Computer Assisted Methods in Engineering and Science, **20**: 325–336, 2013.

TWENTY YEARS OF THE CAMES

Identification in multiscale thermoelastic problems

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The paper deals with the identification in multiscale analysis of structures under thermal and mechanical loads. A two-scale model of porous materials is examined. Direct thermoelastic analyses with representative volume element (RVE) and finite element method (FEM) are taken into account. Identification of material constants of the microstructure and identification of the shape of the voids in the microstructure are considered. Identification functional is formulated on the basis of information obtained from measurements in mechanical and thermal fields. Evolutionary algorithm is used for the identification as the optimization technique. Numerical examples of identification for porous aluminum models are enclosed.

Keywords: multiscale modeling, numerical homogenization, thermoelasticity, evolutionary algorithms, identification, coupled problems, finite element method.

1. Introduction

Multiscale calculations play a key role in the design of novel and advanced materials. The designing of such materials may concern the searching for proper material properties or desired shape of the microstructure. Multiscale calculations allow to simulate a behavior of such materials by means of suitable methods. To take into account all the details of geometry and material structure in one scale only, it would require the creation of very complex models. Numerical simulations in such a case, if possible, would be very time consuming. Multiscale calculations may concern two or more scales, starting from the macro level, taking into consideration external mechanical and thermal loads, through meso- and micro-scale (phase inclusions, porosity), down to the defects in the crystal lattice. A coupling between numerical simulations and the molecular dynamics is also possible [1, 7, 8]. In order to move 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. In transition from the lower to upper scales the efficient material parameters are calculated 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 both geometry and boundary conditions. Very popular and efficient approach is coupling of the numerical homogenization [1, 9] with the finite element method (FEM) [2, 14]. The identification may concern searching for material properties of a structure, shape or position of inclusions or voids etc. If different coupled physical fields are considered, searching for different groups of material properties is required (eg., mechanical, thermal, etc.). In order to perform identification task, a proper functional has to be defined. If numerical methods are used, such functionals

are strongly multi-modal, especially for coupled problems. An efficient optimization requires the usage of techniques, which are resistant to stacking in local optima. Evolutionary algorithms (EAs) are one of the methods which are suitable for solving such problems [10]. In comparison to the other techniques, EAs give a proper balance between two conflicting aspects necessary in successful optimization: the exploitation near the probable optimum and the exploration of the search space.

The paper deals with the identification of parameters of the microstructure for porous materials by means of evolutionary algorithm and the numerical homogenization with FEM. The identification is performed using information about the displacements and the temperatures in the boundary sensor points, measured in the macro level. In order to solve the problem, proper identification functional is formulated.

2. Multiscale modeling by means of numerical homogenization

2.1. Formulation of the problem

The primary purpose of the homogenization is to find homogeneous model for the non-homogeneous medium and thus to determine the relationship between the macroscopic quantities (in practice the mean values) and the so-called efficient material constants. For the thermoelasticity problems, the material constants may include: elastic constants, thermal conductivity constants and thermal expansion coefficients [13, 15]. The two-scale model of the porous structures with global periodicity is examined. Figure 1 shows an exemplary body under thermal and mechanical loads before and after homogenization.

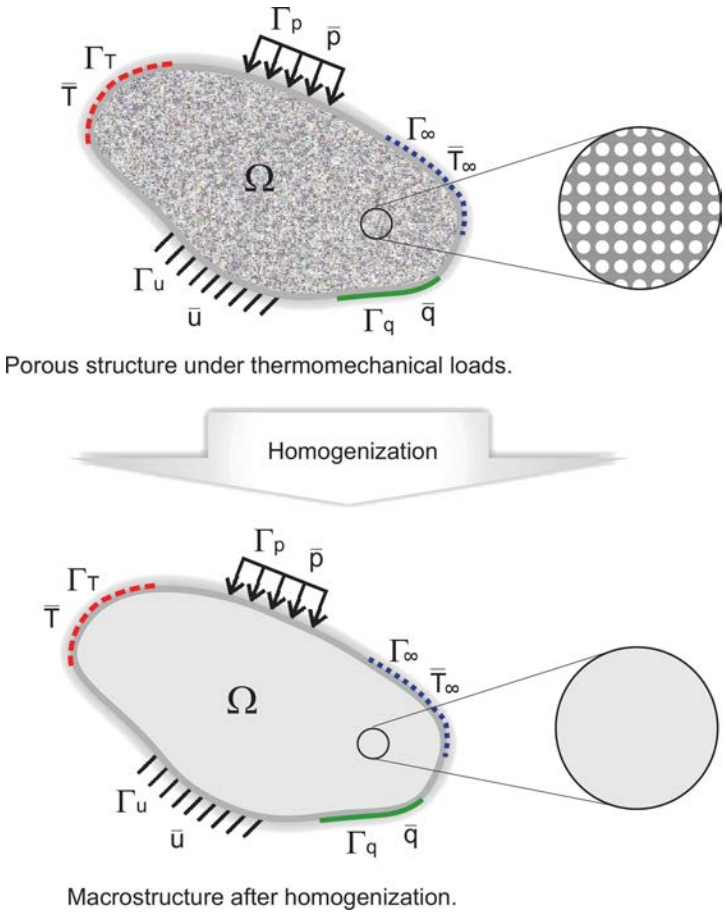


Fig. 1. Homogenization of the thermoelastic porous structure.

The linear thermoelasticity problem is described by differential equation of heat conduction and elastisticity taking into account thermal strains [5, 12].

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

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

where k is thermal conductivity, T is temperature, u is displacement, α_T is linear expansion coefficient, μ and λ are Lamé's constants. These equations have to be supplemented by mechanical and thermal boundary conditions:

$$\Gamma_t \colon t_i = \overline{t}_i, \qquad \Gamma_u \colon u_i = \overline{u}_i, \tag{3}$$

$$\Gamma_T \colon T_i = \overline{T}_i, \qquad \Gamma_q \colon q_i = \overline{q}_i, \qquad \Gamma_c \colon q_i = \alpha(T_i - T^{\infty}), \tag{4}$$

where $\overline{u}_i$, $\overline{t}_i$, $\overline{T}_i$, $\overline{q}_i$, α, T^{∞} are known: displacements, tractions, temperatures, heat fluxes, heat conduction coefficient and ambient temperature, respectively. Γ_t, Γ_u, Γ_T, Γ_u, Γ_q, Γ_{∞} are parts of the boundary, where mechanical and thermal boundary conditions are specified (Fig. 1).

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

- the separation of scales

$$\frac{l}{L} \ll 1, \tag{5}$$

  where l and L are characteristic lengths of the structure for RVE and macro scale respectively,

- volume averaging is done accordingly as follows

$$\langle \cdot \rangle = \frac{1}{|\Omega_{\mathrm{RVE}}|} \int\limits_{\Omega_{\mathrm{RVE}}} (\cdot)\, d\,\Omega_{\mathrm{RVE}}, \tag{6}$$

  where $\langle \cdot \rangle$ denotes the average of a given field over the volume Ω_{RVE} of the RVE,

- the condition for equivalence of energetically and mechanically defined effective properties of heterogeneous materials (Hill's condition)

$$\langle \sigma_{ij} \varepsilon_{ij} \rangle = \langle \sigma_{ij} \rangle \langle \varepsilon_{ij} \rangle , \tag{7}$$

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

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

$$\langle T_{,i} q_i \rangle = \langle T_{,i} \rangle \langle q_i \rangle , \tag{8}$$

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

For the elasticity and heat conduction problems in micro and macro scale, the numerical homogenization by means of FEM is used. Periodic boundary conditions are applied for the RVE. After FEM analysis for the RVE, average stresses and heat fluxes are used to calculate effective constants' values, according to relation (6). Constitutive equation and Fourier's law in the micro scale take the form:

$$\langle \sigma_{ij} \rangle = c'_{ijkl} \langle \varepsilon_{ij} \rangle , \tag{9}$$

$$\langle q_i \rangle = -k'_{ij} \langle T_{,i} \rangle . \tag{10}$$

The tensor of elastic constants c'_{ijkl} is symmetric and has nine independent material constants, for the 3D RVE.

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

For anisotropic non-crystalline materials the tensor of heat conduction coefficients takes the form:

$$k'_{ij} = \begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{bmatrix}. \tag{12}$$

In order to calculate nine independent elastic constants, six analyses of linear elasticity are needed. Each column (or row) of the tensor c'_{ij} is obtained by applying a consecutive initial strain to the RVE model [7, 8]. Respectively, three analyses of heat conduction problem have to be performed in order to calculate all coefficients of k'_{ij}. For the 2D analysis, numerical homogenization consists of three analyses of the elasticity and two analyses of the heat conduction problem, respectively.

2.2. Verification of the developed procedures

Relevant computer programs and procedures which allow to perform the multiscale analysis of porous materials under thermomechanical loading have been developed. The effective elastic and thermal constants are calculated from the microscale. As the linear expansion coefficients are independent of the porosity for the porous materials, it is not necessary to homogenize these parameters. FEM analyses are performed by means of software package MSC.Mentat/Marc [11] in both scales (micro and macro). In-house procedures written in C++ and in an internal script language implemented in the preprocessor Mentat have been developed to perform multiscale analysis.

Accuracy of the developed procedures is examined on different examples. Two numerical examples of verification are included in the paper. The first one concerns determining the effective thermal conductivity for the 3D cube with the spherical void (Fig. 2a).

Material with such a microstructure has isotropic properties. Porous aluminum is considered. Obtained results are compared with the results for reduced analytical models. Thermal conductivity of the air in the microstructure is neglected due to very low value of it in comparison aluminum (thermal conductivity of aluminum is 200 W/mK, whereas for the air it is 0.025 W/mK).

Very popular reduced analytical models for structures with spherical voids are:

- Weiner and Hashin-Strikman model

$$k' = \frac{1-\phi_p}{1+(\phi_p/2)}, \tag{13}$$

- Hashin-Strikman model

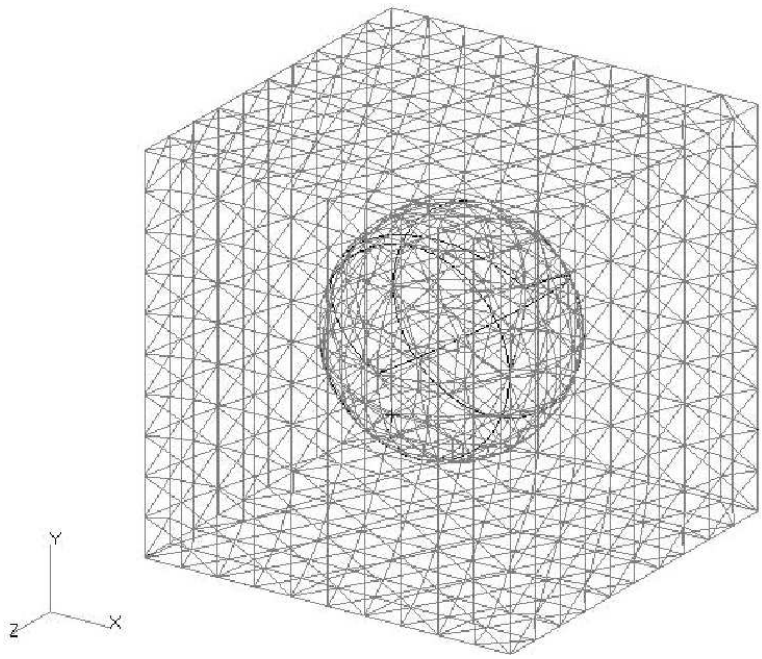
$$k' = e^{\left(\frac{-(3/2)\phi_p}{1-\phi_p}\right)}, \tag{14}$$

- exponential model

$$k' = (1-\phi_p)^{3/2}, \tag{15}$$

where ϕ_p is porosity defined as the ratio of pore volume to the volume RVE.

a)



b)

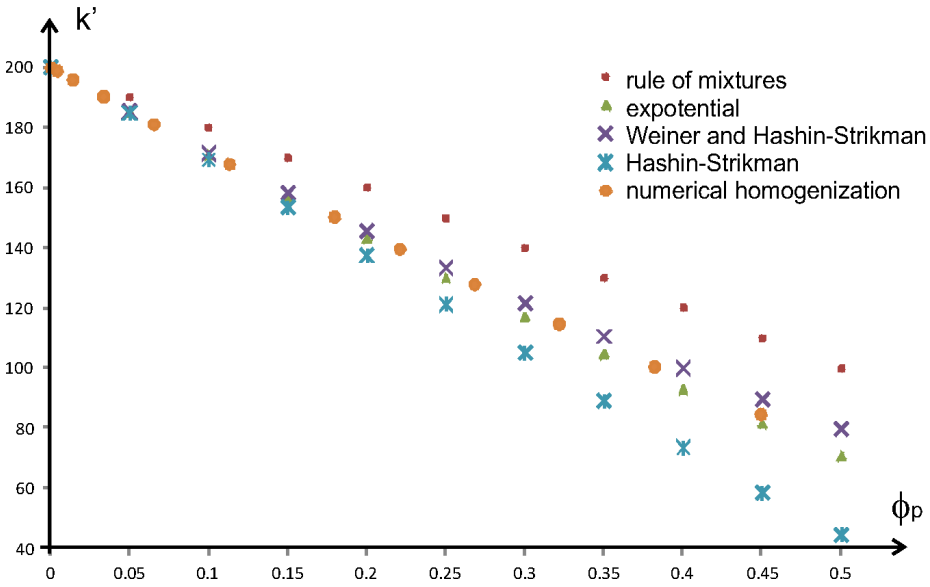


Fig. 2. a) FEM cubic RVE model with spherical void, b) relation between thermal conductivity and porosity of aluminum. Comparison between models: rule of mixtures ($k' = 1 - \phi$), exponential, Weiner and Hashin-Strikman, Hashin-Strikman and numerical homogenization.

Figure 2b shows relation between thermal conductivity and the porosity for the analytical models and the developed numerical homogenization procedure.

Comparison for nonhomogeneous and the developed two-scale models of exemplary structure is considered also. Rectangular plate with global periodicity, for which microstructure includes elliptical voids is examined. The left side of the plate is supported, whereas on boundaries AB and AD temperatures $T_1 = 0°\text{C}$ and $T_2 = 50°\text{C}$ are applied, respectively. Parts of the boundary BC and DE are insulated ($q = 0$). The plate has a thickness of 1 mm and is modeled in plain stress state. The geometry of the plate and the boundary conditions are shown in Fig. 3.

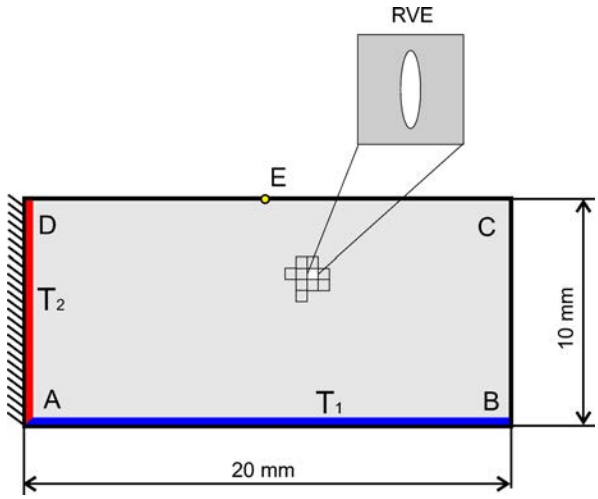


Fig. 3. Rectangular plate with periodical microstructure.

Figures 4 and 5 show the temperature distribution and map of the vertical displacement in the structure for nonhomogeneous and the two-scale models. Value of the temperature at the point E for

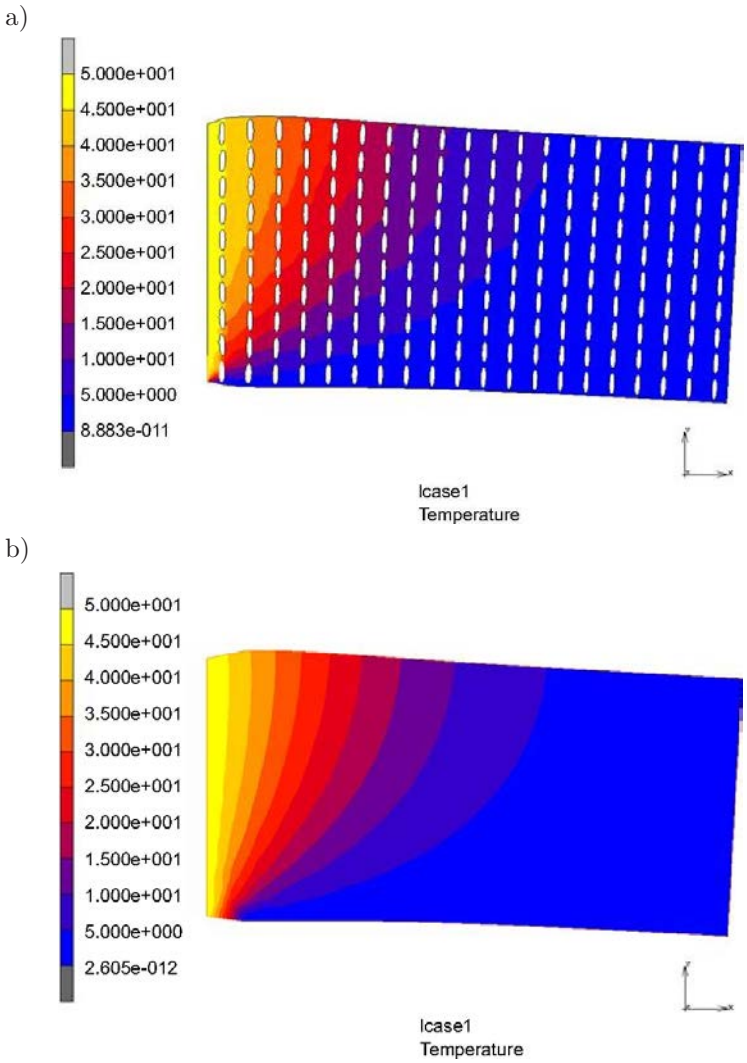


Fig. 4. Temperature distribution in the structure: a)non-homogeneous model, b) two-scale model.

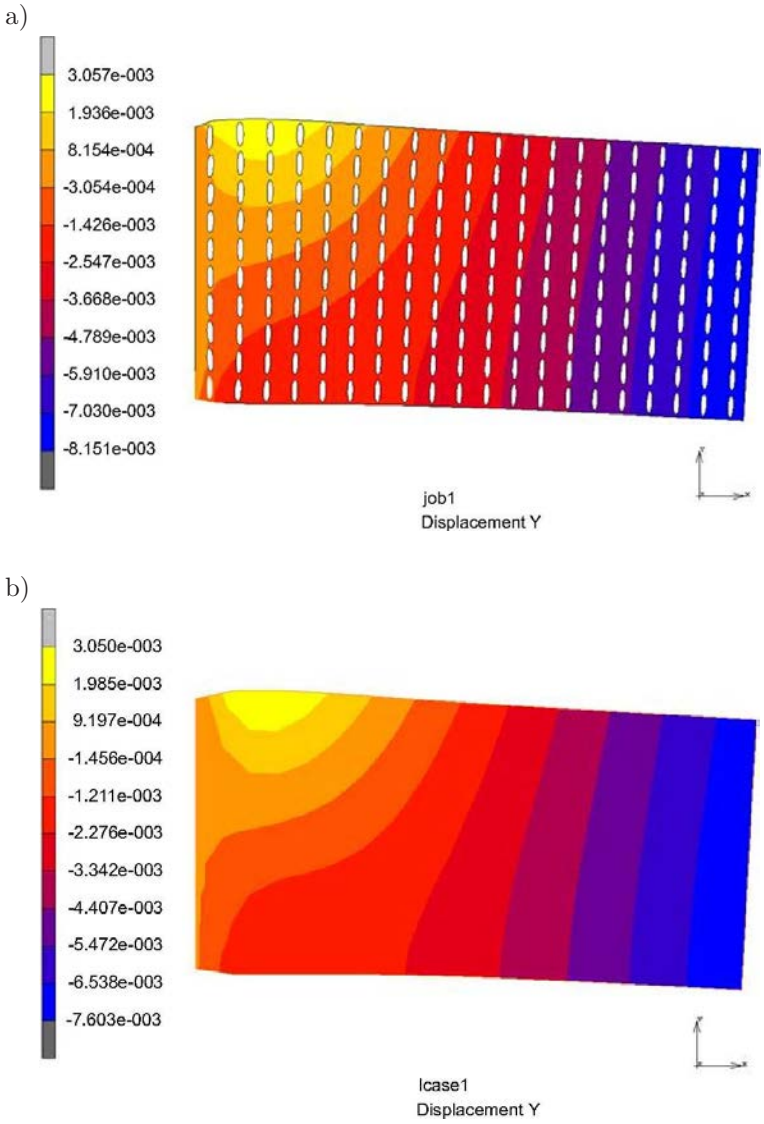


Fig. 5. Vertical displacement in the structure: a)non-homogeneous model, b) two-scale model.

the nonhomogeneous model is equal to 7.99°C, whereas for the two-scale model is 8.06°C. Maximal values of the vertical displacement for the considered models are 0.003057 mm and 0.00305 mm respectively. The results clearly depict good accuracy of the developed homogenization procedures (error in all cases is less than 1%).

In order to conduct full analysis of the two-scale model, the following are necessary: five analyses of RVE, transfer of efficient material constants to the macro model and performance of the analysis in macro scale. Although heterogeneous numerical model requires only a single numerical simulation, the two-scale model allowed to shorten the calculation time approximately 26 times (numerical heterogeneous model consists of 75 000 nodes whereas the two-scale model RVE consists of 300 and macro model consists of 200 nodes). It is obvious that for the more complicated models a reduction of the computational cost would be much greater. It is therefore clear that the identification tasks using heterogeneous models with a large number of degrees of freedom could be difficult or impossible to accomplish, due to the time of computation. It is especially important that the identification evolutionary algorithm is used, because for each individual it is necessary to calculate the objective function value based on the numerical analysis.

3. Identification problem

The goal of the identification is to determine the parameters of the microstructure on the basis of measurements at the macro level. The following assumptions are assumed:

- set of experimental values measured at selected points of the real object is known,
- set of the corresponding theoretical values calculated using the numerical homogenization is computed.

Values of temperatures and displacements are measured at the boundary sensor points. Both the experimental and theoretical values are obtained by means of FEM. Identification belongs to the class of ill-posed problems. In the tasks of this type, the "answer" of the system for the different sets of input parameters may be similar or, in extreme cases, even the same. Thus, obtaining the correct solution becomes very difficult. In such a case the problem can be solved by: changing the location of the sensors, increasing the number of it or taking measurement from different physical fields. The paper [3] demonstrates superiority of a measurement of both the temperature and the displacement in the boundary sensor points, compared to the measurement of only temperatures or displacement separately (assuming the same number of control points).

To solve identification problem the following functional is defined:

$$J_0 = a\sum_{i=1}^{m} |\widehat{u}_i - u_i| + b\sum_{j=1}^{s} \left|\widehat{T}_j - T_j\right|, \tag{16}$$

where m and s are numbers of sensor points of displacement and temperatures respectively, $\widehat{u}_i$ and u_i are measured and computed values of displacement at sensors i, $\widehat{T}_i$ and T_i are measured and computed values of temperature at sensors i, a and b are weight factors. Symbol $|\cdot|$ stands for the absolute value.

Values of the weight factors are selected in a way to assure comparable influence of the displacement and the temperature parts. The identification task is to minimize functional (16) with regard to parameters describing location or shape of the internal void in the RVE or with regard to material constants. The minimum value of the functional is equal to zero, which corresponds to an exact solution.

4. Evolutionary algorithm

In order to solve identification problem, our own implementation of evolutionary algorithm is used. The solution of the problem is given by the best chromosome whose genes represent design parameters responsible for the shape of the void in the microstructure or values of material parameters. Figure 6 shows flow chart of the developed evolutionary algorithm.

The evolutionary algorithm starts with a population of chromosomes randomly generated. For each individual fitness function is determined. On the basis of chromosomes genes, which are design variables in the identification task, the RVE model is created. Creation of the RVE is aided by procedures written for preprocessor Mentat. Then, five FEM analyses are performed by means of MSC.Marc. Efficient thermal and mechanical material constants are transferred to the previously prepared macro model. After numerical analysis of the macromodel, on the basis of the results, functional J_0 is calculated. This value is transferred back to the evolutionary algorithm. Algorithm works until stop condition is not fulfilled (maximal number of generations is assumed in the paper). Real-coded value of genes (not binary strings) are used in the algorithm. Following evolutionary operators are implemented: uniform mutation, mutation with the Gaussian distribution, simple crossover and arithmetic crossover. Ranking selection is used. Implementation of the Gaussian mutation significantly decreases the risk of stacking the algorithm in local minimum [4].

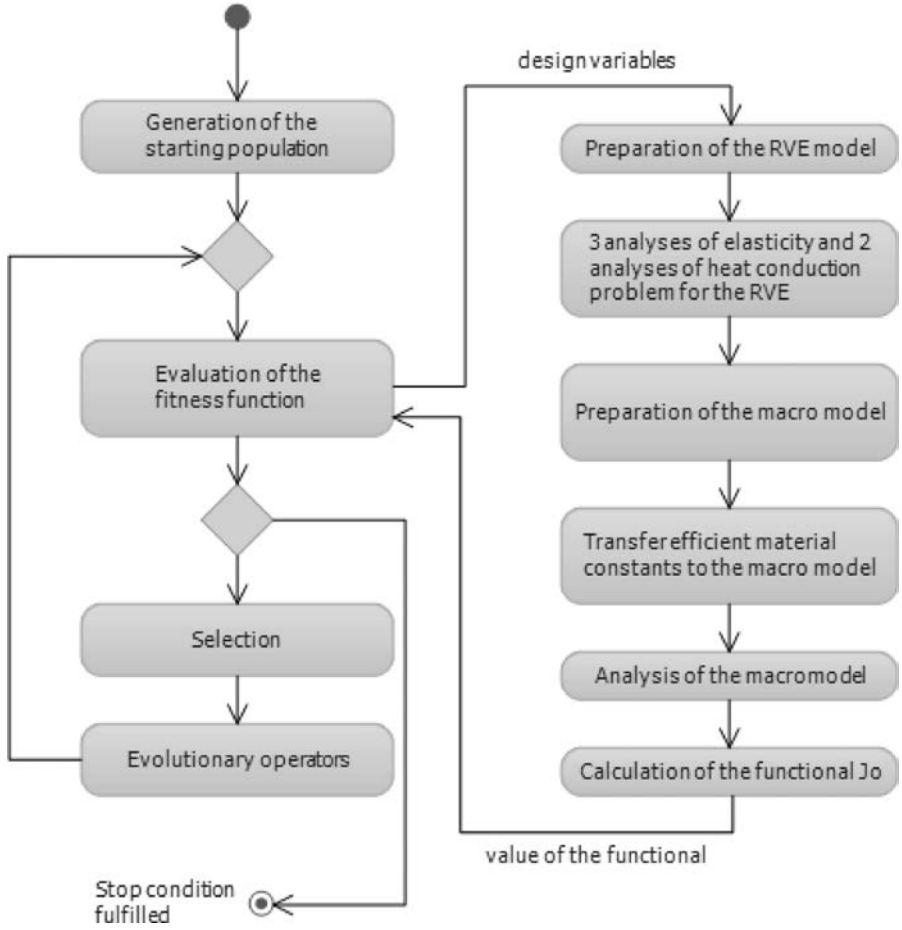


Fig. 6. Flow chart of the evolutionary algorithm combined with two-scale thermomechanical analysis.

5. Numerical example

Square plate of dimension $50 \times 50 \times 1$ mm supported on the left boundary is considered (Fig. 7a). Traction P_0 equal to 10 N/mm is applied on the upper boundary of the length of 10 mm. On the two boundaries temperature boundary conditions are applied ($T_1 = 10°\text{C}$ and $T_2 = 80°\text{C}$). The top and right boundaries of the structure are insulated ($q = 0$). The plate is modeled in plain stress state. On the right and upper boundaries nine sensors are localized. Temperatures and displacements are measured at each sensor. Five variants of identification are performed.

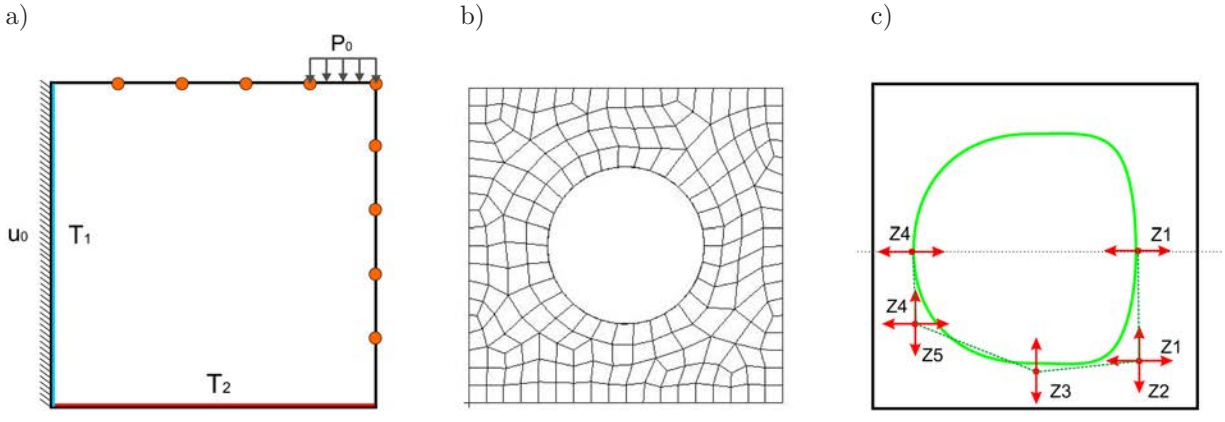


Fig. 7. a) Macromodel of the plate under thermoelastic loading, b) model of the microstructure, c) parametrization of the void in the microstructure.

The first variant of identification microstructure includes circular void (diameter of the void is equal to half the length of the bottom edge). Such a microstructure has isotropic properties. Figure 7b shows numerical model of the microstructure [6]. Three parameters are identified: Young's modulus E, Poisson's ratio ν and thermal conductivity k. Parameters of evolutionary algorithm are as follows: probability of uniform mutation is 0.1, probability of the Gaussian mutation is 0.7, probability of simple crossover is 0.1 and probability of arithmetic crossover is 0.1. Population size is 15 individuals, whereas maximal number of generation is equal to 100. Design variables are identified material parameters on which following box constraints are imposed: E – $[40\,000 \div 80\,000]$, ν – $[0.25 \div 0.35]$, k – $[100 \div 300]$. Table 1 contains results of identification.

Table 1. Results of identification.

Material parameter	Exact value	Value after identification	Error
E [MPa]	70 000	70 111	0.16%
ν	0.3	0.31	3.4%
k [W/mK]	200	222	11%

In further variants the shape of the void in the microstructure is identified. As in variant 1, identification is carried out by measuring temperatures and displacements in boundary sensor points for the macromodel. Void is modeled as an ellipse and closed NURBS curve consists of eight control points. For the elliptical void, design variables are major and minor axis of an ellipse. For the NURBS curve, variables are coordinates of the control points. Symmetry of the void is assumed, the total number of design variables is equal to 5 (Fig. 7c). Parameters of evolutionary algorithm are the same as in the first variant, except the size of the population. For the identification of the elliptical void, population size is 10, whereas for the void modeled as NURBS curve is 20. Table 2 contains results of the identification, whereas Fig. 8 presents shapes of the void for the considered variants of the identification. Figure 9 shows graph of the fitness function value in consecutive generations for the considered variants of identification.

Table 2. Results of the identification – variants 2–5.

Variant/design variable		Exact value	Value after identification	Error
Variant 2 – elliptical void	R1	0.200	0.197	1.6%
	R2	0.800	0.802	0.2%
Variant 3 – elliptical void	R1	0.800	0.801	0.1%
	R2	0.200	0.199	0.4%
Variant 4 – void modeled by NURBS curve	Z1	0.900	0.912	1.4%
	Z2	0.100	0.224	124%
	Z3	0.400	0.342	14.5%
	Z4	0.100	0.099	0.5%
	Z5	0.200	0.153	23.4%
Variant 5 – void modeled by NURBS curve	Z1	0.800	0.787	1.6%
	Z2	0.200	0.090	55.0%
	Z3	0.100	0.117	17.0%
	Z4	0.200	0.166	16.9%
	Z5	0.200	0.317	58.7%

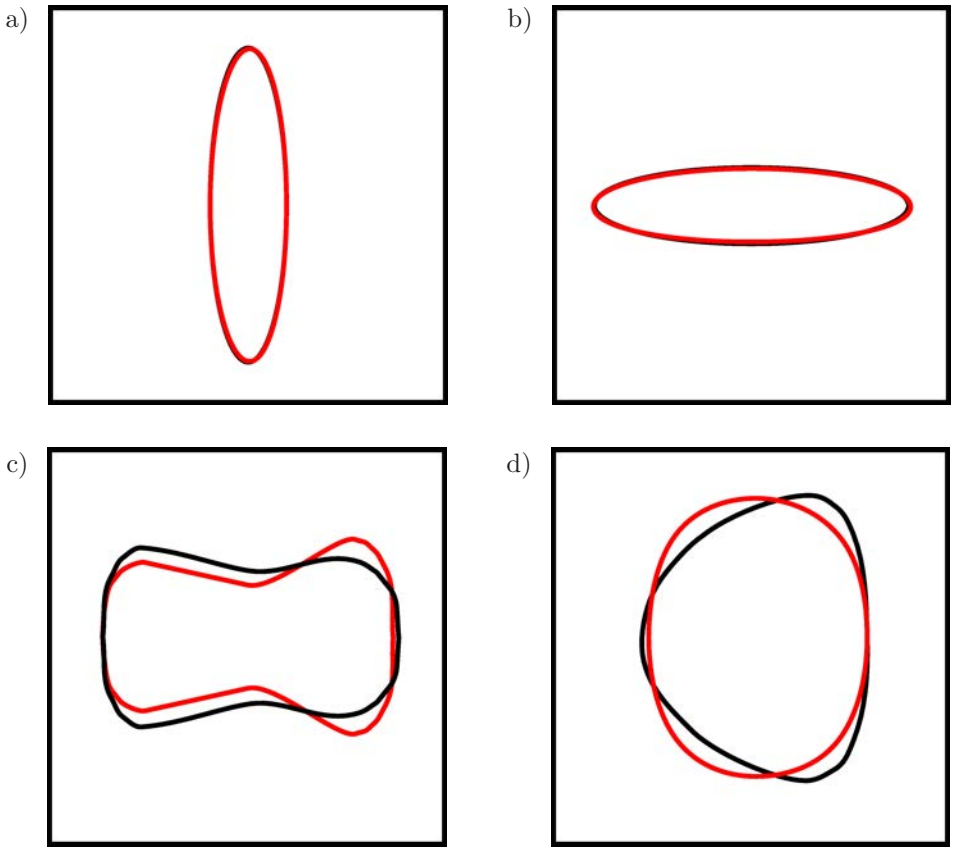


Fig. 8. Results of identification. Red color indicated reference shape, whereas black indicates shape obtained after identification: a) variant 2, b) variant 3, c) variant 4, d) variant 5.

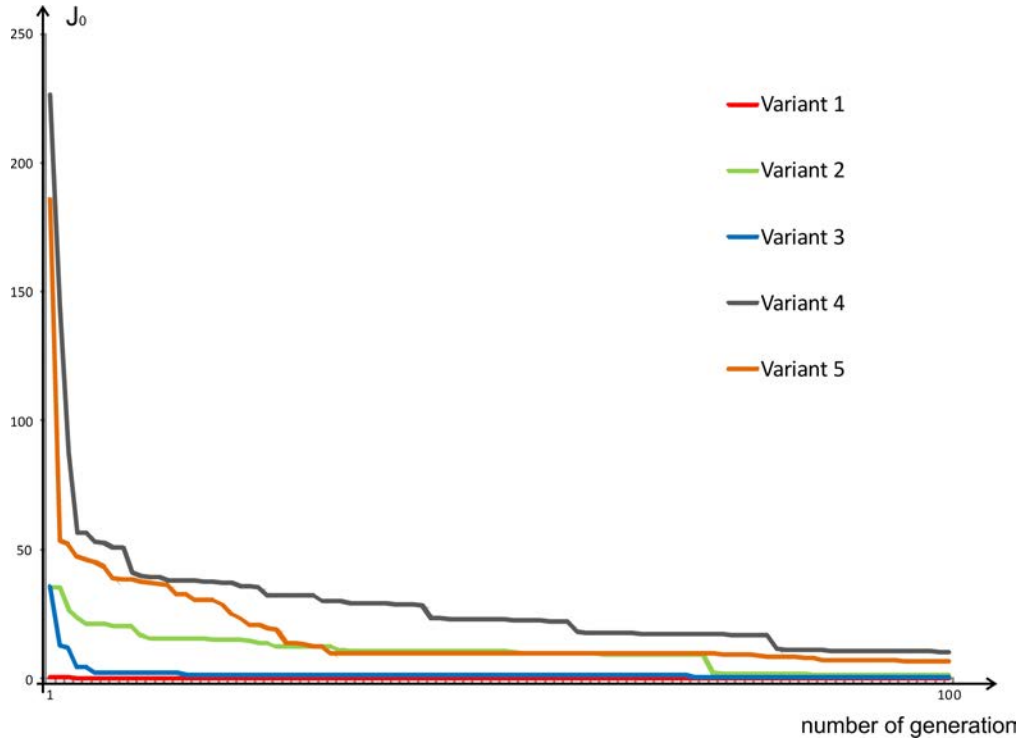


Fig. 9. Graph of the fitness function value in consecutive generations for the considered variants of identification.

6. Conclusions

The coupling of evolutionary computation with multiscale modeling of thermomechanical solid was presented. Numerical homogenization with RVE concept and FEM was used. The two-scale model of porous aluminum was considered. Design variables in identification tasks describe microstructure, whereas functional was formulated on the basis of measured temperature and displacement in a macro scale.

For the evolutionary algorithms there is no need for using the gradient of fitness functions. Such an advantage makes it relatively easy to use in the identification tasks. Presented numerical examples clearly depict pertinence of using EA in the considered type of problem.

Two types of identification were considered: identification of the unknown elastic and thermal constants for the structure with circular void, and identification of the shape of the void in the microstructure. All variants of identification showed high efficiency of the method. For the variant 1 only value of the thermal conductivity was identified with greater error. This due to the low sensitivity of this parameter on the distribution of displacements and temperatures in macromodel. For variants 2 and 3 (elliptical voids), the error of identification is very small, however for variants 4 and 5 the error is greater. Table 2 shows a quite big discrepancy between known and identified values of the position of control points for the last two variants. Nevertheless, Figs. 8c and 8d show a quite good accuracy of identified shapes. It should be emphasized that only nine boundary sensor points were used. In order to identify shape of the void in the microstructure more accurately it is necessary to introduce more sensors.

Acknowledgment

The research is partially financed from the Polish science budget resources as the project no. R07 0006 10.

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