International Journal of Engineering Trends and Technology Volume 70 Issue 5, 317-327, May 2022
ISSN: 2231-5381/ https://doi.org/10.14445/22315381/IJETT-V70I5P235

Original Article

Multiphysics Process Simulation in the Working Area of the Plasma Unit of the Multicomponent Nanocomposite Coating Plant

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Received: 11 March 2022 Revised: 05 May 2022 Accepted: 16 May 2022 Published: 31 May 2022

Abstract *- This research is dedicated to plants for deposition of multicomponent nanocomposite coatings. Increasing the service life of machinery is one of the highest priorities due to the natural limitation of mineral resources used in mechanical engineering. Sputtering techniques of special purpose coatings improving surface strength characteristics, wear resistance, microhardness, corrosion resistance, and many other parameters related to the structural-phase state of the product surface layer have become widespread in recent decades. Such coatings are used in strategically important industries: machine-tool engineering, power engineering, chemical industry, aircraft engineering, automotive industry, shipbuilding, space engineering, and other industries with severe operating conditions. Due to the high complexity, significant materials, and time consumption in the design and development of the plant for multicomponent nanocomposite coatings, modern software and computer complexes for simulating multiphysics processes would seem useful. The cathode-anode assembly of the plant plasmatron unit was simulated with the system of plasma separation from heavy components. The need to consider physical processes in the interelectrode region while designing plasmatron units was shown since the efficiency of the sputtering process and the service life of the plant units largely depend on the discharge parameters and the resulting plasma jet. There is increased wear of copper nozzles at high current density and arc temperature values. The coating characteristics are also affected by structural and flow phase composition. The simulation results confirm the efficiency of the developed plasma separator. The separator configuration, coil arrangement scheme, current strength, and other system efficiency parameters were determined.*

Keywords *- plasma sputtering, nanocomposite coating, complex composition coating, plasma separator, multiphysics processes.*

1. Introduction

The actively developing production field constantly needs more perfect materials and technological processes [1-3]. Meanwhile, the existing recovery mechanisms of material and energy resources are a natural limiting factor of this development. One of the available methods of saving the current resources is to increase the service life of equipment and products [4-6]. The current knowledge about the strength, wear, and fracture of materials allows us to conclude the critical importance of the structural-phase state of the material surface layers in this vein [7-9]. in this regard, a promising technology trend is the modification of the working surfaces of products and tools to give them increased strength, hardness, wear resistance, corrosion resistance, and various special functional characteristics [10-12]. Various kinds of coatings, multicomponent alloying of surface layers, and physical and chemical treatment of working surfaces of products are widespread in technology [13]. Accordingly, the task of developing methods and technological equipment for coating, including composite ones, is relevant [14-16]. It applies to equipment operated in extreme conditions and the tools required to process modern materials.

One method of creating coatings is electrodeposition [17]. For example, nickel-phosphorus coatings can be considered, which help increase wear resistance, corrosion resistance, and microhardness; they have a high hydrogen accumulation capacity and catalytic activity. Additional improvement of characteristics is also possible through the introduction of oxides (TiO_2, Al_2O_3, CeO_2, SiO_2) and carbides (TiC, NbC, TaC, SiC, B_4C, WC), sulfides (MoS_2, WS_2), carbon nanotubes and other inclusions to produce composite coatings. However, the disadvantages of this technology include the complexity of obtaining a stably repeatable distribution of inclusions and the insufficiently studied influence of hydrodynamics, mass transfer, and technological process parameters on the structure and properties of the obtained coatings.

Magnetron sputtering is a variation of the Physical Vapor Deposition (PVD) process [16]. First, a workpiece and a target containing the material components of the future coating are placed in a vacuum chamber, and an electric field is generated between them. Then an inert gas, usual argon, is introduced into the chamber, which is ionized under the electrical action and bombards the target electrode, which causes the material to be ejected toward the workpiece. It is deposited, forming a coating. in addition, this method features magnetic field generators to capture the secondary electrons of the target in the discharge, which enhances the argon ionization process and accelerates the coating deposition process.

Among the disadvantages of the technology are the limitation of the sputtering rate for strongly magnetic materials, rather a low capacity utilization of the target material, and the plasma instability. Conversely, the advantages of the magnetron sputtering technology include sufficiently high productivity at a low degree of workpiece heating, homogeneity, absence of impurities in the coating material, and the relative ease of application.

Double glow plasma surface alloying (DGPSA) is an actively developing technology for product surface treatment. It applies low-temperature plasma generated by a glow discharge to vaporize the target material, containing alloying components, which are subsequently deposited on the working surface of the object workpiece to form a modified layer with the desired set of characteristics determined by the future operating conditions [18]. By varying the process parameters, such as the working gas pressure, the distance between the workpiece and the target electrode, the potential difference between them, and the operating temperature and exposure time, it becomes possible to create a gradient distribution of alloying elements in the surface layer and achieve high bond strength between the coating and the base material. The relatively low required costs make the DGPSA method quite promising. However, this technology is relatively new. Thus, studies addressing specific application issues are still underway, and, as a result, DGPSA has had limited use in existing industrial plants so far.

At the same time, plasma sputtering of functional coatings has proven itself in many industries as a fairly stable technological process for modifying the working surfaces of products and equipment [19, 20). During electric discharge generation, a flow of highly ionized plasma is emitted, which forms the coating of the required thickness in contact with the substrate. The coating material depends on the fed powder mixture and cathode material composition, and the coating thickness is controlled by the ion flux density and exposure time. Magnetic fields can control plasma motion, and the energy of the deposited ions can be adjusted accordingly by applying a negative potential to the substrate. It is also possible to add reaction gas during the sputtering process, which leads to forming on the substrate nitrides from nitrogen, oxides from oxygen, and carbides, from carbon-containing gas, supplied in the working area. By regulating the gas supply and the plasma jet velocity, it is possible to vary the coating porosity, which is essential for some applied tasks, particularly for forming thermal protective coatings. Due to the whole complex adjustable process parameters, it is possible to vary the functional characteristics of the formed coating in a wide range [21-23].

in addition, this method makes it possible to pre-clean the substrate surface. For this purpose, the substrate surface is subjected to ion bombardment, to which a high negative voltage is applied to accelerate charged particles. Consequently, the substrate surface layer is sputtered with the contaminants due to the high energy of the ions. in this pretreatment, the surface is cleaned and becomes activated, and as a result of sputtering, the coating has high adhesion to the substrate material.

Thus, the plasmatron unit is one of the main elements of the multicomponent nanocomposite coating plant. Accordingly, the issues related to its design and simulation of the operation of both separate units and the plant are significant for the plant development.

2. Materials and Methods

2.1. Design Issues of the Plasmatron Working Area Elements

The developed plant is intended for deposition of single- and multi-layer multicomponent nanocomposite coatings with special functional characteristics (hardening, wear-resistance, thermal protection, etc.) on a part surface with a diameter of up to 200 mm and a length of up to 250 mm by vacuum condensation of high-speed gas-metal plasma flow on workpieces. Figures 1 and 2 show the plant's design for depositing multicomponent nanocomposite coatings.

ISSN: 2231-5381/ https://doi.org/10.14445/22315381/IJETT-V70I5P235

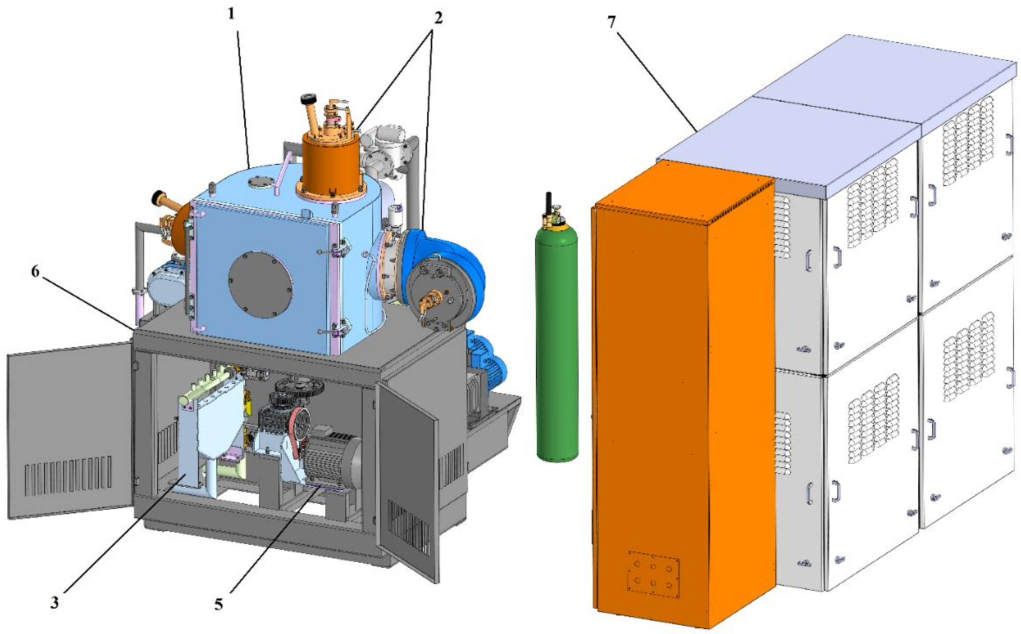

Fig. 1 Plasma sputtering plant for applying multicomponent nanocomposite coatings (front view): 1 – vacuum chamber; 2 – plasmatron cathode-anode assembly and plasma separator unit;3 – water cooling system;4 – vacuum system;5 – workbench rotation mechanism;6 – machine stand;7 – control and monitoring unit

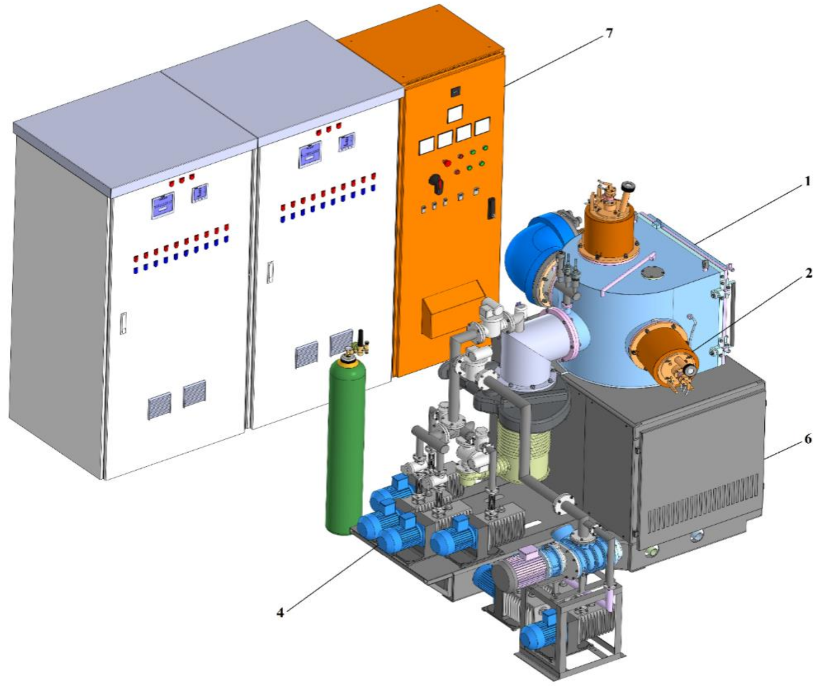

Fig. 2 Plasma sputtering plant for applying multicomponent nanocomposite coatings (back view): 1 – vacuum chamber; 2 – plasmatron cathode-anode assembly and plasma separator unit; 3 – water cooling system; 4 – vacuum system; 5 – workbench rotation mechanism;6 – machine stand;7 – control and monitoring unit

to ensure the main plasmatron function (heating the active substance), it is necessary to provide the required pressure and gas flow rate in the working area, electric discharge formation, formation, and direction of the flow of highly ionized plasma to form a coating with the required characteristics, as well as cooling, and protection against oxidation of structural elements. Based on the above functions, the plasmatron design can be divided into

- Electrical system, which includes power sources, conductors, insulators, cathode and anode assemblies;

- Pneumatic system, which includes nozzles, seals, working chamber, connections to external systems, and devices for input, speed control, feed direction, and changing the gas concentration;
- The vacuum system includes a vacuum chamber and a complex connected system of pumps that create and maintain the desired level of technical vacuum;
- Cooling system includes feed pipes, coolant distribution channels in the heat-loaded elements of the structure, seals and connectors to external removal systems, filtration, and utilization of the used cooling medium.

The main characteristics of the plasmatron, among other technological parameters, including

- Discharge current-voltage characteristics and electric power consumption, determining the requirements for the power supply system;
- Gas pressure and flow rate, determining the requirements for the pneumatic and vacuum systems;
- Operating characteristics such as the degree of ionization, concentration of charged particles, thermal power, enthalpy, average mass temperature, pressure and density of plasma flow, continuous operation time, the cathode anode assembly life;
- Pressure and flow of the cooling medium are required to maintain the specified temperature mode of the structural elements and provided by the cooling system.

The performance of the plasma formation process is determined by the flow rate of the heated substance and the thermal power. That, in turn, is defined as the product of the flow rate and the plasma average mass enthalpy. Thus, the efficiency of the plasmatron could be defined as the ratio of jet thermal power to consumed electric power. Hence, it is quite simple to determine the power losses in the elements of the plasmatron structure.

in addition, an essential performance parameter in addition to the energy efficiency, the adhesive strength of the coating material to the substrate, microhardness, and porosity of the coating is the material ratio specified empirically during the experimental development stage. in addition, the local plasma temperatures, e.g., in the flow axis and their distribution across the jet cross-section, may be of interest in some embodiments. It is also important to consider the plasma velocity at the channel outlet when sputtering. As a rule, in the outlet section, the plasma is in a state of thermodynamic equilibrium, so the plasma composition and degree of ionization are quite unambiguously characterized by temperature and pressure. The technological process determines the selection of the plasma-forming substance. It affects the parameters and features of the structure and the materials of the constituent elements of the plasmatron.

When ions with high energy condense on the substrate surface, the substrate material is heated quite intensively in the sputtering process. If the technological regime is not followed, it can damage the product to which the coating is applied. in this case, for metal parts of machinery, as a rule, overheating above the recrystallization annealing temperature is not recommended. However, it is also important for brittle products to control the temperature difference and thickness since cracks and other defects due to thermal stresses may occur.

Thus, it is necessary to adjust the plasma flow parameters depending on the temperature mode of the processed product. to quantify the values of permissible coating growth rate and plasma concentration near the substrate surface when the product temperature mode is not violated, the following expressions are used:

$$\delta = t\, v_{coat}, v_{coat} = \frac{m_i}{q_i \rho} \sum_{j=1}^{n} \left[j_i \left(I_{arc}, h_{c-p} \right) \cdot \left(\chi(W_i) - k(W_i) \right) \right]_j \quad (1)$$

where δ – coating thickness; t – exposure time; v_{coat} –coating growth rate; $j_i(I, L_{c-p})$ – ion flux density, which is a function of discharge current I_{arc} and the distance from the cathode surface to the substrateh_{c-p} $m_i q_i$; – mass and average charge of the deposited ion; ρ – the specific mass of the deposited substance; χk– deposition and sputtering coefficients, depending on the energy of the particlesW_i.

$$P_s = j_i\, U_s, P_r = \sigma \varepsilon \left(T_{max}^4 - T_0^4 \right) \quad (2)$$

where P_s – power emitted on the substrate; U_s – negative bias voltage; P_s – power outgoing by radiation; T_{max} – product temperature limit.

2.2. Simulation of the Plasmatron Cathode-Anode Assembly

The simulation problem of plasmatron is a multidisciplinary task due to the simultaneous course of many thermophysical, electrophysical, gas-dynamic, and other processes with characteristic times and scales that differ by several orders of magnitude during the operation of the unit [24-26]. That leads to the necessity to consider rather slowly developing microscopic processes with characteristic times from thousandths to tenths of the discharge duration, which requires high computational resources. It is assumed that in the course of self-consistent interaction with the magnetic field and changes in macroscopic parameters, plasma passes from one quasi-uniform state to another. The evolution of the equilibrium of high-enthalpy plasma is generally described by a complex of Maxwell equations, force balance, and kinetic equations for each type of formed particle. This system of equations is simplified in practice, taking into account the peculiarities of a particular problem due to its high complexity, and solved using numerical methods on modern computers with subsequent verification of the model based on experimental data. Argon was considered the working gas, whose flow rate was 60 l/min, and the current strength was 600 A. The working area was divided into a finite-element hexagonal grid. The size of the elements in the near-wall zone was 0.1 mm. The cathode surface current load and the surface temperature distribution were set as the load in the form of dependences.

2.3. *Simulation of the Plant Plasma Separator Unit*

The presence of drop formations in the plasma flow directly impacts the surface treatment results since during the formation of coatings, such formations lead to changes in microrelief, a decrease in microhardness and wear resistance, local stresses, and pore formation, which leads to a violation of corrosion resistance, and in general to uncontrolled changes in coating parameters [27-29]. A study of such formations in coatings shows that particles with a characteristic size of around a micrometer or less have a hemispherical shape. in contrast, a higher ring surrounds the almost flat median part in larger ones. Such formations indicate that before the impact with the substrate surface, the particles were in the form of liquid. to remove such particles from the plasma flow, a system of selective heating and separation is possible. in this case, the separator unit is a system of screens and coils generating a magnetic field, deflecting particles to the chamber walls where they are deposited.

During simulation, a model of plasma mass transfer in an inhomogeneous magnetic field was set by the Monte Carlo method [30]: the initial position, energy, and ion charge are set by random number generation. The limiting factors may be the experimental data, the known preferential direction of the cathode material sputtering in a magnetic field generated by separator coils, and the need for the energy distribution of ions to match the Maxwell equation. Next, the ions iterate their displacement by a value determined using the Born-Mayer potential equation in the quasi-rigid spheres' approximation to within 10-6 of the free path length of the ion in the chamber filled with argon atoms. The probability of an elastic collision is then checked. As a result, the ion either continues its motion or loses part of its energy due to the collision.

3. Results

According to the simulation results of the plasmatron cathode-anode assembly, the pictures of temperature and current density distribution in the working area of the simulation model were obtained. Figures 3-8 show the results for three points in time – 0.014 s, 0.021 s, and 0.028 s. in addition, figures show the deflection of the plasma jet in sputtering. The maximum temperature and the jet velocity values were 32000 K and 1800 m/s, respectively.

Figure 9 presents the deflection of heavy components of the plasma flow to the separator walls. The separation index of plasma flux from heavy components is about 90%. at the same time, its values change rather weakly in the range of current strength in the magnetic field coils from 5 to 20 A. Separation naturally leads to a decrease in flux ions' energy, about 17 %. However, the scattering of ion energy on argon atoms largely causes these losses. Highly charged ions dissipate less energy than relatively low-charged ions due to the free path difference. Its length for highly charged ions is less – about 0.3-0.5 of the length for separate ions. As a result, the amount of energy scattering acts is also less - up to 6, while for ions with energies of 50 eV, it is more than 16.

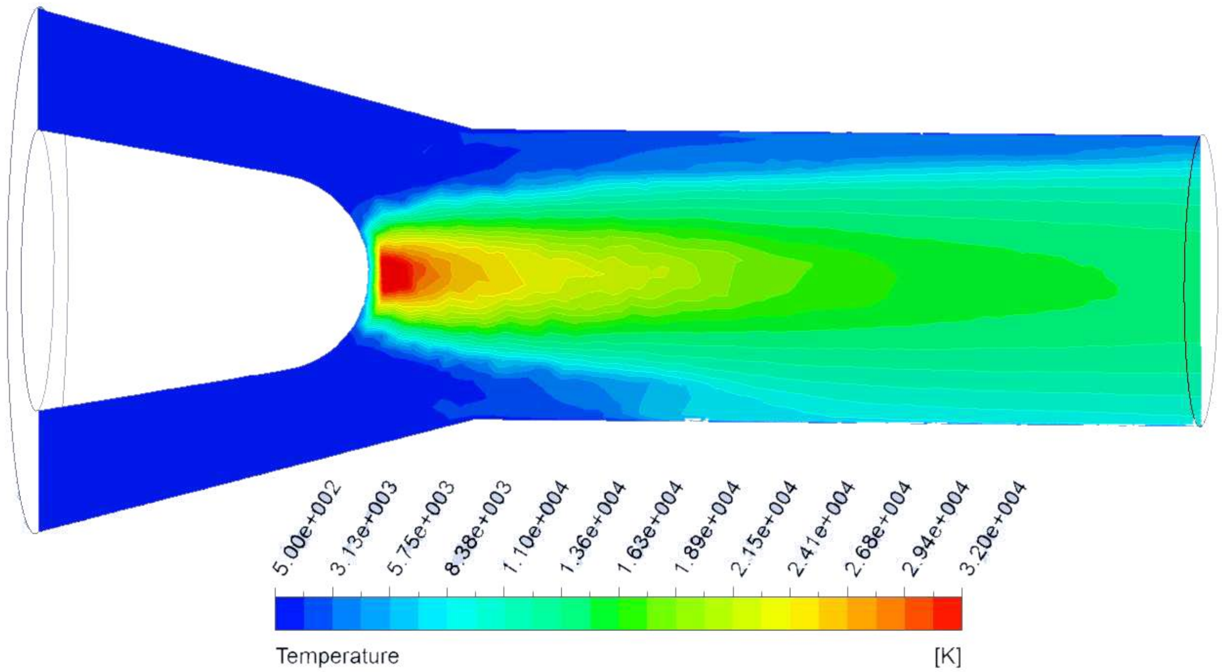

Fig. 3 Temperature distribution in the working area at time 0.014 s

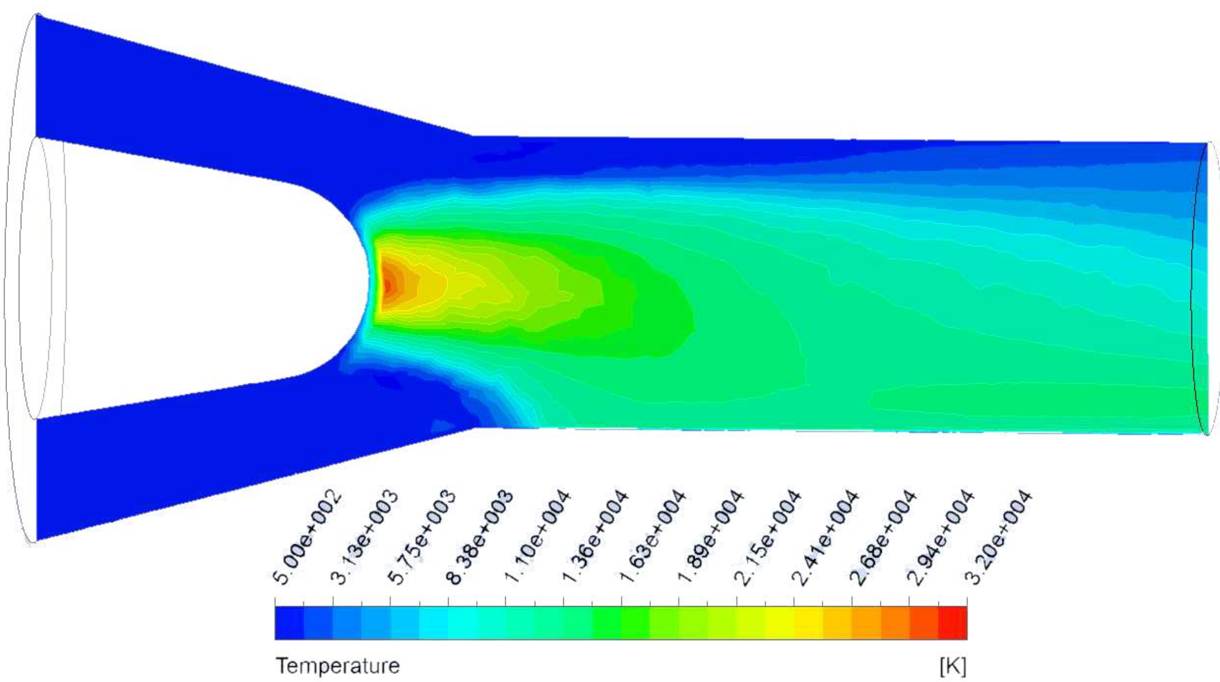

Fig. 4 Temperature distribution in the working area at time0.021 s

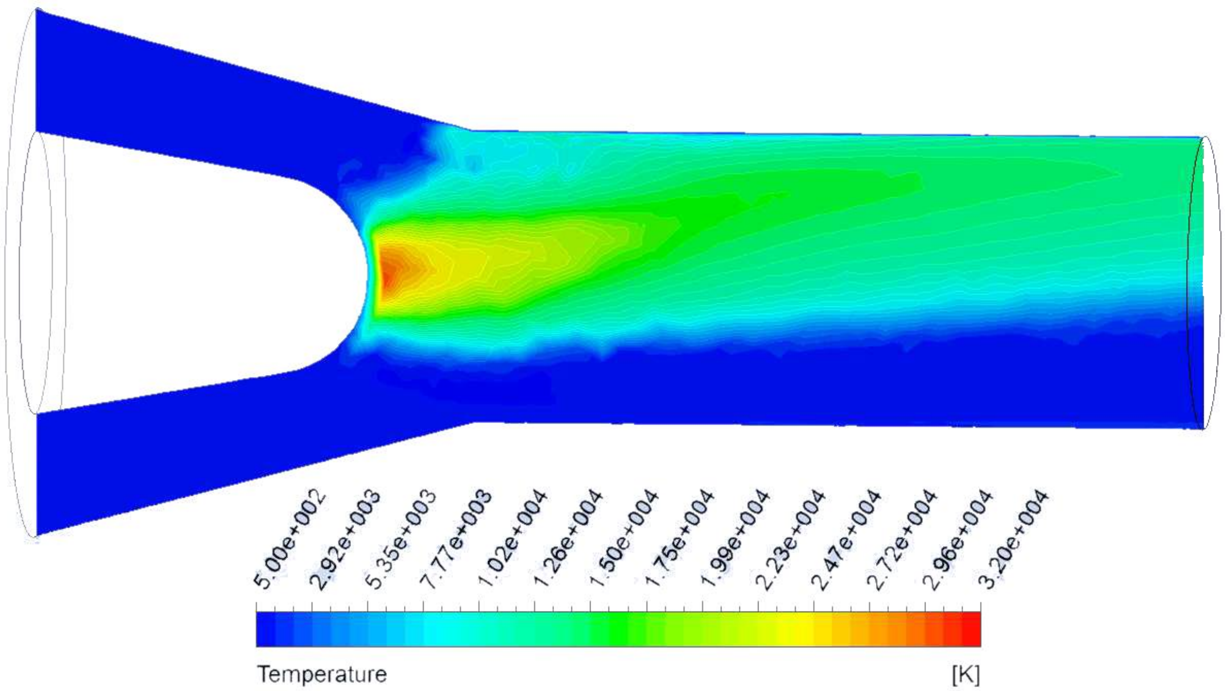

Fig. 5 Temperature distribution in the working area at time0.028 s

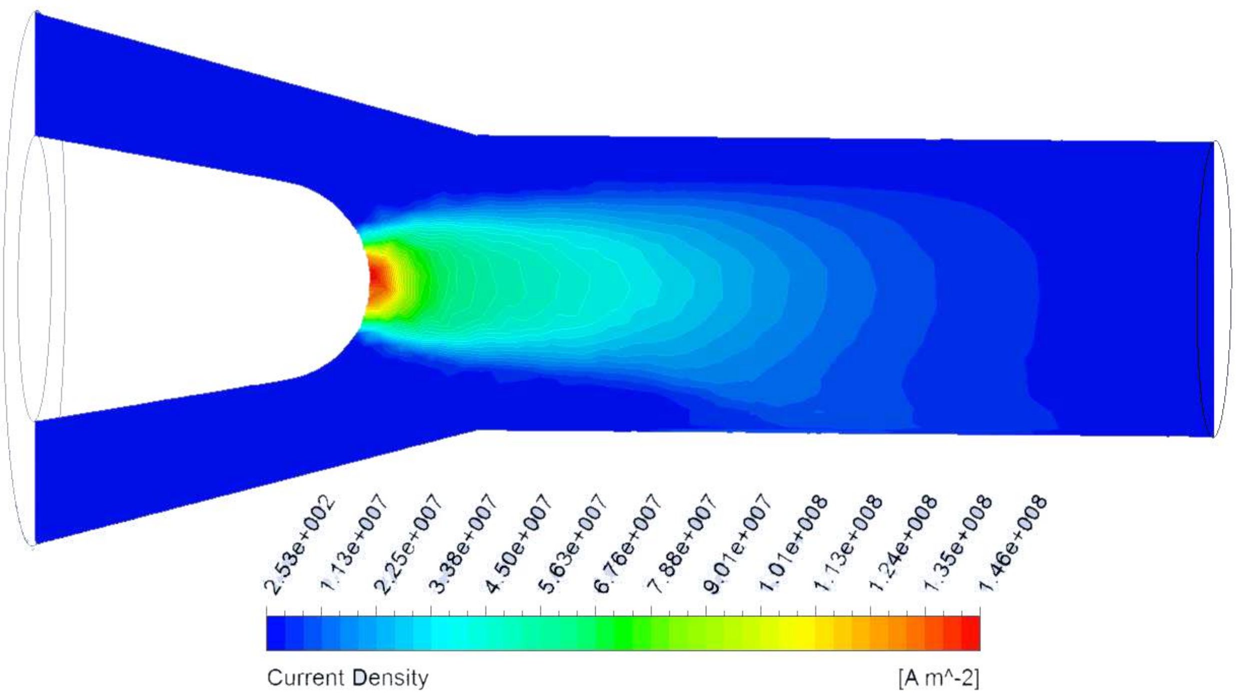

Fig. 6 Current density distribution in the working area at time 0.014 s

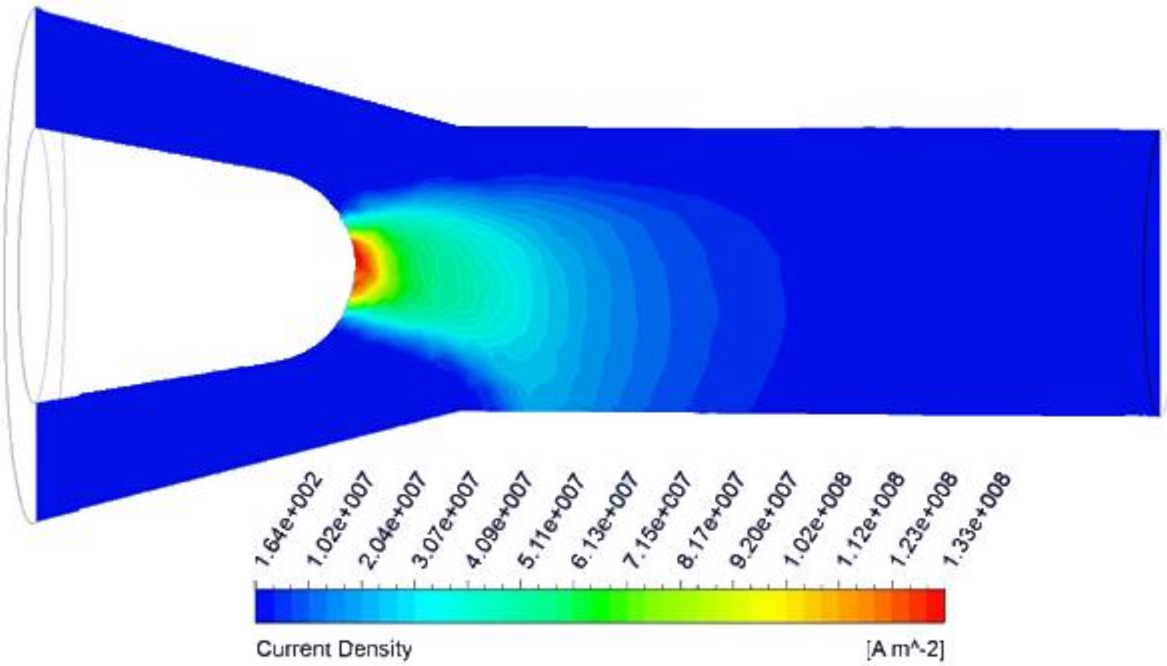

Fig. 7 Current density distribution in the working area at time 0.021 s

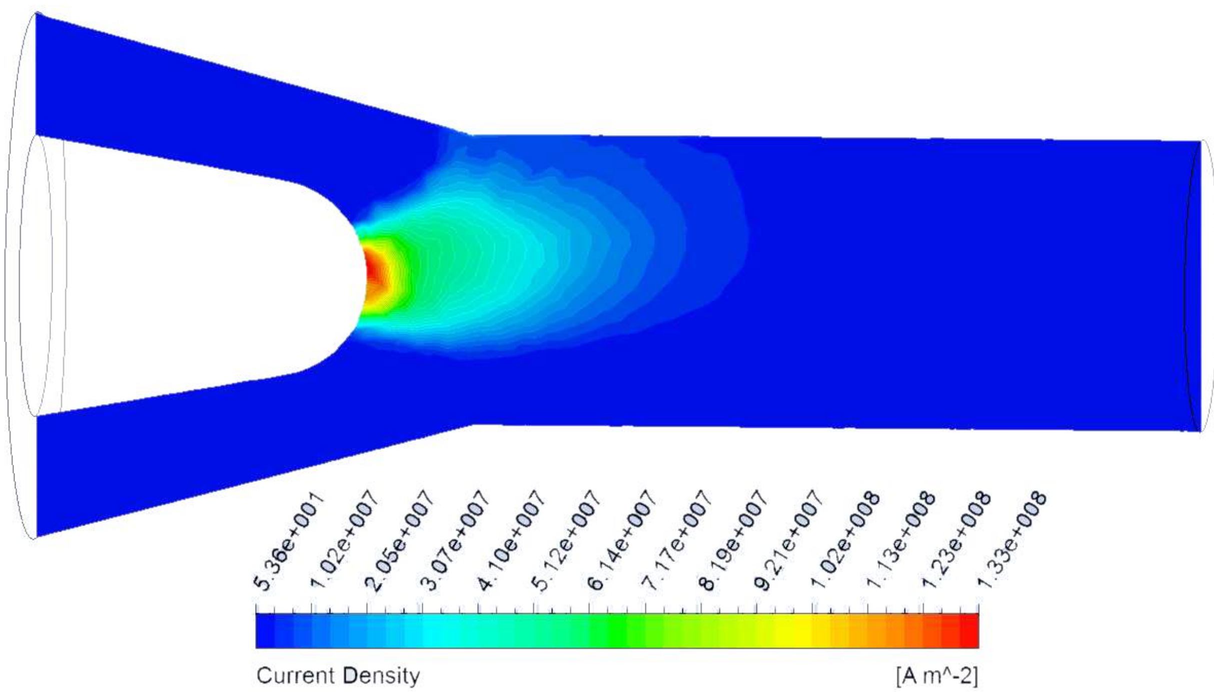

Fig. 8 Current density distribution in the working area at time 0.028 s

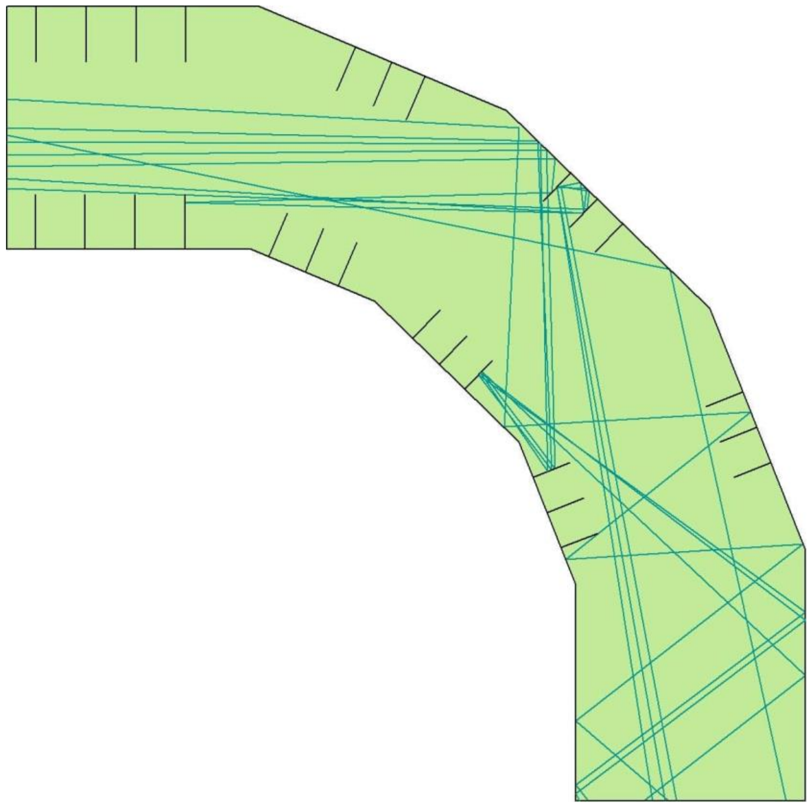

Fig. 9 Schematic image of heavy flow components tracing results as they pass through the plasma separator unit

4. Discussion

Simulation results of the cathode-anode assembly demonstrate the importance of considering the physical processes occurring in the inter-electrode area, which directly affect the efficiency and service life of the plant as a whole. For example, high temperature and current density and the jumping nature of the arc spot motion lead to increased wear of copper nozzles. in addition, the turbulent mixing of plasma flow with ambient cold air affects coating characteristics. As a result, the speed and temperature of sprayed particles in the area of coating formation decrease, and there is a possibility of uncontrolled chemical reactions with ambient gas.

in turn, the calculation of the plasma separator unit showed the picture of displacement of ion flux by the non-uniform magnetic field to the inner wall of drop phase separators with a high density of coil turns. The displacement of plasma flux accordingly affects the concentration distribution profile of plasma components at the outlet of the separator unit and, as a result, the distribution of sputtered components on the substrate, which should be taken into account when developing the technological process. in addition, the height of the substrate installation has an influence, which is associated with a decrease in the plasma flow intensity at the separator outlet.

5. Conclusion

Thus, the methodology of designing the plasmatron unit of the multicomponent nanocomposite coating plant using modern software and computational complexes to simulate the complex multiphysics processes during the operation of the plant is proposed. The developed method makes it possible to reduce the required material and time resources at the design and experimental testing stages due to the exclusion of irrelevant variants of the design of the plant units from consideration. The simulation results confirm that the cathode-electrode unit's durability and sputtering performance directly depend on the discharge parameters and the resulting plasma jet. Thus, copper nozzles have increased wear at high current density and arc temperature values. Patterns of temperature and current density distribution in the interelectrode region were obtained for several points in time. It is shown that the maximum values of the plasma temperature reach 32000 K, and the jet velocity can reach values of 1800 m/s. The unit design for the plasma flow separation from heavy components was also developed. It is shown that at the current strength in the magnetic field coils from 5 to 20 A, the separation index changes weakly enough and is about 90%. Meanwhile, the use of the plasma separator leads to a reduction of ion energy by 17%. in addition, significantly, due to the particles' free path difference, relatively low charged ions scattered more energy than the highly charged ions.

Acknowledgment
Some results of this study were obtained as part of the work under the agreement on the provision of subsidies from Dec14, 2020, No. 075-11-2020-032 (government contract identifier – 000000S207520RNU0002) on the topic: Development and organization of high-tech production of valves for the needs of special and medical equipment with high reliability and durability through the application of multicomponent nanocomposite materials with the Ministry of Science and Higher Education of the Russian Federation.

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