ELECTRON TRANSPORT COEFFICIENT IN SiH_4-He MIXTURES FOR FLUID MODELS

CÁC HỆ SỐ CHUYỂN ĐỘNG ELECTRON TRONG HỖN HỢP SiH_4-He CHO MÔ HÌNH CHẤT LỎNG

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ABSTRACT

The electron transport coefficients with respect to E/N (ratio of the electric field E to the neutral number density N) in the range of 0.1 - 1000Td (Townsend) for 10%, 30%, 50%, 70%, and 90% SiH_4-He mixture (volume mixing ratio), were calculated using the Bolsig+ program. These calculations based on the reliable electron collision cross section set for SiH_4 molecule and He atom. Therefore, the present results will be the necessary data for applications using SiH_4-He mixture, especially in deposition of a-Si:H films using capacitively coupled plasma.

Keywords: *SiH_4-He mixture, a-Si:H film, electron transport coefficients, two-term Boltzmann approximation, Bolsig+.*

TÓM TẮT

Các hệ số chuyển động electron tương ứng với E/N (tỉ lệ điện trường E và mật độ số lượng hạt trung hòa N) trong dải 0,1 - 1000Td (Townsend) cho các hỗn hợp khí 10%, 30%, 50%, 70% và 90% SiH_4-H_e (tỉ lệ trộn theo thể tích) được tính toán sử dụng chương trình Bolsig+. Các tính toán này dựa trên bộ tiết diện va chạm electron đáng tin cậy cho phân tử SiH_4 và nguyên tử He. Do đó, kết quả này sẽ là nguồn dữ liệu cần thiết cho các ứng dụng sử dụng hỗn hợp SiH_4-He, đặc biệt trong lắng đọng màng mỏng a-Si:H sử dụng plasma ghép điện dung.

Từ khóa: *hỗn hợp SiH_4-He, màng a-Si:H, các hệ số chuyển động electron, phương trình xấp xỉ Boltzmann bậc hai, Bolsig+.*

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1. INTRODUCTION

Silane (SiH_4) is widely used in plasma-enhanced chemical vapor deposition (PECVD) using a capacitively coupled plasma (CCP) source to deposit the thin amorphous hydrogenated silicon (a-Si:H) films [1-4]. These CCP-deposited a-Si:H films play vital roles in various semiconductor applications such as solar panels [5], and flat panel displays [6, 7]. Changing the RF or gas mixture ratio is expected to help to increase the deposition rate of the thin film. The properties of the thin films would be also improved with different dilution gas.

Zhang and Zhang controlled the generation of HSRS to improve the photo-induced degradation of hydrogenated amorphous silicon (a-Si:H) films using the mixture of SiH_4 with H_2 ,He, and Ar [8]. H. Park and H. J. Kim [9] investigated the deposition of a hydrogenated silicon (Si:H) film using SiH_4-He CCP discharges using PECVD. Kim [10] investigated the two-dimensional self-consistent fluid model using SiH_4-He discharges. In recent years, several reliable models to model the SiH_4-based CCP deposition process have been successfully developed [1-4, 10-13]. The fluid model for gases or mixture gases typically require the electron transport coefficients and rate coefficients as the input data. In this study, the electron transport coefficients of SiH_4-He mixtures are obtained by using the Bolsig+ program [14]. The results of the research play an important role in understanding and exploiting the properties of plasma in scientific research and technological applications using SiH_4-He gas mixtures.

2. ANALYSIS

Bolsig+ is a Boltzmann solver, which developed by G. J. M. Hagelaar and L. C. Pitchford [14] to compute the electron transport data for gases or gas mixtures. The electron transport data include eletron mobility, mean energy, and diffusion coefficient. The mathematical expressions used to calculate the electron transport using Bolsig+ have been presented in detail in G. J. M. Hagelaar, L. C. Pitchford [14] and are briefly shown below:

Mean energy (eV):

$$<\varepsilon>=\int_0^\infty \varepsilon^{3/2} f_0 d\varepsilon \quad (1)$$

Mobility *N(1/m/V/s):

$$<\mu N>=-\frac{\gamma}{3}\int_0^\infty \frac{\varepsilon}{Q}\frac{\partial f_0}{\partial \varepsilon} d\varepsilon \quad (2)$$

Diffusion coefficient *N(1/m/s):

$$DN=\frac{\gamma}{3}\int_0^\infty \frac{\varepsilon}{Q} f_0 d\varepsilon \quad (3)$$

Here, f_0 is isotropic part of the EEDF and normalized by:

$$\int_0^\infty \varepsilon^{1/2} F_0 d\varepsilon = 1 \quad (4)$$

N is the concentration of atoms, Q is the effective momentum transfer cross section of electrons, $\gamma=(2e/m)^{1/2}$ is a constant and ε is the electron energy in electronvolts. The Bolsig+ freeware[14] is a useful tool to calculate the electron transport coeficients and it has been sucessfully applied for many gases and their mixtures such as He and Ar [15], N_2 and SF_6 [16], SiH_4 and C_2H_4 [17].

The important step in calculating electron transport coefficients is therefore to select the reliable set of cross sections for the gas mixture. The electron collision cross section sets were chosen from T. Itoh and T. Musha [18] for He and from M. Kurachi and Y. Nakamura [19] for SiH_4. The reliability of these sets have been proven in T. Itoh and T. Musha [18] for He and in M. Kurachi and Y. Nakamura [19] for SiH_4 molecules. The electron collision cross section sets for He atom and SiH_4 molecule were shown in Figs. 1 and 2. Information of electron collision cross sections for these molecules were also listed in the Table 1 for He atom and the Table 2 for SiH_4 molecule.

Table 1. Information of electron collision cross sections for He atom

Denoted	Electron collision cross section	Threshold energy
C1	Momentum transfer	
C2	Excitation	19.8eV
C3	Ionization	24.58eV

Table 2. Information of electron collision cross sections for SiH_4 molecule

Denoted	Electron collision cross section	Threshold energy
C4	Attachment	
C5	Momentum transfer	
C6	Excitation	0.11eV
C7	Excitation	0.27eV
C8	Excitation	7.7eV
C9	Excitation	8.4eV
C10	Ionization	11.6eV

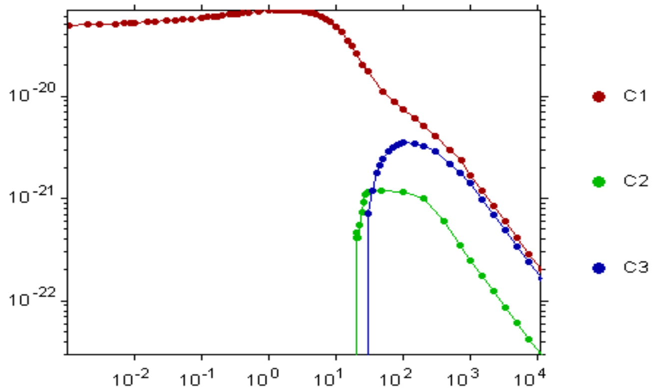

Fig. 1. Electron collision cross section set for He atom

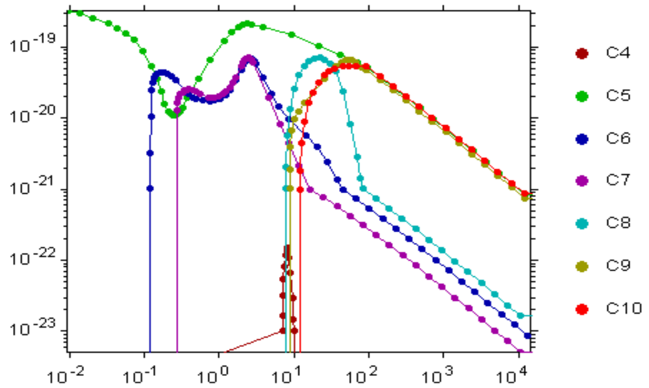

Fig. 2. Electron collision cross section set for SiH_4 molecule

Bolsig+ can calculate for any mixing ratio of the SiH_4-He gas mixture. However, the trends of the electron mobility coefficients in the gas mixture are generally similar, so in this study, the mixing ratios of 10%, 30%, 50%, 70%, and 90% SiH_4-He were chosen as representative.

3. RESULTS AND DISCUSSION

Fig. 3 shows the variation in electron mobility, μ/N, with respect to E/N for several mixing ratios of the SiH_4-He mixtures. The values of μ/N of pure He increase as the values of E/N increase while the values of μ/N of pure SiH_4 decrease as the values of E/N increase. The trend of the curves representing the values of μ/N of SiH_4-He mixture is similar to the curve representing the values of μ/N of pure SiH_4. The values of μ/N decrease rapidly in the E/N range of 0 - 50Td and become almost steady in the further range of E/N, 50 - 1000Td.

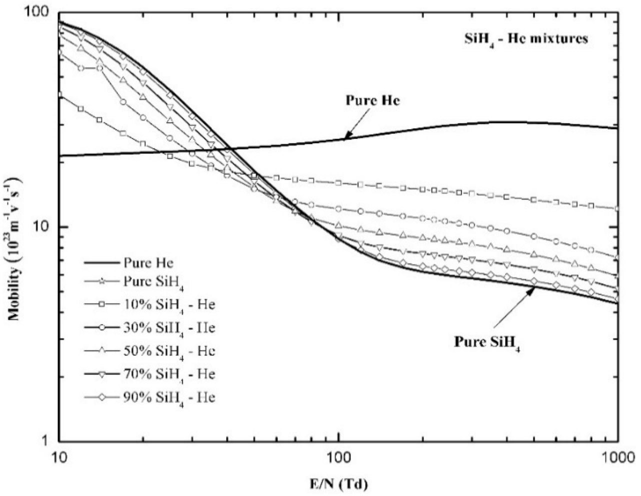

Fig. 3. The mobility μ/N in the SiH_4-He mixtures

Fig. 4 shows the variation in diffusion coefficient, DN, with respect to E/N for several mixing ratios of the SiH_4-He mixtures. The values of DN of pure He increase as the values of E/N increase. The values of DN of pure SiH_4 decrease in the E/N range of 30 - 100Td while increase in the remaining ranges of E/N as the values of E/N increase.

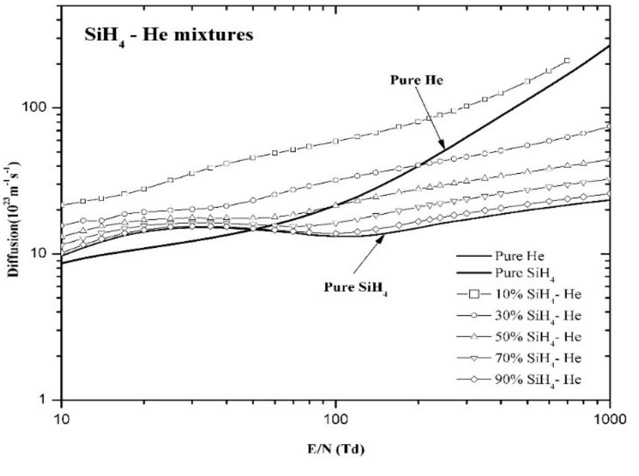

Fig. 4. Diffusion coefficient in the SiH_4-He mixtures

The trend of the curves representing the values of DN of SiH_4-He mixture is also similar to the curve representing the values of DN of pure SiH_4.

Fig. 5 gives the mean energy of SiH_4 molecule by the concentration of SiH_4 molecule in SiH_4-He mixture as functions of E/N. The mean energy of SiH_4 molecule increases with increasing E/N and decreases with increasing percentage of He atom in the mixture.

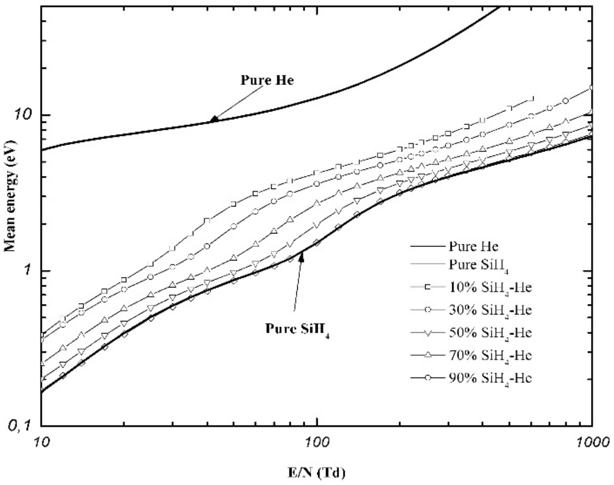

Fig. 5. Mean energy in the SiH_4-He mixtures

4. CONCLUSIONS

In this study, the electron transport, which include the mobility, diffusion coefficient and mean energy with respect to E/N for several mixing ratio of SiH_4-He mixtures, were calculated using the Bolsig+ program. The results were obtained based on the reliable electron collision cross section set for SiH_4 molecule and He atom. Therefore these electron transport of SiH_4-He mixture are useful input data for various applications using SiH_4-He mixture, especially in deposition of a-Si:H films using capacitively coupled plasma.

REFERENCES

[1]. S. Danko, D. Bluhm, V. Bolsinger, W. Dobrygin, O. Schmidt, R. P. Brinkmann, "A global model study of silane/hydrogen discharges," *Plasma Sources Sci. Technol*, 22, 055009, 2013.

[2]. Aman-ur-Rehman, H.C. Kwon, W. T. Park, J. K. Lee, "A study of the role of various reactions on the density distribution of hydrogen, silylene, and silyl in SiH_4/H_2 plasma discharges," *Phys. Plasmas*, 18, 093502, 2011.

[3]. K. D. Bleecker, D. Herrebout, A. Bogaerts, R. Gijbels, P. Descamps, "One-dimensional modelling of a capacitively coupled rf plasma in silane/helium, including small concentrations of O_2 and N_2," *J. Phys. D: Appl. Phys*, 36, 1826, 2003.

[4]. L. Layeillon, P. Duverneuil, J. P. Couderc, B. Despax, "Analysis and modelling of plasma enhanced CVD reactors. I. Two-dimensional treatment of a-Si:H deposition," *Plasma Sources Sci. Technol*, 3, 61, 1994.

[5]. M. Isomura, M. Kondo, A. Matsuda, "Device-grade amorphous silicon prepared by high-pressure plasma," *Jpn. J. Appl. Phys*, 41, 1947, 2002.

[6]. A. A. Howling, B. Legradic, M. Chesaux, C. Hollenstein, "Plasma deposition in an ideal showerhead reactor: a two-dimensional analytical solution," *Plasma Sources Sci. Technol*, 21, 015005, 2012.

[7]. L. Sansonnens, A. Pletzer, D. Magni, A. A. Howling, C. Hollenstein, J. P. M. Schmitt, "A voltage uniformity study in large-area reactors for RF plasma deposition," *Plasma Sources Sci.Technol*, 6, 170, 1997.

[8]. B. Zhang, X. Zhang, "Control of higher-silane generation by dilution gases in SiH_4 plasmas," *Plasma Sources Sci. Technol*, 29, 095012, 2020.

[9]. H. Park, H. J. Kim, "Theoretical Analysis of Si2H6 Adsorption on Hydrogenated Silicon Surfaces for Fast Deposition Using Intermediate Pressure SiH_4 Capacitively Coupled Plasma," *Coatings*, 11, 1041, 2021.

[10]. H. J. Kim, "Importance of Dielectric Elements for Attaining Process Uniformity in Capacitively Coupled Plasma Deposition Reactors," *Coatings*, 12, 457, 2022.

[11]. M. J. Kushner, "A model for the discharge kinetics and plasma chemistry during plasma enhanced chemical vapor deposition of amorphous silicon," *J. Appl. Phys*, 63, 2532, 1988.

[12]. E. Amanatides, S. Stamou, D. Mataras, "Gas phase and surface kinetics in plasma enhanced chemical vapor deposition of microcrystalline silicon: the combined effect of rf power and hydrogen dilution," *J. Appl. Phys*, 90, 5786, 2001.

[13]. A. Salabas, G. Gousset, L. L. Alves, "Two-dimensional fluid modelling of charged particle transport in radio-frequency capacitively coupled discharges," *Plasma Sources Sci. Technol*, 11, 448, 2002.

[14]. G. J. M. Hagelaar, L. C. Pitchford, "Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models," *Plasma Sources Sci. Technol*, 14, 722-733, 2005.

[15]. M. A. Ali, R. H. Majeed, "Calculation of electron transport parameters in noble gases: II. Helium and argon," *AIP Conference Proceedings*, 3097, 090012, 2024.

[16]. S. I. Ibrahim, E. A. Jawad, M. K. Jassim, "Study the effect of mixing N_2 with SF_6 gas on electron transport coefficients," *AIP Conference Proceedings*, 2386, 070003, 2022.

[17]. P. X. Hien, T. T. Son, D. A. Tuan, "Studying Electron Transport Coefficients in C_2H_4-SiH_4 Mixtures Using Bolsig+ Program," *International Conference on Engineering Research and Applications*, Cham: Springer International Publishing, 748-75, 2020.

[18]. T. Itoh, T. Musha, "Monte Carlo calculations of motion of electrons in helium," *Journal of the Physical Society of Japan*, 15(9), 1675-1680, 1960.

[19]. M. Kurachi, Y. Nakamura, "Electron collision cross sections for the monosilane molecule," *Journal of Physics D: Applied Physics*, 22.1, 107, 1989.

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