FAST SELF-CONSISTENT KINETIC MODELLING OF LOW-PRESSURE RF DISCHARGES.

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The principals of the fast self-consistent modelling of low-pressure discharges are proposed.

Introduction.

The numerical modelling of the gas discharge processes is necessary for understanding of the main physical mechanisms and principles, and for design and optimisation of technological processes and devices. It is possible to distinguish two main strategies of modelling:

1. The full-scale modelling. It starts from the first principles: Boltzmann-MC for particles, Maxwell-Poisson for fields. Its merits are: high reliability; any preliminary information and analysis are unnecessary, precise account of all important (and unimportant) processes. Its shortages are: it is very labour-consuming; it is practically impossible to obtain dependencies on external parameters, it is difficult to separate important factors and parameters from non-principal ones.

2. Semi-analytic approach starts from simplified equations. Some important procedures: estimates and neglect of small terms, reduction of order of differential equations, spatial and temporal averaging - are performed analytically before the numerical solution. Its merits are: computational simplicity; as a rule modelling even of comparatively complicated systems can be performed on a PC; dependencies on parameters and scaling laws can be easily obtained; flexibility; the source of main difficulties in the full- scale modelling - a great distinction in the temporal, spatial, and energy scales - gives an opportunity for substantial analytic simplifications; this

approach maximally exploits the previously obtained analytic results. Its shortages consist in the following: the complicated theoretical analysis is necessary; its performance crucially depends on intuition and lucky guess; the principally approximate results are obtained.

Nevertheless, it seems, that for investigation of physical mechanisms, as well, as for the main part of technological applications, the semi-analytic approach is preferable. We shall present here several examples, for which the fast operative modelling schemes can be developed, based on the analytic transformation of the general equations and on the excluding of the steep temporal and spatial scales.

The possibility of a serious reduction of the computational work in the discharge modelling lies, we are sure, in the optimal synthesis of the numerical and analytic approaches. By performing analytically some sort of averaging over the fast plasma motions, by introducing from the beginning the division of the whole discharge volume into the quasineutral plasma and space-charge sheaths, and by replacing the sheaths by some effective boundary conditions, it is possible, at least in the most interesting cases, to eliminate from the beginning the fast time scales, and the sharp transition layers of steep variation of the plasma parameters, which are the main source of the computational problems. The numerical integration of the resulting relatively simple system is, of course, considerably simpler and more physically transparent than the straightforward modelling.

I.High-pressure RF capacitive discharge satisfies typically:

$$\frac{4\pi n e^2}{m\nu_{ea}} >> \omega >> \frac{4\pi n e^2}{\mu\nu_{ia}};\ eU \gg T_e$$

The Debye radius is as a rule small: $r_d \ll L,\ L_{sh}$ .The evolution time of the plasma profile:

$$\tau = L^2 / D_{amb} \gg 1/\omega$$

This great difference in characteristic scales results in considerable numerical difficulties in the full-scale modelling. It can be avoided by temporal averaging. The small scales can be excluded, and averaged equation for the ion motion states

$$\frac{\partial n_i}{\partial t} = \frac{d}{dx}\left[D_{amb}\frac{dn_i}{dx} - \mu_i\langle E\rangle(x)n_i\right] + I - R$$

It contains only the global scales:

$$\langle E\rangle(x) = \frac{4j_0}{\omega}[\sin Z - Z\cos Z]$$

The sharp boundary of $n_e(x,t)$ profile is determined by

$$\sin Z\frac{dZ}{dx} = \frac{e\omega}{j_0}n_i(x)$$

The expressions for the source term can be calculated for the case of uniform plasma. Calculation of one data set demands 3-7 min on a PC.

Non-self-sustained discharge. At the Fig.1 the results of [1] are presented for N_2 , at 7.35 MHz, 90 Torr, 4.5 mA/cm^2, I = 10^{15} cm^{-3}s^{-1}, recombination coefficient 2.10^{7}cm^{3}s^{-1}. The full scale modelling [2] gives practically coinciding curve.

The ion density in the sheathes for self-sustained discharge in N_2 at p = 15 Torr, frequency 13,56 MHz are given at $j_0 = 15\text{ mA / cm}^2$, α-regime (Fig.2). and at $j_0 = 120\text{ mA / cm}^2$, γ-regime (Fig.3; curve 3 - the ionization rate).

At the Fig.4 the VAC for N_2, 15 Torr, 13,56 MHz is given.. Points - from full scale modelling of [3].

The correct description of low-pressure discharges can be performed only on kinetic level (at least for the electrons). The non-local approach turned out to be very effective for description of a dc positive column, cathode and anode regions of dc discharge, and for inductively and capacitevily coupled RF discharges. Its idea is based on the fact, that the electron energy relaxation length can be estimated as $\lambda_\varepsilon = \sqrt{\lambda\lambda^*}$ where λ and λ^* are the mean free paths for elastic and inelastic collisions, respectively. In the non-local approach , which is applicable if discharge gap $L_0 < \lambda_\varepsilon$, the electron kinetics is described by one single isotropic electron distribution function (EDF) of the total electron energy $\varepsilon = u - e\Phi(x)$(u is the kinetic energy, $\Phi(x)$ the space charge potential). This function $F_0(\varepsilon)$ is calculated from a spatially and temporally averaged kinetic equation, where the averaging is performed over the discharge volume, which is available for electrons with a fixed total energy. The spatially averaged coefficients in the averaged kinetic equation also depend only on ε and account for classical and stochastic heating of electrons in RF electric fields, elastic and inelastic energy losses, as well as electron-electron collisions.

The space charge potential profile, which is necessary for the application of the nonlocal approach, is found via a fluid model for the ions. The RF and dc electric fields and the source term in the equation for the ion density are determined by the quasineutrality condition and by the given EDF $F_0(\varepsilon)$. The main results of the existing full-scale modelling calculations and of experiments can be easily reproduced. The criterion of formation of low-energy peak on the EDF has been formulated and relative contribution of the classical and stochastic electron heating mechanisms has been estimated as a function of the external discharge parameters (pressure, gap, current density).

II. Low pressure RFC discharge.

The most complicated is the source in the ion equation. The idea of non-locality and the model of the sharp boundary of $n_e(x,t)$ profile allow to greatly simplify the calculations. One data set takes ~ 10 min on PC 486. In the Fig 5 the electron distribution function for He, p = 0.06 Torr, Lo = 2cm, jo = 7.3 mA/cm^2 is presented. The dotted line corresponds to the full-scale modelling - [4].

III. Low-pressure RFI discharge [5].

The spatial averaging of the Boltzmann equation and dependence of the electron distribution function only on total energy greatly simplifies the problem. The self-consistent calculations for one data set, which includes the solution of the kinetic equation for electrons, of 2D equation for the ion density profile, quasineutrality condition and the Bohm criterion, and of 2D wave equation for the RF field, takes approximately 40 min. on PC 486. At the Fig 6 the experimental and calculated EDF at the discharge center are given for the RFI discharge at 13,56 MHz in Ar in chamber with R=7,5cm, L=6cm.

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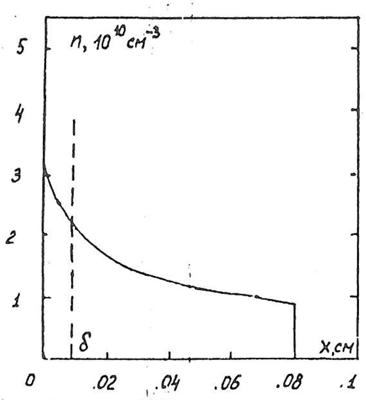

Fig.1 The results of [1] are presented for N_2, at 7.35 MHz, 90 Torr, 4.5 mA/cm^2, $I=10^{15}$ cm^{-3}s^{-1}, recombination coefficient 2.10^7 cm^{3}s^{-1}.

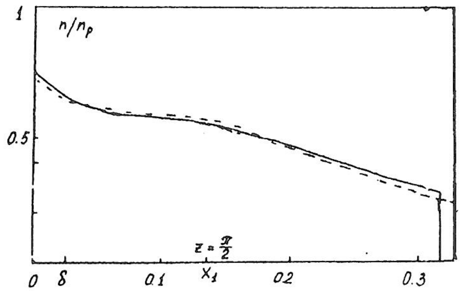

Fig.2 The ion density in the sheathes for self-sustained discharge in N_2 at p = 15 Torr, frequency 13,56 MHz are given at j_0 = 15 mA / cm^2, α-regime.

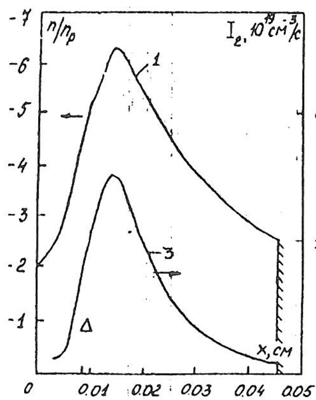

Fig.3 The ion density in the sheathes for self-sustained discharge in N_2 at p = 15 Torr, frequency 13,56 MHz are given at j_0 = 120 mA / cm^2, γ-regime (curve 3 - the ionization rate).

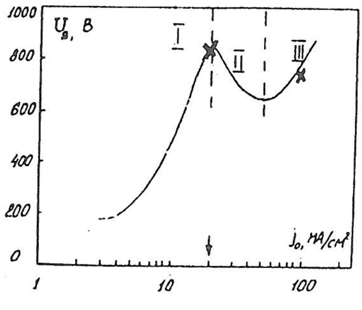

Fig.4 The VAC for N_2, 15 Torr, 13,56 MHz is given. Points - from full scale modelling of [3].

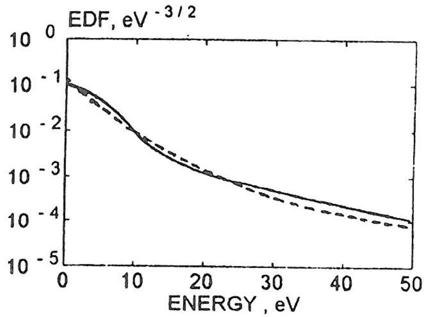

Fig.5 The electron distribution function for He, p = 0.06 Torr, Lo = 2cm, jo = 7.3 mA/cm^2 is presented. The dotted line corresponds to the full-scale modelling - [4].

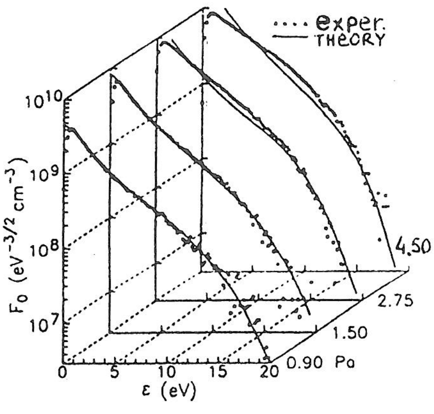

Fig.6 The experimental and calculated EDF at the discharge center are given for the RFI discharge at 13,56 MHz in Ar in chamber with R=7,5cm, L=6cm.