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Simultaneous Design of Optimal Shape and Local Cubic Material Characteristics

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This paper deals with the minimum compliance problem of the femur bone made of a non-homogeneous elastic material with cubic symmetry. The elastic moduli as well as the trajectories of anisotropy directions are design variables. The isoperimetric condition determines the value of the cost of the design expressed as the integral of the trace of the Hooke's tensor. The optimum design is found for a selected design domain and a single load case. The optimal cubic material characteristics are reflected by the properties of the underlying microstructure. Admissible microstructures are reconstructed, thus delivering a deeper insight into the optimum design. The obtained microstructures are second- rank laminates composed of an isotropic material and voids. To eliminate the degeneracy of the design at least three load cases should be considered.

Key words: topology optimization, cubic material design, discrete homogenization.

1. Topology optimization by the cubic material design method

The aim of the cubic material design (CMD) is to construct – within a given feasible domain – the stiffest structure capable of transmitting a given load to a given boundary support by appropriate choice of the material characteristics of the cubic symmetry class. The cubic material design has been recently proposed by Czubacki and Lewiński in [3] in the 3D setting and here its 2D setting is used to study the femur bone problem, which was studied previously within the isotropic material design (IMD) approach in Goda *et al.* [4].

1.1. Description of the cubic material design (CMD) method

In the CMD method, at each point of the structure's six parameters: a triplet $(\mathbf{m}, \mathbf{n}, \mathbf{p})$ of mutually orthogonal unit vectors and three elastic moduli (a, b, c) are to be determined. Since in this paper a 2D setting is dealt with, only two vector fields $(\mathbf{m}, \mathbf{n})$ describing orientation of the material are to be found. The Hooke's tensor of a material with cubic symmetry is represented by the formula (see WALPOLE [6]):

$$\mathbf{C} = a\mathbf{J} + b\mathbf{L} + c\mathbf{M}, \tag{1.1}$$

where a, b, c are elastic moduli and the fourth-rank tensors $\mathbf{J}$, $\mathbf{L}$, $\mathbf{M}$, for 2D case, are expressed as follows:

$$\begin{gathered} \mathbf{J} = \frac{1}{2}\overset{2}{\mathbf{I}}\otimes\overset{2}{\mathbf{I}}, \qquad \mathbf{L} = \overset{4}{\mathbf{I}} - \mathbf{S}, \\ \mathbf{M} = \mathbf{S} - \mathbf{J}, \qquad \overset{2}{\mathbf{I}} = (\delta_{ij}), \qquad \overset{4}{\mathbf{I}} = \left(\frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{kj}\right)\right), \\ \mathbf{S} = \mathbf{n}\otimes\mathbf{n}\otimes\mathbf{n}\otimes\mathbf{n} + \mathbf{m}\otimes\mathbf{m}\otimes\mathbf{m}\otimes\mathbf{m}. \end{gathered} \tag{1.2}$$

In the considered 2D case, the eigenvalues of $\mathbf{C}$ are: $\{a, b, c\}$ and thus $\mathrm{tr}\mathbf{C} = a + b + c$. The cost of the design Λ is assumed as the integral of the trace of the Hooke's tensor over the design domain Ω:

$$\int_\Omega (a + b + c)dx = \Lambda, \tag{1.3}$$

where Λ will be represented as $\Lambda = |\Omega|\, E_0$, with E_0 being a referential elastic modulus.

The minimum compliance problem of the CMD method is formulated as follows: find the layout of elastic moduli a, b, c and the orthogonal trajectories of the vector fields $(\mathbf{m}, \mathbf{n})$ at each point of the feasible domain Ω satisfying the isoperimetric condition (1.3), such that the structure made of material with cubic symmetry is characterized by the smallest total compliance among all the structures designed in the same feasible domain, obeying the same isoperimetric condition and capable of transmitting the same load to the same boundary.

The total compliance of the structure is expressed by the Castigliano formula:

$$Y = \min_{\boldsymbol{\tau}\in\Sigma(\Omega)} \int_\Omega \boldsymbol{\tau}\cdot(\mathbf{C}^{-1}\boldsymbol{\tau})dx, \tag{1.4}$$

where $\Sigma(\Omega)$ is a set of statically admissible stress fields.

Due to an exceptional mathematical structure of the minimum compliance problem, as it has been delivered in [3], the minimization operation over the design variables could be performed analytically and exactly. Upon eliminating all the design variables one finds the final formula for the optimal compliance. Thus, this formula is independent of the material data and can be written as $S = Z^2/\Lambda$, with Z being a number given by the minimization problem:

$$Z = \min\left\{ \int \left(\frac{\sqrt{2}}{2} |\mathrm{tr}\, \boldsymbol{\tau}| + \|\mathrm{dev}\, \boldsymbol{\tau}\| \right) | \boldsymbol{\tau} \text{ being statically admissible} \right\}. \tag{1.5}$$

The latter problem is expressed by the load, kinematic boundary conditions and the design domain.

The integral in problem (1.5) is similar to an integral in a formula that appears in the IMD put forward in [1]. Due to the similarity of CMD and IMD methods a stress field $\boldsymbol{\tau}^*$, which minimizes (1.5), can be found by using the numerical algorithm described in Czarnecki [1] and Czarnecki and Wawruch [2].

According to the main result of [3] the optimal vector fields $\mathbf{m}$, $\mathbf{n}$ follow the trajectories of principal stresses $\boldsymbol{\tau}^*$, and the optimal values of the moduli a, b, c are determined by the minimizer $\boldsymbol{\tau}^*$:

$$a(x) = \frac{\Lambda}{Z} \frac{|\mathrm{tr}\, \boldsymbol{\tau}^*(x)|}{\sqrt{2}}, \qquad b(x) = 0, \qquad c(x) = \frac{\Lambda}{Z} \|\mathrm{dev}\, \boldsymbol{\tau}^*(x)\|. \tag{1.6}$$

Hence the optimal tensor reads

$$\mathbf{C} = a\mathbf{J} + c\mathbf{M}. \tag{1.7}$$

In the optimal frame $\mathbf{m}$, $\mathbf{n}$, the elastic moduli are:

$$C_{1111} = C_{2222} = \frac{1}{2}a + \frac{1}{2}c, \qquad C_{1122} = \frac{1}{2}a - \frac{1}{2}c, \qquad C_{1212} = 0. \tag{1.8}$$

Despite the singularity of the Hooke's tensor, the elasticity problem with optimal moduli is solvable: the stress field in the optimal body is unique and coincides with $\boldsymbol{\tau}^*$.

1.2. Optimal layout of moduli of the cubic material

We consider the 2D model of a femoral bone shown in Fig. 1a. This problem for IMD was discussed by Goda *et al.* [4]. Under the same data, the optimum design of the femur with an assumption that it is made from a material with the pointwise property of cubic symmetry is here constructed by solving the problem (1.5). The optimal moduli are computed by (1.6) at Gauss points and then interpolated to the whole design domain. In this design the stress trajectories determine the pair of unit vectors with cubic symmetry, see Fig. 1b. Irregularities of the trajectories of stresses occur due to the numerical procedure based on the mesh being irregular.

a) b)

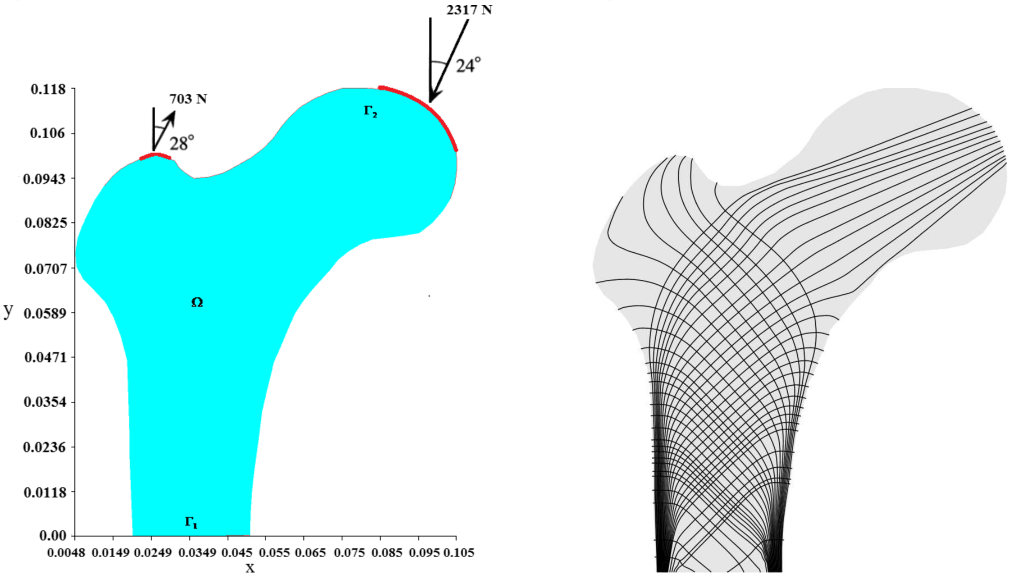

FIG. 1. a) Setting of the static problem, b) trajectories of principal stresses in the optimal body.

Both the moduli a, c assume maximal values along the boundaries close to the fixed lower edge. The violet-coloured domains are empty, indicating that there is no material, cf. Figs. 2a and 2b.

a) b)

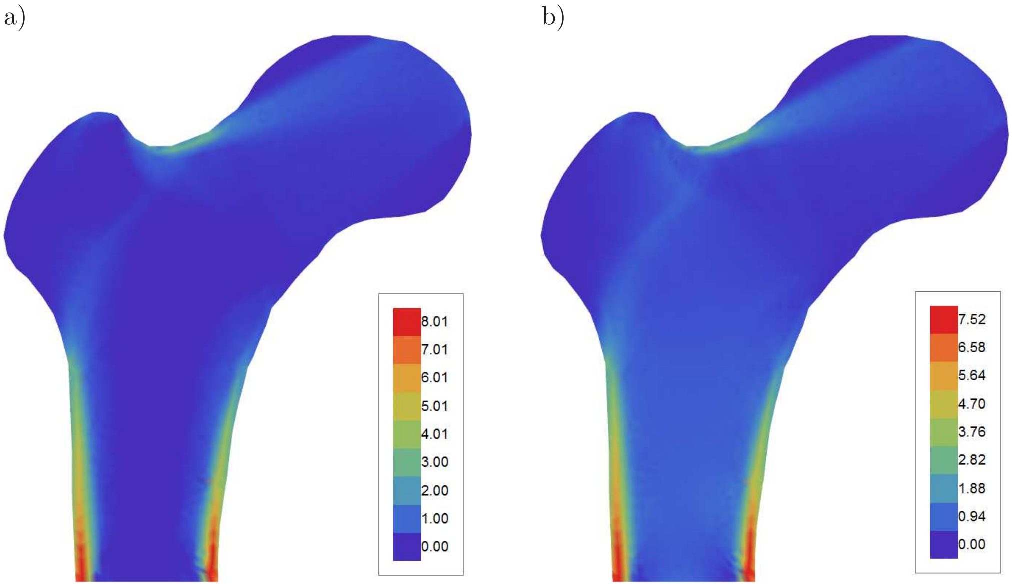

FIG. 2. Optimal layouts of: a) elastic modulus $a/(100E_0)$, b) elastic modulus $c/(100E_0)$.

2. The underlying microstructure

For regions where $a \neq 0$ the material with cubic symmetry can be reconstructed by the second-rank in-plane laminate composed of voids and an isotropic material (denoted as material 2) with bulk modulus k and shear modulus μ. The voids play the role of a core, while material 2 is the coating. This kind of microstructure is called a *stiff laminate* and the formulae for the corresponding effective moduli are derived in Sec. 24.2 in [5]. To be more specific we consider the laminate of second-rank made by stacking together an isotropic material 2 with the homogenized material h which is a first-rank laminate made of material 2 and the voids, with volume fractions θ_2, $\theta_1 = 1 - \theta_2$, respectively. Material 2 is mixed with material h with proportions: ω_2, $\omega_1 = 1 - \omega_2$. The resulting area fraction of the isotropic material equals $m_2 = \omega_2 + \theta_2\omega_1$, while the area fraction of voids is $m_1 = \theta_1\omega_1 = 1 - m_2$, see Fig. 3.

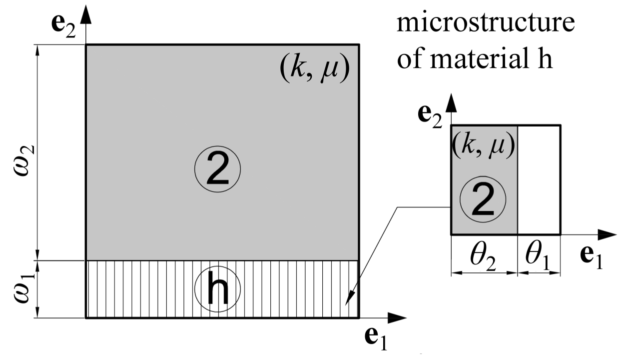

Fig. 3. The second-rank stiff laminate. The isotropic material 2 plays the role of the coating.

Upon finding the optimal layouts of the moduli a and c, see Fig. 2, we proceed to reconstruct the underlying microstructure. Thus, at all points the values of moduli $a > 0$, $c > 0$ are known. Let us introduce a point-wise non-dimensional parameter ε according to the rule presented below:

$$0 < \varepsilon < \varepsilon_0, \qquad \varepsilon_0 = \begin{cases} \dfrac{c}{2(a-c)} & a > c, \\ \infty & a \leqslant c. \end{cases}$$

Let us take

$$\mu_\varepsilon = \left(\frac{1}{2} + \varepsilon\right) c$$

and define

$$k_\varepsilon = \frac{ac\mu_\varepsilon}{ac + 2(c-a)\mu_\varepsilon}, \qquad \theta_1^\varepsilon = \frac{(a+c)\mu_\varepsilon}{c(a+2\mu_\varepsilon)}, \qquad \omega_1^\varepsilon = 2 - \frac{1}{\theta_1^\varepsilon}, \tag{2.1}$$

while

$$m_1^\varepsilon = \theta_1^\varepsilon \omega_1^\varepsilon, \qquad m_2^\varepsilon = 1 - m_1^\varepsilon.$$

Then, the following estimates hold:

$$k_\varepsilon > 0, \qquad 0.5 < \theta_1^\varepsilon < 1, \qquad 0 < \omega_1^\varepsilon < 1.$$

The membrane stiffnesses of the second rank laminate shown in Fig. 3 and with moduli given by (2.1) are equal to the membrane stiffnesses of a plate made of a material with cubic symmetry and elastic moduli (1.8). The basis $(\mathbf{e}_1, \mathbf{e}_2)$ in Fig. 3 coincides with the directions of principal stresses shown in Fig. 1b. Let us define the cost density of material as

$$\Upsilon(\varepsilon) = (2k_\varepsilon + 4\mu_\varepsilon) m_2^\varepsilon \tag{2.2}$$

proportional to the scalar $\mathrm{tr}\mathbf{C}_{\mathrm{iso}}$, where $\mathbf{C}_{\mathrm{iso}}$ is Hooke's tensor for the isotropic material 2.

Let us note that if $\varepsilon \to 0$ then

$$k_\varepsilon \to a/2, \qquad \mu_\varepsilon \to c/2, \qquad \theta_1^\varepsilon \to 0.5, \qquad \omega_1^\varepsilon \to 0.$$

Both the moduli k_ε, μ_ε decrease when ε tends to 0. Moreover,

$$\Upsilon(\varepsilon) \underset{\varepsilon \to 0}{\longrightarrow} a + 2c.$$

Thus, the microstructure of least cost (2.2) corresponds to vanishing values of ε.

3. Final remarks

Bone microstructures corresponding to the class of cubic symmetry can be encountered in the literature on cancellous bones with regular networks of trabeculae with rod-like architecture, as described, e.g., in [7]. In the 2D case such rod-like microstructures may be modelled by the second-rank in-plane laminates discussed in the present paper. They are characterized by zero shear moduli. Despite this degeneracy the presented optimal solution shows a spatial distribution of effective moduli and principal stress directions in good qualitative agreement with those observed in real bone microstructures, and with the results similar to those obtained in [4], although for a different type of material symmetry (isotropic material design and orthotropic classes). This tends to indicate that virtual bone microstructures predicted by such optimality principles are not very sensitive to the assumed class of symmetry.

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