ЕЛЕКТРОНІКА ТА ІНЖЕНЕРІЯ

ANALYTICAL RELATIONS FOR CALCULATION THE CURRENT OF ARG DISCHARGE IN THE METALS' VAPORS AT THE PHYSICAL CONDITIONS OF TECHNOLOGICAL PROCESS OF ELECTRON-BEAM DEPOSITION OF CERAMIC COATINGS

I. Melnyk, S. Tuhai, M. Skrypka, M. Surzhykov, I. Shved

*National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute",
37, Peremogy Avenue, Kyiv, 03056, Ukraine*

Corresponding author: I. Melnyk (e-mail: melnik@phbme.kpi.ua)

(Given 10 November 2022)

The article is devoted to the problem of calculation the value of current of non-self-sustained arc discharge, which is lighting and maintained in the metal vapours and active gases for porviding the chemical reaction between its in the technological process of evaporation of thin coatings. Obtaineed relations are generally based on Poisson equation for defining the distribution of electric field, Mendeleev – Clapeyron equation for defining the concentration of ions in saturated metals' vapours, as well as on equation of current continiouty in gas discharge. Formed set of equations for distribution of electric potential and discharge current in the spatial coordinates is transformed to cubic equation, which was solved analytically. Obtained simulation results are given and analyzed.

1. Introduction

In the modern production of electronic devices, mechanical instrument, as well as details of engines in automotive, aviation and space vessels, the ceramic coatings of different applying are widely used. For example, in electronic industry dielectric coatings for obtaining the high-quality capacitors, as well as for reactive elements for transmitters and receivers' antennas of communication devices are effectively applied today [1–4]. In instrument-making industry the ceramic coatings are effectively applied as hardness protective means for defense at cutting instruments [5–7]. In automation, aviation and space industry ceramic coatings ensure the mechanical strength of machine parts in the presence of friction and protect the metal parts of the engine blades and the walls of the fuel-burning volume from unwanted overheating. Due to this, it is possible to achieve a higher temperature in the engine cylinder, which significantly increases its energy efficiency. In particular, in modern engine models, the temperature in the middle of the cylinder, where the fuel is burned, can be more than 5000 °C [5–7]. As for reinforcing coatings, their use allows you to significantly extend the period of trouble-free operation for important parts of mechanisms that rotate at high speed and are subject to significant friction [5–7].

For obtaining ceramic coatings with high production rate and high quality the electron beam evaporation is widely used today, but since the evaporated ceramic, which is included gas active components, is dissociated in vacuum conditions, maintaining of chemical reaction between metal vapors and active gases is necessary. For providing such reaction effectively the non-self-sustained arc discharge in the metals' vapors, over the crucible, is lighting [8, 9]. With using such kind of discharge the quality of deposited ceramic films is generally improved.

Since the applying of traditional electron guns with heated cathodes for providing evaporation of ceramic materials in the soft vacuum in the medium of active gases is extremely complicated from a technical point of view, for providing this technological operation high voltage glow discharge electron guns are widely used now a day [5–7, 10]. The main advantages of using high voltage glow discharge electron guns in the evaporation technologies are follows [8, 9].

1. Relative simplicity of guns' construction and possibility of its disassembling for repairing and changing spare details.

2. Relative simplicity and cheapness of technological evacuation equipment.

3. High productivity of evaporation technological process.

4. Providing the technological process in soft vacuum in the medium of active gases and possibility of lighting the arc discharge in the technological chamber. Generally, in this aspect the particularities of operation of high voltage glow discharge electron guns are fully corresponded to the singularities of technological process of ceramics films deposition [5–8].

But it should be pointed out, that a restraining factor in the implementation of electron beam technology for obtaining of high-quality ceramic coatings in the production of electronic devices, cutting tools, engines and valuable parts for vehicles is the lack of appropriate methods and means of mathematical modeling of such processes. Particularity, the analytical relations for the preliminary determination of the value of the arc discharge current and the technological modes of electron beam evaporation are absent now a day. If the means of simulation high-voltage glow discharge electron guns were sufficiently fully and thoroughly considered in works [11, 12], simple analytical ratios for determining the arc discharge current in metal vapors do not exist at all. Therefore, obtaining such ratios and analyzing the simulation results is the main goal of this work.

2. Analyze and statement of the problem

A visual illustration of the block of electron-beam technological equipment designed for reactive deposition of a ceramic coating is shown in Fig. 1 [8, 9]. In Fig. 2 shows the construction diagram of the device for the deposition of a ceramic coating, the corresponding geometric dimensions are given as parameters of this device, and also the method of connecting this technological device to the electrical network is shown. As can be seen from Fig. 2, the main design parameters of the technological device under consideration are the following.

1. The cross-sectional radius of the ring electrode r_r.

2. The inner radius of the ring electrode R_r.

3. The distance between the crucible and the ring electrode d.

An important electrical parameter of the mathematical model of the technological device under consideration is also the ignition voltage of the arc discharge U_d. This parameter, according to established physical assumptions and known experimental data on the research of the technological process of reactive electron beam evaporation of metals, can take values in the range from 20 V to 60 V [7–9].

The mathematical model of such an electrode system for the physical conditions of non-self-sustained arc discharge combustion can be built on the basis of the following assumptions and theoretical propositions, which were proposed in the eighties of the 20th century by a leading scientist in the field of gas discharge and discharge plasma physics, Smirnov V. B. and Rayzer Yu. P. [13, 14].

1. The distribution of the electric field between the ring electrode and the surface of the metal being evaporated is determined by analytically solving the Poisson equation in cylindrical coordinates [15]. The corresponding coordinate system (r, z) is shown in Fig. 2.

2. The magnitude of the space charge is determined by the continuity equation for electron and ion currents [16, 17].

3. The energy of metal atoms above the surface of the crucible is determined by Boltzmann's law as kT_{ev}, where k is the Boltzmann constant, and T_{ev} is the evaporation temperature [18].
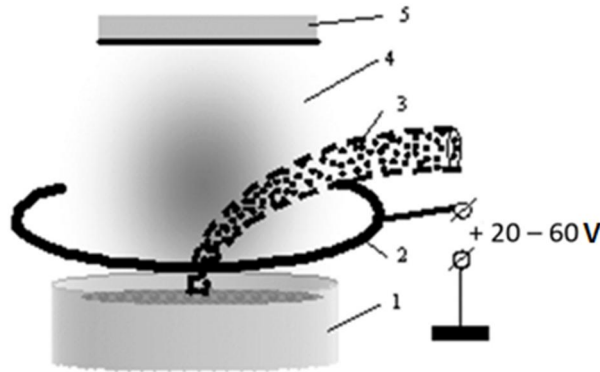

Fig. 1. Visual illustration of technological equipment for reactive electron-beam deposition of ceramic coatings: 1 – crucible; from which metal evaporates; 2 – ring electrode; 3 – electron beam; 4 – metal vapor; 5 –substrate for depositing a ceramic coating
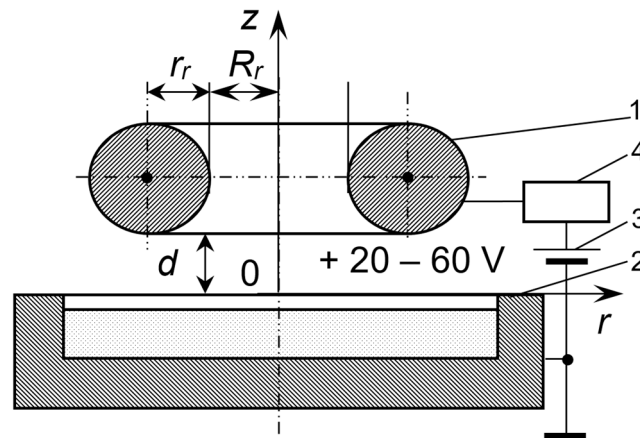

Fig. 2 Structural scheme of the device for maintaining an arc discharge in metal pairs and the method of connecting this device to the electrical circuit: 1 – ring electrode; 2 – crucible; 3 – power source; 4 – electronic system for arc discharge current control

4. Metal vapors above the crucible are saturated. According to this physical assumption, the concentration of metal atoms n_m is determined.

5. The level of metal vapor ionization is determined by the ionization coefficient β_m.

6. The concentration of residual gas atoms is determined by the residual gas pressure in the technological chamber p_g.

7. The level of residual gas ionization is determined by the ionization coefficient β_g.

8. The values β_m and β_g for the mathematical model under consideration are considered constant and do not depend on the arc discharge burning voltage U_d.

9. According to the physical model of singly charged ions, the numbers of ions and electrons in the volume, where the arc discharge maintained, are considered the same.

3. Formation of the basic set of algebraic and differential equations

Corresponding to the formulated assumptions 1 – 9, the basic set of algebraic-differential equations, intended for the formation of analytical relations aimed at solving the given task of mathematical simulation of arc discharge in the metal vapors over the crucible, can be written as follows.

1. Poisson's differential equation for determining the distribution of the electric field in the discharge gap [15]:

$$\frac{d^2\varphi(r)}{dr^2} = \rho \,,$$
(1)

where $\varphi(r)$ is the electric potential; ρ is the space charge density.

2. The Mendeleev–Clapeyron equation for determining the saturated vapor pressure in a technological device for the reactive deposition of ceramic films, the structural scheme of which is shown in Fig. 2 [18]:

$$p_s = \frac{\rho_v}{\mu_v} R T_{ev},$$
(2)

where p_s is the saturated vapor pressure; ρ_v is the vapor density; μ_v is the molecular weight of the vapor; R is the universal gas constant.

3. The equation of the continuity of the arc discharge current, which, according to the boundary conditions for the electrode system, the structural scheme of which is shown in Fig. 2, is written in the following form [13, 14]:

$$j_d = en_{im}\left(\sqrt{\frac{2kT_{ev}}{m_{im}}} + \sqrt{\frac{2e\varphi(r)}{m_{im}}}\right) + en_{ig}\left(\sqrt{\frac{2kT_0}{m_{ig}}} + \sqrt{\frac{2e\varphi(r)}{m_{ig}}}\right) + en_e\sqrt{\frac{2e\varphi(r)}{m_e}},$$
(3)

where j_d is the current density of the arc discharge; m_{im} is the mass of metal ions; m_{ig} is the mass of gas ions; n_{im} is the concentration of metal ions; n_{ig} is the concentration of gas ions; T_0 is the temperature of the external environment in the technological chamber; n_e is the concentration of electrons; m_e is the mass of an electron.

The analytical solution of the system of equations (1–3) will be given in the next sections of the article.

4. Analytical relations for determining the potential distribution

Considering equation (2), it is possible to rewrite the differential equation (1) to determine the potential distribution between the surface of the crucible and the ring electrode as follows:

$$\rho_{\Sigma}(r) = K\sqrt{\frac{1}{\varphi(r)}} \,.$$
(4)

The coefficient K in the equation (4) is defined as follows:

$$K = \sqrt{\frac{e}{k}}\left(\beta_m\sqrt{p_a N_A R} + \frac{\beta_g p_g}{\sqrt{T_0}}\right),$$
(5)

where N_A is the Avogadro constant.

Then, taking into account the obtained relations (4), (5) for the value of the space charge ρ_{Σ}, Poisson's differential equation (1) for the boundary conditions corresponding to the electrode system of the technological device, the structural diagram of which is shown in Fig. 2, can be rewritten in a simplified form as a cubic equation, which is solved analytically using the well-known Cordano formula [19]. The corresponding analytical dependencies are written as follows:

$$p = -\frac{3}{16K^2}, \; q = -\frac{24K^3\left(\frac{2}{3}U_d^{1.5} - (R_r - r)\sqrt{U_d}\right) + 27}{32K^3}, \; D = \left(\frac{24K^3\left(\frac{2}{3}U_d^{1.5} - (R_r - r)\sqrt{U_d}\right) + 27}{64K^3}\right)^2 - \frac{1}{4096K^6},$$

(6)

$$u = \sqrt[3]{-\frac{q}{2} + \sqrt{D}}; \; v = \sqrt[3]{-\frac{q}{2} - \sqrt{D}}; \; y = u + v; \; t = y + \frac{1}{4K}; \; \varphi(r) = \sqrt{t}.$$

5. Analytical relations for determining the arc discharge current

In the case of a known potential distribution function $\varphi(r)$, which is determined by the system of algebraic equations (6), relation (3) for determining the arc discharge current density in the plane of symmetry of the ring electrode is rewritten as follows:

$$j_d(r) = S_1\sqrt{\varphi(r)} + S_2, \; S_1 = \sqrt{2e}\left(C_1\sqrt{\frac{1}{m_{im}}} + C_2\sqrt{\frac{1}{m_{ig}}} + C_3\sqrt{\frac{1}{m_e}}\right), \; S_2 = C_1\sqrt{\frac{2kT_{ev}}{m_{im}}} + C_2\sqrt{\frac{2kT_0}{m_{ig}}},$$

$$C_1 = \frac{e\beta_m}{k}\sqrt{\frac{p_a N_A R}{T_{ev}}}; \; C_2 = \frac{e\beta_g p_g}{kT_0}; \; C_3 = C_1 + C_2.$$

(7)

Then the arc discharge current I_d is determined by integrating the obtained function $j_d(r)$, given by relation (7), along the coordinate r:

$$I_d = 2\pi\left(S_1\left(\int_0^{R_r}\sqrt{\varphi(r)}\,r\,dr\right) + \frac{S_2 R_r^2}{2}\right).$$

(8)

The obtained equation (8) can't be solved in the analytic form, and numerical relation, which corresponded to it, is written as follows [20]:

$$I_d = 2\pi\left(S_1\left(\sum_{i=0}^N i\sqrt{\varphi\left(\frac{iR_r}{N}\right)}\left(\frac{R_r}{N}\right)^2\right) + \frac{S_2 R_r^2}{2}\right),$$

(9)

where N is total amount of discrete points, which are chosen in the range $[0, R_r]$, i is the number of selected point on the corresponded iteration.

The results of simulation the electrode system of the technological device, the structural scheme of which is shown in Fig. 2, obtained by using the analytical ratios (4)–(7), (9), will be considered in the next section of the article.

6. Results of simulation the electrode system of the technological device and their analysis

The results of calculations of current-current characteristics of arc discharge in metal pairs are presented in fig. 3. All results were obtained for the evaporation of titanium in a nitrogen environment. The corresponding values of thermodynamic and electrical coefficients, as internal parameters of the proposed mathematical model, are given in Table 1 [13, 14, 21, 22].

From the graphical dependencies shown in Fig. 3, it is clear, that the current-voltage characteristics of an arc discharge, calculated with using ratios (4)–(7), (9) fully correspond to theoretical ideas about the nature of such dependencies, known from the fundamentals of the physics of a non-independent gas discharge and discharge plasma [13, 14]. In general, the dependences of $I_d(U_d)$ are increasing, but the value of the derivative $\frac{dI_d}{dU_d}$ decreases with increasing discharge voltage U_d. From a theoretical point of view,

this can be explained by the saturation effect of the discharge current, which is limited by the space charge of ions near the ring electrode [13, 14].

Electrical and thermodynamic internal parameters of the mathematical model for the technological process of evaporation of titanium in a nitrogen environment for the purpose of obtaining strengthening ceramic coatings of titanium nitride [13, 14, 21, 22]

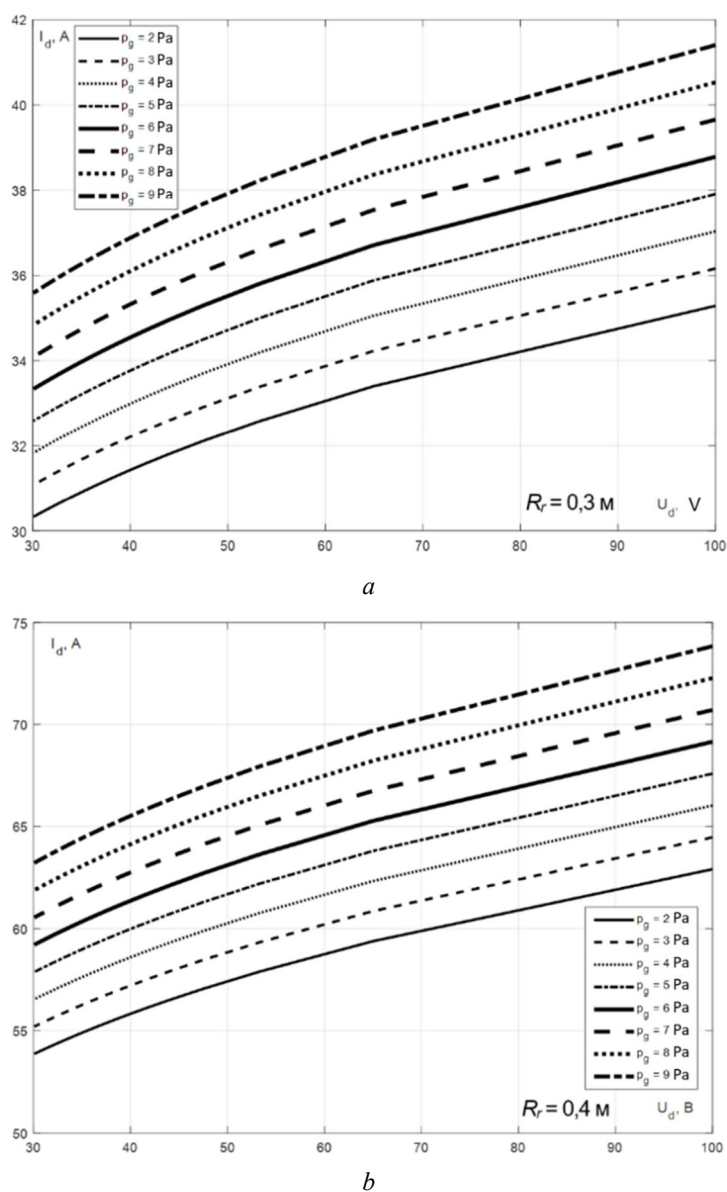| Parameter	Value
Level of ionization of metal vapors, β_m	0.8
Level of ionization of residual gas, β_g	0.75
Temperature in the discharge chamber, T_0, °C	20
Temperature of eavporation, T_{ev}, °C	3600

a

b

Fig. 3 The current-voltage characteristics of non-self-sustained arc discharge for the electrode system of the technological device, the structural scheme of which is presented in Fig. 2. Calculations were provided according to relations (4–7, 9) for residual pressure values in technological chamber p_g from 2 Pa to 9 Pa and for different values of the inner radius of the ring electrode R_r. $R_r = 0.3$ m (a); $R_r = 0.4$ m (b)

The calculated dependences of the arc discharge current derivative $\dfrac{dI_d}{dU_d}$ on the combustion voltage for the considered physical conditions and parameters of the technological process of ceramic coatings deposition are shown in Fig. 4. It should be noted that for small values of the discharge burning voltage, the value of the derivative current-voltage characteristic almost does not depend on the residual gas pressure in the discharge chamber. In addition, as can be seen from the graphic dependencies shown in fig. 4, the saturation effect is more influential for large pressure values than for small ones.

From a mathematical point of view, the effect of a decrease in the rate of current growth with an increase of applied voltage can be explained by the fact, that in the power function $j_d = j_d\left(U_d^{\alpha}\right)$, which is given by relations (6), the largest exponent of the power coefficient α has the value $\alpha = 0.25$, that is, $\alpha < 1$.

It also should be pointed out, that usually in practice the effect of saturation of the discharge current manifests itself to a greater degree and the derivative, under the condition of large values of the discharge burning voltage U_d, has a smaller value [13, 14]. This is primarily due to the dependence of the gas ionization coefficients β_m and β_g on the voltage of the discharge combustion [13, 14]. That is, assumptions 1–9, pointed out in section 2 and based on which the simple mathematical model, have been considered in this paper, was built, are not fully fulfilled. Improvement of the proposed mathematical model in order to take into account $\beta_m(U_d)$ and $\beta_g(U_d)$ dependences, as well as comparison of simulation results with known experimental data [2–4], is the subject of further theoretical research.

As for the dependence of the arc discharge current on the inner radius of the ring electrode, here, according to relation (9), a quadratic function takes place. That is, if it is necessary to obtain a higher value of the arc discharge current, it is worth increasing the inner radius of the ring electrode R_r.

Also, an important conclusion from the obtained simulation results is that, under the condition of saturated steam, for a given value of pressure, the power of the electron beam does not affect the concentration of metal atoms. It determines only by the surface temperature of the liquid metal.

It should be noted also, that in electron beam technologies for deposition of ceramic coatings applying of an arc discharge in metal vapors and active gases, the quality of the obtained coatings and the stoichiometry of their composition directly depend on the voltage of the discharge combustion, the pressure in the technological chamber, and the discharge current [5–7]. Therefore, the simulation results and current-voltage characteristics of the arc discharge, shown in Fig. 3, have extremely important practical significance for applying the electron beam evaporation technologies in industry. Based on the obtained graphical dependencies, the designers of sputtering electron beam equipment can estimate the values of the discharge combustion voltage and the pressure in the technological chamber, which allow obtaining, by the given the known current, the required concentration and degree of activation for both metal vapors and residual gas. Since the pressure in the discharge chamber is an important parameter of the technological process, which largely depends on the quality of the obtained ceramic coating, and the voltage of the discharge combustion significantly affects the degree of gas ionization, the best way to ensure the required amount of discharge current is the correct choice of the inner radius of the ring electrode.

Conclusion

The proposed mathematical model of the arc discharge in metal vapors, which is ignited for the purpose of depositing high-quality ceramic coatings, as well as the obtained graphical dependences for the current-voltage characteristic of the discharge, are extremely important scientific results from a practical point of view. The obtained modeling results allow technologists and designers at the initial stage of designing electron-beam sputtering equipment to preliminary estimate the arc discharge current, which will ensure obtaining high-quality ceramic coatings with high stoichiometry. In general, this approach will

speed up the design of modern electron beam equipment for applying strengthening, heat-resistant and heat-protective coatings, and will also contribute to the introduction of these promising technologies into the production of electronic devices, cutting instruments, as well as engines of different transport vehicles, including cars, ships aircraft and space rockets.
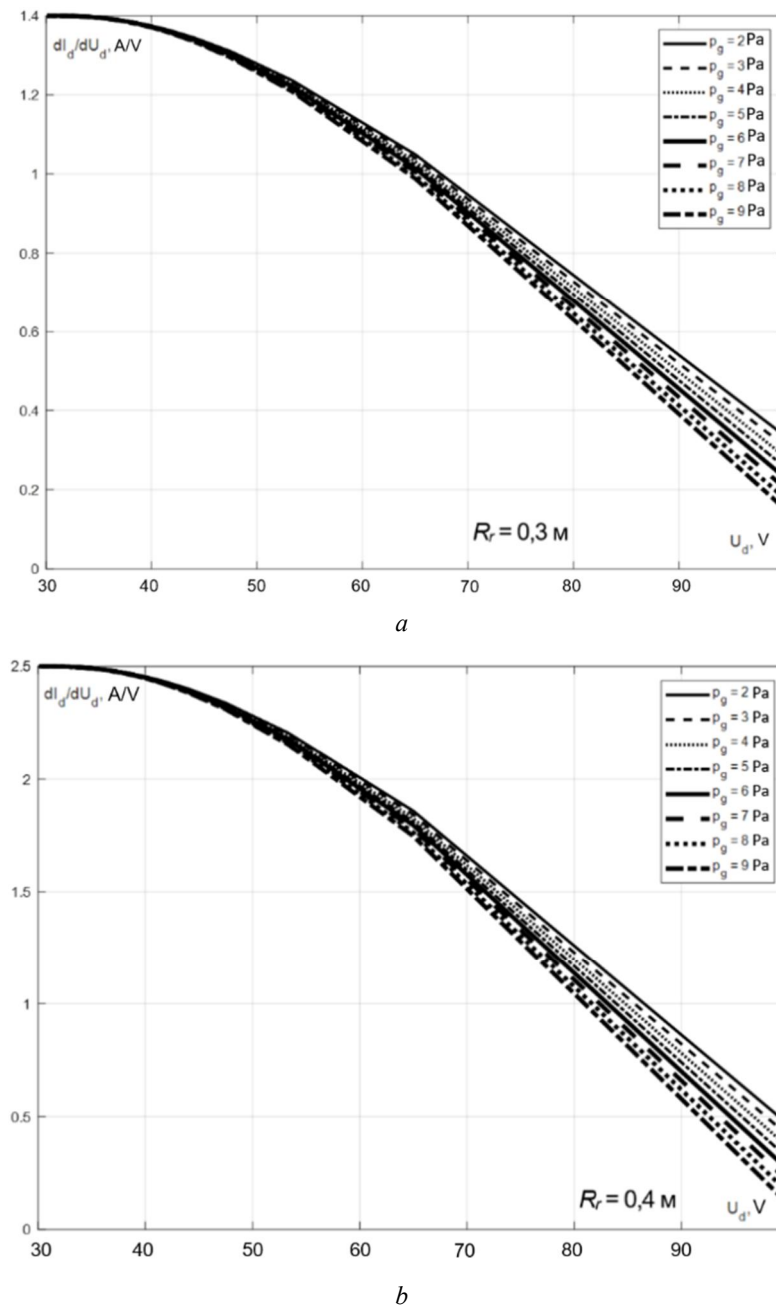

a

b

Fig. 4. The calculated dependences of the derivative of current-voltage characteristic

of the arc $\dfrac{dI_d}{dU_d}$ *on the values of the arc discharge combustion voltage, the pressure*

in the process chamber, and the inner radius of the ring electrode
for the investigated modes of operation of the technological device, the structural diagram
of which is shown in Fig. 2. $R_r = 0.3$ *m (a);* $R_r = 0.4$ *m (b)*

References

[1] *Zakharov A., Rozenko S., Litvintsev S. and Ilchenko M. 2020. Trisection Bandpass Filter with Mixed Cross-Coupling and Different Paths for Signal Propagation, IEEE Microw. Wirel. Compon. Lett. Vol. 30. No. 1. Pp. 12–15, Jan.*

[2] *Zakharov A., Litvintsev S. and Ilchenko M. (2019). Trisection Bandpass Filters with All Mixed Couplings. IEEE Microwave Wireless Components Letter. Vol. 29. No. 9. Pp. 592–594.*

[3] *Zakharov A., Rozenko S. and Ilchenko M. (2019). Varactor-tuned microstrip bandpass filter with loop hairpin and combline resonators. IEEE Transactions on Circuits Systems. II. Experimental Briefs. Vol. 66. No.6. Pp. 953–957.*

[4] *Zakharov A., Litvintsev S. and Ilchenko M. (2020). Transmission Line Tunable Resonators with Intersecting Resonance Regions. Transactions on Circuits Systems. II. Experimental Briefs. Vol. 67. no. 4. Pp. 660–664.*

[5] *Grechanyuk M. I., Melnyk A. G., Grechanyuk I. M. et al. (2014). Modern electron beam technologies and equipment for melting and physical vapor deposition of different materials. Electrotechnics and Electronics (E+E). Vol. 49. No. 5–6. Pp. 115–121.*

[6] *Mattausch G., Zimmermann B., Fietzke F., Heinss J. P., Graffel B., Winkler F., Roegner F. H., Metzner C. (2014). Gas discharge electron sources – proven and novel tools for thin-film technologies. Electrotechnics and Electronics. Vol. 49. No. 5–6 Pp. 183–195.*

[7] *Feinaeugle P., Mattausch G., Schmidt S., Roegner F. H. (2011). "A new generation of plasma-based electron beam sources with high power density as a novel tool for high-rate PVD", Society of Vacuum Coaters, 54-th Annual Technical Conference Proceedings, Chicago. Pp. 202–209.*

[8] *Denbnovetskiy S., Melnyk V., Melnyk I., Tugai B., Tuhai S., Wojcik W., Lawicki T., Assambay A., Luganskaya S. (2017). Principles of operation of high voltage glow discharge electron guns and particularities of its technological application. Proceedings of SPIE, The International Society of Optical Engineering. Pp. 10445–10455.*

[9] *Denbnovetsky S. V., Melnyk V. I., Melnyk I. V., Tugay B. A. (2003). Model of control of glow discharge electron gun current for microelectronics production applications. Proceedings of SPIE. Sixth International Conference on Material Science and Material Properties for Infrared Optoelectronics. Vol. 5065. Pp. 64–76.*

[10] *Schiller S., Heisig U., Panzer S. (1982). Electron Beam Technology. John Wiley & Sons Inc. 508 p.*

[11] *Melnyk I., Tyhai S. and Pochynok A. (2021). Universal complex model for estimation the beam current density of high voltage glow discharge electron guns. Lecture Notes in Networks and Systems: manual book, 152. Edited by Ilchenko M.Yu. Springer. P. 319–341.*

[12] *Melnyk I. V. (2005). Numerical simulation of distribution of electric field and particle trajectories in electron sources based on high-voltage glow discharge. Radioelectronics and Communications Systems, Vol. 48. No. 6. P. 41–48.*

[13] *Raizer Yu. P. (1991). Gas Discharge Physics. New York, Springer, 449 p.*

[14] *Smirnov B. M. (2015). Theory of Gas Discharge Plasma. New York, Springer. 433 p.*

[15] *Schwartz M. (2003). Principles of Electrodynamics. New-York: Dover Publications Inc. 368 p.*

[16] *Lawson J. D. (1988). The Physics of Charged-Particle Beams. 2nd Edition. Oxford University Press. 472 p.*

[17] *Szilagyi M. (2012). Electron and Ion Optics. Springer Science & Business Media. 608 p.*

[18] *Zucker R. D., Biblarz O. (2019). Fundamentals of Gas Dynamics. 3rd Edition. John Wiley and Sons, 560 p.*

[19] *Campbell P., Ellington A., Haver W., Inge V. (2013). The Elementary Mathematics Specialists Handbook. National Council of Teachers of Mathematics, 264 p.*

[20] *Mathews J. H., Fink K. D. (1998). "Numerical Methods. Using MATLAB. Third Edition", Print Hall, Amazon, 336 p.*

[21] *Kuchling H. (2014) Taschenbuch der Physik. 21 Edition. Hanser Verlag (in German).*

[22] *Espe W. (1966). Materials of High Vacuum Technology. Pergamon Press.*

АНАЛІТИЧНІ СПІВВІДНОШЕННЯ ДЛЯ РОЗРАХУНКУ СТРУМУ РОЗРЯДУ АРГ У ПАРАХ МЕТАЛІВ ЗА ФІЗИЧНИХ УМОВ ТЕХНОЛОГІЧНОГО ПРОЦЕСУ ЕЛЕКТРОННО-ПРОМЕНЕВОГО ОСАДЖЕННЯ КЕРАМІЧНИХ ПОКРИТТІВ

І. Мельник, С. Тухай, М. Скрипка, М. Суржиков, І. Швед

Національний технічний університет України "Київський політехнічний інститут імені Ігоря Сікорського",
проспект Перемоги, 37, Київ, 03056, Україна

Стаття присвячена проблемі розрахунку величини струму не самостійого дугового розряду, який запалюється та підтримується в парах металу та активних газах для забезпечення хімічної реакції між ним у технологічному процесі напарювання тонких покриттів. Отримані співвідношення в основному базуються на рівнянні Пуассона для визначення розподілу електричного поля, рівнянні Менделєєва – Клапейрона для визначення концентрації іонів у насичених парах металів, а також на рівнянні неперервності струму в газовому розряді. Сформована система рівнянь розподілу електричного потенціалу та розрядного струму в просторових координатах перетворюється на кубічне рівняння, яке розв'язано аналітично. Наведено та проаналізовано отримані результати моделювання.

Ключові слова: *електронно-променеве випаровування, керамічні покриття, дуговий розряд, розподіл електричного поля, концентрація іонів, насичені пари, кубічне рівняння.*