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Estimating the parameters of a positive column of the halogen-containing glow discharge at moderate pressures

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Abstract

The methodical recommendations for estimating the plasma parameters of an electronegative glow discharge containing halogens at moderate pressures (up to 40 Torr) with the use of simple analytic formulae and without numerical modeling are given. The initial data are easily measureable discharge parameters such as a discharge current, a voltage and a gas mixture pressure and composition as well. It is shown how one can easily consider such important plasma features as non-Maxwellian electron energy distribution function and halogen molecules dissociation by electron impact. As a result, such plasma parameters as the absolute degree of electronegativity, the value of border coordinate between ion–ion and electron–ion plasmas, and the forms of transversal profiles of electron and negative ion concentrations can be evaluated. The comparison of the results with the ones given by a global numerical model shows the suitability of said analytic approach to estimate plasma parameters of real discharges.

Keywords: Gas discharge; Electronegative gas; Halogen; Positive column.

Collision processes between charged particles taking place in the plasma of a positive column (PC) of the direct current (DC) glow of electronegative (EN) discharge at low and moderate pressures (up to 40 Torr) are of undoubted interest. In Ref. [1], simple analytic expressions connecting the elementary collision rates to each other and to energetic and geometric parameters of transversal profiles of charged particles density were presented. This could be very useful for practical calculations of PC plasma parameters since this makes it possible to calculate the values of mentioned plasma parameters fast, easily and without any numerical modeling.

But in fact, as declared in Ref. [1], the improvement of the adequacy of theoretical treatment of EN discharge was reduced to introducing ion diffusion into the theory (indeed, it had not been taken into consideration before). The problem of practical estimation of PC plasma parameters was virtually omitted in Ref. [1]; therefore it remains unclear, how exactly the theory [1] describing the properties of the model discharges is applicable to those of the real ones.

The present paper offers the technique of calculation of the parameters used in the theory. The technique is based on initial, easily measureable discharge characteristics such as a current, voltage and gas composition. As the result, it allows us to estimate the values of some important PC plasma parameters which cannot be measured directly. Hence, the present work completes

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the theoretical paper [1], expanding their practical application area.

Moreover, one of the present work goals was to check the accuracy of PC plasma parameters calculations for real discharges by using analytical expressions obtained in Ref. [1].

In the present paper, the same notation symbols are used as used in Ref. [1]: ν_i, ν_a are ionization and attachment frequencies; ρ_i is an ion–ion recombination constant;

$$\nu = \nu_i/D^*_{ap}; \quad \alpha = \nu_a/D^*_{an}; \quad \eta = n_{e0}\rho_i/D^*_{ap};$$

$$D^*_{ap} = \mu_p T_e/\left(e x_W^2\right); \quad D^*_{an} = D^*_{ap}/\mu;$$

T_j, μ_j are temperatures and mobilities of the particles of the kind j; indices e, p, n correspond to electrons, positive ions and negative ions; $\mu = \mu_p/\mu_n$; x_W is an absolute wall coordinate, and for cylindrical geometry (CG) $x_W = R_t$ (R_t is an inner radius of the discharge tube); n_{e0} is electron density in the discharge center; X is a reduced dimensionless transverse coordinate, in particular, for CG $X = r/R_t$; X_0 is the reduced coordinate of the boundary between e–i and i–i plasmas [1]; $\tau_j = T_j/T_e$; $\tau_S = \tau_p + \tau_n$; $n(X) = n_e(X)/n_{e0}$; $N(X) = n_n(X)/n_{e0}$; N_0 is the ratio of negative ion and electron densities in the discharge center (at $X = 0$), i.e. $N(0)$ at $\tau_S \to 0$; $N_{\tau 0}$ is the same quantity as N_0 but it is taken at $\tau_S > 0$.

From the expressions obtained in Ref. [1] which relate to the values of α, η and ν, it could be hypothetically possible to calculate the electron temperature T_e or even the E/N (the ratio of the longitudinal electric field to the concentration of neutral particles), how it can be made from Schottky's relation for electropositive plasmas [2]. But the information on T_e is not highly profitable for the further calculations, particularly for the estimations of characteristics of plasma radiation, because the electron energy distribution function (EEDF) in plasma containing molecular gases is non-Maxwellian. Checking calculations of the power of excimer UV radiation for the discharge in the mixture of Xe–Cl_2 made by model [4] (if we let the EEDF be Maxwellian there) gave the UV-power values of about 2–3 times lower than the ones obtained experimentally. And since the EEDF is non-Maxwellian, the problem of E/N calculation becomes as complex as a full-scale numerical global discharge model is. It is irrelevant to pose such a problem having a purpose to reach the maximal simplicity of the estimations of transversal density profiles of charged particles.

But if we prescribe the value of E/N as an input parameter, together with the concentrations of neutral components of gas mixture as it will be shown below, the estimation of plasma parameters of glow EN discharge becomes a relatively simple task wherein no any numerical model is needed.

The value of E/N for discharges in halogen-containing gas mixtures can be taken from the published data [5–7] or estimated experimentally, e.g. by the movable electrode method as it was made in Refs. [5–7].

If E/N and gas mixture composition are known, it makes sense to use the free software BOLSIG [8]. There both EEDF and D_e, μ_e, ν_a, ν_i, as well as the other electron collision frequencies, can be calculated by numerical solution of the Boltzmann kinetics equation. It is the simplest way to take the non-Maxwellian EEDF into consideration and hence to improve the adequacy of all following results.

With the known values of μ_e and E/N, it is possible to estimate the n_{e0} value from the measured discharge current, keeping in mind that the transversal electron density profile at strong electronegativity is almost flat in the great part of the discharge cross section [1,3,4] (see also Fig. 1b).

Ionic temperatures, also corrected for ion heating by electric field, can be calculated by using expressions given in Ref. [9]; ion mobilities can be taken from the data of Ref. [10], and ion–ion recombination rates for halogens ρ_i are taken from Refs. [11–13].

Estimating real EN discharge parameters, we should take into account the reduction of halogen molecules concentration (relative to their concentration without the discharge) due to molecule dissociation caused by electron impact taking place even at small discharge currents [4]. Let us describe the iterative procedure of estimating halogen molecules concentration through the example of a discharge in the mixture of Xe–Cl_2.

All the iterations were made with the use of the above-mentioned free software BOLSIG. For the first iteration, we set the initial gas composition as the filling one. After finishing the calculations we should take the sum of excitation collision frequencies for $B^1\Pi$, $B^3\Pi$ and $C^1\Pi$ states of the Cl_2 molecule (in sum they give the total electron impact dissociation frequency) from the BOLSIG output data. In BOLSIG, all the collision frequencies are normalized to the total gas mixture concentration of 3.5×10^{16} cm^{-3}; so we should divide the said sum by 3.5×10^{16} and by the relative fracture of Cl_2 to obtain the rate coefficient for molecule dissociation $\langle \sigma_d v_e \rangle$ in cm^3/s. Then, from the expression [14]

$$N_{Cl_2} = \frac{A + 8BC - \sqrt{A^2 + 16ABC}}{8C} \tag{1}$$

we can find the concentration of remaining chlorine molecules.