

# DEVELOPMENT OF MODELS, ALGORITHMS AND SOFTWARE FOR EVALUATING THE EFFECTIVE CHARACTERISTICS OF MATERIALS OBTAINED BY USING ADDITIVE TECHNOLOGIES USING MULTISCALE PHYSICAL MODELING

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One of the vectors of the development of our country's economy is the transition to the so-called "digital economy". In the message of the President of the Russian Federation to the Federal Assembly on December 1, 2016, "It is necessary to focus on areas where the powerful technological potential of the future is accumulating, and these are digital, other so-called end-to-end technologies that today determine the appearance of all spheres of life" [1]. One of the elements of the digital economy is 3D printing, additive technologies, or layer-by-layer synthesis technologies, one of the most dynamically developing directions of digital production in our country and abroad. These technologies combine one circumstance: the construction of a part occurs by adding material (from English add - "add") in contrast to traditional technologies, where the creation of a detail occurs by removing "excess" material.

In turn, this raises the problem of developing a mathematical, algorithmic and software apparatus for modeling the characteristics of newly created materials. This problem in all industrially developed countries of the world is solved by replacing the real object with its mathematical model, reproducing the basic functions of the original and the like in given relevant aspects.

At present, there is no single generally accepted approach directly linking the features of the microscopic structure of inhomogeneous composites produced using additive technologies with their macroscopic properties, which limits the functionality of the systems of engineering analysis (SAE) (universal strength computational packages). In this regard, the development of new physical models, computational methods and algorithms that would allow to connect the results of modeling at the microlevel with macroscopic properties, is especially urgent [2].

For these reasons, it seems relevant in the framework of the proposed PSI to develop methodologies for approach to computer modeling combined by a common ideology of multiscale modeling and parallel computing technologies, the exchange and processing of input and output data

In the Tula State Pedagogical University. L.N. Tolstoy together with the FKP "Aleksinsky Chemical Plant" are carrying out research within the framework of the Federal Program "Research and Development in Priority Areas for the Development of the Scientific and Technological Complex of Russia for 2014-2020" on the theme "Development of models, algorithms and a prototype of a software module for assessing the effective characteristics of materials produced using additive technologies using multiscale physical modeling "[2].

The overall goal of the work is a significant acceleration and optimization of the process of developing multicomponent materials obtained by using additive technologies with given physical and mechanical properties due to multiscale physical modeling and increasing the efficiency of using modern high-performance computing systems for computer simulation and design of new materials.

Other research objectives are:

- development of scientific and technical software in the field of software for evaluating the effective characteristics of materials obtained by using additive technologies using multiscale physical modeling;

- acceleration and optimization of the process of development of multicomponent materials obtained by using additive technologies with specified deformation-strength properties due to increasing the accuracy of prediction of structure and properties;

– increasing the efficiency of using modern high-performance computing systems for computer modeling and design of new materials and structural elements from them.

Carrying out a multilevel modeling of the processes of deformation and destruction of materials obtained with the use of additive technologies, suggests a study, during which should be:

1. Models have been developed to evaluate the effective characteristics of materials obtained by using additive technologies using multiscale physical modeling.

2. Algorithms have been developed for carrying out scalable computations in multilevel modeling problems of effective characteristics of materials obtained by using additive technologies.

3. Prototypes of software modules are created that implement the developed algorithms for evaluating the effective characteristics of materials obtained by using additive technologies.

4. Experimental verification of the results of theoretical studies, first of all, using methods of numerical simulation of the effective characteristics of materials obtained with the use of additive technologies, and confirmed the possibility of carrying out multilevel calculations combining micro and meso levels.

5. The mechanisms of deformation and destruction of materials obtained using additive technologies using multiscale physical modeling are analyzed, and the efficiency of the proposed modeling techniques is analyzed from the point of view of their use for the development of new materials obtained with the use of additive technologies.

Thus, the object of research are material bodies created from materials obtained with the use of additive technologies (MIAT) with various mechanical and physical properties.

At the micro level, the processes occurring throughout the composite body are described by differential equations with variable coefficients whose values depend on which of the volumes the point belongs to. Moreover, these coefficients undergo finite discontinuities when passing through the boundaries of volumes [3-5].

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