NUMERICAL MODELLING OF FERROMAGMETIC ENHANCED INDUCTIVELY COUPLED PLASMA DISCHARGE PARAMETERS IN OXYGEN

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INTRODUCTION

Ferromagnetic enhanced inductively coupled plasma (FMICP) is of great interest for fundamental research and a lot of applications, such as plasma etching, thin film deposition, plasma chemical synthesis, optical emission spectroscopy, etc.

Recently, FMICP source with a distributed plasma generation in a large discharge chamber was developed (*A. Fedoseev, M. Isupov, N. Demin, and G. Sukhinin, "Large-scale ferromagnetic enhanced Ar/Cl_2 ICP," Plasma Sources Sci. Technol., vol. 29, pp. 045021, April 2020*).

In this work we provide calculations of basic FMICP properties, including densities of neutral and charged plasma components, electronegativity and dissociation fraction in pure oxygen for a large-scale FMICP source.

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NUMERICAL MODEL

The global (volume averaged) model is used. The content of the chamber is assumed to be spatially uniform and the power is deposited uniformly in plasma. Electrons, oxygen atoms and molecules in ground state, oxygen atoms in metastable state $O(^1D)$, oxygen molecules in metastable states $O_2(a^1\Delta_g)$, $O_2(b^1\Sigma_g)$, positive ions O^+ and O_2^+ and negative oxygen ions O^- were considered.

For each type *k* of particle the time-dependent balance equation was solved:

$$\frac{dn^{(k)}}{dt} = \sum_i R^k_{G,i} - \sum_i R^k_{L,i}$$

where $R^k_{G,i}$ and $R^k_{L,i}$ are the rates of generation and loss of particle in *i*-th process.

The reaction set was taken from ***J.T. Gudmundsson et al, "An ionization region model of the reactive Ar/O$_2$ high power impulse magnetron sputtering discharge," Plasma Sources Sci. Technol., vol. 25,*** which includes reactions of electrons with neutral particles, or between gas particles in the plasma volume, recombination or quenching of neutral particles on the chamber wall and neutralization of positively charged ions. It is assumed, that electrons have a Maxwellian energy distribution function. The electrical quasi-neutrality is assumed in the discharge and electron density is calculated from this condition without solving the balance equation.

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NUMERICAL MODEL

The rate of the positive oxygen atomic and molecular ions loss due to their flow to the chamber walls is given as:

$$k_{i^+,wall} = u_{Bohm}^{i^+} \frac{A_{eff}}{V},$$

where $u^{i+}_{\mathrm{Bohm}} = (kT_e/m_i)^{1/2}$ is the Bohm velocity, A_{eff} is an effective ion loss area:

$$A_{eff} = h_L A_L + h_R A_R = 2\pi\left(R^2 h_L + RLh_R\right),$$

where h_L and h_R are the ratios of ion densities at the edge and at the center of the discharge plasma:
where $K_L = 0.86Lu_B/\pi D_a$ and $K_R = 0.8Ru_B/\chi_{01}J_1(\chi_{01})D_a$. Here $\alpha_0 = 3/2\alpha_s$ is the electronegativity in the middle of the discharge, α_s is the electronegativity at the sheath edge, $\eta = 2T_+/(T_+ + T_-)$, $J_1(\chi)$ is the first order Bessel function, $\chi_{01} \approx 2.405$ is the first zero of the zero order Bessel function $J_0(\chi)$, $D_a = D_i(1+\gamma+\gamma\alpha_s)/(1+\gamma\alpha_s)$ is the ambipolar diffusion coefficient, D_i is the mean diffusion coefficient of the positive ions, $\gamma = T_e/T_i$ is the ratio of the electron and ion temperatures, λ_i is the ion mean free path.

$$h_L = \left[\left(\frac{0.86}{1+\alpha_0}\right)^2 \left(\left(3 + \frac{\eta L}{2\lambda_i}\right) + K_L{}^2\right)^{-1} + h_c^2\right]^{1/2},$$

$$h_R = \left[\left(\frac{0.8}{1+\alpha_0}\right)^2 \left(\left(4 + \frac{\eta R}{\lambda_i}\right) + K_R{}^2\right)^{-1} + h_c^2\right]^{1/2},$$

NUMERICAL MODEL

h_c is the scaling factor for one-region flat-topped electronegative profile defined by the expression:

$$h_c = \left[\gamma_-^{1/2} + \gamma_+^{1/2} n_*^{1/2} n_+ n_-^{3/2}\right]^{-1},$$

where $\gamma_- = T_e/T_-$ and $\gamma_+ = T_e/T_+$ are the ratios of electron and ion temperatures, and n_* :

$$n_* = \frac{15\eta^2}{56 k_{rec} \lambda_i} v_i,$$

where $v_i = (8kT_i/\pi m_i)^{1/2}$ is the ions thermal velocity, $k_{rec} = 4\text{x}10^{-14}$ $(300/T_g)^{0.44}$ [m^3s^{-1}] is the rate constant of ion-ion bulk recombination processes. These scaling factors capture the modification to the Bohm velocity due to the presence of negative ions near the sheath edge.

Diffusion losses of oxygen atoms and metastable states of oxygen atom and molecule on the chamber walls are estimated using effective loss factor:

$$k_{n,wall} = \left[\frac{\Lambda_X^2}{D_X} + \frac{2V(2-\gamma_X)}{A v_X \gamma_X}\right]^{-1},$$

where D_X, v_X and γ_X are diffusion coefficient, thermal velocity and recombination coefficient of neutral species X on the walls, respectively.

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NUMERICAL MODEL

Λ_X is an effective diffusion length of each neutral species to cylindrical chamber walls:

$$\Lambda_X = \left(\left(\frac{\pi}{L} \right)^2 + \left(\frac{2.405}{R} \right)^2 \right)^{-1/2}.$$

The processes of neutral oxygen species conversion to oxygen molecules on the discharge chamber wall play an important role. For the metastable states of molecular oxygen recombination coefficient $\gamma[O_2(a^1\Delta_g)] = \gamma[O_2(b^1\Sigma_g)] = 0.007$ is taken from the work of Sharpless and Slanger. For the neutral oxygen atom and metastable state of oxygen atom recombination coefficient in the pressure range of 2−150 mTorr is $\gamma_O = \gamma_{Od} = 0.1438*\exp(2.5069/p)$, where p is the pressure in mTorr, and increases linearly with decreasing pressure from 0.5 at 2 mTorr to 1.0 at vacuum.

The electron temperature T_e is determined by the power balance equation:
i.e. the absorbed power by plasma in the chamber P_{ch} loses in elastic and inelastic electron collisions P_e and by ambipolar flux of charged particles to the chamber walls P_w.

$$\frac{d}{dt}\left(\frac{3 n_e k T_e}{2} \right) = \frac{1}{V}\left(P_{ch} - P_e - P_w \right),$$

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NUMERICAL MODEL

The energy losses in elastic and inelastic collisions of electrons with atoms and molecules are:

$$P_e = Ven_e \sum_X \left(P_{iz}^X + \sum_k^{N_{ex}} n^X k_{ex,k}^X \varepsilon_{ex,k}^X + P_{el}^X \right)$$

where $P_{iz}^X = n^X k_{iz}^X \varepsilon_{iz}^X$, $P_{el}^X = 3m_e/m^X * n^X k_{el}^X * T_e$, ε_{iz}^X and k_{iz}^X are the ionization threshold and the ionization rate constant for particles of type X, ε_{ex}^X and k_{ex}^X are the energy threshold and the rate constant of kth process of exciting particles, k_{el}^X is the elastic scattering rate constant. For oxygen all energy thresholds and rate constants are taken from V.M. Donnelly, and M.V. Malyshev, 2000.

The energy losses by the charged particles flow to the chamber wall P_w are:

$$P_w = e \sum_x n_x k_{i^+,wall} \left(\varepsilon_i + \varepsilon_e \right),$$

where $k_{i+,wall}$ is determined by V. Godyak, 2013, n_x is the positive ion density of type X, $\varepsilon_e = 2T_e$ is the mean kinetic electron energy. The mean kinetic energy per ion lost on the chamber walls is determined by the sum of energies gain by an ion in the sheath and presheath $\varepsilon_i = V_s + V_p$. It depends on the plasma electronegativity as was described in details by Thorsteinsson and Gudmundsson, 2009.

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NUMERICAL MODEL

Taking into account a small electronegativity of the plasma in our conditions we assume $\varepsilon_i \approx 5.5$eV for simplicity. Calculations show that the plasma parameters change by no more than 5% when ε_i changes by 1 eV. For the gas temperature an empirical dependence on the absorbed power measured experimentally in a typical RF ICP by Donelly and Malyshev, 2000, and approximated by Thorsteinsson and Gudmundsson, 2009 was used in this work.

Through the chamber inlets, a constant flow of neutral oxygen molecules is injected into the discharge chamber. The gas pressure *p* in the working chamber is defined as the sum of the partial pressures of all the components of the plasma gas. The evacuation of gas particles {O_2, O, O^+, O_2^+, $O_2(a^1\Delta_g)$, $O_2(b^1\Sigma_g)$, $O(^1D)$} from the chamber by vacuum pumping is also taken into account and it plays the role of a feedback for gas pressure *p* in the chamber. The negative charged ions O^- are not pumped out and cannot reach the discharge walls because they cannot overcome the chamber wall potential.

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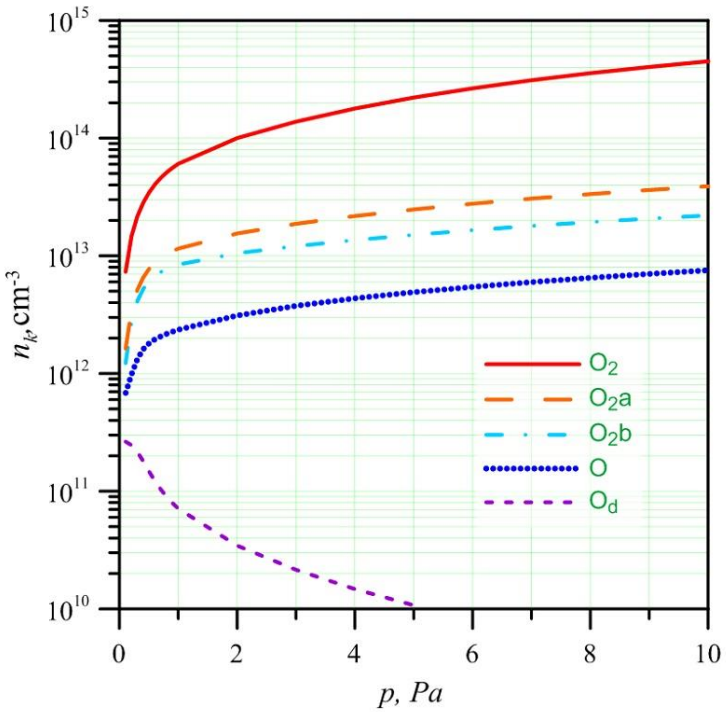
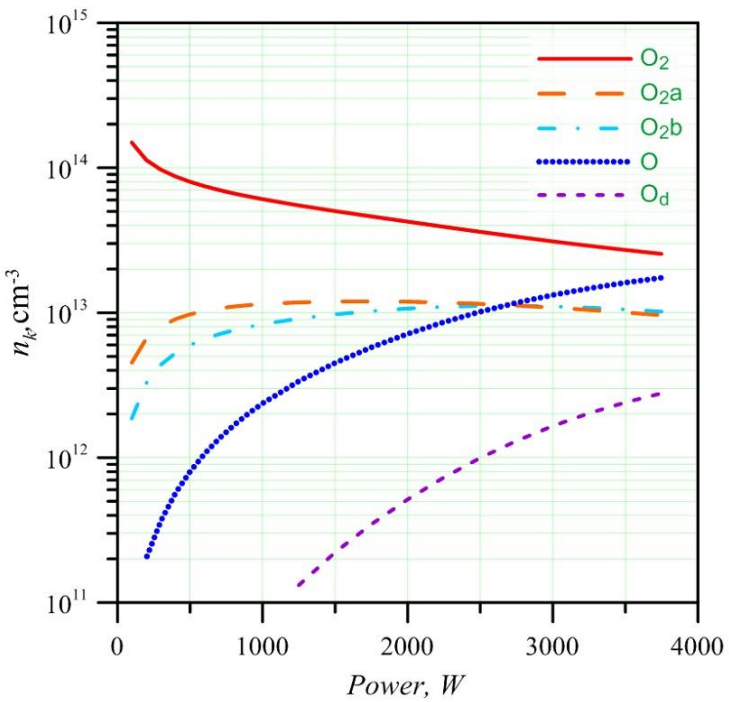
CALCULATION RESULTS. NEUTRALS

Calculations were provided for the large FMICP source with a radius of gas discharge chamber R = 35 cm and a height of L = 50 cm for pure oxygen plasma for the range of pressures of 0.1−10 Pa at discharge power of 1000 W, and for different values of discharge power at gas pressure of 1 Pa.



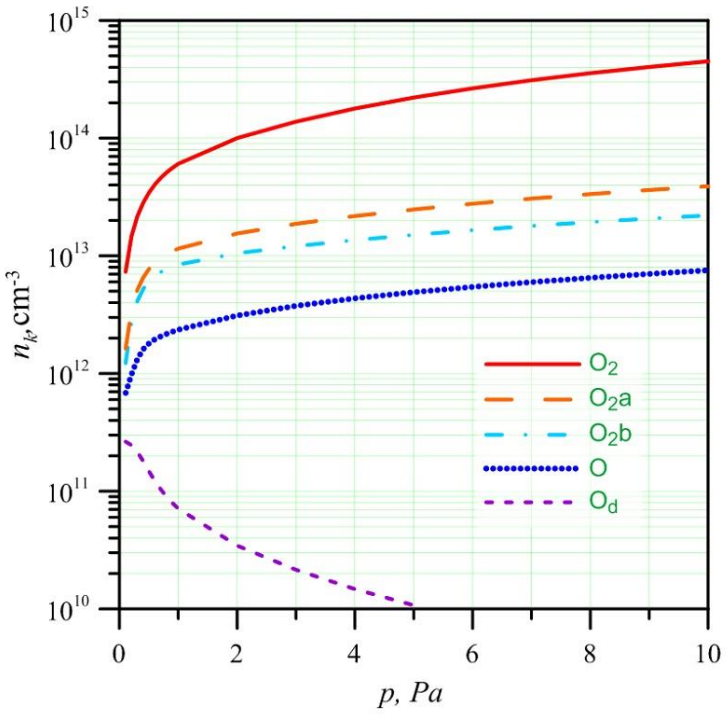
Densities of neutral particles versus gas pressure (at power of 1000W)



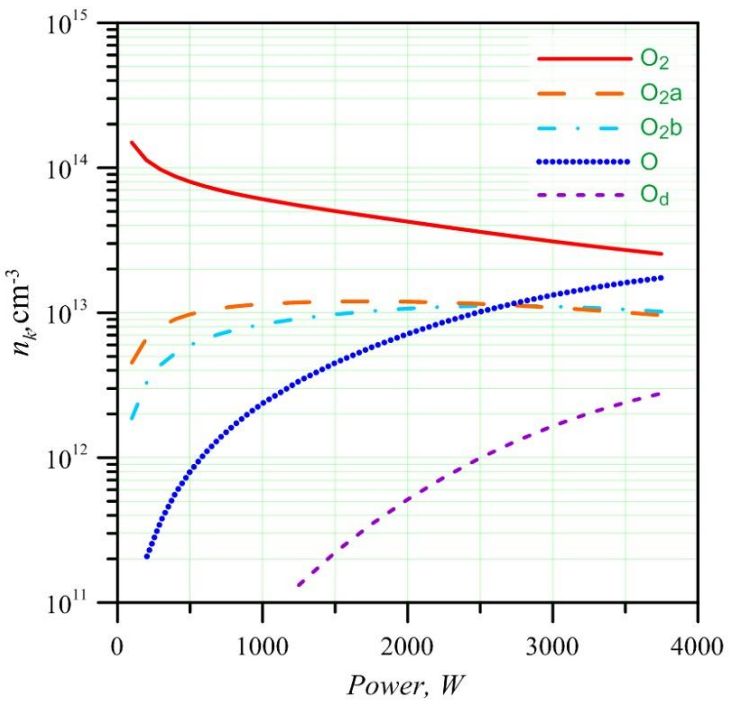
Densities of neutral particles versus discharge power (at pressure 1Pa)

CALCULATION RESULTS. NEUTRALS

With the growth of gas pressure, densities of all neutral plasma components increase except of density of metastable oxygen atom, because of increasing rate of wall recombination. Increase of discharge power leads to the increase of densities of atomic oxygen in ground and metastable states, while concentration of molecular oxygen decreases, which is the result of growth of electron temperature and consequently the growth of rates of volume processes.



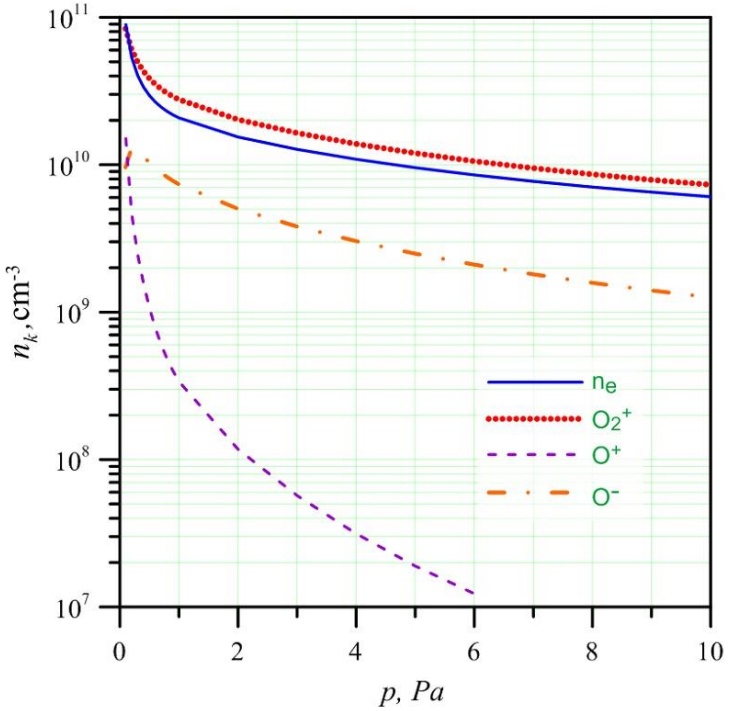
Densities of neutral particles versus gas pressure (at power of 1000W)



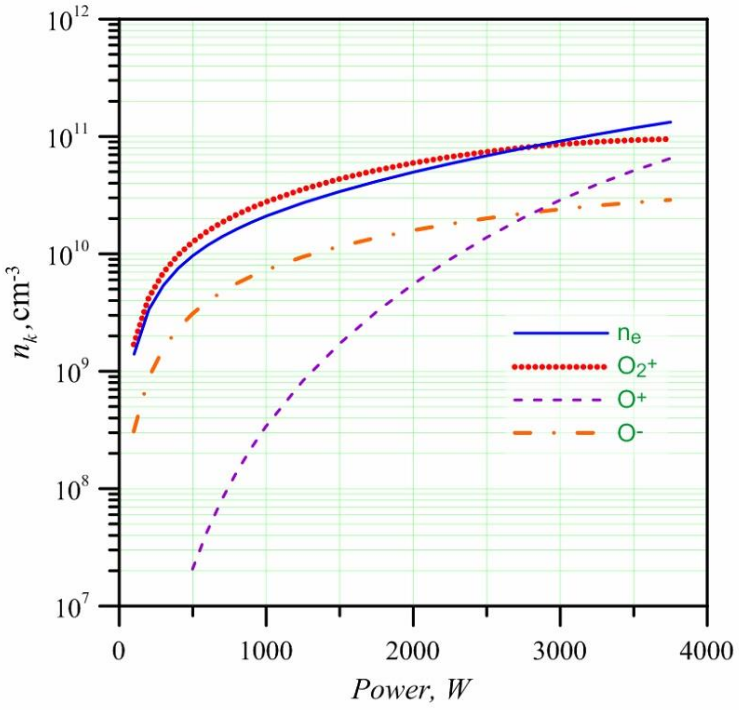
Densities of neutral particles versus discharge power (at pressure 1Pa)

CHARGED PARTICLES

Densities of charged particles decrease with increasing gas pressure, which is the result of increasing rates of wall and volume processes, i.e. recombination, quenching and others. The growth of discharge power leads to the increase of densities of all charged species.



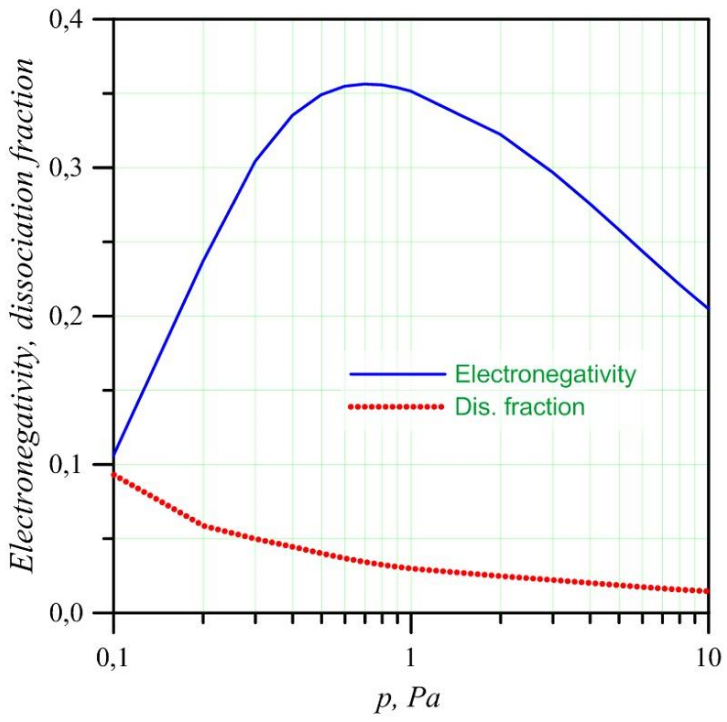
Densities of charged particles versus gas pressure
(at power of 1000W)



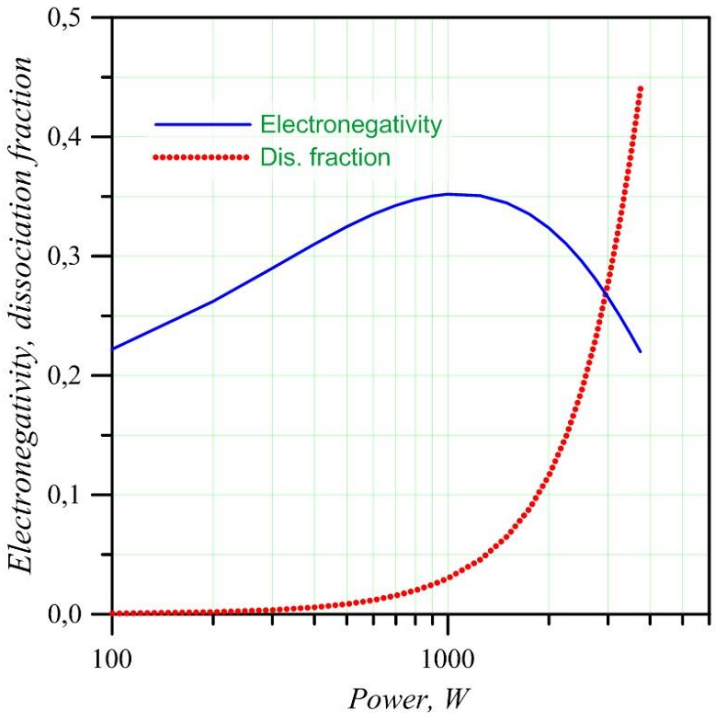
Densities of charged particles versus discharge power
(at pressure 1Pa)

Electronegativity and dissociation fraction

Electronegativity of the discharge ($n[O^-]/n_e$) changes non-monotonously with pressure and have a maximum of 0.35 at the pressure of 0.7 Pa. The dissociation fraction ($n[O+O(^1D)]/n[O_2+O_2(a^1\Delta_g)+O_2(b^1\Sigma_g)]$) decreases with pressure, and have values lower than 0.1 at the whole studied pressure range. The electronegativity of the discharge varies also non-monotonously with discharge power, a maximum is observed at the value of power of 1000 W. The dissociation fraction increases significantly with discharge power and reaches the magnitude of 0.45 at the power of 4000 W.



Electronegativity and dissociation fraction of the discharge versus gas pressure.
(at power of 1000W)



Electronegativity and dissociation fraction of the discharge versus discharge power
(at pressure 1Pa)

CONCLUSION

- **Global model for the low-frequency ferromagnetic enhanced inductively coupled discharge in pure oxygen is presented.**
- **Calculations of all basic plasma parameters are performed for the range of gas pressures of 0.1−10 Pa and the range of discharge power of 100−4000 W.**
- **It was obtained, that electronegativity of the pure oxygen discharge in large chamber varies non-monotonously with gas pressure and discharge power and maximum is appeared at the gas pressure of 1 Pa and power of 1000 W. The dissociation fraction of the discharge substantially increases with discharge power.**

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