limiting the properties of the 3-d materials further by assuming isotropy in each plane of symmetry, and assuming that the moduli in the three principal directions are equal ($E_1 = E_2 = E_3 = E$) we get the constitutive matrix

$$\left[E^{3\text{-d}}_{\text{ort,iso}}\right] = E \begin{bmatrix} \frac{1-\nu_{23}^2}{\Delta} & \frac{\nu_{12}+\nu_{13}\nu_{23}}{\Delta} & \frac{\nu_{13}+\nu_{12}\nu_{23}}{\Delta} & 0 & 0 & 0 \\ \frac{\nu_{12}+\nu_{13}\nu_{23}}{\Delta} & \frac{1-\nu_{13}^2}{\Delta} & \frac{\nu_{23}+\nu_{12}\nu_{13}}{\Delta} & 1 & 0 & 0 \\ \frac{\nu_{13}+\nu_{12}\nu_{23}}{\Delta} & \frac{\nu_{23}+\nu_{12}\nu_{13}}{\Delta} & \frac{1-\nu_{12}^2}{\Delta} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2(1+\nu_{23})} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2(1+\nu_{13})} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2(1+\nu_{12})} \end{bmatrix}, \tag{4}$$

where

$$\Delta = 1 - \nu_{12}^2 - \nu_{23}^2 - \nu_{13}^2 - 2\nu_{12}\nu_{23}\nu_{13}$$

and ν_{ij} are the Poisson's ratios for transverse strain in the j-direction subject to stress in the i-direction.

Finally assuming full isotropy ($\nu_{12} = \nu_{23} = \nu_{13} = \nu$) we have

$$[E_{\text{iso}}^{3\text{-d}}] = E\frac{1-\nu}{(1+\nu)(1-2\nu)}\begin{bmatrix} 1 & \frac{\nu}{1-\nu} & \frac{\nu}{1-\nu} & 0 & 0 & 0 \\ \frac{\nu}{1-\nu} & 1 & \frac{\nu}{1-\nu} & 0 & 0 & 0 \\ \frac{\nu}{1-\nu} & \frac{\nu}{1-\nu} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2(1-\nu)} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2(1-\nu)} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2(1-\nu)} \end{bmatrix} \tag{5}$$

and in 2-d assuming plane stress state we have

$$[E_{\text{iso,pl,stress}}^{2\text{-d}}] = \frac{E}{1-\nu^2}\begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1}{2}(1-\nu) \end{bmatrix} \tag{6}$$

Positive elastic energy requires the constitutive vector to be positive semi-definite thus the Poisson's ratio ν is restricted to the interval $]-1, 1[$ in 2-d and to the interval $]-1, 1/2[$ in 3-d.

In this paper, materials are treated only qualitatively, i.e. the factors outside the matrices in (4), (5), and (6) are considered constant and equal to unity. By simple linear scaling realistic stiffnesses dependent on material type and density should be obtainable.

Materials with extreme parameters such as materials with Poisson's ratio taking the values -1 or 0.5 in (5) are expected to show some kind of mechanism behaviour. Obviously it will be a good choice to model the material as a "thin" structure such as a micro truss structure, which can model mechanism like behaviour, or as a thin micro frame structure which in the limit corresponds to a truss structure. Numerical results in section 5 will show that the described extreme materials in 2-d and 3-d indeed can be generated from microstructures modelled by trusses or thin frames.

3. Homogenization

Structural analysis of bodies composed of materials with complex micro-structural behaviour can become an overwhelming computational task. By using "averaging" methods such as homogenization to determine macroscopic material behaviour, complexity of analysis can be reduced dramatically.

The basic idea of homogenization (or averaging) is to "smear out" complicated micro-structural behaviour of periodic materials, such that the material behaviour can be described by the (macroscopic) homogenized constitutive matrix $[E^{\text{H}}]$.

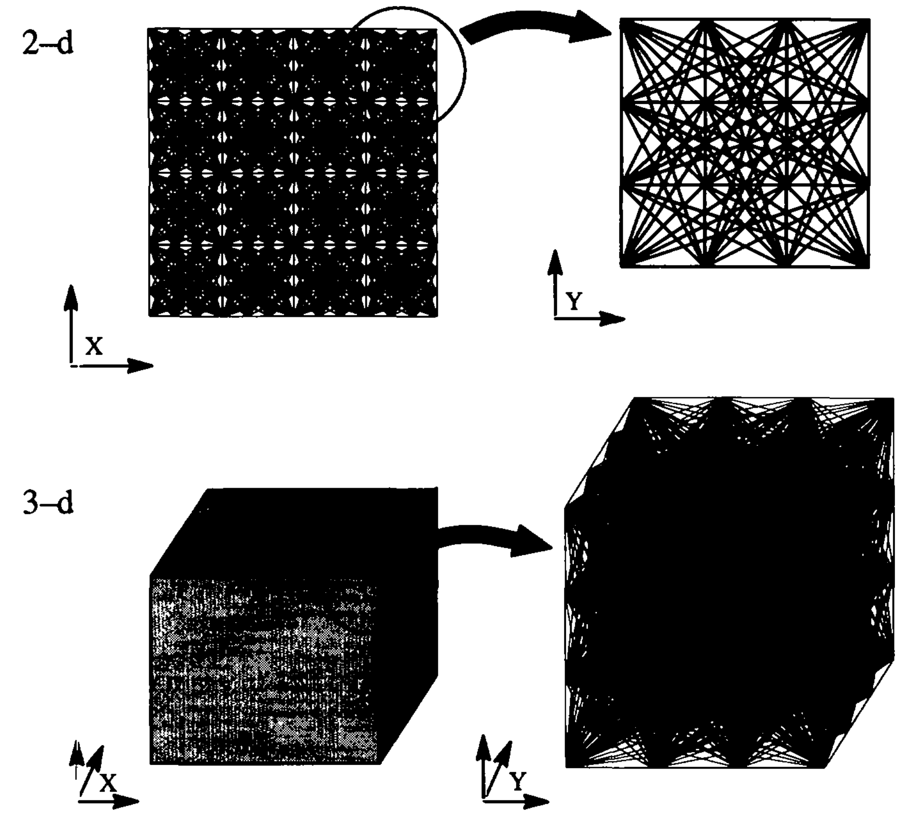


Fig. 1. Composite materials composed of truss or thin frame modelled microstructures in 2 and 3 dimensions.

We will look at the smallest representative unit of the periodic material called the base cell. The base cell represents the microstructure of the material which in this paper is modelled by truss or thin frame elements, as seen in Fig. 1.

The base cell is assumed rectangular in $\mathbb{R}^2$ or $\mathbb{R}^3$, respectively, and is defined as

$$\begin{aligned} &Y =]0, y_1^0[\times]0, y_2^0[\qquad &(2\text{-d}) \\ &Y =]0, y_1^0[\times]0, y_2^0[\times]0, y_3^0[\qquad &(3\text{-d}) \end{aligned} \tag{7}$$

where y_1^0, y_2^0 and y_3^0 are the horizontal length, vertical length and depth of the base cell, respectively.

The homogenized constitutive matrix should satisfy the following condition. The elastic strain energy of a base cell represented by its homogenized constitutive parameters $[E^{\mathrm{H}}]$, subject to any test strain field $\{\varepsilon_0\}$, should be the same as the elastic energy calculated in the microstructure subject to the same test strain field. This condition can be expressed in the following equation

$$\tfrac{1}{2}\{\varepsilon_0\}^T[E^{\mathrm{H}}]\{\varepsilon_0\} = \frac{1}{Y}\int_Y \tfrac{1}{2}(\{\varepsilon_0\} - \{\varepsilon_0\})^T[E](\{\varepsilon_0\} - \{\varepsilon\})\,\mathrm{d}Y, \tag{8}$$

where [E] is the constitutive matrix at a given point in the microstructure. The strain field $\{\varepsilon\}$, which is Y-periodic, is the induced strain field coming from the inhomogeneities of the microstructure, subject to the prestrain field $\{\varepsilon_0\}$. If the microstructure is homogeneous, $\{\varepsilon\}$ will be the zero vector, and the homogenized constitutive matrix will logically be equal to $[E]$.

To find the 6 (2-d) or 21 (3-d) homogenized parameters in $[E^{\mathrm{H}}]$, we must perform an analysis of the base cell subject to three, respectively six, linear independent test strain fields $\{\varepsilon_0^i\}$. By choosing the test strain fields as $\{\varepsilon_0^1\} = \{1, 0, 0\}$, $\{\varepsilon_0^2\} = \{0, 1, 0\}$ and $\{\varepsilon_0^3\} = \{0, 0, 1\}$ in 2-dimensions, and, similarly, with six test strain fields in 3-dimensions, we can find expressions for the individual elements of $[\mathrm{E}^{\mathrm{H}}]$, by simplifying (8) as

$$E_{ij}^H = \frac{1}{Y}\int_Y \left(\{\varepsilon_0^i\} - \{\varepsilon^i\}\right)^T [E] \left(\{\varepsilon_0^j\} - \{\varepsilon^j\}\right) dY, \quad i, j = \begin{cases} 1, \dots, 3 \text{ (2-d)} i \\ 1, \dots, 6 \text{ (3-d)} \end{cases}. \tag{9}$$

The induced strain fields $\{\varepsilon^i\}$ are found as the solutions to the standard Finite-Element equation applied to a base cell with periodic boundary conditions and subject to the test strain fields $\{\varepsilon_0^i\}$. The Finite-Element problem can be written as

$$[S]\{D^i\} = \{A_{\{\varepsilon_0^i\}}\}, \quad i = \begin{cases} 1, \dots, 3 \text{ (2-d)} \\ 1, \dots, 6 \text{ (3-d)} \end{cases} \tag{10}$$

where $[S]$ is the global stiffness matrix of the discretized base cell and $\{A_{\{\varepsilon_0^i\}}\}$ is the vector of equivalent nodal loads corresponding to the initial strain fields $\{\varepsilon_0^i\}$. The solution is given by the global displacement vector $\{D^i\}$, from which $\{\varepsilon^i\}$ is calculated by the usual strain–displacement relations. Periodicity of the displacement vector $\{D^i\}$ is imposed by giving opposing nodes the same node number in the finite-element scheme, thus forcing the opposing nodes to have the same relative displacements.

The homogenization formulas (9) and (10) correspond to the standard numerical homogenization formulas (see, e.g. Bourgat, 1977; Guedes and Kikuchi, 1991). The standard equations are derived for continuum structures under the assumption that no holes intersect the boundaries of the base cell. The truss or thin frame structures handled in this paper are therefore interpreted as "thin" continuum structures, and no elements are allowed to vanish from the ground structures shown in Fig. 1 to prevent holes on the boundaries.

Assuming that the base cell is discretized by NE finite elements (2 noded truss or frame elements) the homogenized coefficients (9) can be written as

$$E_{ij}^{\mathrm{H}} = \sum_{e=1}^{\mathrm{NE}} Q_{ij}^e, \tag{11}$$

where Q_{ij}^e expressing element mutual energies is defined as

$$Q_{ij}^e = \frac{1}{Y}\int_{Y^e} \left(\{\varepsilon_0^i\} - \{\varepsilon^i\}\right)^T [E] \left(\{\varepsilon_0^j\} - \{\varepsilon^j\}\right) \mathrm{d}Y^e, \quad \begin{cases} i, j = \begin{cases} 1, \dots, 3 \text{ (2-d)} \\ 1, \dots, 6 \text{ (3-d)} \end{cases} \\ e = 1, \dots, NE \end{cases} \tag{12}$$

and Y^e is the area of element e. In the finite-element formulation, calculation of the element mutual energies (12) is quite simple. The mutual energies can be written as

$$Q_{ij}^e = \frac{1}{Y}\left(\{d_{0e}^i\} - \{d_e^i\}\right)^T [s^e] \left(\{d_{0e}^j\} - \{d_e^j\}\right), \quad \begin{cases} i, j = \begin{cases} 1, \dots, 3 \text{ (2-d)} \\ 1, \dots, 6 \text{ (3-d)} \end{cases} \\ e = 1, \dots, NE \end{cases} \tag{13}$$

where the vector $\{d_e^i\}$ contains the components of the global displacement vector $\{D^i\}$ associated with element e. Modelling the base cell by truss elements, $[s^e]$ is the 4×4 (2-d) or 6×6 (3-d) element stiffness matrix defined in the global coordinate system. Modelling the base cell by frame elements has only been done in 2-d; in this case $[s^e]$ is the 6×6 element stiffness matrix (4 translational and 2 rotational degrees of freedom).

4. Solving the inverse problem

The aim of this paper is to find the simplest possible material with the prescribed constitutive parameters E_{ij}^{*}. This inverse homogenization problem can be formulated as an optimization problem, where we minimize the amount of material used in the base cell subject to equality constraints on the constitutive parameters E_{ij}^{H}. As shown in the last section, the constitutive parameters of a material can be expressed in terms of element mutual energies. This feature makes the optimization problem well suited for optimality criteria (OC) methods. In the following, a modified version of the OC method proposed in Zhou and Rozvany (1993) will be used.

The prescribed values E_{ij}^{*} of E_{ij}^{H} give us 6 or 21 equality constraints in 2-d and 3-d, respectively. By use of (11) the equality constraints can be written as

$$\sum_{e=1}^{\mathrm{NE}} Q_{ij}^{e} - E_{ij}^{*} = 0 \tag{14}$$

If we by other means make sure that the base cell is symmetric about all half-planes, i.e. we have an orthotropic material, the number of constraints can be reduced to 4 and 9 respectively [given by the non-zero elements in (2) and (3)]. Making use of the abbreviation $ij \to I$ defined by

$$\begin{gathered} 11 \to 1,\ 22 \to 2,\ 12 \to 3,\ 66 \to 4 \quad (\text{2-d}), \\ \left.\begin{matrix} 11 \to 1, & 22 \to 2, & 33 \to 3 \\ 23 \to 4, & 13 \to 5, & 12 \to 6 \\ 44 \to 7, & 55 \to 8, & 66 \to 9 \end{matrix}\right\} \quad (\text{3-d}), \end{gathered} \tag{15}$$

Eq. (14) can be written as

$$\sum_{e=1}^{\mathrm{NE}} Q_{I}^{e} - E_{I}^{*} = 0, \quad I = 1,\ldots,\mathrm{NC} \tag{16}$$

where NC is the number of equality constraints (NC = 4 in 2-d and NC = 9 in 3-d).

As cost function W we choose a modified measure of material volume of the base cell

$$W = \sum_{e=1}^{\mathrm{NE}} \gamma^{e} x^{e}, \quad \text{with } \gamma^{e} = l^{c}\left(\frac{l^{\mathrm{pref}}}{l^{e}}\right)^{\eta} \mu^{e}, \tag{17}$$

where the design variable x^{e} is the eth bar area in the truss case and the eth element depth in the frame case and l^{e} is the length of the eth element. A penalizing term $(l^{\mathrm{pref}}/l^{e})^{\eta}$ is added in order to be able to penalize solutions with long or short elements. l^{pref} is a preferred length of the elements, and elements longer or shorter than l^{pref} will be penalized by choosing η positive or negative, μ^{e} is another penalizing term which makes it possible to penalize elements on the surface of the 3-d base cell. Choosing μ^{e} smaller or greater than 1.0 for elements on the surfaces makes it possible to prefer one solution to another. By choosing μ^{e} smaller than 1.0, we get solutions with only interior elements, and vice versa. In Section 5 different choices of penalty factors and their influence on the solutions will be discussed.

Now we can state the optimization problem as

$$\begin{aligned} &\text{Minimize: } W = \sum_{e=1}^{\mathrm{NE}} \gamma^{e} x^{e} \\ &\text{Subject to: } \sum_{e=1}^{\mathrm{NE}} Q_{I}^{e} - E_{I}^{*} = 0, \quad I = 1,\ldots,\mathrm{NC} \text{ and: } 0 < x_{\min} \le x^{e}, \quad e = 1,\ldots,\mathrm{NE} \end{aligned} \tag{18}$$

where $x_{\min}$ is the lower limit on the design variables.

The Lagrangian function can be written as

$$\mathscr{L}=\sum_{e=1}^{\mathrm{NE}}\gamma^e x^e+\sum_{I=1}^{\mathrm{NC}}\nu_I\left(E_I^*-\sum_{e=1}^{\mathrm{NE}}Q_I^e\right)+\sum_{e=1}^{\mathrm{NE}}\alpha^e(-x^e+x_{\min}), \tag{19}$$

where the ν_I are the NC Lagrangian multipliers for the NC equality constraints and the α^e are the NE Lagrangian multipliers for the NE lower side constraints.

To make an efficient updating scheme for the design variables x^e we will use a commonly used procedure from optimality criteria methods as described in Khot et al. (1979) or Zhou and Rozvany (1993). We will use that the element mutual energies (13) for truss and 2-d frame elements are linearly dependent on the design variables (for fixed strain fields) such that $\partial Q_I^e/\partial x^e=Q_I^e/x^e$. This makes it possible to write stationarity of the Lagrangian function with respect to the design variable x^e in the simple form given by

$$\frac{\partial\mathscr{L}}{\partial x^e}=\gamma^e-\sum_{I=1}^{\mathrm{NC}}\nu_I\frac{Q_I^e}{x^e}-\alpha^e=0,\quad e=1,\dots,\mathrm{NE}. \tag{20}$$

On the basis of (20), we can formulate an updating scheme for the design variable x^e. Assuming the lower side constraint is not active (i.e. $a^e=0$), Eq. (20) can be solved for x^e,

$$x^e=\sum_{I=1}^{\mathrm{NC}}\nu_I\frac{Q_I^e}{\gamma^e}. \tag{21}$$

If (21) takes a value lower than $x_{\min}$, the value of the design variable will be set equal to the lower side constraint. Denoting elements governed by (21) active elements, and elements governed by the lower side constraint as passive, the following updating rule can be used

$$x^e=\begin{cases} x_{\min}, & \text{for } \sum_{I=1}^{\mathrm{NC}}\nu_I\frac{Q_I^e}{\gamma^e}\le x_{\min} \quad\Rightarrow x^e\in R_{\min}\\ \sum_{I=1}^{\mathrm{NC}}\nu_I\frac{Q_I^e}{\gamma^e}, & \text{for } x_{\min}\le\sum_{I=1}^{\mathrm{NC}}\nu_I\frac{Q_I^e}{\gamma^e} \quad\Rightarrow x^e\in R_{\mathrm{act}}\end{cases},\quad e=1,\dots,\mathrm{NW}, \tag{22}$$

where $R_{\min}$ and R_{act} denotes the groups of elements governed by the two updating rules.

Determination of the Lagrangian multipliers ν_I has to be done numerically by a Newton–Raphson procedure. In order to get an implicit set of equations for the Lagrangian multipliers we modify the equality constraints (16) to

$$\sum_{e=1}^{\mathrm{NE}}\frac{x^e}{x_0^e}Q_I^e-E_I^*=0,.\quad I=1,\dots,\mathrm{NC}, \tag{23}$$

where x_0^e is the value of the design variable from the preceding iteration. The factor x^e/x_0^e will be equal to unity when the procedure has converged and will therefore have no effect on the resulting optimal solution. Substituting (22) into the updating formula (23), we get

$$\phi_I=\sum_{e\in R_{\mathrm{act}}}\frac{Q_I^e\sum_{J=1}^{\mathrm{NC}}\nu_J Q_J^e}{x_0^e\gamma^e}+\sum_{e\in R_{\min}}\frac{Q_I^e x_{\min}}{x_0^e}-E_I^*,\quad I=1,\dots,\mathrm{NC} \tag{24}$$

where ϕ_I determines the errors in satisfying the Ith equality constraint. The error is minimized by the standard Newton–Raphson iterative procedure. The recurrence formula is

$$\nu_{k+1}=\nu_k-(\nabla\phi)_k^{-1}\phi_k, \tag{25}$$

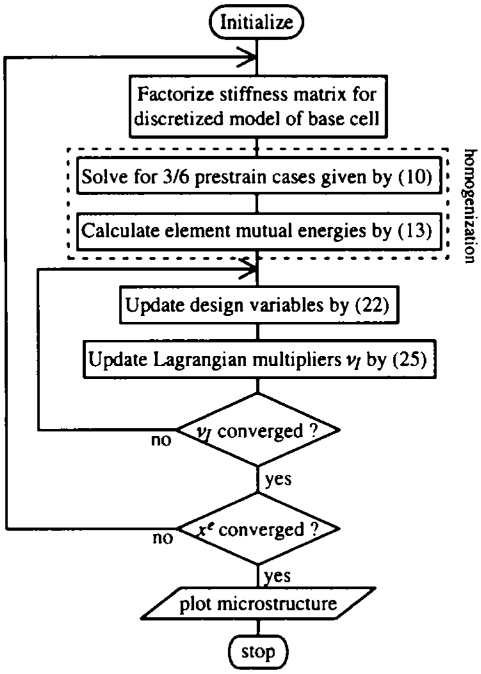


Fig. 2. Flowchart of the optimization algorithm.

where k is the iteration number and $\nabla\phi$ is the NC by NC Jacobian matrix given as

$$\nabla\phi = \frac{\partial\phi_J}{\partial\nu_I} = \sum_{e \in R_{act}} \frac{Q_I^e Q_J^e}{x_0^e \gamma^e}. \tag{26}$$

The Newton–Raphson procedure is continued until satisfactorily accuracy in obtaining the equality constraints is obtained, i.e., the procedure is stopped when $|\phi_I| < \delta$, I = 1,...,NC, where δ is a small number.

The overall computational procedure is summarized in Fig. 2.

To stabilize convergence of the optimization algorithm, design changes in the outer loop of Fig. 2 are constrained by move limits. By limiting changes in design variables to 15% of their initial value, convergence to 5 digits accuracy needed 20–50 iterations depending on the problem.

5. Examples

This section will show a number of examples demonstrating the capabilities of the proposed method. It will be shown that materials with a variety of properties, including materials with Poisson's ratios close to -1 and 0.5 (-1 and 1 in 2-d), can be constructed as truss or thin-frame modelled microstructures in 2 and 3 dimensions.

The presented results are limited to orthotropic materials with axis of symmetry co-aligned with the coordinate system, although all kinds of anisotropic and orthotropic materials with principal axes oriented in different directions can be constructed with the proposed algorithm.

In the 2-d examples all microstructures are constructed from a 4×4 node full ground structure (known from topology optimization), with all nodes connected by bar or beam elements, i.e. there are 120 potential bar members when overlapping is allowed (Fig. 1 upper right). 4 × 4 node seems to be the ideal size of ground structure. Smaller ground structures do not have enough degrees of freedom to model complicated micro mechanical behaviour, and larger ground structures tend to result in more complicated though functionally similar topologies, as will be discussed in a later example. In the 3-d examples a 4 × 4 × 4 ground structure (Fig. 1 lower right) is chosen for the same reasons as in 2-d. Connecting all nodes by bars gives 2016 potential bar members.

The aim of the optimization procedure is to find out which of the potential members of the ground structure should vanish and to find the areas of the non-vanishing members which gives the desired material parameters. As described in the optimization section vanishing members are not removed from the base cell but their areas are set to the minimum value $x_{\min}$. By choosing $x_{\min}$ approximately 10^7 times smaller than the maximum member area, element governed by the minimum constraint in (22) will have no structural significance, and they will not be shown in the examples in order to ensure simplicity of the graphics.

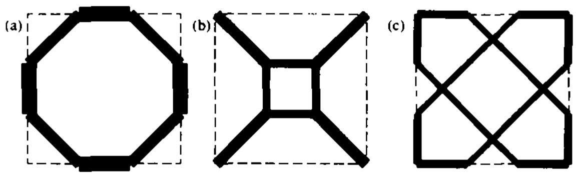
5.1. 2-dimensional examples

This section will show two examples of extreme materials in 2-d, and the difference in modelling the base cell by truss elements and frame elements of varying widths will be discussed.

In the first example we seek the material topology of a material with Poisson's ratio equal to 1. Optimizing a truss modelled base cell for the constitutive parameters obtained by inserting $\nu = 1$ in (6) (ignoring the scaling factor outside the matrix) results in several different solutions with the same structural weight – three of them are shown in Fig. 3(a)–3(c). The three different topologies are obtained by varying the penalty terms in (17) – for instance; topology 3(a) is obtained by penalizing long bars, and topology 3(c) by penalizing short bars.

The microstructure in Fig. 3(a) can be interpreted as an octagonal honeycomb cell. This is in good agreement with literature (see e.g. Ashby and Jones 1986), where standard hexagonal honeycombs are reported to have Poisson's ratio equal to 1.0. The materials represented by the base cell shown in Fig. 3 and the following examples can all be regarded as hierarchical materials (see, e.g. Lakes 1993), and they are expected to have many of the positive features of hierarchical materials pointed out in the review paper.

Another interesting example is the generation of an isotropic material with negative Poisson's ratio. Asking for a material with Poisson's ratio close to −1 the optimization algorithm returns only one simple solution (Fig. 4 left). As shown in the physical interpretation (Fig. 4 right) the base cell consists of two "stiff" quadratic frames (shown in black and grey) rotating about the center, such that expansion in one direction rotates the frames in opposite directions and thereby causes expansion perpendicular to the applied expansion. Subjected to shear, the frames will "lock" because of the periodicity conditions.



$$[E^H] = \begin{bmatrix} 1.0 & 1.0 & 0.0 \\ 1.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix}$$

Fig. 3. Microstructures of materials with Poisson's ratio close to 1.0.

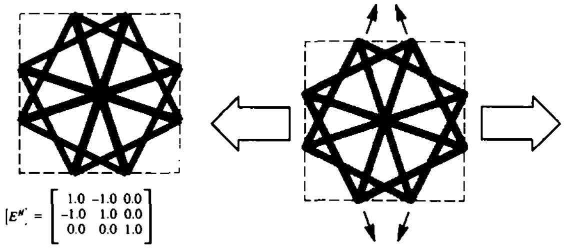


Fig. 4. 2-d base cell of an isotropic material with Poisson's ratio close to -1.0 (left). The physical interpretation (right) shows that the material is composed of two stiff frames (shown in black and grey) free to rotate about their centers. When pulled horizontally (big arrows) the frames will rotate in the directions of the small arrows and thus expand vertically.

To test the function of the negative Poisson's ratio material, a model of the material consisting of an array of 4×4 connected base cells was constructed in the lab (Fig. 5). The model consists of two thin layers of celluloid, put on top of each other, and placed between two stiff transparent plates. Fig. 6 shows the mechanical behaviour of the working model. Comparing the picture of the unstressed material (Fig. 6 left) with the stressed version (Fig. 6 right) the deformation mechanism is seen clearly. A relevant criticism of the proposed microstructures is that, in practice, it is unrealistic to produce trusses on a very small scale. A more realistic possibility is to generate the materials from "micro frames" as encountered in human bone structure (see, e.g. Gibson and Ashby, 1988) or in open-cell polymer foams by Lakes (1987).

It was noted earlier that a more complicated starting guess than the 4×4 node groundstructure does not give rise to better microstructures. Two examples of this are shown in Fig. 7 where the resulting microstructures for a Poisson's ratio 1 (Fig. 7 left) and -1 (Fig. 7 right) material based on a 6×6 node groundstructure with 630 potential bar members are shown. The Poisson's ratio 1 microstructure (Fig. 7 left) can be compared with Fig. 3(c) – only differences are the coordinates of the nodal points. The

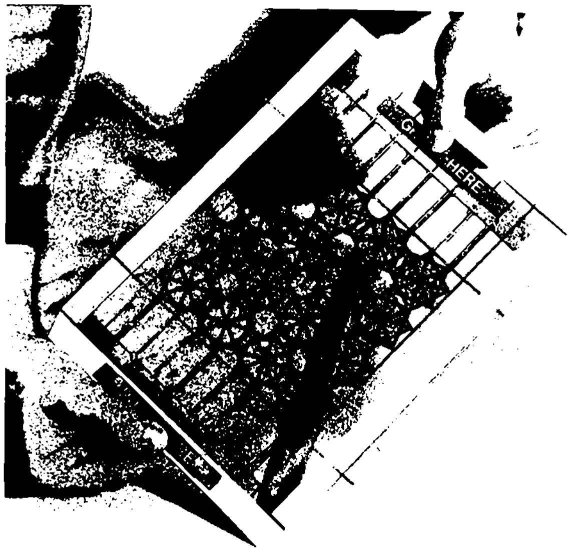


Fig. 5. Working model consisting of an array of 4×4 base cells of the proposed negative Poisson's ratio material from Fig. 4.

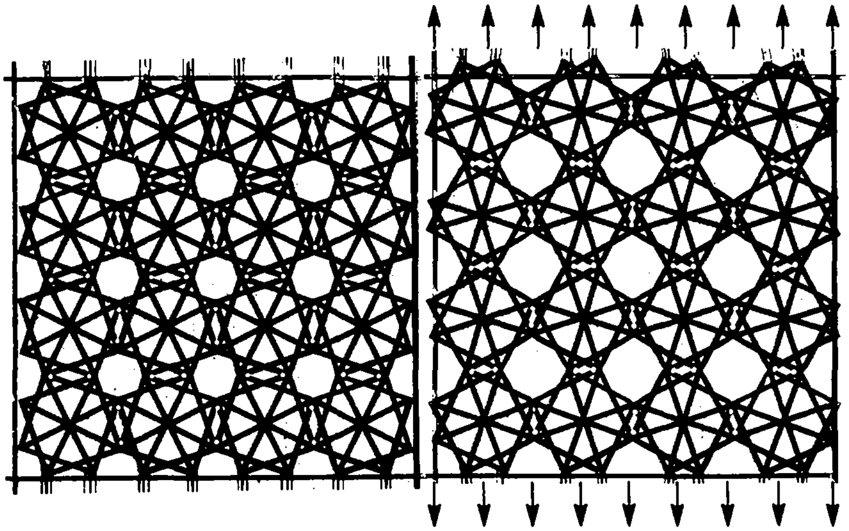


Fig. 6. Working model of the proposed negative Poisson's ratio material from Fig. 4. The undeformed material consisting of an array of 4×4 base cells is shown left. Expanded vertically we get the deformation pattern shown right.

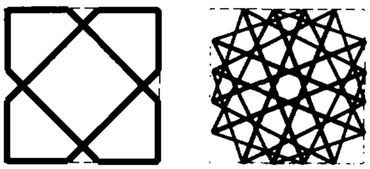


Fig. 7. Effect on choosing more complicated starting guesses. Poisson's ratio 1 (left) and −1 (right) microstructures are based on 6×6 node ground structures with 630 potential bar members.

Poisson's ratio −1 microstructure (Fig. 7 right) can be compared with Fig. 4, in this case we see that starting with a more complicated groundstructure results in a more complicated though functionally similar solution.

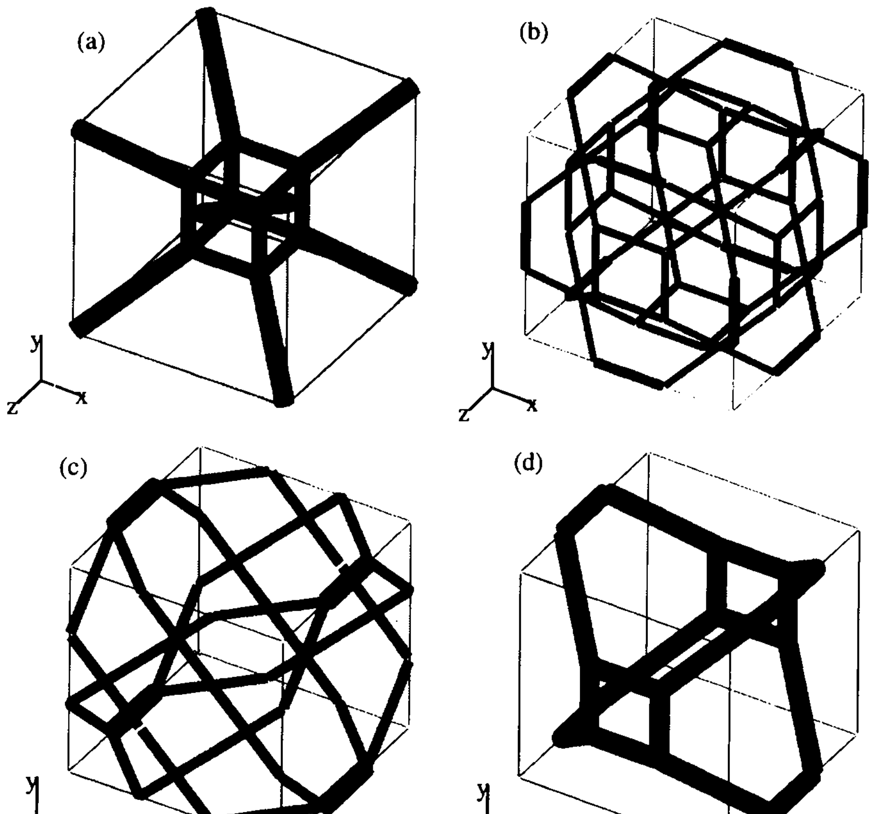
The difference in modelling the base cell as a truss or a frame structure with varying beam thickness is demonstrated in Table 1. The first row in the table shows the attainable Poisson's ratio for a truss modelled base cell. It is seen that the extreme values ($\nu = 1$ and $\nu = -1$) cannot be obtained even for

Table 1
Attainable values of Poisson's ratio from base cells modelled by frame elements with different thicknesses

Beam thickness in % of base cell dimension	$\nu = 1$ Attainable Poisson's ratio	$\nu = -1$ Attainable Poisson's ratio
0 (truss)	0.99996	−0.9998
1	0.9993	−0.997
2	0.997	−0.990
5	0.984	−0.94
10	0.94	−0.80
20	0.79	−0.63

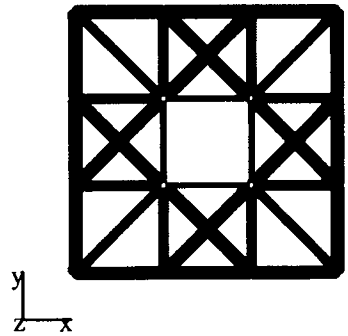
truss modelled materials. This is due to the fact that the elements governed by the minimum thickness constraint $x_{\min}$ prevent the base cell in becoming a true mechanism. The next rows in the table show the attainable values of Poisson's ratio for frame modelled microstructures of increasing thickness. It is seen that modelling the base cell from thick frame elements "damps" out extreme material behaviour as expected. Maximum beam thickness in the table is restricted to 20% of the base cell size. Allowing for thicker beams the microstructure should be thought of as a continuum with small holes (see, e.g. Sigmund, 1994).

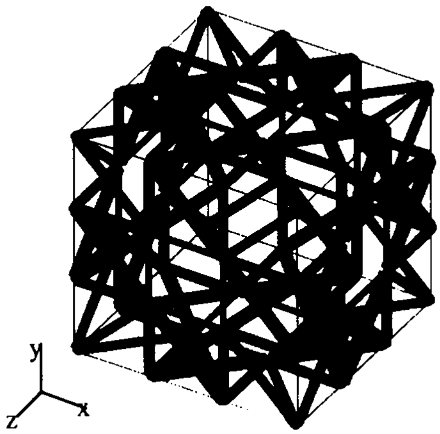
Although not shown graphically, it should be noted that the optimal material topologies for frame modelled base cells are apparently the same as for truss modelled base cells. This means that it is not so important to optimize the base cells using frame elements which, especially in 3-d, is a computationally more complicated task than the truss case (the number of degrees of freedom is twice that of the truss case). Having optimized a truss modelled base cell, we will assume that the frame modelled microstruc-



$$[E^H] = \begin{bmatrix} 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \end{bmatrix}$$

Fig. 8. 3-d base cells of isotropic materials with Poisson's ratio close to 0.5.





$$[E^H] = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.5 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.5 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.5 \end{bmatrix}$$

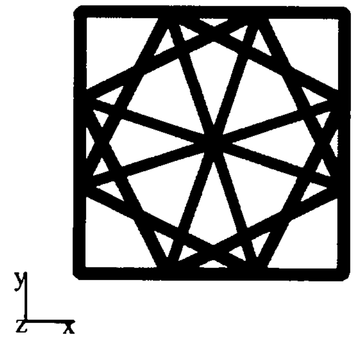
Fig. 9. 3-d base cell of an isotropic material with Poisson's ratio 0.

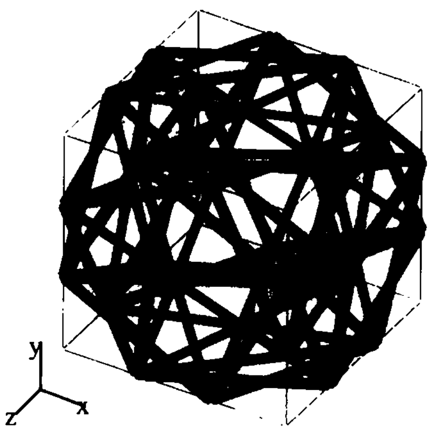
ture can be constructed from the same topology, but it must be taken into account that the material parameters will be "damped" according to Table 1.

For further examples and discussion of 2-d materials with various constitutive properties, the reader is referred to Sigmund (1994).

5.2. 3-dimensional examples

This section will show examples of 3-d microstructures with various material parameters, and their similarity with 2-d microstructures will be discussed.





$$[E^H] = \begin{bmatrix} 1.0 & -.5 & -.5 & 0.0 & 0.0 & 0.0 \\ -.5 & 1.0 & -.5 & 0.0 & 0.0 & 0.0 \\ -.5 & -.5 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.75 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.75 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.75 \end{bmatrix}$$

Fig. 10. 3-d base cell of an isotropic material with Poisson's ratio close to −1.0. The base cell is a cube where the six sides are build up by rotatable frames like in the 2-d case (Fig. 4).

Asking for a 3-d isotropic material with Poisson's ratio close to 0.5, the optimization algorithm returns several different topologies depending on choice of penalty factors, symmetry requirements and starting guess. Four of the resulting microstructures which have equal structural weight are shown in Fig. 8(a)–(d).

Figs. 8(a) and 8(b) show Poisson's ratio 0.5 materials with full cubic symmetry. It is interesting to see that the microstructure in Fig. 8(a) corresponds to a 3-d version of the 2-d microstructure shown in Fig. 3(b). Although Fig. 8(b) has an apparently more complicated microstructure this material too is composed of 2-d microstructures, namely a combination of those from Figs. 3(a) and 3(b). Both Fig. 8(a) and 3(b) have bars in the interior of the base cells. It was tried to find a cubic symmetric Poisson's ratio 0.5 material with surface bars only by choosing the penalty factor μ^e in (17) equal to 0.5, i.e. bars on the surfaces are made "cheaper" than interior bars. This approach does not result in any solution, which was seen in lack of convergence of the optimization algorithm. In order to obtain a "surface" solution, requirements on symmetry are lessened, i.e. only symmetry about the three coordinate planes individually are required instead of the full cubic symmetry. This lessening of symmetry requirement results in the microstructure shown in Fig. 8(c). This microstructure too is seen to be composed of 2-d microstructures, namely Fig. 3(c) in the *xy*-plane and Fig. 3(a) in the *yz*- and *zx*-planes. Lessening the symmetry requirements also results in another "interior" solution shown in figure 8(d) which actually is a simple version of figure 8(b). We note that it is possible to construct isotropic materials which are not cubic symmetric in the microstructure.

A base cell of a material with Poisson's ratio equal to zero is shown in Fig. 9. The solution is obtained by penalizing interior bars, thus the microstructure only has bars on the surface, but still it has a very complex microstructure.

Another interesting example in 3-d is the tailoring of an isotropic Poisson's ratio -1.0 material. The first solution for this problem, which is obtained without any penalty factors, results in a very complicated microstructure with a lot of crossing and overlying bars. The solution is structurally quite expensive and will not be shown here. Experiments with penalty factors ($\mu^e = 0.5$, $\eta^e = -1.0$ and $l^{pref} = 0.5$) leads to a much nicer solution which is shown in Fig. 10. The microstructure in Fig. 10 has only exterior bars, and is seen to be build up by rotatable frames like the 2-d case (Fig. 4).

A $15 \times 15 \times 15$ cm working model of this microstructure was build in the lab, consisting of 72 plastic tubes connected by bent pieces of thin wire (Fig. 11). The test cube works nicely which means that if compressed vertically, it will also compress in the two other directions. The negative Poisson's ratio

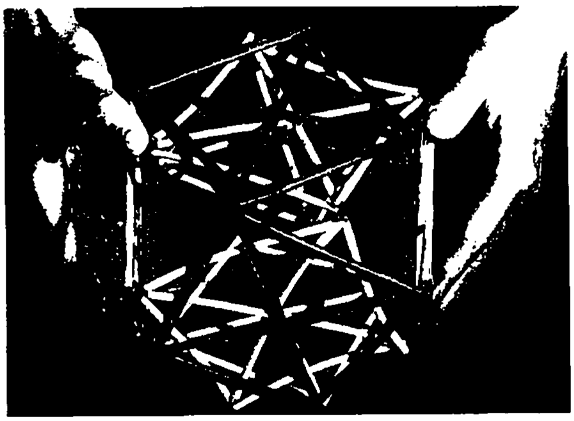
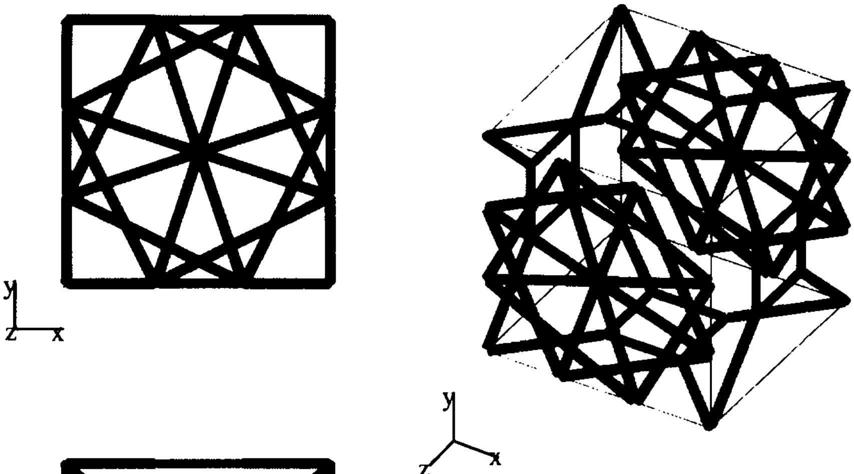
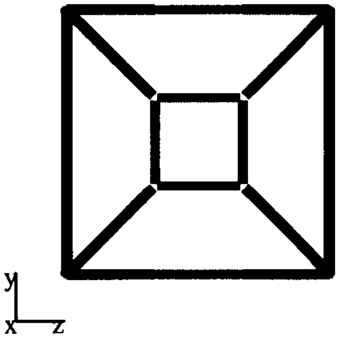


Fig. 11. Working model of the Poisson's ratio -1 material shown in Fig. 10.





$$[E^H] = \begin{bmatrix} 1.0 & -.5 & .5 & 0.0 & 0.0 & 0.0 \\ -.5 & 1.0 & .5 & 0.0 & 0.0 & 0.0 \\ .5 & .5 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.75 \end{bmatrix}$$

Fig. 12. 3-d base cell of an isotropic material with Poisson's ratio -1.0 in the xy-plane and Poisson's ratio 1.0 behaviour in the yz- and zx-planes.

behaviour of the base cell, is, of course, limited to the point where the rotating square frames become parallel.

The last example will show that it is also possible to tailor 3-d materials with different behaviour in different directions. Asking for Poisson's ratio -1.0 behaviour in the xy-plane and Poisson's ratio 0.5 behaviour in the yz- and zx-planes we get the 3-d microstructure shown in Fig. 12. Examining Fig. 12, we notice that the microstructure is composed of the 2-d microstructures in Fig. 3(b) and Fig. 4. It can furthermore be seen that the xy-plane with Poisson's ratio -1 behaviour is not connected to the two other planes.

The 3-d microstructures in this section were obtained independently of the 2-d results and they all came from the 2016 bar ground structure (Fig. 1). Results in this section indicates that 3-d materials with arbitrary structural behaviour can be composed by "braiding" of 2-d microstructures into 3-d microstructures with small modifications.

6. Discussion

As shown in the previous sections, we have obtained a numerical method to tailor materials with prescribed elastic properties.

Material parameters of the truss and frame modelled periodic materials in 2 and 3 dimensions are found by a numerical homogenization procedure. The tailoring problem is formulated as an optimization problem of finding the simplest possible microstructure with constraints given by the specified elastic constants. As a starting guess to the optimization problem we use a groundstructure approach known from topology optimization.

Examples of a variety of materials with prescribed parameters were tailored by the proposed method. Asking for a material with some prescribed constitutive properties generally resulted in several, topologically different solutions depending on starting guess and size of move limits in the optimization algorithm. A penalty term in the cost function of the optimization algorithm makes it possible to penalize solutions with long or short bars, or to prefer solutions without bars in the interior of the base cell. Experimenting with the penalty parameters makes it possible to control the solutions and thereby to find the materials with the simplest possible microstructures.

By examination of the resulting 3-dimensional microstructures, it is concluded that materials with specified constitutive properties can be composed by "braiding" and minor modifications of 2-dimensional microstructures. This conclusion indicates that the study of material mechanisms in porous materials can be concentrated on the 2-dimensional case which is intuitively and computationally simpler than the 3-dimensional case.

Two of the proposed microstructures have been tested in simple experiments. A working model of the proposed Poisson's ratio-1 material was build as a single base cell in 3 dimensions, and as a small array of base cells in 2-d. Both models showed the expected behaviour.

The proposed materials are not readily manufacturable, but a first approach to build them could be by rapid prototyping (suggested in Lakes (1993) for other microstructures). A CAD-model of the repeated microstructure could be given as input to the rapid prototyping machinery and would result in a practical, though still very coarse, model of the material. The author hopes to build such "test-materials" in the near future.

The final step should be to produce the proposed materials in real micro scale. Current progress in the fields of molecular modelling, polymers (see, e.g. Evans, 1990) and crystal growth indicates that it will be possible (in future) for skilled chemists or physicists to synthesize the proposed microstructures.

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