Cross section set and transport properties for Ar^+ in CF_4

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Cross section set for scattering Ar^+ ions in CF_4 is developed by using and extrapolating the available experimental data for charge transfer cross sections. Monte Carlo simulation is employed to calculate transport properties of Ar^+ ions in CF_4.

1. Introduction

In often applied mixtures of argon (dominant gas) and CF_4 (minority gas- 5-10% in the abundance) often overlooked collisions are those of argon ions on minority constituent in the mixture since their transport is dominated by the resonant charge exchange collisions with the parent gas argon. Still one believes that completing the set of data would be welcome and provide more accurate foundation for modelling. In addition, taking in account Ar^+ collisions on CF_4, reactive collisions may provide new channels for some ionic species and alter their kinetics.

Charge transfer reactions of ions with molecules are unavoidable elementary processes in modelling kinetics in terrestrial, industrial, and astrophysical plasmas. In the selected case, charge transfer reactions are known to represent the most significant part of a cross section set. Line spectra of excited atoms obtained in spectrometric measurements in CF_4 [1] indicate that the charge transfer reaction is the dominant process in collisions with inert gas ions. Thus, in this work we assessed cross section set for Ar^+ in CF_4 by using existing experimental data [2] for charge transfer collisions producing radical ions of CF_4.

Since no direct information is found in the literature how mobility of inert ions such as Ar^+ ions behaves in CF_4 we also calculated transport parameters by using Monte Carlo simulations.

2. Cross section set

The cross sections presented by Fisher *et al* [2] were used to determine the elastic momentum transfer cross section ("elastic" in Fig. 1) assuming the total momentum transfer cross section σ_{mt} is known. At low energies we assumed that σ_{mt} is Langevin's cross section and elastic momentum transfer cross section is determined by deducting all reactive cross sections.

Average polarizability of CF_4 is not well established [2] and may produce discrepancy for calculated mobility of ions in CF_4 [3] and thus affect plasma parameters prediction in modelling. We adopted value of 3.86 A^3 used by Stojanović *et al* [3] who found excellent agreement between experimental and calculated mobility of CF_3^+ ions in CF_4. Note that usage of this polarizability increases Langevin's cross section above reaction cross sections of Fisher *et al.* (1990) at least in the region of the validity of polarization potential approximation.

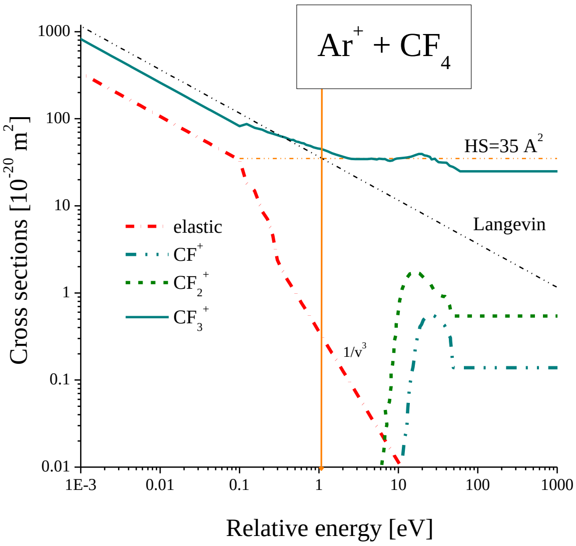

Figure 1. Cross section set for $Ar^+ + CF_4$.

Further, extrapolation of elastic momentum transfer cross section trend approximately beyond the crossing point of Langevin's and hard sphere (HS) cross section [2] is done by smoothly connecting to $1/v^3$ trend [4] where v is the center-of-mass velocity (see Fig. 1).

Reactive cross sections for ions are extrapolated by constant values for kinetic energies above 50 eV following measurements of emission cross section by Motohashi *et al.* [1] where slow oscillatory behaviour of the emission cross sections was found at high projectile energies and almost constant reaction probability was found over a wide energy range.

3. Transport parameters

In this paper Monte Carlo technique was applied to perform calculations of transport parameters. We have used a code that properly takes into account thermal collisions [5]. The code has passed all the relevant benchmarks [6] and has been tested in our work on several types of charged particles [6,7].

Results of Monte Carlo simulations are shown in Figs. 2-5. 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 Ar^+ in CF_4.

The reactive collisions which are spread over the entire energy range affect the drift velocity (as well as other transport coefficients) at all *E/N* values (Fig. 2). Since the total collision frequency for endothermic reactions increases with energy at high *E/N*, the dominant loss of the fast ions happens at the front of the swarm. This shifts the swarm's centre of mass towards the lower values. Thus, the bulk values (real space drift velocity d<x>/dt) are lower than the flux values (velocity space drift velocity <v>).

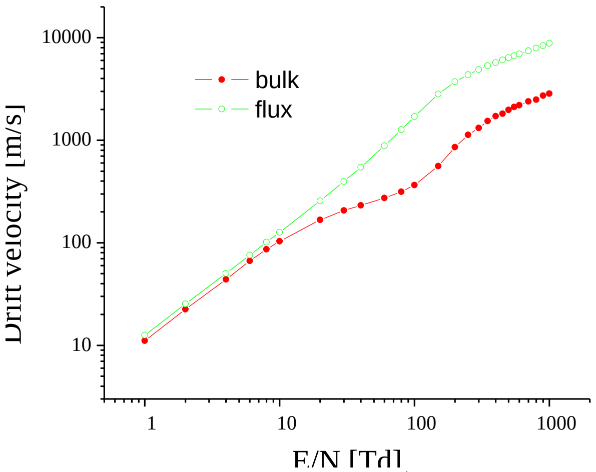

Figure 2. Drift velocities of Ar^+ ions in CF_4 as a function of *E/N*.

Reduced mobility for Ar^+ ions as a function of *E/N*(*E*-electric field, *N*-gas density) compared with Langevin's value K_{pol} is shown in Fig. 3. Values of the reduced mobility as a function of *E/N* shown are obtained by using bulk drift velocities, as those are measured in most experiments, though proper quantities should be applied according to the source of experimental data [8,9]. A significant increase of mobility at low E/N is the result of non-conservative charge exchange at low energy. At about 300 Td another mobility peak appears, representing a significant increase of reactive collisions.

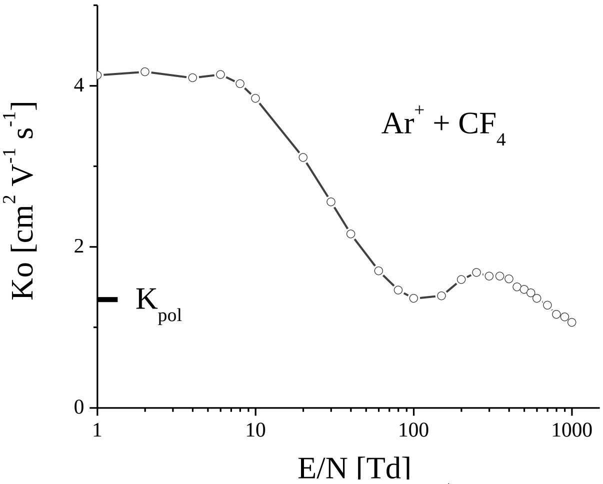

Figure 3. Reduced mobility for Ar^+ in CF_4 at 300 K.

Characteristic energies (longitudinal L and transverse T) and the mean energy, as a function of *E/N*, are shown in Fig. 4. To calculate the longitudinal component properly here and also in the case of diffusion coefficients, one would need a better and more complete information on the anisotropy of scattering.

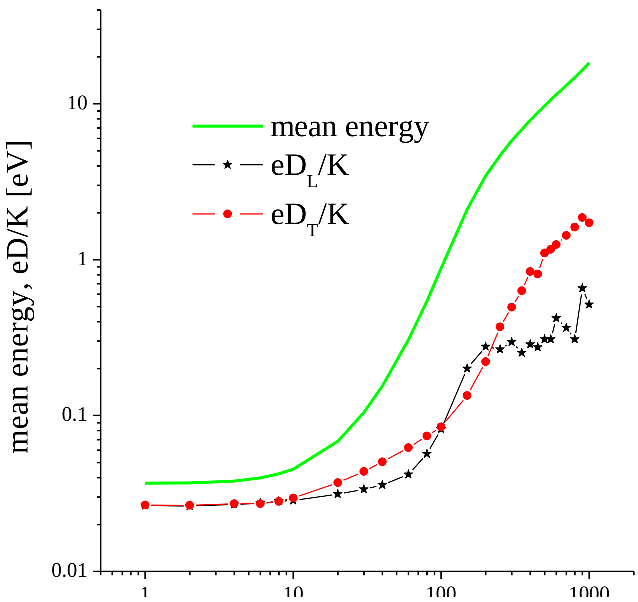

Figure 4. Mean and characteristic energy for Ar^+ in CF_4 at 300 K.

Diffusion coefficients are given in Fig. 5 and one should also notice very large non-conservative effects almost as large as in positron transport [10,11]. Similarly to the results for drift velocity flux diffusion coefficients are significantly larger than the bulk values.

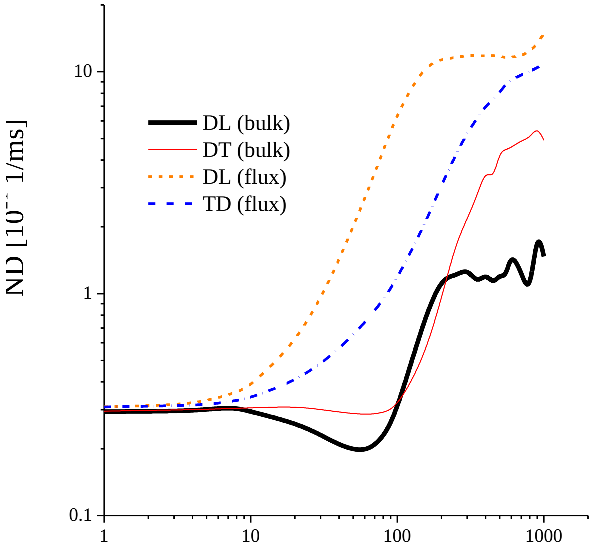

Figure 5. Diffusion coefficients as a function of E/N for Ar^+ in CF_4 at 300 K.

4. Conclusion

In addition to presenting the data we show here effects of non-conservative collisions on ion transport. Due to non-conservative cross sections that are larger than the elastic scattering cross section differences between flux and bulk transport coefficients are quite large - comparable to the strongest cases observed for electrons, even positrons.

Data for swarm parameters for ions are needed for hybrid and fluid codes and the current focus on discharges in liquids or possibly liquids in mixtures with rare gases dictates the need to produce similar data for ions stemming from the liquid vapour .

4. Acknowledgment

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5. References

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