ISSN 1392–1207. MECHANIKA. 2016 Volume 22(5): 337–342

Identification of elastic properties of individual material phases by coupling of micromechanical model and evolutionary algorithm

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crossref http://dx.doi.org/10.5755/j01.mech.22.5.16313

1. Introduction

Development of the novel composite materials leads to obtaining materials with unique properties, sometimes with characteristics opposite to the materials used as phases of the composite. There are many works that are focused on estimation of effective material properties in dependence on properties of individual phases. Various analytical and numerical approaches has already been proposed in literature, therefore the second chapter of this article describes briefly the homogenization procedures applicable for multi-phase materials. However, the main aim of this paper is connected with solving an inverse problem of identifying the individual material phases properties in dependence of known effective properties. The identification can be treated as a minimisation of some functional depending on appropriate variables. There are a few works dealing with the identification of elastic constants of composite materials. For example, Maletta and Pagnotta in work [1] and Beluch and Burczyński in work [2] combined finite element analysis with evolutionary algorithms in order to identify the elastic constants of composite laminates with the use of vibration test data. Moreover, work [2] presents how to solve the same problem with the use of artificial immune systems. Burczyński at. al. [3] identified elastic constants of osseous tissues by combining evolutionary algorithms with finite element method. Similar approach was also applied by Makowski and Kuś [4] in order to optimize periodic structure of bone scaffold. Herrera-Solaz at.al [5] used Levenberg-Marquard method combined with finite element analysis for the identification of single grain properties by using the knowledge of polycrystalline behaviour. This study proposes to solve the identification problem with the use of evolutionary algorithms. Traditional identification methods, such as gradient methods, tend to stack in the local optima or cause problems with the calculation of fitness function gradient. Evolutionary algorithms overcome that problems by taking into account a wide range of exploration directions what is a result of population diversity. Moreover, evolutionary algorithms do not require information about fitness function gradient [2, 6]. To calculate fitness function value, the well known Mori-Tanaka micromechanical method has been used. The original contribution of this paper is a new identification strategy involving a resultant error representing the uncertain character of both the experimental data and model predictions. The error is introduced and magnified gradually during the evolutionary identification up to reaching zero value of fitness function. During this study, several analyses with different assumptions were performed in order to demonstrate this new approach. The identification focuses on a three-phase composite whose matrix is reinforced with spherical particles and long fibers. Experimental data considered as input to analysis is based on results published in work of Duc and Minh [7].

2. Effective stiffness of three phase material

In order to calculate the effective stiffness tensors of multi-phase materials by considering the properties of the individual phases, the use of homogenization procedure is essential. Homogenization involves replacing the heterogeneous material with an equivalent homogeneous material. The stiffness of multi-phase material can be estimated with the help of various approaches that have already been proposed. One of the most versatile method that can deal with the finite number of phases of any morphology is numerical homogenization based on finite [8-10] or boundary [11, 12] element analysis of representative volume element (RVE). On the other hand, this approach generally requires relatively high computational cost. Another popular group of homogenization methods is mean field approach that is based on the well-known equivalent inclusion approach of Eshelby [13]. In comparison with finite element or boundary element based homogenization, mean field methods have got few limitations but the huge advantage of this approach is computational efficiency and simplicity. In case of solving the identification problem, the objective function that contains homogenization procedure has to be computed multiple times. As the computational efficiency of homogenization is one of the crucial issues, the study proposes the use of the well-known, mean field Mori-Tanaka method [14]. In this case, effective elasticity tenor can be determined by using the following relation:

$$C^{EFF} = C_m + f_i\left[\left(C_i - C_m\right)A^{MT}\left(f_m I + f_i A^{MT}\right)\right]^{-1}, \quad (1)$$

where

$$A^{MT} = S\left[\left(1-v_f\right)I + v_f S\right]^{-1} \quad (2)$$

is Mori-Tanaka strain concentration tensor, S is an Eshelby tensor, I is identity tensor, C_m and C_i are stiffness tensors of matrix and inclusion material, f_m and f_i are volume fractions of matrix and inclusion phases respectively. Although Mori-Tanaka method is originally dedicated to the analysis of two-phase materials, it can be easily extended to multi-phase materials by simply performing homogenization several times. The concept of this approach is presented in Fig. 1 using the example of three-phase composite (intentionally similar to the one that was experimentally examined in work [7]). At the first level the matrix material is homogenized with reinforcing particles. Thus obtained effective material plays the role of a fictitious matrix (Matrix II) which is reinforced with fibres. The second homogenization allows to obtain equivalent material properties of composite.

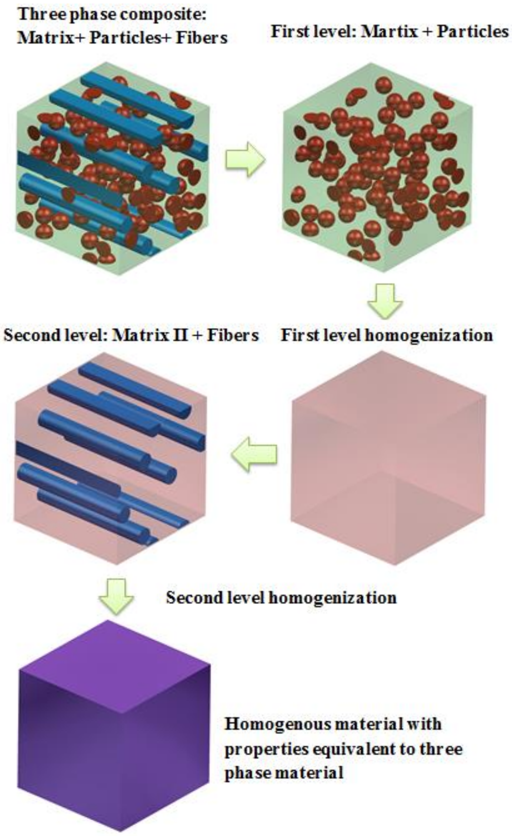

Fig. 1 Multi level homogenization scheme using the example of three-phase material

The material considered during this study is a three-phase composite reinforced with spherical particles and unidirectional long fibers. The properties of each phase are presented in Table 1. The experimental study presented in work [7] contains data for the individual phases and for composites with different volume fraction of phases. These are presented in Table 2 - E_L denotes longitudinal Young modulus, E_T is transverse Young modulus, X_{EL} and X_{ET} denote absolute relative percentage difference between experimental results and models predictions. Table 2 also contains the results of Mori-Tanaka homogenization and the results of finite element based homogenization. During Mori-Tanaka homogenization, different Eshelby solutions were considered: at the first homogenization level, it was the solution for spherical inclusion and at the second homogenization level, it was the solution for infinite fiber. The mentioned Eshelby solutions can be found in closed form, for example, in the work of Mura [15]. As finite element computation is not the main goal of this study, it was conducted only for the first material presented in Table 2, in order to compare the obtained results with Mori-Tanaka and experimental results. Finite element based homogenization was performed for representative volume element containing three phases (similar to the one presented in Fig. 1) in a way presented in the previous works of authors [8, 9]. It should be underlined that, in general, the applicability of multi-phase Mori-Tanaka methods is limited by their tendency to predict non-symmetric stiffness tensors. It may occur, for example, during studying composites reinforced with nonaligned inclusions [16]. To deal with misaligned composites, Pierard et al. proposed to decompose inclusions into the so-called pseudo grains, use Mori-Tanaka method at the first homogenization level for each pseudo grain and then use Voight method at the second homogenization level [17].

Table 1

Elastic constants of individual phases [7]

	Matrix	Particles	Fibers
Young modulus, GPa	1.43	5.58	22.00
Poison ratio	0.345	0.200	0.240

Table 2

Material properties of composites: experimental data [7], analytical and numerical predictions

Composite 20% particles + 15% fibers				
	E_L	X_{EL}	E_T	X_{ET}
Experiment	4685.71		2710.03	
Mori-Tanaka	4927.45	5.16%	2493.86	7.98%
FE homogenization	4941.06	5.45%	2674.40	1.35%
Composite 20% particles+ 20% fibers				
Experiment	6296.40		2874.98	
Mori-Tanaka	5960.41	4.93%	2741.34	4.65%
Composite 30% particles+ 15% fibers				
Experiment	4950.75		2975.76	
Mori-Tanaka	5183.26	4.70%	2844.02	4.43%
Composite 30% particles+ 20% fibers				
Experiment	6448.83		3201.23	
Mori-Tanaka	6222.70	3.51%	3144.98	1.76%

3. Solving identification problem by using evolutionary algorithms

The idea of identification of the individual material phases properties proposed in this work is based on the knowledge of Young modulus of composites determined for the materials with different volume fraction of the reinforcement. In order to solve the identification problem, this study proposes the use of evolutionary algorithm. The scheme of applied algorithm is presented in Fig. 2.

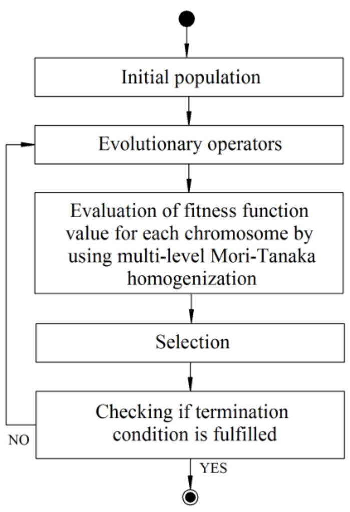

Fig. 2 Scheme of evolutionary algorithm combined with homogenization procedure

The fitness function that is minimized during the optimization is defined as follows:

$$F\left(x\right)=\sum_{i=1}^{n}\left|\frac{\overline{y}_i-y_i}{\overline{y}_i}\right|, \tag{3}$$

where x_i are variables, $\overline{y}_i$ are known elastic constants (for example from experimental data), y_i are elastic constants computed during optimization in dependence of variables x_i, n denotes the number of materials used. Variables x_i that are accounted are Young moduli and Poisson ratios of the individual composite phases. Another issue that is raised in this article is the treatment of uncertain character of experimental data and the material homogenization model. Apart from an experimental test error, in some cases only a few specimens can be examined which very often leads to obtaining relatively large standard deviation of the mean value. On the other hand, homogenization methods are based on some idealised, simplified assumptions (e.g. perfect geometry of inclusions, uniform distribution of inclusions, perfect bonding between matrix and inclusions) and do not reflect real material behaviour exactly. Therefore, a novel method of identification involving resultant error estimation is proposed. Resultant error means that it is neither connected with experimental data nor with homogenization method errors. It is of implicit nature and can be treated as an effective error. Fitness function, accounting for an error, is evaluated in a fashion presented in Fig. 3.

$$for\ \ i=1:n$$

$$\text{if}\ \left|\frac{\overline{y}_i-y_i}{\overline{y}_i}\right|<Error$$

$$f_i=0$$

$$else$$

$$f_i=\left|\frac{\overline{y}_i-y_i}{\overline{y}_i}\right|$$

$$end$$

$$F\left(x\right)=\sum_{i=1}^{n}f_i$$

$$end$$

Fig. 3 Fitness function evaluation, accounting for an error

While the resultant error is of an implicit nature, determining it is no trivial task. The iterative method of error estimation proposed in this paper considers gradual magnification of error during evolutionary computation up to reaching zero value of fitness function, computed in accordance with the scheme presented in Fig. 4. The resultant error value corresponds to the last iteration of the algorithm.

Table 3

Evolutionary algorithm parameters

Population size	100
Crossover fraction	0.9
Selection procedure	Rank selection
Elite count	5% of population size
Crossover	Heuristic
Mutation	Adaptive feasible
Stall generation limit	5

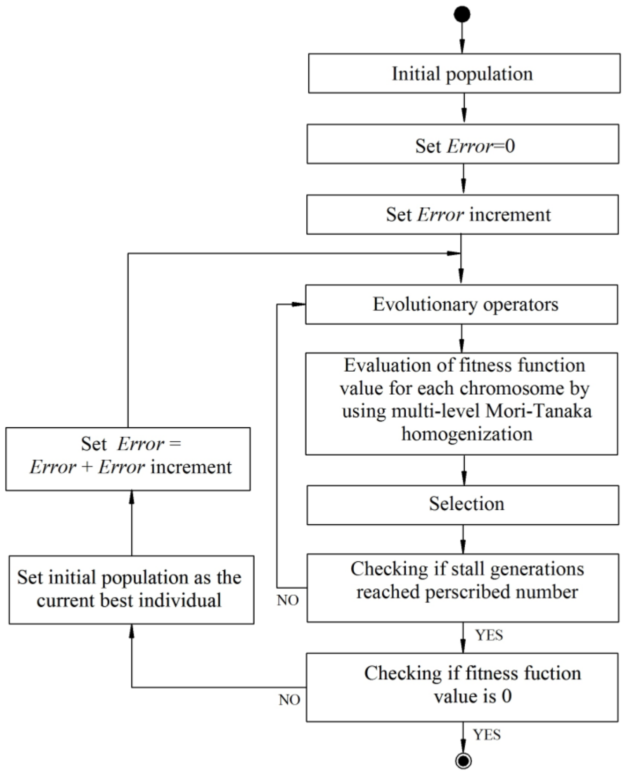

Fig. 4 Scheme of proposed evolutionary algorithm, accounting for resultant error

Evolutionary algorithm parameters, common for all performed analyses, are introduced in Table 3. The paper focuses on three-phase material; therefore the defined fitness function depends on six variables. Table 4 contains information about variables and applied constrains.

Table 4

Variables accounted for during identification and applied constraints

Accounted variables	Min. value	Max. value
Young modulus of matrix	0.5, GPa	1000, GPa
Young modulus of particles	0.5, GPa	1000, GPa
Young modulus of fibers	0.5, GPa	1000, GPa
Poisson ratio of matrix	0.16	0.36
Poisson ratio of particles	0.16	0.36
Poisson ratio of fibers	0.16	0.36

4. Results of identification

At the beginning, in order to verify the algorithm presented in Fig. 2, simple identification of elastic constants of composite constituents was carried out by using the results obtained with Mori-Tanaka method as input data. The input data is generated for four different composites described in Table 2. Two different types of analyses accounting for different input data were conducted. In the first one, all five independent, effective constants of composite are taken into account (transversally isotropic effective behaviour). In this case, fitness function is formulated as follows:

$$F(x)=\sum_{i=1}^{4}\left(\begin{array}{l}\left|\dfrac{\bar{E}_{L_i}-E_{L\,i}}{\bar{E}_{L_i}}\right|+\left|\dfrac{\bar{E}_{T_i}-E_{T\,i}}{\bar{E}_{T_i}}\right|+\left|\dfrac{\bar{\nu}_{L_i}-\nu_{L\,i}}{\bar{\nu}_{L_i}}\right|+\\ +\left|\dfrac{\bar{G}_{P_i}-G_{P\,i}}{\bar{G}_{P_i}}\right|+\left|\dfrac{\bar{G}_{T_i}-G_{T\,i}}{\bar{G}_{T_i}}\right|\end{array}\right), \tag{4}$$

where E_L is longitudinal Young modulus, E_T is transverse Young modulus, ν is in plane Poisson ratio, G_P is in plane shear modulus and G_T is transverse shear modulus. Thus obtained results are presented in Table 5.

The second analysis assumes knowledge only of longitudinal and transverse Young moduli. In this case, fitness function is formulated as follows:

$$F(x)=\sum_{i=1}^{4}\left(\left|\frac{\bar{E}_{L_i}-E_{L\,i}}{\bar{E}_{L_i}}\right|+\left|\frac{\bar{E}_{T_i}-E_{T\,i}}{\bar{E}_{T_i}}\right|\right). \tag{5}$$

Thus obtained results are presented in Table 6.

The next identification was performed by using experimental results, presented in Table 2, as input data, in particular longitudinal and transverse Young moduli were considered. Initially, the identification was performed without including error (in accordance with scheme presented in Fig. 2). The results are presented in Table 7. Then the identification was carried out while accounting for error (in accordance with scheme presented in Fig. 4). Error increment that was taken into consideration equals 0.25%. The results are presented in Table 8 and additional, averaged values in Table 9 - X_E denotes absolute relative percentage error between the identified modulus E and the known one. Moreover, Fig. 5 shows Young modulus errors in a function of resultant error, encountered during the identification of individual phases (for each identification procedure, it was slightly different due to the nondeterministic nature of applied algorithm). Figs. 6-9 present Young moduli identification errors in function of resultant error for matrix, particles and fibres respectively.

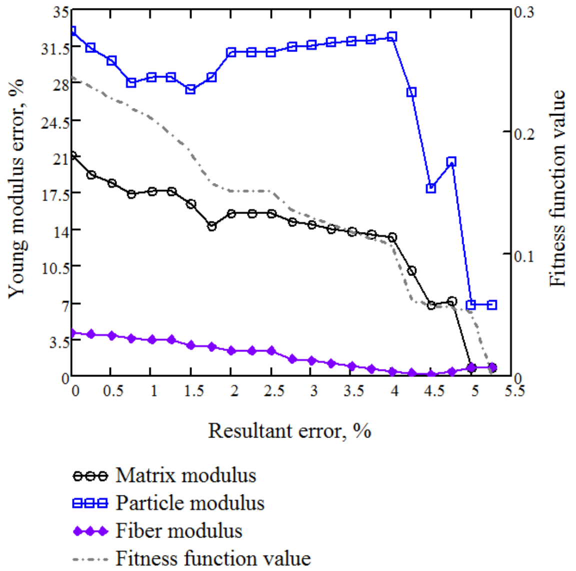

Fig. 5 Young Modulus error in a function of resultant error

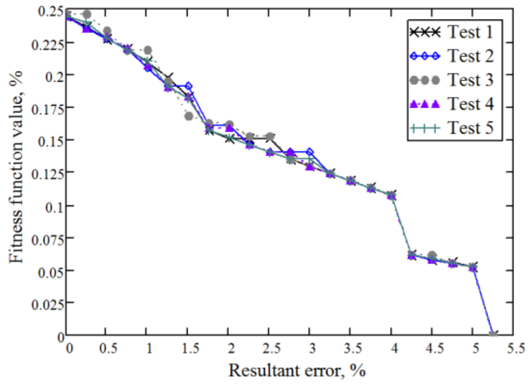

Fig. 6 Fitness function value in a function of resultant error for five independent algorithm executions

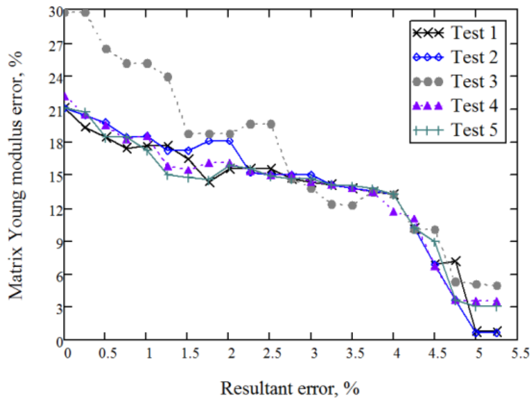

Fig. 7 Matrix Young modulus error in a function of resultant error for five independent algorithm executions

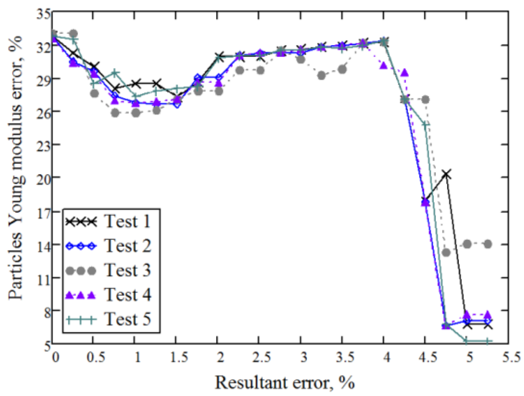

Fig. 8 Particles Young modulus error in a function of resultant error for five independent algorithm executions

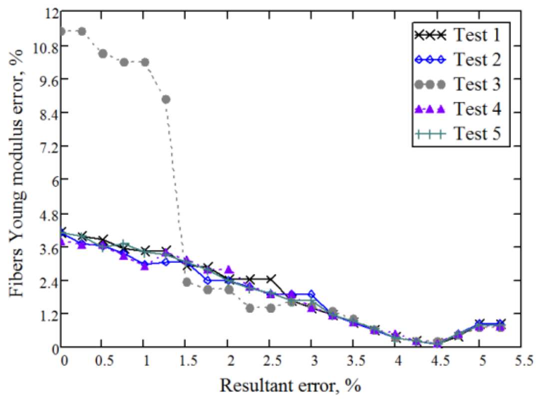

Fig. 9 Fibres Young modulus error in a function of resultant error for five independent algorithm executions

Table 5

Results of evolutionary identification, input data: all five independent, effective constants of four different composites determined by Mori-Tanaka model

Test no.	X_{Em}, %	X_{Ep}, %	X_{Ef}, %	X_{vm}, %	X_{vp}, %	X_{vf}, %	Fitness function value	Total number of generations
1	0.0001	0.0016	0.0003	0.0000	0.0130	0.0069	3.69E-05	148
2	0.0000	0.0009	0.0000	0.0015	0.0118	0.0005	2.16E-05	149
3	0.0011	0.0041	0.0000	0.0010	0.0096	0.0000	3.99E-05	122

Table 6

Results of evolutionary identification, input data: longitudinal and transverse Young moduli of four different composites determined by Mori-Tanaka model

Test no.	X_{Em}, %	X_{Ep}, %	X_{Ef}, %	X_{vm}, %	X_{vp}, %	X_{vf}, %	Fitness function value	Total number of generations
1	0.0613	0.0164	0.0278	0.5026	5.7571	14.3592	2.39E-05	172
2	0.0529	0.0333	0.0454	0.5056	5.1514	13.9351	1.44E-05	183
3	0.0951	0.0092	0.0347	0.6946	8.5994	20.5272	3.92E-05	163

Table 7

Results of evolutionary identification, input data: longitudinal and transverse Young moduli of four different composites determined in experiment [7], errors excluded

Test no.	E_M, MPa	E_P, MPa	E_F, MPa	X_{Em}, %	X_{Ep}, %	X_{Ef}, %	Fitness function value	Total number of generations
1	1731.62	3748.21	22905.88	21.09	32.83	4.12	0.24465	268
2	1731.91	3748.77	22904.82	21.11	32.82	4.11	0.24465	355
3	1855.29	3738.98	19514.68	29.74	32.99	11.30	0.24675	54
4	1747.33	3760.16	22837.15	22.19	32.61	3.81	0.24473	115
5	1731.92	3749.10	22904.43	21.11	32.81	4.11	0.24465	374

Table 8

Results of evolutionary identification, input data: longitudinal and transverse Young moduli of four different composites determined in experiment [7], errors included

Test no.	E_M, MPa	E_P, MPa	E_F, MPa	X_{Em}, %	X_{Ep}, %	X_{Ef}, %	Resultant error, %	Total number of generations
1	1440.51	5955.78	21813.34	0.73	6.73	0.85	5.209	1762
2	1439.32	5976.66	21814.52	0.65	7.11	0.84	5.206	1890
3	1501.38	4799.02	21846.29	4.99	14.00	0.70	5.264	1163
4	1480.78	5155.55	21834.33	3.55	7.61	0.75	5.247	1191
5	1473.54	5289.60	21828.77	3.04	5.20	0.78	5.242	1615
6	1440.80	5967.06	21811.27	0.76	6.94	0.86	5.211	1334
7	1461.77	5497.52	21826.07	2.22	1.48	0.79	5.227	1609
8	1439.64	5974.18	21813.39	0.67	7.06	0.85	5.207	1722
9	1481.37	5204.61	21891.68	3.59	6.73	0.49	5.520	1332
10	1449.33	5756.53	21818.80	1.35	3.16	0.82	5.216	1472

Table 9

Mean values of identified moduli and corresponding errors

E_M, MPa	E_P, MPa	E_F, MPa	X_{Em}, %	X_{Ep}, %	X_{Ef}, %
1460.84	5557.65	21829.85	2.16	0.40	0.77

5. Discussion on the results and conclusions

The results presented in Table 5 show that using all independent elastic constants of analyzed composites as input data leads to only a unsubstantial error between identified elastic constants of the individual material phases and the actual one. The results of the next example in which input data consisted only of longitudinal and transverse Young moduli (results presented in Table 6) point to the fact that Young moduli of the individual phases were identified with slightly less precision than in the previous example (maximum observed error does not exceed 0.1%) and Poisson ratios were not accurately identified. This fact leads to the conclusion that the lack of information about Poisson ratios or shear moduli does not significantly affect the identification of Young moduli of the individual phases. The next problem under consideration was connected with the identification based on experimental input data. The results presented in Table 7 show an unacceptable identification error (about 32% in case of modulus of particles). However, the application of a novel approach, discussed in this paper, that is connected with the introduction of resultant error leads to satisfying results that are presented in Table 8. Moreover, the presented approach, apart from resulting in a relatively small identification error, provides information about the resultant error. The proposed approach should be verified by further work on different materials. Moreover, the method efficiency will be improved by introducing adaptive changes of the resultant error.

Acknowledgement

The results presented in the paper are partially financed from BKM-547/RMT4/2015 (10/040/BKM_15/2016) and 10/990/BK_16/0040.

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IDENTIFICATION OF ELASTIC PROPERTIES OF INDIVIDUAL MATERIAL PHASES BY COUPLING OF MICROMECHANICAL MODEL AND EVOLUTIONARY ALGORITHM.

S u m m a r y

The paper is devoted to an inverse problem of identification of individual material phases properties in dependence of known effective properties. In order to solve the identification problem, combining evolutionary algorithm with Mori-Tanaka method is proposed. In particular, the study focuses on a three-phase composite and takes experimental results from literature as an input data to analysis. The original contribution of this paper is a new identification strategy involving a resultant error that represents the uncertain character of both experimental data and model predictions. The new approach is demonstrated by performing several analyses with various assumptions.

Keywords: identification, multi-phase materials, evolutionary algorithm, homogenization.

Received March 02, 2016
Accepted September 28, 2016