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Calculation and analysis of electron transport coefficients in BF_3-N_2 and TMS-N_2 gas mixtures

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Abstract

The electron transport coefficients in both of pure gases and their mixtures are necessary data for expansion of the choices of proper gases in plasma processing. The electron transport coefficients, which include electron drift velocities, density-normalized longitudinal diffusion coefficients and density-normalized effective ionization coefficients in BF_3-N_2 and TMS-N_2 mixtures, were firstly calculated and analyzed using a two-term approximation of the Boltzmann equation in the E/N (ratio of the electric field E to the neutral number density) range of 0.1-1000 Td (Townsend). These results are very useful to consider for using BF_3-N_2 and TMS-N_2 mixtures with various mixture ratios in plasma processing such as plasma etching, plasma-enhanced chemical vapor deposition and doping plasma.

Keywords: Electron transport coefficients; BF_3-N_2 mixture; TMS-N_2 mixture; gas mixture; plasma processing

1. Introduction

Tetramethylsilane (TMS), $Si(CH_3)_4$, boron trifluoride (BF_3) and N_2 molecules in the form of pure are widely used in plasma processing such as plasma etching, plasma-enhanced chemical vapor deposition and doping plasma [1]-[8]. Moreover, these gases are not only used in the form of pure but also used in the form of mixtures with other gases depending on requirement of specific application. The electron transport coefficients and electron collision cross section set for TMS, BF_3 and N_2 molecules have been determined. However, the electron transport coefficients in BF_3-N_2 and TMS-N_2 mixtures in both experiments and theories are not available. For expansion of the choices of TMS-N_2 and BF_3-N_2 mixtures in plasma processing, these electron transport coefficients are necessary to determine.

For these purposes, the electron transport coefficients, which include electron drift velocities W, density-normalized longitudinal diffusion coefficients ND_L, the first ionization coefficients α/N in BF_3-N_2 and TMS-N_2 mixtures, were firstly calculated and analyzed using a two-term approximation of the Boltzmann equation in the E/N range of 0.1-1000 Td.

2. Analysis

As successfully used in our previous papers [9]-[13], the electron swarm method was also applied in this paper. The electron transport coefficients were calculated using two-term Boltzmann approximation of the Boltzmann equation based on sets of electron collision cross section [14]. Therefore, using the reliable sets of electron collision cross section are necessary for obtaining the accuracy electron transport coefficients. The electron collision cross section set for TMS molecule determined by Hien *et al*. [12], BF_3 molecule determined by Hien *et al*. [11] and N_2 molecule determined by Nakamura [15], were used in this study. The validity of these sets has been proven in [11], [12], [15].

The electron collision cross section set for TMS molecule [12] includes one momentum transfer cross

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section, two vibrational excitation cross sections (threshold energies of 0.15 eV and 0.21 eV), one electronic excitation cross section (threshold energy of 6.5 eV), one dissociative attachment cross section (threshold energy of 3.05 eV) and one ionization cross section (threshold energy of 9.8 eV). The electron collision cross section set for BF_3 molecule [11] includes one momentum transfer cross section, five vibrational excitation cross sections (threshold energies of 0.11, 0.086, 0.18, 0.059 and 1.1 eV), one electronic excitation cross section (threshold energy of 6.5 eV), one dissociative attachment cross sections (threshold energy of 10.1 eV), two dissociation excitation cross sections (threshold energy of 6.48 eV and 11.2 eV) and one ionization cross section (threshold energy of 15.95 eV). The electron collision cross section set for N_2 molecule [15] includes one momentum transfer cross section, seven vibrational excitation cross sections (threshold energies of 0.288 to 2.18 eV), seven electronic excitation cross sections (threshold energies of 6.169 to 12.579 eV) and one total ionization cross section (threshold energy of 15.5 eV).

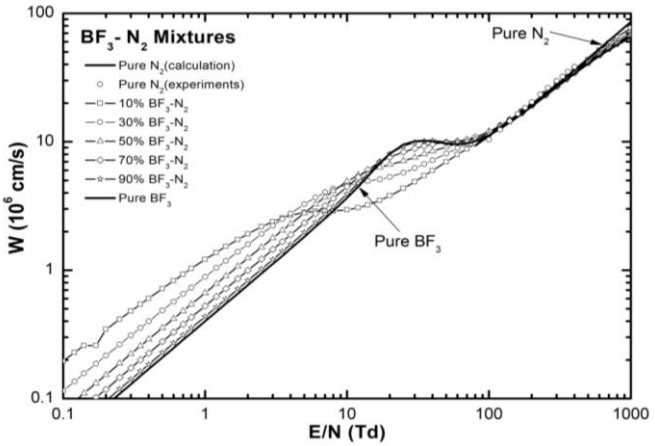

Fig. 1. The electron drift velocity W as a function of E/N in BF_3-N_2 mixtures.

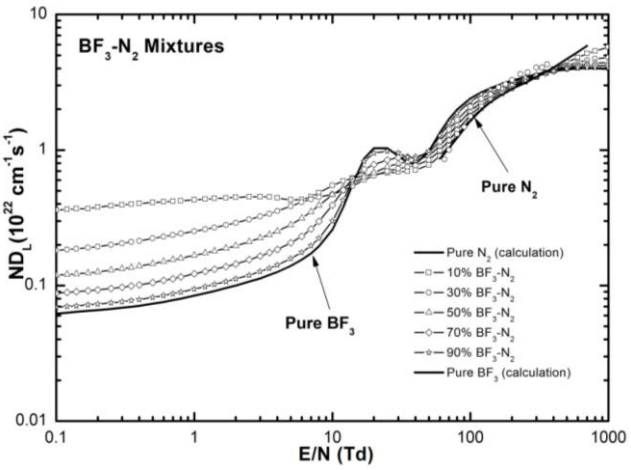

Fig. 2. The density-normalized longitudinal diffusion coefficient ND_L as a function of E/N in BF_3-N_2 mixtures.

3. Results and Discussion

3.1. Electron transport coefficients in BF3-N2 mixtures

The results for the electron transport coefficients, as functions of E/N for the BF_3-N_2 mixtures with 10%, 30%, 50%, 70%, and 90% BF_3, calculated in the wide E/N range by a two-term approximation of

the Boltzmann equation are shown in Fig. 1-Fig. 4. The solid line and symbols show calculated electron drift velocity (W), density-normalized longitudinal diffusion coefficient (ND_L), ratio of the longitudinal diffusion coefficient to the mobility (D_L/μ) and first Townsend ionization coefficient (α/N) for the BF_3-N_2 mixtures. The solid curves show calculated W, ND_L, D_L/μ and α/N for the pure BF_3 and N_2 molecules. There are not significantly differ from the values of the electron transport coefficients in the pure BF_3, pure N_2 and BF_3-N_2 mixtures (E/N > 80 Td for electron drift velocities; E/N > 50 Td for the density-normalized longitudinal diffusion coefficient; E/N > 60 Td for ratio of the longitudinal diffusion coefficient to the mobility). Fig. 4 showed the first ionization coefficient in the BF_3-N_2 mixtures. The values of the first ionization coefficients in the BF_3-N_2 mixtures are found to be between those of the pure gases.

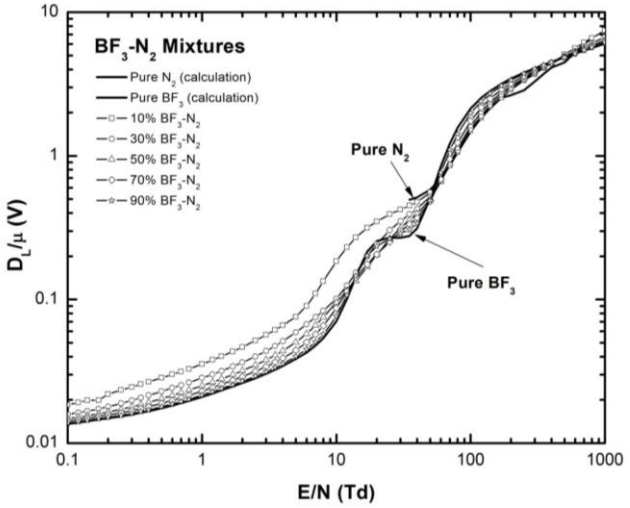

Fig. 3. Ratio of the longitudinal diffusion coefficient to the mobility D_L/μ as a function of E/N in BF_3-N_2 mixtures.

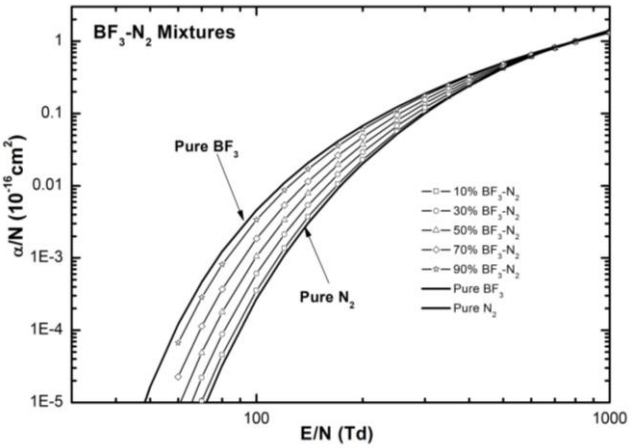

Fig. 4. The first Townsend ionization coefficient α/N as a function of E/N in BF_3-N_2 mixtures.

3.2. Electron transport coefficients in TMS-N2 mixtures

The results for the electron transport coefficients, as functions of E/N for the TMS-N_2 mixtures with 10%, 30%, 50%, 70%, and 90% TMS, calculated in the wide E/N range by a two-term approximation of the Boltzmann equation are shown in Fig. 5-Fig. 8. The solid line and symbols show present W, ND_L, D_L/μ and α/N values calculated using a two-term approximation of the Boltzmann equation for the TMS-

N_2 mixtures. The solid curves show W, ND_L, D_L/μ and α/N values calculated for the pure TMS and N_2 molecules. The open circles show the measured values for pure N_2 molecule [15]. In the TMS-N_2 mixture the values of electron transport coefficients are found to be between those of the pure (E/N > 60 Td for the electron drift velocities and the density-normalized longitudinal diffusion coefficient; E/N > 30 Td for ratio of the longitudinal diffusion coefficient to the mobility).

As shown in Fig. 8, the remarkable synergism in the Townsend first ionization coefficient α/N is displayed in 10%, 30% and 50% TMS-N_2 mixtures. In these cases, the values of α/N in the TMS-N_2 mixture are greater than those in pure TMS and N_2 molecules. Fig. 9 shows the example of the variation of the Townsend ionization coefficient in the TMS-N_2 mixture at 200 Td with the variable mixture ratios of N_2. The changes of the electron energy distribution function in the pure TMS, pure N_2, 10% TMS-N_2 and 90% TMS-N_2 mixtures at E/N = 200 Td are presented in Fig. 10. The calculated electron energy distribution function in the TMS mixtures depends on the mixture ratio of the N_2 molecule. The changes of the electron energy distribution function in the pure TMS, N_2, 10% TMS-N_2 and 90%TMS-N_2 mixtures are presented in Fig. 10. The calculated electron energy distribution in the TMS-N_2 mixtures depends on the mixture ratio of the N_2 molecule. The electron energy distribution in the 90%TMS-N_2 mixture significantly differs from that in the pure TMS, but no significant difference exists in the electron energy distribution between the pure N_2 and TMS-N_2 mixtures containing less than 10%TMS.

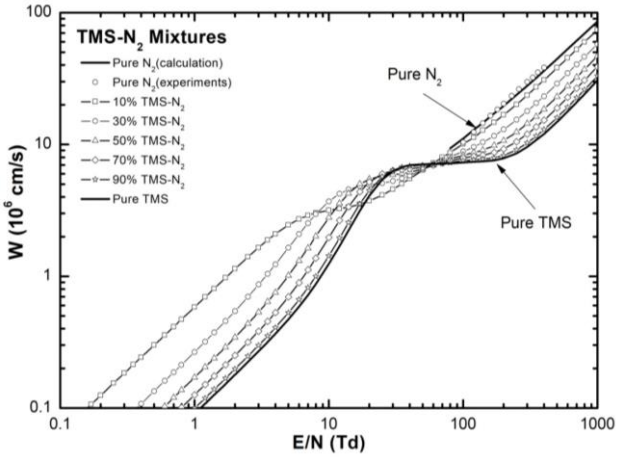

Fig. 5. The electron drift velocity W as a function of E/N in TMS-N_2 mixtures.

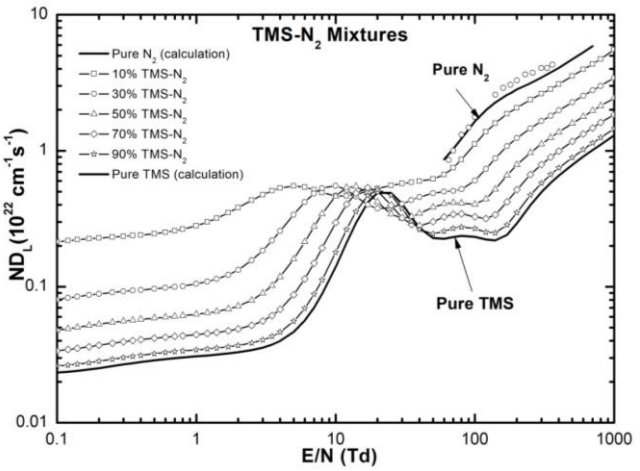

Fig. 6. The density-normalized longitudinal diffusion coefficient ND_L as a function of E/N in TMS-N_2 mixtures.

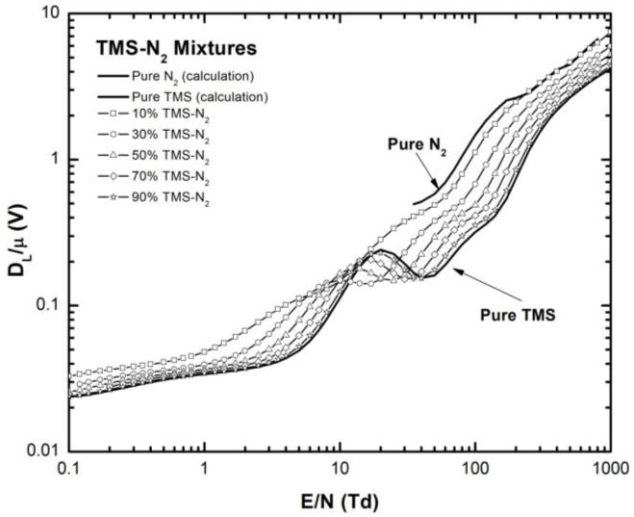

Fig. 7. Ratio of the longitudinal diffusion coefficient to the mobility D_L/μ as a function of E/N in TMS-N_2 mixtures.

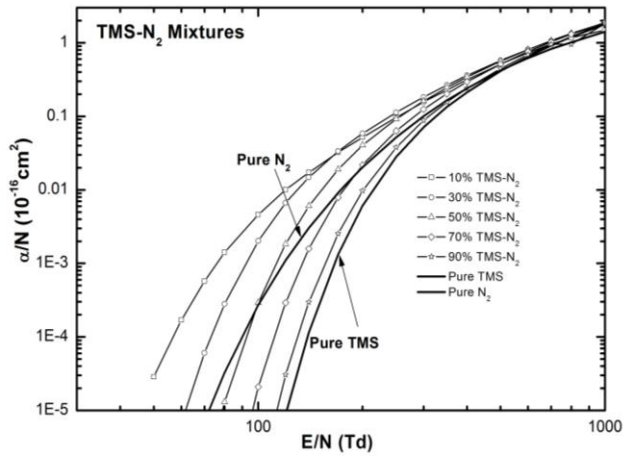

Fig. 8. The first Townsend ionization coefficient α/N as a function of E/N in TMS-N_2 mixtures.

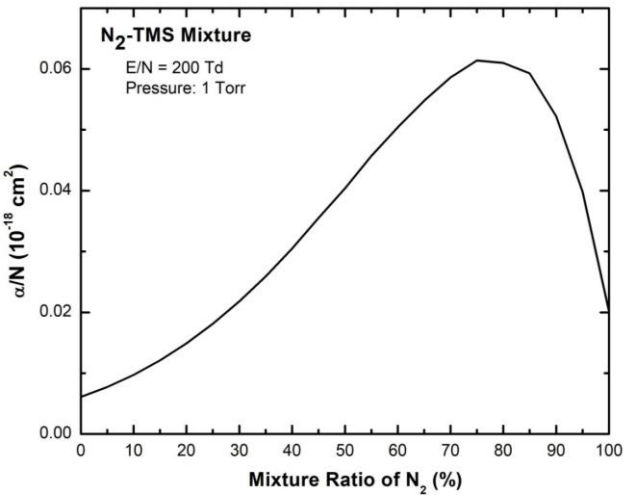

Fig. 9. Variation of the α/N values in TMS-N_2 mixtures at E/N = 200 Td with the mixture ratio of N_2.

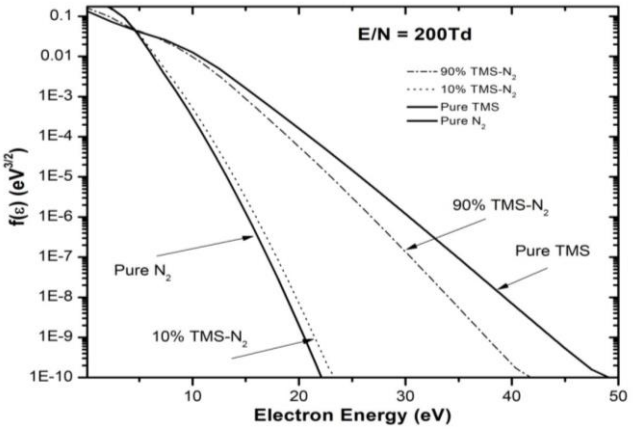

Fig. 10. Electron energy distribution function for pure TMS, pure N_2, a 10%TMS-90%N_2 and a 90%TMS-10%N_2 mixture at E/N = 200 Td.

4. Conclusion

By using two-term approximation of Boltzmann equation, the electron transport coefficients in TMS-N_2 and BF_3-N_2 mixtures were calculated and analyzed in the E/N range of 0.1-1000 Td for the first time. These electron transport coefficients were produced from reliable sets of electron collision cross section for TMS, BF_3 and N_2 molecules. Moreover, the remarkable synergism in the Townsend first ionization coefficient in the TMS-N_2 mixtures was also found out. Therefore, these results are useful and reliable data for expansion of choices of TMS-N_2 and BF_3-N_2 mixtures in many industrial applications, especially in plasma etching, plasma-enhanced chemical vapor deposition and doping plasma.

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