ELECTRON TRANSPORT COEFFICIENTS AND INITIAL ELECTRON COLLISION CROSS SECTIONS FOR TRIETHOXYSILANE MOLECULE

CÁC HỆ SỐ CHUYỂN ĐỘNG VÀ TIẾT DIỆN VA CHẠM ELECTRON BAN ĐẦU CỦA PHÂN TỬ TRIETHOXYSILANE

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ABSTRACT

Triethoxysilane molecule, both in form of pure and mixtures, are widely used in manufacturing processes of semiconductor devices. In this study, the physical and chemical characteristics and important applications of triethoxysilane molecule are presented. The necessary database of electron transport coefficients and electron collision cross sections in triethoxysilane molecule is also collected and analyzed. An initial electron collision cross section set for triethoxysilane molecule is suggested based on comparison of calculated and measured values of electron transport coefficients. This initial electron collision cross section set is useful for obtaining the reliable one for triethoxysilane molecules.

Keywords: *Triethoxysilane, Electron transport coefficient, Electron collision cross sections, Boltzmann equation, Electron swarm method.*

TÓM TẮT

Phân tử triethoxysilane cả ở dạng nguyên chất và hỗn hợp được sử dụng rộng rãi trong công nghệ chế tạo các thiết bị bán dẫn. Trong bài báo này, các tính chất vật lý, hóa học và các ứng dụng quan trọng của phân tử triethoxysilane được trình bày. Các hệ thống dữ liệu quan trọng của các hệ số chuyển động electron và các tiết diện va chạm electron trong phân tử triethoxysilane cũng được thu thập và phân tích. Bộ tiết diện va chạm electron ban đầu của phân tử triethoxysilane được đề xuất dựa trên sự so sánh giá trị tính toán và thực nghiệm của các hệ số chuyển động electron. Bộ tiết diện va chạm electron ban đầu này rất hữu ích cho việc nhận được bộ tiết diện va chạm electron đáng tin cậy cho phân tử triethoxysilane.

Từ khóa: *Triethoxysilane, Hệ số chuyển động electron, Tiết diện va chạm electron, Phương trinh Boltzmann, Phương pháp đám electron.*

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1. INTRODUCTION

Silicon dioxide (SiO_2) films are necessary materials in semiconductor fabrication. In order to build SiO_2 insulating layer, SiH_4 (monosilane) and $Si(OC_2H_5)_4$ (tetraethoxysilane, TEOS) are often used [1-3]. Because of higher quanlity and conformal deposition, triethoxysilane (TRIES), $Hsi(OC_2H_5)_3$ has been suggested to as alternative for these gases [4]. It has also less ethoxy ($-OC_2H_5$) substrate, high growth rate without a heating source material [4]. Moreover, triethoxysilane is an environmentally clean, nontoxic and nonexplosive gas [5]. Therefore, triethoxysilane is a good candidate for SiO_2 film deposition. In the lack of chemical and physical properties, electron transport coefficients and electron collision cross sections, which are necessary in modeling of plasma processing, are in need of determination. The electron transport coefficients and electron collision cross sections of gaseous molecules can be obtained by experimental or theoretical methods. Electron transport coefficients include electron drift velocity, density-normalized longitudinal diffusion coefficient, attachment coefficient and ionization coefficient. Electron drift velocity and density-normalized longitudinal diffusion coefficient can be determined by using time-of-flight (TOF) method and arrival-time spectra (ATS), and attachment and ionization coefficients can be determined by using steady-state Townsend (SST) method. Electron collision cross sections for gaseous molecules such as momentum transfer, vibrational excitation, electronic excitation, attachment, dissociation and ionization cross sections are related to electron transport coefficients. Therefore, electron collision cross sections can be obtained based on measured electron transport coefficients. In order to carry out this procedure, an electron swarm method and analysis of Boltzmann equation are often used [6]. The validity of obtaining electron collision cross sections depends on reliability of collecting data of electron

transport coefficient and electron collision cross sections. Therefore, the analysis and evaluation of collected database of electron transport coefficients and electron collision cross sections for triethoxysilane are necessary.

2. DATABASE OF ELECTRON TRANSPORT COEFFICIENTS AND ELECTRON COLLISION CROSS SECTIONS FOR TRIETHOXYSILANE MOLECULE

As presented in part 1, the reliable electron collision cross sections for gaseous molecules are obtained based on electron transport coefficients using electron swarm method [6]. The basic procedure of electron swarm study has been presented in many articles [6-9] and also shown in Figure 1. In order to obtain the final electron collision cross section set, the measured values of electron transport coefficients and some related database of electron collision cross section are needed to compile before modifying the shape and amplitude of electron collision cross section set. Their information are presented and analyzed as bellow.

Yoshida *et al*. [7] firstly reported the electron transport coefficients in TRIES molecule. The mean-arrival time drift velocity (W_m) and the longitudinal diffusion coefficient (D_L) in E/N (ratio of the electric field E to the neutral number density N) range of 20 - 5000Td (1Td = 10^{-17}V.cm^2) were measured by the ATS method using a double-shutter drift tube. The ionization coefficients (α) in E/N range of 300 – 5000 Td were measured by the SST method. These results were also analyzed in comparison with those for SiH_4 [8] and TEOS [9]. Based on these analyses, Yoshida *et al*. [7] suggested an electron collision crosss section set for TRIES molecule using the Boltzmann equation analysis. This cross section set includes the momentum transfer cross section (Q_m), the ionization cross section (Q_i), the dissociation cross section (Q_d), and two vibrational excitation cross sections (Q_{v1} and Q_{v2}). The threshold values for these electron collision cross sections are listed in Table 1 [7].

Table 1. Threshold of electron collision cross sections for TRIES molecule [7]

Electron collision cross sections	Energy threshold (eV)
Vibrational excitation cross section Q_{v1}	0.16
Vibrational excitation cross section Q_{v2}	0.4
Ionization cross section	7.4
Dissociation cross section	9.9

The electron collision cross section set for TRIES molecule was obtained based on electron collision cross section set of TEOS that was reported by Morgan[12]. Then, electron drift velocity and ionization coefficient in TRIES molecule were calculated. The calculated results are in good agreement with those in experiments. However, density-normalized longitudinal diffusion coefficient for TRIES has been not calculated although measured values are available.

Recently, Tuan and Jeon [9] have been also reported an electron collision cross section set for TRIES molecule by using electron swarm method. As mentioned in [9], the electron collision cross section set for TRIES molecule suggested by Tuan and Jeon [9] are more reliable than those suggested by Morgan[12]. In order to obtain the reliable electron collision cross section set for gaseous molecule, electron swarm method often applied based on measured values of electron transport coefficients. The electron collision cross sections will be modified until the calculated and measured electron transport coefficients are in good agreement. Therefore, it is necessary to choose consistent initial electron collision cross section set for modified procedure. The electron transport coefficients, which include electron drift velocity, density-normalized longitudinal diffusion coefficient, were calculated using the two-term approximation of the Boltzmann equation given by Tagashira *et al*. [6]. This approximation of the Boltzmann equation was successfully used for the TEOS [9], TMS [11], and BF_3 [10] molecules. The mean-arival time drift velocity (W_m), which is calculated by an approximation formula of $(W_r^2 - 4R_iD_L)^{1/2}$ when the constant ω_n ($n \geq 3$) is neglected [6], where W_r is the centre-of-mass drift velocity, R_i is the ionization frequency, and the longitudinal diffusion coefficient (D_L) are calculated in the time-of-flight (TOF) parameters. The electron transport coefficients calculated in the pure TRIES molecule by using the two sets from Yoshida *et al*. [7] and Tuan and Jeon [9] for the TRIES molecule are shown in Figures 2 and 3.

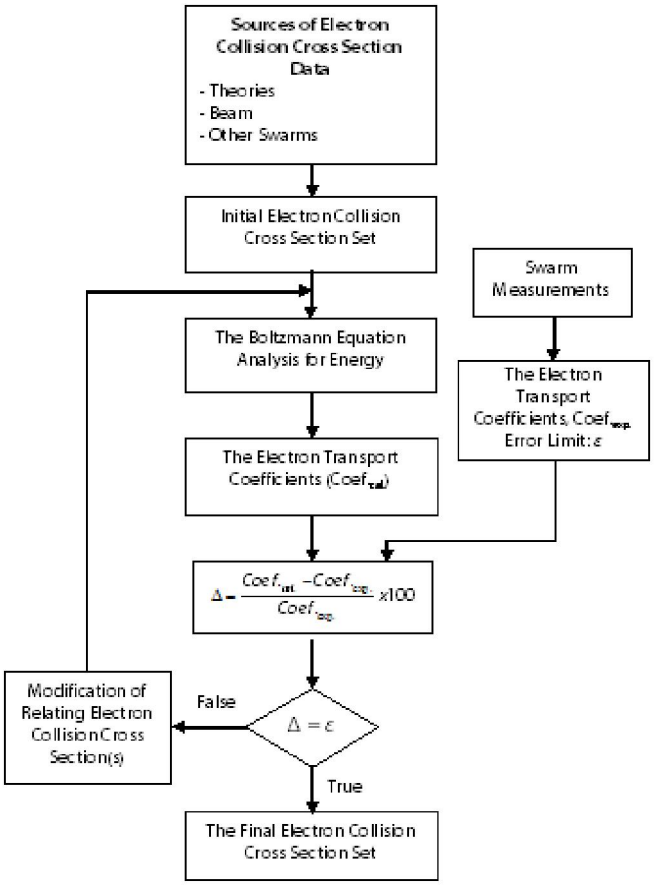

Figure 1. Electron drift velocity W_m as a function of E/N for the pure TRIES molecule

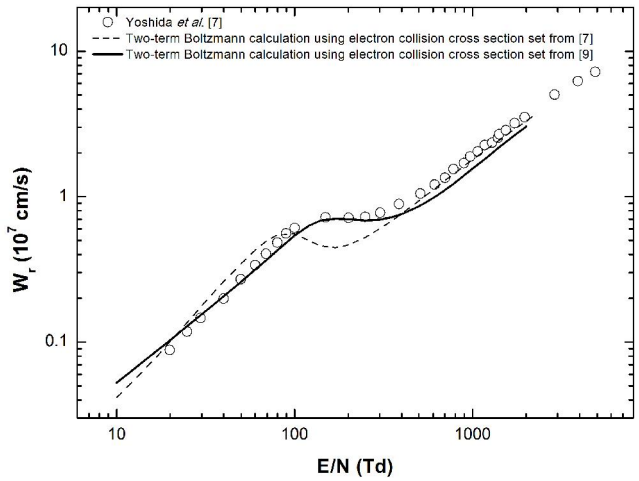

Figure 2. Electron drift velocity W_m as a function of E/N for the pure TRIES molecule. Broken curve shows a two-term Boltzmann calculation using the electron collision cross section set from [7]; solid curve shows a two-term Boltzmann calculation using the electron collision cross section set from [9]; open circles show measurement results of the pure TRIES molecule [7].

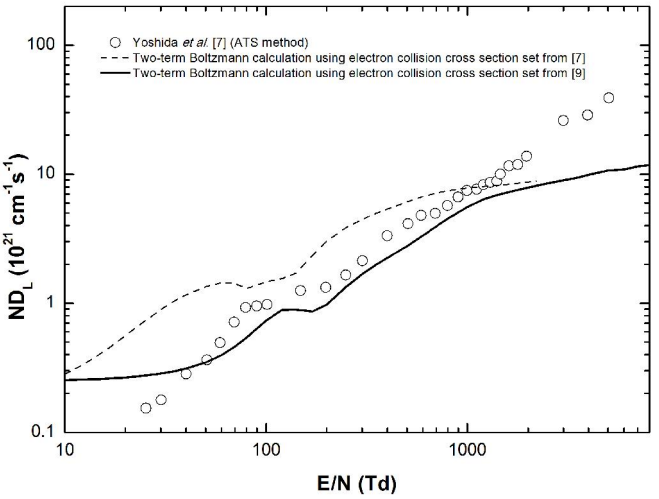

Figure 3. Density-normalized longitudinal diffusion coefficient ND_L as a function of E/N for the pure TRIES molecule. Broken curve shows a two-term Boltzmann calculation using the electron collision cross section set from [7]; solid curve shows a two-term Boltzmann calculation using the electron collision cross section set from [9]; open circles show measurement results of the pure TRIES molecule [7].

3. RESULTS AND DISCUSSION

The mean-arrival time drift velocity and the density-normalized longitudinal diffusion coefficient as functions of E/N for the pure TRIES molecule, calculated by using a two-term approximation of the Boltzmann equation for the energy with the initial electron collision cross section sets of TEOS molecule from [7] and [9] are shown in Figures 2 and 3. As shown in Figure 2, the differences of the electron drift velocity values between calculations using Yoshida's set and measurements are very large, especially in the range of 100-300Td. In Figure 3, there were also significant differences between calculated density-normalized longitudinal diffusion coefficient using electron collision cross section set from [7] and the measurements over the entire range. On the other hand, the electron drift velocity, which were calculated using electron collision cross section set from [9], were agreement with those in measurements. The differences of density-normalized longitudinal diffusion coefficient between calculations using electron collision cross section set from [9] and measurements still exist. However, these differences are smaller than those between calculations using set from [7] and measurements. It is clearly that the agreement between calculated and measured electron transport coefficient in results which calculated using electron collision cross section set from [9] are better than those in [7]. Therefore, the initial electron collision cross section set for TRIES molecule is recommended to use the electron collision cross section of TEOS molecule from [9]. The recommended electron collision cross section set for TRIES molecule was shown in Figure 4. Threshold energies of these electron collision cross sections were also listed in Table 2.

Table 2. Threshold of electron collision cross sections for TRIES molecule

Electron collision cross sections	Energy threshold (eV)
Vibrational excitation cross section Q_{v1}	0.16
Vibrational excitation cross section Q_{v2}	0.37
Ionization cross section	10.6
Dissociation cross section	3.6

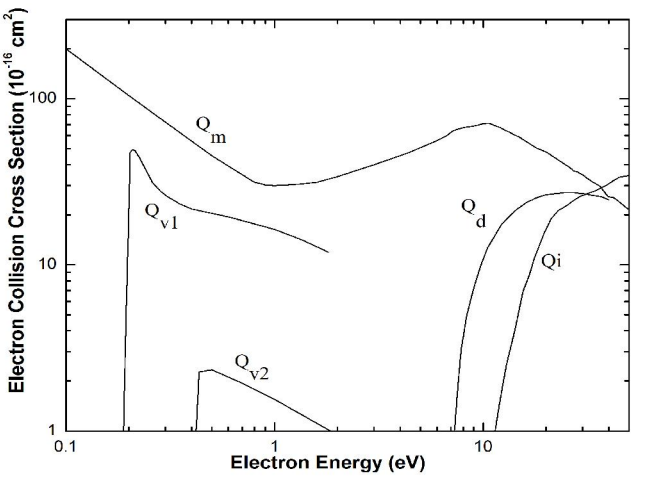

Figure 4. The set of cross sections consists of the momentum transfer cross section (Qm), the ionization cross section (Qi), the dissociation cross section (Qd), and two vibrational excita tion cross sections (Qv1 and Qv2).

4. CONCLUSIONS

The electron transport coefficients, which include mean-arrival time drift velocity W_m, the ratio of the density-normalized longitudinal diffusion coefficient ND_L, were calculated by using two available sets of electron collision cross sections for the TRIES molecule and the two-term approximation of the Boltzmann equation analysis. Based on analyses and comparisons of available electron collision cross sections, the currently best available electron collision cross section set for the TRIES molecule was recommended.

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