TOWNSEND FIRST IONIZATION COEFFICIENT IN SiH_4-O_2 MIXTURES

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SUMMARY

The values of Townsend first ionization coefficient in SiH_4-O_2 mixtures are calculated using two-term Boltzmann equation analysis. The Townsend first ionization coefficient in SiH_4-O_2 mixtures with various ratios are obtained based on reliable cross section sets of SiH_4 and O_2 molecules. Therefore, they are fundamental important data for description of discharge processes and plasma discharge in various applications using SiH_4-O_2 mixtures.

Keywords: *gas discharge; SiH_4-O_2 mixtures; Townsend first ionization coefficient*

INTRODUCTION

The Townsend first ionization coefficient, defined as *the mean number of collisions for an electron per unit length in the direction of the electric field multiplied the ionization propability*, is one of fundamental important coefficient, which is often used in all discharge processes and in the calculation or modeling of gas ionization or plasma discharge [1]. SiO_2 thin films are widely used in various applications. The low temperature SiO_2 film can be deposited using different methods such as plasma-enhanced chemical deposition (PECVD), photo-CVD, Remote-PECVD etc [2]. A SiH_4-O_2 mixture typically applied to deposit SiO_2 on wafer [2-3]. Townsend first ionization coefficient in SiH_4-O_2 mixture is indispensable parameter in simulation of microelectronic processes using SiH_4-O_2 mixtures. However, according to our best knowledge, the measurement for Townsend first coefficient in SiH_4-O_2 mixture is not available. Therefore, the Townsend first ionization coefficient in SiH_4-O_2 mixtures is necessary to be determined. In this study, the Townsend first ionization coefficient in SiH_4-O_2 mixtures with various mixture ratios were calculated using the two-term Boltzmann equation analysis for the first time.

CALCULATION METHOD

In order to obtain the Townsend first ionization coefficient in SiH_4-O_2 mixture, the two-term Boltzmann equation analysis suggested by Tagashira [4] was used throughout in this study. This calculation method has been successfully used in determination of electron transport coefficients for BF_3-Ar and BF_3-SiH_4 mixtures [5] and TEOS-Ar and TEOS-O_2 mixtures [6]. The Townsend first ionization coefficient:

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

where, I is the ionization onset energy, $q_i(\varepsilon)$ is the ionization cross section, W is the electron drift velocity. Therein, the electron drift velocity is obtained based on the electron energy distribution function, $f(\varepsilon, E/N)$, of the Boltzmann equation:

$$W = -\frac{1}{3}\left(\frac{2}{m}\right)^{1/2} \frac{eE}{N} \int_{0}^{\infty} \frac{\varepsilon}{q_m(\varepsilon)} \frac{df(\varepsilon, E/N)}{d\varepsilon} d\varepsilon \quad (2)$$

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.

In order to obtain the electron transport coefficients in mixtures, it is necessary to use the electron collision cross section sets for both of two gaseous molecules. Therefore, the reliability of electron transport coefficients in mixtures depend on the accuracy of electron collision cross section sets of two pure gases. In this study, thus, the electron collision cross section sets for SiH_4 and O_2 molecules were chosen from Kurachi and Nakamura [7] and

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B. H. Jeon [8], respectively. Electron collision cross section set for SiH_4 molecule [7] includes the momentum transfer cross section, two vibrational excitation cross sections, attachment cross section, the electronic excitation cross section and the ionization cross section. Electron collision cross section set for O_2 molecule [8] includes the momentum transfer cross section, four vibrational excitation cross section, the rotational excitation cross section, the three-body attachment cross section, seven electronic excitation cross sections, the ionization cross section. The validity of these electron collision cross section sets have been proved in [7] for SiH_4 and in [8] for O_2 molecules. Thresholds of these electron collision cross sections are listed in Table 1 and 2.

RESULTS AND DISCUSSION

The first Townsend ionization coefficient, α/N, as functions of E/N for SiH_4-O_2 mixtures calculated by a two-term approximation of the Boltzmann equation are shown in Fig. 1. In this study, we calculated and showed the values of α/N in mixtures of SiH_4-O_2 with different percentages of SiH_4 molecule (10%, 30%, 50%, 70%, 90% SiH_4). It is clear that the values of α/N in SiH_4-O_2 mixtures are between those of pure SiH_4 and O_2 molecules.

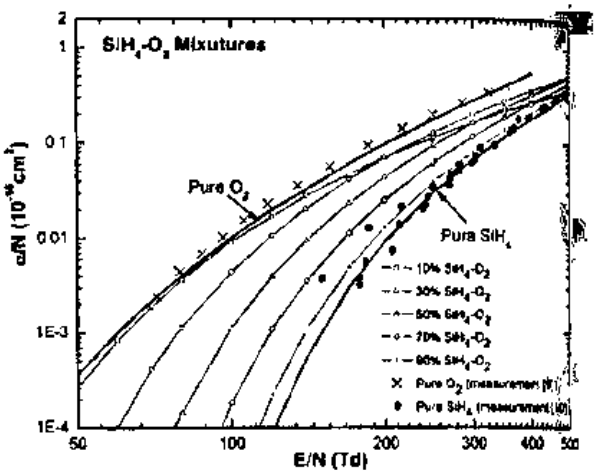

Figure 1. *Townsend first ionization coefficient, α/N as functions of E/N for the SiH_4-O_2 mixtures with 10%, 30%, 50%, 70% and 90% SiH_4. The solid line and symbols show present α/N values calculated using a two-term approximation of the Boltzmann equation for the SiH_4-O_2 mixtures. The solid curves show present α/N values calculated for the pure SiH_4 and O_2 molecules. The symbols show the measured values for pure O_2 and pure SiH_4 molecules from [9] and [10], respectively*

Table 1. *Threshold of electron collision cross sections for O_2 molecule*

Electron collision cross sections	Energy threshold (eV)
Rotational excitation cross section Q_{rot}	0.07
Attachment cross section	0.058
Vibrational excitation cross section Q_{v1}	0.19
Vibrational excitation cross section Q_{v2}	0.44
Vibrational excitation cross section Q_{v3}	0.68
Vibrational excitation cross section Q_{v4}	0.79
Electronic excitation cross section of $a^1\Delta_g$	0.977
Electronic excitation cross section of $b^1\Sigma g$	1.627
Electronic excitation cross section of 6 eV	6
Electronic excitation cross section of SR	8.4
Electronic excitation cross section of LB	9.97
Electronic excitation cross section of SB	10.29
Electronic excitation cross section of 13.3 eV	13.3
Ionization cross section	12.06

Table 2. *Threshold of electron collision cross sections for SiH_4 molecule*

Electron collision cross sections	Energy threshold (eV)
Vibrational excitation cross section Q_{v1}	0.113
Vibrational excitation cross section Q_{v2}	0.271
Attachment cross section	7.05
Electronic excitation cross section	8.4
Ionization cross section	11.6

CONCLUSIONS

The Townsend first ionization coefficient in SiH_4-O_2 mixtures were calculated for the first time using two-term Boltzmann equation analysis based on the reliable electron collision cross sections for SiH_4 and O_2 molecules. These values are useful for description of all discharge processes and calculation or modeling plasma discharge in applications using SiH_4-O_2 mixtures.

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TÓM TẮT

HỆ SỐ ION HÓA TOWNSEND THỨ NHẤT TRONG HỖN HỢP KHÍ SiH_4-O_2

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Giá trị hệ số ion hóa Townsend thứ nhất trong hỗn hợp khí SiH_4-O_2 được tính toán bằng việc sử dụng các phân tích phương trình bậc hai Boltzmann. Hệ số Townsend thứ nhất trong hỗn hợp khí SiH_4-O_2 với các tỉ lệ trộn khác nhau nhận được dựa trên các bộ tiết diện va chạm đáng tin cậy của các phân tử SiH_4 và O_2. Do đó, các kết quả này là các dữ liệu quan trong cho việc mô tả các quá trình phóng điện và phóng điện plasma trong các ứng dung công nghiệp có sử dụng hỗn hợp khí SiH_4-O_2.

Keywords: *phóng điện khí; hỗn hợp SiH_4-O_2; hệ số ion hóa Townsend thứ nhất*

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