ELECTRON TRANSPORT COEFFICIENTS IN TRIES-SiH_4 MIXTURE

Pham Xuan Hien[1], Phan Thi Tuoi[2], Do Anh Tuan[3*]

Abstract: *The electron transport coefficients for the TRIES-SiH_4 mixtures in the E/N (the reduced electric field) range of 0.1-1000 Td (townsend) were calculated for the first time by solving the two-term approximation of Boltzmann equation. The calculation based on the reliable sets of electron collision cross section for the TRIES and SiH_4 molecules. The present results are important data for modelling and simulation of plasma discharge using TRIES/SiH_4 mixtures.*

Keywords: Electron transport coefficients; Boltzmann equation; PECVD; TRIES; SiH_4.

1. INTRODUCTION

SiO_2 and SiN_x films play a vital role in semiconductor manufacturing. The plasma enhanced chemical vapour deposition (PECVD) can be used to deposit SiO_2 on organic based materials. In these PECVD processing, the organosilanes such as tetraethoxysilane (TEOS), triethoxysilane (TRIES), tetramethoxysilane (TMOS), and trimethoxysilane (TRIMOS), are required [1, 2]. Among these organosilanes, TRIES vapour is suggested to as alternative for TEOS vapour and SiH_4 gas for safety and high quality films [3]. Because of above reasons, the electron transport coefficients in the TRIES-SiH_4 mixtures are necessary to determine for modeling and simulation of plasma discharge. The fluid model or hybrid simulations require the input of electron transport coefficients, which include electron drift velocity, the density-normalized longitudinal diffusion coefficient, ratio of the longitudinal diffusion coefficient to the mobility, the density-normalized longitudinal diffusion coefficient, the Townsend first ionization coefficient. Such electron transport coefficients can be obtained by solving the Boltzmann equation based on the electron collision cross section sets of using gases. The accuracies of these electron transport coefficients play a key role in ensuring the ability of plasma simulation. Therefore, the electron collision cross section sets have been chosen from Tuoi [4] for the TRIES molecule and from Kurachi and Nakamura [5] for the SiH_4 molecule. The validity of these set have been proved in [4, 5].

2. THEORY

To desired the electron transport coefficients, the two-term approximation of Boltzmann equation suggested by Tagashira [6] was applied. This method has been successfully used in previous work for [4, 7, 8]. The electron energy distribution function (EEDF), f(ε, E/N), is normalized by

$$\int_0^\infty f(\varepsilon, E/N)d\varepsilon \equiv 1 \tag{1}$$

The EEDF can be obtained theoretically by solving the Boltzmann equation

$$\frac{\partial f}{\partial t} + \vec{v}\nabla_r f + \vec{a}\nabla_v f = \left(\frac{\partial f}{\partial t}\right)_{coll} \tag{2}$$

where f = f($\vec{r},\vec{v},t$) is the distribution function of the positions r and velocities of electrons v, is the acceleration due to external forces and $(\partial f/\partial t)_{coll}$ is the collision induced rate of change of the number of electrons per unit volume of phase space. The electron drift velocity calculated from the solution of electron energy distribution function, f(ε, E/N), of the Boltzmann equation is defined as

$$W = -\frac{1}{3}\left(\frac{2}{m}\right)^{1/2}\frac{eE}{N}\int_0^\infty \frac{\varepsilon}{q_m(\varepsilon)}\frac{df(\varepsilon, E/N)}{d\varepsilon}d\varepsilon \quad (3)$$

where ε is the electron energy, m is the electron mass, e is the elementary charge and $q_m(\varepsilon)$ is the momentum-transfer cross section.

The density-normalized longitudinal diffusion coefficient is defined as

$$ND_L = \frac{V_1}{3N}\left(E\int_0^\infty \frac{\varepsilon}{q_T}\frac{\partial}{\partial\varepsilon}(F_1\varepsilon^{-1/2})d\varepsilon + \int_0^\infty \frac{\varepsilon^{1/2}}{q_T}F_0 d\varepsilon\right) - \left(\varpi_0 A_2 - \varpi_1 A_1 - \varpi_{02}\right) \quad (4)$$

where V_1 is the speed of electron, q_T is the total cross section, here F_n and ϖ_n (n = 0, 1, 2) are respectively the electron energy distributions of various orders and their eigenvalues. V_1, ϖ_n, ϖ_0 and A_n are given by

$$V_1 = \left(\frac{2e}{m}\right)^{1/2} \quad (4.1)$$

$$\varpi_1 = -\frac{V_1 E}{3N}\int_0^\infty \frac{\varepsilon}{q_T}\frac{\partial}{\partial\varepsilon}(F_0\varepsilon^{-1/2})d\varepsilon + (\varpi_0 A_1 - \varpi_{01}) \quad (4.2)$$

$$\varpi_0 = V_1 N\int_0^\infty \varepsilon^{1/2} q_i F_0 d\varepsilon \quad (4.3)$$

$$\varpi_{0n} = V_1 N\int_0^\infty \varepsilon^{1/2} q_i F_n d\varepsilon \quad (4.4)$$

$$A_n = \int_0^\infty F_n d\varepsilon \quad (4.5)$$

$$\alpha/N = \frac{1}{W}\left(\frac{2}{m}\right)^{1/2}\int_I^\infty f(\varepsilon, E/N)\varepsilon^{1/2} q_i(\varepsilon)d\varepsilon \quad (4.6)$$

where q_i is the ionization cross section.

The Townsend first ionization coefficient is defined as where I is the ionization onset energy and $q_i(\varepsilon)$ is the ionization cross section.

3. RESULTS AND DISCUSSION

The electron transport coefficients for the TRIES-SiH_4 mixtures with 1%, 5%, 10%, 30%, 50%, 70% and 90% TRIES were calculated in the E/N range of 0.1-1000 Td by a two-term approximation of the Boltzmann equation. These results are shown in Figs. 1-4 with the electron transport coefficients in the pure TRIES and SiH_4 molecules.

As shown in fig. 1-3 the values of W, ND_L and D_L/μ in TRIES-SiH_4 mixture gases are suggested to be between those of the pure gases over the all range of E/N. However, in fig. 4, the values of ionization coefficient in the TRIES-SiH_4 mixture are to be found not between those of the pure gases. In the fig. 1, the slight regions of the NDC (negative differential conductivity) phenomena in 1%, 5%, 10%, 30% and 50% TRIES-SiH_4 mixtures are observed in the E/N range 20 < E/N < 200 Td. The NDC is relatively shallow in these cases. In fig. 2, the values of ND_L in the mixtures also decrese with increasing E/N for the E/N range of 20-100 Td. The ND_L curves have minima in the E/N range of 90 - 150 Td for these mixtures. The behavior of W and ND_L in the TRIES-SiH_4 mixtures are due to the Ramsauer-Tovmsend minimum (RTM) of the elastic momentum transfer cross sections of the TRIES molecule.

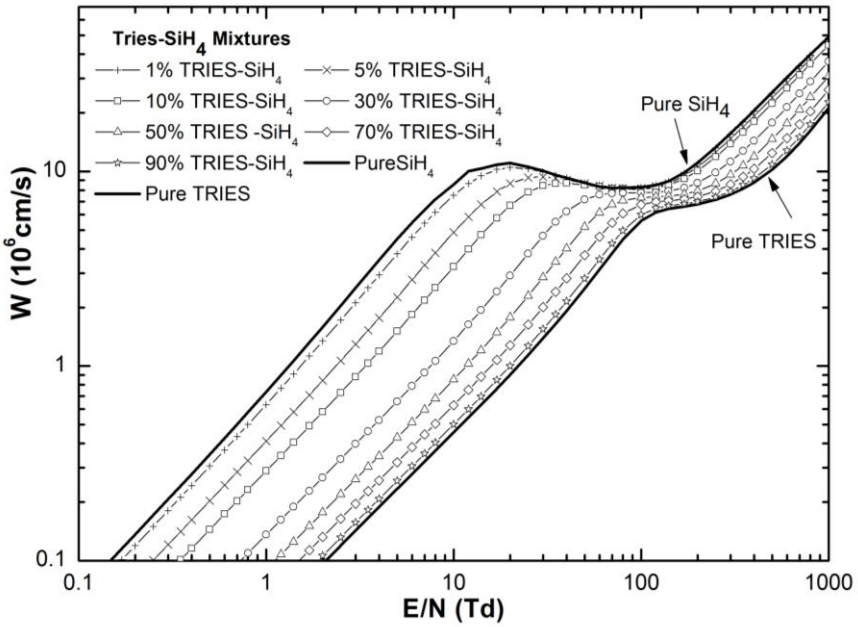


Figure 1. *The electron drift velocity, W, as a function of E/N for the TRIES- SiH_4 mixtures with 1%, 5%, 10%, 30%, 50%, 70%, and 90% TRIES. The solid line and symbols show present W values calculated using a two-term approximation of the Boltzmann equation for the TRIES - SiH_4 mixtures. The solid curves show present W values calculated for the pure TRIES molecule and SiH_4 molecule.*

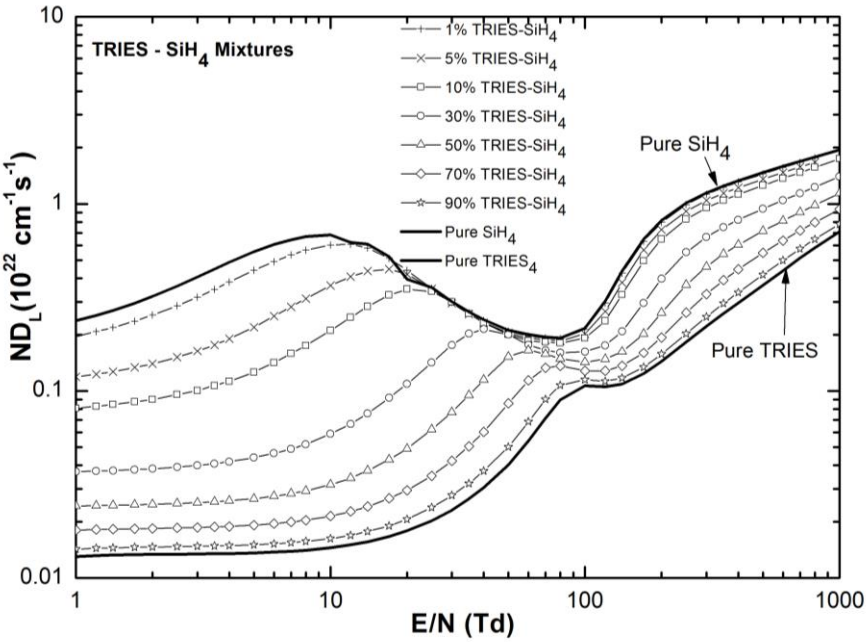


Fig. 2. *The density-normalized longitudinal diffusion coefficient, ND_L, as a function of E/N for the TRIES- SiH_4 mixtures with 1%, 5%, 10%, 30%, 50%, 70%, and 90% TRIES. The solid line and symbols show present ND_L values calculated using a two-term approximation of the Boltzmann equation for the TRIES- SiH_4 mixtures. The solid curves show present ND_L values calculated for the pure TRIES and SiH_4 molecules.*

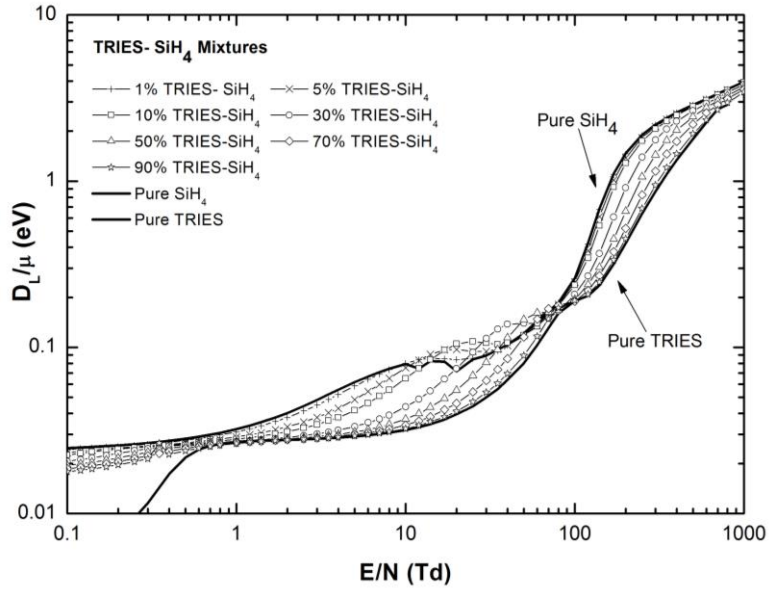


Fig. 3. *Ratio of the longitudinal diffusion coefficient to the mobility, D_L/μ, as a function of E/N for the TRIES- SiH_4 mixtures with 1%, 5%, 10%, 30%, 50%, and 70%, and 90% TRIES. The solid line and symbols show present D_L/μ values calculated using a two-term approximation of the Boltzmann equation for the TRIES - SiH_4 mixtures. The solid curves show present D_L/μ values calculated for the pure TRIES and SiH_4 molecules.*

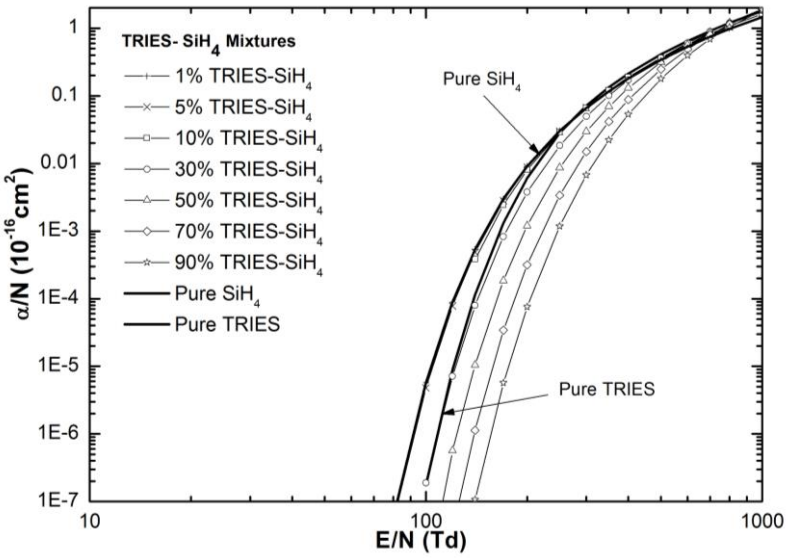


Fig. 4. *Townsend first ionization coefficient α/N as functions of E/N for the TRIES-SiH_4 mixtures with 1%,5%, 10%, 30%, 50%, 70%, and 90% TRIES. The solid line and symbols show present α/N values calculated using a two-term approximation of the Boltzmann equation for the TRIES-SiH_4 mixtures. The solid curves show present α/N values calculated for the pure TRIES and SiH_4 molecules.*

4. CONCLUSIONS

We calculate the electron transport coefficients in TRIES/SiH_4 mixtures in the wide range of E/N for the first time. The electron transport coefficients include electron drift velocity, the

density-normalized longitudinal diffusion coefficient, ratio of the longitudinal diffusion coefficient to the mobility, the density-normalized longitudinal diffusion coefficient, the Townsend first ionization coefficient. These coefficients are calculated by two-term approximation of Boltzmann equation and reliable sets of electron collision cross sections of the TRIES and SiH_4 molecules. Therefore, the calculated eletron transport coefficients has many benefits for modeling and simulation of plasma discharge.

REFERENCES

[1]. G. Franz, "*Plasma Enhanced Chemical Vapor Deposition of Organic Polymers*," Processes, Vol. **9**, no. 6, pp. 980, (2021).

[2]. J. H. Lee, C. H. Jeong, J. T. Lim, N. G. Jo, S. J. Kyung and G. Y. Yeom, "*Characteristic of SiO_2 Films Deposited by Using Low-Temperature PECVD with TEOS/N_2/O_2*," Journal of the Korean Physical Society, Vol. **46**, pp. 890-894, (2005).

[3]. Y. Kudoh, Y. Homma, N. Sakuma, T. Furusawa and K. Kusukawa, "*Directional Plasma CVD Technology for Sub-quarter-micron Feature Size Multilevel Interconnections*," Japanese journal of applied physics, Vol. **37**, pp. 1145-1149, (1998).

[4]. P.T. Tuoi, D. A. Tuan, P.X. Hien "*Electron Collision Cross Sections for the TRIES Molecule and Electron Transport Coefficients in TRIES-Ar and TRIES-O2 Mixtures*" Journal of the Korean Physical Society, Vol. **73**, No. 12, pp. 1855-1862, (2018).

[5]. M. Kurachi and Y. Nakamura, "*Electron collision cross sections for the monosilane molecule*," Journal of Physics D: Applied Physics **22**, pp. 107, (1989).

[6]. H. Tagashira, Y. Sakai, and S. Sakamoto, "*The development of electron avalanches in argon at high E/N values. II. Boltzmann equation analysis*" J. Phys. D. **10**, pp. 1051-1063, (1977).

[7]. P. X. Hien, P. T. Tuoi, T. C. Nhung, D. A. Tuan, "*Studying Effect of Adding Buffer Gases Studying Effect of Adding Buffer Gases Transport Coefficients*", Lecture Notes in Networks and Systems, Vol. **104**, pp. 693-703, (2020).

[8]. P.X. Hien, D. A. Tuan, B.H. Jeon, "*Electron collision cross sections for the BF_3 molecule and electron transport coefficients in BF_3–Ar and BF_3–SiH_4 mixtures*," Journal of the Physical Society of Japan **82**, pp. 034301-034308, (2013).

TÓM TẮT

HỆ SỐ CHUYỂN ĐỘNG ELECTRON TRONG HỖN HỢP TRIES/SIH_4

Các hệ số chuyển động electron cho hỗn hợp TRIES-SiH_4 trong dải 0.1-1000 Td được tính toán lần đầu tiên thông qua việc giải phương trình xấp xỉ bậc hai Boltzmann. Các tính toán dựa trên các bộ tiết diện va chạm electron đáng tin cậy cho các phân tử TRIES và SiH_4. Kết quả trong nghiên cứu này là dữ liệu quan trọng cho việc mô hình hóa và mô phỏng phóng điện plasma sử dụng hỗn hợp TRIES-SiH_4.

Từ khóa: Các hệ số chuyển động electron, phương trình Boltzmann, PECVD, TRIES, SiH_4.

Received date, 15th March, 2021
Revised manuscript, 11th August, 2021
Published, 05th September, 2021

Author affiliations:
[1] University of Transport and Communication;
[2] Hung Yen University of Technology and Education;
[3] National Center for Technological Progress, Vietnam Ministry of Science & Technology.
[*]Email: datuan@most.gov.vn.