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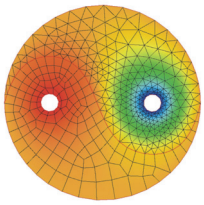
AKAPIT

COMPUTER METHODS IN MATERIALS SCIENCE

Informatyka w Technologii Materiałów

Vol. 14, 2014, No. 1



OPTIMIZATION IN MULTISCALE THERMOELASTIC PROBLEMS

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Abstract

The paper is devoted to the optimization in two-scale thermoelastic problems. The problems are solved by means of evolutionary computation and direct analysis based on a numerical homogenization. Direct thermoelastic analysis with representative volume element (RVE) and finite element method (FEM) is performed. Design variables in optimization tasks describe micro-structure, whereas optimization functionals are formulated on the basis of the quantities derived from a macro scale. Numerical examples of the optimization are included.

Key words: multi-scale modeling, numerical homogenization, thermoelasticity, evolutionary algorithms, multi-objective optimization, coupled problems, finite element method

1. INTRODUCTION

Designing of novel and smart materials in which multiphysics phenomena are considered, requires combination of coupled field analysis, multiscale modeling and optimization methods. The proper functionals for considered criteria have to be defined in order to solve optimization tasks. Such functionals, which depend on quantities derived from different physical fields (e.g. mechanical, thermal, etc.), are very often contradictory. Moreover, for real engineering problems optimization functionals are strongly multimodal. An application of proper optimization methods in such case is essential. Evolutionary algorithms (EAs), as a group of bioinspired methods are resistant for getting stack in local minima (Michalewicz, 1996). Another advantage of such method is there is no need to calculate the gradient of the fitness function. Multicriteria optimization problems are formulated if more than one criterion is considered in the same time and not one, but a set of optimal solutions is obtained for the contradictory criteria. Such solutions are optimal in the Pareto sense (Pareto-optimal solutions). Application of popular optimization methods like EAs is highly desirable in this case, because in a population of solutions is processed in every iteration.

Multiscale calculations may concern two or more scales (Buyrachenko, 2007; Zhodi & Wriggers, 2008). In order to make a transition from higher to lower scales it is necessary to transmit proper quantities (e.g. strains, temperatures), which allow to simulate the behavior of the material in lower scale. The efficient material parameters are calculated in transition from lower to upper scale. Such parameters can be obtain by means of experimental, analytical or numerical homogenization methods. Experimental methods require a real experiment for considered material, whereas analytical methods are limited to structures with simple geometry and boundary conditions. Very popular and efficient attitude (applied in the paper also) is coupling of the numerical homogenization with finite element method (FEM) (Zienkiewicz & Taylor, 2000).

ISSN 1641-8581

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2. MULTISCALE ANALYSIS IN THERMOELEASTIC PROBLEM

Coupling of the global optimization techniques and numerical multiscale models allows to design materials meeting particular requirements. For structures under thermomechanical loading optimization concerns both mechanical and thermal properties (e.g. strength, stiffness, low or high thermal conductivity). Multiscale optimization tasks can be formulated as a designing of a shape of voids/inclusions in the microstructure, selection of the phases properties, etc. In order to calculate effective material constants, numerical homogenization by means of representative volume element (RVE) is used (Kouznetsova et al., 2004; Madej et al., 2008). In general, homogenization consists in the determination of smooth coefficients of partial differential equations which can be applied to the prediction of structure response on the macroscopic scale. In the present paper linear uncouped thermoelasticity is considered (Carter & Booker, 1989; Nowacki, 1972). Two-scale models of porous structures with global periodicity are examined. For the thermoelasticity problems, the numerical homogenization allows to calculate the following effective constants: elastic constantans, thermal expansion coefficients and heat conduction coefficients (Terada et al., 2010). The thermal expansion coefficient is invariant for porous materials, so there is no need to homogenize this parameter. An example of such a structure is presented in figure 1.

Linear thermoelasticity problem is decribed by differential equations of heat conduction and elastosticity, taking into account thermal strains (Nowacki, 1970; Nowacki, 1972):

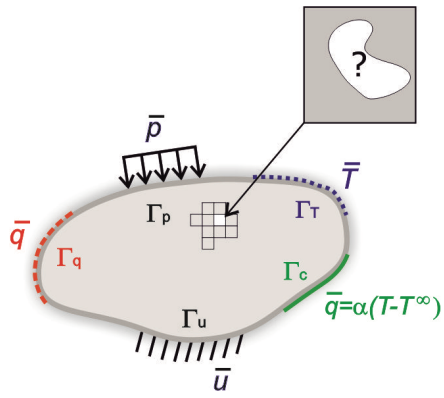

Fig. 1. *The macro-structure under thermal and mechanical loads*

$$kT_{,ii} = 0 \tag{1}$$

$$\mu u_{i,jj} + (\mu + \lambda) u_{j,ji} - (3\lambda + 2\mu)\alpha_T T_{,i} = 0 \tag{2}$$

where: k thermal conductivity, T is temperature, u is displacement, α_T is linear expansion coefficient, μ and λ are Lamé constants.

These equations have to be supplemented by mechanical and thermal boundary conditions, which take the form:

$$\begin{aligned} &\Gamma_t : t_i = \bar{t}_i \ ; \Gamma_u : u_i = \bar{u}_i \\ &\Gamma_T : T_i = \bar{T}_i \ ; \Gamma_q : q_i = \bar{q}_i \ ; \Gamma_c : q_i = \alpha(T_i - T^\infty) \end{aligned} \tag{3}$$

where $\bar{u}_i, \bar{t}_i, \bar{T}_i, \bar{q}_i, \alpha, T^\infty$ are known: displacements, tractions, temperatures, heat fluxes, heat conduction coefficient and ambient temperature, respectively.

Application of numerical homogenization using RVE takes into consideration the following principles:

– the separation of scales

$$\frac{l}{L} << 1 \tag{4}$$

where: l and L are characteristic lengths of the RVE and in the macro scale

– volume averaging is done according to:

$$\langle \cdot \rangle = \frac{1}{|\Omega_{RVE}|} \int_{\Omega_{RVE}} (\cdot)\, \mathrm{d}\Omega_{RVE} \tag{5}$$

where: $\langle \cdot \rangle$ denotes the average of a given field over the volume V of the RVE

– the condition for equivalence of energetically and mechanically defined effective properties of heterogeneous materials (Hill condition):

$$\langle \sigma_{ij}\varepsilon_{ij} \rangle = \langle \sigma_{ij} \rangle \langle \varepsilon_{ij} \rangle \tag{6}$$

where: σ_{ij}, ε_{ij} are stress and strain tensors, respectively.

For the heat conduction problem the Hill condition takes the form:

$$\langle T_{,i} q_i \rangle = \langle T_{,i} \rangle \langle q_i \rangle \tag{7}$$

where: $T_{,i}$ and q_i are temperature gradient and heat flux, respectively.

The FEM is used in the numerical homogenization in order to solve elasticity and heat conduction problems for micro- and macro scales. The periodic boundary conditions are applied for the RVE. After FEM analysis for the RVE average stresses and heat fluxes are used to calculate the effective constants values, according to the equation (5). Constitutive equation and Fourier law in the micro scale take the form:

$$\langle \sigma_{ij} \rangle = c'_{ijkl} \langle \varepsilon_{ij} \rangle \tag{8}$$

$$\langle q_i \rangle = k'_{ij} \langle T_{,i} \rangle \tag{9}$$

Tensor of elastic constants c'_{ijkl} is symmetric. The RVE is described by 9 independent material constants for 3D problems. Using Voight notation, tensor of elastic constants can be written in the form:

$$c'_{ij} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{21} & c_{22} & c_{23} & 0 & 0 & 0 \\ c_{31} & c_{32} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix} \tag{10}$$

Tensor of heat conduction coefficients k'_{ij} for non-crystalline anizotropic materials takes the form:

$$k'_{ij} = \begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{bmatrix} \tag{11}$$

In order to calculate all independent elastic constants, 6 analyses for linear elasticity are needed. Each column (or row) of the tensor c'_{ij} is obtained by applying an appropriate initial strain for the RVE model (Fish, 2006; Fish, 2008). Respectively, 3 analyses of heat conduction problem have to be performed in order to calculate all k'_{ij} values. For the 2D analysis numerical homogenization consists of 3 elasticity and 2 heat conduction analyses. FEM analyses are performed by means of software package – MSC.Mentat/Marc (Marc, 2010) software package in both scales. An in-house procedures written in C++ and in internal script language implemented in preprocesor Mentat were developed to perform multiscale analyses.

3. MULTIOBJECTIVE OPTIMIZATION PROBLEM

3.1. Formulation of the multiobjective optimization problem

The optimization process based on a collection of objective functions is called a multi-objective optimization (MOO). The MOO problem is formulated as follows:

find the vector $\mathbf{x} = [x_1, x_2, \ldots x_n]^T$ which satisfy the m inequality constrains:

$$g_i(\mathbf{x}) \geq 0 \qquad i = 1, 2, \ldots, m \tag{12}$$

and the p equality constrains

$$h_i(\mathbf{x}) = 0 \qquad i = 1, 2, \ldots, p \tag{13}$$

which minimizes the vector of l objective functions:

$$f(\mathbf{x}) = \left[f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_l(\mathbf{x}) \right]^T \tag{14}$$

where n is the number of design variables.

Box constraints are imposed on each design variable:

$$x_i^L \leq x_i \leq x_i^R \tag{15}$$

where x_i^L and x_i^R are minimum and maximum acceptable values for the variable x_i, respectively.

Multi-objective optimization deals with multiple conflicting objectives and usually the optimal solution for one of the objectives is not necessarily the optimum for any of the other ones. For such a case, instead of single optimal solution in single-objective optimization problem, many solutions are simultaneously incomparable and optimal (Abraham et al., 2005; Andersson, 2000).

3.2. Optimization algorithm

Multiobjective evolutionary algorithm based on Pareto concept is used to solve optimization prob-

lems in the present paper. The in-house implementation of such algorithm, called MOOPTIM is developed. It is an improved version of the multiobjective evolutionary algorithm for which some ideas are inspired by Deb's NSGA-II algorithm (Deb et al., 2002). MOOPTIM works on real-coded genes (not binary strings, like in classical genetic algorithms). It uses non-dominated sorting procedure and crowding mechanizm like NSGA-II, but MOOPTIM has modified selection procedure and uses more evolutionary operators. The proposed algorithm has no binary tournament selection operator like in NSGA-II, but selection is performed on the basis of nondomination level and crowding coefficient (Długosz & Burczyński, 2012). Two types of mutation (uniform and Gaussian) and two types of crossover operators (simple and arithmetic) are used. It should be emphasized that Gaussian mutation has significant influence on the effectiveness of searching by the algorithm. This operator requires an additional parameter (besides mutation probability) in the form of the mutation range (from 0 to 1). It was observed that higher values of the probability and range of this operator improved the convergence of the algorithm, especially for more difficult tasks. The MOOPTIM algorithm consists of two parts: an initialization and a main loop. Figure 2 shows the flowchart of the MOOPTIM. MOOPTIM algorithm was tested on several benchmarks (SCH, ZDT1, ZDT2, ZDT3, ZDT4, ZDT6, DTLZ1, DTLZ2, CONSTR, SRN, TNK) (Deb, 1999; Zitzler & Thiele, 1999) and also on engineering problems (Długosz & Burczyński, 2011; Długosz & Burczyński, 2012). The results obtained using MOOPTIM are better in comparison with the results obtained by means of NSGA-II in most cases. Advantage of using MOOPTIM instead of NSGA-II especially appears for functions rather difficult to optimize i.e.: having strong multimodality, non-convex Pareto front or discontinuous Pareto front. Detailed description of MOOPTIM and comparison between MOOPTIM and NSGA-II can be found in (Długosz, 2010).

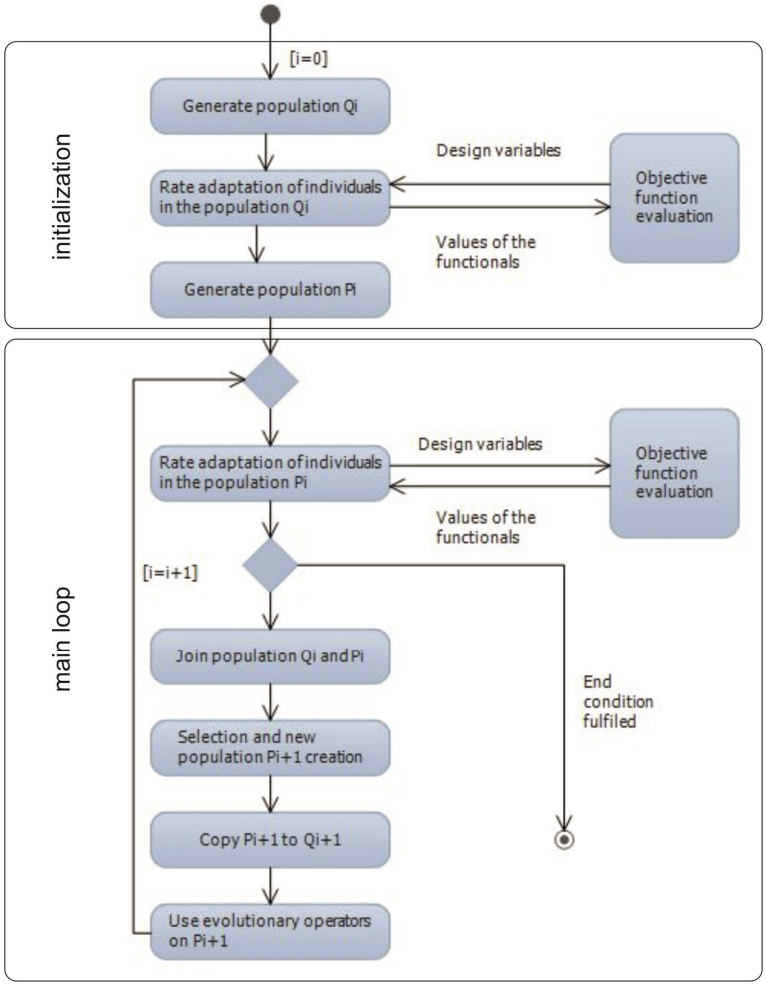

Fig. 2. *Flowchart of the MOOPTIM.*

3.3. Optimization criteria

For structures under thermomechanical loading, the optimization concerns both mechanical, and thermal properties (e.g. strength, stiffness, low or high thermal conductivity). Multiscale optimization tasks can be formulated as a designing of a microstructure (shape of voids or inclusions) or selection of the properties for the particular phases. Optimization criteria can be defined on the basis of thermal or mechanical quantities (displacements, stresses, strains, temperatures, heat fluxes). The following criteria have been defined:

– minimization of the displacement u on the selected part of the boundary Γ_u:

$$\min_{\mathbf{x}} \quad f_1 \overset{def}{=} \int_{\Gamma_u} u \, \mathrm{d}\Gamma_u \tag{16}$$

– minimization of the heat flux q on the selected part of the boundary Γ_q:

$$\min_{\mathbf{x}} \quad f_2 \overset{def}{=} \int_{\Gamma_q} q \, \mathrm{d}\Gamma_q \tag{17}$$

– maximization of the heat flux q on the selected part of the boundary Γ_q:

$$\min_{\mathbf{x}} \quad f_3 \overset{def}{=} \int_{\Gamma_q} q \, d\Gamma_q \tag{18}$$

– maximization of the porosity defined as the ratio of pore volume to the volume of RVE:

$$\max_{\mathbf{x}} \quad f_4 \overset{def}{=} \frac{\int_{\Omega_{por}} d\Omega_{por}}{\int_{\Omega_{RVE}} d\Omega_{RVE}} \tag{19}$$

4. NUMERICAL EXAMPLE

A square plate of dimensions 50 x 50 x 1 mm under thermomechanical loads is considered (figure 3a). The plate is made of porous aluminum. Thermoelastic material constants for aluminium are as follows: Young modulus E = 70000 MPa, Poisson ratio=0.35, thermal conductivity k = 200 W/mK, thermal expansion coefficient $\alpha = 23 \cdot 10^{-6}$ 1/K. A bottom part of the plate is supported, whereas an upper part is uniformly loaded by a traction equal to 100 N/mm. The temperature is equal to 0°C on the left side, whilst 100°C is applied on the right side of the plate. The plate is modelled in plane stress state. Two-scale micro-macro model is considered.

Multiobjective optimization task concerns determining the optimal shape of the void in the microstructure by minimization or maximization of the functionals calculated on the basis of results obtained from macromodel. The microstructure is modeled as RVE with periodic boundary conditions. The effective elastic and thermal constants are obtained from the numerical homogenization. The void in the microstructure is modeled with the use of closed NURBS curve (Piegl & Tiller, 1996) consisting of 8 control points. Five design variables have been defined due to the symmetry (figure 3b).

The multiobjective optimization is performed for functionals defined in section 3.3. Functional (16) concerns minimization of the vertical displacement on the upper side of the structure, whereas functionals (17) and (18) concern minimization or maximization of the total heat flux on the right side of the structure. Two optimization tasks are performed for: functionals (16) and (17), and functionals (18) and (19). Table 1 contains main parameters of MOOPTIM. The set of Pareto-optimal solution is shown in figure 4 and figure 6, whereas shapes of voids in the microstructure for selected points on Pareto front are shown in figure 5 and figure 7. Table 2 contains thermal and elastic material constants after optimization for points indicated in figure 4 and figure 6.

Tab. 1. *Parameters of the MOOPTIM.*

Parameter	Value
size of the population	30.0
no of generation	150
probability of uniform mutation	0.1
probability of Gaussian mutation	0.7
Range of Gaussian mutation	0.5
probability of simple crossover	0.1
probability of arithmetic crossover	0.1

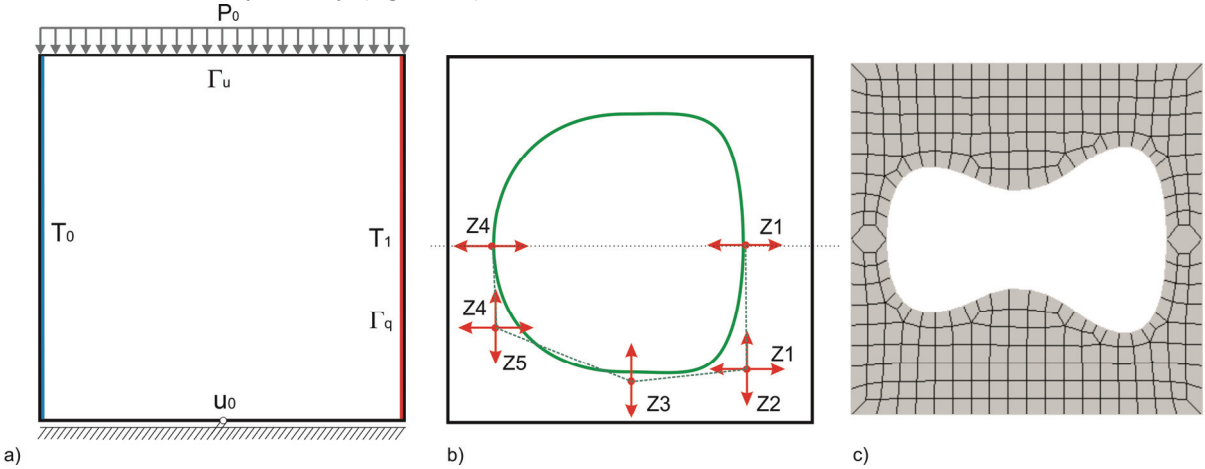

Fig. 3. *a) Macromodel of structure under thermomechanical loading, b) parameterization of the void in the RVE by closed NURBS cure, c) Example model of RVE after discretization*

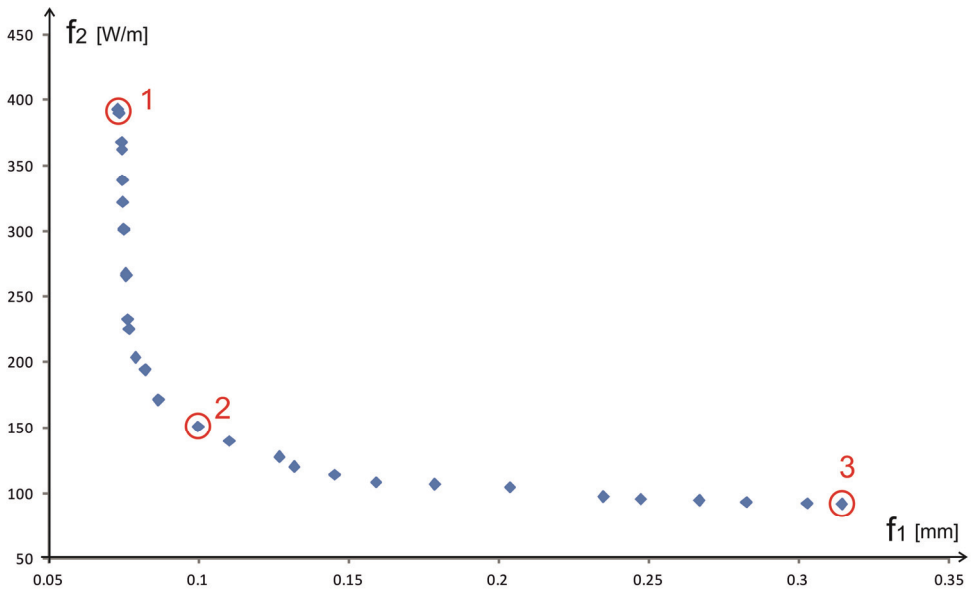

Fig. 4. *The set of Pareto optimal solutions for minimization functional f_1 (16) and minimization functional f_2 (17).*

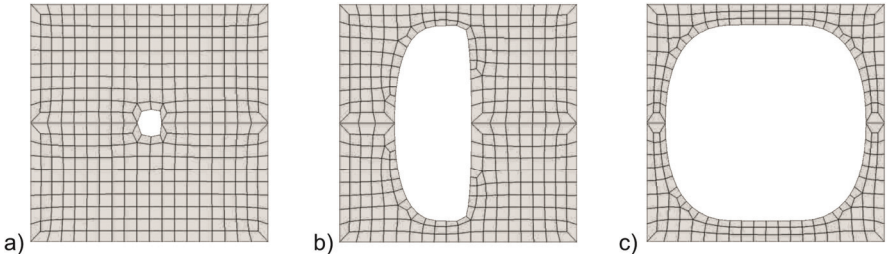

Fig. 5. *Shapes of voids in microstructure after optimization for: a) point 1, b) point 2, c) point 3 (points are indicated in figure 4).*

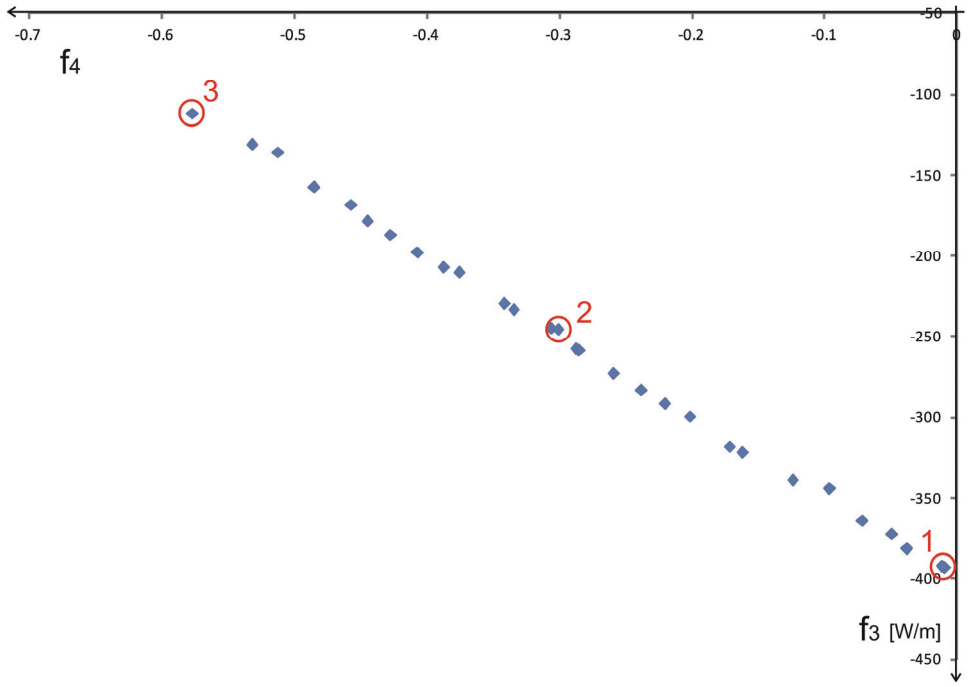

Fig. 6. *The set of Pareto optimal solutions for maximization functional f_3 (18) and minimization functional f_4 (19).*

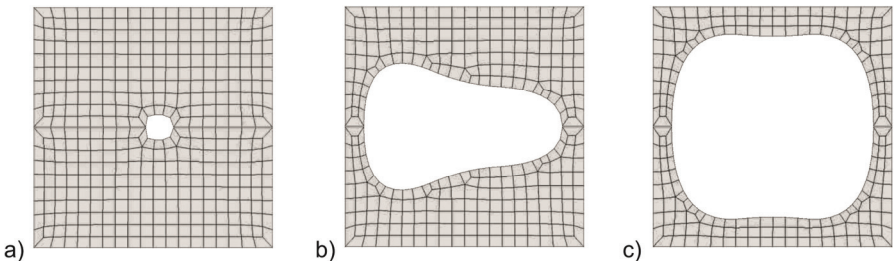

Fig. 7. *Shapes of voids in microstructure after optimization for: a) point 1, b) point 2, c) point 3 (points are indicated in figure 6).*

plication of multiobjective evolutionary algorithm based on Pareto concept is a good choice. Results of optimization have been presented in the form of the sets of a Pareto-optimal solutions and also in the graphical form of optimal microctructures for selected solutions from these sets.

Tab. 2. *Values of design variables and values of material constants after optimization for points indicated in figures 4 and 6.*

Point	Values of design variables					Values of material constants					
	Z1	Z2	Z3	Z4	Z5	c11 [MPa]	c22 [MPa]	c12 [MPa]	c44 [MPa]	k11 [W/mK]	k22 [W/mK]
	minimization functional f_1 (16) and minimization functional f_2 (17)										
1	0.55	0.42	0.45	0.45	0.45	75052.8	75256.0	22493.7	26315.8	196.5	196.8
2	0.55	0.09	0.09	0.23	0.10	23135.3	52017.8	6567.3	6572.1	75.6	143.1
3	0.92	0.09	0.09	0.08	0.09	16130.8	16103.3	1781.6	891.1	46.0	45.5
	maximization functional f_3 (18) and minimization functional f_4 (19)										
1	0.58	0.45	0.45	0.47	0.45	75167.5	74885.3	22468.5	26266.2	196.6	196.2
2	0.91	0.35	0.33	0.08	0.15	41967.4	20895.7	4799.6	4848.29	122.4	67.3
3	0.92	0.09	0.13	0.08	0.09	19801.1	16254.1	2154.13	1113.4	55.9	46.5

The sets of Pareto-optimal solutions, presented in figure 4 and 6 are evenly distributed. For the extreme solutions (points 1 and 3), values of the design variables are close to or even equal to maximal or minimal admissible values. For such points the obtained results may not be surprising. Pairs of functionals (16) and (17) are contradictory, so smaller voids increase the stiffness while improving the thermal conductivity properties. For the functionals (18) and (19), smaller porosity improves thermal conductivity properties. Point 2 in the figure 4 represents the compromise between higher stiffness and better insulating thermal properties, whereas point 2 in figure 6 represents compromise between greater ability to conduct heat and greater porosity.

5. CONCLUSIONS

The coupling of evolutionary computation with multiscale modeling of thermomechanical solid has been presented. Numerical homogenization with RVE concept and FEM has been used. The results of the multiobjective optimization of multiscale thermoelastic models have been presented. The functionals depending on mechanical and thermal properties of the material have been formulated. Considered functionals are typically contradictory, so ap-

ACKNOWLEDGEMENT

The research is financed from the Polish science budget resources as the project R07 0006 10.

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OPTYMALIZACJA W WIELOSKALOWYCH ZAGADNIENIACH TERMOSPRĘŻYSTYCH

Streszczenie

W artykule przedstawiono polaczenie modelowania wieloskalowego dla układów termosprężystych oraz wielokryterialnego algorytmu ewolucyjnego. W pracy przedstawiono przykłady optymalizacji parametrów mikrostruktury porowatej, z której wykonany jest układ poddany obciążeniom termomechanicznym. Zadania polegały na optymalnym doborze kształtu pustki w mikrostrukturze modelowanej za pomocą zamkniętej krzywej NURBS. Zdefiniowano kilka funkcjonałów, zależnych od przemieszczeń i strumienia ciepła w skali makro oraz od porowatości mikrostruktury. Optymalizację wielokryterialną przeprowadzono dla wybranych par funkcjonałów z użyciem opracowanego algorytmu MOOPTIM.

Received: October 02, 2013
Received in a revised form: December 17, 2013
Accepted: December 18, 2013