Cross-Sections and Transport Properties of F^- Ions in F_2

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We present the new results for the simple scattering cross-section set and proposed transport coefficients for F^- ions in F_2 that can be used in such models. Nanbu's theory based on thermodynamic threshold energies and separating elastic and reactive collisions is used to calculate cross-sections for binary collisions of ions with atoms and molecules. Direct MC method is applied to obtain swarm parameters at temperature of $T = 300$ K.

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1. Introduction

The goal of this work is to present data for modeling of complex low temperature collisional plasmas containing F^- ions by using a global [1–3] and other plasma models. The negative halogen ions are abundant in various forms of nonequilibrium plasmas relevant to applications such as excimer lasers [4, 5] and electrical discharges, biomedical devices, nanotechnologies and in radiation chemistry in the atmosphere. For example, it is experimentally found that negative ions are effective for increasing the etch rate and improving the etch profile [6]. F^- ions are also unavoidable part of production of cBN films [7].

For example, F_2 may be produced in pulsed plasma implantation system that is the basis for establishing doping of integrated components. In such a system it is necessary to create uniform plasma over the entire wafer that could be more than 500 mm wide. To achieve such a goal one needs to understand a number of processes of particles interacting with either gas molecules or surfaces. Time resolved measurements of ion energy distributions in the cathode boundary [8] indicated a possible role of charge-transfer collisions between singly charged ions of various masses.

In this paper we study the energy dependent scattering and transport processes for F^- ions in F_2 gas.

2. Monte Carlo technique and the cross-section data

The cross-sections for scattering of F^- on F_2 molecule are calculated by using Nanbu's theory [9, 10] that within same framework treats elastic and reactive endothermic collisions. In Nanbu's theory reactive collision is treated by accounting for thermodynamic threshold energy and branching ratio according to the Rice–Rampsperger–Kassel (RRK) theory [9]. In the RRK theory of uni-molecular reaction rates excited molecular complex is treated as excited activated complex where internal energy is distributed among equivalent oscillators--vibrational modes of the complex.

Our procedure is a direct implementation of this theory and approximation. We have used value 1.2611×10^{-30} m^3, for polarizability of F_2 recommended by Spelsberg and Meyer [11], ionization potentials for F_2 and F^- from [12] and the bond values between atoms in Ref. [13]. One is usually applying procedure where unfolding the cross-sections is coming from the measured transport coefficients and thermo-chemical data known from a separate drift tube and other experiments. According to our knowledge no such data are available.

In Monte Carlo (MC) technique used in this study collision frequency in case of thermal collisions of a test ion particle is not calculated by MC integration technique [14] but by using piecewise calculation [15]. That method is based on assumption that most cross-sections are defined numerically at limited number of points with linear interpolation for mid points.

The MC technique was applied to perform calculations of transport parameters as well as rate coefficients in DC electric fields. In this paper we have used a MC code that properly takes into account the thermal collisions [15]. The code has passed all the tests and the benchmarks that were covered in our earlier studies [15, 16]. For example the distinction should be made between [17, 18] the so called bulk (b) and flux (f) transport properties such as drift velocity

$$\boldsymbol{v}_b = \frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=1}^{n}\boldsymbol{r}_i, \quad \boldsymbol{v}_f = \sum_{i=1}^{n}\boldsymbol{v}_i. \tag{1}$$

3. Discussion and results

In Fig. 1 we show calculated cross-sections for F^- scattering on F_2. Cross-section for charge transfer (CT) producing F_2^- ion measured by Chupka et al. [19] is shown in the same figure.

Transport parameters were calculated for the room gas temperature of $T = 300$ K. The rate for CT with its low threshold of 0.39 eV overlaps with the thermal distribution function of participants in a collision and thus a

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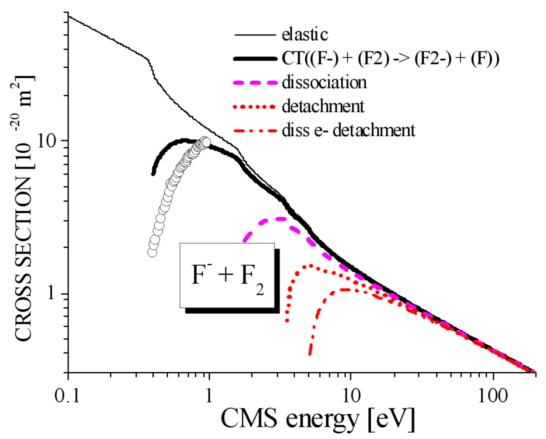

Fig. 1. Cross-section set for F^- ions in F_2. Open circles denote the data of Chupka et al. [19] placed on absolute scale by assuming maximum value as obtained by Nanbu's theory.

plateau exists at low E/N. The value of the plateau is very low but it increases rapidly as the temperature of the gas is increased.

The temperature for the most part does not affect elastic scattering as the total cross-section does not depart much from the cross-section consistent with the constant collision frequency.

As for the rates of inelastic processes the temperature makes a small, hardly observable, effect as the thresholds are considerably higher than the thermal energy.

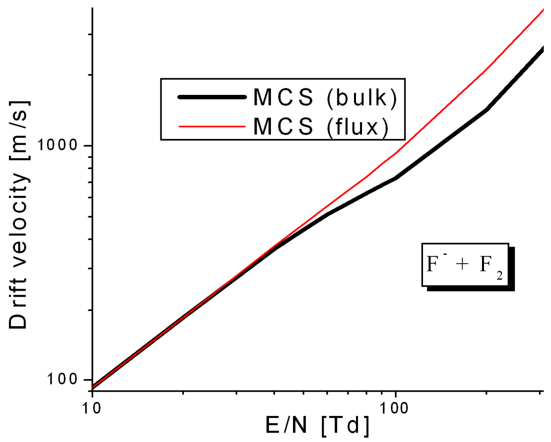

Fig. 2. Flux and bulk values of drift velocity for F^- ions in F_2 as a function of E/N.

Flux and bulk drift velocities [20, 18, 21] as a function of E/N are given in Fig. 2. The drift velocities obtained by MC simulation were calculated in real space (bulk) and in velocity space (flux) values which are obtained as $\langle v \rangle$ and $\mathrm{d}x/\mathrm{d}t$, respectively. In most plasma assisted applications exploiting low temperature conditions the drift velocities are not affected by the gas temperature and ion mobility is almost constant. Yet we observe effect of reactive collisions affecting the splitting of flux and bulk drift velocity components above 40 Td (1 Td = 10^{-21} V m^2). Since accuracy of the ion implantation model is based on the precise determination of the flux and ion velocities at the surface of the electrode, then the difference between bulk and flux drift velocity represents the error in flux calculations. The first mention of non-conservative effects in ion transport was given in [12].

Longitudinal and transverse bulk diffusion coefficients for F^- ions in F_2 as a function E/N are shown in Fig. 3. They are necessary in modeling ionic diffusion losses in global models [3]. Let us note that difference between flux and bulk values of diffusion coefficients since having the same origin have the same initial value as drift velocities. There are no published experimental data for the longitudinal and transverse diffusion coefficients of F^- in F_2.

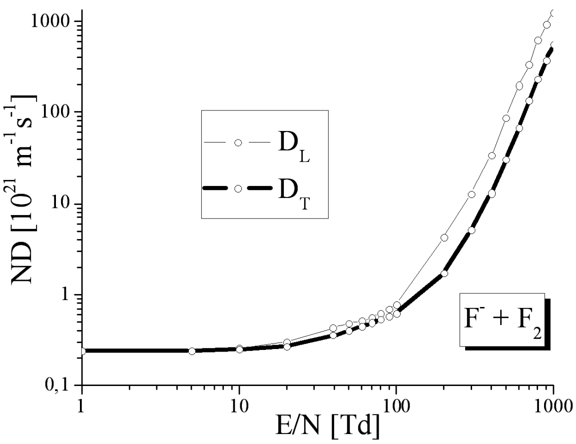

Fig. 3. The diffusion coefficients for F^- ions in F_2 obtained by MC simulation as a function of E/N at $T = 300$ K.

From the modeler's point of view, specifically for purpose of modeling a specific application, distinguishing between flux and bulk transport coefficients affects accuracy of numerical calculations [22].

4. Conclusion

The cross-sections for scattering of F^- ions on molecule are calculated by using Nanbu's theory [9] separating elastic from reactive collisions.

Monte Carlo technique was applied to carry out calculations of the drift velocity and diffusion coefficients as a function of reduced electric field in DC electric fields.

The cross-sections and transport data for technologically very important gas F_2 have been determined by using simple theory. While it is a good basis for modeling it would be much better to add a data base of measured transport coefficients and then to perform the analysis again.

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