*34th EPS Conference on Plasma Phys. Warsaw, 2 - 6 July 2007 ECA Vol.**31F**, P-2.115 (2007)*

Calculation of resonant charge exchange cross-sections of ions Rubidium, Cesium, Mercury and noble gases

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1. Introduction. The present study was stimulated by the oppressive variety (of 10 to 50 %) of the available literature data on the cross sections of ion charge exchange on proper-gas atoms for low collision energy. The aim of the study was the approximation of charge exchange cross sections to an accuracy corresponding to precision of measurement of coefficients of ion diffusion and mobility in weak fields, i.e., ~1 %. We shall restrict our consideration to the data for noble gases, and *Cs, Rb* and *Hg* because our general task here is to create an effective algorithm of simulation of ion-atom collisions that determine the characteristics of dust formations in gas-discharge plasma [1].

A homogeneous external electric field *E* induces ion drift in a gas at a velocity proportional to the field strength:

$$\mathrm{v}_d = \mu E \,, \qquad (1)$$

where the ion mobility coefficient $\mu(E,N,T)$ depends on both the field strength and the gas parameters (temperature *T*, pressure *p* = *NT*, and composition). A large number of experimental and theoretical works (reviews [2 - 5]) are devoted to determination of coefficients of ion diffusion and mobility in a gas, and one can believe that at least in the region of weak and moderately strong fields (*E/N < 1000 Td*) the ion mobility is known with rather high accuracy of < 1 %.

In the weak field approximation, the coefficient of ion mobility does not depend on the field strength because the velocity distribution of ions is close to equilibrium and the ion collision frequency does not depend on the field strength. In this case the drift velocity is proportional to the field strength $\mathrm{v}_d \sim E$ and is determined by the scale of the ion-atom collision cross sections at energies of the order of the thermal energy: 0.01 - 0.1 eV. The ion drift velocity in a strong field is $\mathrm{v}_d \sim E^{1/2}$; it exceeds the thermal velocity of atoms and is determined by the scale of cross sections at collision energies much higher than the thermal energy.

The experimental measurements of the coefficients of mobility and diffusion allow the determination of the collision cross section and the interaction potential. For example, independence of the coefficient of mobility in weak fields of the field strength and gas temperature is possible if the collision frequency is independent of the collision energy and, accordingly, the cross section depends on the relative velocity v_{12} of colliding particles by the law $\sigma_{st} \propto 1/v_{12}$ and the particle interaction force is inversely proportional to the fifth power of spacing between them. Such a case was first considered by Maxwell irrelative of the ion-atom interaction because the Boltzmann collision integral is greatly simplified for only such cross sections (the case of Maxwellian molecules).

2. Ion-atom collisions. We shall determine the collision energy $\varepsilon_r = m v_{12}^2/4 = \varepsilon_{12}/2$, equal to the total kinetic energy of colliding particles in the center-of-mass system, and the effective diameter d of collision related to the diffusion cross section by the relation $\sigma_d = \pi d^2$.

The ion polarizes atoms by its electric field and interacts with induced dipoles. The potential energy of this polarization interaction for distances larger than the atomic diameter and smaller than the mean interatomic distance $N^{-1/3}$ is

$$U(r_{12}) = -\frac{\alpha Ry a_0^4}{r_{12}^4}, \qquad (2)$$

where r_{12} is the distance between the atom and ion, $\alpha = \alpha_0 / a_0^3$, α_0 - is atomic polarizability, $a_0 = 0.529 \cdot 10^{-8}$ cm is the Bohr radius, Ry = 13.6 eV is the Rydberg constant, and N is the atom number density. The polarization collision cross section is $\sigma_{pol} \propto 1/v_{12}$, and the model of a constant ion collision frequency (independent of velocity) is applicable for the determination of ion mobility in the case of prevalence of polarization collisions.

The problem of collision of two rigid spheres with different diameters d_1 and d_2 and masses m_1 and m_2 can be reduced to the problem of one-particle scattering by an immobile center. This cross section depends weakly on the collision energy, and therefore when the ion and atom approach each other to a distance of the order of atomic size, one can use the model of rigid spheres with diameter d_{gas}. The gas-kinetic cross section in the elastic sphere collision model is equal to

$$\sigma_{gas} = \pi d_{gas}^2, \qquad (3)$$

and the effective atomic diameter d_{gas} can be determined from the gas viscosity data.

3. Charge transfer upon ion-atom collision. In the collision between an ion with a parent-gas atom, an electron can be transferred from the atom to the ion without affecting the internal energy of colliding particles. Let us consider the model of this process in more detail.

The probability of electron transition from the atom to the ion falls exponentially with increasing interparticle spacing. If the ion and the atom approach each other so closely that the electron orbits of the atom and ion strongly overlap, the electron will make many transitions from the atom to the ion within the collision time. After collision, the electron will remain with one of the colliding particles with equal probability of 1/2. The resonant charge exchange cross section in atomic units has a functional form [5]:

$$\sigma_{res}(\mathrm{v}) = \frac{\pi}{2\gamma^2}\ln^2\frac{\mathrm{v}_0}{\mathrm{v}}, \qquad (4)$$

where the parameter γ characterizes the velocity of the exponential fall of the electron wave function outside the atom and the parameter v_0 depends weakly on the velocity.

One can determine the effective radius $r_{ct}(\mathrm{v}_{\min})$ of the charge transfer reaction, which is determined by the functional dependence (4) for velocity at the point of closest approach. We shall assume that the charge transfer probability is negligibly small for the closest approach $r_{\min} > r_{ct}$ and is equal to 1/2 for $r_{\min} < r_{ct}$. The charge exchange cross section in this approximation is determined by the relation

$$\sigma_{res} = \frac{1}{2}\pi\rho^2(r_{ct}), \qquad (5)$$

where the impact parameter $\rho(r_{ct})$ corresponds to approach at a distance r_{ct}.

For collision energies $\varepsilon_{12} = m\mathrm{v}_{12}^2/2 >> \varepsilon_d$, where $\varepsilon_d = \frac{\alpha Rya_0^4}{d^4}$ is the polarization interaction energy at a distance of atomic diameter, one can neglect the deflection of the trajectories from linear. Then the charge exchange cross section can be approximated by the dependence

$$\sigma_{res}(\varepsilon_{12}) = \sigma_{res}(\varepsilon_1)[1 + a\ln(\varepsilon_1/\varepsilon_{12})]^2, \qquad (6)$$

where ε_1, a, and $\sigma_{res}(\varepsilon_1)$ are positive approximation constants.

4. Simulation of ion-atom collisions. The problem of construction of an effective algorithm for calculation of the ion-atom collision is important for a correct solution of many problems of gas-discharge physics, involving a simultaneous effect of all the above-mentioned types of particle interactions. Although at low ion energies (< 0.1 eV) the ion-atom polarization interaction cross section usually exceeds the resonant charge exchange cross section, the contribution of collisions with charge exchange to the diffusion cross section is two times greater because in each collision with charge exchange the ion completely loses its velocity.

5. Approximation of cross sections. The proposed algorithm allows obtaining the ion drift velocity for a given charge exchange cross section. The obtained approximation $\sigma_{res}(\varepsilon_{12})$ is based on the choice of the physically grounded dependence (6) for which two fitting constants, $\sigma_{res}(\varepsilon_1), a$, are necessary. To determine them, one can use some two known values of the resonant charge exchange cross section. One of them was the value of $\sigma_{res}(\varepsilon_2)$ for $\varepsilon_2 =$ =10000 eV [4], and so the accuracy of the data on cross sections is high for high energies. The second value of the resonant charge exchange cross section was chosen from the condition that this algorithm should reproduce the mobility and diffusion coefficients known to high accuracy for low fields.

System	$\sigma_{res}(\varepsilon_1)$	$\sigma_{res}(\varepsilon_2)$	*a*
He^+- He	*27.9*	*6.6*	*0.0557*
Ne^+- Ne	*29.0*	*5.9*	*0.060*
Ar^+ - Ar	*55.3*	*13.8*	*0.0543*
Kr^+-Kr	*61.2*	*18*	*0.0497*
Xe^+-Xe	*84.2*	*28*	*0.046*
Rb^+- Rb	*247*	*150*	*0.024*
Cs^+- Cs	*295*	*174*	*0.025*
Hg^+ - Hg	*164*	*45*	*0.052*

The parameters involved in the collision model, as well as the results of adjusting the approximation dependences of charge exchange cross sections are tabulated.

Rresonat charge-exchange cross sections as a function of relative energy:

$$\sigma_{res}(\varepsilon)=\sigma_{res}(\varepsilon_1)[1+a\ln(\varepsilon_1/\varepsilon)]^2 .$$

Cross sections in unit 10^{-16} cm^2,

ε – kinetic energy at eV,

$\varepsilon_1, \varepsilon_2 = 1, 10000$ eV.

The work was supported by Russian Foundation for Basic Research (Grants 05-02-16796, 05-02-17845, 06-02-17520, 06-08-01554) and NWO (Project 047.017.2006.007).

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