Monte Carlo simulation of mercury ion drift characteristics in an inert gas

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Abstract. The Monte Carlo method calculated and tabulated the diffusion-drift characteristics of mercury ions in three inert gases (He, Ar, Xe) depending on the reduced electric field strength - the average energy of the ions, their longitudinal and transverse temperatures, diffusion coefficients along and across the direction of the field. The velocity distribution function of the ions and the angular dependence of the ions bombarding the surface are investigated.

1. Introduction

The ion drift as applied to gas-discharge plasma problems has already been studied in a number of works [1-12]. Plasma-chemical reactions involving ions in various types of gas discharge; the processes taking place in the ionosphere under the influence of the solar wind, the processes of interaction of ion flows with the surfaces of solid and liquid substances are largely determined by the ion velocity distribution function.

On the other hand, it is well known that the transition from the volumetric form of combustion to the spark channel is preceded either by the explosion of the micropoints of the cathode surface or the initiation of the emission center during breakdown of dielectric inclusions [13-14]. Consequently, a certain number of atoms of the electrode material can enter the working gas [15–16]. It is well known [17-18] that the addition of even a small amount of easily ionizable gas (for example, argon to helium [17] or krypton to helium [19]) in an inert gas with a large ionization potential can radically change the kinetic characteristics of the discharge. Therefore, the study of the effect of metal vapor on the ionization-drift characteristics of electrons and ions is of independent interest.

2. Research methods and analysis of the results

2.1. Inert gas numerical simulation algorithm for mercury ion drift

To simulate ion-atom collisions during ion motion in a uniform electric field, the equations of ion motion were integrated according to the second-order Runge-Kutta scheme. At each time step, a collision of an ion with an atom was played out. An algorithm for simulating ion-atom collisions is described in [1].

We list the main stages of the developed algorithm for modeling the ion-atom collision:
for the center of mass of the colliding particles in the system in accordance with the probability of collision, randomly select speeds and impact parameter of the collision;

- when moving in the system of the center of mass of particles with a polarizing interaction potential, the following are determined: distance of closest approach \( r_{\text{min}} \), relative velocity of particles at the point of closest approach \( V_{12}(r_{\text{min}}) \), scattering angle \( \chi \);

- if closest distances \( r_{\text{min}} > d_{\text{gas}} \) (atom diameter), then the velocities of the ion and atom deviate by an angle \( \chi \); otherwise, i.e. if \( r_{\text{min}} < d_{\text{gas}} \), then the velocities of the ion and atom are recalculated in accordance with the law of collision of elastic spheres, the distance of minimal approach is assumed \( r_{\text{min}} = d_{\text{gas}} \), the relative particle velocity at the closest point is determined \( V_{12}(r_{\text{min}}) \);

- recalculated speeds in the laboratory system, statistics are accumulated on various characteristics of collisions.

2.2. The results of calculating the characteristics of the drift of mercury ions in an inert gas. Tables 1-3 show the results of calculation of the drift velocity \( V_{\text{dr}} \), effective temperature \( T_{\text{eff}} \), longitudinal \( T_\parallel \) and transverse temperatures \( T_\perp \), coefficients of longitudinal \( D_\parallel \) and transverse diffusion \( D_\perp \), as well as the drift velocity \( V_{\text{dr}} \) of mercury ions in xenon, argon and helium, respectively.

As can be seen from tables 1-3, the drift characteristics of mercury ions increase with increasing reduced value of the field \( E/N \), depend on the ratio of the mass of the mercury ion to the mass of the inert gas \( M_+/M_\text{g} \) and has the smallest value in xenon.

To demonstrate the effect of atomic temperature on the dependence of the longitudinal and transverse diffusion coefficients on the electric field strength, we calculated the ratio of the longitudinal and transverse diffusion coefficients \( D_\parallel/D_\perp \) of the reduced field \( E/N \) (Figure 1a) and gas temperature (Figure 2b). As can be seen, the anisotropy effect is more pronounced in xenon, and the degree of anisotropy decreases with increasing gas temperature.

**Table 1.** Characteristics of mercury ion drift in xenon at gas temperature \( T_g=300 \) K.

| E/N, Td | \( T_{\text{eff}}, \) kK | \( T_\parallel, \) kK | \( T_\perp, \) kK | \( D_\parallel, \) cm\(^2\)/s | \( D_\perp, \) cm\(^2\)/s | \( V_{\text{dr}}, \) km/s |
|--------|----------------|----------------|----------------|----------------|----------------|----------------|
| 1      | 0.30           | 0.30           | 0.30           | 0.02           | 0.02           | 0.02           |
| 10     | 0.31           | 0.32           | 0.30           | 0.02           | 0.02           | 0.02           |
| 50     | 0.46           | 0.68           | 0.34           | 0.03           | 0.02           | 0.11           |
| 100    | 0.90           | 1.79           | 0.46           | 0.04           | 0.03           | 0.21           |
| 300    | 4.22           | 9.97           | 1.35           | 0.10           | 0.08           | 0.56           |
| 500    | 8.21           | 19.78          | 2.43           | 0.13           | 0.12           | 0.80           |
| 1000   | 18.52          | 45.12          | 5.22           | 0.18           | 0.19           | 1.23           |
| 2000   | 39.31          | 96.18          | 10.87          | 0.24           | 0.30           | 1.80           |

**Table 2.** Characteristics of mercury ion drift in argon at gas temperature \( T_g=300 \) K.

| E/N, Td | \( T_{\text{eff}}, \) kK | \( T_\parallel, \) kK | \( T_\perp, \) kK | \( D_\parallel, \) cm\(^2\)/s | \( D_\perp, \) cm\(^2\)/s | \( V_{\text{dr}}, \) km/s |
|--------|----------------|----------------|----------------|----------------|----------------|----------------|
| 1      | 0.30           | 0.30           | 0.30           | 0.02           | 0.02           | 0.00           |
| 10     | 0.31           | 0.32           | 0.30           | 0.02           | 0.02           | 0.02           |
| 50     | 0.46           | 0.68           | 0.34           | 0.03           | 0.02           | 0.11           |
| 100    | 0.90           | 1.79           | 0.46           | 0.04           | 0.03           | 0.21           |
| 300    | 4.22           | 9.97           | 1.35           | 0.10           | 0.08           | 0.56           |
| 500    | 8.21           | 19.78          | 2.43           | 0.13           | 0.12           | 0.80           |
| 1000   | 18.52          | 45.12          | 5.22           | 0.18           | 0.19           | 1.23           |
| 2000   | 39.31          | 96.18          | 10.87          | 0.24           | 0.30           | 1.80           |
Table 3. Characteristics of the drift of mercury ions in helium at gas temperature $T_\text{g}=300$ K.

| $E/N$, Td | $T_{\text{eff}}$, kK | $T_{\perp}$, kK | $T_\parallel$, kK | $D_{\parallel}$ cm$^2$/s | $D_{\perp}$ cm$^2$/s | $V_{\text{dr}}$, km/s |
|-----------|---------------------|-----------------|-----------------|---------------------|---------------------|------------------|
| 1         | 0.31                | 0.34            | 0.30            | 0.37                | 0.37                | 0.04             |
| 10        | 1.59                | 4.14            | 0.32            | 0.41                | 0.41                | 0.40             |
| 50        | 24.81               | 73.29           | 0.57            | 0.61                | 0.61                | 1.73             |
| 100       | 66.29               | 196.90          | 0.99            | 0.87                | 0.87                | 2.84             |
| 300       | 239.67              | 713.57          | 2.72            | 1.54                | 1.54                | 5.42             |
| 500       | 413.37              | 1231.21         | 4.46            | 1.99                | 1.99                | 7.12             |
| 1000      | 847.29              | 2524.36         | 8.76            | 2.82                | 2.82                | 10.20            |
| 2000      | 1715.35             | 5111.27         | 17.35           | 4.02                | 4.02                | 14.51            |

Figure 1. The ratio of the longitudinal and transverse diffusion coefficients $D_{\parallel}/D_{\perp}$ of the reduced field $E/N$ (a) and gas temperature (b).

2.3. Calculation results distribution function of mercury ions in an inert gas.

Figure 2 shows the distributions of the longitudinal and transverse components of the distribution function of mercury ions in an inert gas over velocity projections for a reduced electric field strength $E/N = 100$ Td and gas temperature $T_\text{g} = 300$ K.

For comparison, the Maxwell distribution for atoms at $T_a = 300$ K is also plotted:

$$ f(u) = \left( \frac{m}{4\pi kT_a} \right)^{1/2} \exp\left( -\frac{mu^2}{2kT_a} \right) $$

And for the longitudinal distribution function, the Maxwell distribution shifted by the value of the drift velocity is plotted. The ion velocity (abscissa axis) is normalized to the characteristic thermal velocity of iron atoms:

$$ V_T = (T_a / m)^{1/2} $$

We note the following features of the drift of mercury ions in an inert gas with increasing field strength:

1) the drift velocity increases and anisotropy of the distribution of ions in directions appears, the dispersion of the distribution function (temperature) increases;

2) in the velocity distribution of ions in the direction along the field and across the field, the deviation is insignificant and is more pronounced in helium.
Figure 2. Distribution functions of mercury ions during drift in helium over velocity projections along (a) and across (b) field directions at $E/N = 100$ Td, $T_a = 300$ K and the corresponding Maxwell distribution functions.

Figure 3. Results of calculation of the angle distribution function $\phi$ between the direction of ion flight and the direction of the electric field for $E/N = 10$ Td (a) and the gas temperature of 300K (b).

To clarify the applicability limits of the two-term approximation, it is of interest to calculate the ion distribution functions over the cosines of the angles between the direction of the ion velocity and the direction of the electric field. In the spherically symmetric case, i.e., with an isotropic distribution of ion velocity, the ion distribution function is constant. In the two-term approximation, the distribution function is expanded in Sonin polynomials, and only the linear term of the expansion is retained, i.e., it is assumed that the dependence of the distribution function on the angle is linear in the cosine of this angle. In figure 3 presents the results of calculating the ion distribution function over the cosine of the angle $\phi$ between the direction of flight of the ion and the direction of the electric field. As the results for mercury ions in all inert gases show at $T_a = 300$ K, starting from reduced electric fields of $\sim 10$ Td and above, the assumption of linearity in the cosine expansion is violated.
The results of calculations of the angular characteristics of the ion flux during drift in a gas can be used to estimate the characteristics of a gas discharge plasma when considering magnetron and barrier discharges, probe characteristics, etc.

3. Conclusions

Thus, the drift of mercury ions in an inert gas has a number of important features that lead to a significant change in the discharge characteristics. All this indicates the complexity of the processes in the discharge and stimulates further studies of the properties of the discharge.

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