Inelastic Cross Sections for the C₃F₈ Molecule from Electron Transport Coefficients in C₃F₈-Ar Mixtures

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1 Introduction

Perfluoropropane(C_3F_8) is frequently used as an effective etchant in semiconductor etching processes, and it is also used as a gaseous medium in gas discharge switches and radiation detectors [1].

Pirgov and Stefanov [2] derived a momentum transfer cross section and a total vibrationally inelastic cross section for the molecule from electron swarm data measured by Hunter *et al.* [3] by using a two-term approximation of the Boltzmann analysis, which may not be valid for molecules with large vibrationally inelastic cross sections. There are also new measurements of the total ionization cross sections including various positive ions of the molecules by Chantry and Chen [4].

In the present study, we measured the drift velocity and the longitudinal diffusion coefficient of electrons in C_3F_8 -Ar mixtures and derived a new set of electron collision cross sections for the C_3F_8 molecule for applications in quantitative modeling of related plasmas.

2 **Experiments**

The apparatus and the data processing procedure used in the present measurement of the drift velocity and the longitudinal diffusion coefficient were the same as those used in the works of Nakamura [5] and Kurachi and Nakamura [6]. The special feature of the apparatus is that the drift distance is variable (1-10 cm). This allows the application of the so-called differential method which is very effective in reducing the effects of the electron energy relaxation, of the finite width of the starting electron swarm, and of the non-uniform electric field around the electron shutters.

Measurements were repeated at least at three different gas densities at each E/N value. All measurements were carried out at room temperature, $300 \pm 2K$.

The mixtures were composed of pure $C_{3}F_{8}$ gas (purity 99.99%) and argon (99.9999%), and the actual mix ratio was determined by using a gas chromatography test.

3 Experimental Results

Electron transport coefficients, the drift velocity, W, and the product of the gas number density and the longitudinal diffusion coefficient, ND_L , of electrons, were measured in 0.526% and 5.05% C_3F_8 -Ar mixtures over the E/N range 0.03 to 100 Td and over the gas pressure range from 0.133 to 122 kPa (1 to 900 torr, 1 torr = 133.322 Pa). Typical scatter of the measured values at different pressures at each E/N was less than 2% for the drift velocity and less than 10% for the ND_L . Fig. 1 shows the electron transport coefficients (W and ND₁) measured in the 0.526% C_3F_8 -Ar mixture (solid squares), and Fig. 2 shows those in the 5.05% C_3F_8 -Ar mixture with the same symbols as in Fig. 1. Both figures also show the respective transport coefficients in pure argon [7], by solid triangles, for comparison.

The drift velocity measured in each mixture was enhanced by more than an order of magnitude from that in pure argon by adding only a small fraction of the C_3F_8 molecule and showed clearly the so-called negative differential conductivity (NDC) over the E/N range from 0.4 to 10 Td in the 0.526% mixture and from 2 to 35 Td in the 5.05% mixture. The ND_L in each mixture showed a similar but pronounced structure over the measured E/N range.

For higher E/N values each transport coefficient approached that of pure argon. This can be explained by the shift of the dominant inelastic collision processes in the swarm from those with C_3F_8 molecules to electronic excitations of the majority of argon atoms.

4 Boltzmann equation analysis

The electron transport coefficients (W and ND_L) were calculated using a multi-term approximation of the Boltzmann equation analysis [8].

The cross section set for Ar atoms determined by Nakamura and Kurachi [7] was used throughout the present study. The initial cross section set for the C_3F_8 molecule consisted of those for elastic momentum transfer (Q_m) cross sections by Pirgov and Stefanov [2], total attachment including various negative ions (Q_{att}) by Hunter and Christophorou [9], total ionization including various positive ions (Q_i) by Chantry and Chen [4], and vibrational excitations (Q_v) by Pirgov and Stefanov [2]. A trial calculation showed the need for inclusion of additional vibrational cross sections, and we also tentatively included the set of vibrational cross sections for C_2F_6 proposed by Hayashi and Niwa [10] because of insufficient information on the vibrational threshold energies of the C_3F_8 molecule.

According to a comparison of the present transport coefficients in the C_3F_8 -Ar mixtures with those in C_2F_6 -Ar mixtures [11], the E/N dependence of the measured transport coefficients for the two mixtures are similar, and we may assume the threshold and the energy dependence of vibrational cross sections of the C_3F_8 molecule to be similar to those of the C_2F_6 molecule, possibly with lower resonance energy.

Electron transport coefficients, W and ND_L , calculated using this initial cross section set, are shown by solid and dashed lines in Figs. 1 and 2.

In Fig. 1, the maximum differences in W and ND_L between the measurements and calculations, shown by solid lines, are 57% and 83%, and those by dashed lines are 21% and 48%, respectively, over the E/N range from 0.03 to 0.2 Td. In Figs. 2 and 3, those differences are 47.6% and 86%, and 16.7% and 56%, respectively, over the E/N range from 0.03 to 1.2 Td. The corresponding mean electron energies for these E/N ranges were 0.09-0.3 eV, and the magnitudes of the vibrational excitation cross sections in this electron energy range were amended so that the calculated results agreed with the experimental results.

The magnitude of the vibrational excitation cross section of about 0.09 eV threshold energy was multiplied by a factor of 5 in the energy range 0.09-0.2 eV. That of about 0.13 eV threshold energy was multiplied by a factor of 3.4 in the energy range 0.13-0.3 eV, and the threshold energy of this cross section was changed by 0.113 eV after numerous trials.

The new set of electron collision cross sections for the C₃F₈ molecule is shown in Fig. 3.

5 Conclusion

We measured electron transport coefficients for 0.526% and 5.05% C_3F_8 -Ar mixtures over the E/N range from 0.03 to 100 Td. The measured transport coefficients were compared with those measured in the $C_nF_{2n+2(n=1,2)}$ -Ar mixtures with similar mixing ratios.

The E/N dependence of the measured transport coefficients clearly indicates possible directions for changes of the vibrational excitation cross sections. We have determined the inelastic cross sections for the C_3F_8 molecule. We started the measurement of transport coefficients in pure C_3F_8 and are going to determine the elastic momentum cross section for the C_3F_8 molecule, after completion of the measurements, by using the present vibrational cross sections.

References

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Figure 1: The electron drift velocity, **W**, and the product of the longitudinal diffusion coefficient and the gas number density, ND_L , as a function of E/N in a 0.526% C_3F_8 -Ar mixture. The broken curves show the analysis using the initial cross section for C_3F_8 molecule. • - Experimental results; Δ - Calculated values using the present cross section set; • - Ar. (Nakamura and Kurachi 1988)



Figure 2: The electron drift velocity, **W**, and the product of the longitudinal diffusion coefficient and the gas number density, ND_L, as a function of E/N in a 5.05% C_3F_8 -Ar mixture. The broken curves show the analysis using the initial cross section for C_3F_8 molecule. \bullet - Experimental results; Δ - Calculated values using the present cross section set; \blacktriangle - Ar. (Nakamura and Kurachi 1988).



Figure 3: The present set of electron collision cross sections for the C_3F_8 molecule. The solid curves show the present cross section set for the C_3F_8 molecule. The dotted curves show initial cross section for the C_3F_8 molecule.