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Modeling of constitutive behaviour of anisotropic composite material using multiscale approach

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1. Introduction

Particle-reinforced metal matrix composites have found application in many areas of engineering practice. They usually provide higher strength, stiffness and weight savings in comparison with conventional metal alloys. Moreover, this group of materials is attractive due to their cost-effectiveness [1]. Estimation of elastic-plastic response in particle-reinforced composites is a complex problem depending on variety of factors such as particle size, shape, distribution or orientation [1, 2]. In this paper, special attention is put into consideration of material anisotropy caused by manufacturing process. One of the most popular ways of manufacturing particle-reinforced composites is through an extrusion. Extrusion is a process connected with creating objects with fixed cross section. It allows to manufacture complex cross sections with brittle materials that in turn result in parts with excellent surface finish [3]. Because extrusion is classified as secondary processing method, it is preceded by one of primary processing methods such as powder metallurgy [3, 4]. In case of application of powder metallurgy, raw composite constituents in the form of powders are mixed, milled, pressed into compacted powder and finally extruded [4]. After extrusion, generally a significant degree of orientation of the reinforcement particles is expected along the extrusion axis. However, the degree of mechanical property anisotropy is related to the volume fraction of particles. In particular, mechanical property anisotropy increases with increasing volume fraction of particles due to the reduction in mean free path between the particles [5]. Therefore, during this study, composite with 0.3 volume fraction of the reinforcement is taken into consideration. In this case, anisotropy of mechanical properties plays a significant role in overall material performance. During this research, spatial distribution of the particles, measured experimenttally, is taken into account by assuming results presented in work [6]. The three dimensional representative volume element (RVE) geometry that represents the material microstructure is created by using Digimat-FE software. The RVE is a statistical representation of material properties. It should contain enough information to describe the behavior of considered composite. The analysis of the RVE is conducted by the finite element method, in particular commercial MSC Marc solver is applied. In addition, different approaches based on the two step homogenization method [7] and the orientation averaging procedure [8] are proposed. Results obtained numerically by using different approaches are presented, compared and related to experimental results that can be found in work [9].

2. Determination of the RVE geometry

The RVE geometry is created by taking into account the spatial distribution of the particles measured experimentally. In particular, results presented in work [6] are considered. In the analyzed case, the shape of the particles is simplified and modeled as ellipsoids with constant size and aspect ratio of 2.68. The histogram that represents the probability distribution of the angle between the particle axis and the extrusion axis is presented in Fig. 1. To create the RVE geometry eight families of particles with angles and probability density corresponding to this histogram were set up. The created RVE that contains 250 particles is presented in Fig. 2, each color indicating different family of the particles, *X* is the axis of the extrusion. Considered RVE is a rectangular cuboid with the dimensions 500x250x500 μm. The orientation of the particles in the extrusion plane *YZ* is usually random. In the other two symmetry planes distribution shows similar trend that is in accordance with the histogram presented in Fig. 1 [6].

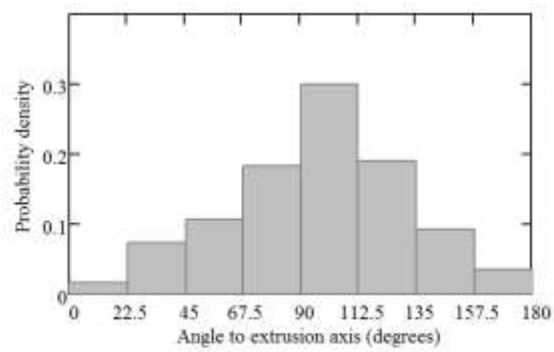

Fig. 1 Angle between particle axis and extrusion axis distribution

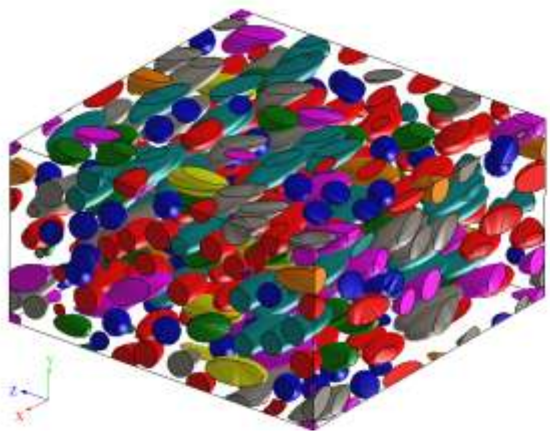

Fig. 2 RVE representing composite microstructure

3. Determination of effective anisotropic properties

3.1. Homogenization based on finite element analysis of the RVE

To calculate the effective elasticity tensors of heterogeneous materials, the usage of homogenization procedure is essential. The homogenization procedure involves replacing the heterogeneous material with an equivalent homogeneous material. Calculating the equivalent material properties requires solving six RVE boundary value problems (BVP) in three dimensional case [2, 10]. For each BVP a prescribed strain is applied in accordance with Eq. (1) (a superscript j = 1-6 indicates the number of analysis, I = 1-6).

$$\varepsilon_i^{(j)} = \delta_{ij} \,. \tag{1}$$

In addition, periodic boundary conditions are introduced [11]. After solving six BVPs, both the stresses Eq. (2) and strains Eq. (3) are averaged in post-processing stage of the analysis.

$$<\sigma_{ij}> = \frac{1}{V_{RVE}} \int_{V_{RVE}} \sigma_{ij} dV_{RVE} \,, \tag{2}$$

$$<\varepsilon_{ij}> = \frac{1}{V_{RVE}} \int_{V_{RVE}} \varepsilon_{ij} dV_{RVE} \,, \tag{3}$$

where $<\sigma_{ij}>$ is average stress, $<\varepsilon_{ij}>$ is average strain, σ_{ij} is stress in the RVE, ε_{ij} is strain in the RVE and V_{RVE} is volume of the RVE.

The relation between stress and strain tensors is expressed by:

$$<\sigma_{ij}> = C <\varepsilon_{ij}> , \tag{4}$$

where C is elasticity tensor.

The presented methodology is applied to the estimation of effective properties of the material which is represented by the RVE presented in Fig. 2, as well as for material with inclusions perfectly aligned with the extrusion axis.

3.2. Orientation averaging

Another approach that deals with determining the effective properties of composite materials with non-homogenous orientation of the reinforcement is orientation averaging. The orientation averaging procedure is based on equation proposed by Advani and Tucker [8]:

$$\begin{aligned} C_{ijkl} &= B_1(a_{ijkl}) + B_2(a_{ij}\delta_{kl} + a_{kl}\delta_{ij}) + B_3(a_{ik}\delta_{jl} + \\ &+ a_{il}\delta_{jk} + a_{jl}\delta_{ik} + a_{jk}\delta_{il}) + B_4(\delta_{ij}\delta_{kl}) + \\ &+ B_5(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \end{aligned} \tag{5}$$

where a_{ij}, a_{ijkl} are second and fourth-order orientation tensors and B_1-B_5 are scalar constants related to the components of stiffness tensor of unidirectional composite.

A drawback of this approach is that the fourth-order tensor a_{ijkl} is required to calculate the effective stiffness. In practice, very frequently only the second order orientation tensor is known. The graphical representation of the second-order orientation tensor is presented in Fig. 3 where λ_i and n_i are eigenvalues and eigenvectors.

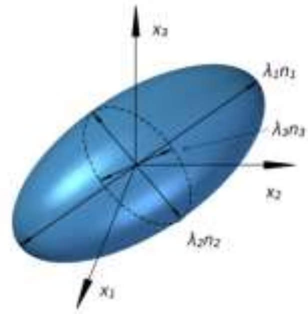

Fig. 3 Graphical representation of second-order orientation tensor

The second-order orientation tensor has the following properties:

$$a_{ii} = 1 \,, \tag{6}$$

$$a_{ij} = a_{ji} \,. \tag{7}$$

Therefore, the second-order orientation tensor has five independent components. To estimate the fourth-order orientation tensor, closure approximations are commonly considered where the fourth-order tensor components are calculated from the components of the second-order tensor. The closure that provide the most accurate results in comparison with experimentally measured fourth-order tensors is the orthotropic closure proposed by Cintra and Tucker [12, 13] in their work [14]. The orthotropic closures are based on the assumption that the principal axes of the approximated fourth order tensors are in alignment with the principal axes of the second order tensor [14]. The definition of orthotropic closure approximation reduces the choice to three scalar functions f, such as $a_{iiii}=f_i(a_1,a_2)$. Cintra and Tucker used in their work second-degree polynomials:

$$a_{iiii} = T_{i1}^1 + T_{i2}^2 a_{(1)} + T_{i3}^3 a_{(1)}{}^2 + T_{i4}^4 a_{(2)} + T_{i5}^5 a_{(2)}{}^2 + T_{i6}^6 a_{(1)} a_{(2)} \,, \tag{8}$$

where there is no sum on i, $a_{(1)}$ and $a_{(2)}$ are the first and the second eigenvalue of the second-order orientation tensor, $T_m{}^i$ is a matrix of coefficients which can be determined by using specific orientation distributions (smooth version) or by fitting it to distributions evaluated for a set of flow fields (fitted version). It requires additional transformation between the global coordinate and the principal coordinate.

To determine the effective properties of the composite from Eq. (2), besides the second and the fourth-order orientation tenors, scalar constants B_1-B_5 also have to be calculated. These constants are related to the components of unidirectional composite stiffness tensor C^U as follows [8]:

$$\left.\begin{aligned} B_1 &= C_{1111}{}^U + C_{2222}{}^U - 2C_{1122}{}^U - 4C_{1212}{}^U , \\ B_2 &= C_{1122}{}^U - C_{2233}{}^U , \\ B_3 &= C_{1212}{}^U + \frac{1}{2}\left(C_{2233}{}^U - C_{2222}{}^U\right), \\ B_4 &= C_{2233}{}^U , \\ B_5 &= \frac{1}{2}\left(C_{2222}{}^U - C_{2233}{}^U\right). \end{aligned}\right\} \tag{9}$$

During this study, unidirectional composite effective properties were determined by using the finite element based homogenization in the same way as for establishing the properties of RVE presented in Fig. 1. The effective stiffness tensor of the misaligned composite is evaluated by considering the average second-order orientation tensor corresponding to the created RVE:

$$a = \begin{pmatrix} 0.618 & 0.065 & -0.057 \\ 0.065 & 0.118 & -0.169 \\ -0.057 & -0.169 & 0.276 \end{pmatrix}. \quad (10)$$

3.3. Two step homogenization

Another approach that allows to consider the spatial distribution of the particles presented in Fig. 1 is the two-step homogenization. Inclusions are divided into different families characterized by different orientation vector similarly as during the preparation of the RVE geometry. In the first step, the stiffness tensors of perfectly aligned composite corresponding to each particle family are computed. In this case, the properties of unidirectional composite determined by the finite element based homogenization are transformed in accordance with the spatial orientation of a particular particle family. At this step the stiffness tensors are evaluated individually for each family of particles. In the second step, stiffness tensors determined in the first step are aggregated by assuming Voigt homogenization model [15]. The two step homogenization approach was proposed with application of mean-filed homogenization methods presented in works [7, 15].

4. Analysis results

The geometry has been divided on a regular mesh of cube shaped finite elements creating discrete system of approximately 3 million degrees of freedom (Fig. 4). The properties of the composite constituents are collected in Table 1. Moreover the stress-strain curve representing matrix material elastic-plastic behavior is shown in Fig. 5.

Table 1

Properties of composite constituents

	Matrix	Particles
Young modulus, GPa	73	410
Poisson ratio	0.34	0.19
Volume fraction	0.7	0.3
Aspect ratio	-	2.68

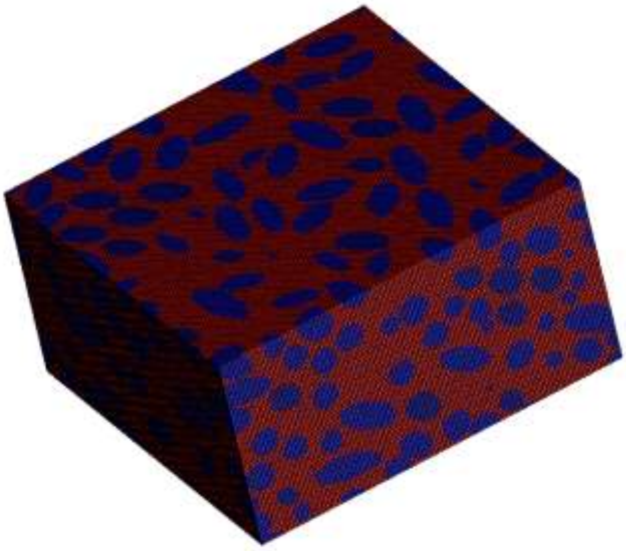

Fig. 4 Finite element discretization of the RVE

The results of the analyses carried out by using different approaches are collected in Table 2. Additionally, Table 3 shows percent relative error between material parameters determined by numerical methods E^{NUM} and experimental data E^{EXP} defined as follows:

$$\chi E = \frac{\left| E^{EXP} - E^{NUM} \right|}{E^{NUM}} \cdot 100\% . \quad (11)$$

Table 2

Effective elastic material properties: *E*-Young modulus, *G*- shear modulus

	Material parameters, GPa					
	E11	E22	E33	G12	G13	G23
Experiment [9]	124.0	112.3	120.4	44.6	47.6	45.3
Microstructure based	128.30	118.80	121.75	46.31	46.98	45.67
Orientation averaging	123.78	119.15	121.02	45.25	45.19	45.09
Two step homogenization	126.76	116.17	119.06	46.21	46.72	45.19
Unidirectional composite	138.13	115.57	116.45	45.27	44.80	42.63

Table 3

Percent relative error between material parameters evaluated by numerical methods and experimental data

	$\chi E11$	$\chi E22$	$\chi E33$	$\chi G12$	$\chi G13$	$\chi G23$	Average percentage error
Microstructure based	3.47	5.79	1.12	3.84	1.30	0.82	2.72
Orientation averaging	2.23	3.45	1.11	3.61	3.19	0.07	2.28
Two step homogenization	1.75	3.94	1.31	3.82	1.85	0.71	2.30
Unidirectional composite	11.40	2.91	3.28	1.49	5.87	5.89	5.14

The investigation of the composite behavior after plasticizing of matrix material is conducted by enforcing uniaxial strain on the RVE presented in Fig. 2. Three analyses, for different strains, are performed: $\varepsilon_{11}^{(1)} = 0.01$, $\varepsilon_{22}^{(2)} = 0.01$, $\varepsilon_{33}^{(3)} = 0.01$.

The results of these analyses are presented in the form of stress-strain curves shown in Fig. 5, additionally curve that represents matrix material behavior is attached. The differences between the curves caused by non-homogenous orientation of the reinforcement can be noticed. Moreover, anisotropic plasticity of metal matrix may have a significant impact on the result. Generally, in the extruded aluminum alloy parts there are differences between yield stress in the extrusion direction and the transverse directions [16]. However, during this research, the plastic behaviour of matrix material is simplified and treated as isotropic so Fig. 5 accounts only for the distribution of particles effects on the material response. In addition micro-fields of equivalent plastic strain (Fig. 6) and maximum principal stress in the extrusion plane (Fig. 7) are presented. In the case of Fig. 7 micro-field is shown in randomly chosen section view. High stress values exceeding even the ultimate stress of the reinforcement material can be noticed, however this phenomenon occurs only locally. It indicates the areas of probable damage or crack initiation. During this study material failure is not considered, it should be investigated in the further, detailed analysis.

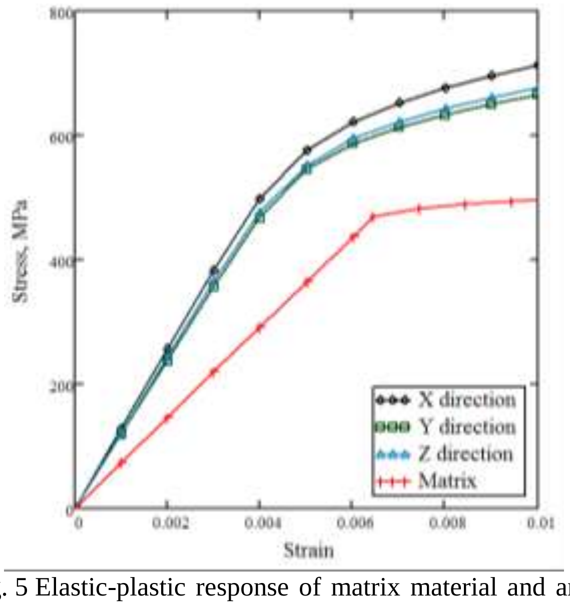

Fig. 5 Elastic-plastic response of matrix material and analyzed composite depending on enforced strain direction

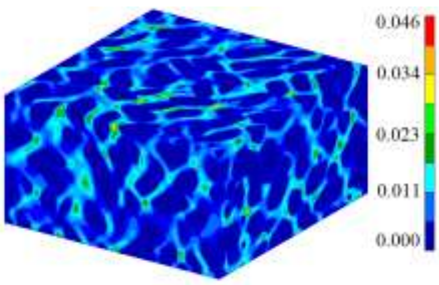

Fig. 6 Equivalent plastic strain caused by uniaxial strain ε_{11}=0.01

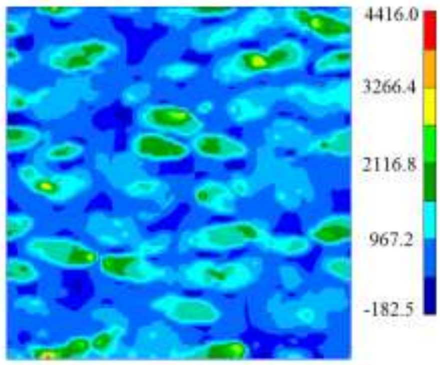

Fig. 7 Maximum principal stress distribution, MPa in the transverse plane caused by uniaxial strain ε_{11}=0.01

The distribution of probability density of maximum principal stress values in the reinforcement and matrix phases in case of prescribed uniaxial strain ε_{11}=0.01 is presented in Fig. 8.

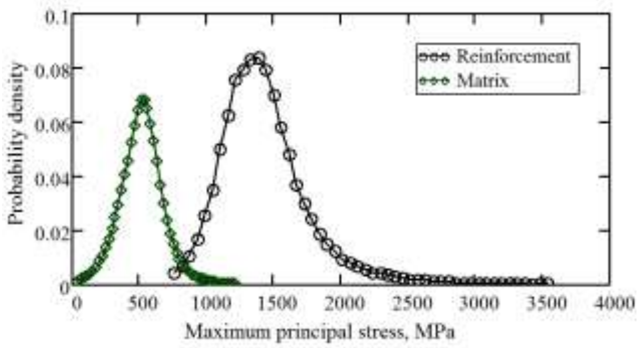

Fig. 8 Probability density distribution of maximum principal stresses in the reinforcement and matrix phases in case of prescribed uniaxial strain ε_{11}=0.01

5. Conclusions

This work presents methodology of determining effective material properties of particle reinforced composites with non-homogenous distribution of orientation of the particles. Three different approaches are presented: homogenization based on analysis of RVE that reflects simplified material microstructure, orientation averaging procedure and two step homogenization method. All presented methods give acceptable results when compared with the experimental data. The first method needs complex geometry preparation which requires the creation of huge discrete models. Therefore, this method is very expensive from the computational point of view. The orientation averaging procedure requires the determination of the effective properties of composite with perfectly aligned inclusions and the second-order orientation tensor. Nevertheless, it also requires an application of closure approximation to compute the fourth-order orientation tensor. The third method, based on two step homogenization, involves determining effective properties of crated sub domains separately in the first step and homogenization of the sub domains in the second step. From the numerical point of view, the orientation averaging and the two step homogenization procedures are more complex than the first method, but on the other hand they are fast and flexible. For example, different orientation distributions can be analyzed by considering the same, previously determined unidirectional material properties. Neglecting the consideration of the actual orientation distribution of the particles and considering the material as orthotropic (unidirectional composite) can lead to unacceptable errors in determining the effective material properties. In particular, the biggest error, amounting to 11.4%, is connected with overestimation of young modulus in the extrusion direction. Although the investigation of composite behavior after plasticizing of matrix material is conducted, improvements - involving the consideration of anisotropic plasticity of matrix material and the damage should be considered in further work.

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MODELING OF CONSTITUTIVE BEHAVIOUR OF ANISOTROPIC COMPOSITE MATERIAL USING MULTISCALE APPROACH

S u m m a r y

The paper is focused on determining the elastic-plastic behavior of anisotropic composite materials. One of the main goals of this study is to compute effective material properties by analyzing material behavior at microstructure level. The effective material properties were investigated with the use of homogenization procedure connected with volume averaging of stress and strain values in RVE (Representative Volume Element). The three dimensional RVE geometry that represents material microstructure is taken into consideration. The spatial distribution of the particles is determined with experimental data. A boundary value problem is solved by using the finite element method and enforcing periodic boundary conditions. In addition, another approaches based on two step homogenization method and orientation averaging procedure are proposed. Results obtained numerically by using different approaches are presented, compared and related to the experimental results.

Keywords: anisotropy, orientation averaging, homogenization, particle-reinforced composite.

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