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Computer Modeling of Technological Processes

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Abstract: *The article is devoted to the developments of authors in the field of technological processes computer simulation and especially ultrasonic flattening, plasma spraying and heat treatment. The proposed conception of integrate simulation is considered. It is based on comprehensive description of physical processes influencing on quality of produced parts, imitation approach and application of ex pert systems elements. The developed mathematical models, software and further developments per spective are discussed. In the article provides an overview of the authors ' developments in the field of computer modeling of technological processes, in particular, the processes of ultrasonic flattening of tapes, plasma deposition of coatings and heat treatment. The proposed concept of complex modeling is presented, which is based on an end-to-end description of physical processes that affect the quality of manufactured products, a simulation approach to modeling, and the use of elements of expert systems. The developed mathematical models are discussed. Models, software packages and prospects for further development of research in this area.*

Keywords – computer modeling, ultrasound, plasma technologies, heat treatment.

1.Introduction

In currently, due to the rapid moral aging of products (especially in the field of electronic and computer technology), it is of great importance to reduce the time of their deposition in production. Therefore, leading companies are increasingly using flexible production systems, integrated computer manufacturing (CIM - Computer Integrated Manufacturing), which are based on automation of the entire product life cycle, starting from their development and ending with operation and disposal [1].

Automation of the stages of scientific research and technological preparation of production is of great importance for the practical implementation of the CIM concept (the creation of automated research systems (ASSR) - automated systems of scientific research, as 11111 - automated systems of technological preparation of production). In addition, due to the expensive cost of materials, research and technological equipment, full-scale study of various processes in laboratory conditions is not always possible and in many cases is associated with significant material and monetary costs. This problem is especially relevant in the study and development of fast-flowing processes associated with electro-physical methods of processing materials at high temperatures and ambient pressures. For example, in the case of plasma deposition of coatings, the temperature of the plasma jet can vary in the range of 2000-15000 K, the velocity up to 800 m/s, which requires a unique expensive aperture for experimental studies [1, 2].

These problems can be solved with the help of modern methods of computer modeling, which, with minimal time and material resources, allow you to study and investigate various processes, optimize them with access to specific design issues of the products themselves, develop technological processes, etc. appropriate organization and technical equipment — for the training of control programs and automated production of products using flexible production systems [1-4].

Over the past 15 years, the laboratory of computer modeling of technological processes of the Department of Electronic Engineering and Technology of BSUIR has been conducting research and development in the field of computer modeling of technological processes, in particular, the ultrasonic method for manufacturing tapes from refractory metals and alloys for MHP, plasma deposition of coatings, and heat treatment of metal parts [1-8].
In this article presents an overview of the developed mathematical models and software tools that implement them.

2. An integrated approach to the modeling of technological processes

The basis of these developments is an integrated approach to modeling technological processes, the main provisions of which are [6, 7]: end-to-end mathematical description of all the main stages and processes in accordance with the logical sequence of their flow, taking into account the dependence of the properties of materials on the conditions of their processing (temperature, pressure, etc.);

implementation of mathematical methods and software tools for solving both direct and inverse modeling problems;

solving problems of optimization of the studied technological process or design by a given objective function;

introduction of elements of expert systems for analysis of research results and selection of the most optimal modes of the studied processes into the software complexes;

creation of automated process control systems based on modeling software tools, as well as automated equipment with flexible software management of the equipment with flexible software control.

To explain the concept described above, we will consider the features of its application to specific thermos-physical and dynamic processes occurring at various stages of plasma deposition of coatings [6].

Prerequisites for the organization of complex modeling of these processes are the ability to transfer data from one stage to another and the commonality of their structure. Based on this, the input data for the plasma jet generation model will be the design parameters of plasma torches, electrical characteristics, composition and mass flow rate of the plasma-forming gas, and data on the temperature dependence of properties. The output of this model should be a distribution of temperature and velocity in an unloaded plasma jet in the area from the introduction of particles into the plasma jet to the base. These data will be input data for the model of the 2nd stage of the process, along with information about the mass flow rate of the sprayed powder, its size and properties, mass flow rate, composition and properties of the transport gas.

The output of the plasma jet model will be an array of data on the time distribution
и space of temperature and velocity of particles and plasma-forming gas. In addition, the input data for the 3rd stage of the process will be the configuration, the base material and its properties, the heat sink to the mounting devices or forced cooling characteristics, the ambient temperature, the thickness of the coating to be sprayed and the material properties, the speed and the law of movement of the spray gun.

Results of modeling the 3rd stage of the process: information about the nature of deformation of molten powder particles upon impact with the substrate; the shape, size and coordinates of the particle hitting a certain point of the substrate; surface roughness of the coating, pore content; distribution of temperature and residual stresses in the coating-substrate system; energy or strength of adhesion of the coating to the substrate.

Complex modeling implements a scheme for end-to-end data transfer from one model (process stage) to another and their dynamic change during calculations. Information that is common to all modeling stages can be stored in a database, a special file, or in RAM and used by each model as needed. – STE. The database can also contain the results of intermediate calculations of all stages of the process, which allows you to independently study a particular stage using data from previous calculations, or the required information is entered by the user from the keyboard.

The most promising mathematical methods of the description considered above processes of plasma spraying of coatings is the so-called "computational fluid dynamics" (Computational Fluid Dynamics (CFD)), based on the solution of equations Navier – Stokes equations the complete formulation (modeling the plasma jet) and the finite element method (simulation of the system "coating-basis") [6].

As noted above, the developed models should be focused on their subsequent practical implementation in the form of software complexes for a certain class of computer technology that is practically used in scientific research and production, as well as take into account the prospects for its further development.

3. Modeling of ultrasonic micro-plastic deformation of metals and alloys

The processes of ultrasonic micro-plastic deformation (UMD) (ultrasonic flattening of tapes for M ill parts) [2], ultrasonic winding of LEV spirals [3], manufacturing of reed switches contact parts [3], developed at BSUIR, have found wide practical application in the technology of electronic equipment products. In the studies conducted by the authors [2, 3], it is shown that the most effective direction for further development of the theory and practice of these processes is the use of computer modeling methods. In the works [2, 3], General regularities are established and the concept and scheme of complex modeling of methods for forming structural elements of electronic devices based on the use of ultrasound are proposed. The concept is based on the use of the principles of end-to-end data transmission, a common database of properties of substances involved in the studied processes, conveyor methods for their processing, and taking into account the temperature dependence of the properties of materials. Based on the proposed concept, interrelated mathematical models of all stages of DMD processes are developed.

To mathematically describe the heating of metal before deformation and heat transfer in the metal-tool system, a model is developed based on the application of the theory of the finite element method, which describes the dynamics of temperature changes in the deformed metal during its heating by infrared radiation and direct current transmission, as well as during interaction with processing tools.

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The temperature field in the problem under consideration is described by the heat conduction equation, which is a special case of the Navier – Stokes equation, which can be represented in matrix form as [9]:

$$\left([K]+\frac{2}{\Delta\tau}[C]\right)\{T\}_1=\left(\frac{2}{\Delta\tau}[C]-[K]\right)\{T\}_0-2\{F\}^*-2\mathrm{V}[C]\frac{\Delta T}{\Delta x}, \qquad (1)$$

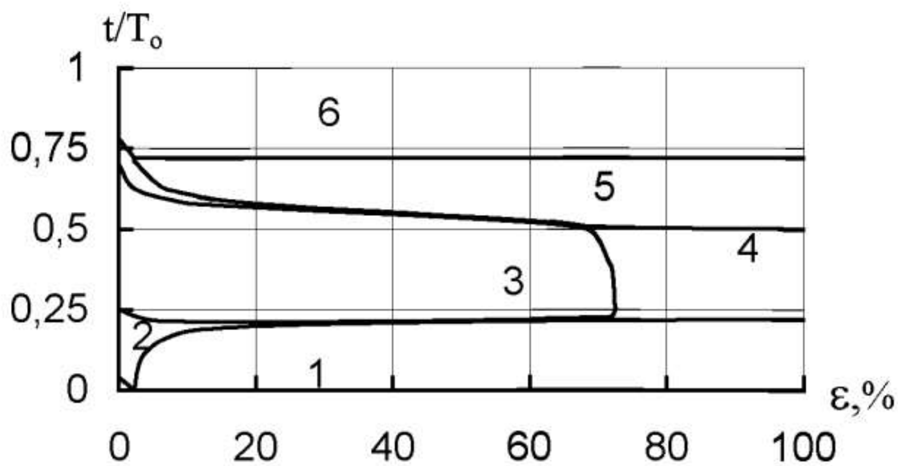
where And $[C]$- the matrix of heat capacity; $[K]-$ is the matrix thermal conductivity; $\{T\}$ vector of nodal points temperatures; $\{F\}-$ load vector.

The numerical solution of the system of equations (1) allows us to study the dynamics of heating and cooling of metal depending on the technological modes of processing, which is necessary for controlling recrystallization processes and, accordingly, the properties of the deformable metal.

In order to analyze the kinematics and dynamics of the DMD process, a model has been developed that takes into account the elastic properties of the deformation zone and the propagation of a longitudinal elastic wave in the work-piece to be processed. This approach made it possible to distinguish two main modes of interaction between metal and tools (with contact break — ultrasonic forging mode and without contact break — ultrasonic drawing mode) and six different phases of the elementary cycle of the DMD: phase I-elastic unloading of a stationary billet; phase II-elastic unloading.
phase III — separate movement of tools and the work-piece; phase IV-elastic compression with sliding; phase V-elastic compression of a stationary work-piece; phase VI-plastic metal precipitation.

An iterative numerical algorithm for calculating the duration of each phase of interaction and the force characteristics of processing is developed based on the basic principles of the theory of vibrational systems and the physics of a solid deformable body [2, 3].

B as a result of the analysis of the elastic characteristics of the deformation process, it is established for the first time that the main contribution to the total value of elastic deformation is made by the elastic deformation of tools. It, in turn, consists of deflection of surfaces and volumetric deformation of tools. It is shown that the value of surface deflection is determined by the contact stress distribution. The volumetric deformation of tools does not depend on the law of distribution of contact stresses over the surface and is determined only by the pressure force of the work-piece, so a model based on the volumetric rigidity of tools, the value of which is determined experimentally, is used to calculate it. The results of modeling kinematic and dynamic characteristics in relation to the ultrasonic flattening process are shown in Fig. 1.



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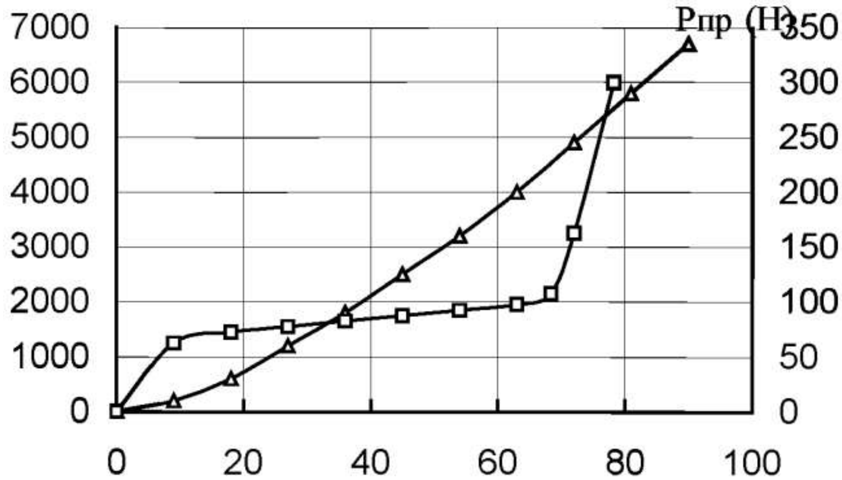

Fig. 1. Dependence of the parameters of the UD kinematics *(a),* flattening forces (R||l), and stretching forces (RPR) (b) on the degree of metal deformation per pass.

When developing a physical and mathematical model of the process of ultrasonic winding of LBW tape spirals, the features of the interaction of tools with the work-piece on a rotating core are taken into account [10].

The mathematical model of metal shape change in the course of UD is developed based on the peculiarities of metal precipitation with ultrasonic instruments. It is established that the studied process (in comparison with traditional methods of metal processing by pressure) is characterized by a higher metal drawing, which is explained by the presence of tensile stresses in the metal surface.

The deformation process and the more complex shape of the deforming part of the tools. The ratio between the expansion and extension deformations of the belt is primarily determined by the ratio of the length and width of the contact area of the tools.

Based on the hypothesis of equality of absolute increments of the length and width of the work-piece in the elementary act of precipitation, taking into account the results of experimental studies, analytical expressions are obtained for calculating the width of the tape and the size of the contact pad during ultrasonic flattening of work-pieces in the form of a round wire and a rectangular tape with tools with an arbitrary approach angle and width of the calibration pad.

The analysis of the developed mathematical models has shown that the determining parameter of the processes of ultrasonic vibration is the ratio of the amplitude of ultrasonic vibrations and the value of elastic deformation. If the range of vibrations is less than the total elastic deformation, then the process of ultrasonic forging switches from the ultrasonic forging mode to the drawing mode, which causes a sharp increase in the power characteristics of processing (see Fig. 1) and degrades the quality of the manufactured tapes. Therefore, in [2, 3] conducted a thorough physical and mathematical analysis of practical operation of the ultrasonic vibrating systems used in UMD, in re the result, which is based on the method of harmonic linearization of the generalized numerical model of a loaded vibrating system and the relation between the oscillation amplitude in the steady state, the dynamic stiffness of the oscillating system and external force action in the following form [11]:

$$A = \frac{A_0 W(j\omega)}{W(j\omega)+k+j\omega b}, \qquad (2)$$

where K and b are harmonic linearization coefficients; $W(j\omega)$ is the dynamic stiffness of the system.

It is established that the force action on the oscillatory system leads to an increase in its resonant frequency and a decrease in the amplitude of vibrations (Fig. 2). it is shown That to calculate the amplitude of steady-state vibrations in the processes of DMA, it is necessary to determine the generalized parameter of the oscillatory system-dynamic stiffness, which is calculated using the run-through method.

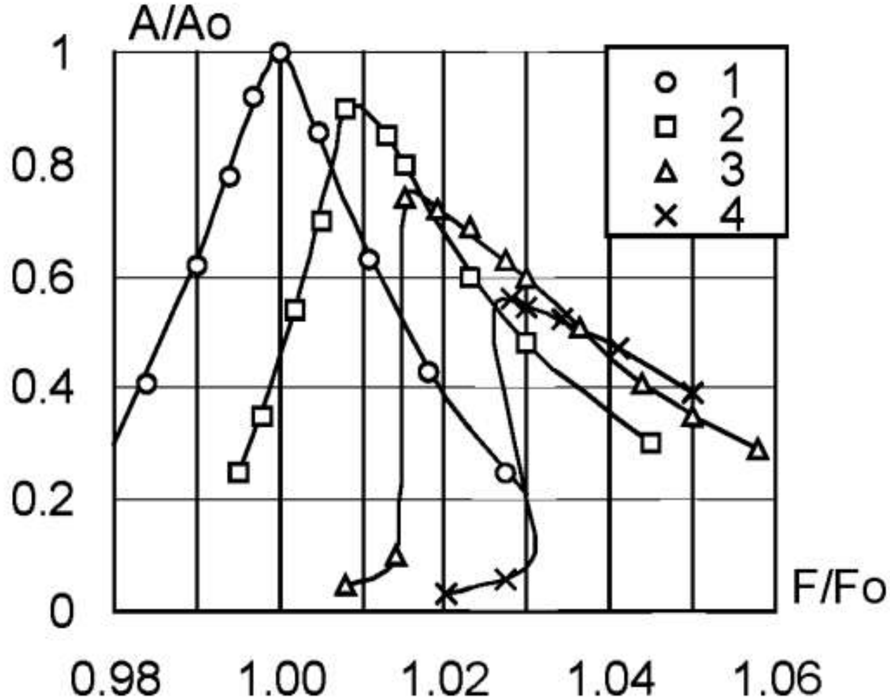

Fig. 2. Amplitude-frequency characteristics of an oscillatory system under load:

1-P=50; 2 — 100; *3* — 200; *4* — 300N

To account for internal friction losses in an oscillatory system, the Feucht-Kelvin model of viscoelastic behavior is used, which is used to derive the equation for the amplitude function:

$$ES\frac{d^2u}{dz^2}(1+nj\omega)+m_0\omega^2u=0\,, \qquad (3)$$

$u(z)$ is a complex amplitude function that characterizes the amplitude and phase of vibrations in the cross-section with the coordinate z; η the coefficient of internal friction; S *is the cross*-sectional area of the rod.

The developed mathematical model makes it possible to analyze and calculate the resonant characteristics of oscillatory systems of arbitrary cross-section depending on the technological parameters of the UMD process. Based on the results of the conducted research, recommendations are formulated for the design of specific rod oscillatory systems used in the developed equipment.

C using the finite element method, an elastic-plastic model of the stress-strain state (SSS) of a metal in the processes of mechanical deformation is developed, based on the analysis of deformations under cyclic loading using the variable stiffness method and an iterative calculation scheme [2]. As applied to the process of ultrasonic winding of tape spirals, the analysis of metal VAT was carried out using the principle of independence of the action of the deforming force, bending moment and counter-tension force [10].

The developed mathematical models are practically implemented as part of the ultrasound software package, which makes it possible to conduct computer studies of heating of the deformable metal, kinematic and force parameters of processing, operating modes of the ultrasonic oscillatory system, geometric characteristics of the manufactured belts, and their stress-strain state during processing in a single cycle [2].

Comparison of the simulation results with experimental data indicates the adequacy of the developed models to the real process, which allows them to optimize the design solutions and technological parameters of the processes of manufacturing structural elements of electronic devices using the UMD method. Ultrasonic technological processes and equipment developed with the use of computer modeling have been put into production at a number of enterprises of the electronic industry of the Russian Federation.

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4. Modeling of plasma deposition of coatings

The analysis of thermos-physical and dynamic processes occurring during plasma sputtering showed their complete correlation with the processes of UD, which made it possible to develop mathematical models according to the General scheme in accordance with the concept of complex modeling. In this paper, for the first time in the theory of plasma sputtering, a simulation model of the plasma sputtering process is proposed and practically implemented, which is based on modeling the behavior of powder particles in a plasma jet and when interacting with the base in accordance with the physical and logical sequence of the processes occurring. A statistical approach to describing the interaction of powder particles with a plasma jet is proposed, which takes into account the distribution of powder particles over the diameter, cross-section of the injector, and the random nature of the initial injection rate [8]. A 3D mathematical model of acceleration and heating of powder particles in a plasma jet is developed, which is distinguished by taking into account the random characteristics of the deposition process, the presence of a temperature gradient across the particle cross section and its evaporation at normal and low pressures, taking into account the temperature dependence of the properties of materials and plasma-forming gases. A model for forming a coating profile on a single passage of a plasma torch is proposed, which differs from the known ones by taking into account the trajectory of the plasma torch and random characteristics of the deposition process.

The laws of the molecular kinetic theory of gases and numerical methods for describing the plasma jet were used to solve similar problems in relation to the conditions of rarefied media, which made it possible to develop algorithms for calculating the dynamics of temperature changes

и particle velocities in a plasma jet depend on the technological parameters of sputtering [12].

Based on the theory of continuous media proposed technique for three-dimensional fashion profiling of the interaction of powder particles with the base, which includes mathematical description of velocity, pressure, temperature, and stress fields, taking into account the crystallization process and the movement of the free surface of a molten particle, which makes it possible to bring the model of formation of the structure of plasma coatings closer to real deposition conditions. This problem is solved on the basis of the Navier-Stokes equation in the Bussynesk approximation [13].

Heat transfer in the particle-base system is described by solving a 2-dimensional heat transfer problem, taking into account hydrodynamic processes in the molten particle and pressure forces. In contrast to previously existing models of particle interaction base (V. V. Kudinov, O. P. Solonenko, F. Fukanuma etal.) in the developed model offers a comprehensive consideration in the mathematical level of interrelated physician processes, such as the impact of particles on a solid base, its spreading, given the crystal of implementation and the determination of the free surface of the melt based on the use of liquid phase volume (F) ($F = l$ in the presence of a liquid phase and $F = 0$ in its absence):

$$\frac{\partial F}{\partial t} + (\vec{V}\nabla)F = 0 \qquad (4)$$

Since the main contribution to the formation of continuity defects in plasma coatings (cracks, delaminations, etc.) is made by stresses of the first kind, interrelated models of heat transfer and the formation of temperature stresses in the coating-base system in one-dimensional and three-dimensional descriptions are developed for their analysis.

The developed models are practically implemented in the Plasma software package, which provides end-to-end modeling of the main thermos-physical and dynamic processes that affect the qualitative characteristics of plasma coatings (Fig.

For a three-dimensional description of the problem, we use the finite element theory implemented in the MARC software package, which is adapted to the conditions of plasma deposition, dynamic changes in the coating thickness, the formation of lamellae, pores, and real dimensions of sprayed parts [15]. To take into account the influence of microstructure on the properties of a hypothetical continuous material, which is a coating, in finite-element VAT calculations of the coating-base system, two families of homogenization algorithms were developed for the first time, which differ in different assumptions about the behavior of the medium in the computational domain [16]. The use of homogenization as a step that precedes the calculation using the finite element method makes it possible to more accurately predict the behavior of various plasma coatings under thermal and mechanical loads.

Based on the proposed concept of end-to-end modeling of plasma coating deposition processes, an integrated technological complex has been developed for the study and practical implementation of plasma coating deposition processes used in electronic and other branches of technology [17]. The complex includes the developed original software and mathematical software, a set of measuring equipment, and tools for computer control of sputtering modes. The practical application of the complex in the experimental production of the R & d Institute (Minsk) makes it possible to reduce the time required for technological preparation of new products, reduce the cost of materials and gases required for research, and improve the working conditions of production engineers.

5. Modeling of heat treatment processes

The developed complex mathematical model of heat treatment processes is based on the provisions of maximum consideration when modeling thermos-physical and dynamic processes that determine the process flow and properties of manufactured parts (stress-strain state, hardness distribution, phase composition, etc.). in Addition, the principle of geometric correspondence of the model to real detail was adopted. that is, the use of three-dimensional modeling [18].

An enlarged logical scheme of complex modeling and the composition of developed models that take into account all stages of the process, end-to-end data transmission, and interaction with the material properties database (DB) are shown in Fig. 4. the Developed models are implemented as part of the software package for modeling and optimizing the processes of heat treatment of parts Thermo-Sim [19]. which is created using the most modern programming technologies, information processing and 3D visualization, and database technologies.

4. the complex consists of three main modules: a preprocessor, a processor, and a postprocessor. The task of the preprocessor is to prepare the input information for the simulation, namely the job:

model geometries (import files for exchanging drawing and graphic data, checking the closeness of surfaces, splitting into finite elements (FE) by surface and volume with setting the number of elements, checking the correct orientation of normal to the FE) (figure 5):

material properties (loading of material properties and thermos-kinetic diagrams (TCD) from the database (DB) and approximation of temperature dependences of properties);

initial and boundary conditions (temperature conditions (initial value of node temperature, node temperature values and their graphical dependences, cooling media)), mechanical conditions (movement of nodes);

words of the heat treatment process (total number of increments, number of periodically stored increments, total process time);

starting the calculation (checking the correctness of constructing the CE model, visualizing the calculation progress (monitoring) , and reporting errors).

The software modules included in the processor block perform mathematical calculations of temperature, strain, stress, and hardness fields. The temperature fields are calculated by solving the heat conduction equation in accordance with the initial values specified in the volume and the boundary values specified on the surface, the nodal temperatures, density, coefficients of heat capacity, thermal conductivity of the material, heat exchange with the environment, and cooling time.

The stress-strain state is determined based on the solution of the elastically plastic problem and the obtained temperature fields, thermos-physical properties of certain phases (austenite, ferrite, carbide and marten-site). The hardness, the start and end temperatures of phase transformations, and the percentage composition of phases can be determined either from the TCD or by approximating the values, taking into account the chemical composition and cooling rate. Interfacial properties assume setting the value of heat (energy) released or absorbed during the phase transition (to take into account the influence of the thermal effect during the phase transition).

B the tasks of the postprocessor include processing the output information of the processor, as well as the output and processing of simulation results (distribution of temperatures, deformations, stresses, and hardness), i.e. constructing graphical dependencies of the above values
and visual distribution of their values over the surface and in the cross-section of the part model. A distinctive feature of the developed models is the accounting of volumetric geo-part metrics (ZO-modeling), as well as phase transformations and stress relaxation due to plastic deformations. The description of the temperature distribution in a heated or cooled part is based on solving a nonstationary heat conduction equation for the three-dimensional case using the finite element method (FEM). At the same time, in contrast to the known developments, the model takes into account the influence of the thermal effect obtained during phase transformation (the condition of the presence of internal heat sources), the dependence of the properties of materials depend on the temperature and phase composition, i.e. the nonlinearity of the material properties is taken into account.

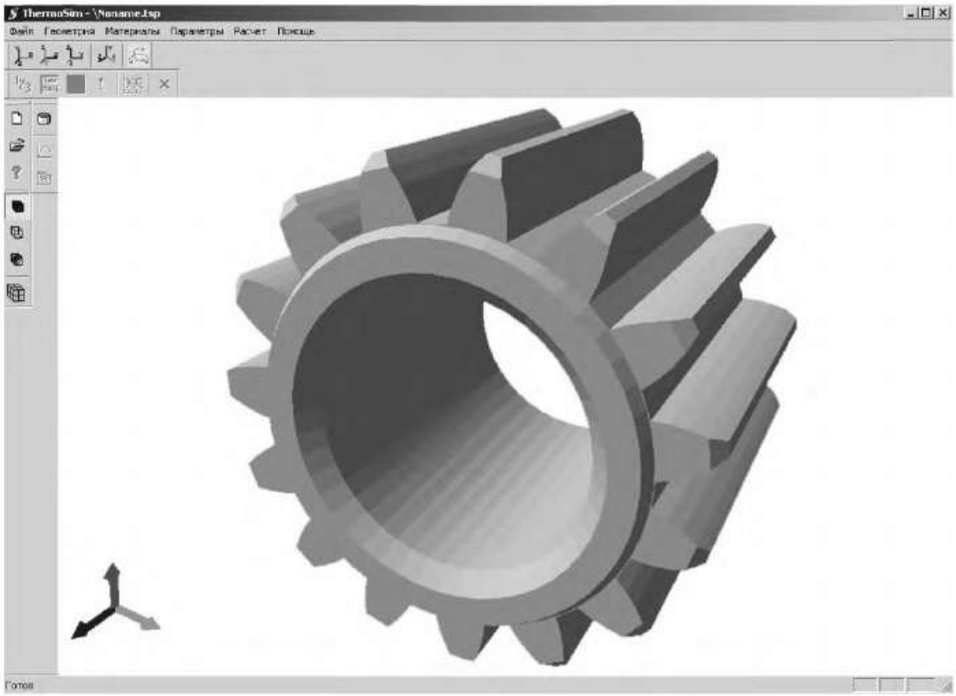

Fig. 3. The working field of the program complex Thermo-Sim

In currently, pilot tests and verification of models are being carried out in the conditions of the Central factory laboratory of the Department of the main Metallurgist of RUE "MAZ".Planned terms of implementation of the first stage of the developed software package in production at MAZ-t in The quarter of 2004 The application of the development will provide end-to-end automation, reducing the time and material costs for the design and technological preparation of parts subjected to heat treatment.

Prospects for further development of methods of computer modeling of technological processes

Further development of methods of computer modeling of technological processes and new developments of the laboratory will go in the following directions:

transition to three-dimensional computer-based design and modeling systems, which allows developers to work with more realistic models, increases productivity and quality of their work;

improving the performance of software tools that implement modeling systems. by applying more efficient algorithms for solving mathematical problems and complex geometric transformations;

further expansion and improvement of databases of material properties, the quality of which largely depends on the possibility of application and accuracy of modeling results;

"intellectualization" of modeling systems by including expert systems and other elements of artificial intelligence systems in their composition.

The latter direction is currently under intensive development, in particular, in relation to the processes of plasma sputtering and heat treatment [20].

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