Third type boundary conditions for steady state ambipolar diffusion equation

V S Zheltukhin\textsuperscript{1}, S I Solov’ev\textsuperscript{2}, P S Solov’ev\textsuperscript{2}, V Yu Chebakova\textsuperscript{2} and A M Sidorov\textsuperscript{2}

\textsuperscript{1}Kazan State Technological University, 68 Karl Marx Street, Kazan, 420015, Russia
\textsuperscript{2}Kazan Federal University, 18 Kremlevskaya Street, Kazan, 420008, Russia

E-mail: vchebakova@mail.ru

Abstract. A third type boundary condition for boundary value problem of electron balance in inductively coupled radio-frequency (ICRF) discharge is described. It is assumed that directions of diffusion and drift flows on boundary through the positive charge layer are coincided. Herein we study the effect of different boundary conditions on the parameters of ICRF discharge by computational solution of eigenvalue problems. It is showed that electronic temperature at boundary conditions derived in this study differ from the electronic temperature at boundary condition which mean a complete recombination of charged particles on the wall of gas discharge chamber (DC). The derived boundary conditions can be used for modelling ICRF discharges to determine optimal parameters of plasmatrons.

1. Introduction

ICRF discharge is widely used in different technological plasma processes. Modes of material processing are extremely sensitive to the main parameters of ICRF discharge. Mathematical modelling is necessary for more efficient and better choice of design solutions RF plasma equipment as some technological characteristics of plasma either evade direct measurements, or such measurements are labor-consuming [1-5].

2. Boundary condition derivation

Magnetic field in inductively plasmatron is directed lengthwise the coil axis, and force electric lines are the circle and plasma density is high; in other words, we can assume that current is vortex and the volume charge does not accumulate in quasineutral plasma, and relatively diffusion is ambipolar. ICRF discharges is modeled at local or non-local of electron distribution function which depends on ratio of electron energy relaxation length with skin-layer thickness. Herein we provide a mathematical model of ICRF discharge in case of non-local function of distribution in total discharge volume.

Evaluation of elementary processes taking place in low pressure ICRF plasma is showed that time of steady state stabilization exceeds a lot an electromagnetic field oscillation period. Correspondingly, fluctuations of plasma properties near average values, taken per the variation period, are negligible. With a glance to this hypothesis, balance equation of electrons in plasma of low pressure ICRF discharge takes the following form

$$\frac{1}{r} \frac{d}{dr} \left( r D_e \frac{d n}{dr} + r V_e n \right) = \nu n - \beta n^2, \quad 0 < r < R.$$ 

Here $R$ is the...
radius, is a coefficient of ambipolar diffusion, \( \beta \) is a recombination coefficient, \( v_i \) is an ionization frequency, \( V_a \) is gas flow velocity. It is supposed that \( D_e \) and \( v_i \) are functions of electron temperature.

Symmetry axis of the chamber stipulates condition that means continuity of flow of the charged particles. The border of the discharge including surface of the discharge chamber (DC) usually stipulates condition that means complete recombination of the charged particles on DC walls. But this condition results in infinite value of electron velocity near DC wall that is in conflict with discharge physics. It is known that double electric layer forms near the surface of a solid in plasma and such solid has negatively potential to plasma. Therefore a condition of equality of diffusion flow from plasma to drift flow through a double layer is more correctly than the condition of complete recombination on DC walls. Evaluations of elementary processes in plasma of low pressure ICRF discharge are showed that the last particle collisions take place approximately at the average free path from the wall surface. At low pressure the double layer thickness is more less than the mean free path of electrons. So we suppose that double layer is collisionless. Let us assume that deviation of the electron energy distribution function from Maxwellian is low at the first approximation. In this case, only those electrons can achieve the surface, which have velocity directed to the surface of electrode and energy of which is sufficient to overcome potential barrier. So, we can point microscopic density of electron and ion flux on the surface as flux density of corresponding particles, energy of which allows overcoming difference of potentials between the wall surface and potential of plasma at the border of plasma and double layer [6]. From the condition of continuity of particle flows, it follows that microscopic values of density of charged particle flux shall be equal to the corresponding values of flux density, when \( x = X_b \):

\[
U_e = -\frac{\mu_e}{\mu_e + \mu_i} J_b \frac{d n_e}{d x} - \frac{D_e}{n_b} \left( \frac{d n_e}{d x} \right)_b, \quad U_i = -\frac{\mu_i}{\mu_e + \mu_i} J_b \frac{d n_i}{d x} - \frac{D_i}{n_b} \left( \frac{d n_i}{d x} \right)_b
\]

where \( n_b \) is density of particles at the border of plasma and double layer, \( \mu_e, \mu_i \) is electron and ion mobility ratios, \( J_b \) - density of charged particle flux.

As a result, we get the system

\[
\begin{align*}
\frac{n_b C_e}{4} h_e &= -\frac{\mu_e}{\mu_e + \mu_i} J_b \frac{d n_e}{d x} - \frac{D_e}{n_b} \left( \frac{d n_e}{d x} \right)_b, \\
\frac{n_b C_i}{4} h_i &= -\frac{\mu_i}{\mu_e + \mu_i} J_b \frac{d n_i}{d x} - \frac{D_i}{n_b} \left( \frac{d n_i}{d x} \right)_b.
\end{align*}
\]

After having divided the first equation of the system by \( \mu_e \), the second – by \( \mu_i \) and after having summed them, as a result we get the following boundary condition:

\[
D_a \left( \frac{d n}{d x} \right)_b = n_b \frac{\mu_e C_e h_e + \mu_i C_i h_i}{4(\mu_e + \mu_i)}
\]

Here \( C_{e,i} = (8kT_{e,i} / \pi m_{e,i})^{1/2} \) are the average velocity of electrons and ions, correspondingly is, \( T_{e,i} \) - temperature of electrons and ions, \( m_{e,i} \) - weight of electrons and ions correspondingly, functions \( h_e, h_i \) are determined by the following way:

\[
h_e = \begin{cases} 
\exp \left[ \frac{e(\phi_e - \phi_p)}{kT_e} \right] & \text{when } \phi_e \geq \phi_p, \\
1 & \text{when } \phi_e \leq \phi_p
\end{cases} \quad h_i = \begin{cases} 
\exp \left[ \frac{e(\phi_i - \phi_p)}{kT_i} \right] & \text{when } \phi_i \leq \phi_p, \\
1 & \text{when } \phi_i \geq \phi_p
\end{cases}
\]

Here \( \phi_p \) is potential at the surface, \( \phi_e, \phi_i \) is potential of plasma at the border of plasma and surface, which is necessary to calculate \( h_{e,i} \).
Let us consider the surface as an electrode with instantaneous value of the potential to plasma (at lower boundary of ambipolar zone), which is equal to $V_p$. In this case the constant potential of plasma to the electrode can be calculated from dependences of average instantaneous potential fall through the layer for period of E-vibrations on a shift of fluctuating motion of electrons which equal to thickness of positive charge layer and on the difference $\phi_p - \phi_b = \frac{9KTe}{4e}$.

3. Numerical modelling

The paper work [7-8] describes balance problem of the charged particles of ICRF discharge, which is non-linear problem of eigenvalues, although a spectral parameter is absent in explicit form; as well this paper work gives explanation for origin and nature of the spectral parameter. It is shown that, as eigenvalues of differential problem can be in full accounted due to equation ratios and boundary conditions, so the sole free parameter is the value of electronic temperature in the center of the discharge, which meets some balance between ambipolar diffusion ratio, ionization frequency, recombination ratio and radius of plasmatron. This balance sets condition, necessary to support stationary low-pressure ICRF discharge. It is obvious that, by analogy with linear case, the eigenvalues of non-linear problem, forms function from electronic temperature too, but condition to calculate such case cannot be taken out in similar form. The paper work [9] describes the condition, which assumes existence of minimal eigenvalue that satisfies positive eigenfunction of non-linear problem toward eigenvalues with the ratios, which depend on spectral parameter aimed to determine concentration of the charged particles of the stable ICRF discharge. To resolve stationary and non-stationary non-linear problems, we can use methods proposed in [10-13].

Mathematical model, which takes into account the processes described in this study was implemented was realized numerically. We compared results of numerical calculations used to resolve model boundary value problems as including condition of equality to zero concentration on the wall of the gas discharge chamber and including the condition (1), by means of numerical modelling. Both problems are non-linear eigenvalue problems, spectral parameter of which is maximum value of the electronic temperature owing to dependencies $D_a$ and $\nu_i$. It has been established that distribution of the charged particles concentration, which is rated to 1, under use of genus first boundary condition and genus third boundary condition, differs obviously near boundary of gas discharge chamber. But maximum value of electronic temperature, obtained due to resolving problem with third genus boundary condition, is far less then maximum value of electronic temperature obtained due to resolving the problem with the condition of complete recombination of the charged particles. As a result, the boundary condition, set on DC wall, provides more significant impact on maximum value of electronic temperature in the interelectrode interval, than on distribution of the charged particles concentration. This is caused owing to non-linearity of mathematical model of ICRF discharge and dependency of spectral parameter from electronic temperature, which in its turn can be presented as function set obviously from the least eigenvalue.

Acknowledgments

The work is performed according to the Russian Government Program of Competitive Growth of Kazan Federal University and this work was supported by Russian Science Foundation, project no. 16-11-10299.

References

[1] Abdullin I Sh, Zheltukhin V S and Kashapov N F 2000 Radio-Frequency Plasma-Jet Processing of Materials at Reduced Pressures: Theory and Practice of Applications (Kazan: Izd. Kazan. Univ.) [in Russian]

[2] Chebert P and Braithwaite N 2011 Physics of radio-frequency plasmas (Cambridge: Cambridge Univ. Press)
[3] Fridman A 2008 *Plasma chemistry* (Cambridge: Cambridge Univ. Press)

[4] Lebedev Y A, Tatarinov A V, Epstein I L and Averin K A 2015 Mathematical modeling of the gas bubbles in the microwave discharge of boiling n-heptane *Contemporary Engineering Sciences* **8** (21) 1057-65.

[5] Chebakova V Ju, Zheltukhin V S and Dubrovin V T 2016 Problem of radio-frequency discharge at atmospheric pressure in local statement *Applied Mathematical Sciences* **8** (21) 1013-22.

[6] Micher M and Kruger CH 1976 *Partially ionized gases* (Moscow: Mir)

[7] Zheltukhin V S 1999 On the solvability of a nonlinear spectral problem in the theory of high-frequency discharges of reduced pressure *Russ. Math*. **43** (5) 24–9

[8] Zheltukhin V S 2005 On conditions for the solvability of a system of boundary value problem in the theory of a high-frequency plasma of reduced pressure *Russ. Math*. **49** (1) 47–52

[9] Zheltukhin V S, Solov’ev S I, Solov’ev P S and Chebakova V Yu 2014 Computation of the minimum eigenvalue for a nonlinear Sturm–Liouville problem *Lobachevskii J. Math.* **35** (4) 416–26

[10] Badriev I B and Banderov V V 2014 Numerical method for solving variation problems in mathematical physics *Mechanical components and control engineering III* **668–669** 1094-97

[11] Badriev I B 1983 Difference-schemes for linear-problems of the filtration theory with discontinuous law *Izvestiya Vysshikh Uchebnykh Zavedenii Matematika* **5** 3-12

[12] Solov’ev S I 1997 The finite element method for symmetric nonlinear eigenvalue problems *Comput. Math. Math. Phys.* **37** (11) 1269–76

[13] Solov’ev S I 2014 Approximation of differential eigenvalue problems with a nonlinear dependence on the parameter *Differ. Equations* **50** (7) 947–54