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Mean field homogenization in multi-scale modelling of composite materials

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Analysis and modelling

ABSTRACT

Purpose: The paper is focused on testing of the capabilities of the mean field homogenization scheme in numerical analysis of composite materials. Another goal of this research is an attempt of coupling of mean field homogenization procedure with finite element computations to carry out a multi-scale analysis

Design/methodology/approach: This research is based on the application of the DIGIMAT software which is material modelling platform. The Mori-Tanaka homogenization scheme implemented in DIGIMAT code was applied to obtain the average composite's mechanical properties. Additional aspect is coupling of DIGIMAT material modeller with finite element solver.

Findings: Application of mean field homogenization allows to obtain the effective properties of heterogeneous material very efficiently. Process of assigning material parameters to each composite's phase on the micro level is operative and fast. Coupling homogenization procedure with finite element solver leads to full multi-scale analysis where material nonlinearities can be taken into account

Research limitations/implications: Mean field homogenization gives approximate results, therefore detailed stress and strain fields in microstructure can not be analysed.

Practical implications: Methodology presented in present article shows efficient approach to finding effective composite properties and in addition allow to carry out nonlinear multi-scale analysis.

Originality/value: The paper presents new methodology which is intensively developed in the field of numerical simulation of structures and materials. The material parameters are not treated as the constant input data, but are obtained as results of the material parameters modelling process on the micro-scale level.

Keywords: Mean field homogenization; Multi-scale modelling; DIGIMAT

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1. Introduction

Due to increasing popularity of composite materials in industrial applications new computational strategies was developed. Very important and practical issue is estimation of effective properties of heterogeneous materials. Homogenization of composite's properties can be achieved by analysis of the RVE (Representative Volume Element). RVE is a statistical representation of material properties. It should contain enough information to describe behaviour of considered composite [1]. At macro scale, each material point is interpreted as the centre of RVE. Application of homogenization procedure is essential to find the macro constitutive response of RVE that represents the microstructure. Very popular approach is based on direct finite element [2,3] or boundary element [1,4] analysis of RVE. Another approach, on which this paper focuses, is application of mean filed homogenization [5,6]. To test an influence of microstructure properties on macro behaviour of machine's parts or structures multi-scale analysis is essential. In the present paper two scale analysis is presented. The first, microscopic scale, is connected with the composite heterogeneous microstructure. The second scale is the macroscopic one where the whole considered body can be seen as homogenous. Those complicated procedure is conducted in the numerical way. Till now it required preparing an own code in most cases, but lately some commercial codes are also able to conduct this procedure. In this research composite's effective properties are estimated by mean filed homogenization procedure implemented in the DIGIMAT software [7]. Then structural analysis is carried out by finite element method. In this paper conceptions of strong and weak multi-scale strategies are presented.

2. Numerical homogenization

2.1. Mean field homogenization

Homogenization techniques, as stated before, are often based on direct finite element analysis of RVE at micro scale using macroscopic values as the boundary conditions. Then computed results are returned to macro scale by averaging techniques. This approach is very accurate and gives detailed micro fields. However, especially for nonlinear problems, it is computationally very expensive. In addition, the creation of discrete model of RVE is also necessary. Preparation of discrete representation of composite's microstructure can lead to additional difficulties. Another method is mean field homogenization (MFH). MFH is based on analytical models and gives only approximations of the volume averages of stresses and strains, both at the macro level and in each micro phase [7]. The main advantage of MFH method is computational efficiency. Generally, homogenization procedure is divided into three steps (Fig. 1). In the first step given macroscopic strain tensor $\bar{\varepsilon}$ is localised in each phase of the composite material. The second step is connected with application of constitutive laws of each phase. As a result per phase stress tensors σ are computed. In the last step phases stress tensors are averaged and macroscopic stress tensor $\bar{\sigma}$ is obtained.

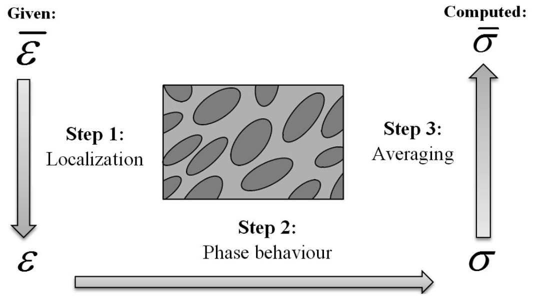

Fig. 1. Homogenization scheme

Let us take into consideration two-phase composites in which inclusions that extend on domain ω_1 and have volume V_1 are reinforcing the matrix which extends on domain ω_0 and has a volume V_0. Volume fraction of matrix and inclusion can be expressed as:

$$v_o = \frac{V_0}{V} \tag{1}$$

$$v_1 = \frac{V_1}{V} = 1 - v_0 \tag{2}$$

where V is the volume of RVE.

The average quantity over a RVE is defined by:

$$\langle f(x,\bar{x}) \rangle = \frac{1}{V}\int_{\omega}(x,\bar{x})dV \tag{3}$$

where integration is carried out with respect to micro coordinates and $f(x,\bar{x})$ is the micro field inside the RVE.

In case of two phase composites volume average can be expressed as:

$$\langle f \rangle = v_1 \langle f \rangle_{\omega_1} + v_0 \langle f \rangle_{\omega_0} \tag{4}$$

As a result the volume averages of the strain field over the RVE, the matrix phase and the inclusion phase are related as:

$$\langle \varepsilon \rangle_{\omega} = v_1 \langle \varepsilon \rangle_{\omega_1} + v_0 \langle \varepsilon \rangle_{\omega_0} \tag{5}$$

The per phase strain averages are connected by a strain concentration tensor B^{ε} :

$$\langle \varepsilon \rangle_{\omega_1} = B^{\varepsilon} \langle \varepsilon \rangle_{\omega_0} \tag{6}$$

The per phase strain averages are related to the macroscopic strain by:

$$\langle \varepsilon \rangle_{\omega_0} = \left[v_1 B^{\varepsilon} + (1 - v_1) I \right]^{-1} : \langle \bar{\varepsilon} \rangle \tag{7}$$

$$\langle \varepsilon \rangle_{\omega_1} = B^{\varepsilon} : \left[v_1 B^{\varepsilon} + (1 - v_1) I \right]^{-1} : \langle \bar{\varepsilon} \rangle \tag{8}$$

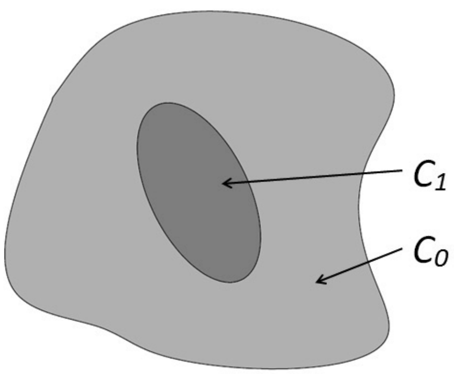

Fig. 2. Single-inclusion problem description

In the most relevant mean field homogenization models fundamental role plays the Eshelby's solution [8]. Eshelby's solution allows solving the single-inclusion problem. Considering single-inclusion problem, an infinite body is subjected to linear displacements on its boundary corresponding to a uniform far-field strain ε. The body is made of an ellipsoidal inclusion (I) of modulus C_I which is embedded in an infinite matrix of modulus C_0 (Fig. 2).

Using Eshelby's solution, it can be found that strain inside inclusion is uniform and related to the remote strain:

$$\varepsilon(x) = H\left(I, C_0, C_1\right) : E, \quad \forall \in (I) \tag{9}$$

where H is the single-inclusion strain concentration tensor defined as follows:

$$H\left(I, C_0, C_1\right) = \left\{I + \zeta(I, C_0) : C_0^{-1} : \left[C_1 - C_0\right]\right\}^{-1} \tag{10}$$

where $\zeta(I, C_0)$ is Eshelby tensor.

Mori-Tanaka homogenization model, which is used in further computations, assumes that strain concentration tensor $B^{\square}$ is equal to strain concentration tensor of single inclusion problem H [5,6,7]. Benveniste [9] gives the following interpretation of Mori-Tanaka's model: each inclusion behaves like an isolated inclusion in the matrix seeing average matrix strain $\langle \varepsilon \rangle_{\omega_0}$ as a far-field strain.

2.2. DIGIMAT-MF software

DIGIMAT is the nonlinear multi-scale material and structure modelling platform. In this article capabilities of DIGIMAT-MF module are presented. DIGIMAT-MF is the mean field homogenization software used to predict the nonlinear constitutive behaviour of composite materials. Macro material properties are defined as a function of the matrix and inclusion constitutive relations and inclusion of the volume fraction and shape. DIGIMAT contain variety of micro materials models which can be assigned to each micro phase, for example: thermo-elastic, elasto-plastic, viscoelastic, elasto-viscoplastic, and hyperelastic models [7].

3. Application of mean field homogenization

As an example of application of mean field homogenization, estimation of average composite mechanical properties is presented. Mori-Tanaka homogenization scheme implemented in DIGIMAT-MF software is used. Composite taken into account is aluminium alloy 6061 reinforced with SiC particles. Aluminium alloy is modelled as elasto-plastic matrix material. SiC reinforcement is modelled as linear elastic ellipsoidal particles. Random orientation of particles was considered. Table 1 shows assumed properties of matrix material and Table 2 shows properties of inclusion material, respectively.

Table 1.
Properties of Al 6061 alloy

Property	Value	Units
Density	2.7	g/cm^3
Modulus of elasticity	68.9	GPa
Poisson's ratio	0.33	
Yield stress	276	MPa
Hardening constant	255	MPa
Hardening exponent	0.3	

Table 2.
Properties of SiC

Property	Value	Units
Density	3.21	g/cm^3
Modulus of elasticity	450	GPa
Poisson's ratio	0.17	

Several analyses which different volume fraction of the reinforcement were carried out. Fig. 3 shows tensile responses of matrix material, reinforcement material and composite in form of stress-strain curves. Fig. 4 presents the influence of volume fraction of reinforcement on composite's tensile response. Obtained Young modulus and Poisson ratio values for analysed composite are collected in Table 3. Fig. 5 shows composite's Young modulus in function of volume fraction of reinforcement. It can be observed that in this case Young modulus dependence on reinforcement volume fraction is approximated by the second order polynomial.

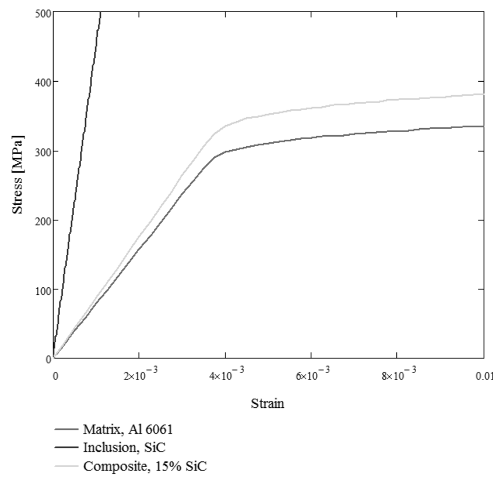

Fig. 3. Stress-strain curves of matrix material, inclusion material and composite material

Table 3.
Linear material properties of analysed composite

SiC volume fraction	Young modulus, GPa	Poisson ratio
10%	80.88	0.3192
15%	87.54	0.3138
20%	94.73	0.3085

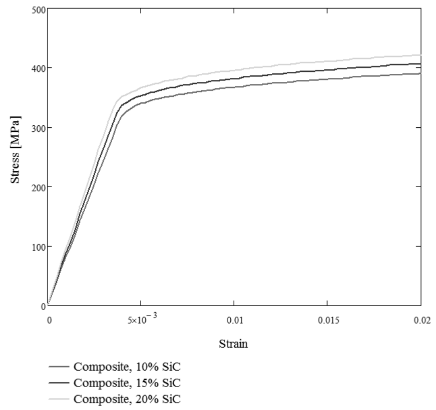

Fig. 4. Estimated stress-strain curves of composites with different volume fraction of reinforcement

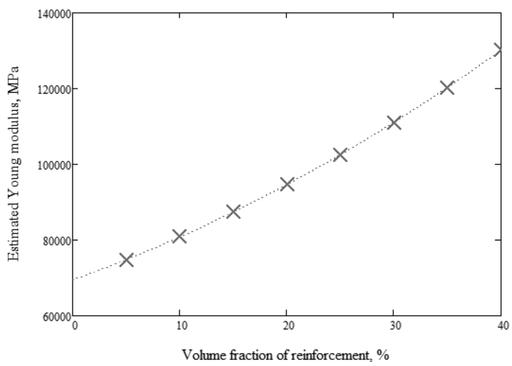

Fig. 5. Composite's Young modulus in function of volume fraction of SiC particles

Fig. 6 shows plastic strain of matrix phase in function of composite's macro strain in case of composite with 15% volume fraction of SiC reinforcement.

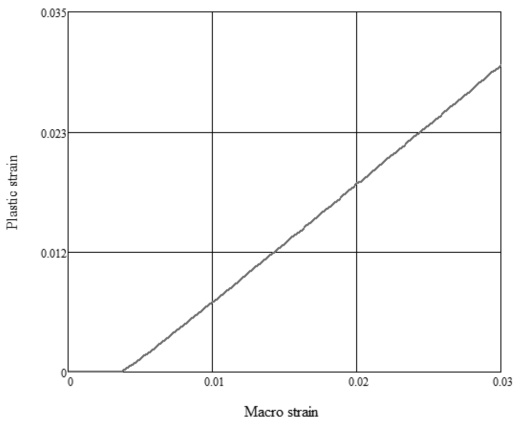

Fig. 6. Plastic strain of matrix phase in function of macro strain in uniaxial state of stress

4. Multi-scale modelling

Multi-scale modeling [2,3] is connected with calculation of material properties or system behavior on one level using information or models taken from different levels. In this article two scale analysis is presented. Micro scale which represents composite's microstructure is analyzed by means of mean field homogenization procedure implemented in DIGIMAT software. The finite element method with applied effective properties of material from micro scale is used in macro scale. Two different multi-scale strategies can be recognized: weak and strong scales coupling. In weak coupling, homogenized composite's properties are transferred to finite element integration points just once and during the finite element computation any further data exchange between scales does not take place (Fig. 7). In strong coupling, data exchange between scales is permanent (Fig. 8). For example in each iteration or time step, material data prescribed to integration points is actualized. In case of linear analyses weak coupling approach is sufficient. However, to model nonlinear problems with taking into account microstructure's behavior, strong coupling should be used.

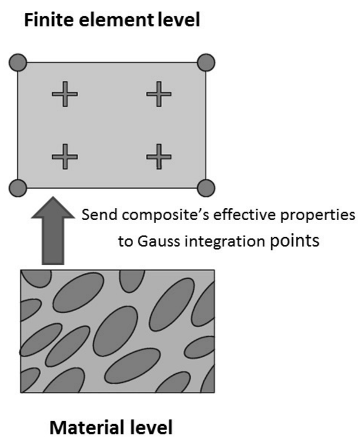

Fig. 7. Weak coupling strategy

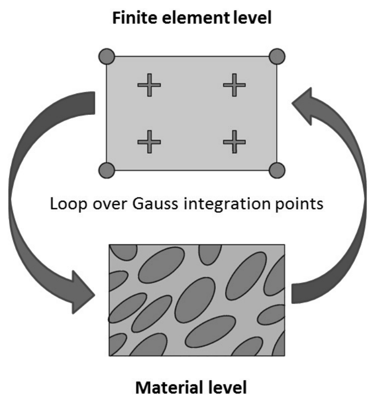

Fig. 8. Strong coupling strategy

In this research strong coupling was applied. DIGIMAT as homogenization module was strongly coupled with finite element solver.

5. Case study

As the example of presented methodology the numerical multiscale simulation of tensile test was carried out. Finite element mesh of exemplary flat specimen is shown in Fig. 9. Aluminium alloy 6061 matrix composite reinforced with 15% volume fraction of SiC particles was taken into consideration. After plasticizing of specimen the information about stress fields in composite, matrix phase and reinforcement phase were collected (Fig. 10). Stresses values in each phase were compared at arbitrary chosen state. Comparison is illustrated in Table 4.

Fig. 9. An exemplary specimen's finite element mesh

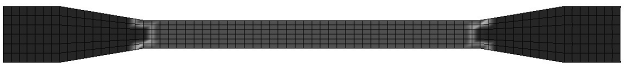

Fig. 10. Plastic region in matrix phase at arbitrary chosen state, red colour indicates plasticized material

Table 4.
Normal stress in the specimen

	Stress, MPa
Composite	324.6
Matrix phase	301.5
Reinforcement phase	531.9

It can be observed that reinforcement supports the highest stress values and matrix material exceed the yield stress.

To show the capabilities of presented methodology, a more complex example is also presented. Nonlinear response of the composite cantilever presented in Fig. 11 is analysed. The same material as in previous example is taken into account.

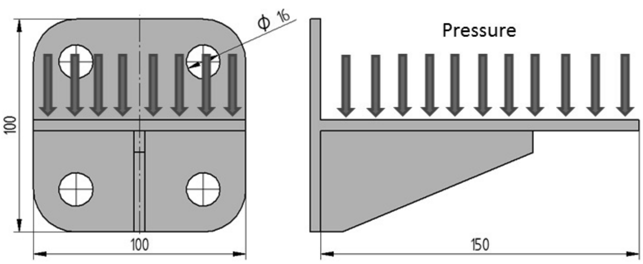

Fig. 11. Exemplary cantilever

Cantilever's geometry was discretised using shell finite elements (Fig. 12). The cantilever of the same geometry but made of homogenous aluminium alloy was considered to compare the analyses results.

Fig. 12. Finite element discretization

Fig. 13 presents predicted accumulated plastic strain in matrix phase of composite material and Fig. 14 respectively presents plastic strain in homogenous aluminium alloy made cantilever.

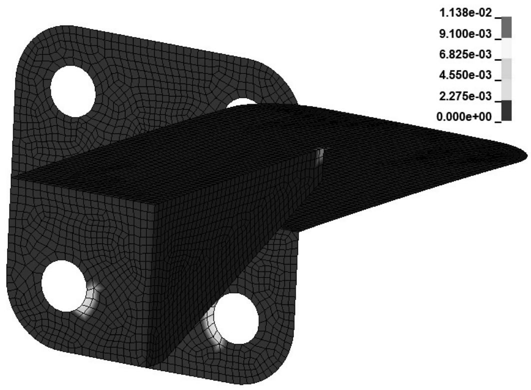

Fig. 13. Accumulated plastic strain in matrix phase of composite cantilever, maximum value equals $8.232 \cdot 10^{-3}$

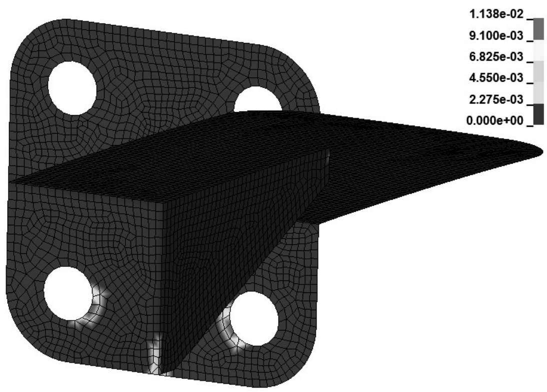

Fig. 14. Accumulated plastic strain in aluminium alloy part, maximum value equals $1.138 \cdot 10^{-2}$

The comparison between stiffnesses of composite and aluminium alloy cantilever is presented in Fig. 15. In this case finite element computation had iterative character so cantilever displacement is presented as a function of analysis step.

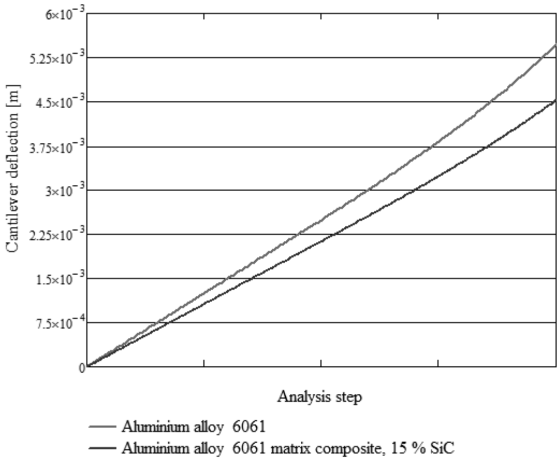

Fig. 15. Deflection comparison of cantilever made of aluminium alloy and cantilever made of aluminium matrix composite

Presented results showed an influence of SiC particles reinforcement on mechanical response of analysed exemplary part. Plastic strain reached higher values in case of homogenous aluminium alloy part. Composite's cantilever is stiffer than aluminium alloy made one.

6. Conclusions

Presented paper shows capabilities, advantages and limitations of mean field homogenization method in estimation of effective properties of composite materials. As an example of MFH practical application, metal matrix composite's effective properties were evaluated. In addition an influence of reinforcement phase volume fraction on composite macroscopic response was tested. Applied MFH procedure is very efficient from the computational point of view. This advantage allows to carry out full strongly coupled multi-scale analysis in reasonable CPU time. Proposed methodology of nonlinear multi-scale analysis is based on coupling of MFH scheme with finite element solver. Presented exemplary analysis results give more information about behaviour of the composite part than standard finite element approach. Averaged macro and per phase micro stresses and strains fields can be observed. The material parameters are not treated as the constant input data, but they are obtained as results of the material parameters modelling process on the micro-scale level. On the other hand MFH gives only approximate results, therefore detailed stress and strain fields in microstructure can not be analysed. In addition, the microstructure's size influence is neglected in MFH scheme.

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