KINETIC THEORY OF IONIZATION IN A CATHODE SHEATH OF ABNORMAL GLOW DISCHARGE

A. A. GURIN

Scientific Center 'Institute for Nuclear Research“, Nat. Acad. Sci. of Ukraine
(*47, Nauky Prosp. Kyiv 03038, Ukraine*)

533.951

‰ 2001

The exact integral term of ionization in the electron kinetic equation taking into account the semi-empirical differential cross section of ionization by electron impact is derived. An efficient algorithm of solution of the kinetic equation is given in the one-dimensional case in the cathode sheath of dc glow discharges in helium. The electron current density distribution over energy and the space distribution of ionization efficiency in the cathode fall region are calculated. The results obtained for a set of parameters up to the kilovolt range show the detailed picture of forming a beam-like electron flow within the cathode fall region as well as the sharp localization of the ion/electron production rate near the cathode in kilovolt discharges.

Introduction

The cathode sheath of a dc glow discharge is well known to be responsible for main physical parameters of discharge characteristics. Near the cathode, the presence of a strong electric field is resulted in a significant complicacy of the simultaneous electron acceleration and swarming processes, so the determination of the electron distribution function (EDF) turns out to be a very difficult problem. Therefore, in spite of the exceedingly ancient age that problem of self-consistent cathode sheath description numbers, attempts to develop a more detailed cathode sheath picture are not terminating (the modern comprehensive review of the cathode sheath theory and kinetic models for various regions within a cathode sheath are presented in the analytic work [1]).

Two directions in researches of the cathode physics seem to be of interest up today. Technological applications of dc glow discharges for ion treatment of metal surfaces have stimulated the studying of ion energy spectra of cathode bombardment. Some features of the spectra are tightly connected with the electron behavior inside the cathode fall region (CFR). In particular, the localization of ion production at a short distance from the cathode within the CFR in the kilovolt discharges in He, first displayed by the computer simulation [2], can be resulted in arising a low-energy peak in ion spectra [3].

Another research direction concerns the formation of a cathode sheath structure outside the CFR far off the cathode, where the negative glow is being observed and the field reversal occurs [1]. The reason for the reversal and a bump-like potential distribution in the negative glow region is given by the arrival of a group of fast electrons at the boundary between the cathode fall region and the negative glow one. There, the electric field has become weak and even passes zero. The beam-like shape of the electron distribution function at the exit from the CFR is well studied in low discharges [1]. However, the formation of a high-energy electron flow depends quantitatively on the detailed energy and particle balance of electron inelastic scattering and swarming processes inside the CFR.

The complexity of the kinetic theory for various cathode sheath zones stipulates for researchers to use simplified models. The basic assumption well convenient in CFR is one-dimensionality of EDF. Even with this approximation, subsequent simplifications have been used such as a simplification of the energy-loss function (so-calles Bethe – Bloch's formula for high-energy electron losses), the neglect of the cross section dependence on the electron energy, etc. [1]. A surprising fact consists in that the correct entire form of the collision term for ionization in the electron kinetic equation has not described up-today (at least no one reference in review [1] contains such an information). This situation seems to be inadequate especially as the exact differential cross-section of ionization in He, for example, is well known [4]. (In the 'cascade“ computer model [2] close by a Monte-Carlo procedure, with using of data [4], the most full results for the EDF had been obtained without any analysis of an electron kinetic equation).

In this work, the exact entire form of an electron kinetic equation appropriate for cathode layer conditions is given. Moreover, it is shown that the

kinetic equation can be solved in a finite way. Although the algorithm proposed does not give a possibility to have a solution in a transparent analytic form, it enables the numerical calculations of the EDF to be the sufficiently exact and fast procedure.

Here, with the assumption of the parabolic distribution of electric potential within the CFR, that is, for the generally accepted picture of a cathode sheath [1], a solution of the electron kinetic equation is given. The problems of constructing the self-consistent electric field inside the CFR as well as arising the potential bump beyond this zone are not considered. We have limited ourselves to show efficiency of the theory for ion production rate calculations and detailed description of the EDF in the CFR. The simulation of the electron kinetics in a cathode sheath region has been carried out for the same values of the cathode fall as in [2] and has confirmed the quantitative results of this work.

1. Electron Kinetic Equation for the CFR.

The kinetic theory of ionization in the CFR can be based on the differential cross-section $\sigma(E, \varepsilon)d\varepsilon$ for a total energy loss ε within the interval $d\varepsilon$ of an electron whose kinetic energy before ionizing impact is equal to E. The process may be recognized as a decrease of the energy E down to $E - \varepsilon$ for the 'primary" electron and the generation of a 'secondary" electron with the energy $\varepsilon - I$, where I is the ionization threshold ('potential") of an ambient gas. The two-variable function $\sigma(E, \varepsilon)$ is not equal to zero only under conditions $I \le \varepsilon \le E$. The cross-section for helium used in this paper is determined by the semi-empirical formula derived in [4] (with the additional coefficient $1/2$ whose the meaning will be explained below):

$$\sigma(E, \varepsilon) = \frac{4}{EB(E)}\left\{\frac{1}{\varepsilon^2} - \frac{1}{(E + I - \varepsilon)^2} - \frac{E + I}{E + W}\times\right.$$

$$\left.\frac{1}{\varepsilon\,(E + I - \varepsilon)} + 0.98I^2L(E)\left[\frac{1}{\varepsilon^3} + \frac{1}{(E + I - \varepsilon)^3}\right]\right\}, \qquad (1)$$

where $W = 67.7$,

$$L(E) = \ln(1.6 + [0.15(E - I)]^{1/2}),$$

$$B(E) = 1 + \frac{5.34}{E}\,\frac{1 + 5.34/E}{1 + (0.027E)^3}.$$

Here, the energy and cross-section are gauged in the atomic units $\mathrm{Ry} = 13.6$ eV and $\pi a^2 = 0.88 \cdot 10^{-16}\,\mathrm{cm}^2$ correspondingly (that is, $I = 1.81$ for He in formula (1)).

The differential cross-section (1) can be normalized to the integral cross-section as follows:

$$Q(E) = \int_I^E d\varepsilon\sigma(E, \varepsilon) \qquad (2)$$

or, when $E > I$,

$$Q(E) = \frac{8}{EB(E)}\left\{\frac{1}{I} - \frac{1}{E} - \frac{\ln(E/I)}{E + W} + 0.49L(E)\left[1 - \frac{I^2}{E^2}\right]\right\}. \qquad (3)$$

Usually, in [4] too, the same expression (3) for the integral cross-section is determined by integrating within the interval $I \le \varepsilon \le (E + I)/2$ that is half narrower than the integration area in Eq.(2). However, the value σ is determined twice as much the σ given by expression (1). Generally, the formulae for σ represent the group of terms in such a manner to provide the indistinguishability, of two electrons after impact through the symmetry property $\sigma(E, \varepsilon) = \sigma(E, E - \varepsilon + I)$. That is why the normalization of the differential cross-section to the integral one could be carried out only between the limits of integration I and $(E + I)/2$ that is only over half the validity interval (I, E) in which the differential cross-section σ is defined as a positive function of ε. In this case, the cross-section σ would be doubled in comparison with the defined above (1), and the faster electron after impact would be considered conventionally as a 'primary" one, whilst the slower electron as a 'secondary" one [2]. Our definitions (1) – (3) give the possibility to classically consider the primary and secondary electrons with arbitrary energy as distinguishable ones taking into account the indistinguishability only by means of the symmetry $\sigma(E, \varepsilon) = \sigma(E, E - \varepsilon + I)$. Such a manner is more natural for the classical kinetic theory to obtain the correct integral formulas for the energy and particle balance under ionization.

Let the cathode sheath occupy the space $x > 0$, where $x = 0$ is ascribed to the cathode surface, and let the width of the CFR be equal a. Suppose the electric gradually growing potential $\Phi(x)$ inside the interval $(0, a)$ under the conditions $\Phi(0) = 0$, $\Phi(a) = U_c$, where U_c is the cathode fall. With the assumption of one-dimensionality of the electron motion problem, we denote as $\Gamma(x, E)dE$ the flow density of electrons with energy within the interval $(E, E + dE)$ at a point x. (The kinetic theory given below for the 'current density" Γ could be formulated in terms of the usual velocity distribution function f in accordance with the definition $\Gamma(x, E)dE = \nu f(x, \nu)d\nu$, where $E = m\nu^2/2$. Therefore, the value Γ will be named elsewhere also as 'EDF").

The ionization collisional term in the kinetic equation for Γ does not conserve the number of particles, because each primary electron frees an additional 'secondary" one. The structure of the collisional term could be described by three items: two positive ones representing the quantity of electrons generated in the unit volume per unit time within the energy interval dE, correspondingly, as decelerated primary electrons or arbitrary secondary ones, the third negative item takes into account the energy loss rate owing to ionization in this interval. The appearance of the primary electron in the energy interval $(E, E + dE)$ occurs when an electron with the energy $E + \varepsilon$ losses its component ε. The differential contribution to this quantity by the scattering channel $d\varepsilon$ is $\Gamma(x, E + \varepsilon)dE \cdot N_0 \sigma(E + \varepsilon, \varepsilon)d\varepsilon$, where N_0 is the gas density. Summing over all energy losses gives the primary electron production rate:

$$(S_{i0}^{+})_{\text{prim}}dE = N_0 dE \int_{I}^{E_{\max}-E} \Gamma(x, E + \varepsilon)\sigma(E + \varepsilon, \varepsilon)d\varepsilon. \quad (4)$$

The upper integration limit in this integral follows from the condition that, in the CFR, the maximal energy $E_{\max}(x)$ exists for which $\Gamma(x, E) = 0$ when $E \geq E_{\max}$. The existence of the upper electron energy limit is justified by the physical observation that such a limitation takes place under the cathode emission caused by ion bombardment. Otherwise, the boundary condition for the EDF can be represented in the form

$$\Gamma(0, E) = j_0 F_0(E), \ 0 \leq E < E_0;$$

$$\Gamma(0, E) = 0, \ E_0 \leq E, \quad (5)$$

where the initial distribution is normalized to 1, that is, $\int dE F_0(E) = 1$ with integrating over the interval $(0, E_0)$. This definition makes j_0 to have the sense of emission current density and E_0 to be the upper energy boundary for electrons starting at the cathode face after ion impacts. Since the collisions diminish only the electron energy in our model, a further motion, for $x > 0$, of some amount of electrons realizes the probability to run away any inelastic collisions and gains the kinetic energy as much as possible in the electric field throughout CFR. Therefore, the $E_{\max}$ turns out to be dependent on x as consistent with the simple rule

$$E_{\max}(x) = E_0 + e\,\Phi(x). \quad (6)$$

The limitation of the validity area of the EDF with energy (6) is of importance to find a solution of the kinetic equation. As concerns the lower limits in integral (4), its value I is conditioned by the threshold dependence of the cross-section σ on the variable ε.

The secondary electron emerges in the interval $(E, E + dE)$ when an energetic primary electron with energy $E' > E + I$ losses the portion of its energy in the interval $(E + I, E + I + dE)$. The differential secondary electron production rate is $\Gamma(x, E')dE'N_0\sigma(E', E + I)dE$. With the same arguments in regard to the integration limits, integration over E' gives the positive secondary electron contribution into the electron production rate

$$(S_{i0}^{+})_{\text{second}}dE = N_0 \left[\int_{E+I}^{E_{\max}} dE' \Gamma(x, E')\sigma(E', E + I) \right] dE. \quad (7)$$

Expressions (4), (5) look quite different being identical indeed, as is demanded with the indistinguishability principle. This can be verified by changing $E' = E + \varepsilon$ in integral (4) and taking into account the fundamental symmetry $\sigma(E, \varepsilon) = \sigma(E, E - \varepsilon + I)$. Taking into account as usually the negative component of the total electron balance within the interval $dxdE$ under ionized impacts and the gain of electron density owing to acceleration in the field of electric potential $\Phi(x)$, the electron kinetic equation can be written by

$$\left[\frac{\partial}{\partial x} + e\Phi(x) \frac{\partial}{\partial E} \right] \Gamma(x, E) = 2S_{i0}^{+} - N_0 Q(E)\Gamma(x, E). \quad (8)$$

Here, it does not matter what positive source (4) or (5) may be written on the right-hand side in Eq.(8) in view of their identity. The integral cross-section $Q(E)$ obeys definitions (2), (3).

If it is necessary to take into account the accompanying process of inelastic excitations, the ionization term ought to be added by the source S_{ex} of the well-known form:

$$S_{\text{ex}} = \Sigma \left[N_0 Q_{\text{ex}}(E + I_{\text{ex}})\Gamma(x, E + I_{\text{ex}}) - N_0 Q_{\text{ex}}(E)\Gamma(x, E) \right], \quad (9)$$

where Q_{ex} and I_{ex} are the cross section and threshold energy of the excitation process, correspondingly, the sum is over all types of excitations.

The integration of Eq.(8) over energy gives the particle density balance in the static cathode sheath defined exclusively by ionization:

$$\alpha(x) = \frac{d}{dx} j(x) = N_0 \int_{I}^{E_{\max}(x)} dE Q(E)\Gamma(x, E), \quad (10)$$

where $j(x) = \int E d(x, E)$ with integration within the same limits $(I, E_{\max})$. In such a way, the ionization efficiency (the ion/electron production rate) α is

defined through the spatial current increment or by integral (10).

2. Solution of the Kinetic Equation

Eq.(8) becomes the most convenient for integration when one tries to find the EDF as a function of the total energy: $\Gamma(x, E) = F(x, \varepsilon)$ where $\varepsilon = E - e\Phi(x)$. In accordance with remarks concerning the upper limit (7) for the kinetic energy of electrons in the CFR, the validity area of the function $\Gamma(x, E)$, $0 \le E \le E_{\max}(x)$, transforms into the interval $-e\Phi(x) \le \varepsilon \le E_0$. So the $F(x, \varepsilon)$ must be found for the preferable negative total energies because of really $E_0 << eU_c$ for abnormal disharges. The gauge to units a and σ_0 for x and cross-sections in the expressions written above gives the most general kinetic equation available for numerical integration:

$$\left[\frac{\partial}{\partial x} + Q_{\text{tot}}(\varepsilon + e\Phi(x))\right] F(x, \varepsilon) = 2S^+_{i0} + S^+_{\text{ex}}, \qquad (11)$$

where $\lambda = a\sigma_0 N_0$,

$$S^+_{i0}(x, \varepsilon) = \lambda \int_{\varepsilon + I}^{E_{0\max}} d\varepsilon' F(x, \varepsilon')\sigma(\varepsilon' + e\Phi(x),\ \varepsilon' - \varepsilon), \qquad (12)$$

$$S^+_{\text{ex}}(x, \varepsilon) = \lambda \sum_{\text{ex}} Q_{\text{ex}}(\varepsilon + e\Phi(x) + I_{\text{ex}}) F(x, \varepsilon + I_{\text{ex}}), \qquad (13)$$

Q_{tot} is the total cross-section, $Q_{\text{tot}}(E) = Q(E) + \Sigma Q_{\text{ex}}(E)$ (the sum is over excitations taken into account).

The boundary condition (5) becomes $F(0, \varepsilon) = j_0 F_0(\varepsilon)$ because of $\Phi(0) = 0$. So the solution $F(x, \varepsilon)$ is defined by two constituents: the EDF for positive energies of order of a few eV for the transit electrons being emitted by cathode, and the EDF in the negative energy region within the range of the cathode fall eU_c (≈ 1 keV) which is filled from the top by electrons due to inelastic scattering of primary and secondary electrons.

A solution of the kinetic equation (11) can be born on the observation that the positive integral sources S^+_{i0} and S^+_{ex} at a point (x, ε) are not depend on values $F(x, \varepsilon)$ within a finite vicinity of ε for any x. Indeed, the lower limit in integral (12) defines the shift of the integration interval up to more high energies $\varepsilon' \ge \varepsilon + I$ as well as the excitation source (13) depends evidently on F at the energy enlarged by the excitation threshold I_{ex}. Therefore, if the values of EDF would be calculated in the total energy area $(\varepsilon + I_{\min}, E_0)$ where $I_{\min} = \min\{I, I_{\text{ex}}\}$, the solution $F(x, \varepsilon)$ is determined from the Eq.(11) with the known right part. Really the value E_0 is not high comparably with I_{ex} (in [2], it was assumed $E_0 = 0.6I$ whereas the minimal threshold for lowest singlet levels, $I_{\min} = \min\{I_{\text{ex}}\}$, is equal to $\approx 0.88I$). This implies that, for the highest values ε which belong to the interval $E_0 - I_{\min} < \varepsilon \le E_0$, the EDF is governed by the elementary homogeneous equation (11) with zero source because the ε-interval $(E_0, E_0 + I_{\min})$ is empty for particles. In particular, if $E_0 \le I_{\min}$, it follows for any x that

$$F(x, \varepsilon) = F_0(\varepsilon) \exp\{-\lambda \int_0^x ds Q_{\text{tot}}(\varepsilon + e\Phi(s))\},$$

$$0 \le \varepsilon \le E_0. \qquad (14)$$

Thus, the entire procedure of resolution proceeds in two steps. After the EDF in the positive energy area is found at first by Eq.(14), $F(x, \varepsilon)$ can be computed for a succession of negative energies given, for example, by the equidistant grid $\varepsilon_j = -j\delta\varepsilon$, where j is integer: $j = 1, 2, \ldots, N$ (N is the round off ratio $eU_c/\delta\varepsilon$),

$$\delta\varepsilon \le I_{\min}. \qquad (15)$$

For this, the simple zero-boundary problem $F(0, \varepsilon_j) = 0$ must be resolved with the nonzero right part of Eq.(11) calculated on the known EDF's values for higher energies and any x. Moreover, since $F(x, \varepsilon)$ is represented only inside the region $-e\Phi(x) \le \varepsilon \le E_0$, the closed interval $[0, x_\varepsilon]$ whose boundary x_ε obeys the condition $\varepsilon + e\Phi(x_\varepsilon) = 0$ for a negative ε, turns out to be empty. Thus, the actual initial condition for EDF in the negative energy region is

$$F(x_\varepsilon, \varepsilon) = 0, \quad \varepsilon < 0, \qquad (16)$$

and a positive EDF is found only for $x > x_\varepsilon$.

The sole restriction (15) that the procedure having been correct is easy to be complied with a discrete representation $x \to x_i$, $\varepsilon \to \varepsilon_j$, $F(x, \varepsilon) \to F_{ij}$ providing the sufficient accuracy of numerical integration in Eq.(12). The value $\delta\varepsilon = (1/20)I$ used in calculations has answered all the requirements of approximation. It was most convenient for our problem to use the grid being inhomogeneous over x_i answering the constraints $e\Phi(x_i) = i\delta\varepsilon$. The simplest code resolving problem (11) is given by the recurrent formula

$$F_{ij} = F_{i-1,j}\, e_{ij} + 0.5\lambda\delta x_i (S^+_{ij} + e_{ij} S^+_{i-1,j}), \qquad (16)$$

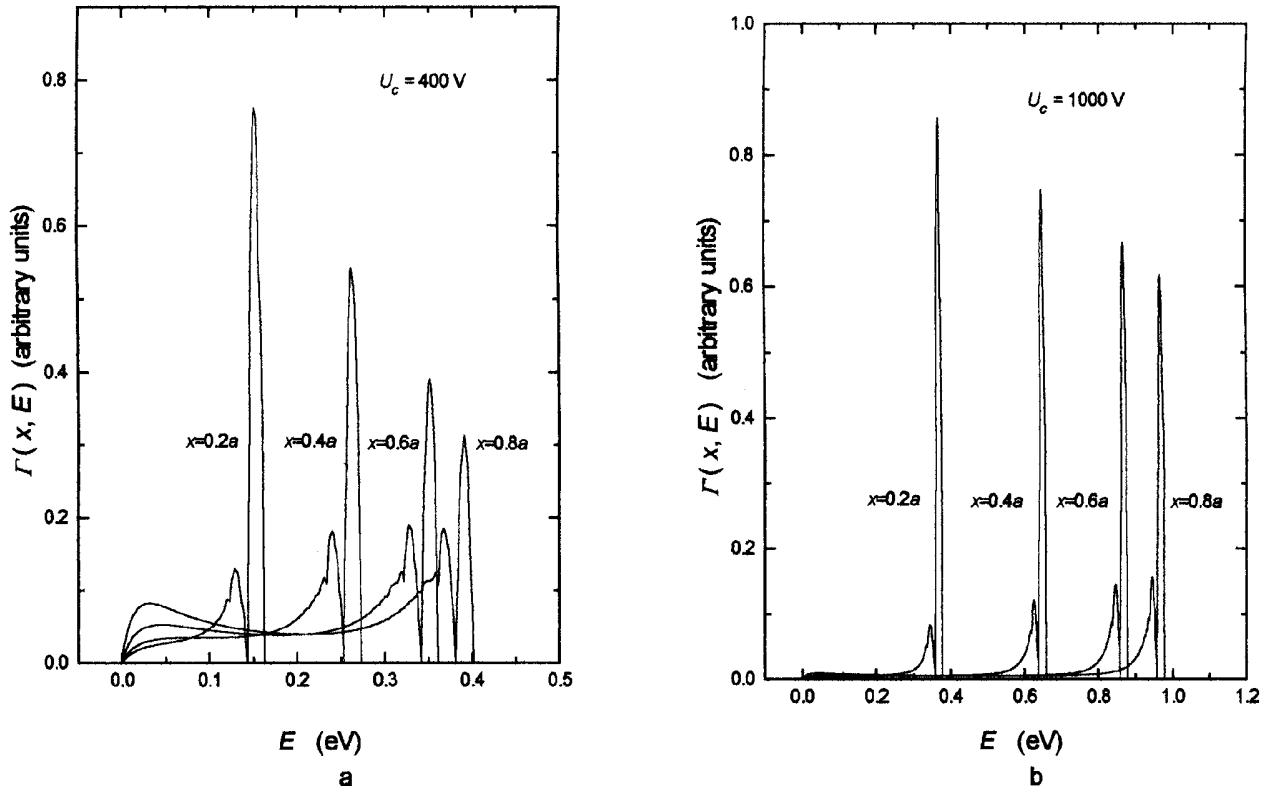

Fig.1. Spatial evolution of the EDF through various positions (x is shown against each curve in units of a) in the cathode sheath region: a – for a cathode fall U_c = 400 V; b – U_c = 1000 V

where $\delta x_i = x_i - x_{i-1}$, $S_{ij}^{+} = 2S_{i0}^{+}(x_i, \varepsilon_j) + S_{\rm ex}^{+}(x_i, \varepsilon_j)$,

$$e_{ij} = \exp\{-\lambda \int_{x_{i-1}}^{x_i} ds Q_{\rm tot}(\varepsilon_j + e\,\Phi(s))\}. \qquad (17)$$

Procedure (16) begins from the 'diagonal" $i = j$ where $F_{jj} = 0$ in accordance with the initial condition (15). It is equivalent to the account of electron groups involved into one, two, three, ... etc. ionizations while the energy ε_j passes the zones of width I down to the negative limit $\varepsilon_N = -eU_c$. With the definitions, the algorithm contains no problems of convergence or stability.

3. Results and Discussion

To provide a sufficient accuracy of calculations, the cross-sections $Q_{\rm tot}$ and $Q_{\rm ex}$ in formulas (12), (13) must be specified. We constrain the consideration with the summary cross-section $Q_{\rm ex}$ over all excitations corresponding the common lowest value $I_{\rm ex} = I_{\rm min}$ in helium (that is, $I_{\rm ex} = 0.88I$ or ≈ 21.6 eV). This constituent of the total cross-section $Q_{\rm tot}$ was depicted from the data of [2], where the cross-sections are presented in absolute units.

The calculations have been carried out with the parabolic distributions $\Phi(x)$ and $F_0(E)$:

$$\Phi(x) = U_c\, x(2a - x)/a^2, \quad 0 \le x \le a; \qquad (18)$$

$$F_0(E) = 6E(E_0 - E)/E_0^3, \quad 0 \le E \le E_0. \qquad (19)$$

Choice (18) is usual in the cathode sheath theory [1, 2]. The initial distribution (19) is normalized to 1 over the area $(0, E_0)$, as it is necessary. The parabolicity is not obligatory for the E_0 taken usually as a trapezoid or like δ-function at $E = 0$ [2]. The F_0's form defines only the front shape of the EDF for the most fast transient electrons crossing the CFR without scattering. Such insignificant details are not visible for the EDF gauged to the cathode fall U_c because of always $U_c >> E_0$.

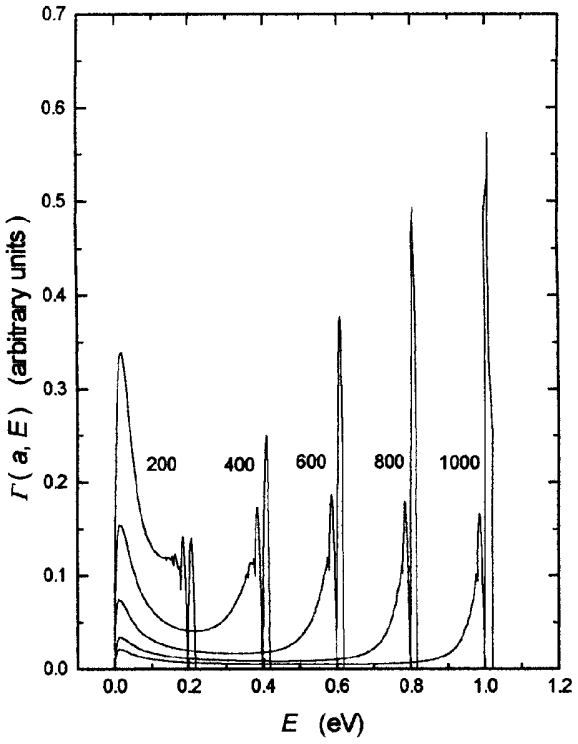

Fig.2. Shape of the EDF at the exit from the cathode sheath region for five values of the cathode fall U_c (shown against each curve in volts)

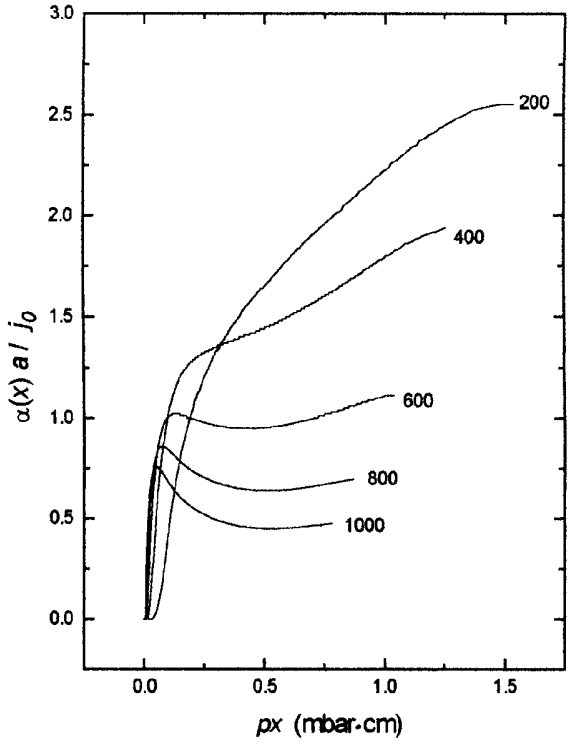

Fig.3. Spatial distribution of ionization efficiency within the cathode fall region (the curves break against the values of ap corresponding the cathode falls U_c shown besides in volts)

The dimensionless parameter $\lambda = \sigma_0 a N_0$ can be expressed also through the physical discharge characteristics: $\lambda = 0.35ap$, where p is the gas pressure (mbar) at a temperature of 273 K, a is the CFR's width (cm). The choice of ap (mbar · cm) for corresponding cathode falls $U_c(V)$ is taken from phenomenological diagrams for abhormal discharges in He [5]. We have used the following set of parameter pairs: ($U_c = 200$ V, $ap = 1.65$), ($U_c = 400$ V, $ap = 1.3$), ($U_c = 600$ V, $ap = 1.05$), ($U_c = 800$ V, $ap = 0.9$), ($U_c = 1000$ V, $ap = 0.8$).

Fig.1, *a* and *b*, shows the forming of the EDF at four distances from the cathode ($x/a = 0.2, 0.4, 0.6, 0.8$) for two values of U_c: *a* – $U_c = 400$ V (an intermediate discharge), *b* – $U_c = 1000$ V (a high-voltage discharge). There is an evident demonstration of the EDF's evolution from the initial peak to a beam-like shape at CFR's end. The dependence of the beam-like form of EDF at the exit from CFR on cathode falls is depicted in Fig.2. The high energy peak prevails mainly in the high-voltage discharges that agrees well with the results of all previous examinations [1, 2].

The ionization efficiency α can be calculated as the derivative of the current $j(x)$ or by formula (10). Both ways were used to verify the reliability of calculations. In Fig.3, the space distributions $\alpha(x)$ are depicted for five cathode falls and the corresponding values of discharge parameters ap. The results agree qualitatively with the data of Monte-Carlo simulations [3] and are in excellent agreement with calculations within the cascade method [2], especially for high-voltage discharges. Fig.2 demonstrates the effect of localization of the ion/electron production rate near by the cathode inside the CFR while the cathode fall increases up to one kilovolt.

The accuracy of our calculations is restricted in our cathode sheath model, as far as the width a and potential distribution $\Phi(x)$ being taken as external parameters. However, the efficiency of the method proposed gives the possibility for a self-consistent determination of the discharge characteristics in the wider cathode sheath range. The revealed main features of the electron behavior in the CFR have be peculiar to a more general model.