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Geometric modeling of the microstructure of the surface based on the theory

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Annotation. The microstructure of the surface is an important characteristic associated with properties such as microhardness, wear resistance, fatigue strength, coefficient of friction, thermal and power loads, aero and gas dynamic resistances, etc. Solving problems of gas dynamics in the absence of data on the real structure of the surface with which gas molecules interact makes it difficult to formulate boundary conditions for calculation the transfer of energy and momentum during the flow of bodies .

Keywords: surface, resistance, problems, structure, calculation, nano, coatings, modeling, geometry.

Mathematical models of surfaces of metals, alloys, and nano-coatings used in modeling physical processes such as scattering of light fields, laminar-turbulent transition, or interaction of gas molecules with a surface, contain in most cases strong simplifications. The assumption of surface smoothness leads to a number of physically unfounded conclusions, because it has been experimentally proven that the microstructure of the surface at the nanometer and atomic levels has a significant impact on the calculation results. As studies in recent years have shown, an effective way to model rough (non-differentiable) surfaces for solving problems of gas dynamics is to use fractal geometry methods that take into account roughness at the micro and nano levels and are based on the validity of the statement that the structure of a natural surface is equally fractal at all levels.

The task of constructing a geometric model of a microsurface has both theoretical and applied aspects. As you know, the physical processes that occur when atoms and molecules of a gas interact with a surface are very complex. Therefore, a theoretically justified interpretation of the results of ground-based experimental testing of fragments of aircraft is required. The applied value is determined by the need to optimize flow diagnostics tools in high-enthalpy installations in which thermal loading acting on aircraft during flight occurs, as well as technological processes for creating heat-shielding materials and coatings for rocket and space technology (RCT) products.

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1. The choice of the fractal dimension parameter as an effective characteristic of the development of the micro- and nanostructure of a rough surface is justified. Fractal dimension equivalently replaces a whole range of amplitude and step characteristics of surface roughness. The use of the fractal dimension parameter is proposed in relation to the problems of heat transfer in high-enthalpy nonequilibrium flows

2. Improved algorithms for modeling the microstructure of the surface by introducing a geometrically ordering component, which made it possible to effectively approximate the roughness of the surface with irregularities at the micro and nano levels simultaneously. The advantage of constructing fractal surfaces over classical models of non-smooth shapes is the completeness of the description of the surface geometry.

3. The possibility of using fractal surface models to determine the properties of heat-shielding materials of aviation and rocket and space technology products is investigated. It has been experimentally confirmed that fractal models make it possible to simplify and reduce the cost of calculating the interaction of gas with a wall by eliminating the stage of direct investigation of the geometric characteristics of a real surface.

The fractal surface model obtained using the proposed construction algorithms is designed to refine experimental data on the catalytic activity of thermal protection materials and transfer these data to the conditions of full-scale aircraft flight in the atmosphere. The practical significance of the study is the results obtained by modeling non-differentiable shapes for the needs of gas dynamics, including to reduce the measurement error of the enthalpy of gas deceleration in high-temperature installations and stands through the use of highly catalytic (metal) coatings with a highly developed structure of the surface layer. It has been experimentally proved that physical quantities such as the measured heat flux and the specular reflection coefficient are influenced by the micro- and nano geometry of the surface.

The practical application of the work was the introduction of the research results into the process of experimental testing of the structural elements of the docking unit of the apparatus in terms of interpreting the effect of reducing convective heat flows on protruding elements coated with high-temperature paint. Validity and reliability. The research was carried out taking into account the current state of knowledge of the problem of the influence of the geometric properties of micro- and nano-roughness of materials on the physico-chemical processes of their flow with a high-enthalpy gas. The

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construction of a mathematical model of a rough surface using fractal principles is theoretically justified, experimentally confirmed and is the basis for the study of the influence of the geometry of the micro- and nanostructure of the surface on the physical properties of the materials under study. Data on the geometry of the micro- and nanostructure of the surface of the studied materials were obtained using a scanning tunneling microscope, for calibration of which a test surface with known relief parameters was used.

A review of the geometric characteristics of the surface that affect the results of ground-based testing of heat-protective materials is carried out. It is shown that the scanning tunneling microscope (STM) most fully satisfies the conditions of non-contact investigation of the spatial microstructure of the surface layer. The theoretical and applied issues of studying the geometry of the surface at the micro and nano levels and the problem of taking into account the roughness of the surface with irregularities at the micro and nano levels at the same time are studied. It has been found out that in recent years there has been a tendency to switch from working with a two-dimensional model to a three-dimensional model with a simultaneous reduction in the number of parameters taken into account without loss in their information completeness.

It is established that the fractal dimension parameter replaces the set of classical roughness parameters. It is proved that the fractal dimension does not depend on the magnification scale. This indicates that the geometry of real surfaces is close to fractal. The second chapter examines existing approaches to creating models of non-differentiable shapes and describes improved algorithms based on fractal theory for modeling surface microstructure. In his work, de Carpentier describes the creation of a surface model using Brownian motion, the geometric meaning of which is to project sections of a linear surface onto a plane. At each iteration, the elevation of the resulting "fragments" changes.

However, in this work it was found that when constructing a microsurface model in this way, after 48 iterations and adding filtering in accordance with the normal law of probability distribution, the value of the fractal dimension corresponds more to the dimension of the plane than to the "highly developed" surface. This led to the need to improve the algorithm by using a cyclic surface instead of a linear surface with a parallelism plane.

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The design task was to obtain a fractal surface similar to the surface of a copper alloy having D = 2.47. Thus, the required value of D was achieved only at 186 iterations. Volumetric visualization of the image of the micro surface of the copper alloy.

However, the most interesting modifications of the method were algorithms based on the use of projections of the torus section and the torus node (Fig. 1)

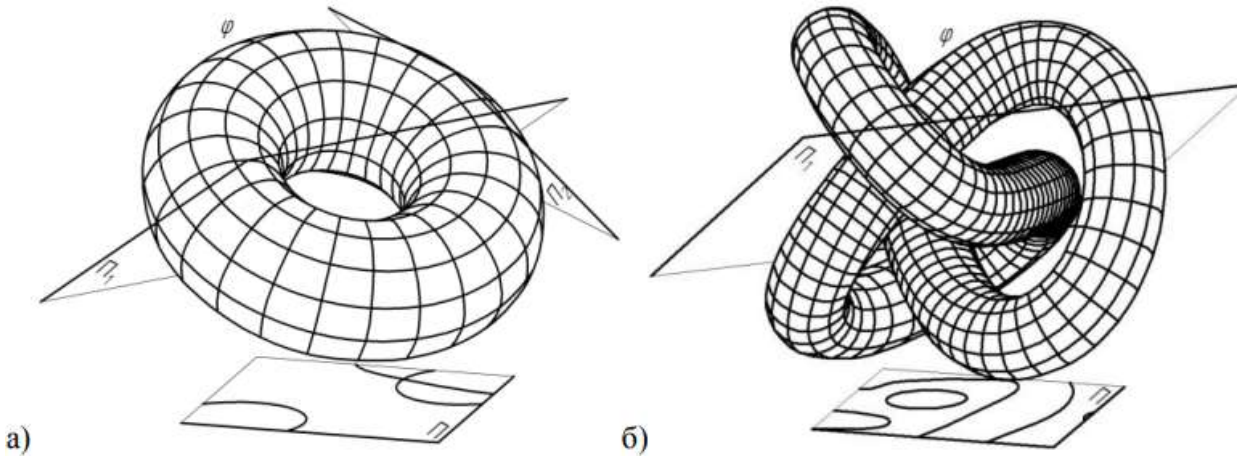

Fig. 1

The results of the algorithms for projecting torus sections and torus node sections also lead to the construction of a fractal surface with dimension D≈2.47.

It should be noted that the number of iterations to achieve the fractal dimension D≈2.47 for each algorithm is a quantitative characteristic.

The shaded area indicates the optimal ratio of the number of variables taking a random value in an iteration to ensure a minimum of the iterations themselves. To verify the simulation results and calculate the fractal dimension, the algorithms of construction and calculation were tested. This revealed a correspondence between the theoretical and calculated values.

The verification of the calculation method based on the calculation of the fractal dimension of the surface for simple fractal surfaces has a good correspondence with the theoretical results. It should be noted that a comparison of the real micro-surface of a copper alloy and an artificial fractal surface obtained using an improved Brownian motion algorithm only on the basis of equality of their fractal dimension D would look incorrect. Therefore, a comprehensive calculation of the roughness characteristics was

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carried out in accordance with: – the height characteristics of the profile (Ra, Rz, Rmax); – the step characteristics of the profile (Sm, S); – the parameter of the relative reference length of the profile (tp).

It is established that the fractal dimension parameter, calculated for a local surface area by the cubic dimension method, replaces a whole complex of amplitude and step parameters of the surface profile. Fractal dimension, as a measure of the development of the structure of the surface layer, 17 correctly describes the geometric characteristics of roughness and harmoniously fits into the calculations of heat transfer in high-enthalpy nonequilibrium flows, which allows us to solve the problem of the influence of microstructure on the speed of heterogeneous processes occurring on the surface of a heat-shielding material.

Algorithms have been improved to build a model approximating the roughness parameters at the micro and nano levels simultaneously. The introduction of a geometrically ordering component in the iterative process in the form of linear and cyclic surfaces with a plane of parallelism made it possible to reduce the number of iterations to achieve the necessary values of fractional dimension by almost half. By means of verification of modeling methods and calculation of fractal dimension, it is established that the fractal model qualitatively describes the roughness parameters of a real surface.

Numerical simulation of the interaction of an incoming atom with atoms of the crystal lattice of the surface by the PSM method shows that the average number of collisions is proportional to the surface area. A formula is derived to determine the relationship between the fractal dimension of the surface and the average number of multiple reflections of a molecule from the surface.

It has been experimentally confirmed that the heat flow in chemically nonequilibrium dissociated gases is influenced by the catalytic properties of the surface, which depend both on the chemical composition of the material and on the structure of the surface layer.

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