Cross-Section and Transport Parameters of Ne^+ in CF_4

Ž. Nikitović*, V. Stojanović and Z. Raspopović
Institute of Physics, University of Belgrade, POB 68, 11080 Belgrade, Serbia

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A cross-section set for scattering Ne^+ ions in CF_4 is assessed by using available experimental data for charge transfer cross-sections. In this paper we present new results for the mean energy, reduced mobility and diffusion coefficients for low and moderate reduced electric fields E/N (N — gas density) and account for the non-conservative collisions. The Monte Carlo method is used to calculate transport properties of Ne^+ ions in CF_4 at temperature of $T = 300$ K.

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1. Introduction

Charge transfer reactions of ions with molecules are unavoidable elementary processes in modeling kinetics in terrestrial, industrial, and astrophysical plasmas in dark matter detection [1]. Motivational factors for this study are identified and this paper reports on a topic important both for fundamental studies and for applications.

Tetrafluoromethane or CF_4 molecule which has widely been used in aluminium manufacturing and semiconductor industries has an extremely long life time (≈ 50000 years) and the highest atmospheric abundance of all perfluorocarbons [2]. It is, therefore, very important to develop replacing materials or methods to decompose efficiently CF_4 molecules in order to reduce man-made greenhouse gases.

Line spectra of excited atoms obtained in spectrometric measurements in CF_4 indicate that the charge transfer reaction is dominant process in collisions with inert gas ions. In selected cases charge transfer cross-sections is representing the most significant part of a cross-section set.

The cross-section data for dissociative excitation of CF_4 [3] are essential in estimating the degree of importance of many related processes. In this work we assessed cross-section set for Ne^+ in CF_4 by using existing experimental data [4] for charge transfer collisions producing radical ions of CF_4.

Since no direct information is found in the literature how mobility of high recombination energy ions such as Ne^+ ions behaves in CF_4 we also calculated transport parameters by using the Monte Carlo simulation technique [5].

2. Cross-section set

The experimentally measured reaction cross-sections presented by Fisher et al. [4] were extrapolated toward lowest energies according to Langevin's cross-section trend (curves with labels CF^+, CF_2^+, CF_3^+) and shown in Fig. 1. These curves were used to determine the elastic momentum transfer cross-section ("EL" in Fig. 1) assuming the total momentum transfer cross-section σ_{mt} is known. At low energies less than 1 eV we assumed that σ_{mt} is Langevin's cross-section and elastic momentum transfer cross-section is determined by deducing all reactive cross-sections.

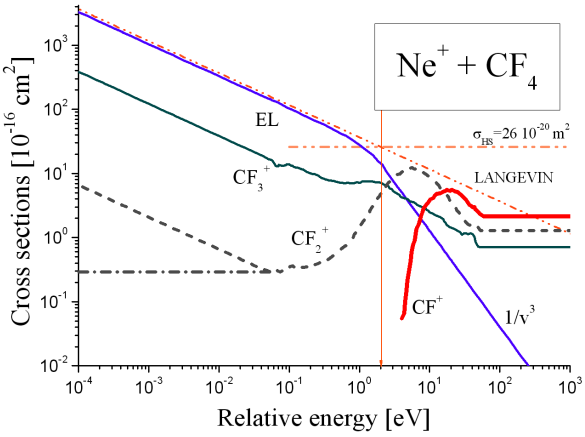

Fig. 1. Cross-section set for $Ne^+ + CF_4$.

The Langevin cross-section was determined by using the polarizability of the gas. The average polarizability of CF_4 is not well established [4] and may produce discrepancy for calculated mobility of ions in CF_4 [6, 7] and thus affect plasma parameters prediction in modeling. We adopted value of 3.86×10^{-30} m^3 used by Stojanović et al. [6] who found excellent agreement between experimental and calculated mobility of CF_3^+ ions drifting in CF_4 gas. Extrapolation of the elastic momentum transfer cross-section trend beyond crossing point (see vertical arrow in Fig. 1) of the Langevin and hard sphere (σ_{HS}, see dash-dot-dot line in Fig. 1) cross-section [1] is done by smoothly connecting to $1/v^3$ trend [8] where v is the center-of-mass velocity (see Fig. 1).

At all ion kinetic energies above 50 eV reactive cross-sections are extrapolated by constant values taking into account measured ratio of reactive cross-sections at high energies [9].

*corresponding author; e-mail: zeljka@ipb.ac.rs

The effects of various extrapolations (short dot-dashed and dashed line in Fig. 1) of unusual behavior at low energy, observed for measurements of the cross-section leading to formation of CF_2^+ (where irrespective of the Ne^+ spin state exothermic behavior of reaction is expected) is found negligible on mobility.

3. Transport parameters

The Monte Carlo technique was applied to perform calculations of transport parameters. Information about the cross-sections is used during the integration of the collision frequency to get kinematics after the collisions. By using the statistical methods transport parameters (mean energy, drift velocity and diffusion coefficients) were determined after their temporal relaxation.

We have used a Monte Carlo code that properly takes into account thermal collisions [10]. The code has passed all the relevant benchmarks [11] and has been tested in our work on several types of charged particles [11, 12].

Results of Monte Carlo simulations are shown in Figs. 2–4. Note that these transport parameters are the only information present in the literature up to now, there are no published experimental data for the transport coefficients of Ne^+ in CF_4.

In Fig. 2 we show the mean energy, which cannot be directly measured in experiments but a map of mean energy versus E/N may be used directly to provide the data in fluid models especially when local field approximation fails. The mean energy having thermal value of 0.039 eV increases above 10 Td.

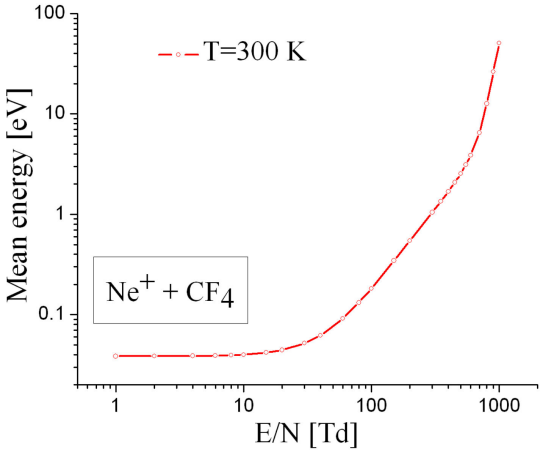

Fig. 2. The mean energy for Ne^+ in CF_4 as a function of E/N.

Generally, the presence of non-conservative collisions causes the drift velocity to be more complex i.e. one may define bulk drift velocity as a measure of center of mass displacement in time ($W = \mathrm{d}\langle x\rangle/\mathrm{d}t$) [13] and flux drift velocity $w = \langle v\rangle$ that describes ion flux. Bulk drift velocity is reaction corrected flux drift velocity: $w = W + S$, where S is the term representing a measure of the effect of reactions on the drift velocity.

Reduced mobility for Ne^+ ions as a function of E/N (E — electric field, N — gas density) compared with Langevin's value is shown in Fig. 3.

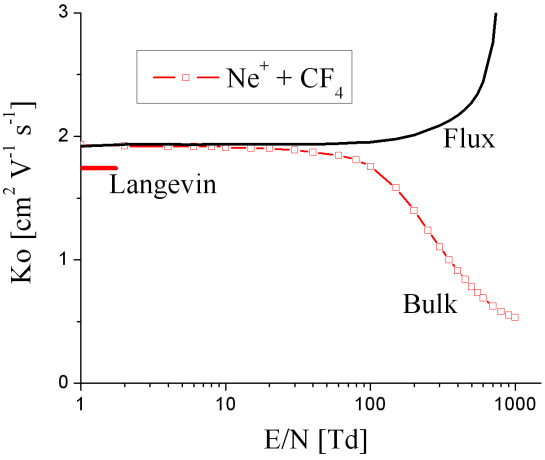

Fig. 3. The bulk and flux reduced mobility for Ne^+ in CF_4 as a function of E/N.

For $E/N < 50$ Td, exothermic collision frequency is approximately corresponding to the energies below 0.1 eV. This causes the equality of the bulk and flux reduced mobilities [14, 15] since the ions from the front and the tail are removed with equal rate [16].

For higher E/N the bulk reduced mobility is decreasing with E/N because of an increasing number of ions removed from the regions of higher energy (from swarm front). That results in a shift in the centre-of-mass position. At the same time, flux reduced mobilities increase with E/N since number of elastic collisions decrease.

Due to exothermal collisions mobility is 10% higher than the polarisation limit ($E \to 0$ and $T \to 0$) value (see the mark "Langevin" in Fig. 3) predicted by the Langevin theory. The mobility which is shown is the same at smaller temperatures because of the constant collision frequency on small energies.

Bulk and flux longitudinal diffusion coefficients [13] were calculated by time averaging the position (x) and velocity (v_x) (direction of the electric field) of each swarm particle

$$D_L(\text{bulk}) = 0.5\frac{\mathrm{d}}{\mathrm{d}t}\left(\langle x^2\rangle - \langle x\rangle^2\right),$$

$$D_L(\text{flux}) = \langle x v_x\rangle - \langle x\rangle\langle v_x\rangle,$$

respectively. The same procedure is used for transversal diffusion coefficients ($\langle y\rangle = \langle z\rangle = 0$, $\langle v_y\rangle = \langle v_z\rangle = 0$). All calculated diffusion coefficients are shown in Fig. 4.

One should notice the very large non-conservative effects, almost a reminder of the positron transport [17]. Similarly to the results for drift velocity flux diffusion coefficients are significantly larger than bulk values. The decrease of the bulk longitudinal diffusion from 200 Td to 600 Td is especially interesting due to a significant increase of the collision frequency for reactive collisions.

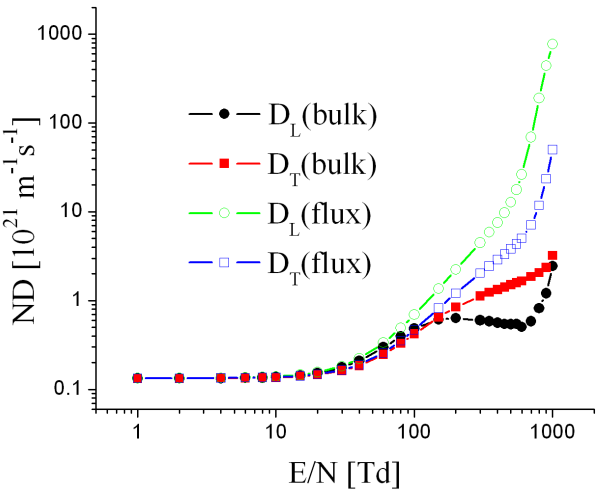

Fig. 4. The transversal and longitudinal diffusion coefficients for Ne^+ in CF_4 as a function of E/N.

4. Conclusion

By using measured charge transfer cross-sections we assessed the complete cross-section set for Ne^+ions in CF_4 that is used as an input in Monte Carlo simulations in order to calculate transport parameters.

Focusing on calculated reduced mobility data as a function of E/N, in this paper we found that is necessary to discuss both flux and bulk reduced mobility data.

Data for swarm parameters for ions are needed for hybrid and fluid codes and the current focus on liquids or liquids in the mixtures with rare gases dictates the need to produce data compatible with those models.

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