DIFFUSION AND MOBILITY OF IONS IN THEIR OWN GAS

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Submitted to JETP editor March 14, 1963; resubmitted July 13, 1964

J. Exptl. Theoret. Phys. (U.S.S.R.) 48, 133-137 (January, 1965)

The diffusion and mobility of ions of an inert gas in the gas itself are calculated by taking into account resonance charge exchange and polarization capture of the ions by the gas atoms. Exact values of the cross sections for resonance charge exchange of an ion on its own atom are employed, and the dependence of the resonance charge exchange cross section on the elastic scattering and on the polarization ion capture by the atom is taken into account. The ion mobility values at room temperature are in satisfactory agreement with the experiments.

1. The essential characteristics of a plasma are the mobility of the plasma ions and the diffusion of the ions to the walls. These parameters are determined by the ion-ion or ion-atom collision cross sections: the elastic scattering cross sections, the polarization capture cross section, and especially the resonance charge exchange cross section. The diffusion and mobility of ions in their parent gas were calculated by Holstein [1] and Dalgarne et al [2-4], who used the resonance charge exchange cross sections derived by a semi-empirical method. The calculations in the present paper are based on knowledge of the exact values of the charge exchange cross sections. We calculate the diffusion and mobility of the inert-element ions in their parent gas, with allowance for the resonance charge exchange and polarization capture of the ions by the atoms. We take into consideration here the dependence of the cross section for resonance charge exchange of the ions with the parent atoms on the elastic scattering and on the polarization capture of the ions, a factor which becomes important at low collision velocities.

The diffusion and mobility of ions in their parent gas are determined essentially by the resonance charge exchange of the ions even at low temperatures.

2. The diffusion coefficient D is [5]

$$6D=\frac{1}{h^2}\left\langle\frac{d(\Delta\mathbf{p})^2}{dt}\right\rangle=\frac{\mu^2}{e^2}M^2\left\langle\frac{d(\Delta\mathbf{v})^2}{dt}\right\rangle. \tag{1}$$

Here h—friction force, $\mu = e/h$—ion mobility, M—mass of ion and atom, e—charge of ion, and $\langle d(\Delta v)^2/dt\rangle$—mean square of the change in the ion velocity per unit time.

In the case of an ideal gas, the diffusion and mobility are connected by the Einstein relation[6,7] $\mu = eD/T$, where T = gas temperature. Hence

$$D=6\left(\frac{T}{M}\right)^{1/2}\Big/\left\langle\frac{d(\Delta\mathbf{v})^2}{dt}\right\rangle. \tag{2}$$

The mean square of the change in the ion velocity per unit time is

$$\left\langle\frac{d(\Delta\mathbf{v})^2}{dt}\right\rangle=\int(\Delta\mathbf{v})^2|\mathbf{v}-\mathbf{v}'|\sigma(\mathbf{v},\mathbf{v}')nf(\mathbf{v}')f(\mathbf{v})\,d\mathbf{v}d\mathbf{v}'.$$

Here $\sigma(\mathbf{v}, \mathbf{v}')$—cross section for the collision of the ion $\mathbf{v}$ with the atom $\mathbf{v}'$, $\Delta\mathbf{v}$—change in ion velocity resulting from such a collision, $f(\mathbf{v})$ and $f(\mathbf{v}')$—distribution functions of the ions and the atoms, normalized per unit time, and n—density of the atoms. Neglecting the collisions of the ions with the ions and the small-angle elastic scattering of the ions by the atoms, which make a small contribution to the diffusion coefficient, we obtain

$$\left\langle\frac{d(\Delta\mathbf{v})^2}{dt}\right\rangle=\int\Big[\,|\mathbf{v}-\mathbf{v}'|^2\sigma_{\mathrm{res}}(|\mathbf{v}-\mathbf{v}'|)$$
$$+\frac{|\mathbf{v}-\mathbf{v}'|^2}{4}\cdot 2(1-\cos\theta)\,\sigma_{\mathrm{cap}}(|\mathbf{v}-\mathbf{v}'|)\Big]$$
$$\times|\mathbf{v}-\mathbf{v}'|nf(\mathbf{v}')f(\mathbf{v})\,d\mathbf{v}'d\mathbf{v},$$

where $\sigma_{\mathrm{res}}(|\mathbf{v}-\mathbf{v}'|)$ is the part of the resonance charge exchange cross section of the ion $\mathbf{v}$ by the atom $\mathbf{v}'$ not connected with the capture of the ion, $\sigma_{\mathrm{cap}}(|\mathbf{v}-\mathbf{v}'|)$—cross section for the capture of the ion by the atom, and θ—angle between $\mathbf{v}$ and the direction of emission of the initially captured ion, in the c.m.s. of the colliding atom and ion (we assume that the ions are isotropically distributed relative to the emission angles).

Assuming that the ions and atoms have a Maxwellian distribution, we obtain

$$\left\langle \frac{d(\Delta \mathbf{v})^2}{dt} \right\rangle = \frac{4n}{\sqrt{\pi}} \left(\frac{T}{M} \right)^{3/2}$$

$$\times \int_0^\infty e^{-u^2/2} u^5 du \left[\sigma_{\text{res}}(u) + \frac{1}{2} \sigma_{\text{cap}}(u) \right],$$

where $u = |\mathbf{v} - \mathbf{v}'| (M/2T)^{1/2}$.

The diffusion coefficient and the mobility are equal to

$$D = \frac{3(\pi T)^{1/2}}{16 n \bar{\sigma} M^{1/2}}, \quad \mu = \frac{3\pi^{1/2} e}{16 n \bar{\sigma} (TM)^{1/2}}; \tag{3}$$

$$\sigma = \frac{1}{8} \int_0^\infty e^{-u^2/2} u^5 \left[\sigma_{\text{res}}(u) + \frac{1}{2} \sigma_{\text{cap}}(u) \right]. \tag{4}$$

If capture can be neglected, these expressions coincide with those customarily used[2–4]. The problem of determining the diffusion coefficient and the mobility reduces to a determination of a certain mean value $\bar{\sigma}$.

3. The cross section for ion-atom resonance charge exchange, in the case when the elastic scattering of the ion can be neglected, is equal to $\sigma_{\text{ce}} = \pi R_0^2/2$, where R_0 is given by[8]

$$\left(\frac{R_0}{a_0} \right)^{2/\gamma - 1/2} e^{-R_0 \gamma / a_0} = \frac{0.22}{A^2} \frac{v}{v_0}, \tag{5a}$$

a relation valid under the following condition, which is satisfied in almost all cases:

$$R_0 \gamma^2 / 2a_0 \gg 1. \tag{5b}$$

Here $\gamma = \sqrt{-2\epsilon\hbar^2/me^4}$, m—electron mass, ϵ—binding energy of the electron in the atom, $\hbar$—Planck's constant, $v_0 = e^2/\hbar$, $a_0 = h^2/me^2$, v—relative velocity of collision between the ion and the atom, and A—constant determined by the behavior of the electron in the atom.[1]

Allowance for the elastic scattering in the calculation of the resonance charge exchange cross section yields[3]

$$\sigma_{\text{res}} = \begin{cases} \frac{1}{2} \pi R_0^2 [1 - U(R_0)/E], & R_0(v) \geqslant R_{\text{cap}} \\ \sigma_{\text{cap}}/2 & R_0(v) \leqslant R_{\text{cap}} \end{cases}. \tag{6}$$

Here U(R)—potential for the interaction between the ion and the atom, assumed to be a polarization potential at large distances between the nuclei ($U = -\alpha/2R^4$, α—polarizability of the atom), E—kinetic energy of the nuclei in the c.m.s., R_{cap}—minimum approach at which capture is still possible. In the case of polarization interaction

$$R_{\text{cap}} = (\alpha / 2E)^{1/4}, \qquad \sigma_{\text{cap}} = 2\pi (\alpha / 2E)^{1/2}.$$

4. As can be seen from (5a), $R_0(u) = \gamma^{-1} \times \ln(A/u)$, where A(u) is a smooth function of the velocity at large values of R_0. Consequently, when calculating the mean value $\bar{\sigma}$ for each temperature, A(u) can be regarded as constant. For the mean values $\langle R_0^2 \rangle$ and $\langle U(R_0) R_0^2/E \rangle$ we have

$$8\langle R_0^2 \rangle = \frac{1}{\gamma^2} \int_0^\infty e^{-u^2/2} u^5 \ln^2 \frac{A}{u} du = \frac{1}{\gamma^2} \ln^2 \frac{A}{u_0} \int_0^\infty e^{-u^2/2} u^5 du$$

$$- \frac{2}{\gamma^2} \ln \frac{A}{u_0} \int_0^\infty e^{-u^2/2} u^5 du \ln \frac{u}{u_0} + \ldots,$$

$$8 \left\langle \frac{1}{u^2 R_0^2} \right\rangle = \gamma^2 \int_0^\infty e^{-u^2/2} u^3 du \ln^{-2} \frac{A}{u} = \gamma^2 \ln^{-2} \frac{A}{u_1} \int_0^\infty e^{-u^2/2} u^3 du$$

$$+ 2\gamma^2 \ln^{-3} \frac{A}{u_1} \int_0^\infty e^{-u^2/2} u^3 du \ln \frac{u}{u_1} + \ldots.$$

We choose u_0 and u_1 in these expressions such that the second integral vanishes. This corresponds to determining these quantities accurate to the first two terms of the expansion in powers of $a_0/R_0\gamma \ll 1$. For the mean values $\langle R_0^2 \rangle$ and $\langle U(R_0) R_0^2/E \rangle$ we obtain, with the accuracy indicated,

$$\langle R_0^2 \rangle = R_0^2(u_0), \qquad u_0 = 2.24,$$

$$-\langle U(R_0) R_0^2 / E \rangle = \alpha / 4TR_0^2(u_1), \qquad u_1 = 1.75. \tag{7}$$

From (4) and (6) we have for the mean cross section $\bar{\sigma}$

$$\bar{\sigma} = \frac{1}{24} \int_0^\infty \sigma_{\text{cap}} e^{-u^2/2} u^5 du + \frac{\pi R_0^2(u_0)}{16} \int_z^\infty e^{-u^2/2} u^5 du$$

$$+ \frac{\pi\alpha}{16TR_0^2(u_1)} \int_z^\infty e^{-u^2/2} u^3 du + \frac{1}{16} \int_0^z \sigma_{\text{cap}} e^{-u^2/2} u^5 du, \tag{8}$$

where z is given by

$$R_{\text{cap}}(z) = R_0(z), \qquad z = (\alpha / R_0^4 T)^{1/4},$$

and the values of the arguments u_0 and u_1 depend, generally speaking, on z ($u_0 = 2.24$, $u_1 = 1.75$ when $z = 0$). However, in calculating the mean cross section we can, with accuracy sufficient for practical purposes, regard u_0 and u_1 as constants, inasmuch as σ is much less sensitive to u_0 and u_1 than to z, and wherever u_0 and u_1 deviate noticeably from the values used in (7) the integrals that contain these quantities make no contribution to the mean cross section $\bar{\sigma}$.

We thus obtain ultimately

$$\bar{\sigma} = \frac{\pi}{4} \left(\frac{2\alpha}{T} \right)^{1/2} \left[\frac{\sqrt{\pi}}{2} + \frac{3\sqrt{\pi}}{4} \Phi(\sqrt{x}) - e^{-x} x^{1/2} \left(1 + \frac{3}{2} x \right) \right.$$

$$\left. + \frac{1}{4} \pi R_0^2 (2.24 v_T) e^{-x} (x^2 + 2x + 2) \right] + \frac{\pi \alpha e^{-x} (x+1)}{8TR_0^2(1.75 v_T)}, \tag{9}$$

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[1] In the case of inert gases A is equal to 2.1, 1.41, 1.92, 2.02, and 1.31 for helium, neon, argon, krypton, and xenon, respectively [7].

Table I

$\bar{\sigma}$, 10^{-16} cm^2

Gas		log *T*, °K						
		2	2,5	3	3,5	4	5	6
H	our data	94	76	64	56	48	38	27
	data of [2]			78	68	61	47	34
He	our data	46	34	27	23	20	17	11
	data of [2]			46	42	38	28	22
Ne	our data	58	42	34	28	24	18	12
	data of [2]			54	48	44	34	26
Ar	our data	108	82	67	56	49	38	28
	data of [2]			96	90	83	73	63
Kr	our data	132	101	83	72	63	50	38
	data of [2]			119	111	104	92	79
Xe	our data	143	108	88	75	65	50	37
	data of [2]			140	134	126	112	98

where $x = z^2/2 = (\alpha/R_0^4T)^{1/2}/2$, $\Phi(\sqrt{x})$ is the probability integral, and $v_T = \sqrt{2T/M}$.

When $x \ll 1$ (case of high temperatures), (9) goes over into

$$\bar{\sigma} = \frac{\pi}{8}\left(\frac{2\pi\alpha}{T}\right)^{1/2} + \frac{1}{2}\pi R_0^2(2.24 v_T) + \frac{\pi\alpha}{8TR_0^2(1.75 v_T)}. \qquad (10)$$

The mean values calculated by formulas (9) and (10), in units of 10^{-16} cm^2, are listed in Table I. The values of the cross sections for the resonance charge exchange $\pi R_0^2/2$, obtained without allowance for elastic scattering, are taken from the paper by Chibisov and one of the authors [10]. The lower figures in the table correspond to the values of $\bar{\sigma}$ calculated by Dalgarno [2] by a semi-empirical method and therefore deviate noticeably from our result.

The mobility is usually related to a gas density $n = 2.69 \times 10^{19}$. If the gas temperature is measured in degrees, the ion mass M in proton-mass units, and the mean cross section $\bar{\sigma}$ in units of 10^{-16} cm^2, then the mobility is given by

$$\mu = \frac{1{,}3 \cdot 10^4}{(MT)^{1/2}\bar{\sigma}} \frac{\text{cm}^2}{\text{V} \cdot \text{sec}}. \qquad (11)$$

Comparison of the results calculated from (11) with the experimentally measured values of the mobility [11-17] is given in Table II.

In conclusion, the authors are deeply grateful to O. B. Firsov for valuable discussions and for interest in the work.

Table II

μ, cm^2/V · sec

Gas	*T* = 77° K	*T* = 195° K	*T* = 300° K
He	15.1 13.5 [11] 13.8 [12]	12.2 12.1 [11] 11.1 [12]	10.9 10.8[11], 9.6 [12] 10.5[13], 10,7 [14]
Ne	6.1 5.2 [11,12]	4.3 4.5 [11,12]	3,9 4.2 [11,12], 4.0 [13] 4.1 [14]
Ar	1.92 2.2 [11] 1.88 [16]	1.68 1,95 [11]	1.41 1,6 [13,14] 1,63 [15], 1.38 [16]
Kr			0,8 0,9 [13] 0.9—0,95 [17]
Xe			0.56 0,58 [13]

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Translated by J. G. Adashko
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