Determination of the Inelastic Cross Sections for C_3F_8 Molecule by Electron Swarm Study

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We measured the electron transport coefficients, the electron drift velocity, W, and the longitudinal diffusion coefficient, D_L, over the E/N range from 0.03 to 100 Td and gas pressure range from 0.133 to 122 kPa in the 0.526% and 5.05% C_3F_8-Ar mixtures by the double shutter drift tube with variable drift distance. And we calculated these electron transport coefficients by using multi-term approximation of Boltzmann equation analysis. We determined the electron collision cross sections set for C_3F_8 molecule by the comparison of measurement and calculation. Our special attention in the present study was focused upon the inelastic collision cross sections of the C_3F_8 molecule.

Keywords : C_3F_8 molecule, multi-term approximation of Boltzmann equation, electron drift velocity, longitudinal diffusion coefficient, electron collision cross section

1. INTRODUCTION

Perfluoropropane(C_3F_8) and other perfluoroalkanes, C_nF_{2n+2}(n=1,2,3,4), satisfy the requirements of a gaseous medium for use in a diffuse discharge switches for pulsed-power inductive energy storage application C_3F_8 also show a similar etching property for SiO_2 as C_2F_6.[1]

Because of physical and industrial importance of Perfluoropropane(C_3F_8), there have been a small number of investigations on electron transport coefficients in C_3F_8 gas[2, 3] and on electron collision cross sections of the C_3F_8 molecule[4]. Recently Christophrou and Olthoff [5] compiled a set from available cross sections data, but their compilation was rather scanty for use in any quantitative computer modeling of related plasma phenomena.

In our previous paper[6] (hereafter referred to as paper I), first, we measured electron drift velocity and the longitudinal diffusion coefficient in the 0.526% and 5.05% C_3F_8-Ar mixtures and, secondly, the derived vibrational excitation cross sections for the C_3F_8 molecule from the electron transport coefficients measured in the two mixtures by using the multi-term Boltzmann.

But calculated results by using cross sections set derived in the paper I is especially much different from measurements of D_L in 0.526% and 5.05% C_3F_8-Ar mixture over the E/N range from 0.2 Td and up and 0.4 Td and up, respectively.

In the present study, therefore, for determination of the more exact set of the inelastic collision cross sections for the C_3F_8 molecule, we re-amended determined set in the paper I by using the trial and error amendment procedure.

2. ANALYSIS

We took our general scheme outlined in the paper I : we determined the vibrational excitation cross sections from the drift velocities and the longitudinal diffusion coefficients measured in the C_3F_8-Ar mixtures by electron swarm study.

First, we were compared calculations using multi-term approximation of Boltzmann equation analysis[7, 8]

code developed by Robson and Ness in James-Cook university[9] with measurements reported in paper I .

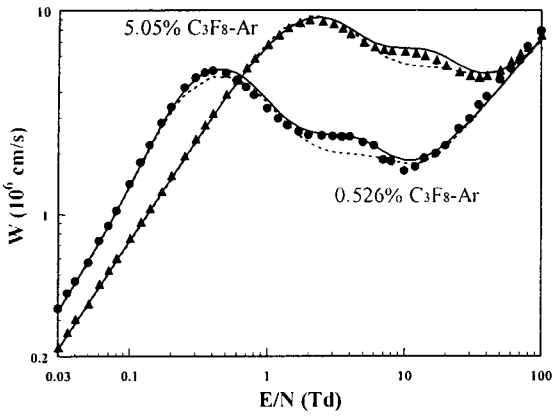

Fig. 1. The electron drift velocity, W, as a function of E/N in 0.526% and 5.05% C_3F_8-Ar mixtures. The broken and the solid curves show calculated values using an initial and the present cross sections set, respectively, for C_3F_8 molecule. ● and ▲ are measured results in the 0.526% and 5.05% C_3F_8-Ar mixtures, respectively.

The cross sections set for argon atom was also used that determined by Nakamura and Kurachi[10], and we did that the cross sections set derived in the paper I was chosen as the starting cross sections set for the C_3F_8 molecule (hereafter referred to as initial cross sections set): the cross sections set derived in paper I was based on the elastic momentum transfer (Q_m) by Pirgov and Stefanov[4], the total attachment (Q_{att}) by Hunter and Christophorou[11], the total ionization (Q_i) by Chantry and Chen[12], the total vibrational excitation (Q_v) by Pirgov and Stefanov[4] and vibrational cross sections for the C_2F_6 molecule proposed by Hayashi and Niwa[13].

Secondary, the trial-and-error amendment procedure [14, 15] for further agreement of the electron transport coefficients in the C_3F_8-Ar mixtures between the measurement and the calculation was started.

3. RESULTS AND DISCUSSIONS

3.1 Electron Transport Coefficients

The calculated results of electron drift velocity, W, the product of the gas number density and the longitudinal diffusion coefficient, ND_L, and the ratio of the longitudinal diffusion coefficient to the electron mobility, D_L/μ, as a function of E/N in the 0.526% and 5.05% C_3F_8-Ar mixtures using the set of initial cross sections for C_3F_8 molecule are shown in figures 1 to 3, respectively.

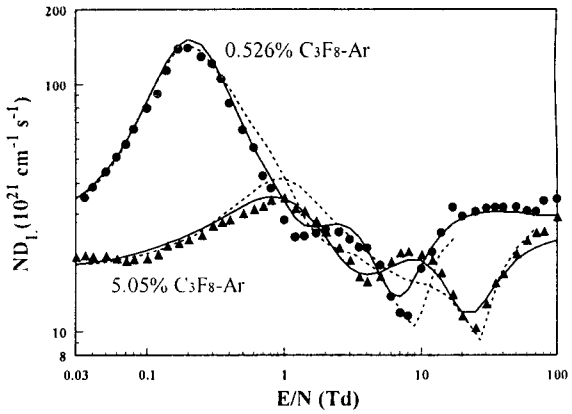

Fig. 2. The product of the longitudinal diffusion coefficient and the gas number density, ND_L, as a function of E/N in 0.526% and 5.05% C_3F_8-Ar mixtures. The each curves and symbols same as shown in Fig. 1.

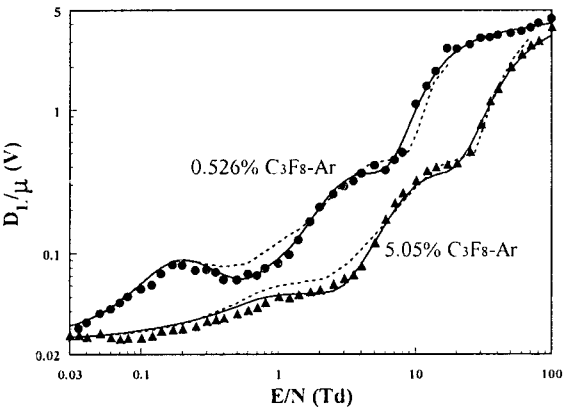

Fig. 3. The ratio of the longitudinal diffusion coefficient to the electron mobility, D_L/μ, as a function of E/N in 0.526% and 5.05% C_3F_8-Ar mixtures The each curves and symbols same as shown in Fig. 1.

The broken and solid curves show calculated values using an initial and the present cross sections set for C_3F_8 molecule, respectively. And the solid symbols show mean values of each electron transport coefficients measured at several gas densities as shown in paper I .

3.2 Present Set of Electron Collision Cross Sections

The initial set of electron collision cross sections for the C_3F_8 molecule was actually necessary for better agreement between measurements and calculations over the E/N between the two peaks in ND_L in the two mixtures as shown in figure 2.

The cross sections set for the C_3F_8 molecule is determined, which is fairly consistent with experimental transport coefficients, but the initial set still has two difficulties. : First, its utilized threshold energies of vibrational excitation cross sections ($Q_{v=1,2,3}$) are

necessary to amend in order to meet the reported twenty-two fundamental frequencies of vibration of C_3F_8 (316, 339, 350, 382, 462, 537, 546, 624, 664, 731, 766, 778, 809, 1006, 1032, 1155, 1210, 1250, 1264, 1313, 1350 and 1369 cm^{-1}) which have confirmed by the Raman and Infrared absorption spectrum of C_3F_8[16]. And, secondly, there are still considerable disagreements between measurements and calculations of electron transport coefficients over the E/N range from 0.3 to 30 Td in the two mixtures. It is, therefore, necessary to determine the more exact set of cross sections for C_3F_8 molecule by the re-amendment of the vibrational excitation cross sections or an addition of other inelastic cross sections to the initial set.

For these reasons, the threshold energies were lowered for the Q_{v3} from 0.27 eV to 0.17 eV (1369 cm^{-1}), for the Q_{v2} from 0.113 eV to 0.1 eV (809 cm^{-1}), and for the Q_{v1} from 0.089 eV to 0.082 eV (664 cm^{-1}), respectively, in order to meet the reported vibrational thresholds, and the magnitude of the Q_{v3} is also amended in part. The ravine or dip of the Q_{v3} over the electron energy range 0.7-2 eV are especially responsible for the E/N range 0.3-1 Td and 0.6-4 Td of the ND_L in 0.526% and 5.05% C_3F_8-Ar mixtures, respectively. After these amendment, the maximum difference between the calculations and the measurements reduced from 45% to 20% at near of 1 Td of the ND_L, and from 40% to 8% at near of 1 Td of the D_L/μ, but, on the contrary, the difference in the drift velocity increased from 6% to 10% at near of 1 Td.

And two new inelastic cross sections labeled as Q_{ex1} and Q_{ex2} are responsible for the second peak of the ND_L and the smaller hump in the drift velocity after numerous trials.

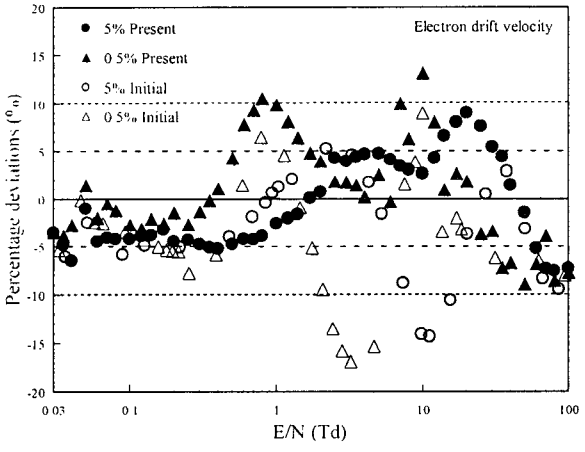

Fig. 4. The percentage deviations of electron drift velocity, W, from the experimental values. The solid symbols are those calculated with the present set and the open symbols are those with an initial set in the 0.526% and 5.05% C_3F_8-Ar mixtures, respectively.

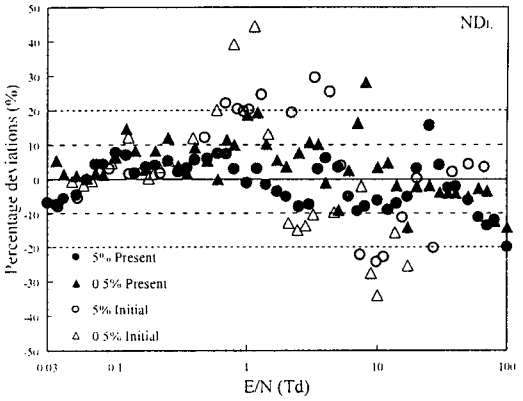

Fig. 5. The percentage deviations of the product of the longitudinal diffusion coefficient and the gas number density, ND_L, from the experimental values The symbols same as shown in figure 1.

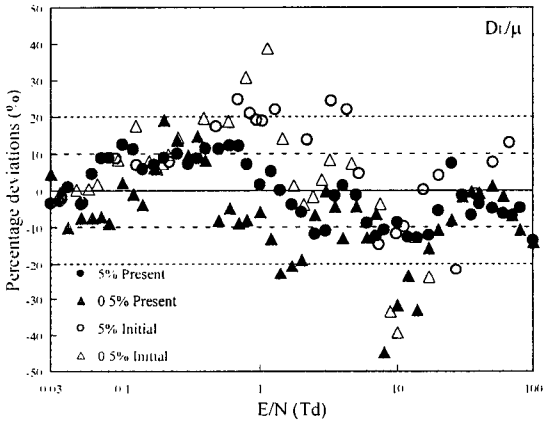

Fig. 6. The percentage deviations of the ratio of the longitudinal diffusion coefficient to the electron mobility, D_L/μ, from the experimental values The symbols same as shown in figure 1.

The maximum difference between the calculations and the measurements by addition of them reduced from 17% to 2% of drift velocity, from 30% to 4% of the ND_L, and from 24% to 2% of the D_L/μ over the E/N range 1.2-20 Td in the 0.526% C_3F_8-Ar mixture, and 3.5-100 Td in the 5.05% C_3F_8-Ar mixture.

No such inelastic cross sections have been reported and the present swarm study cannot identify the origins of such inelastic processes. Only plausible explanation for them is vibrational excitations of higher vibrational modes because the Q_{ex1}, in particular and the dissociation attachment cross section overlap each other in energy.

The each percentage deviations of W, ND_L and D_L/μ in 0.526% and 5.05% C_3F_8-Ar mixtures using the present cross sections set are shown in figures 4 to 6, respectively.

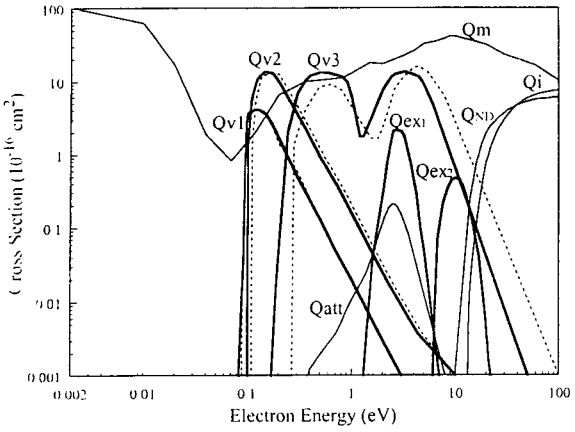

Fig. 7. The present set of electron collision cross sections for C_3F_8 molecule (by the solid and the thick solid curves). The broken and the solid curves show initial cross sections for C_3F_8 molecule.

The present set of electron collision cross sections for C_3F_8 molecule by the solid and the thick solid curves is shown in figure 7 including the cross section of the momentum transfer compiled by Christophorou and Olthoff[5] over the electron energy range 1.5-100 eV and of the neutral dissociation by Harold and Mitio[17], both of which did not have appreciable effect on the electron transport coefficients in the 0.526% and 5.05% C_3F_8-Ar mixtures in the measured range. And this figure also shows initial cross sections set by broken and solid curves.

4. CONCLUSIONS

We have re-amended a new set of electron collision cross sections for C_3F_8 molecule by using electron transport coefficients, such as electron drift velocity and longitudinal diffusion coefficients (ND_L and D_L/μ), in the 0.526% and 5.05% C_3F_8-Ar mixtures by multi-term approximation of the Boltzmann equation analysis.

The electron transport coefficients in these mixtures sensitively reflect the cross section of vibrational excitations and excitations, and are nearly insensitive to the elastic momentum transfer cross section for the molecule.

By utilizing this advantage, the measured transport coefficients were used to determine the inelastic collision cross sections for the C_3F_8 molecule over the energy range where the electron beam experiment may be difficult to carry out.

For a complete set of cross sections of the C_3F_8 molecules, it is further necessary to measure the electron transport coefficients in pure C_3F_8 and to determine the elastic momentum transfer cross section by analyzing them, when the present inelastic cross sections should be utilized.

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