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## Computer modeling and verification of mechanical properties of metal-polymer composite materials used in the technological process of layer-by-layer growing of parts used in the technological process of layer-by-layer growing

**Abstract.** The article presents the results of computer modeling of the microstructure of a composite material consisting of a polyamide matrix and metal inclusions. The researched composition is one of the advanced trends in the production of materials for advanced MIM technologies. This paper describes the design of a new pressing device to produce composite rods. Computer modeling of mechanical properties of composite metal-polymer material was performed in the high-level CAD system DIGIMAT module MF. Micro-level modeling of the composite made it possible to establish the relationship between the percentage of inclusions and the upper yield strength of the material and the influence of the shape of the inclusions on the tensile strength of the designed material. The computational experiment results were verified with the results of the field experiment for the samples produced by the injection molding technology and the 3D printing technology.

**Keywords:** feedstock, MIM technology, 3D printing, injection molding, flow limit, material mechanical properties.

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### Introduction

Identifies and defines two main technological development stages of mechanical engineering products and devices. These are: improving the quality of materials used for products and reducing the cost of the technological process of manufacturing products. To meet this requirement, for the development of materials and products, it is necessary to qualitatively strengthen production technologies and achieve the possibility of changing the composition of the material at the stage of product development. One of the main methods for developing the method of manufacturing products is the method of heating metal powders or powders of refractory materials by mixing them into the binding material (composite materials), changing its composition, condition, structure pressing them into a certain form. In the production of small-scale, complex-shaped products, one of the modern methods is considered to be the technology of filling composite materials by pressure [1, 2, 3, 4].

Currently, additive technologies are widely used in the production of products with complex geometric shapes, and their large-scale research. In the works [5, 6], a thread was made from a metal-polymer composite material (feedstock), that is, a thread. In addition, the product was developed by layer-by-layer pressing by the method of Fused Filament Fabrication (FFF) using the resulting filament, determining the mechanical characteristics of the filament, and researching the connections between the products. In many scientific studies, it was found that additive technologies using feedstock brand 316L, that is, the production of products on a 3D printer and the main parameters at the stage of printing on a 3D printer directly affect the quality of the product. In addition, studies [7] showed that the quality of the filament is relatively high compared to the Metal Injection Molding (MIM) method. The cost of filament

(for 316L stainless steel composite material) made by MIM technology is about 15-18 euros/kg, as well as BASF Ultra fuse, showed that in the manufacture of filament (for 316lx) the cost is about 200 euros/kg. Moreover, the cost of filament from carriers or suppliers is 100 euros/kg. Currently, it is aimed at reducing the price of filaments and optimizing the printing parameter on a 3D printer, as well as analyzing the optimal compatibility of metal powder binders in the feedstock.

In the development of filament compositions for a 3D printer, BASF used 316LW steel feedstocks [8]. Many studies have shown that the percentage of powder Binder is in the ratio of 60% to 40%, and this percentage of feedstock contains 90% or more powders. If the material contains a high percentage of powder, this leads to a low instability index [13], and leads to a high viscosity during the melting period of feedstock [14]. In their research [9], the authors said that the quality of the filament can be determined by two main parameters, which are the limits of tensile and bending strength. The tensile parameter means that when the thread is fed to a 3D printer through an extruder, we mean the tensile break of the thread [10], and bending strength means that when the thread is fed, we estimate the elasticity of the thread [11]. Widely considered in the experiment, for example, in MIM technology, tests were carried out for the bending period of a filament made of 316LW feedstock material. In order to improve the elasticity of the filament, polyacetal (rum) and polyethylene (LDRE) polymers were mixed by heating at a temperature of 170 °C. With a higher percentage of binder, the elasticity of the filament improves. However, as the percentage of binders, i.e. polymers, increases, metal powders begin to decrease. This leads to the external and internal structure of the product during the cooking process, as well as incorrect unification of powders. It was found that the choice of POM, and LDPE polymers as binders with a certain percentage, affects the strength of the filament.

Taking into account the scientific research, we can conclude that for the MIM method with a rational complex, it is necessary to conduct experiments with composition materials and conduct research with additional calculations.

**The main purpose of this scientific paper** is computer modeling of microstructures of a material to determine the mechanical characteristics and additional parameters of metal polymer composite materials.

### Research methods

A continuous reverse pressing device has been designed and developed to create a thread from a metal-polymer composite material. With this device, powder materials can be obtained by mixing them into a binder without breaking them to a certain length. There is a hopper, extruder, auger, burners, movable and immovable plates, press stamp, reverse press form, and hydraulic cylinders that load the material into the continuous reverse pressing device. As shown in figures 1 and 2 below, the extruder of this continuous reverse pressing device has three different burners, and along this extruder, the material is melted in stages at three different temperatures. It is kept in a specially designed container at a temperature of 120-150 °C, and the material is released by pressing with a press-stamp, giving a reverse pressure using a hydra cylinder, and through a hole in the center of the press-stamp [16].

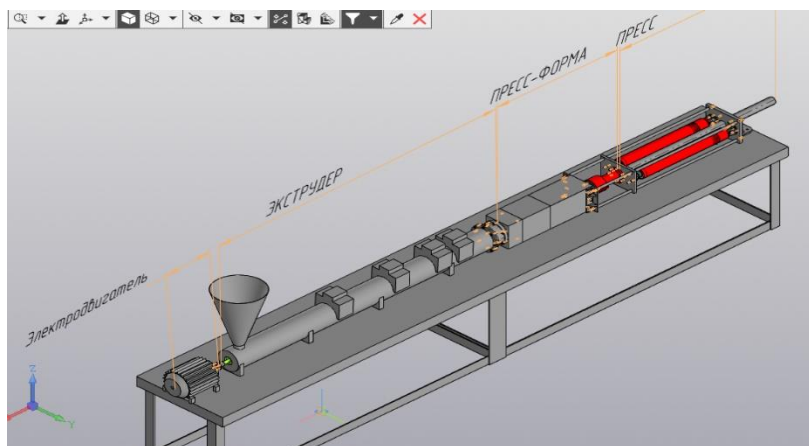


Figure 1. 3D model of the continuous reverse pressing device



Figure 2. The continuous reverse pressing device

The main factors affecting the physical and mechanical characteristics are, in particular, the presence of a single size of powders by the percentage volume of binders, and the interaction of the physicochemical process at the boundary of the binders phases. However, the most basic depends on the type of binder, i.e. polymer. Due to the increase in molecular weight, the hardness and strength of the metal polymer composite material increase. However, in this case, the physical and chemical characteristics are not determined, since it is considered a dispersed polymer composite material with high binding content.

Depending on the manufacturing technologies, various polymers are used, and there is very little information about their physical and mechanical characteristics [11].

In the process of performing calculations of the thermal conductivity property of a metal polymer composite material and as a dispersed capacity, as well as the calculation of physical and mechanical characteristics, it is possible to perform calculations by two different methods [12], which are carried out based on the Hashin-Strikman and Foigta-Reiss ratio. At the same time, there is a lack of practical value due to the wide range of possible values of two different micro-characteristics, and the only way to narrow the calculated "fork" is to show the relative location and geometry of The Shape of the phase zones that make up the metal-polymer composite. Such methods and approaches lead to individual computational analysis of material structures, under the influence of which a method of direct calculation of the mechanics of the medium of a metal-polymer composite material arises, which gives rise to the theory of averaging [13, 14, 15].

Such calculations are now widely developed in connection with the development of computer programs, such as MSC. Digimat and the program also include the structural foundations of materials. One of the most convenient programs for determining the nature of various composite materials is the DIGIMAT program.

The DIGIMAT program allows you to analyze the properties of materials and each phase, the volumetric mass composition of the material, as well as the microstructure of composite materials. In the MSC.Digimat program, the FE module should be selected for modeling, since it determines the microstructural properties of composite materials, and it is necessary to use the homogenization method to determine the reactions of materials at the macro level.

The main goal of these methods is to find an equivalent homogeneous (homogeneous) material that has the same effective characteristics at the macro level as a heterogeneous material at the micro-level. Indicators of parameters based on modeling are shown in Table 1.

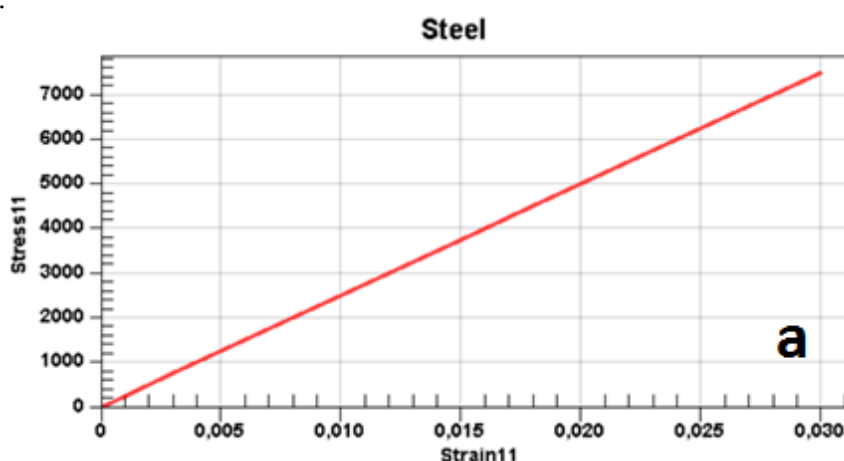
Basic information:

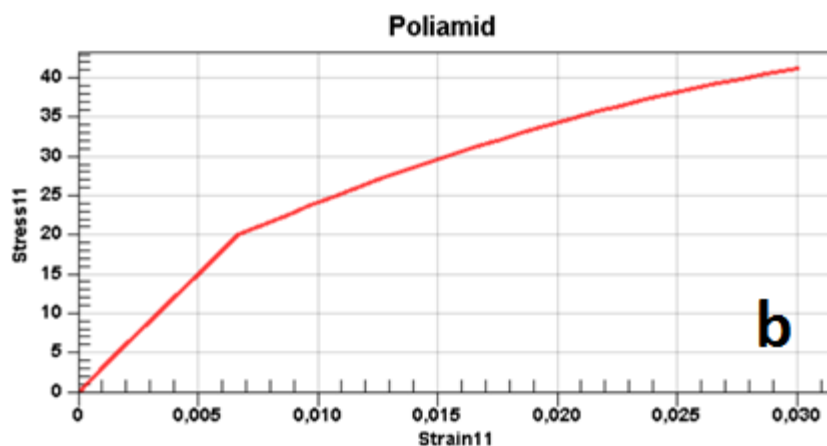
- mechanical characteristics of 38CrMA stainless steel
- mechanical characteristics of Catamold 42CrMo4
- the number of metal impurities
- the percentage of metal impurities

Table 1. Parameter indicators for the experiment

Parameters	Units of measure
Modulus of elasticity of polyamide, MPa	2700
The density of polyamide, kg/mm <sup>3</sup>	1,14· 10 <sup>-9</sup>
Poisson's ratio of polyamide	0,37
Modulus of elasticity of steel, MPa	210000
Steel density, kg/mm <sup>3</sup>	7,8· 10 <sup>-9</sup>
Poisson's ratio of steel	0,3
Particle size, mm	1

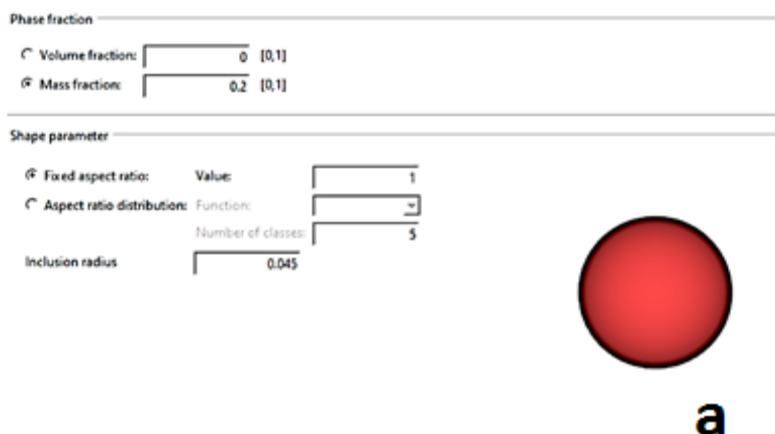
Figure 3 shows the stress-strain resistance curves of the composite matrix material developed in the DIGIMAT program.

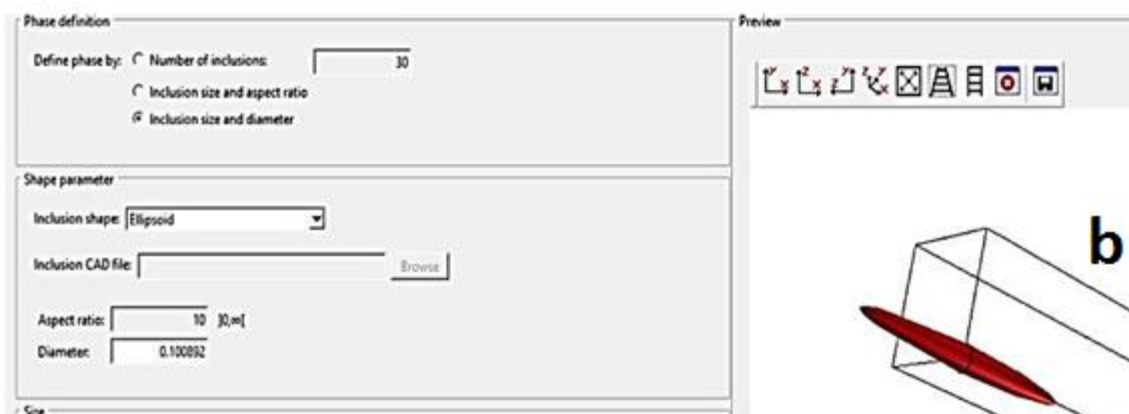




**Figure 3.** Stress-deflection diagram: a) Steel material; b) PA6-polyamide, which is the matrix in the composition.

Figure 3 shows the resistance curves generated in DIGIMAT for the deformation of the matrix material and inclusions. The next step in modeling the composite material is to create the microstructure. Using the option "Ratio coefficient", it is possible to vary the size of the inclusion particles, we chose "Ratio coefficient" equal to 25, so the particle size of metal inclusions is 1 mm. The option "Shape" allows us to change the shape of inclusions, we chose two shapes of inclusions elliptical and spheroidal. Since we had the task to compare the mechanical properties of the material with needle and spherical inclusions, by changing the parameters we simulated two kinds of particles, respectively after mechanical treatment (grinding in ball mills) and treatment by gas atomization. Figure 4 shows the simulated shapes of inclusions.





**Figure 4.** Parts modeled in the MSC.Digimat program:  
a) Spherical shape; b) elliptical shape

Metal polymer composite is considered one of the main factors that have a direct impact on the mechanical properties of the material, and the orientation of the fibers in space. An indicator of this parameter is the orientation tensor  $T$ .

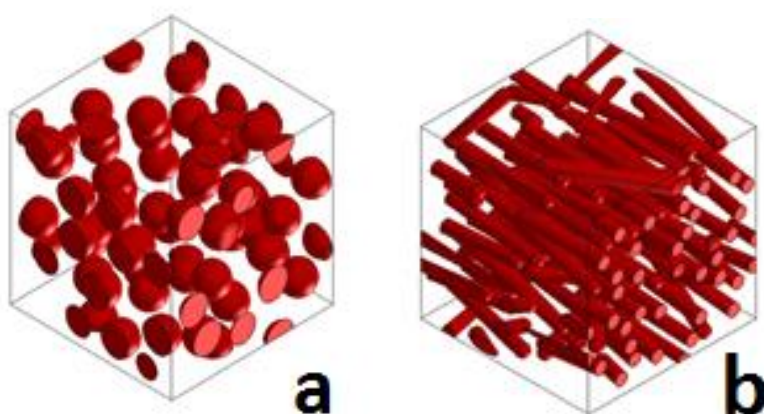
$$T = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

Where  $a_{ij}$  are the components of the orientation tensor corresponding to the direction of the direction along the  $x$ ,  $y$ , and  $z$  axes.

For the model of a metal polymer composite, the orientation  $a_{11} = 0.5, a_{22} = 0.5$  was chosen when reinforced with short elements and aimed at the isotropy of the projected material.

In the MSC.Digimat software information, a model of the material element Catamold 42CrMo4 metal polymer composite was developed.

For the article, we conducted a comparative study of the mechanical properties of a metal polymer composite material by steel powder and an analysis of its microstructure, including processing methods related to The Shape of the powders. In addition, the spherical shape of the steel powder (shown in figure 5. a) and the needle-shaped shape (shown in figure 5. b) were modeled.



**Figure 5.** Elementary models of metal polymer composite material developed in the MSC.Digimat program, a) spherical shape b) needle shape

We also took a sample printed on a 3D printer with a metal polymer composite material and a sample pressed into a molten form, compared the mechanical characteristics of the two samples, and conducted experimental work on stretching and bending by volume. The metal polymer composite material consists of 316L grade stainless steel powders with a carbon content of 0.018 %, and 90 % percent.

FILABOT EX2 with a filament diameter of 1.75 mm for printing on a 3D printer, Filabot made a filament at a temperature of 180 °C at a speed of 15 rpm. Using the PrintBox3D one 3D printer, we obtained the following G-code parameters in the special Repetier Host software management. They are extruder temperature 230 °C, working table temperature 60 °C, floor height 0.6 mm, filling 100 %, printing speed 25 mm/s.

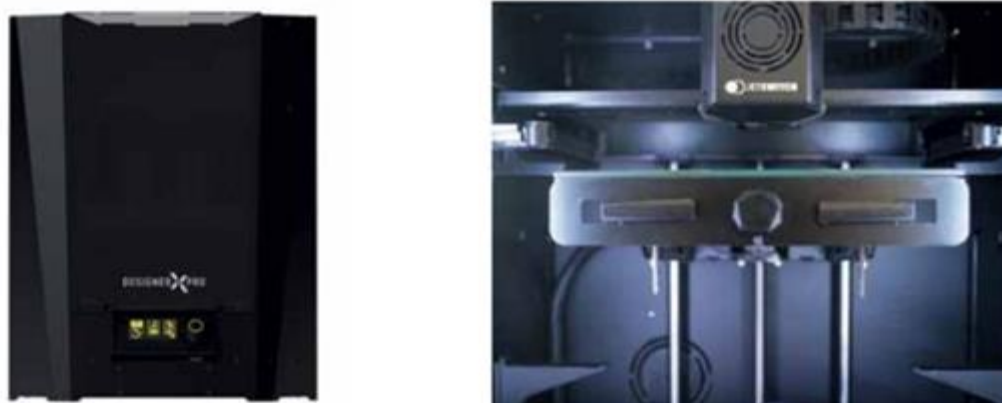


Figure 6. PrintBox3D printer



Figure 7. Specially prepared samples: a) sample obtained by casting by soldering; b) sample printed on a 3D printer

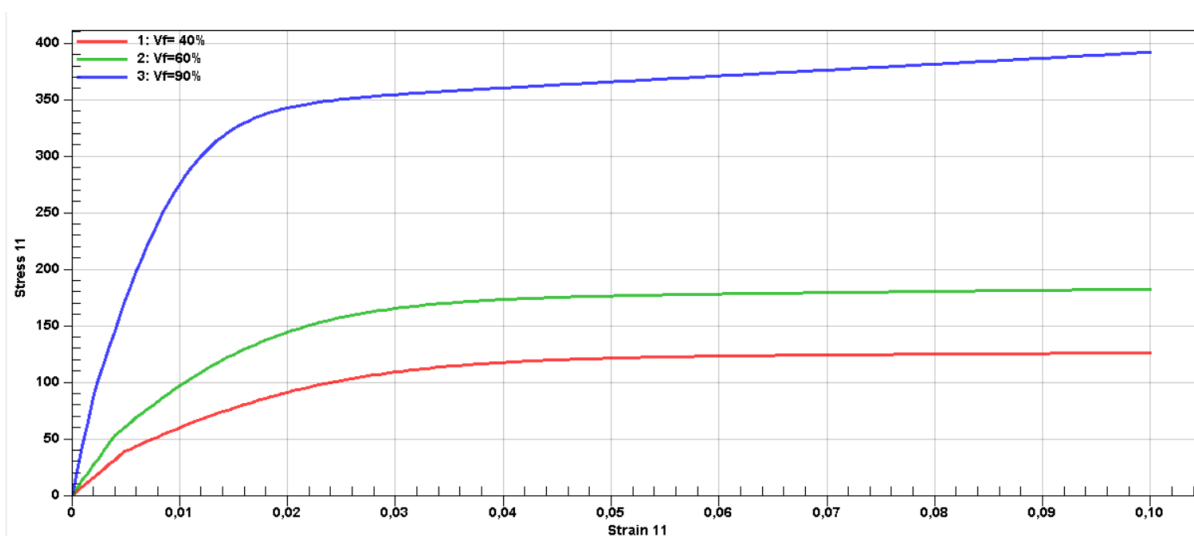
3D printer specifications include print speed: up to 100 cm<sup>3</sup> /H; nozzle diameter: 0.3 mm; maximum print temperature: 380 °C; maximum table temperature: 150 °C.

If we talk about the form for the soldering method, the form is made on a single screw extruder with a diameter of 55 mm, L: D = 25, produced by Esmos. Electric heating. Thermocouples and a thermostat regulate the temperature. The temperature regime of extrusion is as follows: Zone I-260 °C; Zone II - 265 °C; Zone III-270 °C, and Zone IV-260 °C.

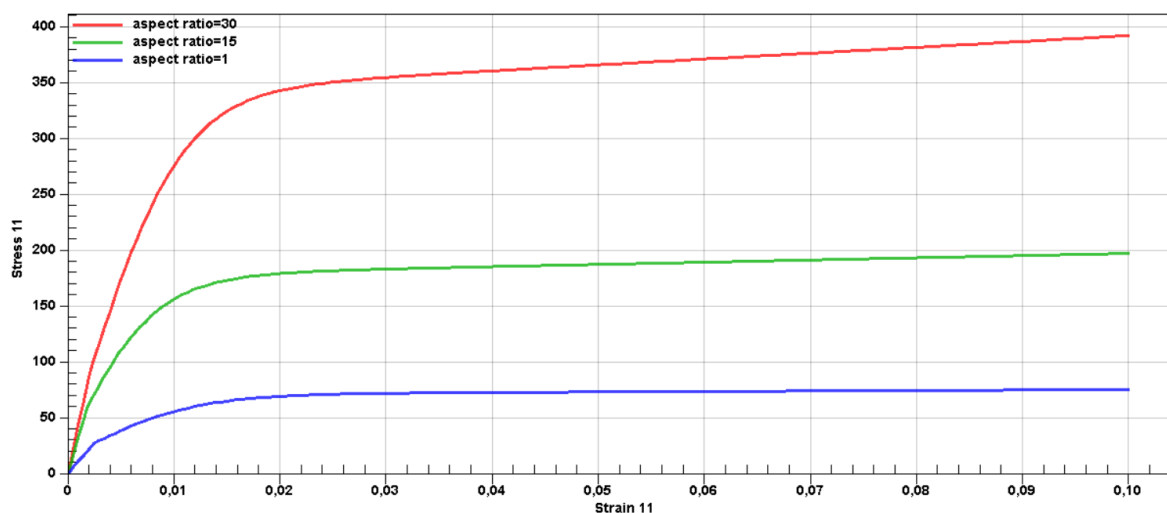
## Results and discussion

The results of the calculation of the diagram of mechanical characteristics of a material consisting of a combination of different percentages of binders and metal powders were obtained by the DIGIMAT program.

A diagram of the mechanical properties of composite materials with glass fibers is shown in figure 8. The results of the calculation revealed an increase in the flexibility limit of the needle-shaped composite material. The flexibility limit of the spherical Composite is 100 MPa. The limit of elasticity of the material with mechanical inclusions of the needle is 380 MPa. These results can be seen in figure 9.



**Figure 8.** Diagram of deformation resistance for samples with needle inclusions when filling 40%, 60%, 90%



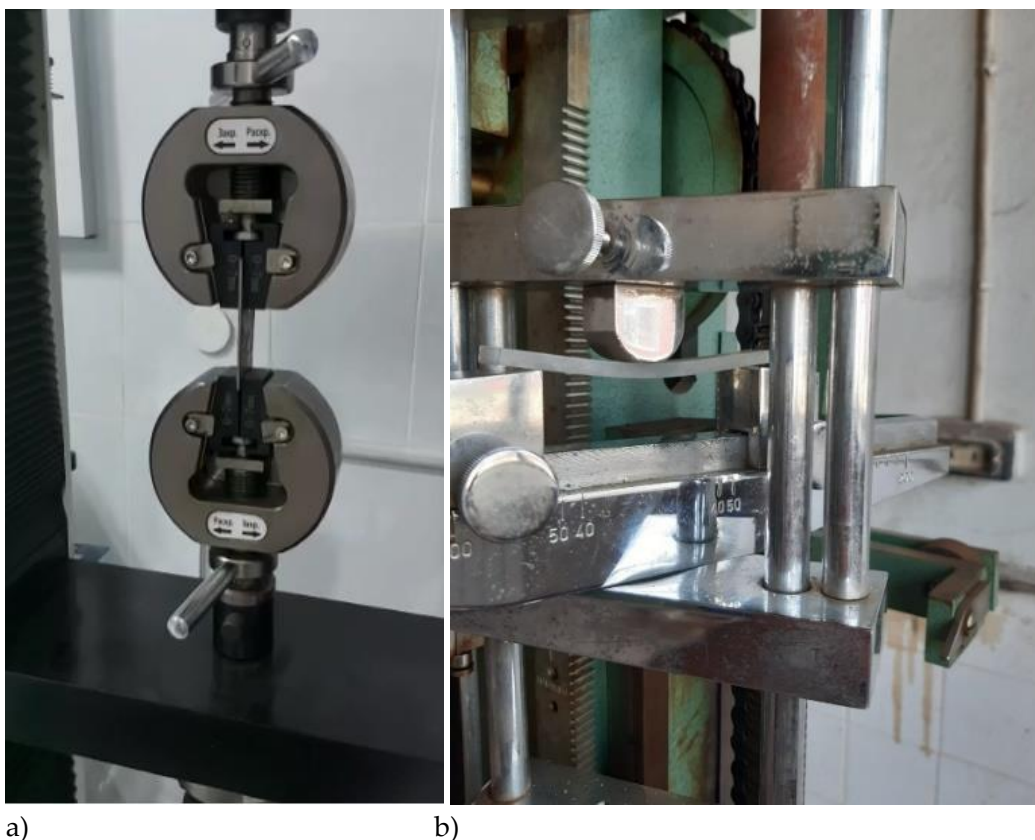
**Figure 9.** Diagram of deformation resistance for samples with a coefficient of the ratio of the radii of the shape, needle shape 30 (red curve), needle shape 15 (green curve), ball shape 1 (blue curve)

In the analysis of the diagram in Figure 8, you can see the linear dependence of the strength of composite material on the percentage of metal powders. Also, meal polymer composite material, that is, feedstock 316LW traditional MIM technology in the production of a filament with a percentage of metal powders up to 90 %, the filament breaks down by bending. If a large amount of metal powders is added, which increases the strength, the composite material loses its elasticity. For samples with a coefficient of



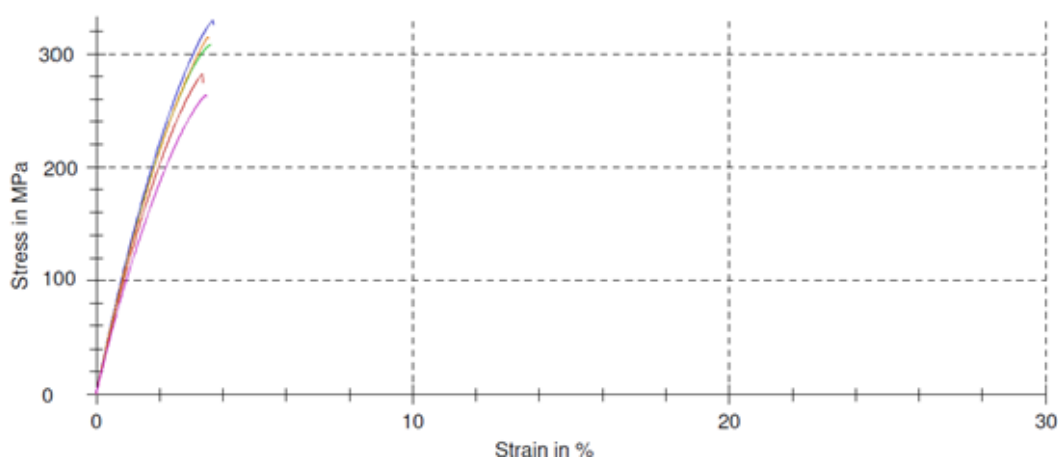
the ratio of the radii of the form, it allows us to assume that the specification of metal powders in the deformation resistance diagram improves the quality of the layer-by-layer pressing process [13, 14, 15], but on the other hand, reduces the strength characteristics of the composite, this fact contributes to a further deepening of the study of optimal parameters of the ratio of inserts and matrices. As shown in figure 9.

According to the results of the study, the strength values depend on the parameters of the method of filling samples with molten pressure. The casting temperature is 270 °C. The main goal is to evaluate the relative values of strength during the creation period using two methods of unburned samples. The figures and diagrams during the experiment were shown below.



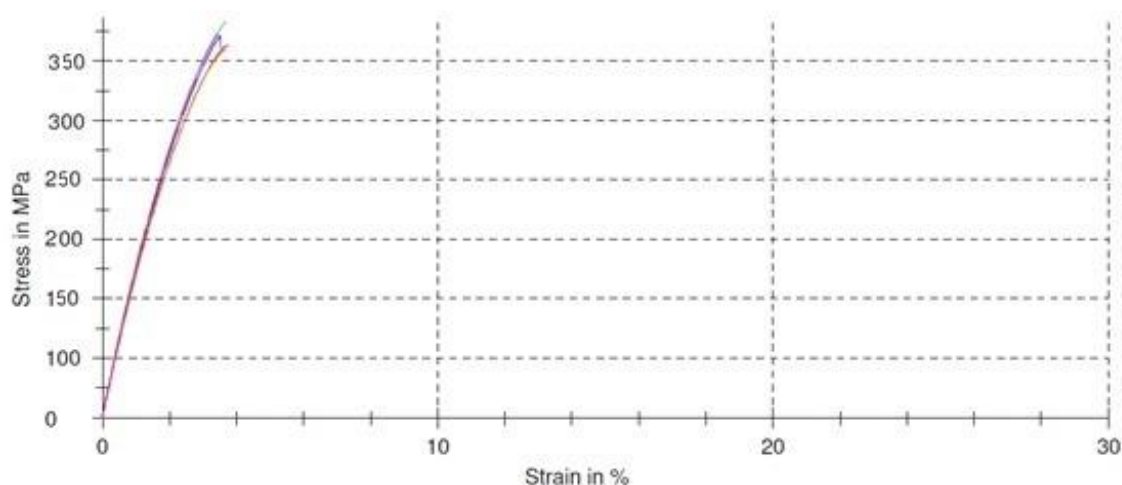
**Figure 10.** a) Stretching tests; b) bending tests

**Series graph:**



**Figure 11.** Voltage-deformation diagram of a sample printed on a 3D printer with a metal polymer composite material

**Series graph:**



**Figure 12.** Voltage-deformation diagram of a sample made by soldering pressure-casting technology with a metal polymer composite material

A comparison of the diagrams presented in figure 11, figure 12 indicates a difference in the magnitude of the rupture stress for samples made by different technology (casting and 3D printing), it is obvious that with the technology of printing samples, the rupture voltage  $\sigma = 320$  MPa and with casting  $\sigma = 380$  MPa. The results of bending are shown in Table 2.

Table 2. Flexural stress of the composites

№	MP %	Flexural stress, MPa	
		3D printing technology	casting technology for soldering
1	90	341.2	360
2	90	357.7	352
3	90	360	375
4	90	388.4	356
5	90	370.5	368

The tensile strength of the product printed on a 3D printer decreased by 18 %, which is directly related to the parameter at the time of printing. It is possible to increase the mechanical properties by selecting the desired parameter. The metal showed a satisfactory level of mechanical properties of the sample printed on a 3D printer with a polymer composite material.

### Conclusion

A new reverse pressure Press device has been developed to create a thread that will be applied to a 3D printer. To determine the microstructure of a metal polymer composite material, compounds with needle and spherical shapes were obtained, and a method of modeling the modulus of strength and elasticity of composite materials was proposed. This method allows you to obtain a stable and accurate prediction of mechanical properties.

Numerical modeling of the percentage dependence of metal powders on the fluidity limit and modulus of elasticity of a metal polymer composite material was carried out. A comparative study of a sample printed on a 3D printer, a sample obtained by melting pressure casting, was carried out.

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**Бөлшектерді қабатты өсірудің технологиялық процесінде пайдаланылатын металл полимерлі композитті материалдардың механикалық қасиеттерін компьютерлік модельдеу және верификациялау**

**Аңдатпа.** Мақалада полиамидті матрицадан және металл қоспалардан тұратын композиттік материалдың микроструктурасын компьютерлік модельдеу нәтижелері келтірілген. Зерттелетін композиция прогрессивті МІМ технологияларға арналған материалдар өндірісіндегі алдыңғы қатарлы бағыттардың бірі болып табылады. Мақалада композициялық шыбық өндіруге арналған жаңа престоу құрылғысының құрылымы келтірді. Композитті металл полимерлі материалдың механикалық қасиеттерін компьютерлік модельдеу MF модулі DIGIMAT жоғары деңгейдегі АЖЖ-да жүргізілді. Шағын деңгейдегі композитті модельдеу қосылымдардың пайыздық құрамы мен материалдың ағымдылығының жоғарғы шегі арасындағы өзара байланысты, сондай-ақ жобаланатын материалдың беріктігі шегіне қосу нысанының әсерін орнатуға мүмкіндік берді. Есептеу экспериментінің нәтижелері инъекциялық құю технологиясымен және 3D баспа технологиясымен дайындалған үлгілер үшін табиғи эксперимент

нәтижелерімен тексерілді.

**Кілт сөздер:** фидсток, МІМ технологиялар, 3D басып шығару, инжекциялық құю, аққыштық шегі, материалдың механикалық қасиеттері.

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**Компьютерное моделирование и верификация механических свойств  
металлополимерных композитных материалов, используемых в технологическом  
процессе послойного выращивания деталей**

**Аннотация.** В статье приведены результаты компьютерного моделирования микроструктуры композитного материала, состоящего из полиамидной матрицы и металлических включений. Исследуемая композиция является одним из передовых направлений в производстве материалов для прогрессивных МІМ технологий. Приведена конструкция нового прессового устройства для производства композитного прутка. Компьютерное моделирование механических свойств композитного металлополимерного материала проводилось в САПР высшего уровня DIGIMAT MF. Моделирование композита на микроуровне позволило установить взаимосвязь между процентным содержанием включений и верхним пределом текучести материала, а также влияние формы включений на предел прочности проектируемого материала. Результаты вычислительного эксперимента были верифицированы с результатами натурального эксперимента для образцов, изготовленных технологией инжекционного литья и технологией 3D печати.

**Ключевые слова:** фидсток, МІМ технологии, 3D печать, инжекционное литье, предел текучести, механические свойства материала.

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