CALCULATIONS OF PLASMA PARAMETERS FOR HIGH POWER IMPULSE REFLEX DISCHARGE

Yu.V. Kovtun

National Science Center "Kharkov Institute of Physics and Technology", Kharkov, Ukraine E-mail: Ykovtun@kipt.kharkov.ua

The temporal behavior of the plasma parameters in a high power impulse reflex discharge are investigated using a time dependent global (volume averaged) model. The density of neutral atoms and cathode material ions coming into the discharge by the cathode sputtering mechanism is determined. The comparison between the calculation data and experimental results is provided.

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INTRODUCTION

The gas discharge plasma formed in the reflex discharge (Penning discharge) is used in many technical devices which are widely used for solving both physical and applied problems, for example, in the charged particle sources [1], ion pumps and vacuum gauges [2] etc. The reflex discharge was first proposed by Penning F.M. [3] in 1936 for developing a vacuum manometer. During the many-year history a large number of various reflex discharge models were offered and investigated. However, despite the long-term and numerous researches, there is no satisfactorily complete physical model that would describe the reflex discharge. This circumstance is partially connected with the fact that the reflex discharge has a number of modes depending on the working gas pressure and the magnetic field [4]. In the case of low gas pressure $(p \le 1.33 \cdot 10^{-2} \text{ Pa})$ in the interelectrode space a negative volume charge is predominant. Under higher gas pressures $(p > 1.33 \cdot 10^{-2} \text{ Pa})$ the whole interelectrode space is filled with plasma. The reflex discharge under pressures above $p > 1.33 \cdot 10^{-2} \,\mathrm{Pa}$ is often used as a base for formation of plasma sources.

Global (volume-averaged) models of steady-state and pulse plasma discharges [5] are simple but rather powerful tools to analyze. They have less computational load and results of simulation can be analyzed relatively easily. In [6], a model of stationary reflex discharge on the basis of the volume-averaged (global) model [5, 7] was proposed and analyzed. The difference between experimental results with calculated data in [6] was within a factor ~2. The model proposed in [6] was further developed in [8]. The model takes into account the Penning ionization of sputtered cathode atoms and their influence on the balance of charged particles in plasma.

The authors of [9] investigated the behaviour of argon plasmas produced by time-modulated power in high-density plasma reactors using a spatially averaged (global) model. A global plasma model for an ionized physical vapor deposition (IPVD) system is described in [10]. The ionization mechanism and the temporal behavior of the plasma parameters in a high power impulse magnetron sputtering (HiPIMS) discharge was investigated in [11] using a time dependent global model. A time-dependent global plasma model for ionization region (IRM model) in a HiPIMS discharge was proposed and analyzed in [12]. The processes of modulated pulsed power magnetron sputtering (MPPMS) discharge are numerically modeled (time-dependent global plasma model) and experimentally investigated in [13].

The previous experience [14, 15] testifies that the high power impulse reflex discharge is an effective instrument for producing a multicomponent gas-metal plasma. In this case, the metal plasma component is formed as a result of the ionization of particles sputtered from cathode that penetrate into the discharge. The processes of injection of a sputtered and ionized working material into the impulse reflex discharge plasma have been considered in [16] at an initial stage of dense gasmetal plasma formation. A calculation model has been proposed to estimate the parameters of the sputtering mechanism for the required working material to be injected into the discharge.

In the present paper the modeling of a high power impulse reflex discharge is provided on the base of the time dependent global (volume-averaged) model.

1. EXPERIMENTAL DETAILS

The parameters of the multicomponent gas-metal plasma of a high-power impulse reflex discharge were investigated at the "MAKET" facility [14] representing the stainless steel vacuum chamber with the internal diameter of 20 cm and the length of 200 cm. A maximum magnetic field induction is $B_0 \leq 0.9$ T, magnetic field pulse duration – 18 ms. The vacuum chamber was pumped down to a pressure of $1.33 \cdot 10^{-4}$ Pa; then the igniting gas Ar was let into the chamber. The plasma was produced by discharging a capacitor bank ($C = 560~\mu\text{F},~U_0 = 3.8~\text{kV}$) between two cold cathodes with diameter $\emptyset = 10~\text{cm}$, and the anode (vacuum chamber). The cathodes were made from metallic Ti. The gas-metal plasma was produced in the mixture of the igniter gas and the sputtered cathode material.

The multicomponent gas-metal plasma density was investigated by microwave interferometry method. The plasma probing was performed across the plasma column using the ordinary O-wave with the wavelengths $\lambda=8$ mm and $\lambda=4.13$ mm. Besides, the current-voltage characteristic of the discharge was regularly measured, giving possibility to estimate the energy deposited in plasma.

2. THE PULSED-POWER MODEL

The calculation is done by utilizing a time dependent global model of a cylindrical plasma discharge, assuming uniform spatial distributions of plasma parameters over the plasma volume. All species densities are volume averaged. The electron density $N_{\rm e}$ is directly given by the ion densities N_i assuming quasineutrality of the plasma $N_{\rm e} = \Sigma Z_{\rm i} N_{\rm i}$, where $Z_{\rm i}$ is ion charge. In the reflex

discharge the most part of electrons go away in the radial direction to the anode, and ions are axially directed to the cathodes. The fluxes of ions and electrons are assumed to be equal. The electrons are assumed to be in thermal equilibrium and have a Maxwellian-like energy distribution function.

The total heat balance of the rotating plasma was considered in [17, 18] with assumption that the power is deposited uniformly into the plasma volume. The absorbed power was assumed equals to $P_{abs}(t) = P_d(t)F_d$, where $P_{\rm d}(t)$ is discharge power input, $P_{\rm d}(t) = I_{\rm d}(t) \ U_{\rm d}(t)$, and $F_{\rm d}$ is the adjustable parameter. The discharge voltage $U_d(t)$ and the discharge current $I_d(t)$ were determined experimentally. A fitting parameter F_d represents the fraction of the discharge power input that goes into heating of electrons. In the paper [18] the components of the energy balance in rotating plasma were calculated. Taking into account the results of [18], the adjustable parameter was taken as $F_{\rm d}=0.35$. The plasma is described by a set of nonlinear equations: particle balance equation for each of the species and one power balance equation were calculated in sections 3 and 4.

3. PARTICLE BALANCE

In generalized form, the particle balance equation is given by:

$$\frac{dN}{dt} = \sum_{i} R_{\text{Gener, i}} - \sum_{i} R_{\text{Loss, i}}, \qquad (1)$$

where $R_{\rm Gener,i}$ and $R_{\rm Loss,i}$ are the characteristic particle generation rate and loss rate, respectively, with including of variety of processes running in plasma – such as ionization, excitation, recombination, diffusion, charge exchange, and others.

3.1. PARTICLE BALANCE FOR Ar SPECIES

The rate equation for the working gas Ar is

$$\begin{split} &\frac{dN_{\rm Ar}}{dt} = \frac{1}{V_{\rm p}} \left(N_{\rm Ar^{+}} V_{\rm B}^{\rm Ar^{+}} A_{\rm eff} + N_{\rm Ar^{2+}} V_{\rm B}^{\rm Ar^{2+}} A_{\rm eff} \right) + \\ &+ N_{\rm Ar^{+}} \left(N_{\rm e} \left(N_{\rm e} \alpha_{\rm 3} + \alpha_{\rm RR} + N_{\rm Ar} \alpha_{\rm tb} + \alpha_{\rm DR} \right) + N_{\rm Ti} K_{\rm CT}^{\rm Ar^{+}-Ti} \right) - \\ &- N_{\rm Ar} \left(N_{\rm e} K_{\rm iz}^{\rm Ar} + N_{\rm Ar^{2+}} K_{\rm CT}^{\rm Ar^{2+}-Ar} \right) \end{split}$$
(2)

where $N_{\rm Ar}$, $N_{\rm Ti}$, $N_{\rm Ar}^+$, $N_{\rm Ar}^{2+}$, $N_{\rm e}$ are densities of: neutral atoms Ar and Ti, ions Ar⁺ and Ar²⁺, electrons; $\nu_{\rm B}^{{\rm Ar}^+}$, $\nu_{\rm B}^{{\rm Ar}^2-}$ the Bohm velocity of ions Ar⁺ and Ar²⁺; $K_{\rm CT}^{{\rm Ar}^+-{\rm Ti}}$, $K_{\rm CT}^{{\rm Ar}^2-{\rm Ar}}$ are the rate constants of gas ion charge transfer; $V_{\rm p}$ – the plasma volume; $A_{\rm eff}$ is the effective area for charged particle loss; $K_{\rm iz}^{{\rm Ar}}$ is the rate constant for the neutral particle ionization; α_3 – the rate constant for the collisional three-body (e – e – ion) recombination; $\alpha_{\rm tb}$ – the rate constant for the electron-ion radiative recombination; $\alpha_{\rm RD}$ – the rate constant for the dielectronic recombination.

For Ar⁺ ions the rate equation can be written as

$$\frac{dN_{Ar^{+}}}{dt} = N_{Ar}N_{e}K_{iz}^{Ar} + N_{Ar^{2+}}\left(N_{e}\left(N_{e}\alpha_{3}^{1} + \alpha_{RR}^{1} + \alpha_{DR}^{1}\right) + 2N_{Ar}K_{CT}^{Ar^{2+}-Ar}\right) - N_{Ar^{+}}\left(N_{e}\left(N_{e}\alpha_{3} + \alpha_{RR} + N_{Ar}\alpha_{tb} + \alpha_{DR}\right) + K_{iz}^{Ar^{2+}}\right) + N_{Ti}K_{CT}^{Ar^{+}-Ti}\right) - N_{Ar^{+}}N_{e}K_{iz}^{Ar^{+}} - \frac{1}{V_{o}}N_{Ar^{+}}V_{B}^{Ar^{+}}A_{eff},$$
(3)

where α_3^1 ; α_{RR}^1 α_{RD}^1 are the rate constants for recombination of Ar^{2+} ions; $K_{iz}^{Ar^+}$ is the rate constant for the ionization ion Ar^+ .

The rate equation for Ar²⁺ ions is

$$\frac{dN_{Ar^{2+}}}{dt} = N_{Ar^{+}}N_{e}K_{iz}^{Ar^{+}} - N_{Ar^{2+}}\left(N_{e}\left(N_{e}\alpha_{3}^{1} + \alpha_{RR}^{1} + \alpha_{DR}^{1}\right) + A_{RR}K_{CT}^{Ar^{2+}-Ar}\right) - \frac{1}{V_{a}}N_{Ar^{2+}}V_{B}^{Ar^{2+}}A_{eff}.$$
(4)

The rate constants, cross-sections, and various process parameters used in the calculations were taken from [19 - 28]. They are quoted in Table.

3.2. PARTICLE BALANCE FOR Ti SPECIES

The interaction of plasma formed in the reflex discharge with the cathode surface results in destruction of a cathode material owing to sputtering; the eroded material goes into the plasma and is subsequently ionized.

The rate equation for Ti atoms is:

$$\begin{split} &\frac{dN_{\text{Ti}}}{dt} = \frac{1}{V_{p}} \left(Y_{g} N_{\text{Ar}^{+}} v_{\text{B}}^{\text{Ar}^{+}} A^{1}_{\text{eff}} + Y_{g} N_{\text{Ar}^{2+}} v_{\text{B}}^{\text{Ar}^{2+}} A^{1}_{\text{eff}} + \right. \\ &+ Y_{\text{m}} N_{\text{Ti}^{+}} v_{\text{B}}^{\text{Ti}^{+}} A^{1}_{\text{eff}} + Y_{\text{m}} N_{\text{Ti}^{2+}} v_{\text{B}}^{\text{Ti}^{2+}} A^{1}_{\text{eff}} + \\ &+ Y_{\text{m}} N_{\text{Ti}^{3+}} v_{\text{B}}^{\text{Ti}^{2+}} A^{1}_{\text{eff}} \right) + N_{\text{Ti}^{+}} \left(N_{e} \left(N_{e} \alpha^{11}_{3} + \alpha^{11}_{\text{RR}} + \alpha^{11}_{\text{DR}} \right) \right) - \\ &- N_{\text{Ar}^{+}} N_{\text{Ti}} K_{\text{CT}}^{\text{Ar}^{+} - \text{Ti}} - N_{\text{Ti}} N_{e} K_{\text{iz}}^{\text{Ti}} - \frac{N_{\text{Ti}}}{\tau_{\text{D}}}, \end{split}$$
(5)

Here N_{Ti}^{+} , N_{Ti}^{2+} , N_{Ti}^{3+} are, respectively, density of ions Ti⁺, Ti²⁺ and Ti³⁺; $\nu_{\text{B}}^{\text{Ti}}$, $\nu_{\text{B}}^{\text{Ti}^{2+}}$, $\nu_{\text{B}}^{\text{Ti}^{3+}}$ are Bohm velocity of ions Ti⁺, Ti²⁺ and Ti³⁺; $K_{i\epsilon}^{\text{Ti}}$ is the rate constant for the neutral particle ionization; α_{3}^{-11} ; α_{RR}^{-11} , and α_{RD}^{-11} are the rate constant for recombination of ion Ti⁺; Y_{m} and Y_{g} – the sputtering coefficients of the cathode material by metal and gas ions, correspondingly; A_{eff}^{-1} is the effective area of charged particle loss on cathodes; τ_{D} – the characteristic diffusion time of a sputtered particle, $\tau_{\text{D}} = \Lambda/D_{\text{m}}$, with Λ as the characteristic time of sputtered particle diffusion and D_{m} – as its diffusion coefficient in the gas or plasma. To calculate the ratio of sputtering, the diffusion time of a neutral atom and the time of its ionization we use the model proposed in [16].

For Ti ions the rate equation can be written as

$$\begin{split} & \frac{dN_{\text{Ti}^{+}}}{dt} = N_{\text{Ti}} N_{\text{e}} K_{\text{iz}}^{\text{Ti}} + N_{\text{Ar}^{+}} N_{\text{Ti}} K_{\text{CT}}^{\text{Ar}^{*}-\text{Ti}} + \\ & + N_{\text{Ti}^{2+}} N_{\text{e}} \left(\alpha^{21}_{\text{RR}} + \alpha^{21}_{\text{DR}} \right) - N_{\text{Ti}^{+}} N_{\text{e}} K_{\text{iz}}^{\text{Ti}^{+}} - \\ & - N_{\text{Ti}^{+}} \left(N_{\text{e}} \left(N_{\text{e}} \alpha^{11}_{3} + \alpha^{11}_{\text{RR}} + \alpha^{11}_{\text{DR}} \right) \right) - \frac{1}{V_{\text{p}}} N_{\text{Ti}^{+}} V_{\text{B}}^{\text{Ti}^{+}} A_{\text{eff}} , \end{split}$$

$$(6)$$

where α_{RR}^{2l} , α_{RD}^{2l} are the rate constants for recombination of Ti^{2+} ; $K_{iv}^{Ti^{+}}$ the rate constant for ionization ion Ti^{+} .

$$\frac{dN_{\text{Ti}^{2+}}}{dt} = N_{\text{Ti}^{+}} N_{\text{e}} K_{\text{iz}}^{\text{Ti}^{+}} + N_{\text{Ti}^{3+}} N_{\text{e}} \left(\alpha^{31}_{\text{RR}} + \alpha^{31}_{\text{DR}} \right) + \\
- N_{\text{Ti}^{2+}} N_{\text{e}} K_{\text{iz}}^{\text{Ti}^{2+}} - N_{\text{Ti}^{2+}} N_{\text{e}} \left(\alpha^{21}_{\text{RR}} + \alpha^{21}_{\text{DR}} \right) - \frac{1}{V_{\text{p}}} N_{\text{Ti}^{2+}} V_{\text{B}}^{\text{Ti}^{2+}} A_{\text{eff}},$$
(7)

The α_{RR}^{31} , α_{RD}^{31} are rate constants for recombination of ion Ti³⁺; $K_{iz}^{Ti^{2+}}$ – the rate constant for ionization of ion Ti²⁺.

$$\frac{dN_{\text{Ti}^{3+}}}{dt} = N_{\text{Ti}^{2+}} N_{\text{e}} K_{\text{iz}}^{\text{Ti}^{2+}} - N_{\text{Ti}^{3+}} N_{\text{e}} \left(\alpha^{31}_{\text{RR}} + \alpha^{31}_{\text{DR}} \right) - \frac{1}{V_{\text{p}}} N_{\text{Ti}^{3+}} V_{\text{B}}^{\text{Ti}^{3+}} A_{\text{eff}}.$$
(8)

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		Dun	Rate	Cita-	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Process		coefficient	tion	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$					
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1		$K_{ m iz}^{ m Ar}$	19	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	2			19	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3		$K_{\mathrm{iz}}^{\mathrm{Ti}}$	19	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	•	$oldsymbol{K}_{ m iz}^{ m Ti^+}$	19	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	$e + Ti^{2+} \rightarrow Ti^{3+} + 2e$	$K_{\rm iz}^{{ m Ti}^{2+}}$	19	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	6	$2e + Ar^+ \rightarrow Ar + e$	α_3	20	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	$2e + Ar^{2+} \rightarrow Ar^{+} + e$		21	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	8	$Ar^+ + Ar + e \rightarrow Ar + Ar$	$\alpha_{ m th}$	22	
Radiative recombination 10	9		a_3^{11}	23	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Radiative recombination				
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	10	$e + Ar^+ \rightarrow Ar + hv$	$\alpha_{ m RR}$	24	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	11	$e + Ar^{2+} \rightarrow Ar^{+} + hv$	α_{RR}	24	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	12	$e + Ti^+ \rightarrow Ti + hv$	α_{RR}	23	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	13	$e + Ti^{2+} \rightarrow Ti^{+} + hv$	$\alpha_{\rm RR}^{21}$	23	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	14	$e + Ti^{3+} \rightarrow Ti^{2+} + hv$	$\alpha_{\rm RR}^{31}$	23	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Dielectronic recombination				
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	15	$e + Ar^+ \rightarrow Ar^* \rightarrow Ar$	$\alpha_{ m RD}$	25	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	16	$e + Ar^{2+} \rightarrow Ar^{+*} \rightarrow Ar^{+}$	$\alpha_{ m RD}$	25	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	17	$e + Ti^+ \rightarrow Ti^* \rightarrow Ti$	I ORD	25	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	18	$e + Ti^{2+} \rightarrow Ti^{+*} \rightarrow Ti^{+}$	a_{RD}^{21}	25	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	19	$e + Ti^{3+} \rightarrow Ti^{2+*} \rightarrow Ti^{2}$	a_{RD}^{31}	25	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Charge transfer				
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	20		$K_{\mathrm{CT}}^{\mathrm{Ar}^{2+}-\mathrm{Ar}}$	26	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	21	$Ti + Ar^+ \rightarrow Ti^+ + Ar$		27	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Sputtering				
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	22	$Ar^+ \rightarrow Ti$		28	
$ \begin{array}{c ccccc} 24 & Ti^+ \rightarrow Ti & Y_m & 28 \\ \hline 25 & Ti^{2+} \rightarrow Ti & Y_m & 28 \end{array} $	23	$Ar^{2+} \rightarrow Ti$		28	
$25 \qquad \text{Ti}^{2+} \rightarrow \text{Ti} \qquad Y_{\text{m}} \qquad 28$	24	$Ti^+ \rightarrow Ti$		28	
	25	$Ti^{2+} \rightarrow Ti$		28	
	26	$Ti^{3+} \rightarrow Ti$	$Y_{ m m}$	28	

^{*} excited atoms and ions

3.3. PARTICLE BALANCE FOR ELECTRONS

The continuity equation for the electrons is determined by quasineutrality, the electron flux across the boundary is obtained as the sum of all ion fluxes. Accordingly, for equation 1, the characteristic rates of generation and loss of electrons are similar to those described in equations 2-8.

4. POWER BALANCE

In the power balance equation the absorbed power equates to power losses. The time-dependent electron temperature $T_{\rm e}$ can be obtained by solving the energy balance equation of the system:

$$V_{\rm p} \left(\frac{d}{dt} \left(\frac{3}{2} \cdot q \cdot N_{\rm e} \cdot T_{\rm e} \right) \right) = P_{\rm abs}(t) - P_{\rm loss}(t), \quad (9)$$

Here P_{abs} is the absorbed power, $P_{abs}(t) = P_{d}(t)F_{d}$; $P_{\rm loss}(t)$ – power losses defined as

$$P_{\text{los}} = P_{\text{Ve}} + P_{\text{le}} + P_{\text{li}} + P_{\text{R}} + P_{\text{ll}},$$
 (10)

where P_{Ve} is the power released in the volume due to energy loss in collisions of electron with neutral particles; P_{le} is plasma power taken by electrons; P_{li} – plasma power taken by ions; P_R – power of recombination (free-bound) radiation [23]; P_{\parallel} – power lost in electronion collisions.

A part of the input power is also lost as kinetic energy loss of particles (electrons and ions) to the walls, what can be described as

$$P_{\rm le} = q \cdot N_{\rm e} \cdot v_{\rm B} \cdot A_{\rm eff} \cdot W_{\rm e}, \tag{11}$$

$$P_{\rm li} = \sum q \cdot Z_{\rm i} \cdot N_{\rm i} \cdot v_{\rm R} \cdot A_{\rm eff} \cdot W_{\rm i}. \tag{12}$$

$$\begin{split} P_{\text{le}} &= q \cdot N_{\text{e}} \cdot v_{\text{B}} \cdot A_{\text{eff}} \cdot W_{\text{e}}, \\ P_{\text{li}} &= \sum q \cdot Z_{\text{i}} \cdot N_{\text{i}} \cdot v_{\text{B}} \cdot A_{\text{eff}} \cdot W_{\text{i}}. \\ \text{In these equations } q \text{ is electron charge; } W_{\text{e}} - \text{the av-} \end{split}$$
erage kinetic energy taken by electrons, in the Maxwell distribution assumption its value is $2T_e$; W_i – average kinetic energy taken by ions, which equals to the sum of ion energies before coming into the sheath (Debye sheath) and obtained in the sheath, $W_i = (T_e/2) + V_s$, where V_s is the cathode potential drop approximately equals to the discharge voltage U_d .

The power lost in electron-ion collisions is defined according to:

$$P_{\rm ll} = V_{\rm p} \sum_{\rm q} \cdot Z_{\rm i} \cdot N_{\rm i} \cdot (3 \ m_{\rm e} / m_{\rm i}) \cdot (T_{\rm e} - T_{\rm g}) \cdot W_{\rm i} \cdot v_{\rm ei}$$
. (13) Here $m_{\rm e}$ and $m_{\rm i}$ are mass of electron and ion; $v_{\rm ei}$ – is the electron-ion collision rate, $T_{\rm g}$ is the gas temperature.

The power released in the volume due to the electron energy loss during collision with neutral particles defined as:

$$P_{\text{Ve}} = q \cdot N_{\text{e}} \cdot N_{0} \cdot V_{\text{p}} \cdot W_{\text{iz}} \cdot K_{\text{iz}}. \tag{14}$$

 $P_{\rm Ve} = q \cdot N_{\rm e} \cdot N_0 \cdot V_{\rm p} \cdot W_{\rm iz} \cdot K_{\rm iz}.$ For ions this equation takes the form:

$$P_{\text{Ve}} = \sum q \cdot N_{\text{e}} \cdot N_{0} \cdot V_{\text{p}} \cdot W_{\text{iz}} \cdot K_{\text{iz}}, \qquad (15)$$

where W_{iz} is the average energy spent for ion-electron pair formation or the ionization cost. For neutral titanium and ions (Ar⁺, Ti⁺, Ti²⁺, Ti³⁺), the value W_{iz} was taken equal to the ionization potential.

4.1. MEAN ENERGY EXPENDED PER ION PAIR BY ELECTRONS

For partly ionized plasma, it is necessary to take into account all processes associated with direct, cascade, and nonradiative transitions, and the ionization cost in this case depends not only on the temperature, but also on the electron number density. The calculations taking into account all the processes are rather complicated. In the model proposed in [7], cascade and nonradiative transitions are ignored. Thus, the mean energy expended per ion pair by electrons for an atom can be determined from the relation [7]:

$$W_{iz}(T_{e}) = E_{iz} + \sum_{i} E_{exc,i} \frac{K_{exc,i}(T_{e})}{K_{iz}(T_{e})} + \frac{K_{elas}(T_{e})}{K_{iz}(T_{e})} \frac{3m_{e}}{m_{M}} T_{e},$$
(16)

where $E_{\rm exc,i}$ and $K_{\rm exc,i}$ denote, respectively, the energy and the excitation rate constants of electronic levels of the atom; E_{iz} and K_{iz} are the energy and the rate constant of ionization, $K_{\rm elas}$ is the rate constant of elastic collisions. In the calculations are used the cross sections of the elementary processes: elastic scattering [29], excitation of 43 electron levels of Ar atoms [29, 30], ionization [19]. The results of the calculation are shown in Fig. 1.

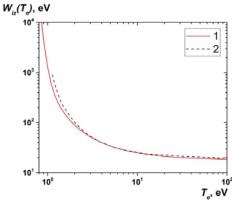


Fig. 1. Mean energy per electron-ion pair for Ar on electron temperature: present results (curve 1), data [31] (curve 2)

5. RESULTS AND DISCUSSION 5.1. CALCULATION RESULTS

Let us calculate the density and electron temperature in the high power impulse reflex discharge. The initial conditions are as follows: plasma column radius R = 0.1 m; its length – L = 1.35 m; Ar pressure $p = 0.267 \text{ Pa } (N_0 = 7.075 \cdot 10^{19} \text{ m}^{-3}); \text{ the plasma volume}$ $V = 0.042 \text{ m}^3$; cathode surface area -0.016 m^2 , area of the end surface of the plasma cylinder – 0.063 m². Initial electron density $N_e = 4 \cdot 10^{16} \text{ m}^{-3}$, $T_e = 1 \text{ eV}$.

A system of 9 ordinary differential equations was solved numerically, using the fourth-order Runge-Kutta fixed-step method. The results of calculations are shown in Figs. 2-4. By convention, the time behavior of the gas-metal plasma density can be divided into three stages. The first stage consists in the plasma creation and its density rise. The second stage presents the existence of the dense highly ionized plasma. The degree of ionization of argon and titanium is, respectively $\approx 84\%$ and ~ 100% (see Fig. 4). The third stage - when plasma density is decreasing and decays. The maximum electron temperature (see Fig. 2,b) was 7 eV (first stage), the minimum 0.38 eV (third stage). The maximum particle density was (see Fig. 3): electrons N_e = $7.15 \cdot 10^{19} \text{ m}^{-3}$; argon ions $5.96 \cdot 10^{19} \text{ m}^{-3}$ (Ar⁺) and $3.3 \cdot 10^{17} \,\mathrm{m}^{-3} \,(\mathrm{Ar}^{2+})$; titanium ions $4.43 \cdot 10^{17} \,\mathrm{m}^{-3} \,(\mathrm{Ti}^{+})$, 1.33·10¹⁸ m⁻³ (Ti²⁺) and 3.29·10¹⁶ m⁻³ (Ti³⁺). The density of titanium ions Ti²⁺ is greater than that of ions Ti⁺. In Penning-type plasma source [32], the density of Ti²⁺ is less than that of Ti⁺. This is due to the failure to take into account a number of elementary processes, the cross sections of which are absent in the literature.

These are the processes: of charge transfer (Ti, Ar – neutral atoms, Ar* - excited atoms, Arm - metastable atoms)

$$Ti^{2+} + Ti \rightarrow Ti^{+} + Ti^{+},$$
 (17)

$$Ti^{2+} + Ar \rightarrow Ti^{+} + Ar^{+},$$
 (18)

$$Ti^{2+} + Ar^* \rightarrow Ti^+ + Ar^+$$
. (19)

$$Ti^{2+} + Ar \rightarrow Ti^{+} + Ar^{+},$$
 (18)
 $Ti^{2+} + Ar^{*} \rightarrow Ti^{+} + Ar^{+},$ (19)
 $Ti^{2+} + Ar^{m} \rightarrow Ti^{+} + Ar^{+},$ (20)

and three-body recombination

$$2e + Ti^{2+} \rightarrow Ti^{+} + e,$$
 (21)

$$Ti^{2+} + Ti + e \rightarrow Ti^{+} + Ti,$$
 (22)

$$Ti^{2+} + Ar + e \rightarrow Ti^{+} + Ar.$$
 (23)

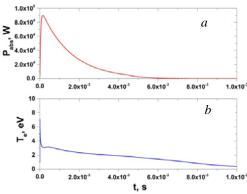
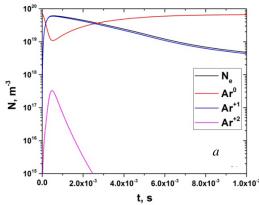


Fig. 2. Modeled time evolution of the adsorbed power $P_{abs}(a)$ and electron temperatures (b)



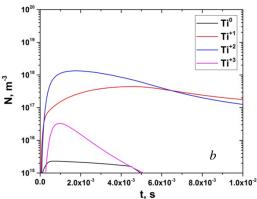


Fig. 3. Modeled time evolution of the density of electrons, argon atoms, species ions (a) and titan atoms, species ions (b)

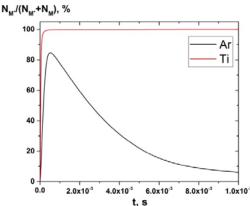


Fig. 4. Degree of ionization of Ar atoms, and sputtered metal (Ti) atoms

The density of neutral argon atoms is greater than of titanium. Accordingly, the reactions (18) - (20), (23) with neutral argon will make a significant contribution. Process (18) is endothermic, respectively, under the given conditions is unlikely. The lifetime of the excited states of argon atoms is small in comparison with the collision time. Therefore, the contribution of process 19 is apparently insignificant. In contrast, the processes of 20 (the lifetime of metastable levels Ar^m is longer than the collision time), 21, and 23 make the greatest contribution to the decrease of the Ti^{2+} ions charge. In calculations there were not taken into account the concentrations of metastable atoms Ar^m and the dimers $(Ar_2^+, ArTi^+, Ti_2^+)$, which can be formed in the discharge plasma [33]. Thus, the decrease of Ti^{2+} ions density (see Fig. 3) can be explained if accounting all processes enumerated above.

5.2. COMPARISON WITH MEASUREMENTS

Fig. 5 shows the comparison of electron density measured in a high-power impulse reflex discharge and that found by calculations (the initial stage of the discharge). As can be seen, the results of the calculations differ from the experimental data by no more than a factor of ~2. Such difference can be the result of some unaccounted factors in the considered model. For example, in the calculations the electron energy distribution function was assumed to be Maxwellian, whereas in reality, several groups of electrons with different energy can exist in plasma of such discharge.

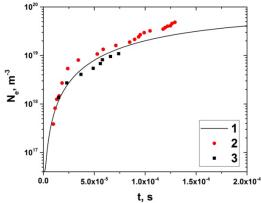


Fig. 5. Comparison of the calculated (1) and experimental (2), (3) electron density at the initial stage of the discharge. Microwave interferometer $\lambda = 4.13$ mm (2) and $\lambda = 8$ mm (3) $(p = 0.267 \ Pa, \ U_0 = 3.8 \ kV)$

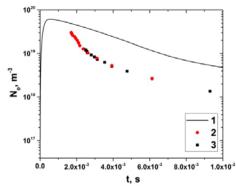


Fig. 6. Comparison of the calculated (1) and experimental (2), (3) electron density. Microwave interferometer $\lambda = 4.13$ mm (2) and $\lambda = 8$ mm (3) (p = 0.267 Pa, $U_0 = 3.8$ kV)

During the whole time of the discharge (Fig. 6), the values of calculated and measured electron density dif-

fer within factor 2-5: the calculated values are larger than the experimental ones. This fact may be explained by failure to take account of all loss channels for radiative losses and losses of plasma particles. To more fully take into account the radiation losses, it is necessary to create a collisional-radiative plasma model. Besides, classic plasma diffusion across magnetic field was assumed for calculation, but in practice in the reflex discharge an anomalous diffusion with the transverse diffusion coefficient close to the Bohm diffusion coefficient was observed.

CONCLUSIONS

Within the framework of the model under consideration, the plasma density (ions and electrons) and temperature in the high-power impulse reflex discharge are calculated. The processes of cathode material sputtering with subsequent ionization of sputtered atoms in the plasma are investigated. The density of neutral particles and sputtered cathode material atomic ions are determined. The comparison between the calculation data and experimental results has been performed. In general, the modeled densities are in satisfactory agreement with the experimental data. Further development of the model can give more accurate coincidence between the experimental and calculation results.

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РАСЧЕТ ПАРАМЕТРОВ ПЛАЗМЫ МОЩНОГО ИМПУЛЬСНОГО ОТРАЖАТЕЛЬНОГО РАЗРЯДА *Ю.В. Ковтун*

Исследовано изменение параметров плазмы во времени в мощном импульсном отражательном разряде с использованием зависящей от времени глобальной (усредненной по объему) модели. Определена плотность нейтральных атомов и ионов материала катода, поступающих в разряд за счет механизма катодного распыления. Проведено сравнение расчетных данных с результатами эксперимента.

РОЗРАХУНОК ПАРАМЕТРІВ ПЛАЗМИ ПОТУЖНОГО ІМПУЛЬСНОГО ВІДБИВНОГО РОЗРЯДУ $\emph{Ю.В.}$ Ковтун

Досліджено зміну параметрів плазми в часі в потужному імпульсному відбивному розряді з використанням залежної від часу глобальної (усередненої за об'ємом) моделі. Визначена густина нейтральних атомів та іонів матеріалу катода, що надходять у розряд за рахунок механізму катодного розпилення. Проведено порівняння розрахункових даних з результатами експерименту.