Development of a Mathematical Model of an Arc Plasma Discharge in Vacuum, Describing the Joint Solution of the Navier-Stokes Equations, Heat Transfer, with Equations of Plasma Theory

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Abstract. This article is devoted to the description of arc processes in a vacuum, relevant today for the melting of wire materials in the implementation of hybrid technologies of layer-by-layer synthesis. The directions of using an electric arc as a source of heat in creating arc additive technologies are indicated. One of the most promising methods for creating an arc discharge in vacuum using a non-consumable thermoelectronic hollow cathode is presented. A two-dimensional model has been developed for studying a hollow-cathode arc discharge in vacuum, where argon was used as the plasma-forming gas. All calculations were carried out in an axisymmetric formulation. To obtain a numerical solution, the COMSOL Multiphysics application software package was used. The obtained simulation results showed a satisfactory agreement with the literature and experimental data.

1. Introduction

The use of arc and plasma sources for melting wire material in the implementation of hybrid technologies of layer-by-layer synthesis has been actively developing in the world in recent years.

A promising area today is combining the capabilities of technologies from companies such as Sciaky [1, 2] and NorskTitanium, which will combine the effectiveness of vacuum protection and the properties of an electric arc as a heat source to create arc additive technologies in vacuum on their basis. Moreover, the degree of rarefaction in a vacuum chamber can be significantly less than when using an electron beam as a heat source, and the quality of protection will be higher than when using shielding gases or chambers with a controlled atmosphere, as with traditional arc methods.

The process of generating an arc discharge in a rarefied atmosphere for welding or single-layer surfacing is known [3, 4]. In work [5], welding with a consumable electrode in a low pressure argon medium is considered. In [6], the issues of the formation of metal compounds by arc welding methods in high vacuum are considered. Known results are primarily preliminary and represent mainly experimental results.

Speaking of layer-by-layer synthesis of materials, the process of arc melting of wire material in vacuum has not yet been considered. One of the factors that complicate the development of this
technology is the lack of mathematical models. With the development of the computational capabilities of modern technical means in modeling processes associated with arc welding, the results presented in [7–9] were obtained, however, such studies for processes in a rarefied medium are practically absent. At the same time, the formation of metal in this case is fundamentally different in many ways, starting with the features of the formation of a plasma discharge [10, 11], ending with the pressure of the plasma arc on the melt [12] and increased evaporation under conditions of uncertainty in the boiling point [13]. In describing the arc discharge in a rarefied atmosphere, the model developed in [14] for a non-self-sustained plasma discharge in electron beam welding will be used.

2. Mathematical model

One of the most promising methods for creating an arc discharge in vacuum is a circuit with a non-consumable thermoelectronic hollow cathode. The industrial application of a hollow cathode arc (HCA) discharge requires an understanding of the processes of plasma interaction with the cathode and anode, as well as related processes. (HCA) discharge can stably exist even at very low pressures, which is especially important when working with chemically active alloys [15–18]. Earlier, in [19], a mathematical model was developed for the formation of an arc discharge at low pressures using a hollow cathode. The mathematical formulation of the problem of forming an arc discharge in vacuum at low pressures (100 Pa and below) is based on solving a system of transport equations for the concentration and average energy of electrons, taking into account the description of mass transfer of heavy plasma particles (ions, neutral unexcited and excited atoms). At the same time, the distribution of neutral particles, which is used as input in the calculation, was taken from general considerations. Plasma properties are important in modeling the formation of an arc discharge based on the solution of the heat equations and the Navier-Stokes equations together with the equations of electrodynamics. In the proposed work, the models are combined to determine the transfer directly in the course of a joint solution.

Figure 1 shows the design scheme (the design scheme is rotated 180° relative to that used in practice). The calculations were performed in cylindrical coordinates in an axisymmetric formulation. Parameters of the hollow cathode: inner radius $r_c = 1.5$ mm, cathode thickness $\delta_c = 1$ mm, length $l_c = 10$ mm.

![Figure 1. Schematic of the HCA discharge model: 1 – axis of symmetry, 2 – anode (U=0), 3 and 6 – gas outlet (S=100 [l/s]), 4 – cathode (U=U0), 5 – gas inlet (Qm).]
2.1. Governing equations

The electron density and mean electron energy are calculated by solving the drift-diffusion equations:

\[
\frac{\partial n_e}{\partial t} + \nabla \cdot \Gamma_\epsilon + (\mathbf{u}_g \cdot \nabla) n_e = \mathbf{R}_\epsilon,
\]

\[
\frac{\partial n_\epsilon}{\partial t} + \nabla \cdot \Gamma_\epsilon + \Gamma_\epsilon \cdot \mathbf{E} + (\mathbf{u}_g \cdot \nabla) n_\epsilon = \mathbf{R}_\epsilon,
\]

where \( n_e \) and \( n_\epsilon \) are the electron density and electron energy density, respectively, \( \Gamma_\epsilon \) and \( \Gamma_\epsilon \) are the electron flux and the electron flux energy.

The \( \mathbf{R}_\epsilon \) component determines the emission or loss of electrons and the electron impact reactions presented in Table 1 [20, 21]. In these equations, \( \mathbf{R}_\epsilon \) represents the change in electron energy in these reactions, \( \mathbf{u}_g \) is the flow rate of the neutral gas, \( \mathbf{E} \) is the electric field strength.

Table 1. Plasma chemical reactions.

| No. | Formula | Data od reaction | Type of interaction |
|-----|---------|-----------------|--------------------|
| 1   | \( e + Ar \rightarrow Ar + e \) | cross-section | elastic |
| 2   | \( e + Ar \rightarrow Ar^* + e \) | cross-section | excitation |
| 3   | \( e + Ar^* \rightarrow Ar + e \) | cross-section | excitation |
| 4   | \( e + Ar^* \rightarrow Ar^+ + 2e \) | cross-section | ionization |
| 5   | \( e + Ar \rightarrow Ar^+ + 2e \) | cross-section | ionization |

The mass transfer equation for a multicomponent mixture is used to describe the mass transfer of heavy plasma particles [22, 23]:

\[
\rho \frac{\partial \omega_k}{\partial t} + \rho (\mathbf{u}_g \cdot \nabla) \omega_k + \nabla \cdot \Gamma_k = \mathbf{R}_k,
\]

where \( \rho \) is the mass density of the working gas, \( \omega_k \) is the mass fraction of the \( k \)th component, \( \mathbf{R}_k \) is the collision component of heavy particles obtained from plasma-chemical reactions in Table 1, \( \Gamma_k \) is the flux of the \( k \)th component.

To calculate the electric field strength, the Poisson’s equation is used:

\[
\varepsilon_0 \nabla \cdot (\nabla U) = \varepsilon_0 \nabla \cdot \mathbf{E} = \rho
\]

where \( U \) is the electrostatic potential of the plasma, \( \rho \) is the volume charge density, \( \varepsilon_0 \) is the dielectric constant of the vacuum.

A plasma discharge is accompanied by the emission of secondary electrons from the surface of the cathode. The boundary conditions take into account the loss of charge on the walls of the chamber and on the surface of the product as a result of chaotic motion resulting from thermionic effects [23]:

\[
-n \cdot \Gamma_\epsilon = \frac{1}{2 \nu_e n_e} + n_e \mu_e \mathbf{E} \cdot \mathbf{n} - n \cdot \Gamma_\epsilon
\]

and for the electron energy flux:

\[
-n \cdot \Gamma_\epsilon = \frac{1}{2 \nu_e n_e} + n_e \mu_e \mathbf{E} \cdot \mathbf{n}
\]
where \( v_{e,t} \) is the thermal velocity of electrons, \( \Gamma_t = J_t/e \) is the flux of thermal emission of electrons and \( n \) is normal, \( \mu_e \) and \( \mu_\epsilon \) are the mobility and energy coefficients of electrons. The boundary condition for the electron flux, electron energy flux, and heavy particle flux at the boundaries 2, 3, 4, 5, 6 is described in detail in [24].

A neutral gas flow, considered as a laminar flow, is described by the system of Navier-Stokes equations. The mass continuity equation and the momentum balance equation have the following form:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}_g) = 0
\]

\[
\rho \frac{\partial \mathbf{u}_g}{\partial t} + \rho (\mathbf{u}_g \cdot \nabla) \mathbf{u}_g = -\nabla p + \mu_d (\nabla \mathbf{u}_g + (\nabla \mathbf{u}_g)^T) - \frac{2}{3} \mu_d (\nabla \mathbf{u}_g) I
\]

where \( p \) is the pressure of the mixture of the gaseous medium, \( \mu_d \) is the dynamic viscosity, \( I \) is the tensor unit. The right term of the equation is the force of the pressure gradient and the tensor of viscous stresses, respectively. The superscript \( T \) represents the displacement of the matrix.

The heat transfer equation is a classic convection-diffusion equation, it looks like this:

\[
\rho c_{p,g} \frac{\partial T_g}{\partial t} + \rho c_{p,g} \mathbf{u}_g \cdot \nabla T_g + \nabla (-k_g \nabla T_g) = Q_{eh} + Q_{J,ion}
\]

where \( T_g \) is the temperature of the neutral gas, \( c_{p,g} \) and \( k_g \) are the specific heat at constant pressure and the thermal conductivity of the working gas, respectively. The terms of the heat source include the expression of the exchange of energy between electrons and heavy particles:

\[
Q_{eh} = \frac{3}{2} k_g \left( \frac{2m_e}{m_i} \right) (T_e - T_g) v_{eh}
\]

and the expression of the Joule heating of ions:

\[
Q_{J,ion} = J_{ion} \cdot E
\]

In equation (10), the coefficient \( k_g \) is the Boltzmann constant, \( m_e \) and \( m_i \) are the mass of one electron and one heavy particle, \( v_{eh} \) is the total frequency of collisions between electrons and heavy particles, which can be obtained by plasma chemical reactions. In equation (11), \( J_{ion} \) is the ion current density at which only (Ar +) ions are considered in this study [24].

The gas flow in the hollow cathode and directly at the exit from it is described by an intermediate flow regime called the «slip mode» (Knudsen number \( 0.01 < Kn < 0.1 \)). In the intermediate mode, the Navier-Stokes equations are still applicable, but special modified boundary conditions are applied. When moving away from the end of the hollow cathode towards the surface of the product, the jet spreads in cross section, the flow is characterized by an intermediate Knudsen number \( (Kn \sim 1) \). When moving away from the weld zone, the flow passes the molecular flow regime \( (Kn >> 1) \) and can be described using the Monte Carlo method. In the deposition zone (the cathode cavity and the zone below it), an intermediate mode \( (Kn \sim 1) \) is realized. In the studies known in the open literature, in this case both the description by the “sliding mode” using the Navier-Stokes equations and the molecular flow description are used, sometimes correcting the obtained solutions by introducing some calibration coefficients. A numerical experiment showed a satisfactory convergence between the results obtained using both the first and second approaches.

3. Results
The calculations were carried out in an axisymmetric cylindrical formulation. To obtain a numerical solution, we used the COMSOL 4.4 application software package, the Plasma Module, Molecular Flow, and Rarefied Flow modules. The simulation results show a satisfactory agreement with the literature and experimental data.
The pressure inside the hollow cathode depends on the flow rate of the supplied gas and decreases almost linearly as it approaches the outlet (Figure 2). In the zone of interaction between the plasma flow and the anode, the distribution is close to Gaussian (Figure 3).

![Figure 2. Pressure in the cavity of the hollow cathode.](image1)

![Figure 3. Distribution of plasma pressure on the surface of the anode, calculated as part of the description of the flow by free molecular flow.](image2)

The distribution of the concentration of neutral particles obtained from the description of the gas flow is an input parameter for the description of the plasma using equations (1) - (11). The values of the energy released as a result of solving equations (1) - (11) are used in solving the problem of describing a gas flow. Solving the system of equations (1) - (11) also allows you to calculate the transfer coefficients, such as plasma conductivity, diffusion coefficients, etc.

Figure 4 shows the calculated distribution of electron density in the case of HCA discharge in vacuum with a microflow of a plasma-forming gas (argon) through the cathode cavity. The maximum electron density is near the end of the hollow cathode [19].
Figure 4. Distribution of electron density at HCA discharge (discharge current $I_d = 96$ A, electric potential $U_0 = 30$ V, gas flow rate $Q_m = 3$ mg / s).

Figure 5. Change in electron temperature (eV) in the space under the hollow cathode.
Figure 6. Change in plasma concentration in the cavity of the hollow cathode and under it.

Figures 5, 6 show the distribution of electron temperature and plasma concentration in the cavity of the hollow cathode and below it along the axis of symmetry.

4. Conclusion
A mathematical model has been developed that describes a method for creating an arc discharge in vacuum using a non-consumable thermoelectronic hollow cathode.

As a result of the simulation, the following results were obtained:
- data on the pressure in the cavity of the hollow cathode;
- distribution of plasma pressure on the surface of the anode;
- distribution of electron density in HCA discharge;
- data on changes in electron temperature in the space under the hollow cathode;
- data on changes in plasma concentration in the cavity of the hollow cathode and under it.

The solution of the associated mathematical problem for an arc plasma discharge in vacuum, which describes the joint solution of the Navier-Stokes equations, heat transfer, and equations of plasma theory, was obtained for the first time.

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