Electron drift characteristics in argon with iron vapor: coefficient of mobility, ionization and runway

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Abstract. The kinetic characteristics of electron drift in argon in the presence of iron fumes at an electric field strength $E/N=1$-$100$ Td with allowance for inelastic collisions are calculated by the Monte Carlo method and the effect of the metal vapor concentration on the drift velocity, average electron energy, diffusion and mobility coefficients are analyzed. In addition, the ionization coefficient of Townsend and electron runaway, the energy distribution functions of electrons are calculated and their comparison with the Maxwell and Druvestein distributions is given. It is shown that even insignificant additions of iron atoms in argon, starting with a fraction of a percent, strongly influence the discharge, in particular, the characteristics of inelastic processes and the charge composition.

1. Introduction

As it is known, the transition from the volumetric form of combustion to the spark channel is preceded by either the explosion of micro-points on the cathode surface or the initiation of the emission center in the breakdown of dielectric inclusions. Therefore, a certain amount of the atoms of the material from which the electrodes are made can enter the source gas [1, 2]. It was shown in [3, 4] that the addition of an even small fraction of an easily ionizable gas to an inert gas with a large ionization potential (for example, with the addition of small fractions of argon to helium [3] or krypton to helium [4]) can radically change the kinetic characteristics of discharge. Two factors play a decisive role: 1) easily ionizable additives lead to a change in the charge composition; 2) impurity ions do not collide with resonant charge exchange when moving in an improper gas, so their distribution function differs radically from the case when ions drift in the parent gas [5].

In this paper we have investigated the effect of low iron vapor concentrations on the kinetic characteristics of a discharge in argon, since the question of the effect of iron vapor additives due to the sputtering of the cathode material during ion bombardment is not given due attention (for example, for small mercury impurities in argon, see [6]).

2. Modeling of electron drift characteristics

Let us consider the drift of electrons in a stationary, spatially homogeneous electric field. In a typical case for a gas discharge, the average electron energy is much higher than the energy of the atoms. So the energy received by the electron from the electric field is lost in elastic collisions with colder atoms,
and it is also expended on excitation of atomic levels and ionization. In addition, electrons lose or acquire energy in collisions with excited atoms and in recombination (see, for example, books and reviews [7-11]).

When drifting in a constant and uniform electric field due to Joule heating per unit time, the electron acquires, on the average, energy

$$Q_{EW} = eEW,$$

where

$$e - \text{electron charge, } E - \text{electric field strength, } W - \text{drift velocity.}$$

The electron energy balance can be written in the following form:

$$Q_{EW} = Q_{\text{excitation}} + Q_{\text{ionization}} + Q_{\text{recombination}},$$

where on the right side the corresponding energy losses of one electron per unit of time are presented as a result of elastic collisions, the costs of excitation, ionization and recombination. The kinetics of electrons can be greatly complicated by such effects as stepwise ionization, the presence of metastable atoms, the transfer of resonant radiation, the superelastic collisions, etc. For example, in recombination, an electron can acquire energy in the energy balance of a supercooled plasma, recombination heating plays a decisive role [12].

Let us consider a swarm of electrons, which in a constant and uniform electric field move uniformly accelerated, experiencing collisions with gas atoms. The collision model is based on the procedure for generating random numbers—a method such as Monte Carlo. The realization of electron-atom collisions by the Monte Carlo method allows one to take into account the energy balance of electrons on the basis of elementary acts, including inelastic collisions. Based on the analysis of the trajectories of various electrons, the values of the drift velocity, mean electron energy, Townsend characteristic energy, Townsend ionization coefficient, and electron runaway are calculated. The electron runaway coefficient is defined similarly to the Townsend ionization coefficient, which is the number of acts of electron runaway when it passes 1 cm of path in the direction of the field.

In the realization of electron-atom collisions, we will assume that:

- the gas atoms have a Maxwellian velocity distribution and do not change their temperature due to collisions with electrons;
- elastic electron—atomic collisions occur as collisions of hard spheres, i.e. in the collision, isotropic scattering occurs in the center of mass system, but the collision cross section is assumed to depend on the energy of their relative motion;
- the loss of electrons to the excitation of atomic levels is irreplaceable, i.e. it is assumed that the excited atoms lose their excitation energy in the volume de-excitation regime, and the metastable atoms diffuse rapidly beyond the limits of the volume under consideration and do not affect the energy distribution of the electrons;
- in the case of ionization by electron impact, an electron incident on an atom loses energy equal to the sum of the ionization energy and the kinetic energy of the knocked out electron;
- Recombination processes of electrons and atoms, quenching of excited levels and transfer of resonant radiation do not change the energy of electrons: $Q_{\text{recombination}} = 0$.

The probability of ionization and excitation is determined by the corresponding cross sections for which the Thomson approximation, characterized by linear growth, beginning with the threshold of the reaction, is used and fallen at large energies [8-11], compared with the ionization potential.

The electron energy distribution function determines many properties of electron drift and is the most important characteristic of a gas discharge. To determine it, various theoretical models are developed, but most often a two-term approximation of the kinetic Boltzmann equation (two term approximation – TTA) is used for numerical solution.

If the electron drift in a constant and homogeneous field is determined only by elastic collisions with atoms, and the field strength is such that the average kinetic energy of an electron is much higher
than the temperature of the atoms, then the solution of the two-term approximation of the Boltzmann equation is the electron velocity distribution function looks as follows:

\[ f_0(v) = A \exp \left( -\frac{3m}{M} \left( \frac{mN}{eE} \right)^2 \int_0^v c^2 \sigma_{el}(c) dc \right), \tag{3} \]

here \( m, M \) – mass of an electron and an atom, \( \sigma_{el} \) cross section for elastic collisions, constant \( A \) – is determined from the normalization condition:

\[ 1 = 4\pi \int_0^\infty c^2 f(c) dc. \tag{4} \]

With a power-law dependence of the cross section on the velocity:

\[ \sigma_{el}(c) = \sigma_0 (c / c_0)^\nu \tag{5} \]

the integral in (3) is calculated in explicit form \([9, 10]\). At a constant collision frequency, the dependence of the cross section on the velocity has the form

\[ \sigma_{el}(c) = \sigma_0 (c / c_0)^{-\nu/2}, \tag{6} \]

then (3) goes over into the Maxwell distribution:

\[ f_{Maxwell}(\varepsilon) = \varepsilon^{\nu/2} \exp\left(-\varepsilon / T\right). \tag{7} \]

At a constant cross section \( \sigma_{el}(c) = \sigma_0 \) the free path length does not depend on the velocity and the distribution (3) goes over into the distribution of the Druvestain:

\[ f_{Druvestain}(\varepsilon) = \varepsilon^{\nu/2} \exp\left[-(\varepsilon / \varepsilon_0)^2\right], \tag{8} \]

The dependence of the collision cross section on velocity has a complicated character, and for it in the energy range \( 0<\varepsilon \leq E_1 \), \( I \) the approximation of a constant mean free path is more likely. Therefore, experimental data on the energy distribution of electrons in a gas discharge are usually better described by the Druvestain distribution, rather than by Maxwell.

The distributions of Druvestain and Maxwell are often used in the analysis of various problems of gas-discharge physics. But all these models do not take into account the death and production of electrons, so in principle they cannot be applied, for example, to the case of a stratified discharge in a tube under a reduced gas pressure. Nevertheless, as shown in \([13]\), the periodic field of the stratum can lead to a maxwellization of the electron distribution (see also \([14-16]\)).

The unlimited flow model (pipe-line model) \([8, 11]\) takes into account the creation of an electron with zero energy, the drift along the kinetic energy axis with a constant diffusion coefficient and instantaneous death upon reaching the ionization or excitation energy. The corresponding distribution function has the form:

\[ f_{pipe-line}(\varepsilon) = 1.5(1 - \varepsilon / I)^{\nu/2} I. \tag{9} \]

As a result of using these approximations, only the drift velocity is often determined for the distribution functions, and other factors important for modeling the gas discharge kinetics, such as the diffusion coefficients along and across the field, the energy and the first Townsend ionization coefficients, are not determined by the complexity of the problem. Therefore, the numerical experiment is practically the only reliable tool for studying the characteristics of electron drift, especially when discharged in a gas mixture, when small additives can significantly affect the discharge.
3. Results of calculations and their discussion.
A Monte Carlo-based algorithm was used to simulate collisions. It was developed to simulate the drift of ions and electrons in a gas [5, 17]. In the course of the collision, the known dependences of the collision cross-sections on energy were taken into account [9-11, 18]. A detailed description of the procedure for modeling electron drift in a gas and the results for drift in neon are presented in [17], the results of calculations of the integral characteristics of a discharge in neon are given in [19].

In figures 1-4 are graphs of the dependence of the electron drift characteristics on the reduced electric field strength $E/N$.

Figure 1 is the dependence of the drift velocity of electrons in argon, in argon with 0.1%, 1%, 10% and 50% content of iron atoms, as well as in pure iron. The graphs of the drift velocity dependences show that the addition of iron fumes to argon up to 0.1% of the concentration of their atoms does not lead to a noticeable change in the drift velocity, but with the addition of even 1% percent of iron, the drift velocity of the electrons varies noticeably.

It should be noted that the electron drift velocity at low iron concentrations is determined mainly by elastic collisions of electrons with argon atoms. However, we should note an interesting fact that Blank's law for this mixture is not held. Addition of 1% of iron atoms to argon at field strength $3\text{Td}<E/N<20\text{Td}$ leads to approximately a twofold increase in the drift velocity. This effect of a significant increase in the mobility of electrons is due to a decrease in their average energy due to high energy costs for ionization and excitation of iron atoms and a dip in the cross section for elastic collisions of electrons in argon in the low-energy region (Ramsauer effect).

Figure 2 shows the dependence of the reduced Townsend ionization coefficient, which is determined by the ratio of the number of pairs generated per 1 cm to the numerical density of atoms. The calculations were performed in pure argon, in iron vapors, as well as with 0.1%, 1%, 5% and 10% iron impurity atoms in argon.

These graphs show that even 0.1% of the concentration of iron atoms at $10\text{Td}<E/N<20\text{Td}$ completely changes the charge composition and significantly reduces the value of the field at which ionization of the gas begins.

In figures 3 and 4 are graphs of the energy characteristics of electron drift as a function of the reduced electric field strength $E/N$. Figure 3 shows the characteristic energy of Townsend, which is determined by the ratio of the coefficients of transverse diffusion and mobility $eD_{\perp}/\mu$. The calculations were performed in pure argon, in iron vapors and with 0.1%, 1%, 2%, 5%, 10% and 50% iron impurity atoms in argon. There are graphs of the dependence of the average electron energy in figure 4. The designations are similar to the previous figure.
The energy characteristics of electron drift, given in these two figures, allow us to draw two important conclusions:

- small additions of iron atoms to argon exert a strong influence not only on the charge composition of the plasma, but also on the electron energy distribution function, while changing in an essential way its average characteristics;

- there is a significant deviation from the widely used Nernst-Townsend-Einstein ratio, so there can be a large difference between the temperature and the characteristic Townsend energy, $eD_\perp/\mu$ which is usually the experimentally determined value.

The results of the calculations give a fairly complete picture of the mechanism of the effect of small additions of iron vapors on the characteristics of a gas discharge.

**Figure 3.** The graphs of characteristic energy dependency Townsend, $eD_\perp/\mu$ from $E/N$.

**Figure 4.** Graphs of the dependences of the average electron energy from $E/N$.

**Figure 5.** Electron energy distribution functions in a mixture with 1% Fe content at $E/N=15$ Td, as well as the Maxwell EECDE, Druyvestein and the distribution corresponding to the instantaneous flow approximation.

**Figure 6.** The coefficient of electrons runaway as a function of $E/N$.

The most interesting and important fact, from a practical point of view, is a strong increase in the ionization frequency with an insignificant (on the order of fractions of a percent) addition of iron fumes. In addition, it should be noted that in this case, iron atoms will predominantly be ionized, respectively, iron ions will be mainly represented in the discharge.
Figure 5 shows the distribution of electrons in energy at 1% iron fraction in a mixture of argon and iron vapor at $E/N=15$ Td, for comparison, the distributions of Maxwell (7) and Druvestain (8) with an average energy equal to the Monte Carlo, as well as pipeline distribution (9) (unlimited flow model). This figure clearly demonstrates the great difference between the real energy distribution of electrons and the commonly used Maxwell and Druvestain distributions.

A detailed analysis of the energy distribution functions of electrons shows that they cannot be described in any way by any single-parameter function with an effective temperature determined by $K_{\text{eff}}=1.5T_{\text{eff}}$.

The question of the maximum energy efficiency of maintaining the discharge is of interest. As an example, we point out that, at $E/N=10$ Td, the largest fraction of the ionization energy is consumed by an electron at 1% iron atom concentration, and at $E/N=20$ Td the maximum fraction of the ionization cost is reached at 2% iron concentration.

In figure 6 shows the dependence of the runaway coefficient of electrons in pure argon, in iron vapors and with 0.1%, 5%, 10% and 50% iron impurity content in argon. Here, too, we see the effect of metal impurities on the electron drift characteristics.

The main purpose of this paper is to present new data on the characteristics of the drift of electrons in argon in the presence of iron vapors, which can be useful in various applications of gas-discharge plasma. The presented calculation results allow one to follow the influence of the percentage composition of iron atoms in argon on the characteristics of electron drift in a constant, uniform electric field with the intensities in the range from 1 to 100 Td, characteristic for discharges under reduced gas pressure.

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