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Kinetic Characteristics of Electron Drift in Gas Discharge Plasma

Abstract. An electron drift in a monatomic gas was studied for a spatially uniform electric field. Functions of the electron energy distribution are found by solving the Boltzmann equation in the two-term approximation and applying the Monte Carlo method. We take into account both elastic and non-elastic collisions of electrons with atoms, recombination at the walls. Integral characteristics of the electron drift in the gas were calculated, allowing to analyze the drift of electrons on a qualitative level. The results of calculations of the energy balance of electrons and drift characteristics in argon are shown at the values of reduced field 1<E/N <28 Td.
Keywords: Electron drift, gas discharge plasma, the Boltzmann equation, Monte Carlo method, Electron energy distribution function.

Introduction

Diffusion and drift of electrons in gases have been well studied both theoretically and experimentally [1, 2]. But in recent years there has been a great interest in simulation of kinetics of electrons in low-temperature plasma, due to numerous technological applications. It is the numerical simulation that gives accurate and complete information about the characteristics of gas-discharge plasma, which is necessary for understanding and interpreting the properties of dust structures in plasma.

In many papers on the study of dusty plasma in the gas dc discharge at low gas pressure it is assumed that the plasma electrons have a Maxwellian distribution with a temperature which is determined from probe measurements [3]. Druyvesteyn distribution is sometimes used as an alternative model which does not lead to a significant difference in the characteristics of dusty plasmas (see the recent paper [4]). But it is well known that Maxwell and Druyvesteyn distributions are significantly different from the actual distributions of the electron energy in the gas discharge, because in a self-discharge, a decisive contribution to the electron velocity distribution is made by the ionization and recombination processes.

Let's consider the simplest statement - the drift of an electron in a uniform and constant electric field. We assume that the electron moves under the influence of a uniform electric field, suffering only elastic collisions with atoms. Then, in very weak fields, the deviation of the mean energy of electrons is small from the energy of atoms; the function of the electron energy distribution (EEDF) is close to the distribution of atoms, which can be assumed Maxwellian. But in a strong field, there is a sharp imbalance between the electron and nuclear subsystems, and the average electron energy is much higher than the energy of atom. In this case, the electron distribution function in absolute velocity (taking into account only elastic collisions) is determined by the balance between Joule heating and losses in elastic collisions with cold gas [1, 2, 5]:

$$f_0(\mathrm{v}) = A\exp\left(-\frac{3m}{M}\left(\frac{mN}{eE}\right)^2\int_0^{\mathrm{v}} c^3\sigma_{el}^2(c)dc\right), \quad (1)$$

where *m, M* are the masses of electron and atom, σ_{el} is a cross section of elastic collisions, the constant *A* is determined from the normalization condition $1 = 4\pi\int_0^{\infty} c^2 f(c)dc$.

In the case of a power-law dependence on the rate of cross-section: $\sigma_{el}(c) = \sigma_0(c/c_0)^r$ - integral in eq.(1) is calculated. If $\sigma_{el}(c) = \sigma_0(c/c_0)^{-1/2}$, when the collision frequency is constant, the distribution (1) reduces to the Maxwell distribution, when cross-section is constant: $\sigma_{el}(c) = \sigma_0$ the distribution (1) becomes Druyvesteyn distribution [1, 2, 5].

Maxwell distribution is presented as:

$$f_{Maxwell}(\varepsilon) \propto \varepsilon^{1/2}\exp(-\varepsilon/T_e), \quad (2)$$

and Druyvesteyn distribution can be written as:

$$f_{Druwestain}(\varepsilon) \propto \varepsilon^{1/2}\exp(-\varepsilon^2/\varepsilon_D^2). \quad (3)$$

They describe the electron distribution function only in the absence of non-elastic collisions birth or death of the electrons. Then the solution accuracy of eq. (1) is determined only by the error with which the collision cross section is approximated by a power-law dependence on velocity (under the condition that the average energy of electrons is much higher than atomic one).

It should be noted that the Druyvesteyn distribution generally has better agreement with experimental data than the Maxwell distribution. This is due to two factors. Firstly, the cross section of elastic collisions is often better approximated by a constant rather than by decreasing function of velocity. Secondly, at high collision energies, the constant cross-section better corresponds to the real situation, when the tail of the distribution function is cut off due to the appearance of threshold processes - excitation and ionization.

In the steady-state current flow through the discharge tube, whose length is much greater than its diameter, ions and electrons from the positive column in consequence drift and diffusion reach the walls of the tube and there perish. Moreover, for ions in addition to the diffusion the drift in the radial field of the positive column becomes important.

Electrons are trapped in the potential pit, but reach the walls of the tube almost immediately, as their energy exceeds the potential barrier. Completion of dying electrons on the wall occurs due to ionization of atoms by electron impact. In this case an electron loses a significant fraction of its energy and the energy of the emerging electron is close to zero.

Thus, the self-discharge electron drifts and gains energy due to Joule heating, and then loses it at non-elastic collision, then when drifting again begins to gain power. If its energy is greater than the potential barrier, it almost immediately reaches a wall and recombines on it. But both Maxwell (2) and Druyvesteyn (3) distributions, as well as more general one (1) do not take into account the constant electron drift upward along the energy axis. Since it is the non-elastic processes that determine the nature of current flow through the discharge tube the use of solutions (1) in this case is not correct.

Another limit for the EEDF is a "pipe-line" (pipe) model in which formation of the EEDF is determined by the Joule heating model and non-elastic collisions, while the energy loss of electrons at elastic collisions with atoms are assumed to be negligible [2, 4]. In the pipeline model Joule heating is a drift of energy in the positive direction (i.e., the electron energy increases continuously). The drift velocity is determined by the diffusion of energy

$$D_e = \frac{e^2E^2\lambda^2\nu}{3}. \quad (4)$$

The boundary conditions in the pipeline model are selected according to the assumption that the electrons drift from the original zero energy up to some maximum energy, $\varepsilon_{\max}$, where they lose it all making the act of ionization or excitation.

At a constant frequency of electron collisions with atoms, we obtain the following distribution of electron energy [3, 4]:

$$f(\varepsilon,\varepsilon_{\max}) = [1-(\varepsilon/\varepsilon_{\max})^{1/2}]/3\varepsilon_{\max} . \quad (5)$$

The average energy of the electrons in the distribution (5) is equal to

$$<\varepsilon> = \int_0^{\varepsilon_{\max}} \varepsilon f(\varepsilon,\varepsilon_{\max}) d\varepsilon \Big/ \int_0^{\varepsilon_{\max}} f(\varepsilon,\varepsilon_{\max}) d\varepsilon = \frac{3}{10}\varepsilon_{\max} . \quad (6)$$

The maximum energy $\varepsilon_{\max}$ can be put equal to either energy of the first excited level $\varepsilon_{\max} = E_1$ or to ionization potential $\varepsilon_{\max} = I$. Some refinement of this model can be done, if we consider the different levels of excitation and ionization. Then the distribution function will be equal to the superposition of the N-solutions (5) with weights that take into account the share of this type of collisions:

$$f_N(\varepsilon) = \sum_n \alpha_n f(\varepsilon,\varepsilon_n) \quad (7)$$

where the summation is over all levels, and weight $\alpha_n = <\sigma_n \varepsilon^{1/2} f_N(\varepsilon)> / \sum_i <\sigma_i \varepsilon^{1/2} f_N(\varepsilon)>$ is determined by the relative share of the excitation frequency from the ground level to the level *n* in the total number of non-elastic collisions of electrons with atoms.

Monte Carlo Model

Consider the problem of modeling at the independent gas discharge. It should include consideration of the motion of electrons in an electric field, elastic collisions of electrons with atoms, non-elastic collisions and loss of electrons. For the gas discharge tube DC at reduced pressure it is necessary to record the impact ionization, energy consumption for the excitation of atoms and the recombination of electrons on the walls of the tube.

The processes of excitation, ionization and recombination in real experimental conditions often cannot be taken into account in the spatially homogeneous (zero-dimensional) model, since the electrons appear in the tube and die on its surface. Therefore, the distribution of electrons and ions in the coordinates, even in the steady state is inhomogeneous. However, a model of spatially homogeneous drift and take into account loss of electrons on the tube walls by introducing a characteristic time of the withdrawal of electrons on the wall (the lifetime of electrons) can be taken. The introduction of the lifetime, which is the same for electrons with different energies, was not very well done in many papers. Because of the electron with low energy cannot overcome the potential barrier of the wall and stays inside the hole as long as its energy is sufficiently large to overcome the potential barrier. If the electron has sufficient energy to overcome the potential barrier, it almost immediately goes to the wall and dies (recombines) on it.

Therefore, in this paper a different approach [6-8] was used to account for the birth and loss of electrons. For the process of electron drift in the positive column one can assume that total number of births and deaths of electrons are equal. Then the death of electrons on the walls can be taken into account by introducing into the algorithm a rule that for each act of ionization one electron is removed from the whole ensemble. The most logical for the problem of electron drift in the positive column is assumption that only a most energetic electron, which appears in an act of ionization, can leave the ensemble. The average energy of electrons that leave the system, can provide a good estimation of the potential of the wall. Thus, the wall potential is determined from the condition that the number of ionization events is equal to that of particles' escapes from the system (number of acts of destruction at the wall).

To calculate the drift characteristics of electrons in the gas the Monte Carlo method was used [6,8]. After each collision we integrated the equations of electron motion in a constant field, and in accordance with the known cross sections for elastic and non-elastic processes, the probability of an event was determined.

The processes of excitation, ionization and recombination in real experimental conditions often cannot be taken into account in the spatially homogeneous model. Nevertheless, we adopt the following model, which considers spatially-homogeneous stationary flow of electrons under the following assumptions:

1) Gas atoms have a Maxwellian velocity distribution and do not change their temperature by collisions with electrons;

2) Elastic electron-atom collisions occur as collisions of hard spheres, i.e. at collisions isotropic scattering in the center of mass occurs, but the collision cross section is assumed to depend on the energy of their relative motion;

3) The loss of electrons on the excitation of atomic levels is irretrievable, that means that the excited atoms lose their energy of excitation in the surround mode emission, metastable atoms diffuse beyond the boundaries of the volume;

4) In electron-impact ionization one electron colliding with an atom loses energy equal to the sum of ionization energy and the kinetic energy of the second electron. After the act of ionization energy is assumed to be equal to: $\varepsilon_1^{'} = \varepsilon_1 - I - \varepsilon_2^{'}$. We assume that the energy of the first electron is equally likely to take all possible values, and the energy of the second electron is determined from the energy conservation law:

$$\varepsilon_1^{'} = (\varepsilon_1 - I)R \ , \varepsilon_2^{'} = (\varepsilon_1 - I)(1 - R), \qquad (8)$$

where $0 < R < 1$ is a random number.

5) The processes of recombination of electrons and atoms, quenching of excited levels and the transfer of resonance radiation do not change the electron energy.

Let's consider the energy balance of electrons. During the drift in electric field, electrons gain energy from the electric field. In a constant and uniform electric field due to Joule heating an electron acquires an average energy per time unit

$$Q_{EW} = eEW, \qquad (9)$$

here e is electron charge, E is electric field strength, W is the drift velocity.

Let's consider the case when the electrons energy is much higher than the energy of atoms. Then in the stationary, spatially homogeneous case, the energy acquired by an electron is lost in elastic collisions with atoms, is spent on the excitation and ionization of atomic levels, in addition, electrons carry away or obtain energy by recombination:

$$Q_{EW} = Q_{ea} + Q_{ex} + Q_{ion} + Q_{rec}. \qquad (10)$$

The right side of this equation shows the corresponding average energy loss per time unit of a single electron (electron may also gain energy for example, three-body recombination). In the following calculations we have neglected the influence of recombination processes on the electrons energy i.e. $Q_{rec} = 0$.

Model of the Boltzmann equation

In an electric field E one-particle distribution function of the electron velocity *F (r,v,t)* is determined by solving the Boltzmann equation [1, 2, 5]:

$$\frac{\partial F}{\partial t} + \vec{v}\frac{\partial F}{\partial \vec{r}} - \frac{e}{m_e}\vec{E}\cdot\frac{\partial F}{\partial \vec{v}} = S_t(F), \qquad (11)$$

where *St (F)* is a collision integral, $\vec{r}$ and $\vec{v}$ are coordinate and velocity of electrons, t is the time.

Since the solution of Boltzmann equation (11) is a very difficult task, for describing the kinetics of electrons in a gas discharge binomial approximation is often used. The Boltzmann equation in the binomial approximation in a uniform and constant electric field is as follows:

$$\begin{aligned} -\frac{eE_z v}{3\varepsilon}\frac{\partial(\varepsilon f_1)}{\partial \varepsilon} &= S^{el}(f_0) + \sum_j S_j^{in}(f_0) + S^{ion}(f_0) + S_w(f_0), \\ -eE_z\frac{\partial(f_0)}{\partial \varepsilon} &= -N_g\sigma_m(\varepsilon)f_1(\varepsilon) \end{aligned} \qquad (12)$$

where, $S_{el}(f_0)$, $S_j^{in}(f_0)$, $S_{ion}(f_0)$ are integrals of elastic, non-elastic and ionizing collisions of electrons with atoms, $S_w(f_0)$ is a term describing the process of electron loss to the walls of the discharge tube [1, 2, 5-7].

In this paper, the system of equations (12) was solved by iteration method [7, 8]. Then obtained distribution functions were used to calculate various characteristics of the electron drift. We determined the drift velocity, average electron energy, etc. (For more detailed description of the problem and the method of solution obtained with the help of this model characteristics, see [9, 10]).

There are reasonable doubts about the applicability of the binomial approximation to describe the properties of the discharge [2]. In any case it is impossible to carry out equality (as is often done) between the solution of Boltzmann equation and the binomial approximation. Since Monte Carlo method gives as accurate description as the Boltzmann kinetic equation, it is of great methodological interest to compare these two solutions to determine the accuracy of binomial approximation method.

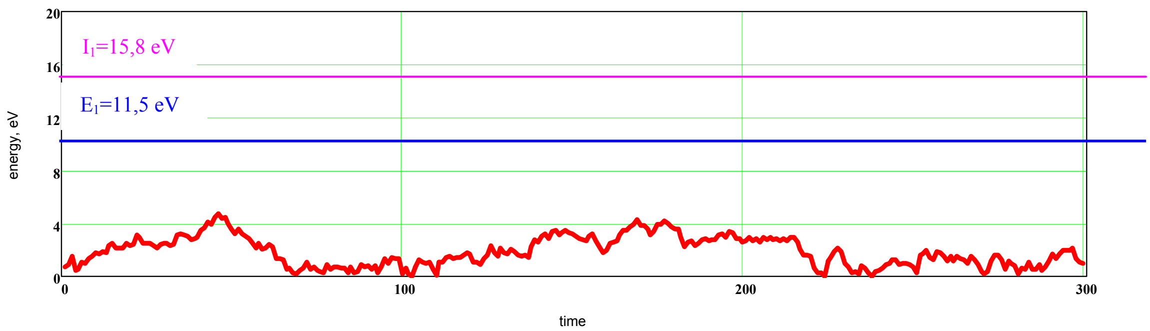
Results of calculations and discussion

Let's consider at first the results of simulation of electron drift at different values of electric field, which may be in different parts of the gas discharge. In calculations by the Monte Carlo method we used the condition of death on the walls only for electrons with high energy and determined the wall potential. In calculations, obtained by solving the Boltzmann equation, the loss of electrons on the walls was taken into account by introducing recombination time [2 - 10].

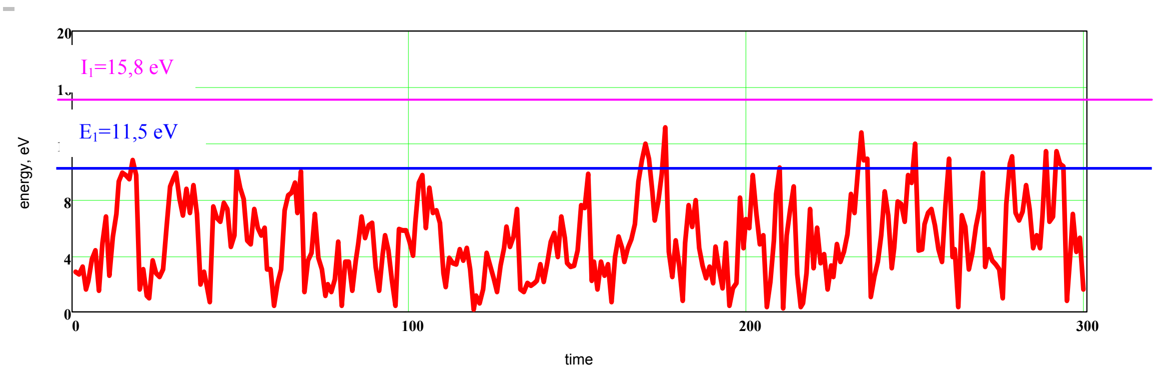
Figure 1 show a typical dependence of the electron energy on the time when the values of reduced electric field are 1, 10 and 28 Td. In Figure 1a - a regime of "weak" field (E /N = 1 Td), when the electron energy reaches up to the energy of excitation and ionization. In this case the electron makes a chaotic movement along the energy axis only due to elastic collisions with atoms, in which, on average lose energy ~ m / M per collision and acquires energy by Joule heating. The distribution function of electron energy in this case is determined by (1).

Figure 1b represents the mode of "moderately strong" field (E / N = 10 Td), when the field becomes strong enough, so that an electron can reach up the excitation energy, but there is not impact ionization from the ground state yet. In this case, self-discharge can exist due to stepwise ionization.

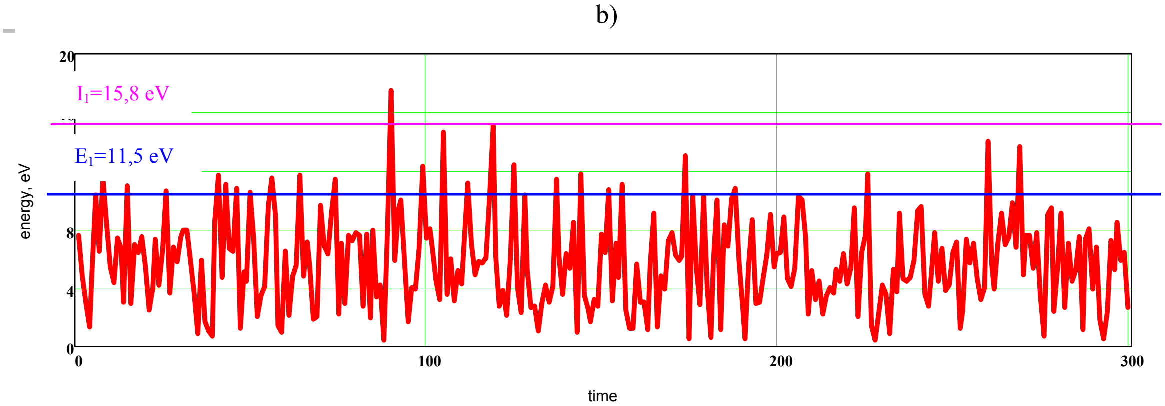
Figure 1c shows the dependence of the electron energy on time for the case of a strong field, the electron can reach up the energy of excitation and ionization. In this case, the discharge will be maintained through the field without additional sources of ionization, i.e. it will be independent.



a)



b)



c)
a) – a case of "weak" field (E / N = 1 Td), there are only elastic collisions;
b) – a case of "moderately strong" field (E / N = 10 Td), excitation energy is high;
c) – a case of "strong" field (E / N = 28 Td) – ionization starts.
Figure 1 – The electron energy as a function of time

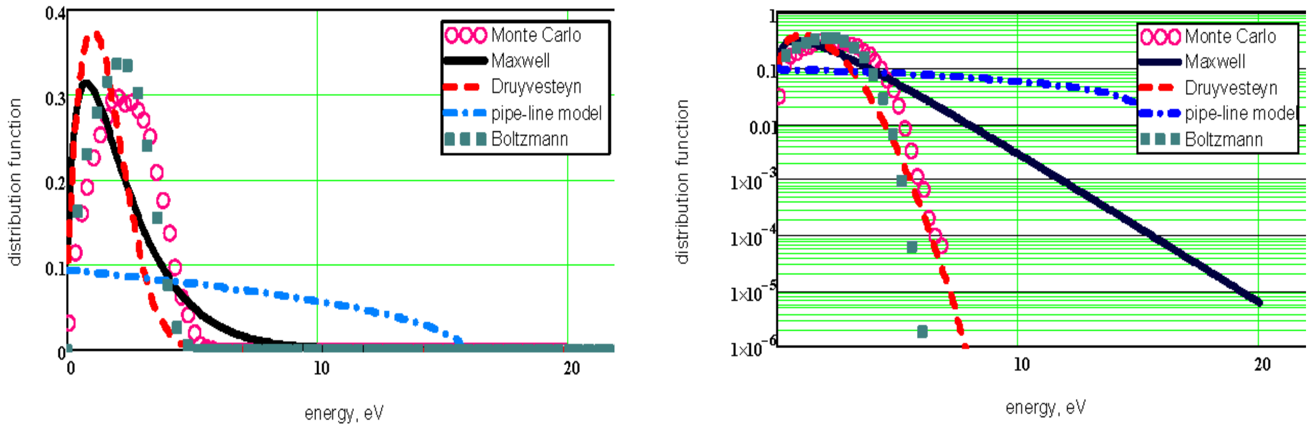
In Table 1 for these three typical cases integral characteristics of the electron drift in a uniform external electric field are shown surface potential of the tube φ_{wall} *(V),*the drift velocity *W(km / s)*, average energy $<\varepsilon>$ *(eV),* the energy factor of Townsend $eD_{\perp}/\mu$ *(eV),* reduced ionization coefficient of Townsend - α / N_a $(10^{-16}$ cm^2*),*the rate of input energy for the elastic losses in the gas $((Q_{ea}/Q_{EW})$ * 100%), ionization $((Q_{ion}/Q_{EW})$ * 100%) and excitation $((Q_{ex}/Q_{EW})$ * 100%) of argon atoms and the average energy after the act of excitation $(<\varepsilon - E_1>)$, ionization $(<\varepsilon - I>)$. Note that in cases of moderately strong and strong-field excitation demands at several times much energy than gas heating and ionization.

Table 1 - Characteristics of the electron drift in argon (E_1 = 11,5 eV, I = 15,8 eV) depending on the reduced field E/N = 1, 10, 28 Td., P = 1 Torr, T = 298 K.

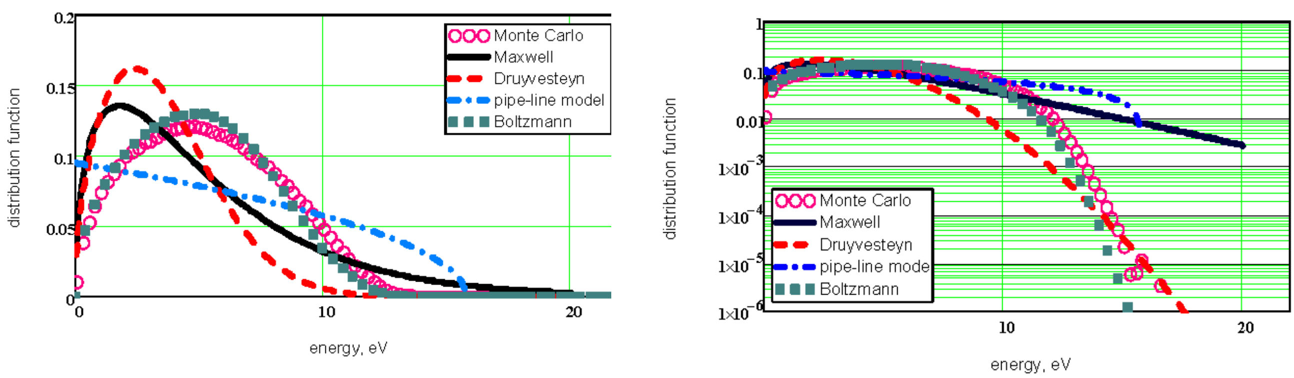
E/N, Td	*1.0*	*10.0*	*28.0*
φ_{wall}	-	*13.0*	*15.0*
W, km/s, MC	*32.4*	*97.1*	*240.0*
W, km/s, Boltzmann	*30.1*	*95.3*	*237.8*
$eD_{\perp}/\mu$ *,eV, MC*	*3.3*	*6.9*	*6.0*
$<\varepsilon>$ *,eV, MC*	*2.4*	*5.4*	*5.3*
$<\varepsilon>$ *,eV, Boltzmann*	*2.2*	*5.1*	*5.6*
α / N_a *, 10^{-16} cm^2, MC*	-	*2.8E-05*	*5.8E-03*

(Q_{ea} / Q_{EW}) *100%, MC	100	26.6	10.3
(Q_{ex} / Q_{EW}) *100%, MC	0	73.3	86.4
(Q_{ion} / Q_{EW}) *100%, MC	0	0.043	3.3
$< \varepsilon - E_1 >$,eV, MC	0	1.1	2.2
$< \varepsilon - I >$,eV, MC	0	0.9	1.3

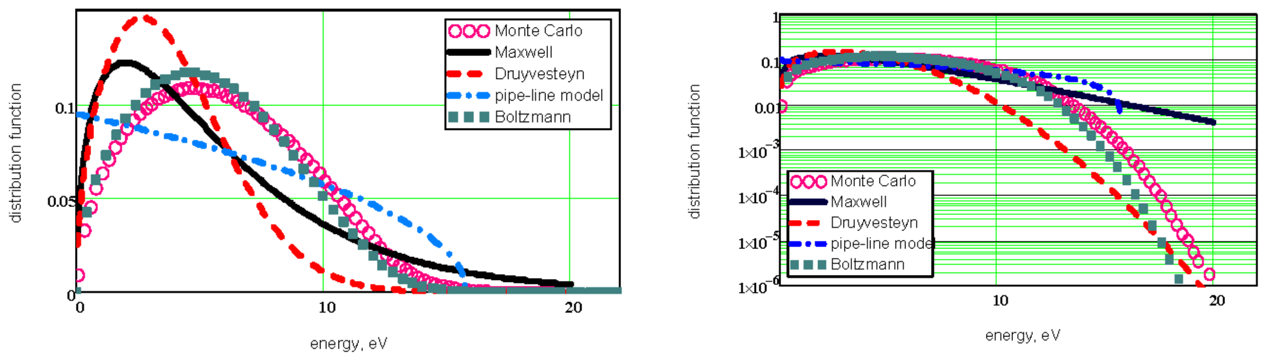
To illustrate the accuracy of various models figure 2 presents the results of calculations of electron energy distribution functions for three variants of reduced field from the Table I. Monte Carlo simulation took into account the finiteness of wall potential and the loss of electrons on it; when solving the two-term approximation of the Boltzmann equation we used the model of ambipolar diffusion of electrons on the wall. For comparison, the distributions of Maxwell and Druyvesteyn are also shown with the same average energy of electrons, as in Monte Carlo calculations. The figures prove that results of EEDF calculations with the Boltzmann equation have a good agreement with calculations by Monte Carlo method.



a) - a case of "weak" field (E / N = 1 Td), there are only elastic collisions.



b) - a case of "moderately strong" field (E / N = 10 Td), excitation energy is high.



c) - a case of "strong" field (E / N = 28 Td) - ionization starts.

Figure 2 - The distribution functions of electron energy for different values of the field

Table 2 shows the characteristics of electrons and experimental results from [11]. The results of calculations by Monte Carlo method gives slightly better agreement with experimental data for the electron temperature, calculations for two-term approximation have also a good agreement with experiments. It should also be borne in mind that experimental methods usually determine not the electrons' temperature and their average energy, but the energetic Townsend coefficient, which for Maxwell distribution coincides with the temperature [1].

Table 2 - Characteristics of the electron drift in argon (E_1 = 11,5 eV, I = 15,8 eV) at different values of gas pressure. The results of calculations and comparison with experiments [11]

Pressure, torr	*0,32*	*0,22*	*0,12*
E/N, Td	*19.0*	*27.0*	*51.0*
φ_{wall} *,eV, MC*	*16.0*	*17.0*	*18.0*
W, km/s, MC	*17.3*	*23.6*	*40.5*
W, km/s, Boltzmann	*22.8*	*32.4*	*58.0*
$eD_{\perp} / \mu$ *,eV, MC*	*6.8*	*6.8*	*7.0*
$eD_{\perp} / \mu$ *,eV, Boltzmann*	*9*	*8.9*	*8.8*
$< \varepsilon >$ *,eV, MC*	*5.7*	*6.0*	*6.5*
$< \varepsilon >$ *,eV, Boltzmann*	*5.4*	*5.6*	*6.0*
α / N_a *, 10^{-16} cm^2, MC*	*0.00084*	*0.0046*	*0.034*
(Q_{ea} / Q_{EW}) **100%, MC*	*11.6*	*10.0*	*16.6*

(Q_{ex} / Q_{EW}) *100%, MC	87.7	87.3	73.0
(Q_{ion} / Q_{EW}) *100%, MC	0.7	2.7	10.4
$<\varepsilon - E_1>$,eV, MC	1.7	2.2	3.0
$<\varepsilon - I>$,eV, MC	0.9	1.2	1.5
T_e ,eV, MC	3.8	4.0	4.3
T_e ,eV, Boltzmann	3.6	3.7	4.0
T_e ,eV, experiment[12]	3.2 ± 1	4.0 ± 1	5.0 ± 1

Conclusions

The model of electron drift in a uniform static electric field was constructed taking into account non-elastic processes and loss of electrons on the walls of the tube. A comparison of results by Monte Carlo simulation with the solutions of the Boltzmann equation in a two-term approximation was made. Calculated data were compared with experimental results of probe measurements.

Acknowledgments

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References

1. Huxley L., Crompton R. Diffusion and drift of electrons in gases – Moscow: Atomizdat. – 1977. – 154 p.
2. Tsendin L.D. Nonlocal electron kinetics in gas discharge plasma // UFN. – 2010. – №180. – 139 p.
3. Fortov V.E., Khrapak A.G., Khrapak S., Molotkov V.I., Petrov O.F. Dusty plasmas // UFN – 2004. – №174. –P. 495.
4. Khrapak S.A. // Floating potential of a small particle in a plasma: Difference between Maxwellian and Druyvesteyn electron velocity distributions // Phys. Plasm. – 2010. – Vol. 17. – P. 104502.
5. Golant V.E., Žilina A.P., Sakharov I.E. Fundamentals of Plasma Physics. – Moscow: Atomizdat. – 1977. – 240 p.
6. Mayorov S.A. Calculation of electron drift in neon at a constant electric field // Brief reports on physics LPI. – 2009. – Vol. 10. – P. 22-27.
7. Antipov S.N., Vasilev M., Mayorov S.A., Petrov O., Forts V.E. Plasma-dust structures in the He-Kr dc glow discharge // JETP. – 2011. – Vol. 139. – P. 554-567.
8. Golyatina R.I., Mayorov S.A. Characteristics of the electron drift in a constant electric field for the inert gases // Applied Physics. – 2011. – Vol. 5. – P. 22-27.
9. Sukhinin G.I., Fedoseev A.V. Influence of dust-particle concentration on gas-discharge plasma //Phys. Rev. E. – 2010. – Vol. 81. – P. 016402.
10. Sukhinin G.I., Fedoseev A.V., Ramazanov T.S., Amangaliyeva R.Zh., Dosbalayev M.K., and Jumabekov A.N. Nonlocal effects in a stratified glow discharge with dust particles // J. Phys. D: Appl. Phys. – 2008. – Vol. 41. – P.245207.
11. Ramazanov T.S., Kodanova S.K., Dzhumagulova K.N., Bastykova N.Kh. The new method for measuring of dust particles charge in glow discharge plasma // EPL. – 2009. – Vol. 96. – P. 45004.