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SOLID MECHANICS

NUMERICAL STRESS STATE EVALUATION OF POWDER NANOFILLED METAL-POLYMER COMPOSITE MATERIALS AT ELECTROCONTACT SINTERING

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ABSTRACT: The technique, design schemes and adaptive finite element models for an assessment of the stress states are developed. Processes of contact interaction of components of powder systems of "microdispersed metal–plated polymer–carbon nanostructures" have been researched with application of approaches of computer modeling. The regularities of formation of fields of internal stresses in the zone of contact interaction components at electrocontact sintering on the multicomponent system are investigated.

KEY WORDS: consolidation of components, carbon nanostructures, metal-polymer systems, metal powder matrix, microdispersed polymer, copper-plated polymer, stress state, electrocontact sintering, nanocomposite, finite element model.

1 INTRODUCTION

Materials used for the manufacture of parts of friction units, largely determine the life of machines and mechanisms. At the same time, the problem of developing such materials is of scientific and practical interest both from the point of view of engineering and materials science [1, 2]. Instead of traditionally used metals and alloys, composite materials are becoming increasingly common. It is the production of composites, developed on the basis of the methods of managing the structure and properties, in order to ensure the reliability and safety of the operation of technical systems, are among the priority areas of scientific and technical activity [3, 4].

In recent years, the objects of the nanometer scale such as fullerenes, nanotubes, nano-onions, and composite materials with their application – nanofilled composites

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has been acquired interest in practical use in various fields of science and technology. Such composites are of great interest, since they combine a number of parameters unattainable for traditionally obtained materials on the basis of mono- and polycrystalline structures [5–7].

The properties of composite materials with a metal matrix are due to the influence of a number of factors: the properties and the type of the matrix; type and amount of filler; the nature of the filler distribution in the matrix; the structure of the composite and the technology of production [8,9]. Therefore, knowledge of the properties of composites will allow rational use of existing composite materials. And the ability to predict and control the formation of the structure, as well as the physical processes during the contact interaction of the dispersed components of nanofilled metal-polymer systems will allow the creation of new adaptive composites.

Electrocontact sintering is accompanied by the appearance of a number of physical and technological effects: a cumulative effect, pinch effect, skin effects, intensive doping and the appearance of new phases. Thereby, the development of new multicomponent composites and coatings based on a metal matrix with a nanostructured carbon filler poses serious problems [10, 11]. It is very important that depending on such technological parameters of electrocontact sintering as pressure on a dispersed medium, amplitude and duration of electric current pulses, the process of forming composites can proceed in different ways, predetermining the change in their structure and properties. Therefore, from the point of view of materials science, the study of the processes of consolidation of the components of nanofilled metal-polymer powder systems activated by cumulative and pinch-effects during electrocontact sintering is a very complex problem. The research of the mechanism of diffusion processes and the formation of the structure of wear-resistant metal-polymer composites structured by carbon nanoparticles, and the patterns of formation of internal stress fields and microdeformations in zones of contact interaction of components at technological impact is an unconventional task.

Progress in the field of physical methods of studying solids has led to more in-depth notions of both the structure and properties of composite materials and their components. Nevertheless, for the detailed description of the processes of structure formation, as well as various mechanisms of interphase interaction, the use of only experimental approaches is insufficient. The effectiveness of the obtained experimental results largely depends on the adequacy of their evaluation, that is, in establishing correct relations between the composition, structure, and characteristics of the composites. Therefore, physical methods of research also require the use of consistent theoretical approaches and the development of effective computer models. Compared with known experimental methods, model representations are of independent value, since with sufficient correctness they can provide more complete information about the features of the structure of the material, and also to predict its possible properties and applications. In this connection, the application of adaptive computer modeling methods in the study of the processes of consolidation of components of nanofilled metal-polymer powder systems and wear-resistant materials when applying technological impact is very relevant.

Thus, the study of the stress state of powder composite materials by computer simulation methods will make it possible to predict effective ways to increase the strength and tribological characteristics of a given kind of materials.

The purpose of this work was to investigate the stress state of powder nanofilled metal-polymer composite materials at electrocontact action on the initial components by computer modeling methods.

2 Design Schemes and Finite Element Models

Calculation schemes and adaptive finite element computer models for studying the stress state, as well as studying the mechanism of the development of the consolidation processes of the components of nanofilled metal-polymer powder systems containing carbon nanotubes (CNTs) and carbon nano-onions (CNOs) in the course of electrocontact sintering have been developed. The most functional means of research using finite-element approach to computer modeling is the ANSYS software package. Modeling is reduced to solving a two-dimensional non-stationary conjugate thermostressed problem. The most optimal in this case is a sequential method of solving a related problem.

The main methodological stages of the conducted model studies are the following:

1. Definition of the object of modeling. At this stage, based on the results of microstructural studies and literature data, information on the geometry and properties of the modeling object is collected.
2. Development of design schemes. Based on the analysis of available information on the structure of nanofilled metal-polymer powder systems and their components, the geometry of the model is constructed.
3. Enter the modeling parameters.
4. Input of data of physical and mechanical characteristics of materials of components of nanofilled metal-polymer powder systems.
5. Development of adaptive computer finite element models. Formation of the finite element meshes on the developed design schemes.
6. Establishment of conditions for the uniqueness of models.
7. Enter the boundary conditions.
8. Carrying out a series of computational experiments and obtaining results.

9. Analysis and interpretation of modeling results.

The developed design schemes and computer finite-element models of mesofragments of contact interaction zones of components of metal-polymer wear-resistant materials by carbon nanoparticles include the following structural elements:

1) Fragments of the copper particles with a size of 100 μm, one particle of plated polymer with the size of 150 μm with the copper layer thickness of 6 μm, and also CNTs and CNOs located in contact areas of surfaces of micrometer components (Fig. 1);

2) Fragment of the copper particle with the size of 100 μm, a fragment of the 150 μm plated polymer particle with the copper layer thickness of 6 μm, one CNT with the internal diameter of 30 nm and the outer diameter of 60 nm disposed horizontally, and two CNOs 100 nm in diameter, each on opposite sides relative to CNTs (Fig. 2);

3) Fragment of the copper particle with the size of 100 μm, fragment of the 150 μm plated polymer particle with the copper layer thickness of 6 μm, one CNT with the internal diameter of 30 nm and the outer diameter of 60 nm horizontally and two CNOs with the diameter of 100 nm located on one side relative to CNTs (Fig. 3);

4) Fragment of the copper particle with the size of 100 μm, fragment of the 150 μm plated polymer particle with the copper layer thickness of 6 μm, two CNTs with the internal diameter of 30 nm and the outer diameter of 60 nm arranged vertically and horizontally, and two CNOs with a diameter of 100 nm (Fig. 4).

The computer models are developed in interactive mode. The advantage of the interactive mode is simplicity and visibility. The complexity of models developed is compensated by the possibility of their multiple solutions when specifying various parameters.

The deformation of the particles of the powder nanofilled metal-polymer material takes place in accordance with the elastic-plastic model: copper particles (Young's modulus $E_c = 110$ GPa, Poisson's ratio $\upsilon_c = 0.37$), CNT ($E_{CNT} = 2000$ GPa, $\upsilon_{CNT} = 0.18$), CNO ($E_{CNO} = 2210$ GPa, $\upsilon_{CNO} = 0.15$), polytetrafluoroethylene (PTFE) ($E_p = 0.49$ GPa, $\upsilon_p = 0.45$). The yield point of copper is 214 MPa, and of polytetrafluoroethylene is 42 MPa.

Taking into account the assumption that the copper particles and the applied compressive force are uniformly distributed, a compressive force of 1.2×10^{-3} N acts on each extracted mesofragment of the material. The value of 1.2×10^{-3} N is determined from the condition that the compression force in the formation of a powder composite of this class at the pilot plant for electrocontact sintering is 12 000 N, and the area of the sintering zone is about 15 mm^2. The computer models developed have a limited ability to move the lower boundaries. The stress state was evaluated on the

(a)

(b)

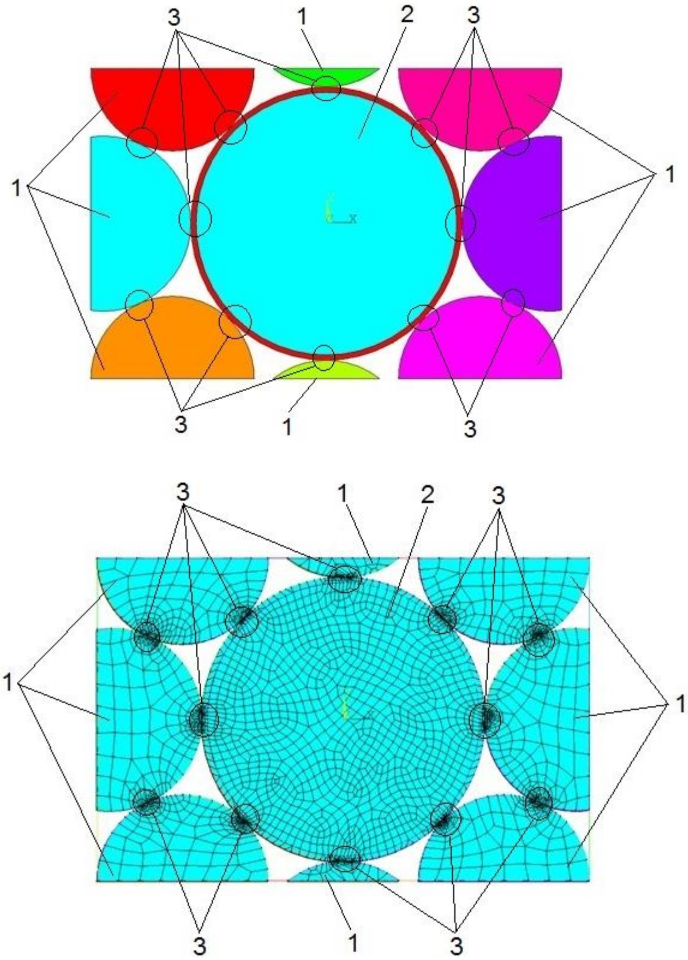


Fig. 1. Design scheme (a) and finite element model (b) of the mesofragment of the metal-polymer powder system containing fragments of copper particles (1), plated polymer particle (2), CNTs and CNOs located in contact areas of surfaces of micrometer components (3).

basis of the solution of the plane problem of the theory of elastoplasticity.

The principal stresses (σ_1, σ_2, σ_3) are obtained from the stress components by the following cubic equation:

$$\begin{vmatrix} \sigma_x - \sigma_0 & \frac{1}{2}\sigma_{xy} & \frac{1}{2}\sigma_{xz} \\ \frac{1}{2}\sigma_{xy} & \sigma_y - \sigma_0 & \frac{1}{2}\sigma_{yz} \\ \frac{1}{2}\sigma_{xz} & \frac{1}{2}\sigma_{yz} & \sigma_z - \sigma_0 \end{vmatrix} = 0\,, \tag{1}$$

(a)

(b)

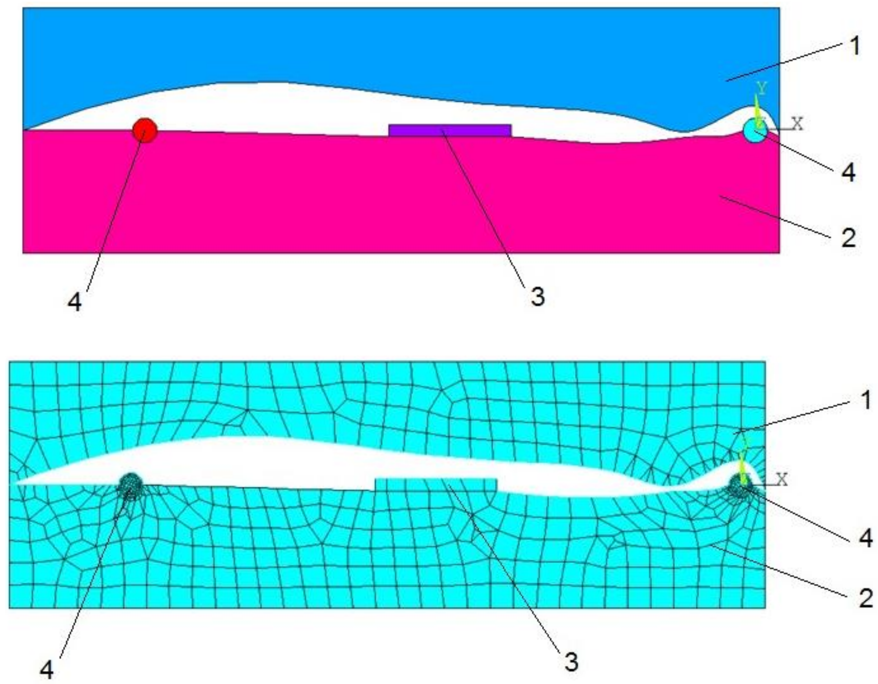


Fig. 2. Design scheme (a) and finite element model (b) of the mesofragment of contact interaction of surfaces of microsize components containing fragment of the copper particle (1), fragment of the plated polymer (2), one CNT (3) and two CNOs (4).

where σ_0 is the principal stress (3 values).

The principal stresses σ_1, σ_2 and σ_3 are designated so that the stress σ_1 is the highest and σ_3 is the lowest.

Equivalent or von Mises stresses σ_e are calculated using the formula

$$\sigma_e = \left(\frac{1}{2}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right]\right)^{\frac{1}{2}}, \tag{2}$$

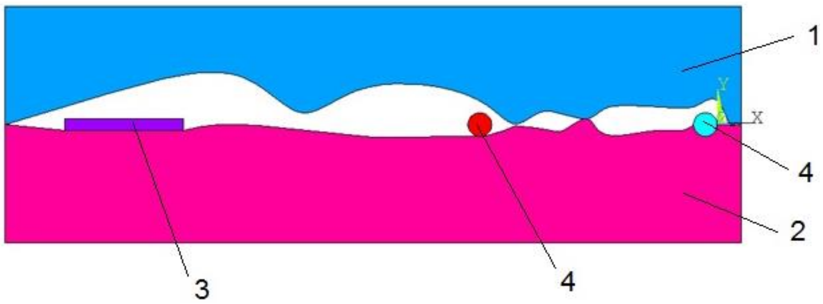
or

$$\sigma_e = \left(\frac{1}{2}\left[(\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + 6\left(\sigma_{xy}^2 + \sigma_{yz}^2 - \sigma_{xz}^2\right)\right]\right)^{\frac{1}{2}}. \tag{3}$$

In supposition that the material is isotropic and linearly elastic, we have for the plane stress state $\sigma_3 = 0$.

To investigate the stress state of the contact interaction zones of powder nanofilled metal-polymer systems, the finite element method implemented in the ANSYS computer program was used. Numerical modeling allows to define and optimize both

(a)



(b)

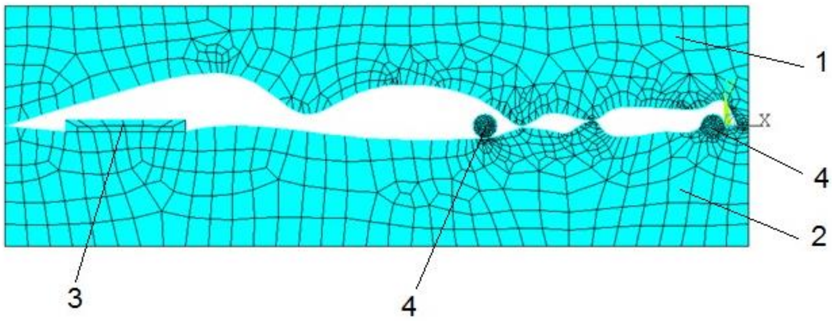


Fig. 3. Design scheme (a) and finite element model (b) of the mesofragment of contact interaction of surfaces of microsize components containing fragment of the copper particle (1), fragment of the plated polymer particle (2), one CNT (3) and two CNOs (4).

strength and thermophysical characteristics of a material, and also to reveal its weak points at the design stage. Partitioning the model into finite elements is done in semi-automatic mode using the ANSYS 14.5 Mesh Tool subroutine. When creating a finite element mesh, it was taken into account that the accuracy of the finite-element method depends on the correct choice of the type and size of the discretization elements. For example, a more frequent grid was used where a large gradient of strains, stresses, and temperatures was expected. At the same time, a rare grid was used in zones with more or less constant stresses or strains, as well as in areas of no particular interest. To solve this problem, a finite element grid of flat quadrangular elements PLANE182 and PLANE223 containing four nodes was created on the copper particles. Each node had two degrees of freedom. The application of these discretization elements turned out to be the most convenient for modeling the nonuniform grid of a flat model. Also in the flat quadrangular element PLANE182 the possibility of plastic deformation is laid. When modeling the process of contact interaction of the initial components of powder materials, special elements TARGE169 and CONTA172 were used, which describe the contact boundary of a plane stress-strain body.

(a)

(b)

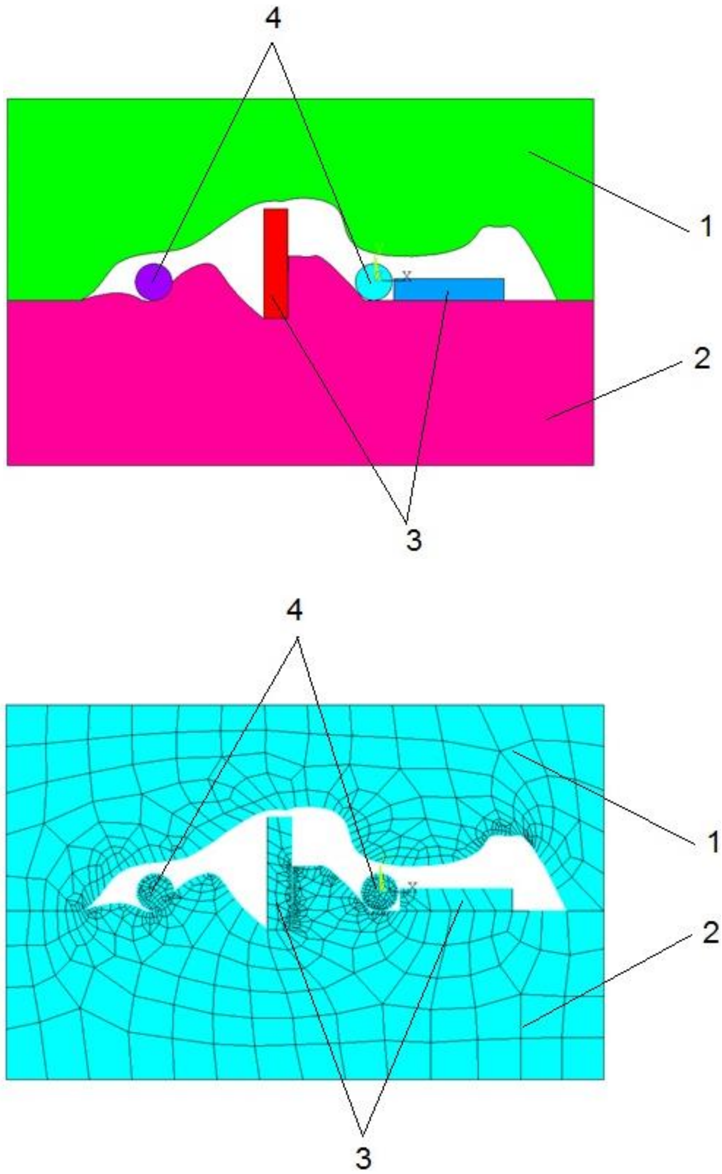


Fig. 4. Design scheme (a) and finite element model (b) of the mesofragment zone of contact interaction of surfaces of microsize components containing fragment of the copper particle (1), fragment of the plated polymer particle (2), two CNTs (3) arranged vertically and horizontally, and two CNOs (4).

3 Investigation of the Influence Of Structure on the Stress State of Nanofilled Metal-Polymer Composites

The influence of structure on the formation of a stress state of wear-resistant materials are studied using the approaches of computer modeling of the flat stress-strains state of mesophragments of the contact interaction of particles of a polycomponent nanofilled metal-polymer powder system, and the patterns of formation of internal stress fields are established.

Analyzing the character of the formation of the stress state of the mesofragment of a powder material containing copper particles of 100 μm in size, one particle of a plated polymer with a size of 150 μm with a thickness of the copper layer of 6 μm can be noted as follows (Fig. 5).

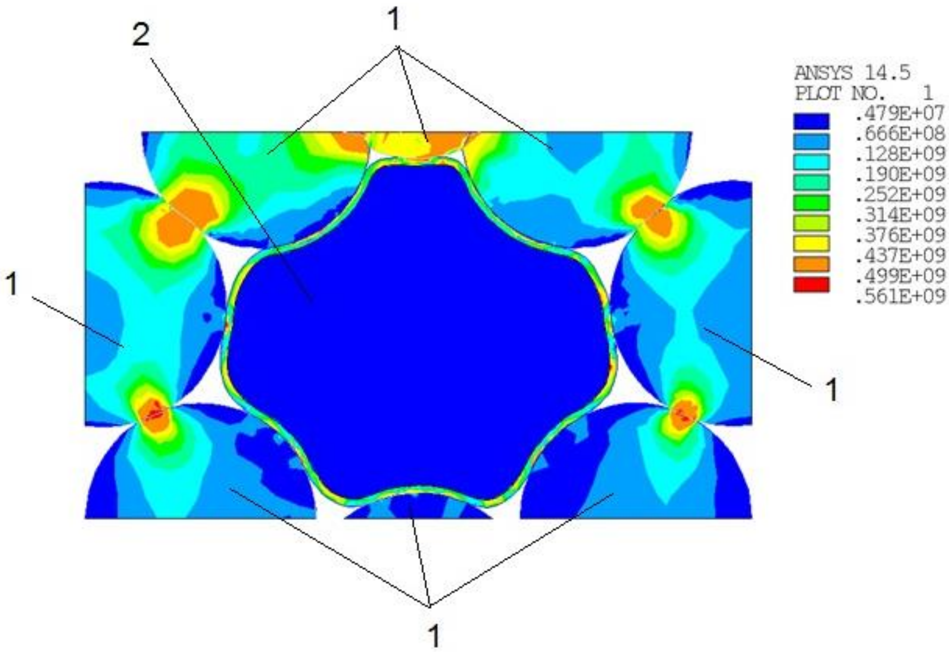


Fig. 5. Distribution of the equivalent Mises stresses in the zone of contact interaction of the components of the powder metal-polymer system containing fragments of copper particles (1), particle of plated polymer (2), CNTs and CNOs located in contact areas of surfaces of microsize components, Pa.

The distribution of equivalent stresses in the micro-dimensional components of the metal-polymer material is heterogeneous. The maximum equivalent stresses occur in contact zone of copper particles and at some points reach a value of 500 MPa. The average value of equivalent stresses in copper particles is in the range from

128 MPa in the lower fragments of copper particles and up to 250 MPa in the upper copper particles. At the same time, the stress in the plated PTFE reaches a yield point equal to 25 MPa, and in some areas exceeds this value. As a result, local compression occurs in some areas of polytetrafluoroethylene plated with a copper shell. The polymer filler is plastically deformed. However, the equivalent stresses in the copper shell of the polymer filler are equal to 190–252 MPa. In some sections of the copper shell, the values of equivalent stresses exceed 300 MPa, but in view of the insignificant size of these sections, it can be stated that this local stress increase does not affect the strength of the copper shell. Analysis of the pattern of stress fields shows that the processes of destruction of component materials in this powder system do not occur. Plastic deformation of copper particles and plated polymer filler is observed in zones of contact interaction of copper particles both with each other and with plated polymer filler.

In studying the consolidation processes of the components of the powder system in the pore space containing a fragment of a copper particle with a size of 100 μm, a fragment of a 150 μm plated polymer particle with a copper layer thickness of 6 μm, one CNT with an inner diameter of 30 nm and an outer diameter of 60 nm disposed horizontally , and two CNOss with a diameter of 100 nm, each of which is located on opposite sides of CNT, we can note the following features of the formation of stress state (Fig. 6). The maximum equivalent stresses occur in the carbon nanostructured filler, the stresses in both the surface layer of the copper particles and the metal-plated polymer filler reach the yield point of copper.

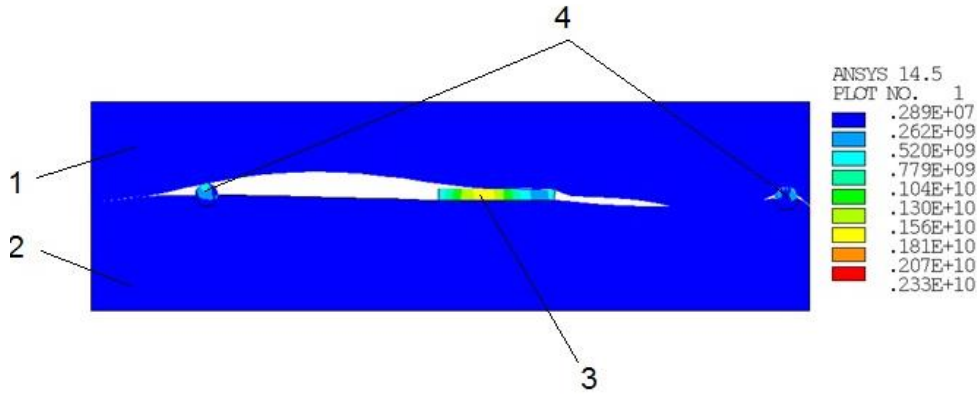


Fig. 6. Distribution of equivalent Mises stresses in the area of contact interaction of surfaces of microsize components of the powder metal-polymer system containing fragment of a copper particle (1), fragment of the plated polymer particle (2), one CNT (3) disposed horizontally, and two CNO (4), each on opposite sides of CNT, Pa.

Upon closer consideration of the CNO located on the left side of the CNT, it is possible to establish the features of the stressed state of the fragment of the powder system (Fig. 7). So the stresses in the surface layers of both the copper particles and the copper shell of the plated polymer filler are 240–250 MPa. The stress distribution pattern in CNO is not homogeneous. Maximum equivalent stresses in CNO occur in the contact zone of a carbon nanostructure with a copper particle. The maximum value of equivalent stresses is 2000–2300 MPa. The average value of these stresses is 500–700 MPa.

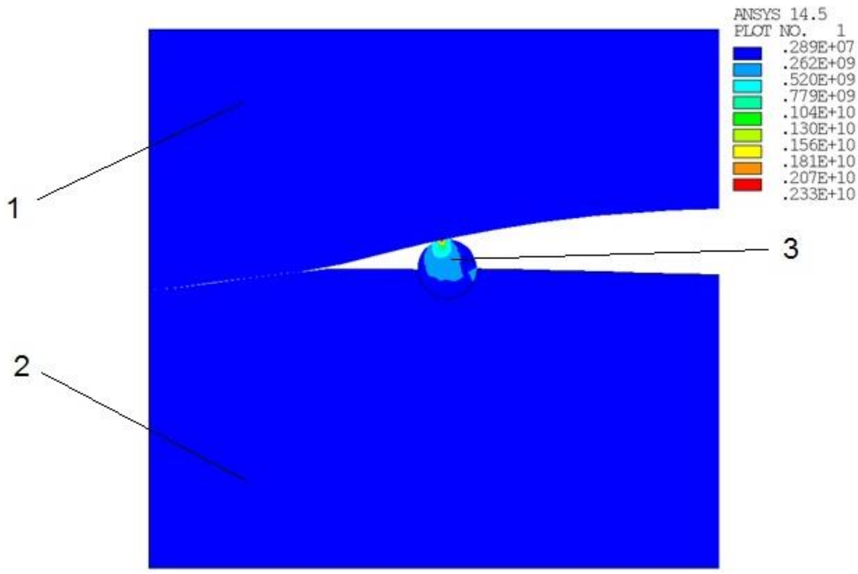


Fig. 7. Enlarged image of the distribution of equivalent Mises stresses in the fragment of the powder metal-polymer system containing fragment of a copper particle (1), fragment of the plated polymer particle (2), CNO (3), Pa.

While considering the pore space of the powder metal-polymer system containing CNT with an inner diameter of 30 nm and an outer diameter of 60 nm and placed horizontally, it was established that the maximum equivalent stresses in CNTs do not exceed 1560 MPa. The average values of equivalent stresses in the nanotube are 780–1000 MPa (Fig. 8).

When considering the fragment of the powder metal-polymer system containing the second CNO located on the right side of the CNT, it was found that the maximum equivalent stresses in a given nanoparticle reach a value of 779 MPa (Fig. 9). The average equivalent stresses are from 400 to 550 MPa.

Investigation of the stress state of the powder system containing a 100 μm copper

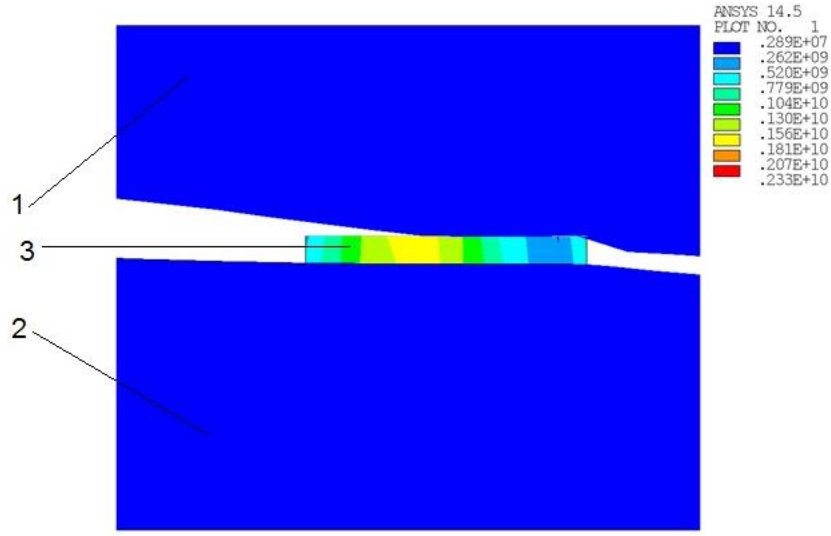


Fig. 8. Enlarged image of the distribution pattern of equivalent Mises stresses in the fragment of the powder metal-polymer system containing fragment of a copper particle (1), fragment of the plated polymer particle (2), CNT (3), located horizontally, Pa.

particle fragment, a fragment of a 150 μm plated polymer particle with a copper layer thickness of 6 μm, one CNT with an internal diameter of 30 nm and an outer diameter of 60 nm disposed horizontally and two CNO with a diameter of 100 nm, located on one side relative to CNT, made it possible to establish that the stresses both in the copper shell of the polymer filler and surface layer of copper particles is 240–250 MPa (Fig. 10). The maximum stresses are observed in the nanostructured filler.

Upon closer consideration of the stressed state of CNT, it should be noted that the average value of equivalent stresses is from 432 to 846 MPa. On some sections of CNT, the values of equivalent stresses reach 1260 MPa (Fig. 11).

Investigation of the distribution of stress fields in CNO located both in the central part of the fragment and on the right side has made it possible to establish that the values of the equivalent stresses in the two nanoparticles differ significantly from each other (Fig. 12).

So the average value of equivalent stresses in CNO located in the central part of the fragment of the powder composite is 846–1260 MPa, while the average value of the equivalent stresses in CNO located on the right side of the fragment of the composite powder is 450–820 MPa. In this case, the maximum value of the stresses arising at one of the points of the nanoparticle located in the central part is 3500 MPa,

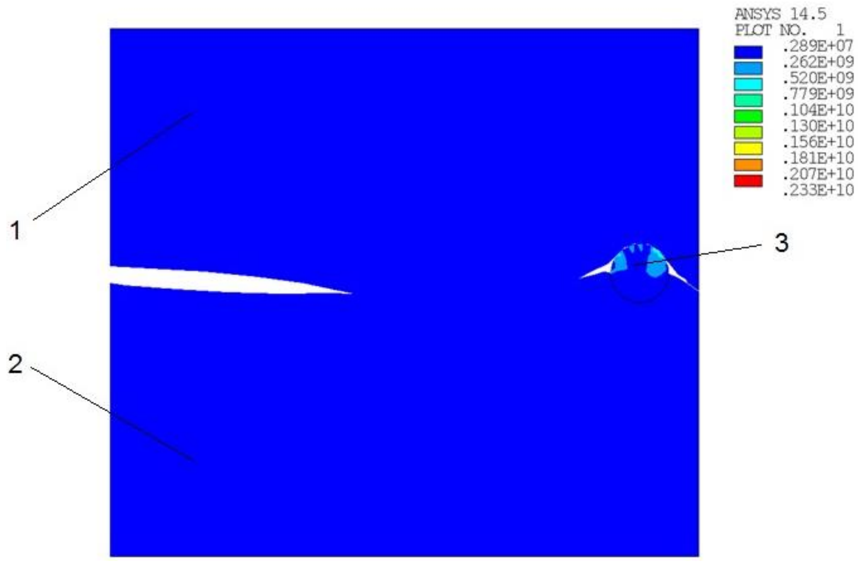


Fig. 9. Enlarged image of the distribution of equivalent Mises stresses in the fragment of the powder metal-polymer system, containing fragment of a copper particle (1), fragment of the plated polymer particle (2), CNO (3), Pa.

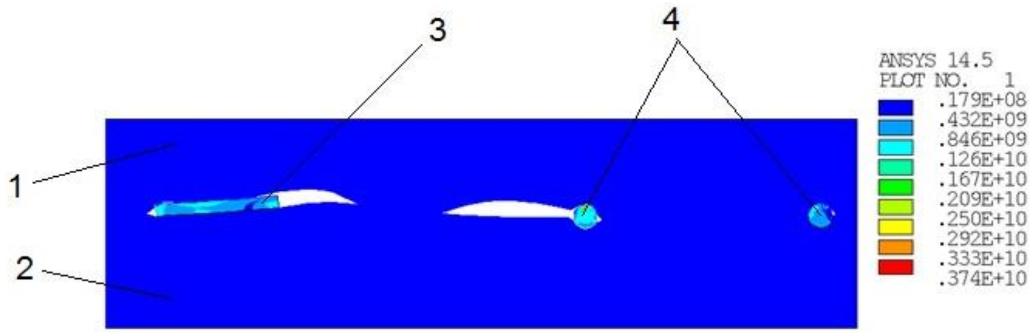


Fig. 10. Distribution of the equivalent Mises stresses in the zone of contact interaction of the surfaces of the microsize components of the powder metal-polymer system containing fragment of the copper particle (1), fragment of the plated polymer particle (2), one CNT (3) disposed horizontally, and two CNO (4) located on one side relative to CNT, Pa.

and the nanoparticle located on the right is 1200 MPa.

Some similarities with the results obtained on the investigated nanosized models have the results obtained in the study of the stress state on a finite-element model containing a fragment of a copper particle with a size of 100 μm, a fragment of a 150

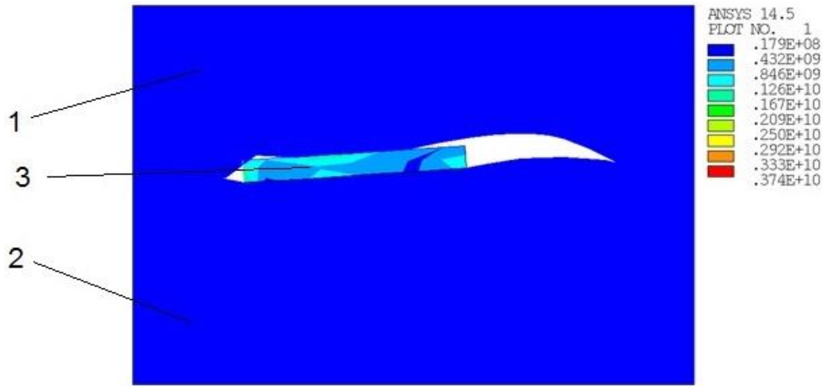


Fig. 11. Enlarged image of the distribution of equivalent Mises stresses in the fragment of the powder metal-polymer system, containing fragment of a copper particle (1), fragment of the plated polymer particle (2), CNT (3), Pa.

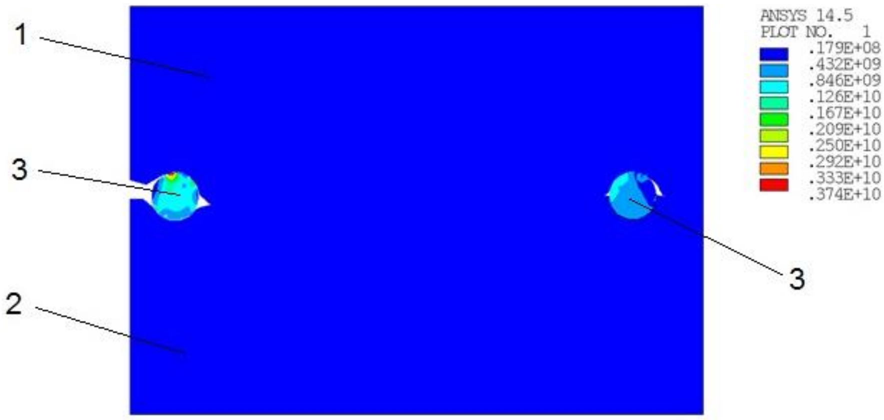


Fig. 12. Enlarged image of the distribution pattern of equivalent Mises stresses in the fragment of the powder metal-polymer system, containing fragment of a copper particle (1), fragment of the plated polymer particle (2), two CNOs (3).

μm plated polymer particle with a copper layer thickness of 6 μm, two CNTs with an internal diameter of 30 nm and an external diameter of 60 nm, located vertically and horizontally, and two CNOs a diameter of 100 nm (Figs. 13 and 14).

At the same time, the stresses in both the surface layer of copper particles and the copper-plating polymer particle do not exceed 230–250 MPa, and the maximum values are equal to 250 MPa. The stresses occurring inside the carbon nanostructures, except for CNTs located vertically also do not exceed 500–600 MPa, which is explained by the initial large porosity. The maximum equivalent stresses reach values

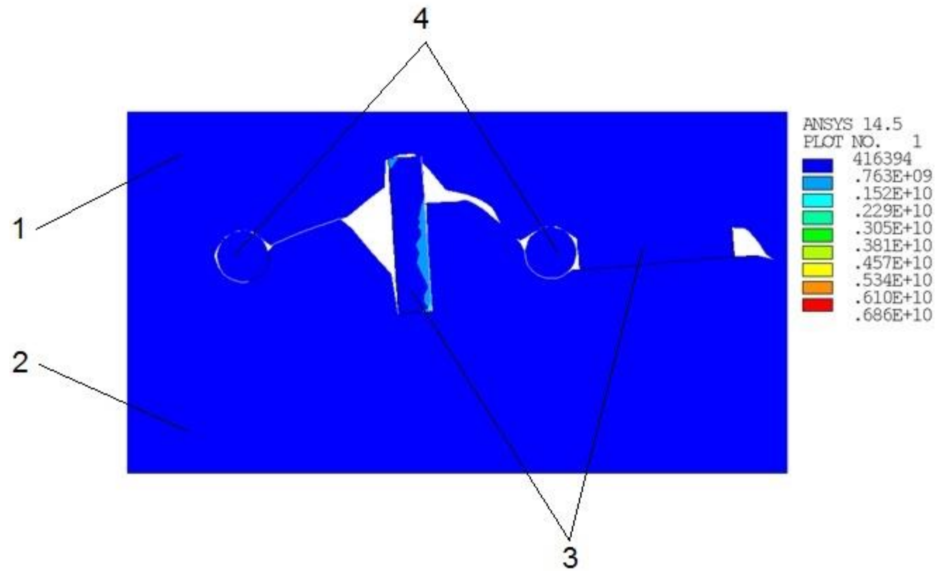


Fig. 13. Distribution of equivalent Mises stresses in the zone of contact interaction of surfaces of micrometer components of the powder metal-polymer system containing fragment of the copper particle (1), fragment of the plated polymer particle (2), two CNTs (3) arranged vertically and horizontally, and two CNOs (4), Pa.

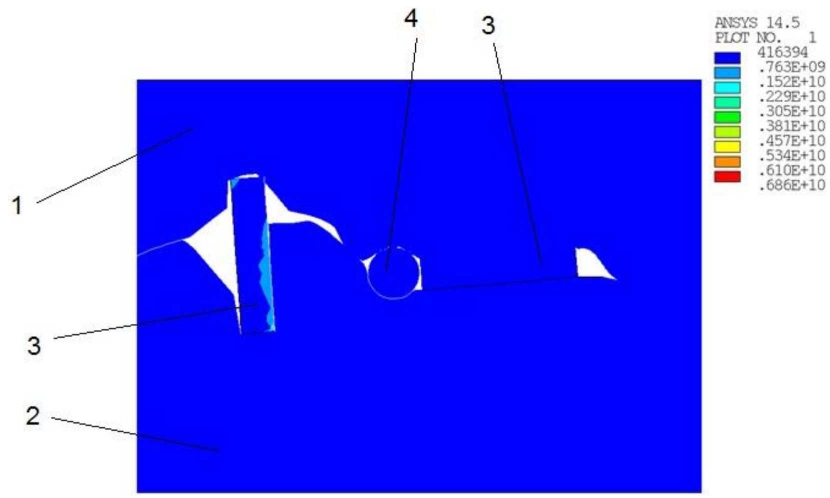


Fig. 14. Enlarged image of the distribution of equivalent Mises stresses in the fragment of the powder metal-polymer system, containing fragment of a copper particle (1), fragment of the plated polymer particle (2), two CNTs (3), CNO (4), Pa.

of 1000 MPa, which does not affect their elastic work, but makes it difficult for the metal to flow when the stresses exceed the yield point.

Based on the obtained results of the research, it can be noted that the stresses arising in CNTs and CNOs during the technological process of producing powdered nanofilled composite materials do not reach the ultimate strength, which indicates their elastic work. As a result of this effect, CNTs and CNOs are not subjected to critical deformations or fractures.

It should be noted that after reaching the stresses in the copper and plated polymer particles that exceed the yield strength of the material, they are subjected to plastic deformation and stress relaxation. The particle material tends to fill the pore space. As a consequence, the pore size is reduced and the density of the material is increased. At the same time, increasing the dimensions of the contact areas on the surface of the particles leads to a decrease in the contact resistance between the particles.

4 Conclusion

A technique, design schemes and adaptive finite element models for estimating the stress state of the components of the "microdispersed metal – metal-plated polymer – carbon nanostructure" powder systems with the use of computer modeling approaches are developed.

In the course of the research, a general picture of the stress state of a multicomponent powder metal-polymer material containing carbon nanostructures in the form of carbon nanotubes and carbon nano-onions was obtained. The analysis of the results of the investigations made it possible to obtain new data on the nature of the stress distribution, to reveal the most loaded zones of the powder systems, including microsize copper particles, plated PTFE particles and carbon nanostructures at electrocontact sintering on the initial components.

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