34th EPS Conference on Plasma Phys. Warsaw, 2 - 6 July 2007 ECA Vol.**31F**, P-5.033 (2007)

Ion–atom collisions simulation in DC plasma

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1. Introduction. In experiments with direct-current discharge, dust particles are located in the electric field of the stratum. The mean velocity of ions (the drift velocity) can be as small and large compared with thermal velocity of gas atoms. We consider here the effect of ion - gas atom collisions upon the ion flow characteristics, namely, upon the relation between the directed velocity and the random thermal velocity of ions in the spatially homogeneous case.

A numerical model of ion collisions with gas atoms is constructed with allowance for the ion resonant charge exchange, the polarization interaction, and the elastic (gas-kinetic) interaction [1].

2. Ion-atom collisions model. 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 $U(r_{12}) = -\alpha Ry a_0^4 / r_{12}^4$, where r12 is the distance between the atom and ion, $\alpha = \alpha_0 / a_0^3$, α_0 - is atomic polarizability, $a_0=0.529\ 10^{-8}$ 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 $\sigma_{pol} \propto 1/\mathrm{v}_{12}$, 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}.

In the collision between an ion with a parent-gas atom, an electron can be transferred from the atom to the ion. 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. One can determine the effective radius $r_{ct}(\mathrm{v}_{\min})$ of the charge transfer reaction, which is determined by 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 $r_{\min} < r_{ct}$.

3. 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. We shall list the main stages of the proposed algorithm:

1) in the center-of-mass system of colliding particles, in accordance with collision probability one chooses the velocities and the impact parameter of collision;

2) in the center-of-mass system of moving particles with the polarization interaction potential (2) one determines the closest approach $r_{\min}$,the relative particle velocity $\mathrm{v}_{12}(r_{\min})$ at the point of closest approach, and the scattering angle χ;

3) if $r_{\min} > d_{gas}$, the ion and atom velocities decline by the angle χ;

4) if $r_{\min} < d_{gas}$, the ion and atom velocities are recalculated according to the law of elastic sphere collision, the closest approach is assumed to be $r_{\min} = d_{gas}$, and the relative particle velocity is determined at the point of closest approach $\mathrm{v}_{12}(r_{\min})$;

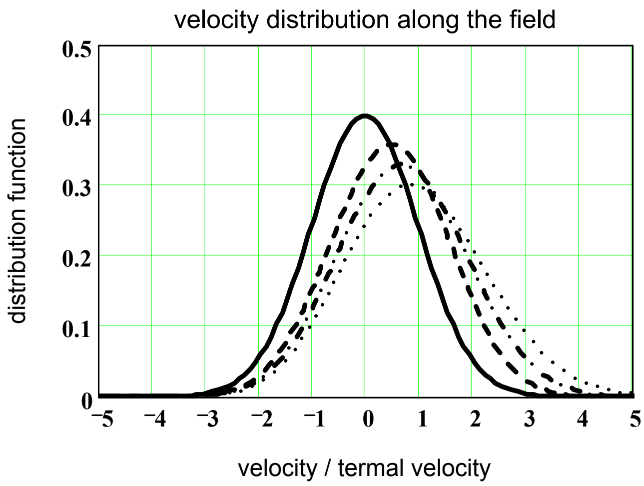
5) the resonant charge exchange cross section $\sigma_{res}(\mathrm{v}_{12}(r_{\min}))$ is determined for the relative particle velocity $\mathrm{v}_{12}(r_{\min})$ at the point of closest approach;

6) for the closest approach $r_{\min} < r_{ct} = (2\sigma_{res}(\mathrm{v}_{12}(r_{\min}))/\pi)^{1/2}$, the ion and atom velocities change with probability of 1/2;

7) the velocities are recalculated in the laboratory frame and statistics for various collision characteristics is accumulated.

On the basis of experimental data on ion mobility and the results of simulation of ion collisions with proper-gas atoms in a homogeneous electric field, the approximations of the ion resonant charge exchange cross sections for noble gases were fitted which are applicable for the description of the ion drift in any fields [2].

4. Example for weak field. The charge of grain in a plasma-dust cloud in a direct-current discharge in room-temperature neon was measured directly in the experiment [3]. We calculated the ion drift by the Monte Carlo method with allowance for resonant charge exchange and polarization interaction of ions with finite-radius particles (the solid core model). The results of these calculations are presented in fig. 1 (*P*=20, 30, 50 Pa) and Table 1.



P, Pa	10	20	30	50	100
M	1.99	1.13	0.79	0.49	0.28
M_{eff}	1.57	1.01	0.74	0.48	0.28
T_{eff}	862	490	393	333	306
T_i	668	427	362	321	303
$T_{\parallel}$	1237	628	463	362	316
$T_{\perp}$	383	328	312	301	296

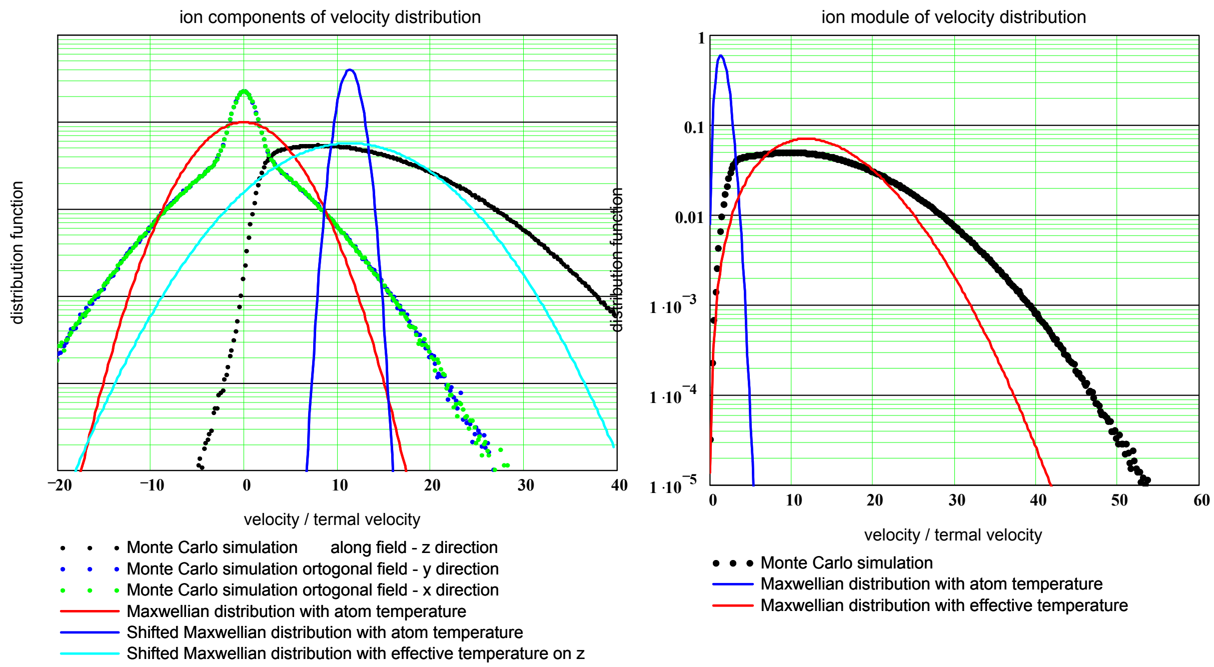
Table 1. Results of Monte Carlo calculations of characteristics of Ne^+ ion flow in *Ne* for the electric field strength $E = 2$ V/cm at a gas temperature of T_a=293 K and at different gas pressures. Temperature unit is K. The Mach number $M^2 = mu_d^2 / T_a$, the effective Mach number $M_{eff}^2 = mu_d^2 / T_i$, ion temperature is defined from $\frac{3}{2}T_i = \frac{1}{2}m\langle u^2\rangle - \frac{1}{2}m\langle u\rangle^2$. Ion temperature, effective ion temperature T_{eff}, temperatures $T_{\parallel}$ and $T_{\perp}$ are defined from $\langle\varepsilon\rangle = \frac{3}{2}T_{eff} = \frac{3}{2}T_i + \frac{1}{2}T_{\parallel} + T_{\perp}$.

A consideration of the effect of deviation of the distribution function of ions from equilibrium upon the charging of macroparticles made it possible to come to agreement between the experimental data and the calculations of the dust particle charge by the method of molecular dynamics with an error of less than 10%.

4. Example for strong field. The charge of grain in a plasma, self-consistent kinetic approach and experimental data for RF discharge in *Ar* are considered in [4]. We calculated the ion drift and ion flow characteristics for different models. Data are collected in Table 2. Fig. 2 presents ion distribution functions for the Monte Carlo method with allowance for resonant charge exchange and polarization interaction of ions in the solid core model. Field strength E = *17* V/cm at a gas temperature of T_a=293 K and at gas pressures 2.7 Pa ($E/N = 2513\,Td$).

	MC [2]	*MC [2,4]*	*MC [4]*	*fit [4]*
u_d , km/s	2.798	2.789	2.349	
M	11.382	11.341	9.55	
M_{eff}	2.16	2.34	2.46	
T_i , eV	0.69	0.593	0.38	
$T_{\parallel}$, eV	1.26	1.73	1.09	3.8
$T_{\perp}$, eV	0.42	0.0255	0.0255	0.025
T_{eff} , eV	1.79	1.676	1.15	1.28

Table 2. Results of Monte Carlo calculations of characteristics of Ar^+ ion flow in Ar for the electric field strength E = *2* V/cm at a gas temperature of T_a=293 K. ***MC [2]*** – Monte Carlo run in full model [2] (precision 1-2 %), ***MC [2, 4]*** – Monte Carlo run in case only resonant charge exchange collisions with cross section fit from [2], ***MC [4]*** – Monte Carlo run in case only resonant charge exchange collisions with constant cross section [4], ***fit [4]*** - fit and theory from [4].



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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