ISSN 1068-3356, Bulletin of the Lebedev Physics Institute, 2015, Vol. 42, No. 10, pp. 294–298. © Allerton Press, Inc., 2015.
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Approximation of Ion Drift Velocity in Own Gas

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Received July 13, 2015

Abstract—The results of Monte Carlo calculations of the drift velocity of noble gas and mercury ions in a constant uniform electric field are presented. The dependences of the ion mobility on the field strength and gas temperature are analyzed. The parameters of the drift velocity approximation by the Frost formula for gas temperatures of 4.2, 77, 300, 1000, and 2000 K are presented. A universal drift velocity approximation depending on the reduced electric field strength and gas temperature is obtained.

DOI: 10.3103/S1068335615100048

Keywords: ion drift, electric field, own gas, noble gases, mercury vapor, Frost formula, approximation, drift velocity.

Ion drift and diffusion in an electric field (e.g., ambipolar ion diffusion from a positive column of a glow discharge) control to a large extent the gas discharge properties. The literature contains many experimental and calculated data on ion drift in gases; however, there are almost no data on the dependence of ion drift characteristics on the gas temperature [1–5].

It is clear that the effect of the atom temperature on ion drift characteristics is very strong, and the gas temperature can differ from room temperature even in laboratory plasma. Modern plasma technologies often use discharge modes in which gas temperatures significantly exceed room temperature.

The use of lower gas temperatures in the cryogenic discharge also leads to a significant change of its characteristics [6]. An addition of minor impurities of argon, krypton, and xenon to helium has the same effect on the discharge, as a gas temperature decrease [7]. Low gas temperatures are characteristic of ionosphere, interplanetary and interstellar space. In experimental studies of properties of ultracold plasma in Pauli traps, ion drift also occurs in a very cold (much lower than 1 K) gas [8].

In the present study, ion drift characteristics in own gas were calculated for helium, neon, argon, krypton, xenon, and mercury at gas temperatures of 4.2, 77, 300, 1000, 2000 K and in a wide range of the reduced electric field strength, from 1 to 10000 Td. The model of ion–atom collisions implemented by the Monte Carlo method [9–12] was used in the calculations. It considered the polarization interaction of ions with atoms, resonant charge transfer, and short-range repulsion of electron shells (see a more detailed description in [9, 10, 12]).

Almost all integral characteristics of ion drift, i.e., the drift velocity and mobility, average ion energy, longitudinal and transverse diffusion coefficients, mean free path, collision frequency, velocity and energy distribution functions, were calculated. Furthermore, the frequency of different collision types, i.e., isotropic scattering in the center-of-mass system, backscattering, deflection to small angles at long transits, was analyzed.

The data obtained make it possible to analyze, refine, and determine ranges of application of various approaches and approximations. Among all kinetic characteristics, only the drift velocity is a directly measured value. The others are obtained by using various relations and models. For example, to determine the longitudinal and transverse diffusion coefficients, the Nernst–Townsend–Einstein relation, modified Einstein relation, or Schottky theory describing ambipolar diffusion in a tube are used. From the Wannier theory, energy characteristics of ion flux are usually obtained [4, 5, 13]; from the first Chapman–Enskog approximation, the effective collision frequency and transport cross sections are calculated [4, 13, 14].

Numerous experimental data show that the ion drift velocity in own gas is very well described by the semi-empirical Frost formula [13, 14]

$$u = a\left(1 + b\frac{E}{N}\right)^{-1/2}\frac{E}{N}. \tag{1}$$

This dependence of the drift velocity on the reduced electric field strength has two parameters: a is the mobility in the weak field limit and $b = 1/(E/N)_{\mathrm{heating}}$. The quantity $(E/N)_{\mathrm{heating}}$ is the reduced strength of the electric field in which the mobility according to the Frost formula decreases by a factor of $\sqrt{2}$ due to ion heating.

Based on an analysis of the calculations of all kinetic characteristics, the approximation parameters in the Frost formula (1) were determined for various gas temperatures. We note that the values of these parameters are published only for room temperature (300 K). There are also little experimental data about drift characteristics at cryogenic temperatures near 77 K and 4.2 K [3–5].

Table 1 lists the parameters a in the units of cm/(s·Td), which corresponds to the drift velocities at 1 Td; these data can be recalculated to the mobility at the normal density often used in reference books using the formula $K_0[\mathrm{cm}^2 V^{-1} s^{-1}] = 268.6763 \times a[\mathrm{cm} Td^{-1} s^{-1}]$.

Table 1. Parameter a in the units of cm/(s·Td) at various gas temperatures

System	$T = 4.2$	$T = 77$	$T = 300$	$T = 1000$	$T = 2000$
He^+ in He	5632	4162	2774	1787	1374
Ne^+ in Ne	1888	1605	1117	771	591
Ar^+ in Ar	668	588	409	280	207
Kr^+ in Kr	377	346	258	176	130
Xe^+ in Xe	236	213	159	101	75
Hg^+ in Hg	165	108	68	44	34

Table 2 lists the parameters $1/b = (E/N)_{\mathrm{heating}}$ in the units of Td. For each gas temperature, the dependence of the mobility on the reduced electric field strength was analyzed. The value of $(E/N)_{\mathrm{heating}}$ at which the ion mobility decreases by a factor of 1.414 in comparison with the mobility in a very weak field was determined by fitting.

Table 2. Parameter $1/b$ (Td) at various gas temperatures

System	$T = 4.2$	$T = 77$	$T = 300$	$T = 1000$	$T = 2000$
He^+ in He	17	33	85	210	410
Ne^+ in Ne	35	45	103	240	450
Ar^+ in Ar	75	95	200	480	1030
Kr^+ in Kr	108	120	225	520	1080
Xe^+ in Xe	125	145	260	730	1450
Hg^+ in Hg	70	170	470	1200	2200

Figure 1 shows the dependences of the parameter a, i.e., the mobility in the weak field limit, on the gas temperature for all noble gases (without mercury). Symbols indicate the mobilities obtained by the

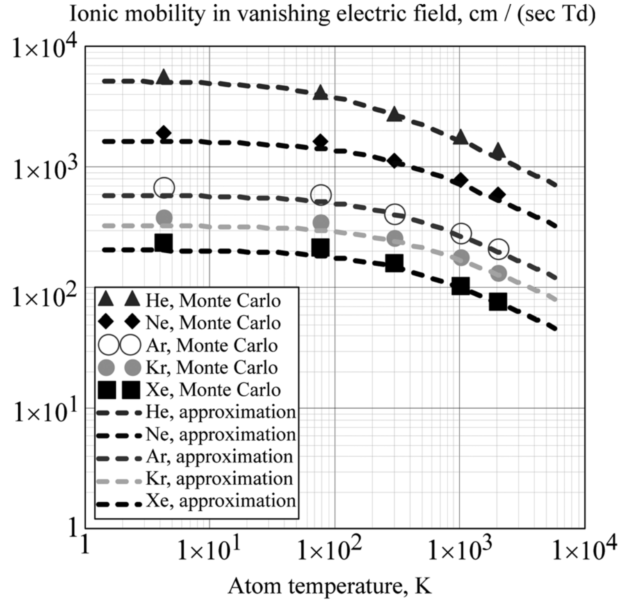

Fig. 1. Dependences of the parameter a, i.e., the mobility in the weak field limit, on the gas temperature for all noble gases. Curves correspond to various gases.

Monte Carlo method; dashed curves are the approximations of the dependence of the mobility on the gas temperature in weak field,

$$a = K_{\rm pol}(N_0/N)(1 + T_{\rm atom}/\varepsilon_0)^{-1/2}, \tag{2}$$

where $K_{\rm pol} = 13.853(\alpha_d \mu)^{-1/2}$ is the polarization mobility in the units of cm^2/(V s) at the standard gas density $N_0 = 2.686763 \times 10^{19}$ in cm^3 (Loschmidt number), α_d is the polarizability in cubic Angströms, and μ is the reduced mass in g per mol [5]. The functional dependence (2) was derived by analogy with the Frost formula (1) under the assumption of identical character of influence of the field strength and gas temperature on the mobility. It is natural that the ion mobility should be equal to the polarization mobility $K_{\rm pol}$ at a zero gas temperature.

The physical meaning of the parameter ε_0 in Eq. (2) consists in that it defines the upper limit of the applicability of constant collision frequency approximation. In the case of $T_{\rm atom} \ll \varepsilon_0$, the polarization interaction of the ion with atoms is determining.

Let us introduce the new parameter

$$\langle \varepsilon \rangle_{\rm pol} = \frac{1}{2} m [K_{\rm pol}(E/N)_{\rm heating}(N_0/N)]^2 \tag{3}$$

equal to the average energy of directional motion of the ion with mass m in the field with the reduced strength $(E/N)_{\rm heating}$. The approximation of the ion mobility in a weak field by formula (2) was found by fitting to the calculated data; good agreement is observed at the choice

$$\varepsilon_0 = 0.6 \langle \varepsilon \rangle_{\rm pol}, \tag{4}$$

where the value of $\langle \varepsilon_0 \rangle_{\rm pol}$ was chosen from a calculation version at an atom temperature of 4.2 K. Table 3 lists the values of $K_{\rm pol}$ and parameter ε_0.

Figure 2 shows the similar dependences of the parameter $b^{-1} = (E/N)_{\rm heating}$ on the gas temperature. Symbols are the values of the heating field $(E/N)_{\rm heating}$ obtained by analyzing Monte Carlo calculations; dashed curves are constructed by the approximation formula

$$1/b = (E/N)_0(1 + 1.5 T_{\rm atom}/\varepsilon_0). \tag{5}$$

Table 3. Approximation parameters for various gases

System	K_{pol} cm^2/s V	ε_0, K	$(E/N)_0$, Td
He^+ in He	21.6	111	16.1
Ne^+ in Ne	6.8	237	34.1
Ar^+ in Ar	2.42	271	73.3
Kr^+ in Kr	1.36	371	106.2
Xe^+ in Xe	0.85	307	122.5
Hg^+ in Hg	0.61	76	64.6

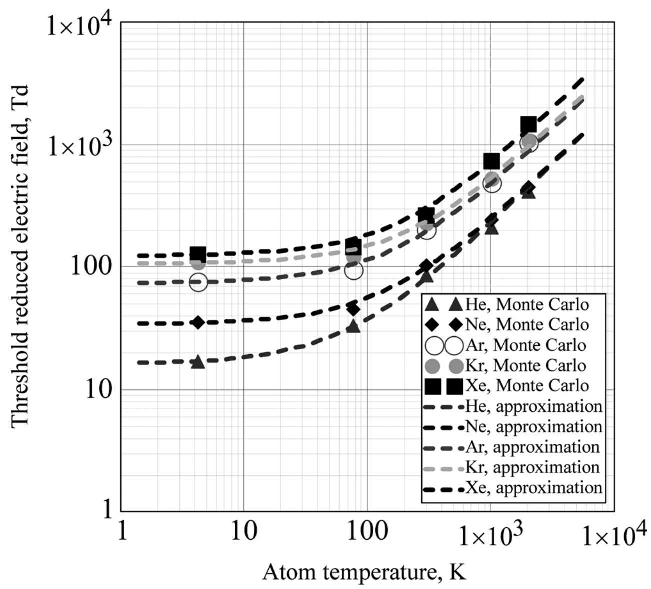

Fig. 2. Dependences of the threshold reduced electric field strength, i.e., the parameter $b^{-1} = (E/N)_{\rm heating}$ on the gas temperature for all noble gases. Curves correspond to various gases.

Here $(E/N)_0$ is the heating field at a zero gas temperature. The parameter $(E/N)_0$ for this approximation was determined from the relation

$$(E/N)_{4.2} = (E/N)_0(1 + 1.5 \times 4.2/\varepsilon_0), \tag{6}$$

i.e., by extrapolating the dependence (5) from the point of 4.2 K to zero. Here the notation $(E/N)_{4.2}$ is introduced for the heating field at an atom temperature of 4.2 K. Table 3 also lists the values of the parameter $(E/N)_0$.

The obtained parameters of the approximation of the ion drift velocity can be used to estimate other gas-discharge plasma characteristics, to analyze and design experiments with dusty plasma under conditions of the cryogenic discharge, to consider the discharge in the mixture of heavy and light gases [6, 7], and to analyze experiments with ultracold ion bundle expansion to an ambient gas [8].

ACKNOWLEDGMENTS

This study was supported by the Russian Science Foundation, project no. 14-50-00124.

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