One-dimensional numerical model of a low-frequency inductively coupled plasma

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Abstract. A simplified model of low-frequency inductively coupled plasma generated in a U-shaped discharge tube has been developed. The model is based on the simultaneous solution of radial continuity equations for electrons and metastable atoms, gas temperature and electron mean energy. New data on plasma parameters of a low-frequency inductively coupled gas discharge have been obtained, for the case of argon plasma forming gas, in the range of discharge currents from 1 to 10 A and low argon pressures from 1 to 20 Pa. The numerical results agree with the present experimental and numerical data and describe the main discharge features, i.e. the low values of electric field strength from 0.2 to 0.6 V/cm, the decreasing voltage-current characteristics, and the decreasing electric field strength pressure dependencies.

1. Introduction
Active use of a low-temperature plasma in many technological processes stimulates the development of new gas-discharge devices that expand the capabilities of existing technologies and allow overcoming their inherent limitations. The radio frequency inductively coupled plasma (RF ICP) devices are widely used for ion-plasma etching to obtain the pure plasma of halogen-containing gases with a high concentration of active species at low (~1–10 Pa) pressures of the plasma forming gas [1]. However, the RF ICPs have a number of disadvantages that limit the efficiency of their use in modern technological processes for the future 450 mm standard of the semiconductor industry [2]. One of the most effective ways to overcome the physical limitations of the RF ICPs is the transition to ferromagnetic enhanced low-frequency (~100 kHz) inductively coupled plasma (FMICP) with the magnetic coupling between the inductor and plasma enhanced with ferromagnetic materials [2–4]. It is proposed to use a distributed principle of the FMICP generation to produce large volumes of dense uniform plasma for plasma treatment [2–4]. A substrate to be treated is placed in a main discharge chamber with a number of U-shaped discharge tubes installed on the main chamber. Every U-shaped discharge tube has its own ferromagnetic core with primary winding (inductor) connected to a power supply, which is used to induce a vortex electric field driving the FMICP. Every U-shaped tube, together with the main discharge chamber, forms a closed discharge current path of the FMICP. Having a cross-section of a few orders less, the plasma resistance in the U-shaped tube is much larger than that in the main chamber. Therefore, practically all power delivered to the ferromagnetic inductor generates plasma in the U-shaped tube. Since plasma density in the U-shaped tube is considerably larger than that in the main chamber, the predominant source of plasma in the main chamber is the diffusion of charged and excited particles from the U-shaped tube into the main chamber [3, 4]. Therefore, knowing the plasma parameters in the U-shaped discharge tube is very important for predicting the plasma parameters in the main chamber.
The aim of the paper is to develop a model to describe plasma in the U-shaped tube of the distributed FMICP under conditions of interest for plasma processing (plasma forming gas pressure of about 1–10 Pa and high electron densities). The model is based on the previously developed models of the FMICP [5–7], and the calculations are performed for the following discharge conditions. The FMICP is generated in a U-shaped discharge tube 5 cm in diameter in argon with the pressure range lower than that in [5–7], i.e. from 1 to 20 Pa, and discharge currents range from 1 to 10 A.

2. Model
In order to understand which physical processes play an important role in the U-shaped discharge tube of the distributed FMICP, a simple model was developed. At the first step only argon is considered as a plasma-forming gas to test the model. The gas discharge plasma is assumed to be in a steady state; it is homogeneous in the longitudinal direction and cylindrically symmetric (i.e. the U-shaped tube is replaced with a cylindrical tube with an equivalent length and diameter). The model is based on a simultaneous solution of the balance equations for electrons and metastable argon atoms densities, balance equations for electron energy and gas temperature. The losses of electrons and metastable argon atoms in the processes of diffusion to the discharge tube wall were taken into account. The gas heat conduction to the discharge tube wall was also taken into account. In this paper for simplicity we assume that the electrons have a Maxwellian distribution function \( f(U, r) \), due to the high frequency of electron-electron collisions at high electron densities in the U-shaped tube:

\[
f(U, r) = \frac{2}{\sqrt{\pi} (kT_e)^{3/2}} \exp(-U / kT_e(r)) ,
\]

where \( U \) is the electron kinetic energy, \( T_e(r) \) is the electron temperature radial distribution.

The electron macroscopic parameters (electron density \( n_e \) and mean energy \( u_e \)) are the integrals of the electron energy distribution function (EEDF) over the energy:

\[
n_e(r) = \int_0^\infty U^{1/2} f(U, r) dU ,
\]

\[
u_e(r) = \frac{1}{n_e(r)} \int_0^\infty U^{3/2} f(U, r) dU .
\]

The axial electron current density \( j_z(r) \) is defined as follows:

\[
j_z(r) = \frac{1}{3} e_e E_z \sqrt{2 / m_e} \frac{U}{H(U)} \frac{\partial f(U, r)}{\partial U} dU ,
\]

where \( E_z \) is the axial component of the electric field strength, \( H(U) = N_g Q_d(U) + \sum_{i} N_g Q_{ik}^m(U) \) is summarized electron momentum losses, \( N_g \) is the neutral gas density, \( Q_d \) and \( Q_{ik}^m \) are the cross sections of elastic and inelastic collisions, correspondingly (see e.g. [7]). The total discharge current is equal to the integral \( I_d = 2 \pi \int_0^R j_z(r) dr \), where \( R \) is the discharge tube radius.

The electron energy balance equation has the form:

\[
\frac{\partial u_e}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (ru_e(r) j_z(r)) = P_e^i(r) - \sum_k P_{ik}^{en}(r) + k_{mn} N_m^2(r) \cdot \varepsilon_{mn} ,
\]

where the energy gain from the electric field (\( E_z \) is the radial electric field component) is:

\[
P_e^i(r) = -e_e E_z j_z(r) - e_0 E_z(r) j_z(r)
\]

the energy loss in elastic collisions:

\[
P_{ik}^{en}(r) = \frac{2 m_e}{M} U^2 N_g^0(r) Q_{ik}^0(U) f(U, r) dU ,
\]

and in inelastic collisions:

\[
P_{ik}^{en}(r) = U^2 \frac{2 m_e}{M} \sqrt{U N_g^0(r) Q_{ik}^0(U) f(U, r) dU} .
\]

The last term in equation (5) describes the electron energy gain (\( \varepsilon_{nm} \)) in metastable-metastable collisions.
For the electron density radial distribution \( n_e(r) \) the following balance equation is used:
\[
\frac{\partial n_e(r)}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left( r D_e \frac{\partial n_e(r)}{\partial r} \right) = S_i(r) + S_w(r) + k_{im} N^2_m(r) - k_{im} n_e(r) n_i(r),
\]
where the rate constant of direct electron impact ionization of argon is:
\[
S_i(r) = \sqrt{2/m_e} \int_0^\infty U N_e(r) Q_i(U) f(U, r) dU,
\]
and the rate constant of stepwise ionization from the metastable argon atom is:
\[
S_w(r) = \sqrt{2/m_e} \int_0^\infty U N_m(r) Q_w(U) f(U, r) dU.
\]
Here \( k_{im} \) is the rate constant of penning ionization as a result of two metastables collision, \( k_{im} \) is the rate constant of recombination in electron-ion collisions (\( n_i \) is the ion density). The quasi-neutrality of the discharge plasma is assumed, i.e. the densities of electrons and ions are equal to each other. \( D_e \) is the electrons and ions ambipolar diffusion coefficient:
\[
D_e = \frac{\mu_e D_e + \mu_i D_i}{\mu_i + \mu_e} = \frac{\mu_i (T_e + T_i)}{e},
\]
where \( T_i \) is the ion temperature and \( \mu_i \) is the ion mobility coefficient. At the axis of the discharge tube the condition \( \frac{dn}{dr} = 0 \) was taken due to the cylindrical symmetry, and at the gas discharge tube wall it was assumed the electron velocity is equal to the Bohm velocity, \( v_d(R) = v_B = (kT_e/M)^{1/2} \), where \( M \) is the ion mass.

The balance equation for metastable argon atoms density \( N_m(r) \) has the form:
\[
\frac{\partial N_m(r)}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left( r D_m \frac{\partial N_m(r)}{\partial r} \right) = S_m(r) + k_{im} n_e(r) n_i(r)
\]
\[- S_w(r) - 2k_{im} N^2_m(r) - k_{2B} N_m(r) N_g(r) - k_{3B} N_m(r) N^2_g(r) \]
where \( D_m \) is the metastables diffusion coefficient, \( k_{2B} \) and \( k_{3B} \) are the coefficients of two-body and three-body recombination, \( S_m(r) \) is the rate of argon metastable atoms excitation by an electron impact:
\[
S_m(r) = \sqrt{2/m_e} \int_0^\infty U N_g(r) Q_m(U) f(U, r) dU.
\]

The rate constants and coefficients were taken as in [7].

The gas heating by the electron current and heat conduction to the discharge tube were taken into account. For this purpose the following thermal balance equation used:
\[
\frac{\partial T_g(r)}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa_g(T_g) \frac{\partial T_g(r)}{\partial r} \right) = P_{el}(r),
\]
where \( \kappa_g(T_g) = 4.17 \times 10^6 T_g^{2.3} \text{[W/(cm·K^{2.3})]} \) [7]. We assume the \( dT_g/dr = 0 \) at the axis and \( T_g = T_w = 300 \text{K} \) at the discharge tube wall. The equation (15) was solved iteratively improving the dependence \( \kappa_g(T_g) \) at each iteration. In the right part of equation (15) it is assumed that the \( P_{el}(r) \) has radial dependence due to the non-uniformity of gas density \( N_g(r) \) and electron density \( n_e(r) \). The gas heating leads to a non-uniform gas density distribution \( N_g(r) \) across the discharge tube:
\[
N_g(r) = \frac{P}{k_g T_g(r)}.
\]

Finally, a feed-back analogous to the Ohm law between the discharge current \( I_d \) and the electric field strength \( E_z \) was used. If the calculated discharge current was smaller than the needed value, the electric field strength was increased, and vice versa. In such a way we can obtain the voltage-current characteristics of the discharge. All the balance equations were solved together by the relaxation method starting with some initial conditions. For the given discharge parameters, i.e. the discharge current \( I_d \) and gas pressure \( p \), we obtained the final set of all the parameters (electron and metastable densities and all rate constants) which do not depend on initial conditions. All the balance equations were totally fulfilled at the final stage.
3. Results
In figure 1, the numerical results concerning the electric field strength dependencies on argon pressure are presented for different discharge currents, \( I_d = 1, 2.5, 5 \) and \( 10 \) A. The data coincide rather well with the experimental results for the low-pressure argon FMICP [6-8] in the whole range of argon pressures from 1 to 20 Pa. The behavior of the numerical results as well as experimental data is as follows. a) The voltage-current characteristics show the negative resistance of the FMICP. b) The pressure dependences are the decreasing functions and approach minima at the same argon pressures \( (p \sim 50 \text{ Pa}) \) as the experimental results. c) Absolute values of the electric field strength are 0.2–0.6 V/cm in the described range of argon pressures.

![Figure 1](image1.png)

**Figure 1.** The dependencies of electric field strength \( E_z \) on argon pressure \( p \) for different discharge currents \( I_d \) (circles for 1 A, squares for 2.5 A, triangles for 5 A, rhombus for 10 A).

![Figure 2](image2.png)

**Figure 2.** The pressure dependencies of electron density \( n_e \) (dashed lines) and argon metastable states \( N_{m} \) (solid lines). \( I_d = 10 \) A (circles), 5 A (triangles), 1 A (rhombus).
For the given value of the discharge current, the electron density $n_e$ increases monotonously with gas pressure $p$, while the argon metastable states density $N_m$ have maximum at low discharge currents (1 and 5 A) and is decreasing function for high discharge current 10 A (see figure 2). It should be noted that the electron density $n_e$ is almost a linear function of the discharge current $I_d$. The minimum value of electron density is $n_e \sim 2 \cdot 10^{10}$ cm$^{-3}$ for the discharge current $I_d = 1$ A and argon pressure $p = 1$ Pa, and the maximum value $n_e \sim 7 \cdot 10^{12}$ cm$^{-3}$ for $I_d = 10$ A, $p = 20$ Pa. The density of argon metastable states has the order of about $N_m \sim 10^{12}$ cm$^{-3}$.

**Figure 3.** The ionization balance terms of equation (9) at the discharge tube axis. Sum of all terms (solid line), direct electron impact ionization $S_i$ (dashed line), stepwise ionization $S_{sw}$ (dash dotted line), Penning ionization $k_{mm}N_m^2$ (dotted line). Discharge current is 1 A.

Figure 3 presents the terms of the electrons balance equation (9) for the discharge current $I_d = 1$ A. It is seen that under low argon pressures the direct electron impact ionization plays the major role in the electron production process. Under high pressures, the stepwise ionization from the argon metastables states becomes the leading ionization mechanism. The bulk recombination is negligible under considered conditions and is not presented in figure 3. However, the higher the discharge current, the greater role is played by the bulk recombination. The losses of electrons are mainly determined by their flux toward the discharge tube. The results also show that this flux increases with the increase of gas pressure and discharge current. All processes excepting the Penning ionization are almost linear functions of the discharge current.

Figure 4 presents the terms of the argon metastable states balance equation (13). The main process leading to production of argon metastable states is the excitation of argon atoms by an electron impact and the consequent cascading to the argon metastable states. The metastables losses are determined by the collisions in stepwise ionization and in Penning ionization. At the considered range of gas pressure, the rate constant of stepwise ionization increases with pressure, and rate constant of Penning ionization have a maximum in pressure dependence.
Figure 4. The terms of argon metastable states balance equation (13) at the discharge tube axis. Sum of all terms (solid line), excitation by electron impact $S_{im}$ (dotted line), losses in stepwise ionization $S_{sw}$ (dashed line), losses in Penning ionization $k_{mm}N_m^2$ (dash dotted line). $I_d = 1$ A.

4. Conclusion

A simplified model of ferromagnetic enhanced low frequency inductively coupled argon plasma generated in a U-shaped discharge tube of a distributed FMICP has been developed. The model is based on the assumption of Maxwellian electron distribution function. Simultaneous solution of radial continuity equations for electrons and metastable argon atoms, gas temperature and electron mean energy was performed. New data on plasma parameters of the FMICP have been obtained for discharge currents in the range from 1 to 10 A, and low argon pressures from 1 to 20 Pa. The radial profiles for the metastable and electron densities, gas and electron temperatures were calculated. The ionization balance and the argon metastable states balance were analyzed. The numerical results agree with the present experimental and numerical data and describe the main discharge features, i.e. the low values of electric field strength from 0.2 to 0.6 V/cm, the decreasing voltage-current characteristics, and the decreasing electric field strength pressure dependencies.

Acknowledgements

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