18th International Conference
ENGINEERING MECHANICS 2012
Svratka, Czech Republic, May 14 – 17, 2012

pp. 1073–1080
Paper #198

BEM SHAPE OPTIMIZATION OF A HOLE IN COMPOSITE FOR MINIMUM LAGRANGIAN

P.P. Prochazka*

Abstract: *In composite materials a problem of optimal shape of hole is of great interest to designers and researchers. This problem seems to be theoretical but good application can be found in soil, fiber reinforced concretes, even steel structures, and, of course, in classical composites fabrication. Since an iteration process has to be constructed the problem can be identified as the problem of moving boundaries. From this conclusion the advantages of finite element method are suppressed and boundary elements should be prioritized. They do not require any improvement of the meshes in an arbitrary iterations step; the mesh can be selected in a reasonable way as it is auxiliary created only for necessary integration over the domain. The boundary element method appears to be extraordinarily advantageous in case the shape optimization is to be treated, although for classical arrangement fiber – matrix it also provides us with many affirmative properties. It had been proved elsewhere by the author that the minimum for Lagrangian of the material system leads to minimization of both the stresses and displacements. Consequently, minimization of Lagrangian is probably the best cost functional ever. Certain examples iteration process and of optimal shapes depending on the volume ratios of the hole will accompany the theoretical considerations.*

Keywords: ***Composite structures, shape optimization, heat transfer, homogenization of coefficient of conductivity.***

1. Introduction

The optimal shape of fiber is studied in a composite structure for optimal overall coefficient of conductivity. For the sake of simplicity a symmetric 2D unit cell is cut out of the structure, where one of the phases is a hole while the rest of the domain describing the unit cell is matrix with given material property, i.e. with given matrix conductivity. Heat transfer or harmonic problem is solved in this paper so that the linear conductivity equation mediates a representative formulation. The design parameters of the optimization problem are connected with the inner shape of matrix, which is assumed to be star-shaped. In this way, the optimization turns to a moving boundary problem so that boundary element method appears to be the most appropriate here. Using homogenization to get the overall properties the problem is not solvable uniquely and, moreover, can exceed the realistic situation. This is why reasonable constraints, or side conditions, should be defined, i.e. the admissible set of possible domains of the hole should be defined in realistically put forward. First of all, a reasonable condition is the restriction of volume (in 2D area) of the hole. Note that this restriction can be changed in next steps according to the requirements of user. On the other hand, this still must not be enough to meet a realistic situation, since the constraints are mostly formulated in integral form (potential energies, surface energies, volume – area, etc.), i.e. positive and negative signs appearing in these formulations can lead to a nonrealistic geometry. For that, additional restrictions on the shape characteristics should be applied to the admissible shape of the hole. Among such the length of diameters of the domain of the hole, tangential slope the inner boundary of the hole, vertical and/or horizontal restrictions on the length of rays starting from the center of the unit cell, etc. The mathematical formulation of homogenization of the heat transfer problem and the subsequent optimization will be suggested and numerical treatment of the problem envisaged provide a reasonable, fully usable in practice, layout.

As mentioned in many publications, e.g. Callis et al (2008), Kaminski (2003), plenty of approaches are available on how to solve these problems. Hereinafter similar procedure, established for elastic

* Prof. Ing. RNDr. Petr Prochazka, DrSc.: Czech Technical University in Prague, Civil Engineering, dept. Mechanics, Thakurova 7, 166 29 Prague 6; CZ, e-mail: petrp@fsv.cvut.cz

optimization problem in Prochazka (2009) will be applied for creating appropriate functional and calculating the optimal shape of the hole.

Classical approach in localization and homogenization of elastic composites belongs to Suquet (1985), and that of steady state heat transfer can be found also in Lévy (1985), in which periodic composites are studied. More or less this procedure is applied in this paper to unit cell concept. Optimization of the fiber shape in a composite structure due to heat load is discussed in Dvorak (1996), where the problem of a variance between given overall properties and calculated from the given material properties of phases is as small as possible.

2. Optimization problems in composite structures

General microstructure identification problem is treated in such a way that for given conductivity of both fiber and matrix (and, of course zero value of conductivity of the hole) with the given volume fractions of phases in the unit cell it is sought arrangement of the phases (in our case the hole) in a periodic cell so that the effective material constants of the periodic composite are as close as possible to maximum or minimum values. The problem in this study is considered for the linear conduction equation. It is necessary to note that although much more complicated problems occur in theory and practice, such as non-linear behavior of the conductivities, time-dependent behavior, high temperature effects, etc. The optimization itself belongs to the wide set of optimal control theories. Existence of solution can be proved under suitable hypotheses, as well as the convergence of numerical approximations. In the conduction case, the full characterization of G_δ-closure set (the set of all effective conductivities that result from taking the given phases in the given volume fraction mixed in any feasible micro-geometry) is known. The concept of composite media not only comes directly from the physical world but also provides a theoretically sound means for relaxation of variational problems - the problem of optimum topology design (see Delgado & Allaire (2011), Suzuki & Kikuchi (1991), for example). It is a classical result of the homogenization theory that composites can be replaced by a macroscopically homogeneous medium its material constants - the so called effective of overall constants or effective modules – depend on the micro-geometry in which the constituent phases form the mixture. Note that in classical theories of composites no respect had been taken to the shape of the phases. Modern theories deny this assumption and show that the shape of the phases can basically influence the properties of the composite at the macro-level. The set of all effective constants of mixtures of a given number of phases taken in a given proportion is called the G_δ-closure set and its knowledge is essential for the relaxation procedure. In the case of a scalar linear elliptic partial differential equation (the steady heat transfer equation), one of the phases may degenerate, i.e., a void or hole can be considered. However, for the case of the system of PDE's of linear elasticity, only a partial information about the G_δ-closure sets is available so far; namely we know how to minimize the complimentary energy for a given single macroscopic stress field. For the design with other (non-compliance) objective functions, the fu11 knowledge of the G_δ-closure set seems inevitable. So far, the following principal constructions are known:

Multiple rank laminates. The microstructure is a laminate (- layered composite) whose one or both components are again laminates that in turn can consist of laminates, etc. The layered rnicrostructure has the advantage that one can calculate the effective constants analytically. However, the scale levels of the subsequent laminations must be well separated which prohibits practical realization of these microstructures. For an example see Delgado & Allaire (2011), for example.

Coated ellipsoids construction. This construction is based on the fact that having a medium with the material constants that are equal to those of our desired microstructure, one can insert an ellipsoid of one phase with an ellipsoidal inclusion of the other phase where the ellipsoids have appropriately balanced dimensions, and the effective properties of the medium are not changed upon this insertion. Thus, one fills up the whole body with coated ellipsoids, but using infinitely many length scales, this time not even separated from one another. As a consequence, one cannot manufacture but a rough approximation of such a microstructure.

Vidgergauz' microstructure. One of the theories aiming to an extreme microstructure is the Vidgergauz microstructure, Vidgergauz (1989). It has the form of a properly shaped (oval-like) inclusion of one phase within the matrix of the other phase. The shape of the inclusion is found from

the optimality conditions that in this setting have the form that "the inclusions are equally strong", no one is preferred. However, the shapes of the inclusion have to be evaluated using elliptic integrals or other non-elementary functions. We note that although it is presented in the elasticity setting, similar results hold for the harmonic equation.

The aim of this work is to establish a numerical technique for the microstructure identification problem considering heat transfer as a typical for the Laplace equation. The optimal control theory is formulated as the problem of microstructure identification: Given the effective modules, what microstructure has its optimal from the point of view of the best overall conductivity - ideally, what microstructure attains the target? The last question is meaningful, as additional constraints may lead to restriction of the goal to ensure the realistic solution. As here the classical optimal shape design approach is based on the boundary variation technique, the class of admissible micro-geometries is restricted to a single inclusion (the hole).

3. Basic considerations and equations

Let the body representing the composite is denoted V and a unit cell is given as $\Omega \subset V \in R^2$ with its boundary $\partial\Omega$, which is supposed to be Lipschitz continuous, such as if the shape of the unit cell Ω is a square $(0,1)\times(0,1)$, for example. Isotropic phases $\Omega_{\mathrm{f}} \subset \Omega$ and $\Omega_{\mathrm{m}} \subset \Omega$ represent the fiber (hole) and matrix, respectively. The boundary of the fiber (i.e. the interfacial boundary Γ_{C}) is star shaped. Note that more general shapes are mentioned in Dvorak (1996), where a special treatment on how to simplify complicated unit cells is also discussed based on body transformations. The transformations create a group of base bodies.

The conservation law is assumed in the standard divergence form applied to temperature $u(y)$ as,

$$\frac{\partial}{\partial y_i}\left(c\frac{\partial}{\partial y_i}u\right) = 0 \tag{1}$$

where $c = c(y)$ is dependent on the position in Ω, consisting of two subdomains, fiber and matrix, which are equipped by different conductivity values $c_{\mathrm{f}} = 0$ (fiber) and c_{m} (matrix), where c_{m} is also constants. Note that the hole bears a negligible conductivity although this assumption is not an obstacle for generality. This means that the coefficient of conductivity c is defined as:

$$c(y) = c_{\mathrm{f}} \quad \text{for} \quad y \in \Omega_{\mathrm{f}} \quad \text{and} \quad c(y) = c_{\mathrm{m}} \quad \text{otherwise} \tag{2}$$

or

$$c(y) = c_{\mathrm{f}}\chi(y) + c_{\mathrm{m}}(1-\chi(y)) \tag{2a}$$

where χ is the characteristic function of the fiber.

The partial equations are written as

$$\nabla q = 0\,, \qquad q = c\nabla u \tag{3}$$

where ∇ is the nabla operator, and q is the flux vector, gradient of u.

For statistically isotropic material with the periodic boundary conditions an analog of the well known Hill condition holds valid as:

$$< q\nabla u >= \frac{1}{\operatorname{meas}\Omega}\int_{\Omega} q\nabla u \,\mathrm{d}\Omega =< q >< \nabla u >= \frac{1}{\operatorname{meas}\Omega}\int_{\Omega} q \,\mathrm{d}\Omega \times \frac{1}{\operatorname{meas}\Omega}\int_{\Omega} \nabla u \,\mathrm{d}\Omega \tag{4}$$

where meas Ω is the volume in 3D or area in 2D, mostly considered equal to unit.

4. Homogenization

In order to get relations between local and overall properties of the composite apply the overall flux q_0 to the composite and the real flux is then equal to

$$q = q_0 + q_1(u_1) \tag{5}$$

where the average of the fluctuation term u_1 is zero, similar to the elasticity problem. From (1) and (5) one gets:

$$\frac{\partial}{\partial y_i}\left[c(y)\left(\frac{\partial u_1}{\partial y_i}+q_0\right)\right]=0 \Rightarrow \frac{\partial}{\partial y_i}\left[c(y)\frac{\partial u_1}{\partial y_i}\right]=-\frac{\partial}{\partial y_i}\left[c(y)q_0\right] \tag{6}$$

in the sense of distributions. Eq. (6) is the starting equation for solving u_1 with u_0 given. This is an elliptic equation being defined in Ω. If comparing with the elasticity problem q_0 is a unit impulse and u_1 is the standard fluctuating term. Since also the Laplace equation (1) is linear, similar approach to that used in linear elasticity can also be applied hereinafter to decode the generalized terms, mainly see in the right hand side, for details see Prochazka & Valek (2012). From the detailed procedure it immediately follows instead of (6):

$$\frac{\partial}{\partial y_i}\left[c(y)\frac{\partial u_1}{\partial y_i}\right]=-q_C\delta_{\Gamma_C} \qquad \text{and the periodic boundary conditions,} \tag{7}$$

where q_C is a jump in the interfacial flow equals to

$$q_C(y)=[c_f-c_m]\,q_0 n^f(y)=[c_f-c_m]\,n^f(y) \tag{8}$$

as q_0 is considered as a unit impulse. Symbol δ_{Γ_C} is the distribution of Dirac's function along the interface between the phases. The formula is in compliance with Suquet (1987).

In the next text axisymmetry and star-shaped hole are supposed, i.e. there is a point (origin of the coordinate system) the rays from which cross the interfacial segment only and only once. For this reason the problem is solved in the first quadrant only.

5. Boundary element formulation

Since the shape optimization is closely related with a moving boundary problem the boundary element formulation seems to be extremely advantageous. Multiplying (7) by a function u_1^*, integrating successively over Ω_f and Ω_m, applying linear approximations over boundary elements and splitting the boundaries into that merging Γ_C and the remaining parts finally yields:

$$\begin{bmatrix} K_{11}^{\mathrm{f}} & K_{12}^{\mathrm{f}} \\ K_{21}^{\mathrm{f}} & K_{22}^{\mathrm{f}} \end{bmatrix} \begin{Bmatrix} u_{\mathrm{f}}^{\mathrm{out}} \\ u_{\mathrm{f}}^{\mathrm{in}} \end{Bmatrix} = \begin{Bmatrix} q_{\mathrm{f}}^{\mathrm{out}} \\ q_{\mathrm{f}}^{\mathrm{in}} \end{Bmatrix}, \quad \begin{bmatrix} K_{11}^{\mathrm{m}} & K_{12}^{\mathrm{m}} \\ K_{21}^{\mathrm{m}} & K_{22}^{\mathrm{m}} \end{bmatrix} \begin{Bmatrix} u_{\mathrm{m}}^{\mathrm{in}} \\ u_{\mathrm{m}}^{\mathrm{out}} \end{Bmatrix} = \begin{Bmatrix} q_{\mathrm{m}}^{\mathrm{in}} \\ q_{\mathrm{m}}^{\mathrm{out}} \end{Bmatrix}, \quad K_{ij} = B_{ik}^{-1} A_{kj} \quad \text{where} \quad A_{ij} u_j = B_{ij} q_j \tag{9}$$

where u and q are vectors of temperature and fluxes, respectively, their components are values at nodal points of the corresponding boundaries, A and B are square, generally not symmetric matrices of approximations, and quantities with superscript in are assigned to the nodal points at Γ_{C} and that with the superscript out are connected with the values outside of Γ_{C}. Since on Γ_{C} it holds $u_{\mathrm{f}}^{\mathrm{in}} = u_{\mathrm{m}}^{\mathrm{in}}$ and $q_{\mathrm{f}}^{\mathrm{in}} + q_{\mathrm{m}}^{\mathrm{in}} = q_C$, one eventually gets:

$$\begin{bmatrix} K_{11}^{\mathrm{f}} & K_{12}^{\mathrm{f}} & 0 \\ K_{21}^{\mathrm{f}} & K_{22}^{\mathrm{f}} + K_{11}^{\mathrm{m}} & K_{12}^{\mathrm{m}} \\ 0 & K_{21}^{\mathrm{m}} & K_{2}^{\mathrm{m}} \end{bmatrix} \begin{Bmatrix} u_{\mathrm{f}}^{\mathrm{out}} \\ u_{\mathrm{f}}^{\mathrm{in}} \\ u_{\mathrm{m}}^{\mathrm{out}} \end{Bmatrix} = \begin{Bmatrix} q_{\mathrm{f}}^{\mathrm{out}} \\ q_{\mathrm{C}} \\ q_{\mathrm{m}}^{\mathrm{out}} \end{Bmatrix} \tag{10}$$

where the matrix of the system is banded but generally not symmetric. Using periodic boundary conditions u and q follows from the previous equation for unit impulse q_0. Moreover,

$$q(y) = c(\frac{\partial u_1}{\partial y_i} + q_0) \Rightarrow < q >= c^* < \nabla u >,$$

where

$$c_i^* = \int_{\Omega} c(y)(1 + \frac{\partial u_1}{\partial y_i})\, \mathrm{d}\Omega(y) = c_{\mathrm{m}} \int_{\Omega_{\mathrm{m}}} (1 + \frac{\partial u_1}{\partial y_i})\, \mathrm{d}\Omega(y), \; i = 1,2 \tag{11}$$

and $c_{\mathrm{f}} \doteq 0$.

Now the main advantage of the boundary element formulation appears: applying the Green theorem to the latter relation leads us to interface integrals as:

$$c_i^* = c_{\mathrm{m}}\, \mathrm{meas}\, \Omega_{\mathrm{m}} + c_{\mathrm{m}} \int_{\Omega_{\mathrm{m}}} u_1 n_{\mathrm{i}}^{\mathrm{m}}\, \mathrm{d}\Omega(y) = c_{\mathrm{m}}\, \mathrm{meas}\, \Omega_{\mathrm{m}} + c_{\mathrm{m}} \int_{\Omega_{\mathrm{m}} \div \Gamma_{\mathrm{C}}} u_1 n_i^{\mathrm{m}}\, \mathrm{d}\Omega(y) + c_{\mathrm{m}} \int_{\Gamma_{\mathrm{C}}} u_1 n_i^{\mathrm{m}}\, \mathrm{d}\Omega(y) \tag{12}$$

so that the unpleasant volume integrals disappear. Note that $c_1^* = c_2^* = c^*$ because of the symmetry considered.

6. Optimization

Similarly to the optimization of beams, Prochazka & Lok (2009), the energy functional is formulated using Lagrangian multiplier λ bounding the given area of the hole. Hence, the problem can be established as:

$$= \frac{1}{2} \int_{\Omega} q \nabla u\, \mathrm{d}\Omega(y) - \lambda(\int_{\Omega^{\mathrm{f}}} d\Omega - \mathrm{meas}\, \Omega_{\mathrm{f}}) = \frac{1}{2} < q >< \nabla u > -\lambda(\int_{\Omega^{\mathrm{f}}} d\Omega - \mathrm{meas}\, \Omega_{\mathrm{f}}) \rightarrow \text{stationary} \tag{13}$$

which means that the above functional is minimum with respect to u but maximum in λ.

The shape of the hole is identified by radii p_s , s = 1,2,…,n of nodes located at the interface Γ_C . Because of the considered symmetry only the first quarter of unit cell (shaded) is observed.

In this way we obtain n triangles T_s, s = 1,...,n, which approximate the domain Ω_f . It obviously holds:

$$\int_{\Omega^\mathrm{f}} d\Omega = \text{meas } \Omega_\mathrm{f} = \sum_{s=1}^{n} \text{ meas } T_s \,. \tag{14}$$

In certain cases of fiber volume ratio with combination of the given phase conductivities restrictive conditions have to be applied to the admissible beams of nodes at the interfacial boundary. This can be done in various ways. A typical lowest value of the length of any node at Γ_C is bounded from below by a given value $0 < p < p_s$ and the highest length is constrained by the conditions as $y_i < h < 1$, p, h are reals selected in advance.

If the above bounds on the beams are attained a special procedure needs to be used, see [3]. It requires an internal iteration, as the improvement of the boundary using collinear mapping to ensure the condition about constant fiber volume fraction.

7. Euler's equations

The stationary requirement leads to differentiation of the functional by the shape (design) parameters p_s

$$\lambda = \lambda_s \frac{\frac{1}{2} < \nabla u > \frac{\partial}{\partial p_s} < q >}{\frac{\partial}{\partial p_s} \int_{\Omega^\mathrm{f}} d\Omega} \quad , \quad s = 1,\ldots,n \tag{15}$$

The equation (15) requires λ to have the same value for any s. In other words, if this requirement were attained at any point on the "moving" part of the interfacial boundary the optimal shape of the trial body would be reached. For this reason the body of the composite structure should increase its area (in 3D its volume) at the nodal point of the boundary identified by p_s if λ is larger than the true value of the target, while it should decrease its value when λ is smaller than the correct Lagrangian multiplier. As, most probably, real value of the target is not known a priori, its estimate is done by averaging the current values at the nodal points. So, approximation of λ will be expressed as:

$$\lambda_{\text{approx}} = \frac{1}{n} \sum_{s=1}^{n} \lambda_s \tag{15}$$

Differentiation by λ completes the system of Euler's equations.

It remains to ensure that the fiber volume friction is constant with the value given a priori. For this aim a collinear mapping is applied after completing the shift of nodes at the interface. It can be done in such a way that assuming the current value of $\text{meas}\,\Omega^\mathrm{f}_\mathrm{curr}$, which is calculated from the current positions of the nodes mentioned, the prescribed $\text{meas}\,\Omega^\mathrm{f}$ is reached by improving the triangles T_i by the value of

$$s = \sqrt{\frac{\text{meas}\,\Omega^{\text{f}}_{\text{curr}}}{\text{meas}\,\Omega^{\text{f}}}} \tag{16}$$

Brief description of algorithm:

1 set up the starting configuration fulfilling the condition of constant area of the hole

2 calculate c^* for the current configuration

3 set a successive unit shifts to nodal points p_s at Γ_C, calculate $c^*(p_s)$ the appropriate λ using substitution of derivatives by differences (central difference is used here and the step of difference is 0.0001)

4 compute λ_{approx} to get new positions of nodes at Γ_C

5 from the new positions get the area of the current Ω_{f}

6 using collinear mapping improve the positions of nodes to ensure the original fiber volume ratio

7 check up the constraint of the beams p_s and if fail occurs apply local iteration

8 Euclidean distance between current and previous energies λ_s should be less then given admissible error; if not, go to 2 and stop otherwise

8. Examples

Unit cell is considered with various fibers volume ratios. Since we compare energy densities at nodal points of the interfacial boundary, the relative energy density may be regarded as the comparative quantity influencing the movement of the boundary Γ_{C} in a proper direction. As said in the previous section, the higher value of this energy, the larger movement of the nodal point of Γ_{C} should aim at the optimum. The process of iterations will end if the Euclidean distance between current and previous energies be less then given admissible error. In the following examples $\text{meas}\,\Omega_{\text{m}}$ and also the conductivity and c_{m} are prescribed.

In the tests considered here $c_{\text{m}} = 1$, $\text{meas}\,\Omega_{\text{m}} = 0.6$ and $\text{meas}\,\Omega_{\text{m}} = 0.5$ with resulting optimal shape presented in Fig. 1 and being attained with relative error 1.8e-04 and 2.5e-04 after twenty seven and twenty two iterations using the step of iteration 0.1 to 0.005.

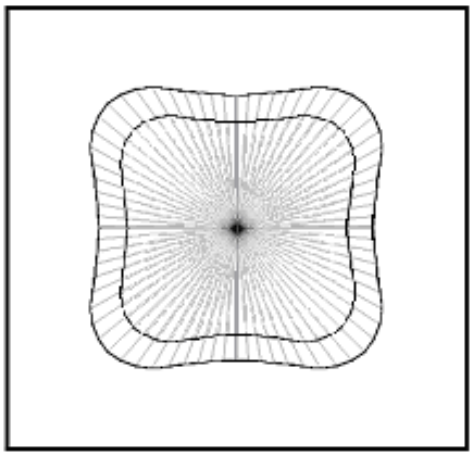

Fig. 1: Optimal shapes of holes for various area fractions

9. Conclusions

New optimization procedure is put forward in this paper based on homogenization technique. The problem which has been solved deals with homogenization of coefficients of the linear harmonic equation. The optimization is formulated in term of energy. A special constraint is adopted, which is involved in the formulation of optimal shape by Lagrangian multiplier, enabling us to show that the stationary point is attained for energy density being equal at each nodal point of the interfacial boundary. This condition leads us to an elegant and efficient numerical approach.

Acknowledgment

Financial support of the Grant agency of the Czech Republic, grant number P105/00/0266 is gratefully acknowledged.

References

Challis, V.J., Roberts, A.P. & Wilkins A.H. (2008) Design of three dimensional isotropic microstructures for maximized stiffness and conductivity. *Int. J. Solids and Structures*, **45**, (14-15), pp.4130-4146.

Kaminski, M. (2003) Homogenization of transient heat transfer problems for some composite materials. *Int. J. Engng. Sci.* **41**, pp. 1-29.

Prochazka, P.P., Dolezel, V. & Lok, T.-S. (2009) Optimal shape design for minimum Lagrangian. *Eng. Anal. with Bound. Elem*. **33**, pp. 447–455.

P.M. Suquet, P.M. (1985) Homogenization techniques for composite media. *Lecture Notes in Physics 272* (eds. E. Sanches-Palencia and A. Zaoi) Part IV, Sprinter Verlag Berlin, pp. 194-278.

Lévy, T. (1985) Fluids in porous media and suspensions. *Lecture Notes in Physics 272* (eds. E. Sanches-Palencia and A. Zaoi) Part II, Sprinter Verlag Berlin, pp. 64-119.

Dvorak, J. (1996) Optimization of composite materials, *PhD thesis*, Charles University, June 1996.

Delgado, G. & Allaire, G. (2011) Shape and Topology Optimization of Composite Materials with the level-set method. *EADS-Innovation Works.* Center of Applied Mathematics - Ecole Polytechnique, Jussieu, France.

Suzuki, K. & Kikuchi, N. (1991) A homogenization method for shape and topology optimization. *Comp. Meth. Appl. Mech. Engng*, **93**, pp. 291-318.

Vidgergauz, S.B. (1989) Regular strucutres with extremal elastic properties, *MTT* 24, pp. 57-63.

Prochazka P.P. & Valek, M (2012) Optimal Shape of Fibers in Composites Exposed to Combustion. To appear in *BETEQ 2012*.