Studying Electron Transport Coefficients in C_2H_4-SiH_4 Mixtures Using Bolsig+ Program

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Abstract. For the first time the electron transport coefficients in C_2H_4-SiH_4 mixtures were calculated by using the Bolsig+ freeware for the E/N (ratio of the electric field E to the neutral number density N) range of 0.1–1000 Td (Townsend). The electron collision cross section sets for C_2H_4 and SiH_4 molecules were chosen and modified to ensure reliability before calculation. Therefore, the electron transport coefficients in C_2H_4-SiH_4 mixtures are useful for plasma modeling.

Keywords: Bolsig+ · Electron transport coefficients · C_2H_4-SiH_4 mixture

1 Introduction

The electron transport coefficient and the electron collision cross section set data are necessary for the fluid model of gas discharge. The electron transport coefficients include the mean electron energy, the mobility, the electron diffusion coefficient, the electron drift velocity, the ionization coefficient. These coefficients can be obtained by measurement or theoretical approaches. The estimation of transport coefficients is not easy to do experimentally, thus the theoretical calculation is the preferred method. The electron transport coefficients depend on the electron energy distribution function (EEDF), which can be found by solving the Boltzmann equation for gases. One of them is Bolsig+ freeware, which solves the Boltzmann equation to obtain the electron transport coefficients from the electron collision cross sections [1]. Especially, these electron transport coefficients are suitable for the fluid model of gas discharge.

C_2H_4-SiH_4 gas mixture is widely used in chemical vapor deposition (CVD) processes [2–5]. However, there is no report of electron transport coefficients in the C_2H_4-SiH_4 mixture both in measurement and existing theory. Therefore, the calculation of the electron transport coefficients in the C_2H_4-SiH_4 mixture are necessary for purposes of understanding or modeling of discharge plasma.

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2 Analysis

In this study, the Bolsig+ freeware was used to generate the electron transport parameters in the C_2H_4-SiH_4 mixture from the reliable set of electron collision cross section for C_2H_4 and SiH_4 molecules. Bolsig+ freeware has been developed by G. J. M. Hagelaar and L. C. Pitchford [1] and briefly discussed here. In ionized gases, the Boltzmann equation for an ensemble of electrons is given as:

$$\frac{\partial f}{\partial t} + v \cdot \Delta f - \frac{e}{m} E \cdot \nabla_v f = C[f] \tag{1}$$

Where f is the electron distribution in six-dimensional phase space, v is the velocity coordinates, e is the elementary charge, m is the electron mass, E is the electric field, ∇_v is the velocity-gradient operator and C represents the rate of change in f due to collisions. After solving this equation, the electron transport coefficients are calculated as follows:

Mean energy:

$$\overline{\varepsilon} = \int_0^\infty \varepsilon^{3/2} F_0 d\varepsilon \tag{2}$$

Energy mobility:

$$\mu_\varepsilon N = -\frac{\gamma}{3} \int_0^\infty \frac{\varepsilon}{\sigma} \frac{\partial F_0}{\partial \varepsilon} d\varepsilon \tag{3}$$

Energy diffusion coefficient:

$$D_\varepsilon N = \frac{\gamma}{3} \int_0^\infty \frac{\varepsilon}{\sigma} F_0 d\varepsilon \tag{4}$$

Rate coefficient:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k F_0 d\varepsilon \text{ (for each collision process)} \tag{5}$$

Here, F_0 is isotropic part of the EEDF and normalized by:

$$\int_0^\infty \varepsilon^{1/2} F_0 d\varepsilon = 1 \tag{6}$$

N is the concentration of atoms, σ is the effective momentum transfer cross section of electrons, $\gamma = (2e/m)^{1/2}$ is a constant and ε is the electron energy in electron volt, σ_k is the effective momentum transfer cross section accounting for possible anisotropy of the elastic scattering.

Bolsig+ generates the electron transport coefficients by using the electron collision cross section sets for gases as input data. Therefore, the accuracy of these coefficients depends on the reliable sets of electron collision cross section. In this study, the electron collision cross section sets were chosen from [6] for C_2H_4 and from [7] for SiH_4. These sets were obtained by modifying the electron collision cross section until the calculated and the measured electron transport coefficients agreed. The electron transport coefficients are calculated by solving the Boltzmann equation based on the electron collision cross section set. However, the definition of electron transport coefficients in [6, 7] and those generated by Bolsig+ are not completely same. To produce the reliable electron transport coefficient from Bolsig+ freeware, the electron collision cross section sets for using gases are needed to be modified. Therefore, before the calculations of the electron transport coefficient in the C_2H_4-SiH_4 mixtures is carried out, the data of the electron collision cross section sets are under minor changes so that the calculated and measured electron transport coefficients in each pure gas are in good agreement.

3 Results and Discussion

The variances of the electron transport coefficients in pure C_2H_4, pure SiH_4, and their mixtures for various concentration mixtures, were shown in Figs. 1, 2, 3, 4 and 5.

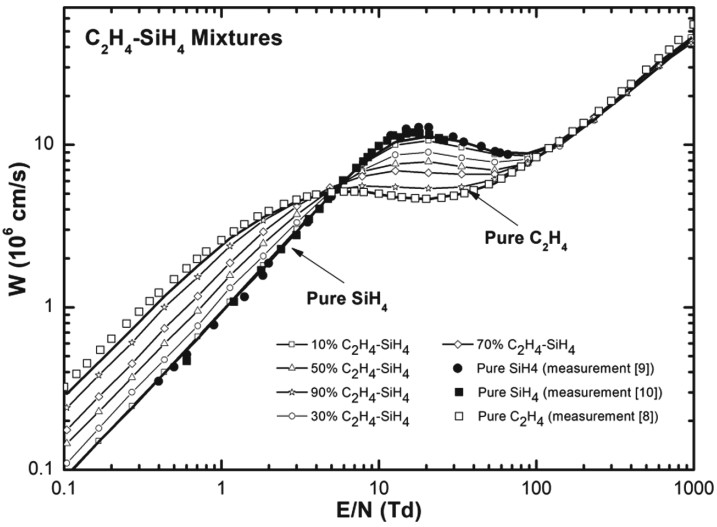

Fig. 1. The electron drift velocity, W, in the C_2H_4-SiH_4 mixtures

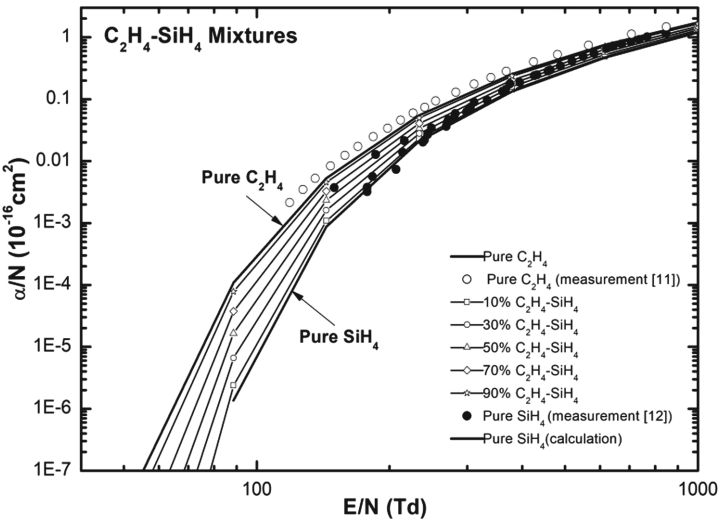

Fig. 2. The townsend ionization coefficient, α/N, in the C_2H_4-SiH_4 mixtures

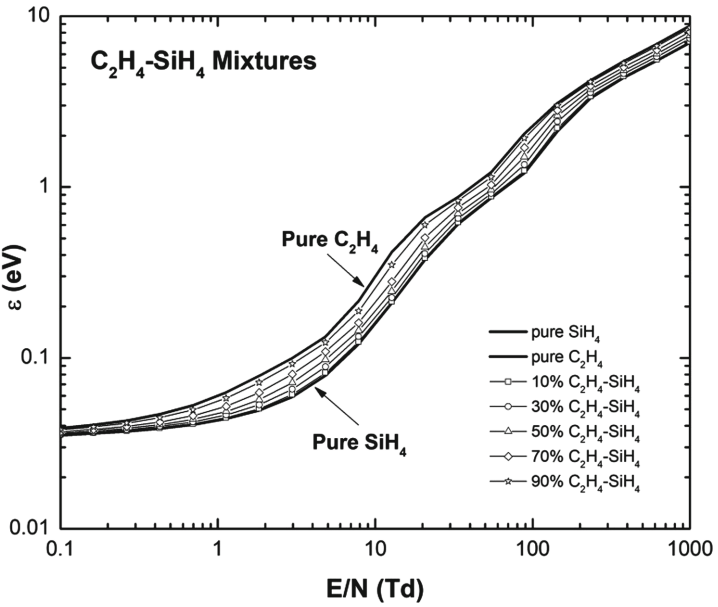

Fig. 3. The electron mean energy, ε, in the C_2H_4-SiH_4 mixtures

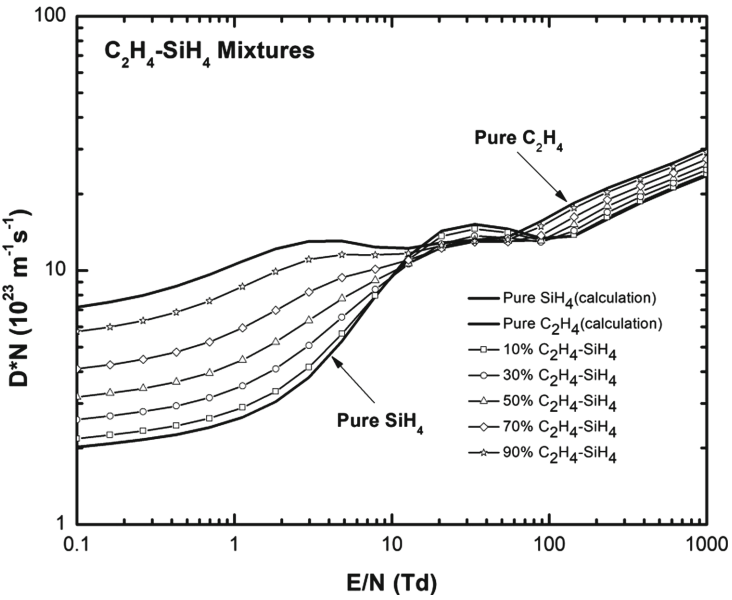

Fig. 4. The electron diffusion coefficient D multiplied by N in the C_2H_4-SiH_4 mixtures

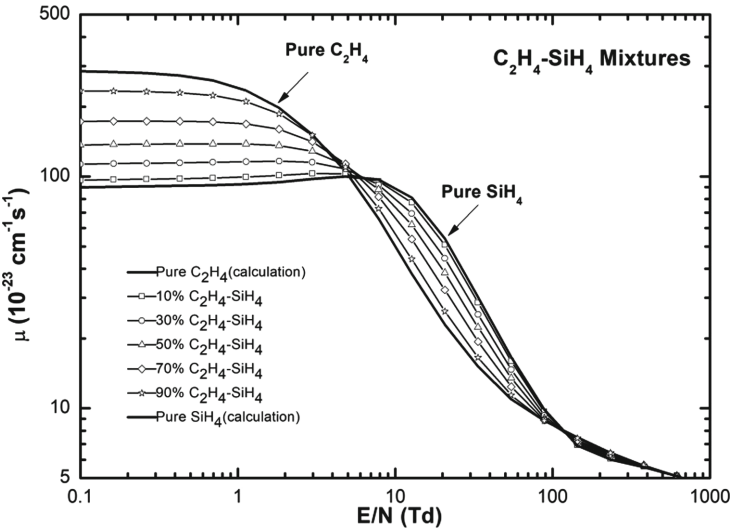

Fig. 5. The mobility μ multiplied by N in the C_2H_4-SiH_4 mixtures

The electron drift velocities, W, in the C_2H_4-SiH_4 mixtures as functions of E/N, were shown in Fig. 1. In this figure, the calculated and measured values of W for the pure C_2H_4 and the pure SiH_4, were also included. It is clear that the calculated values of W are in good agreement with experiment for the pure C_2H_4 [8] and the pure SiH_4 [9,

10]. At the same E/N, the values of W in the pure C_2H_4 are smaller than those in the pure SiH_4, and the mixtures W stand between them in the range of E/N < 5 Td. However, in the range of E/N over 5 – 140 Td, the values of W in pure C_2H_4 are larger than those in pure SiH_4, and the mixtures W also stand between them. In the range of E/N > 140 Td, the differences between the values of W for both pure and mixture are not significant.

Figure 2 shows the relationship between the ionization coefficient, α/N, for the pure of C_2H_4, SiH_4, and their mixtures against E/N. The calculated ionization coefficients are in generally good agreement with experimental values for the pure C_2H_4 [11] and the pure SiH_4 [12]. The α/N in the C_2H_4-SiH_4 mixtures are suggested to be between those of the pure gases over the entire range of E/N.

Figure 3 and Fig. 4 show the electron mean energy, ε, and electron diffusion coefficients, D, in the C_2H_4-SiH_4 mixtures, respectively. The coefficients in the mixtures are suggested to be between those of the pure gases over the entire range of E/N.

Figure 5 shows the mobility multiplied by N, μ * N, for the pure between, pure SiH_4, and their mixtures versus the E/N. The values of two pure gases and their mixtures gradually decrease in the range of E/N < 5 Td. However, in the range of E/N > 5 Td, the values of μ * N significantly decrease when increasing the E/N. The variation of the mobility and the electron drift velocity has the same tendency.

4 Conclusions

The electron transport coefficients in C_2H_4-SiH_4 mixtures for the fluid model were calculated and analyzed using the Bolsig+ freeware for the first time. The data of electron collision cross section sets for C_2H_4 and SiH_4 molecules were minor modified for suitable with the Bolsig+ program. The calculated electron transport coefficients in pure C_2H_4 and SiH_4 are in good agreement with those in measurement. Therefore, the electron transport coefficients in C_2H_4-SiH_4 mixtures are reliable data for understanding and modeling of plasma discharge.

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