Electron Collision Cross Sections for the CF_4 Molecule by Electron Swarm Study

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1 Introduction

Tetrafluoromethane(CF_4) is widely used as working gas for gas discharge opening switches and in etching plasmas for material processing [l]. Thus it is important to know an accurate electron collision cross section set for the CF_4 molecule in order to quantitatively understand the plasma phenomena occurring in the above mentioned area. But the cross section data for CF_4 in the low energy region is not sufficiently reliable at present. Magnitudes and energy dependence of vibrational excitation cross sections and the momentum transfer cross section, in particular, are considerably different according to various researchers [1,2]. We therefore have tried to determine low energy electron collision cross sections for the CF_4 molecule mainly from our own experimental results for the electron transport coefficients.

2 Experimental Description

We used a double shutter drift tube with variable drift distance (1-10 cm) and measured the arrival time spectra of electrons at each E/N value. From those spectra, the electron drift velocity, W, and the product of the gas number density and the longitudinal diffusion coefficient, ND_L, were obtained [3]. The electron transport coefficients were measured in pure CF_4 and two CF_4-Ar mixtures. All the measurements were carried out at room temperature, and at each E/N, the measurements were repeated at three different pressures, at least. The advantages of using both dilute molecular-rare gas mixtures and a pure molecular gas to determine the set of cross sections for the molecular gas are mentioned in Ref. [4].

The mixing ratios of the gases and the range of the measurements are shown in Table 1.

Table 1: Mixing Ratios and the Range of the Measurements

	E/N (Td)	Gas Pressure (Torr)
pure CF_4 (99.99%)	0.04-300	0.03-700
5.08% CF_4-Ar	0.14-100	1.45-300
0.495 CF_4-Ar	0.04-100	1.5-700

3 Results of the Measurements

Fig. 2 shows the electron drift velocity, W (solid squares), and ND_L (solid circles) measured in pure CF_4. In this figure, the measured drift velocity (crosses) by Hunter [5] is also shown for comparison. Figs. 3 and 4 show W and ND_L with the same symbols as in Fig. 2 measured in the 5.08 % and 0.495% CF_4-Ar mixtures, respectively.

4 Boltzmann Equation Analysis

A multi-term code of the Boltzmann equation analysis [6] and a Monte Carlo simulation (MCS) were used, and an initial set of the cross sections for the CF_4 molecule was modified by trial and error until consistency between the electron transport coefficients and the experimental results was obtained while applying the following steps:

Step 1 Modify inelastic cross sections (mainly vibrational excitation cross sections) until the calculated W and ND_L in the two mixtures agree with the experimental results in the CF_4-Ar-mixtures.

Step 2 Modify elastic momentum transfer cross sections so that the calculated W and ND_L for the pure CF_4 molecule agree with the experimental results in pure CF_4.

Step 3 Modify inelastic cross sections except vibrational excitation cross sections until the calculated attachment and ionization coefficients agree with the experimental results for pure CF_4.

The cross section set for the Ar atom determined by Nakamura and Kurachi [7] was used throughout the study. The W and ND_L calculated using the latest cross sections (Fig. 1) are shown in Figs. 2-4 by solid lines. The calculated attachment and ionization coefficients are shown by solid lines in Fig. 5, with the experimental results from [8-13].

As is seen in Figs. 2-5, the agreement between measurements and calculations is fairly good.

5 A Set of Cross Sections for the CF_4 Molecule

The latest cross section set for the CF_4 molecule is summarized in Fig. 1. This cross section set includes momentum transfer (Q_m), vibrational excitation (Q_v), electron attachment (Q_a), neutral dissociation (Q_{dn}), and ionization (Q_i). Also shown in this figure is the total scattering cross section by L. G. Christophorou, J. K. Olthoff, and M. V. V. S. Rao [7].

In this cross section set, four vibrational excitation cross sections, v4 (degenerate deformation, 78meV), v1 (symmetric stretch, 112meV), v3 (asymmetric stretch, 157meV), and 2v3 (the second harmonics of v3) were considered in accordance with the energy loss spectra measured by an electron beam experiment [14] at a resonance peak centered at 8eV, and the relative magnitude was also maintained in the present vibrational cross sections.

The Ramsauer-Townsend minimum of the momentum transfer cross section is similar to that of L. G. Christophorou, J. K. Olthoff, and M. V. V. S. Rao [15]. The present attachment cross section is about 20% smaller than given by them, but the neutral dissociation cross section is much larger.

6 Conclusion

The drift velocity, W, and the product of the gas number density and the longitudinal diffusion coefficient, ND_L, were measured in pure CF_4 and CF_4-Ar mixtures over a wide E/N range.

A cross section set for the CF_4 molecule being consistent with the measured electron transport coefficients (drift velocity, longitudinal diffusion coefficient, attachment coefficients, ionization coefficients) was obtained.

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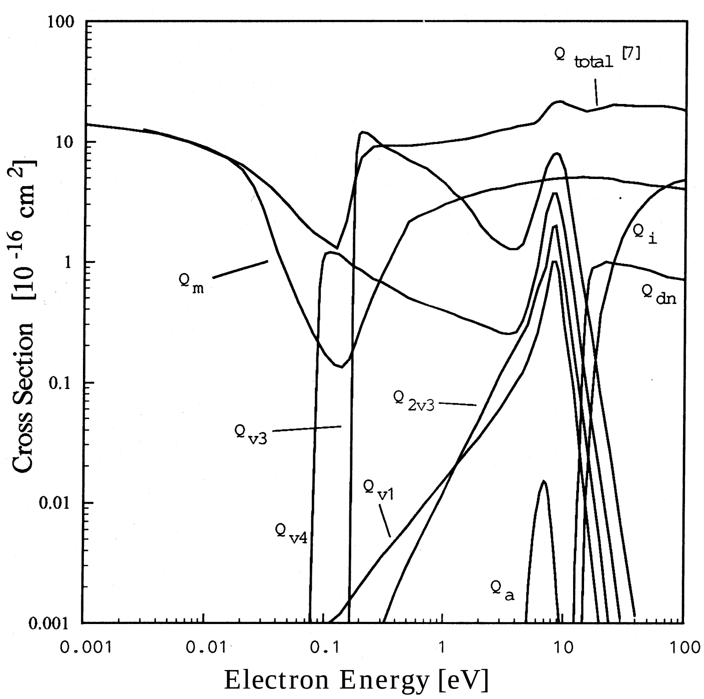

Figure 1: A set of electron collision cross sections for the CF_4 molecule.

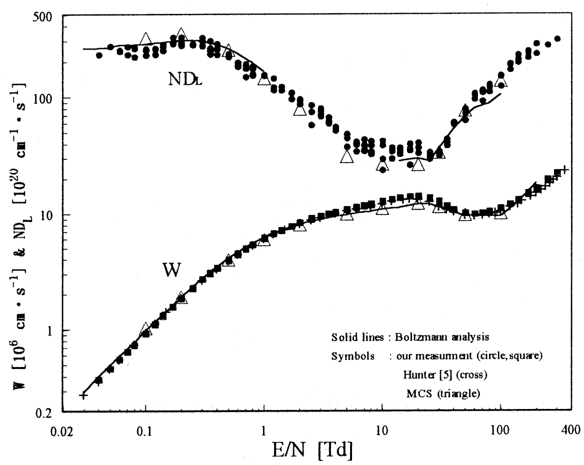

Figure 2: W and ND_L in pure CF_4.

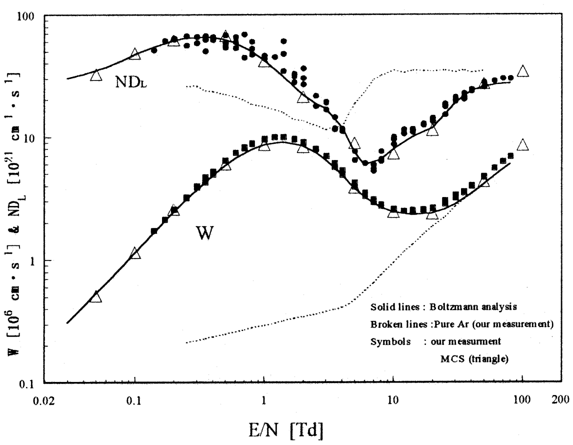

Figure 3: W and ND_L in the 5.08% CF_4-Ar mixture.

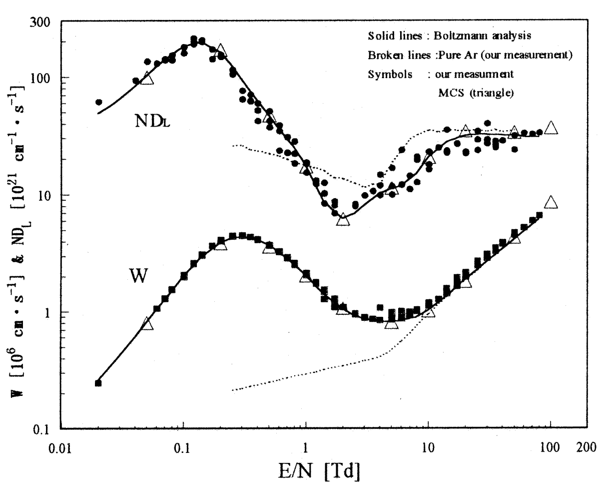

Figure 4: W and ND_L in the 0.495% CF4-Ar mixture.

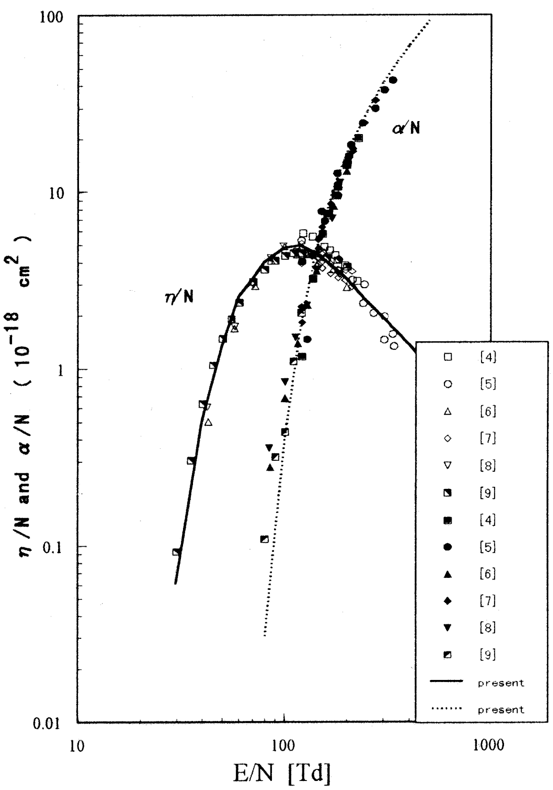

Figure 5: Attachment and ionization coefficients in pure CF_4.