Materials Physics and Mechanics 32 (2017) 74-82 Received: July 5, 2017

MULTISCALE SIMULATIONS OF NOVEL ADDITIVE MANUFACTURED CONTINUOUS FIBER-REINFORCED THREE-COMPONENT COMPOSITE MATERIAL

A.U. Zobacheva*, A.S. Nemov, A.I. Borovkov

Peter the Great St. Petersburg Polytechnic University, Polytechnicheskaya 29, St. Petersburg, 195251, Russia

*e-mail: zobacheva@compmechlab.com

Abstract. The paper is dedicated to simulation of novel three-component composite material obtained by layer-by-layer 3D printing mechanical behavior on the basis of detailed reproduction of its microstructure. Results of numerical study of the microstructure parameters influence on the mechanical characteristics of the composite material produced by 3D printing are presented and discussed.

1. Introduction

One of the key industry trends throughout the twentieth century is the transition from using of traditional materials in the industry to using advanced materials with pre-defined properties which include a wide range of artificial materials designed and manufactured to respond a set of functional requirements. Such materials can be monolithic or represent alloys of several metals, but most often we are talking about composite materials (they are "by definition" considered to be materials with specified properties).

The main advantage of composite materials is that, despite the higher cost, they have a number of basic qualities: 1) a fundamentally higher achievable specific strength; 2) the materials themselves can be "smart": a product made of them can possess different qualities programmed in advance on a plane or in a volume, which is difficult to do with metals; 3) practically zero corrosion; 4) in one operation it is possible to produce much more complex shapes (the technology makes it possible to make a knot that in a metal would consist of 80 mechanical joints).

Currently, composite materials based on carbon fibers and polymer matrices are widely used in rocket-space and aviation engineering. The structures made of such materials have high strength and low mass. One of the modern approaches to composite materials manufacturing is 3D printing (additive technologies). This method is expected to allow in future obtaining the composite materials with almost any developed in advance complex microstructure, optimized for the specific product. Polymers used as matrix in composite material can be classified in two general categories: thermoset and thermoplastic materials, each of which has essential benefits and disadvantages. The simultaneous use of thermoplastic and thermosetting binders makes it possible to achieve good adhesion of the components (mostly due to low viscosity of thermoset material) while maintaining the inherent elasticity and maintainability of the thermoplastic material.

The developed at Skolkovo Institute of Science and Technology additive manufacturing process for production of such novel three-component material [1] is carried out in two stages. At the first stage, the carbon fibers are impregnated with a thermosetting binder and obtained composite (microplastic) is completely cured, at the second stage the microplastic is coated with a melt of a thermoplastic binder in the process of 3D printing. When manufacturing composite products using the described technology, a certain spread of parameters inevitably arises in their microstructure and defects are also formed. The scope of the study is development of an approach to simulation of three-component composite material obtained by 3D printing, as well as estimation of the possible microstructure parameters variation influence on the composite mechanical characteristics.

2. The method of multiscale modeling

Performing mechanical simulations for composite structures has a significant feature in comparison with case of structures made of homogenous materials – it is practically impossible to implement in the numerical model whole microstructure. Due to this reason, various simplifications based on the idea of replacement of the heterogeneous structure with equivalent homogenous one are usually used during simulation of composite structures. This replacement procedure is usually called homogenization and is described in more details further.

The considered in this paper 3D printed three-component material is a particular case of layered composites based on carbon or glass fibers and polymer matrix, one of the most widely used composite type. There are various approaches to finite element simulation of layered composite materials, and most widespread of them are discussed below.

The first approach is based on usage of three-dimensional solid finite elements. In this case, the geometric model is directly divided into the necessary number of layers and each of them is treated like a homogeneous material. The advantages of this method are caused by direct modeling of separate layers that allows to describe correctly the complex stress-strain state of a layered structure, including interlaminar effects. Besides, when using this approach any three-dimensional joints of structural elements can be described correctly. Disadvantages of this method are the complexity of finite element model preparing, usually large amount of finite elements, which increases the calculation time, and the absence of possibility to obtain stresses and strains at the level of single filament.

The second approach assumes usage of shell elements. This approach is based on the theory of multilayer shells, has all the limitations of this theory, and is applicable of cause only to a shell-like structures. An obvious advantage of this approach is the relative simplicity of finite element model preparation, including setting the properties of layers and their orientation. Another advantage of this approach is the smaller dimension of the finite element model in comparison with the previous method. A significant lack of this approach in addition to the limitations imposed by the multilayer shell theory is the impossibility to obtain a correct stress-strain state in the areas of joints and other local structure elements. The disadvantages connected with absence of stress-strain information at level of filaments remain the same as for first approach.

The other approach is a more advanced one and can be called “multiscale modeling”. Treating composite materials and structures it is convenient to introduce the concept of micro (μ), meso (m) and macro (M) levels. As a rule, under the microlevel the features of the microstructure of the composite material and, accordingly, features of considering the stress-strain state at the level of microinhomogeneities are understood. Speaking about the macrolevel, we mean the consideration of the composite structure as a whole, without going into the description of the microstructure features and the stress-strain state at the micro level. In addition to the introduction of macro- and microlevels, in many cases it is expedient to introduce some intermediate levels, which are called mesolevels. When considering the behavior of a composite materials or composite structure on macro, micro and meso levels on the basis of finite element modeling, the concept of a multiscale finite element model naturally arises. At the meso level, a homogenization operation is frequently introduced (replacing the microinhomogeneous composite material with an equivalent material with effective physical and mechanical characteristics), which is one of the necessary tools for linking the stress-strain state at various levels [2-5]. The reverse procedure - heterogenization - is necessary for determining real microstresses and microstrains on the basis of stresses and strains of the global model. It should be noted that some of the mathematical methods outlined in [2-5] allow, in addition to finding effective characteristics of the composite material, also to obtain the distribution of stresses and strains at the microlevel, that is, to solve the heterogenization problem. In particular, the problem of heterogenization can be solved numerically with the help of this method of submodeling. In cases where the allocation of a larger number of levels is rational in the structure of the composite material (for example, when the inhomogeneities considered at the microlevel themselves have an inhomogeneous structure), it is meaningful to consistently perform homogenization at several levels, which can be called multiscale homogenization [6]. In so doing, the inverse problem of multilevel heterogenization can be formulated in a natural way, and combined application of multiscale homogenization and heterogenization procedures allows solving the problem simultaneously at several levels, transferring information about the stress-strain state of the material between them (multiscale modeling).

3. Parametric model of three-component composite material structure

The structure of composite material at the micro- and mesolevels is determined by the preliminary carrying out of full-scale tests of samples using X-ray tomography and microscopic research. Analysis of the material structure at mesolevel indicates presence of the defects such as non-adhesive zones and delamination between the layers of the thermoplastic matrix and the layers of the carbon fiber impregnated with the epoxy binder, as well as changes in the thickness and shape of the layers. Figure 1 shows the results of X-ray tomography (tests were carried out on the X-ray microtomograph MT5 at National Research Tomsk Polytechnic University), red marks shows non-adhesive zones and delamination.

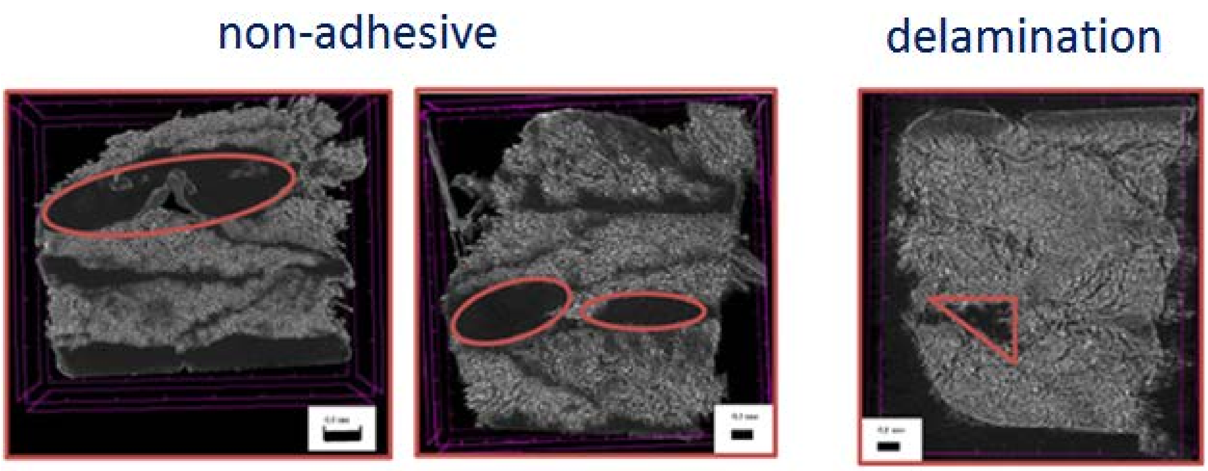

Fig. 1. 3D reconstruction of the cross sections of a sample of a three-component material 10x10x7 mm. Types of defects.

Figure 2 shows the cross sections of several samples of three-component materials with different thicknesses of layers and the mutual arrangement of the layers of the matrix and the carbon fiber impregnated with the epoxy binder (micro photos made at National University of Science and Technology “MISIS”).

A parametric finite element model of composite at mesolevel was created by use of APDL programming language (the programming language used in the ANSYS software environment). The geometrical and materials physico-mechanical characteristics were used as model parameters.

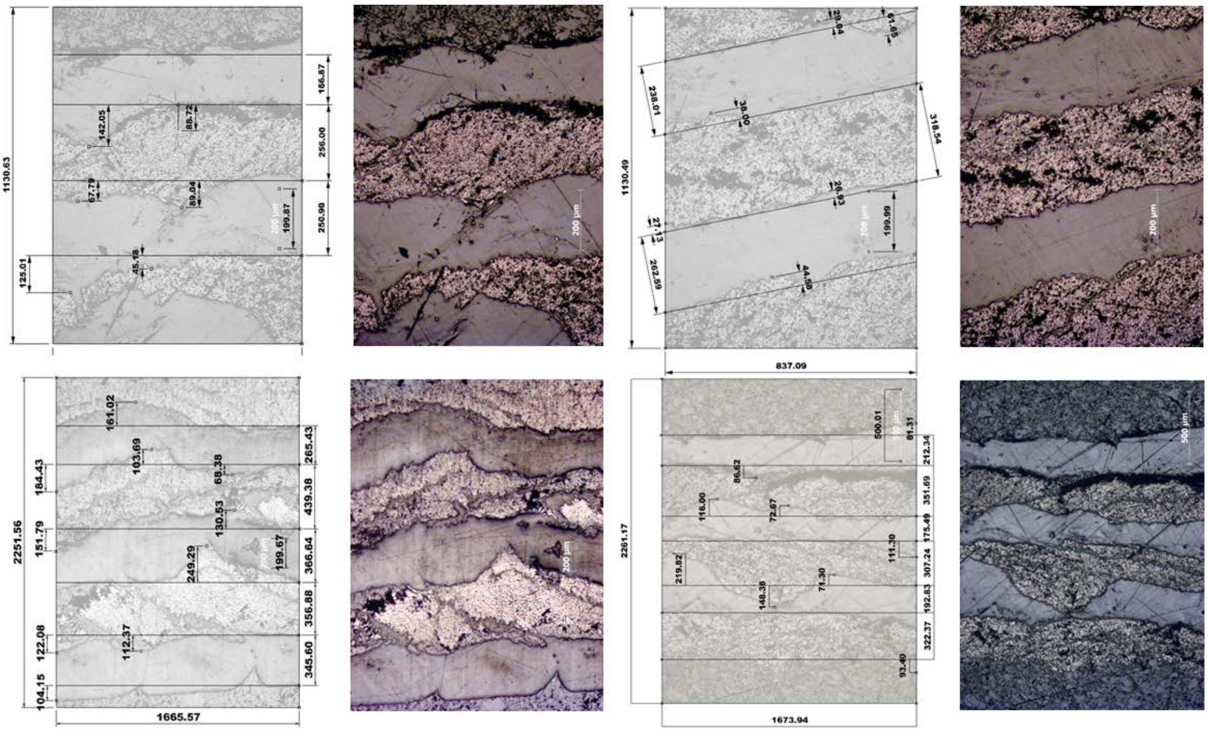

Fig. 2. Analysis of geometric characteristics of mesostructure of a three-component material.

Parameters for controlling the shape and size of the fiber layers are given as an example in Fig. 3: thicknesses of the matrix layers and carbon fibers impregnated with the binder (hm1, hv1, hm2, hv2, hm3), spread of control point coordinates (r1, r2, r3, ... rn), overall dimensions of the mesostructure sample A, B, and L.

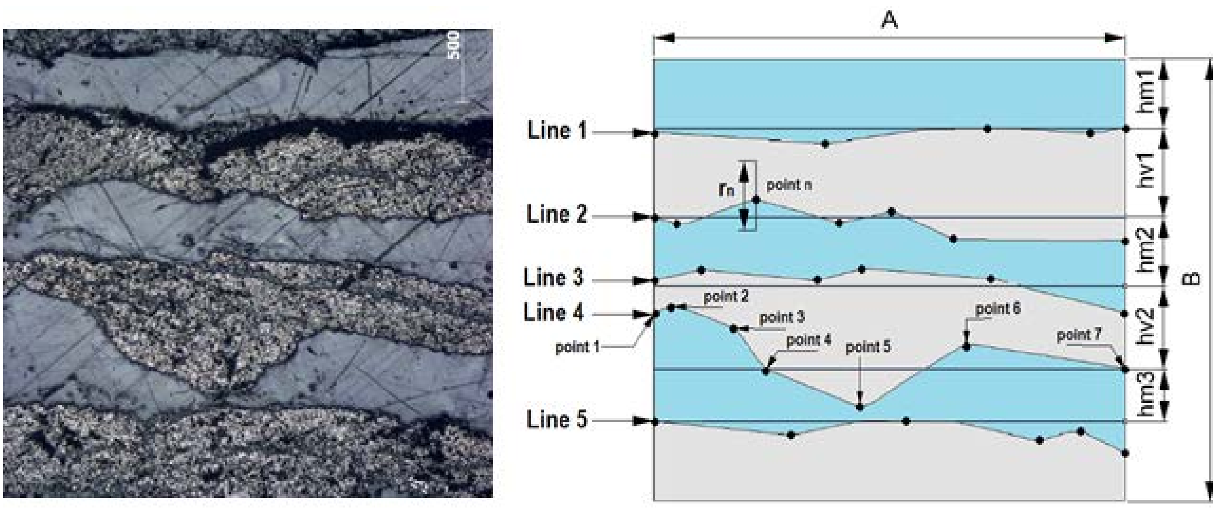

Fig. 3. Parameters for controlling the shape and size of fiber layers.

By change of parameters value within the observed during microstructure research ranges, finite element models of mesostructure samples with various shape of fiber layers and defects and percentage content of fibers were generated. Figure 4 presents some of generated mesostructure models of a composite material.

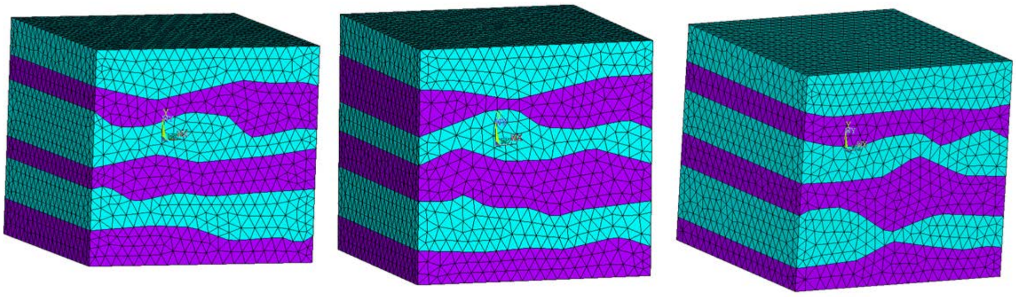

Fig. 4. FE models of mesostructure with variation of parameters.

Figure 5 shows mesostructure models with a different location and percentage content of defects.

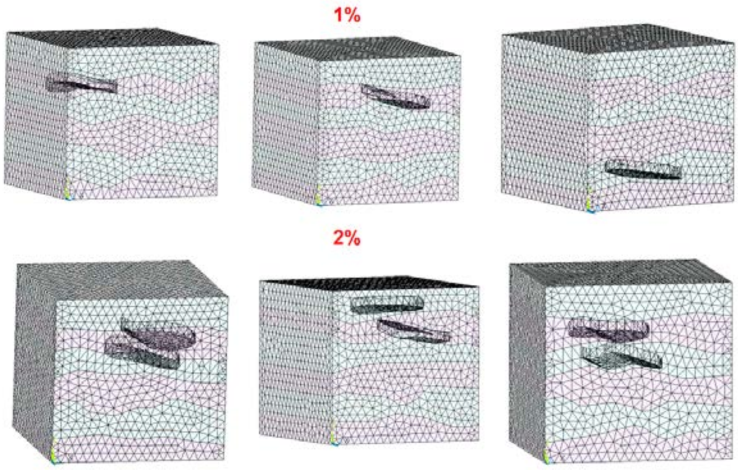

Fig. 5. Variants of defects location in mesostructure models.

4. Research of the influence of layers geometry

A series of virtual tests was performed using the procedure of two-level homogenization and heterogenization. Exactly, virtual tests were carried out by solving continuum mechanics boundary value problems at three levels: macrolevel (level of the specimen), mesolevel (level of composite structure at which layers of fiber impregnated with epoxy binder are represented by a homogeneous material) and the microlevel (microstructure level inside the fiber layers). The relationship between stress-strain states at three levels is realized by means of the developed modules of multiscale modeling. On the basis of single multiscale computation, considering the relationship between the load and the stress as linear, the obtained values are interpolated and a load corresponding to stresses at microlevel reaching the ultimate value is determined (Fig. 6).

During virtual testing, the influence of the composite microstructure parameters on the strength characteristics of the material obtained in tensile and bending tests was investigated.

Virtual tensile tests of composite material are carried out in accordance with the requirements of GOST 25.601 [8] standard and correspond to experimental full-scale tests carried out by the Institute of strength physics and materials science [7]. Table 1 shows the obtained modulus of elasticity and tensile strength values for different fiber concentrations in the sample, and the relative deviations of the calculated values in percent are indicated in parentheses. With an increase in the number of defects in the samples, the values of the modulus of elasticity and the ultimate strength are generally reduced in accordance with expectations, while the range of values variation (due to random positions of the defects) increases.

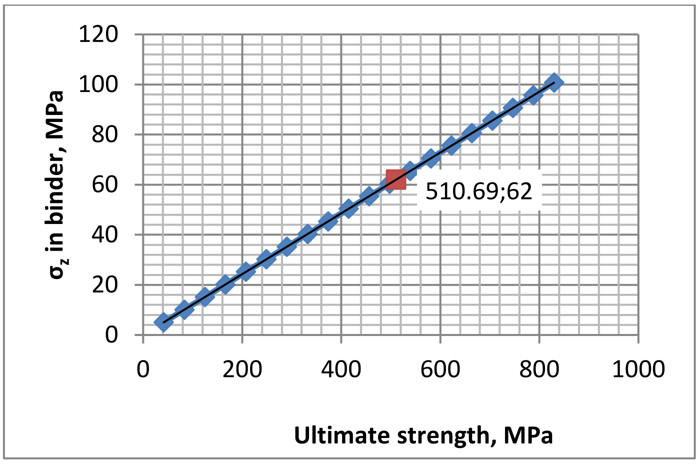

Fig. 6. Determination of ultimate strength.

Table 1. Study of the influence of the layers geometry during tensile tests.

	Without defects	1 % of defects	2 % of defects	Results of full-scale tests
Concentration of fibers in the sample, %	24,72-30,57	24,64-30,34	24,5-29,11	-
Elastic modulus, GPa	57,6-71,2	56,3-70,6	56,8-66,7	62,6
Tensile strength, MPa	461-568	450,5-564,2	453,9-533,1	510,7

Plots of the obtained during all virtual tests values of elastic modulus and tensile strength are presented in Fig. 7. With the number of defects increase, the variation of results due to microstructure parameters variation increases.

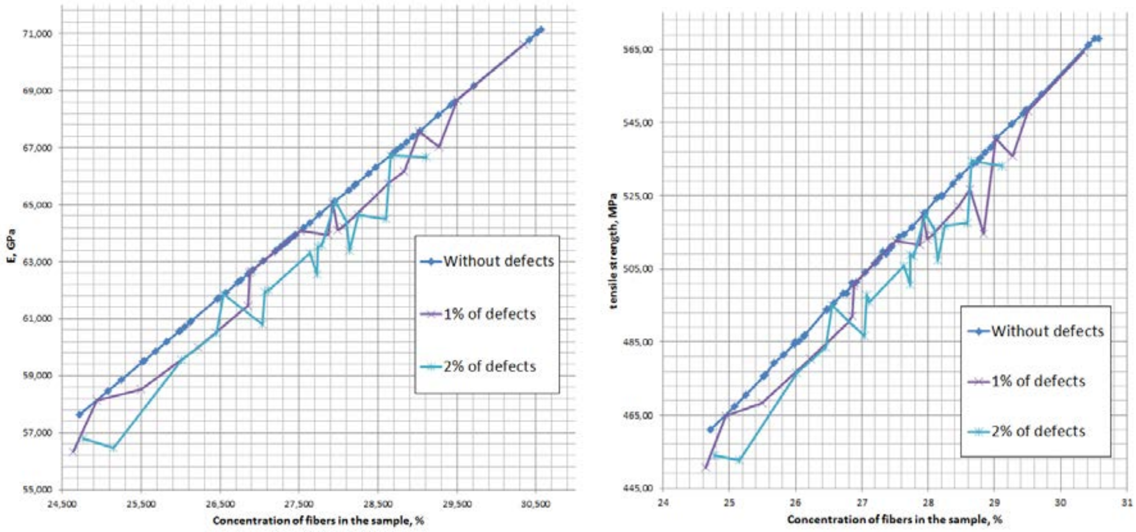

Fig. 7. Influence of defects on strength characteristics during tensile tests.

Virtual bending tests of experimental samples of the composite material are conducted in accordance with the requirements of GOST 25.604 [9] and correspond the experimental full-scale tests. Results indicate that failure during bending tests is initiated at the lower layer of fiber impregnated with epoxy binder due to tensile stresses.

Figure 8 shows the effect of the layers geometry influence on the stress-strain state at mesolevel.

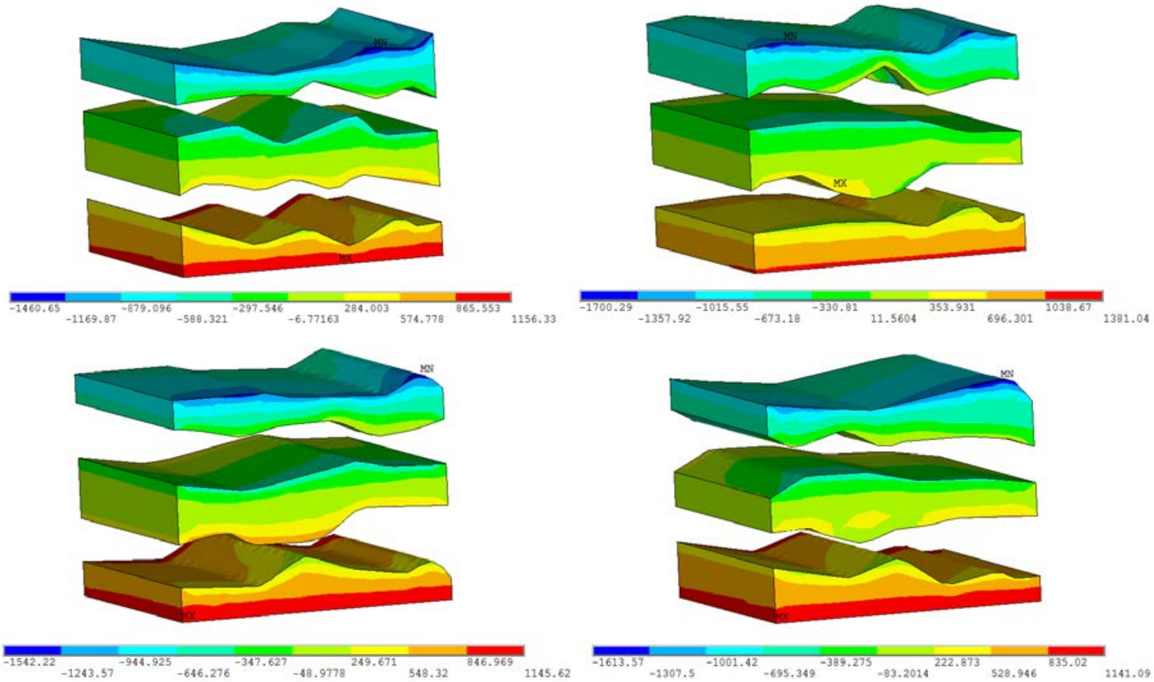

Fig. 8. Effect of the layers geometry on the stress-strain state during bend tests.

Table 2 presents the obtained values of the modulus of elasticity and tensile strength at different fiber concentrations in the sample, and the relative deviations of the calculated values in percent are indicated in parentheses. With an increase in the number of defects in the samples, the values of the modulus of elasticity and the ultimate strength are generally reduced in accordance with expectations, while the range of characteristics variation due to random position of defects increases.

Table 2. Study of the influence of the layers geometry during bending tests.

	Without defects	1 % of defects	2 % of defects	Results of full-scale tests
Concentration of fibers in the sample, %	24,72-30,57	24,64-30,34	24,5-29,11	-
Elastic modulus, GPa	50,78-62,36	49,79-61,68	49,77-58,27	55,3
Bending strength, MPa	424,11-528,8	423,15-520,18	416,46-483,1	524,2

Just as in the case of tensile tests, with an increase in the number of defects, the spread in the values of the strength characteristics also increases, while the spread of the values is more chaotic (Fig. 9) - this is due to the effect of the layers arrangement on the mechanical characteristics during the bend tests.

Plots of the obtained during bending virtual tests values of elastic modulus and tensile strength are presented in Fig. 9. With the number of defects increase, similar to the case of tensile tests, the variation of results due to microstructure parameters variation increases.

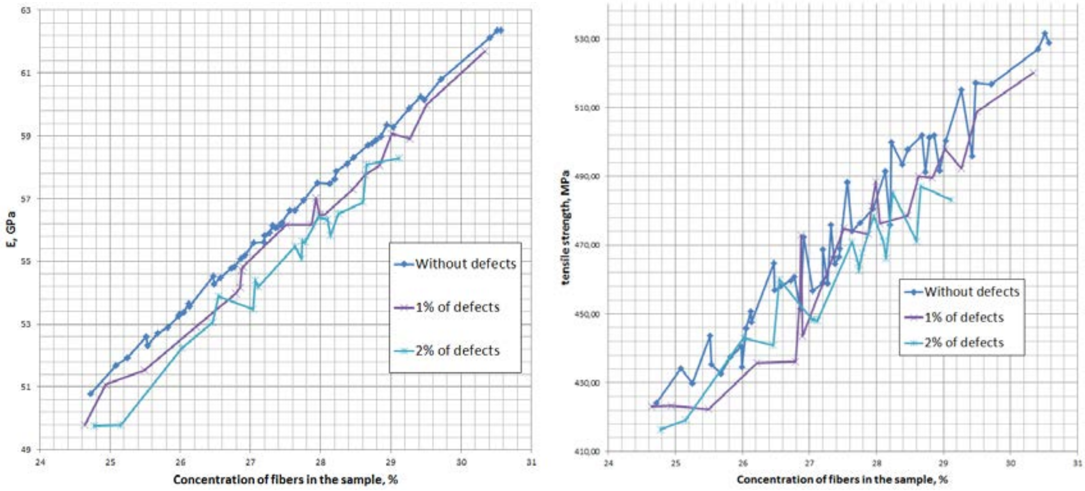

Fig. 9. Influence of defects on strength characteristics during bending tests.

It should be noted that in case of bending tests the results are much more affected by microstructure parameters variation not associatied with fibers fraction change (points with same or very similar absciss on the plots) that makes obtained curves much more "chaotic". Table 3 presents the quantitative analysis of mentioned microstructure influence on the results for both tensile and bending simulations – values in percent represent the maximum observed difference between the results obtained for models with same fibers volume fraction.

Table 3. Analysis of microstructure influence on the results for both tensile and bending simulations.

	Tensile tests		Bending tests	
	Elastic modulus	Tensile strength	Elastic modulus	Bending strength
Without defects	0,03 %	0,06 %	0,44 %	4,86 %
1 % of defects	1,45 %	0,89 %	1 %	7,8 %
2 % of defects	2,64 %	3,18 %	2,07 %	3,89 %

Presented in Table 3 results indicate that strength of the specimen can be affected not only by volume fraction of fibers and defects, but also by uncertainties in microstructure of 3D printed three-component material. This effect is much stronger for the case of bending test – up to 8 % for the specimen strength. In should be noted also that for the case of bending test (unlike the tensile test) the uncertainty in specimen mechanical strength due to microstructure variation is observed even for the specimens without defects.

5. Conclusions

Parametric finite element model of composite mesostructure representative volume with ability to vary fibers volume fraction, geometry and arrangement of layers and percentage of defect was developed. By use of this model and developed procedures of multiscale modeling (homogenization and heterogenization), a parametric study of the mechanical characteristics of novel 3D printed three-component composite material was performed. Results indicate that for the bending test strength of the composite is strongly affected by microstructure parameters even in case when they do not lead to fibers and defects volume fraction variation. Unlike the case of tensile tests, during bending this effect is observed even for the case of defects absence. The estimated uncertainty in three-component composite strength of approximately 8% thus should thus be taken into account when designing 3D printed composite structures.

The developed multiscale models can be used in the calculation of large-sized structures by use of implemented multiscale technique.

Acknowledgments
This work has been supported by RF Ministry of Education and Science (Contract № 14.581.21.0005, RFMEFI58114X0005).

References

[1] A.V. Azarov, F.K. Antonov, V.V. Vasil’ev, M.V. Golubev, D.S. Krasovskii, A. F. Razin, V. A. Salov, V. V. Stupnikov, A. R. Khaziev // Polymer Science, Series D **10** (2017) 87.
[2] N.S. Bahvalov, G.P. Panasenko, *The averaging of the processes in the periodical media* (Nauka, Moscow, 1984).
[3] A. Bensoussan, J.L. Lions, G. Papanicolaou, *Asymptotic analysis for periodic structures* (Amsterdam, North-Holland Publ. Comp., 1978).
[4] A.I. Borovkov, *Effective Physical and mechanic properties of fiber composites* (VINITI, 1985).
[5] V.A. Palmov, A.I. Borovkov // *Applied Mechanics and Materials* **56** (2006) 551.
[6] A.S. Nemov, A.I. Borovkov, B.A. Schrefler // *St. Petersburg Polytechnic University Journal of Engineering Science and Technology* **3** (2009) 153.
[7] A.V. Chumaevskii1, E.A. Kolubaev, S.Yu. Tarasov, A.A. Eliseev // *Key Engineering Materials* **712** (2016) 232.
[8] GOST 25.601, *Design calculation and strength testings. Methods of mechanical testing of polymeric composite materials. Test for tensile properties on plane specimens at normal, elevated and law temperatures* (1980).
[9] GOST 25.604, *Design calculation and strength testings. Methods of mechanical testing of polymeric composite materials. Test for bending properties at normal, elevated and low temperatures* (1982).