ASPECTS OF TOPOLOGY OPTIMIZATION AND BONE-REMODELLING SCHEMES

Martin P. Bendsøe
Department of Mathematics, Technical University of Denmark,
DK-2800 Lyngby, Denmark

January 2003

1 Introduction

The basic idea of the material distribution method for topology design of structures is to describe a structure by a "raster representation" of grey scales, where grey is interpreted as a density of material. This allows the simultaneous optimization of the topology, shape and sizing of a structure, see, for example, Bendsøe & Sigmund (2003)[1].

Models for bone remodelling and optimal design have mutually provided inspiration for new developments in either area, (see for example Pedersen & Bendsøe (1999) for a collection of papers dealing with such aspects and the brief litterature survey at the end of these notes). There is a close similarity between the well-known optimality criteria algorithm for minimum compliance design and schemes for bone remodelling. Also, in many isotropic remodelling algorithms, the relationship between density and the elasticity modulus of cancellous bone is modelled exactly as in the popular SIMP scheme for topology design. Furthermore, when orthotropy is taken into account, Wolff's law for bone predicts that stresses and material axes are aligned, exactly as for minimum compliance design.

Even though it is commonly agreed that *bone does not attain, from a structural optimization point of view, a stable optimal configuration with respect to any given static loads*, the similarity between the two types of modelling has suggested that *optimal remodelling*, that is, a step-wise optimization process, will provide a useful framework for the simulation the bone-adaptation.

2 The topology optimization framework

The purpose of topology optimization is to find the optimal layout of a structure within a specified region. The topology and shape of the structure is represented by a parametrization of the stiffness tensor and it is this parametrization which leads to the design formulations that we will briefly address in the following.

2.1 Minimum compliance design

We consider a mechanical element as a body occupying a domain $\mathsf{D}^{\mathrm{mat}}$ which is part of a larger reference domain D . Referring to D we define the optimal design problem as the problem of finding the optimal choice of elasticity tensor E which is a variable over the domain.

When solving optimal design problems by computational means a typical approach is to

[1] Further literature can be found in the bibliography section at the end of this brief note.

discretize the problem using finite elements as

$$\begin{aligned} \min_{\mathbf{u},\mathbf{E}=(E^1,\dots,E^N)} \quad & \mathbf{p}^T\mathbf{u} \\ \text{s.t.}: \quad & \mathbf{K}(\mathbf{E})\mathbf{u} = \mathbf{p} \ , \\ & E^e \in \mathsf{E}_{\text{ad}}, \ e = 1,\dots,N \ . \end{aligned} \tag{1}$$

Here $\mathbf{u}$ and $\mathbf{p}$ are the displacement and load vector, respectively, and we use the same finite element mesh for both fields of interest, $\mathbf{u}$ and $\mathbf{E}$, and discretize E as constant in each element. The stiffness matrix $\mathbf{K}$ depends on the stiffness E_e in element e, numbered as $e = 1,\dots,N$, and we can write $\mathbf{K}$ in the form $\mathbf{K}(\mathbf{E}) = \sum_{e=1}^{N} \mathbf{K}_e\,(E_e)$, where $\mathbf{K}_e$ is the (global level) element stiffness matrix.

In problem (1), E_{ad} denotes the set of admissible stiffness tensors for our design problem. which in the case of "black-white" topology design consists of all stiffness tensors that attain the material properties of a given isotropic material in the (unknown) set D^{mat} and zero properties elsewhere.

3 An isotropic material model

In the design of the topology of a structure we think of the geometric representation of a structure as similar to a black-white rendering of an image. In discrete form this then corresponds to a black-white raster representation of the geometry, with "pixels" (or "voxels") given by the finite element discretization. The most common approach to solve this problem is to use so-called penalized, proportional stiffness model (the SIMP-model, SIMP: Solid Isotropic Material with Penalization), where one works with continuously varying stiffnesses given as:

$$E^e_{ijkl} = \rho_e^p E^0_{ijkl}, \quad p > 1 \ ; \quad \sum_{e=1}^{N} \rho_e v_e \le V; \quad 0 \le \rho_e \le 1, \ e = 1,\dots,N \ . \tag{2}$$

Here the "density" $\rho_e, \ e = 1,\dots,N$ is then the design variables. One refers to ρ_e as a density of material by the fact that the volume of the structure is evaluated as $\sum_{e=1}^{N} \rho_e v_e$. The density interpolates between the material properties 0 and and E^0_{ijkl}, meaning that if a final design has density zero or one in all elements, this design is a black-and-white design for which the performance has been evaluated with a correct 0-1 FE model. In SIMP one will choose to use $p > 1$ so that intermediate densities are unfavourable in the sense that the stiffness obtained is small compared to the cost (volume) of the material, i.e., specifying $p > 1$ makes intermediate densities uneconomical.

We note that the topology design problem is defined on a fixed reference domain and this together with the SIMP-interpolation means that the optimal topology problem takes on the form of a standard sizing problem on a fixed domain.

3.1 SIMP as a material model

It is interesting to note that the SIMP-model can actually be interpreted in physical terms and that one can find a material (a composite), which realizes the interpolation model. Central in such considerations is a comparison with the Hashin-Shtrikman bounds for two-phase materials, which expresses the limits of possible isotropic material properties one can achieve by constructing composites (materials with microstructure) from two given, linearly elastic, isotropic materials. Without further elaboration we note that the SIMP-model can indeed be considered as a material model if the power p satisfy certain simple conditions, see Bendsøe & Sigmund (1999). In brief, for dimension 2, the smallest possible p is 3, which is admissible for $\nu^0 = 1/3$) In dimension 3 the smallest admissible p is 2, but for $\nu^0 = 1/3$ one should also in 3-D choose p greater than 3. See Figure 1.

We remark here that in *bio-mechanical* models the stiffness of trabecular bone (as an isotropic material) is actually modelled as in SIMP and with $p = 3$!!

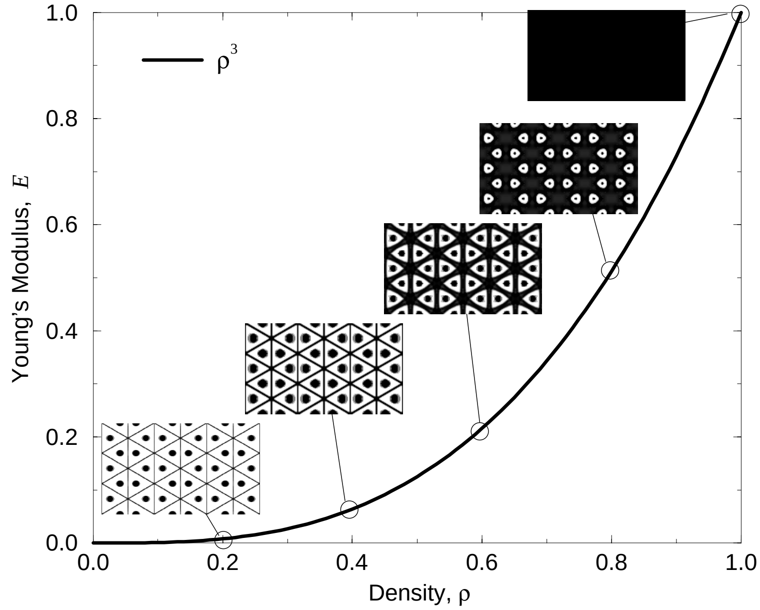

Figure 1: Microstructures of material and void realizing the material properties of the SIMP model with $p = 3$, for a base material with Poisson's ratio $\nu = 1/3$. As stiffer material microstructures can be constructed from the given densities, non-structural areas are seen at the cell centers (from Bendsøe & Sigmund 1999).

3.2 Realizing SIMP by inverse homogenization

We will now describe a methodology that can generate a material model that realizes SIMP. The fundamental notion is that any material is a structure if you look at it through a sufficiently strong microscope. Assuming that the material is periodic, its effective properties may be found by homogenization (see for example Guedes & Kikuchi (1991)). The design problem then consists in assigning a material type to each element used to discretize the base cell. As the microstructure does not exist ab initio we call the process an inverse homogenization method. The goal of material design may be to synthesize a material with prescribed constitutive properties or it may be to synthesize materials with extreme constitutive properties.

If we seek to design a material with a prescribed elastic tensor E^*_{ijkl}, a suitable objective function for the design process is the error between the homogenized elasticity tensor E^H_{ijkl} and the wanted stiffness tensor E^*_{ijkl}. A more general design formulation is

$$\begin{aligned} &\min_{\rho} \; c(E^H_{ijkl}(\rho)) \\ &\text{s.t.}: \frac{1}{|\text{Y}|}\sum_{e=1}^{N} v_e \rho_e \le \vartheta, \\ &\quad g_i(E^H_{ijkl}(\rho)) \le g^*_i, \quad i = 1, \ldots, M \;, \\ &\quad 0 < \rho_{min} \le \rho_e \le 1, \quad e = 1, \ldots, N \;, \end{aligned} \tag{3}$$

where the objective function $c(E^H)$ and constraints $g_i(E^H)$ are functions of the homogenized tensor E^H and M is the number of constraints. Also, ϑ is a bound on the volume fraction and E^H is evaluated via homogenization (d is the dimension of space). The tensor E^H is thus given via the solution of a number of unit cell analysis problems (cf., e.g., Guedes & Kikuchi (1991)) and problem (3) is similar in structure as the original design problem (1).

The constraints in (3) may take different forms. For example minimum Poisson's ratio is obtained for very soft structures and to prevent too flimsy homogenized materials a lower bound constraint on the effective bulk modulus κ_{min} may therefore be added, i.e. $g_1 = -\kappa^H$ and $g_1^* = -\kappa_{min}$. Also, it may be desired to impose a constraint that ensures symmetries in the resulting material properties. Orthotropy (i.e. $E^H_{1112} = E^H_{2212} = 0$) may be obtained by imposing one or more lines of symmetry in the base cell. Square symmetry may for example be obtained by imposing one line of symmetry and adding the constraint $g_2 = (E^H_{1111} - E^H_{2222})^2/(E^H_{1111} + E^H_{2222})^2$ with $g_2^* = \epsilon^2$, where ϵ is a small tolerance number. The problem formulation (3) was first suggested in Sigmund & Torquato (1997) and has since then been used successfully in the design of material with extremal elastic, thermoelastic, piezoelectric and other physical properties. Also, the material design methodology of the inverse homogenization method allows us to construct concrete realizations of the SIMP model, as seen in Fig. 1.

The technique of inverse homogenization was first developed with truss models Sigmund (1994a), Sigmund (1994b), Sigmund (1995), and then for continuum elasticity, see, for example, Sigmund (1994a), Sigmund (1996), Terada & Kikuchi (1996). For recent development consult Neves, Rodrigues & Guedes (2000), Sigmund (2000), Sigmund (2001) and references therein.

4 Computations for topology design

4.1 Necessary conditions

In the following we briefly describe the necessary conditions of optimality for the density ρ_e of the minimum compliance design problem that employs the SIMP interpolation scheme. It here turns out that the condition of optimality reduce to a simple form. Thus, for intermediate densities ($\rho_{\min} < \rho_e < 1$) the conditions can be written as (cf., e.g., Bendsøe & Sigmund (2003)):

$$\frac{p\rho_e^{p-1}}{v_e}\mathbf{u}^T\mathbf{K}_e\mathbf{u} = \Lambda \ , \tag{4}$$

which expresses that the strain energy density-like left-hand side term is constant and equal to a constant Λ for all intermediate densities (Λ is a Lagrange multiplier for the volume constraint of the optimization problem). This is thus a condition that is similar to the fully stressed design condition in plastic design.

As we expect areas with high energy to be too low on stiffness, one can, on the basis of (4), devise the following fix-point type update scheme for the density which should generate an optimal design[2]:

$$\rho^{(K+1)} = \begin{cases} \max\{(1-\xi)\rho^{(K)}, \rho_{\min}\} & \text{if} \ \ \rho^{(K)}B_K^\eta \leq \max\{(1-\xi)\rho^{(K)}, \rho_{\min}\} \ , \\ \min\{(1+\xi)\rho^{(K)}, 1\} & \text{if} \ \ \min\{(1+\xi)\rho^{(K)}, 1\} \leq \rho^{(K)}B_K^\eta \ , \\ \rho^{(K)}B_K^\eta & \text{otherwise} \ . \end{cases} \tag{5}$$

Here $\rho^{(K)}$ denotes the value of the density variable at iteration step K, and B_K is given by the expression

$$B_K = \Lambda_K^{-1}\frac{p(\rho_e^{(K)})^{p-1}}{v_e}\mathbf{u}_K^T\mathbf{K}_e\mathbf{u}_K \ ,$$

where $\mathbf{u}_K$ is the displacement field at at the iteration step K, determined from the equilibrium equation and dependent on ρ_K. Note that a (local) optimum is reached if $B_K = 1$ for densities ($\rho_{\min} < \rho_e < 1$). The update scheme (5) adds material to areas with a specific strain energy that is higher than Λ (that is, when $B_K > 1$) and removes it if the energy is below this value; this only takes place if the update does not violate the bounds on ρ_e. From summing over all elements in (4) one can see that Λ is proportional (by a factor p) to the average strain energy density of the part of the structure that is given by intermediate values of the density.

The variable η in (5) is a tuning parameter and ξ a move limit. Both η and ξ controls the changes that can happen at each iteration step and they can be made adjustable for efficiency

[2] We drop the index e for convenience.

of the method. Note that the update $\rho^{(K+1)}$ depends on the present value of the Lagrange multiplier Λ, and thus Λ should be adjusted in an inner iteration loop in order to satisfy the active volume constraint. It is readily seen that the volume of the updated values of the densities is a continuous and decreasing function of the multiplier Λ. Moreover, the volume is strictly decreasing in the interesting intervals, where the bounds on the densities are not active in all elements of the FE discretization. This means that we can uniquely determine the value of Λ, using a bisection method or a Newton method. The values of η and ξ are chosen by experiment, in order to obtain a suitable rapid and stable convergence of the iteration scheme. A typical useful value of η and ξ is 0.5 and 0.2, respectively.

The type of algorithm described above has been used to great effect in a large number of structural topology design studies and is well established as an effective (albeit heuristic) method for solving large scale problems. The effectiveness of the algorithm comes from the fact that each design variable is updated independently of the update of the other design variables, except for the rescaling that has to take place for satisfying the volume constraint.

It is interesting to note that many models used in bio-mechanics for *bone adaptation* have a form which is similar to the optimality criteria algorithm described above (see for example Cowin (1990) and the paper in Pedersen & Bendsøe (1999)). These models are usually based on energy arguments and are not derived from an optimization principle. This similarity in approach to material redistribution updates has also lead to bone adaptation models being proposed as topology redesign methods (see e.g., Pettermann, Reiter & Rammerstorfer (1997)), as well as optimization models being the base for bone remodelling studies, see section on literature.

4.2 Mathematical programming approach

The standard procedure for using mathematical programming algorithms for solving problems in structural optimization is to consider the design problem as an optimization problem in the design variables only. Thus the displacement field is regarded as a function of these design variables. The displacement fields are given implicitly in terms of the design variables through the equilibrium equation and finding the derivatives of the displacements with respect to the design variables is termed sensitivity analysis. This technique carries over to topology design as well, and is a more general approach than the one described above. We refer to the litterature for details (e.g., Bendsøe & Sigmund (2003)).

5 Design with anisotropic materials

Topology optimization for continuum structures was first developed around the employment of composite materials as an interpolation of void and full material. This was founded on the understanding that the existence of solutions to general shape design problems requires the consideration of relaxed designs in the form of composites.

5.1 Parametrization of design

In the following we introduce a design space obtained by also considering composite materials constructed from the given isotropic material (as defined by E^0_{ijkl}). The design variable is then the continuous density of the base material in these composites. This provides (as SIMP) an interpolation for use in computations. In the setting of composites we have a set of admissible E_{ad} stiffness tensors given in the form:

$$\begin{aligned}
&\text{Geometric variables } \mu_e, \gamma_e, \ldots, \text{ angle } \theta_e \ , \\
&E_{ijkl}(x) = E^H_{ijkl}(\mu_e, \gamma_e, \ldots, \theta_e), \\
&\text{density of material } \rho_e = \rho_e(\mu_e, \gamma_e, \ldots) \ , \\
&\sum_{e=1}^{N} \rho_e v_e \leq V; \quad 0 \leq \rho_e \leq 1, \ e = 1, \ldots, N \ ,
\end{aligned} \tag{6}$$

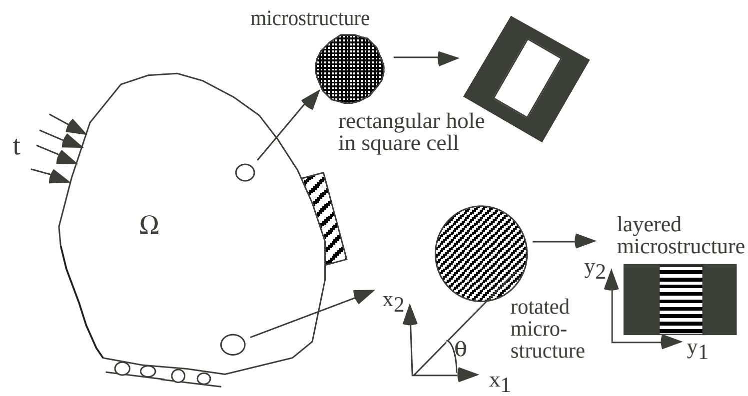

Figure 2: A structure made of materials with micro structure. Notice how the micro structure is rotated by a rotation of the unit cells.

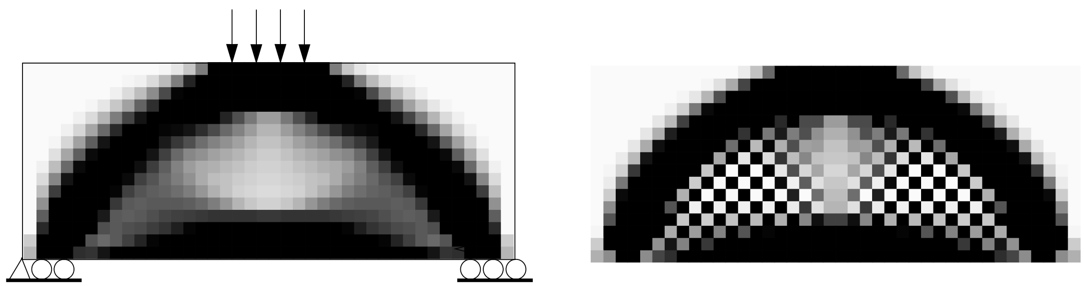

Figure 3: Optimal design using a rank-2 material. Left: The optimal design using an element wise constant density function and a 8-node displacement model. Right: The unstable checkerboard solution obtained when using a 4-node displacement model (from Jog et al. 1994).

where E^H_{ijkl} are the effective material parameters for the composite that are obtained through homogenization. The composite material will, in general, be anisotropic (or orthotropic) so the angle of rotation θ of the directions of orthotropy enters as a design variable. Figure 2 shows a two-dimensional continuum structure made of a material with microstructure and illustrates how the rotation of the unit *cells* influences a microscopic view of the material.

The use of designs spaces defined as in 6 has given raise to the use of the phrase "the homogenization approach" to topology design. This method can be implemented using the same flow of computations as for the material distribution method with isotropic materials. However, two additional aspects have to be considered. First, a database of material properties as functions of the design variables should be generated. However, if layered materials are used one has analytical formulas for this data (see for example Bendsøe & Sigmund (2003)). Second, the optimization routine should also cater for the angles of rotations of the unit cells.

5.2 Optimal rotation of orthotropic materials

The materials with cell symmetry that are typically used in topology optimization are orthotropic, and the angle of rotation of the material axes of this material will influence the value of the compliance of the structure. It turns out that the optimal rotation can be found analytically and this is of great importance for computations and it is interesting in its own right. Thus the optimal rotation of an orthotropic material is not only of importance for the present setting, but is equally significant in the design of composite structures, laminates, etc. , and is also analogous to Wolff's law for *bone-adaptation*. For this reason we will here derive the conditions of optimality for material rotations in plane stress/strain problems (i.e. 2-D).

Assume an orthotropic material as given. Then in the frame of reference given by the material axes of this material we have a stress-strain relation $\sigma_{ij} = E_{ijkl}\varepsilon_{kl}$ with E_{1111}, E_{2222}, E_{1122}, and E_{1212} being the only non-zero components of the stiffness tensor E_{ijkl}. We assume that $E_{1111} \leq E_{2222}$, and work with a given strain ε. With compliance design in mind, our interest is to *maximize* the strain energy density (cf., Pedersen (1989)):

$$W = \frac{1}{2}\left[E_{1111}{\varepsilon_{11}}^2 + E_{2222}{\varepsilon_{22}}^2 + 2E_{1122}\varepsilon_{11}\varepsilon_{22} + 4E_{1212}{\varepsilon_{12}}^2\right] \ .$$

We now express the strains in terms of the principal strains ε_I, ε_{II}, where we choose $|\varepsilon_I| \geq |\varepsilon_{II}|$ for convenience:

$$\begin{aligned}
\varepsilon_{11} =& \frac{1}{2}\left[(\varepsilon_I + \varepsilon_{II}) + (\varepsilon_I - \varepsilon_{II})\cos 2\psi\right] \ , \\
\varepsilon_{22} =& \frac{1}{2}\left[(\varepsilon_I + \varepsilon_{II}) - (\varepsilon_I - \varepsilon_{II})\cos 2\psi\right] \ , \\
\varepsilon_{12} =& -\frac{1}{2}(\varepsilon_I - \varepsilon_{II})\sin 2\psi \ .
\end{aligned}$$

Here ψ is the angle of rotation of the material frame relative to the frame of the principal strains. Inserting the expressions for the strains expressed in terms of the reference principal strains into the equation for W and differentiating, we get the condition of stationarity as:

$$\begin{aligned}
&A\sin 2\psi + B\sin 2\psi\cos 2\psi = 0 \ , \\
&A = ({\varepsilon_I}^2 - {\varepsilon_{II}}^2)(E_{1111} - E_{2222}) \ , \\
&B = (\varepsilon_I - \varepsilon_{II})^2(E_{2222} + E_{1111} - 2E_{1122} - 4E_{1212}) \ .
\end{aligned}$$

For the single load case we can thus express directly the stationary angle ψ:

$$\begin{aligned}
&\sin 2\psi = 0 \ , \quad \text{or} \quad \cos 2\psi = -\gamma, \text{ with } \gamma = \frac{\alpha}{\beta}\frac{\varepsilon_I + \varepsilon_{II}}{\varepsilon_I - \varepsilon_{II}}, \text{ and} \\
&\alpha = (E_{1111} - E_{2222}) \geq 0 \ , \quad \beta = (E_{2222} + E_{1111} - 2E_{1122} - 4E_{1212}) \ .
\end{aligned}$$

Inserting these values in the second variation of W with respect to ψ (Pedersen (1989)), it can be seen that the maximizing ψ (i.e. the compliance minimizer) depends on the sign of the parameter β. The parameter β is a measure of the shear stiffness of the orthotropic material. For low shear stiffness, that is, $\beta \geq 0$ (this holds for materials typically used in topology design), the globally minimal compliance is achieved for $\psi = 0$, i.e. the intuitive result that the numerically largest principal strain is aligned with the stiffer material axis; also, from the stress-strain relation, we see that in this case these axes are aligned with the axes of principal stresses. This is similar to Wolff's law for *bone-growth* (cf. Cowin (1990)).

6 Free material design

In this section we go one step further and represent the material properties in the most general form possible for a (locally) linear elastic continuum namely as the *unrestricted* set of positive semi-definite constitutive tensors. This very general framework results in developments which provide an attainable global lower bound on the performance of any structure designed for the same loads, boundary conditions and ground structure. At the same time, it provides an attainable global upper variational bound on the effective moduli of any elastic material, within the cost measures defined.

This setting of locally unconstrained material properties gives insight into the nature of efficient local structures. This is useful for theoretical as well as practical purposes. As an example of the latter, recent work has thus employed the framework of free material design to generate procedures for tape-lay-up in composites (see Hörnlein, Kocvara & Werner (2001)).

Initial studies on the use of a free parametrization of material can be found in Ringertz (1993), Bendsøe, Guedes, Haber, Pedersen & Taylor (1994), Bendsøe, Díaz, Lipton & Taylor (1995). The development of fast algorithms for these problems (based on interior point methods) is described in, for example, Kocvara, Zowe & Nemirovski (2000).

6.1 Problem formulation

For physical reasons, the possible stiffness tensors in the design formulation are restricted to the set of positive semi-definite, symmetric tensors. Also, suitable cost functions must have the property of frame indifference. Since the goal is to optimize the local material properties as well as the global structural response, we choose to consider cost in terms of invariants of the constitutive tensor itself. Specifically, we choose two invariants as examples of local cost (cf., Bendsøe et al. (1994))

$$\text{Case A}: \ \Psi_{\mathrm{A}}(E) = E_{ijij} \ , \qquad \text{Case B}: \ \Psi_{\mathrm{B}}(E) = [E_{ijkl}E_{ijkl}]^{\frac{1}{2}} \ ,$$

i.e., respectively, the trace and the Frobenius norm of the 4-tensor E. This means that we consider a design parametrization (a definition of E_{ad}) in the form

$$E \succeq 0 \text{ in } \Omega \ , \quad E_{ijkl} \in L^{\infty}(\Omega), \text{ for all } ijkl \ , \quad \int_{\Omega} \Psi(E)\mathrm{d}\Omega \le V \ .$$

where we use the notation $E \succeq 0$ to signify that E is positive semidefinite. We thus optimize over all positive, semi-definite stiffness tensors E_{ijkl} (with the usual symmetry properties) and use the integral over the domain of some invariant $\Psi(E_{ijkl})$ of the stiffness tensor as the measure of cost.

Note that the measures Ψ are homogeneous of degree one. Thus comparing to the conventional 2D problem for the design of material distribution in a sheet (where total cost is proportional to the volume of material), the above "cost measures" correspond in their role to the sheet thickness. More general considerations are also possible, combining several invariants of the tensor to provide for generalized cost measures which can be varied to cater for specific design goals, for example governed by available fiber composites (see for example Rodrigues, Soto & Taylor (1999), and Taylor (2000) and references therein).

It is here also notable that a similar development on the use of any positive semi-definite tensor in the description of material has also been employed in *bone-remodelling* studies, see Jacobs, Simo, Beaupre & Carter (1997).

6.2 Problem reduction

The problem we consider is the minimum compliance problem, now written for a continuum

$$\begin{aligned} &\max_{\substack{\text{density } \rho \\ 0 \le \rho_{\min} \le \rho \le \rho_{\max} < \infty \\ \int_{\Omega} \rho \mathrm{d}\Omega \le V}} \ \max_{\substack{\text{stiffness } E \succeq 0 \\ \Psi(E) \le \rho}} \ \min_{u \in U} \int_{\Omega} W(E,u)\mathrm{d}\Omega - l(u) \\ &W(E,u) = \frac{1}{2} E_{ijpq}(x)\varepsilon_{ij}(u)\varepsilon_{pq}(u) \ , \quad l(u) = \int_{\Omega} f u \mathrm{d}\Omega + \int_{\Gamma_T} t u \mathrm{d}s \ , \end{aligned} \tag{7}$$

with body forces f and boundary traction t. Here we have here provided a separation between the properties of the tensor E that can be optimized locally (at each point in the structure) and those that must be treated as a distributed parameter problem over the full domain. Also, we have introduced an upper bound on the resource densities in order to ensure that the problem is well posed. A possible non-zero lower bound is also catered for. Note that the resource constraints are convex for both case A and B.

In the developments to follow, we show that an analytical optimization actually can reduce the number of free design variables from 6 in dimension two and 21 in dimension three to only *one* in both dimensions (in any dimension that is).

We can now rearrange problem (7) and split it into two coupled optimization subproblems. First we interchange of min and max for the inner problems of (7) and obtain an equivalent formulation (problem (7) satisfies the conditions for existence of a saddle point, see for example Bendsøe et al. (1995)). Then we move the pointwise maximization of strain energy under the integration and study the problem

$$\breve{W}_0(u) = \max_{\substack{E \succeq 0 \\ \Psi(E) \leq \rho}} \frac{1}{2} E_{ijpq}(x)\varepsilon_{ij}(u)\varepsilon_{pq}(u) \ .$$

The optimal energy reduce for both the trace and norm case to the same expression, namely

$$\breve{W}_0(u) = \frac{1}{2}\rho\varepsilon_{ij}(u)\varepsilon_{ij}(u) = \frac{1}{2}\rho I_{ijkl}\varepsilon_{ij}(u)\varepsilon_{kl}(u) \ ,$$

corresponding the energy of an isotropic, zero-Poisson-ratio material, with stiffness tensor ρI, which is ρ times the identity tensor. This matrix has norm $\Psi_B(\rho I) = \sqrt{N}\rho$ and trace $\Psi_A(\rho I) = N\rho$ ($N = 3$ in dimension 2 and $N = 6$ in dimension 3). Note however, that the bound $\breve{W}_0$ is achieved with the (unique) tensor

$$E^*_{ijkl} = E^A_{ijkl} = E^B_{ijkl} = \rho \frac{\varepsilon_{ij}(u^1)\varepsilon_{kl}(u^1)}{\varepsilon_{pq}(u^1)\varepsilon_{pq}(u^1)} \ ,$$

which has norm as well as trace equal to ρ. The optimized material represented by E^* is orthotropic, with axes of orthotropy given by the axes of principal strains (and stresses) for the field $\varepsilon_{ij}(u)$, in analogy to the results on optimal rotations of orthotropic materials (and Wolff's law!) as described above.

7 Implementation issues

The computational results that can be produced with the material distribution based topology design methodology are strongly dependent on the implementation of means that control the appearance of checkerboards and that give mesh-independenct results. The former refers to the formation of regions of alternating solid and void elements ordered in a checkerboard like fashion and is related to the discretization of the original continuous problem. Such patterns are also seen in *bone-remodelling simulations.*

7.1 The checkerboard problem

Patches of checkerboard patterns appear often in solutions obtained by a direct implementation of the material distribution method that use the displacement based finite element method (see Fig. 3). Such patterns are also observed in the spatial distribution of the pressure in some finite element analyses of Stokes flows. It is now well understood that also for topology design the origin of the checkerboard patterns is related to features of the finite element approximation, and more specifically is due to bad numerical modelling that overestimates the stiffness of checkerboards (see Díaz & Sigmund (1995)).

Restriction methods that via filters or other "devices" limit the geometric variability of the designs in the topology optimization setting (see Bendsøe & Sigmund (2003)) also has the effect that checkerboarding is reduced or removed. The reason for this is that when one enforces a constraint on geometry (generally speaking in terms of the length of the boundary or in terms of gradient variation) that assure that solutions exist, one also obtains FE-convergence and checkerboards cannot be present for a fine enough mesh (more precisely, they can be made arbitrarily weak).

There are situations where one does *not* wish to enforce a fixed scale geometric restriction on the designs. This is the case when one uses numerical methods to obtain an understanding of the behaviour of optimal topologies at a fairly fine scale, but in a macroscopic representation. This is

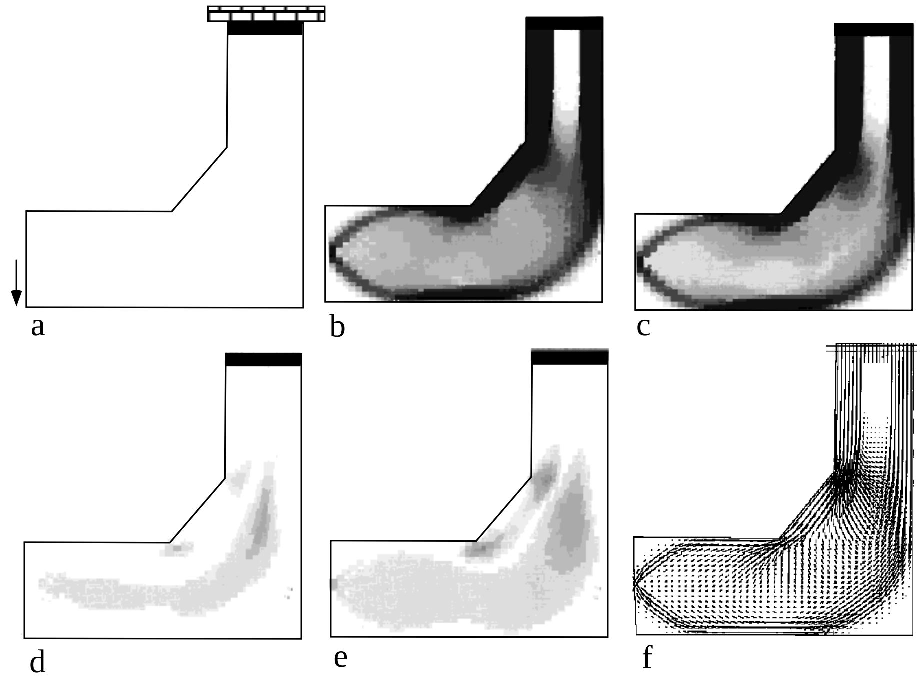

Figure 4: The design of a L-shaped cantilever a) using optimal materials. Single load case. The upper, black part at the support is considered as fixed. b): Distribution of resource. c): Distribution of E_{1111} . d): Distribution of E_{2222} . e): Distribution of $|E_{1122}|$. f) Directions and sizes of principal strains; directions correspond to direction of material axes (from Bendsøe & Guedes 1994).

of theoretical interest for obtaining insight in for example solutions to problems involving Michell type continua and when treating *bone-remodelling.* Geometric restriction is also unwanted when using a design parametrization with composites and free material.

There are several ways to remove checkerboards. One is to use higher-order elements for the displacements, another is to use a patch technique that effectively filters the checkerboards. Filtering the sensitivities is also possible[3] as is the use of a nodal representation of the density. Finally, a direct constraint on checkerboard patterns or a design description by wavelets are also possible. For further details we refer to the literature, see Bendsøe & Sigmund (2003) for an overview.

8 Biomechanics

The structure of bone and of the bone material itself is intricate, and, furthermore, the bone material evolves and adapts to the actual load conditions. Normally, actual bone shows a very specific layout in terms of distribution of densities and material orientations. Can we postulate an objective that leads to these layouts, such as the postulate of maximum stiffness for minimum material? In general the answer is NO, but we can learn from such a postulate – and we have already seen that many elements of "classical" bone-remodelling schemes have analogues in optimal compliance design with varying topology and material.

[3]This idea has also been used to ensure mesh-independence for simulations of *bone-remodelling* (Mullender, Huiskes & Weihnans. (1994).

Figure 5: Bone remodelling simulation for multiple loads. Femur longitudinal cuts. Two sets of results depending on cost of bone creation. By courtesy of P. A. Fernandes, J. M. Guedes and H. C. Rodrigues

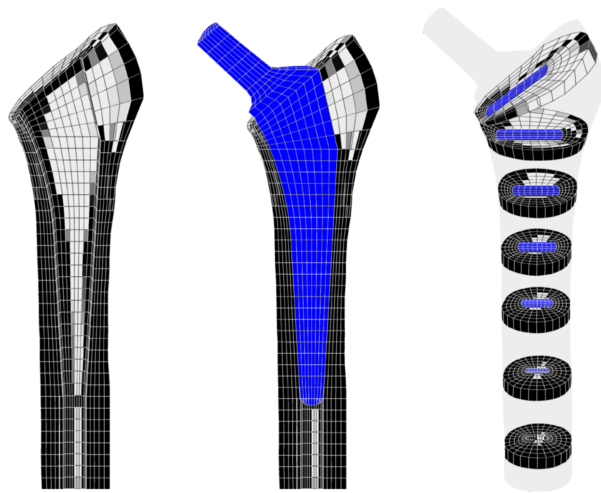

Figure 6: Bone remodelling with tapered hip prosthesis, contact conditions, for multiload case and bone ingrowth modelling. By courtesy of J. Folgado, J. M. Guedes and H. C. Rodrigues.

8.1 Remodelling of bone

The load conditions on a bone change with time due to the different activities of the total body. The bone adapts to these changes, and we need a model for this adaptation. In Bagge (2000) the analogies outlined in the developments above are applied to the development of a model for bone-remodelling based on elements of optimal design. The material of bone is modelled via homogenization as an orthotropic material (based on a frame model) and the principal (extreme) material directions of this material align directly with the principal stress axes (Wolff's law – or optimal choice of material axes for minimum compliance?). The time-stepping procedure consists of an iteratively determined material distribution based on the tendency to move towards an optimal solution of maximizing the total stiffness (minimize the stored elastic energy) for a given total amount of material (this involves optimality criteria steps that involves similar updates as used in other remodelling schemes). Much attention should here, of course, be paid to the modelling of the non-stationary loads on the bone due to various load scenarious, such as compressive body weight forces and tension forces from the muscles. Moreover, one can include a memory function in the formulation to cater for a time-lag.

8.2 An investigation of bone microstructures

If a 3D material is optimized for stiffness (e.g. maximum bulk modulus), the resulting microstructures are close-walled (c.f. Fig. 7), while it has been observed that most bone structures are built up as open walled cells Gibson & Ashby (1988). This indicates that bone structure is not "designed by nature" specifically with optimal stiffness as the objective, and other requirements must also govern the growth of bone.

In order to find mechanisms (phenomena?) that will will result in bone-like high stiffness microstructures with open cell walls, a constraint on the permeability of the cell could be imposed. Permeability is essential for the flow of nutritients that is necessary for maintaining the steadily active bone growth or degradation. Instead of setting up a complicated flow model we can add an extra constraint to the material optimization problem related to the conductivity of the base cell. Here a void element should have a high conductivity and a solid element should have a low (zero conductivity). The interpolations of Young's modulus E and the conductivity ζ, respectively, may thus be written as a maximization of the bulk modulus

$$E(\rho_e) = \rho_e^p E_0 \quad \text{and} \quad \zeta(\rho_e) = (1 - \rho_e)^p \zeta_0 \ .$$

The optimization problem is then be written as

$$\begin{aligned} & \max_{\rho} \ \kappa(\rho) \\ & \text{s.t.} : \zeta^H(\rho) \geq \zeta^* \ , \\ & \qquad \frac{1}{|\mathrm{Y}|} \sum_e v_e \rho_e \leq \vartheta \ , \\ & \qquad 0 < \rho_{min} \leq \rho_e \leq 1, \quad e = 1, \ldots, N \ , \end{aligned}$$

where ζ^* is the lower bound constraint on the effective conductivity. Obviously, this optimization problem only makes sense for 3D problems where both phases may be connected from cell to cell.

By specifying a lower bound on the conductivity of respectively 0%, 10% and 20% of the conductivity of a totally void cell, the open-walled microstructures shown in Fig. 7 are obtained. Comparisons of the objective functions (bulk moduli) for the closed and the open-walled structures show that the close-walled microstructures are significantly stiffer than the open-walled structures (cf., Sigmund (1999)). Thus stiffness is apparently only one of more objectives that governs the lay-out of of bone microstructures. Here a conductivity constraint for allowing flow of nutrition has been applied, but many other objectives of biological or mechanical nature may also play a role; for the latter, minimum size constraints and buckling sensitivity may well be significant (for details on design with buckling constraints, consult Neves, Sigmund & Bendsøe (2002a) and Neves, Sigmund & Bendsøe (2002b)).

9 Notes on relevant literature

Background material on topology design can be found in the monograph Bendsøe & Sigmund (2003)[4] which covers topology design based on the material distribution method. One may also consult the book Hassani & Hinton (1999), which emphasizes the so-called homogenization approach. Recent titles which cover the field in a broad sense are Rozvany (1997) and Rozvany & Olhoff (2000), with Cherkaev (2000), Allaire (2002) emphasizing more the mathematical aspects of the field. These latter books also cover aspects related to composites and relaxation of functionals. The most recent survey on topology design, covering the area in great detail, is the very thorough paper Eschenauer & Olhoff (2001), which contains 425 references. Other example survey papers on classical lay-out theory and topology design are Sigmund & Petersson (1998), and Rozvany (2001).

[4] This is a substantially revised version of the book Bendsøe (1995).

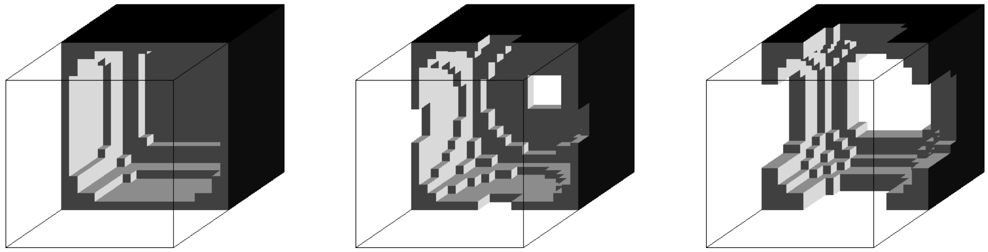

Figure 7: Investigation of "bone" microstructures. All pictures show one half of the resulting base cell topologies. Left: close-walled cell obtained from stiffness optimization without conductivity constraint and center right: open-walled cells obtained from stiffness optimization with conductivity constraints. The local conductivity is inversely proportional to the local stiffness (from Sigmund 1999).

The numerical implementation of the material distribution idea (based on homogenized materials) was first described in Bendsøe & Kikuchi (1988). The idea using a penalized variable density approach (SIMP) for numerically approximating the 0-1 design problem was tested in Bendsøe (1989), Rozvany, Zhou & Sigmund (1994) and Yang & Chuang (1994) and has since been used extensively.

The relation between optimality criteria update schemes, optimal design and models for bone adaptation (adaptive bone-remodelling), has been dealt with in quite a number of papers, see, for example, Cowin (1990), Weinans, Huiskes & Grootenboer (1992), Cowin (1995), Pettermann et al. (1997), Jacobs et al. (1997), Rodrigues, Jacobs, Guedes & Bendsøe (1999), Fernandes, Rodrigues & Jacobs (1999), Huiskes (2000), Bagge (2000), and Fernandes, Folgado, Jacobs & Pellegrini (2002). Moreover, further papers on the close correspondence between bone remodelling schemes and optimal design can be found in Pedersen & Bendsøe (1999).

Acknowledgements

The authors would like to thank Ole Sigmund, Pauli Pedersen, Mette Bagge and Helder Rodrigues for many useful discussions on bone-remodelling and optimal design. The support by the Villum Kann Rasmussen Foundation (MPB) is gratefully acknowledged.

References

Allaire, G. (2002). *Shape Optimization by the Homogenization Method*, Springer, New York Berlin Heidelberg.

Bagge, M. (2000). A model of bone adaptation as an optimization process, *Journal of Biomechanics* **33**(11): 1349–1357.

Bendsøe, M. P. (1989). Optimal shape design as a material distribution problem, *Structural Optimization* **1**: 193–202.

Bendsøe, M. P. (1995). *Optimization of Structural Topology, Shape and Material*, Springer Verlag, Berlin Heidelberg.

Bendsøe, M. P., Díaz, A. R., Lipton, R. & Taylor, J. E. (1995). Optimal design of material properties and material distribution for multiple loading conditions, *International Journal for Numerical Method in Engineering* **38**(7): 1149–1170.

Bendsøe, M. P. & Guedes, J. M. (1994). Some computational aspects of using extremal material properties in the optimal design of shape, topology and material, *Control and Cybernetics* **23**(3): 327–349.

Bendsøe, M. P., Guedes, J. M., Haber, R. B., Pedersen, P. & Taylor, J. E. (1994). An analytical model to predict optimal material properties in the context of optimal structural design, *Transactions of the ASME, Journal of Applied Mechanics* **61**(4): 930–937.

Bendsøe, M. P. & Kikuchi, N. (1988). Generating optimal topologies in structural design using a homogenization method, *Computer Methods in Applied Mechanics and Engineering* **71**(2): 197–224.

Bendsøe, M. P. & Sigmund, O. (1999). Material interpolation schemes in topology optimization, *Archives of Applied Mechanics* **69**(9-10): 635–654.

Bendsøe, M. P. & Sigmund, O. (2003). *Topology Optimization - Theory, Methods and Applications*, Springer Verlag, Berlin Heidelberg.

Cherkaev, A. V. (2000). *Variational Methods for Structural Optimization*, Springer, New York Berlin Heidelberg.

Cowin, S. C. (1990). Structural adaptation of bones, *Appl. Mech. Rev.* **43**: 127–133.

Cowin, S. C. (1995). On the minimization and maximization of the strain energy density in cortical bone tissue, *Journal of Biomechanics* **28**(4): 445–447.

Díaz, A. R. & Sigmund, O. (1995). Checkerboard patterns in layout optimization, *Structural Optimization* **10**(1): 40–45.

Eschenauer, H. A. & Olhoff, N. (2001). Topology optimization of continuum structures: A review, *Appl Mech Rev* **54**(4): 331–390.

Fernandes, P. R., Folgado, J., Jacobs, C. & Pellegrini, V. (2002). A contact model with ingrowth control for bone remodelling around cementless stems, *Journal of Biomechanics* **35**(2): 167–176.

Fernandes, P. R., Rodrigues, H. C. & Jacobs, C. (1999). A model of bone adaptation using a global optimization criterion based on the trajectorial theory of wolff, *Computer Methods in Biomechanics and Biomedical Engineering* **2**: 125–138.

Gibson, L. J. & Ashby, M. F. (1988). *Cellular Solids, Structure and Properties*, Pergamon Press, Oxford, England.

Guedes, J. M. & Kikuchi, N. (1991). Preprocessing and postprocessing for materials based on the homogenization method with adaptive finite element methods, *Computer Methods in Applied Mechanical Engineering* **83**: 143–198.

Hassani, B. & Hinton, E. (1999). *Homogenization and Structural Topology Optimization – Theory, Practice and Software*, Springer, New York Berlin Heidelberg.

Hörnlein, H. R. E. M., Kocvara, M. & Werner, R. (2001). Material optimization: Bridging the gap between conceptual and preliminary design, *Aerospace Science and Technology* **5**(8): 541–554.

Huiskes, R. (2000). If bone is the answer, then what is the question?, *J. Anat.* **197**: 145–156.

Jacobs, C. R., Simo, J. C., Beaupre, G. S. & Carter, D. R. (1997). Adaptive bone remodeling incorporating simultaneous density and anisotropy considerations, *Journal of Biomechanics* **30**(6): 603–613.

Jog, C. S., Haber, R. B. & Bendsøe, M. P. (1994). Topology design with optimized self-adaptive materials, *International Journal for Numerical Methods in Engineering* **37**(8): 1323–1350.

Kocvara, M., Zowe, J. & Nemirovski, A. (2000). Cascading - an approach to robust material optimization, *Computers & Structures* **76**(1-3): 431–442.

Mullender, M. G., Huiskes, R. & Weihnans., H. (1994). A physiological approach to the simulation of bone remodelling as a self-organizational controll process, *Journal of Biomechanics* **11**: 1389–1394.

Neves, M. M., Rodrigues, H. C. & Guedes, J. M. (2000). Optimal design of periodic linear elastic microstructures, *Computers & Structures* **76**: 421–429.

Neves, M. M., Sigmund, O. & Bendsøe, M. P. (2002a). Topology optimization of periodic microstructures with a buckling criteria, *in* H. A. Mang, F. G. Rammerstorfer & J. Eberhardsteiner (eds), *Proceedings of the Fifth World Congress on Computational Mechanics*, WCCM V, pp. on CD–rom.

Neves, M. M., Sigmund, O. & Bendsøe, M. P. (2002b). Topology optimization of periodic microstructures with a penalization of highly localized buckling modes, *International Journal of Numerical Methods on Engineering* **54**(6): 809–834.

Pedersen, P. (1989). On optimal orientation of orthotropic materials, *Structural Optimization* **1**: 101–106.

Pedersen, P. & Bendsøe, M. P. (eds) (1999). *Synthesis in Bio Solid Mechanics*, Kluwer Academic Publishers, Dordrecht.

Pettermann, H. E., Reiter, T. J. & Rammerstorfer, F. G. (1997). Computational simulation of internal bone remodeling, *Archives of Computational Methods in Engineering, State of the art reviews* **4**(4): 295–323.

Ringertz, U. (1993). On finding the optimal distribution of material properties, *Struct. Optim.* **5**: 265–267.

Rodrigues, H. C., Jacobs, C., Guedes, J. M. & Bendsøe, M. P. (1999). Global and local material optimization models applied to anisotropic bone adaption, *in* P. Pedersen & M. P. Bendsøe (eds), *Synthesis in bio solid mechanics*, IUTAM, Kluwer, Dordrecht.

Rodrigues, H. C., Soto, C. A. & Taylor, J. E. (1999). A design model to predict optimal two-material composite structure, *Structural Optimization* **17**(2-3): 186–198.

Rozvany, G. I. N. (2001). Aims, scope, methods, history and unified terminology of computer-aided topology optimization in structural mechanics, *Structural and Multidisciplinary Optimization* **21**: 90–108.

Rozvany, G. I. N. (ed.) (1997). *Topology optimization in structural mechanics*, Springer-Verlag, Vienna.

Rozvany, G. I. N. & Olhoff, N. (eds) (2000). *Topology Optimization of Structures and Composite Continua*, Kluwer Academic Publishers, Dordrecht.

Rozvany, G. I. N., Zhou, M. & Sigmund, O. (1994). Topology optimization in structural design, *in* H. Adeli (ed.), *Advances in Design Optimization*, Chapman and Hall, London, chapter 10, pp. 340–399.

Sigmund, O. (1994a). *Design of material structures using topology optimization*, PhD thesis, Department of Solid Mechanics, Technical University of Denmark.

Sigmund, O. (1994b). Materials with prescribed constitutive parameters: an inverse homogenization problem, *International Journal of Solids and Structures* **31**(17): 2313–2329.

Sigmund, O. (1995). Tailoring materials with prescribed elastic properties, *Mechanics of Materials* **20**: 351–368.

Sigmund, O. (1996). Some inverse problems in topology design of materials and mechanisms, *in* D. Bestle & W. Schielen (eds), *Symposium on optimization of mechanical systems*, IUTAM, Kluwer, Netherlands, pp. 277–284.

Sigmund, O. (1999). On the optimality of bone microstructure, *in* P. Pedersen & M. P. Bendsøe (eds), *Synthesis in Bio Solid Mechanics*, IUTAM, Kluwer, pp. 221–234.

Sigmund, O. (2000). A new class of extremal composites, *Journal of the Mechanics and Physics of Solids* **48**(2): 397–428.

Sigmund, O. (2001). Recent developments in extremal material design, *in* W. A. Wall, K.-U. Bletzinger & K. Schweizerhof (eds), *Trend in computational Mechanics*, CIMNE, pp. 228–232.

Sigmund, O. & Petersson, J. (1998). Numerical instabilities in topology optimization: A survey on procedures dealing with checkerboards, mesh-dependencies and local minima, *Structural Optimization* **16**(1): 68–75.

Sigmund, O. & Torquato, S. (1997). Design of materials with extreme thermal expansion using a three-phase topology optimization method, *Journal of the Mechanics and Physics of Solids* **45**(6): 1037–1067.

Taylor, J. E. (2000). A formulation for optimal structural desig with optimal materials, *in* G. I. N. Rozvany & N. Olhoff (eds), *Topology Optimization of Structures and Composite Continua*, Kluwer Academic Publishers, Dordrecht, pp. 49–59.

Terada, K. & Kikuchi, N. (1996). Microstructural design of composites using the homogenization method and digital images, *Mat. Sci. Res. Int.* **2**: 65–72.

Weinans, H., Huiskes, R. & Grootenboer, H. J. (1992). The behavior of adaptive bone-remodeling simulation models, *J. Biomechanics* **25**: 1425–1441.

Yang, R. J. & Chuang, C.-H. (1994). Optimal topology design using linear programming, *Computers and Structures* **52**(2): 265–276.