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TRANSPORT COEFFICIENTS FOR ELECTRON SCATTERING IN MIXTURES OF CF_4, Ar AND O_2

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Abstract. We present transport coefficients for electrons in mixtures of CF_4 with Ar and O_2 for ratios of the electric field to the gas number density *E/N* from 1 Td to 1000 Td ($1Td=10^{-21}$ Vm^2). We then add a certain percentage of radicals produced by dissociation of CF_4. Our analysis of non-conservative collisions revealed a range of *E/N* where electron attachment introduced by radicals significantly changes electron kinetics obtained for mixtures without dissociation of CF_4 gas. Results are obtained by using a simple, two term solutions for Boltzmann's equation and by a Monte Carlo simulations.

1. INTRODUCTION

Carbon tetrafluoride is commonly used for plasma etching in today's semiconductor industry. It is primarily applied for etching of SiO_2. It is also important for formation of fluorinated polymer films.

CF_4 has a role in other technological applications such as development of gaseous circuit breakers Hunter et al. (1985) and for development of particle detectors (James et al. 1980, Kopp et al. 1982, Yamashita et al. 1992) CF_4 belongs to freons that have a global warming potential of over 50 000. Because of all these arguments it is important to continue research related to the kinetics of CF_4 in ionized gases in order to improve plasma etching applications and facilitate removal of this gas from the atmosphere by applying gas discharges (e.g. by focused microwave radiation Bzenić et al. (1995)). Pure CF_4 plasmas are rarely used in material processing and instead are diluted with Ar and O_2 to control electron energy, production of fluorocarbons and provide selectivity in etching.

Oxygen plasmas are widely used in material processing such as photo resist aching, surface modification, chemical vapor deposition and oxidation. In oxygen plasma, the density of atomic oxygen and its distribution are significant since the processing speed and the process uniformity in a wafer depend on the flux distribution of atomic oxygen onto a wafer. Kitajima et al.(2006) showed that the density of metastable atomic oxygen O (^{1}D) increases in highly Ar diluted oxygen CCP- capacitively coupled plasma.

2. MONTE CARLO CODE AND TWO TERM APPROXIMATION

Requirement to establish reliable transport coefficients for CF_4 plasmas is especially demanding for conditions that include many reactive species. Free radical species, such as CF_y (y=1-3) and fluorine atoms, need to be included to represent properly the realistic conditions in plasma processing. We calculated electron transport coefficients for a ternary mixture of 80 % Ar with 10% of O_2 and CF_4. This is mixture is usual in plasma etching applications. In order to determine the role of radicals, we added up 1 % of radical X species (X= F, F_2, CF, CF_2 and CF_3) replacing the equivalent amount of CF_4. Calculations were made for conditions overlapping with those found in plasma technologies for semiconductor device manufacturing.

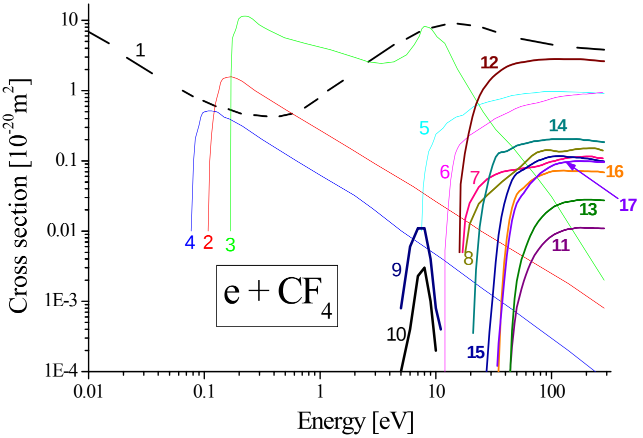

Figure 1: Electron impact cross sections for scattering on CF_4 (1-el. mom. transfer,2-vib.exc. v=1, 3-vib.exc. v=3, 4-excitation v=4, 5-electronic excitation, 6-dissociation to products CF_3, 7-dissociation to products CF_2, 8-dissociation to products CF, 9-dissociative attachment (F^-), 10- disssociative attachment (CF_3^-), 11-CF_2^{2+} + 2F + 2e (ionization), 12-CF_3^+ + F + 2e, 13-CF_3^{2+} + F + 3e, 14-CF_2^+ + 2F + 2e, 15-CF^++ 3F + 2e, 16-C^+ + 4F + 2e, 17-F^+ + CF_3 + 2e.

Electron kinetics in CF_4 is well described by the set of cross sections of Kurihara et al. (2000) extended by Georgieva et al. (2003) and also by Donko (2006). Complete cross section set is shown in Fig. 1. Set of cross sections for O_2 is from Phelps (2009) and for Ar modified cross section set of Hayashi (1992) as used in Raspopović et al. (2005).

Transport coefficients are obtained by using a Two Term approximation (TTA) to the electron Boltzmann equation Morgan and Penetrante (1990) and by a Monte Carlo simulations Petrović and Stojanović (1998).

3. RESULTS AND DISCUSSION

A ternary mixture $Ar/CF_4/O_2$ mixture consisting of 80 % Ar and 10 % CF_4 and 10% O_2 is the object of our calculations. Electron drift velocity in mixtures $Ar/CF_4/O_2$ as a function of *E/N* (E-electric field, N-gas density) are shown in Fig. 2. a)

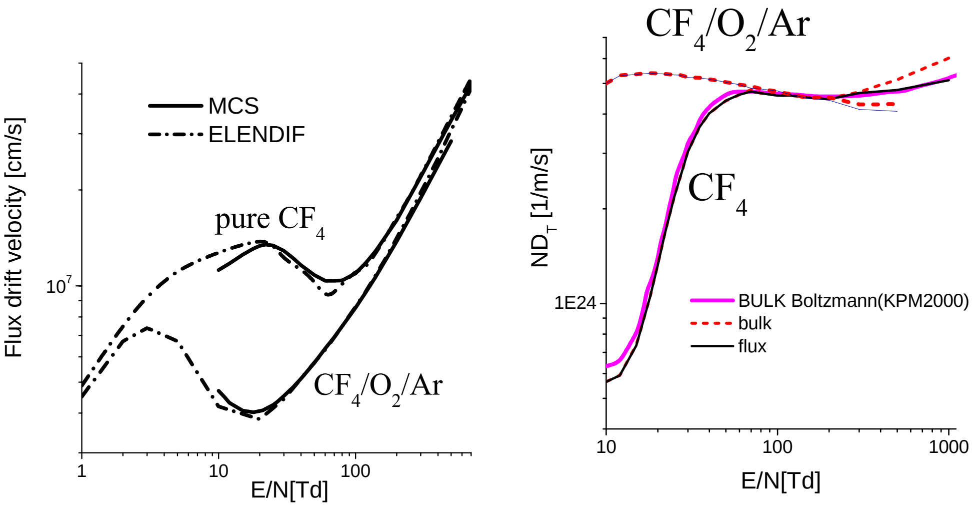

Figure 2: a) Drift velocity and **b)** longitudinal diffusion coefficients as a function of *E/N* for $Ar/CF_4/O_2$ mixture.We also show results for the pure CF_4.

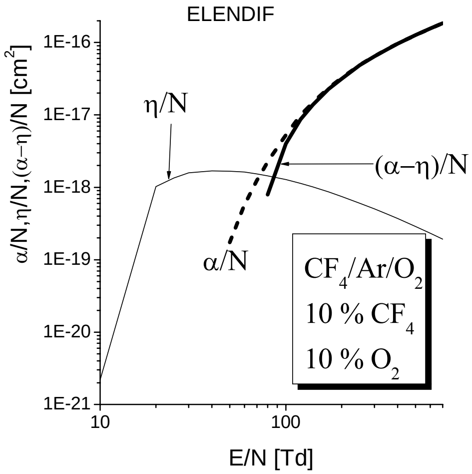

Figure 3: Ionization coefficients for mixture of 80% Ar with 10% CF_4 and 10% O_2.

In Fig. 2.b) we show longitudinal diffusion coefficients in the $Ar/CF_4/O_2$ mixture obtained both by Monte Carlo and two term approximation. In Fig. 3. we show ionization coefficients with 80 % of Ar, 10 % CF_4 and 10% O_2 obtained by TTA.

We have also made calculations of transport coefficients where up to 1% of CF_4 was replaced by the corresponding amount of radicals that are commonly found in plasma processing equipment. Dissociative attachment cross sections in CF_4 and O_2 have high thresholds and three body attachments in oxygen are not effective at typical plasma etching pressures. Thus even a small amount of radicals with low attachment thresholds will change the rates for attachment considerably and will change the nature of the plasma to electronegative. In plasma modeling it is thus necessary to include radicals even when their effect on the mean energy and most transport properties is negligible.

Acknowledgements

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