CALCULATION OF ELECTRON TRANSPORT COEFFICIENTS IN SiH_4-Xe USING BOLSIG$^+$ PROGRAM

Tính toán các hệ số chuyển động của electron trong hỗn hợp khí SiH_4 – Xe sử dụng chương trình Bolsig$^+$

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Abstract:

Microwave-excited plasma enhanced chemical vapor deposition using SiH_4-Xe to create polycrystalline silicon is grown at a temperature of 300 °C. The Bolsig+ program has been used to solve the Boltzmann equation (BE) using the direct simulation Monte Carlo (DSMC) method which is based on the Monte Carlo (MC) simulation for the limited number of fluid-flows. The plasma properties, which include energy mobility, energy diffusion coefficient and ionization coefficients in various concentrations of SiH_4-Xe mixture. In this paper, 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 10 -1000 Td (Townsend) were calculated using the Bolsig+ program for 10%, 30%, 50%, 70%, and 90% SiH_4-Xe mixture. Electron transport coefficients include mobility, electron energy distribution function (EEDF), diffusion coefficient, and ionization coefficient.

Keywords: SiH_4-Xe mixture, Polycrystalline silicon, Electron transport coefficients, Two-term Boltzmann approximation, Bolsig+ program.

Tóm tắt:

Lắng đọng hơi hóa học tăng cường plasma kích thích bằng vi sóng sử dụng SiH_4-Xe để tạo ra Silic đa tinh thể ở nhiệt độ 300°C. Phần mềm Bolsig+ đã được sử dụng để giải phương trình Boltzmann (BE) bằng phương pháp mô phỏng trực tiếp Monte Carlo (DSMC) dựa trên mô phỏng Monte Carlo (MC) cho dòng chất lỏng hữu hạn. Các đặc tính plasma, bao gồm độ linh động năng lượng, hệ số khuếch tán năng lượng và hệ số ion hoá ở các nồng độ khác nhau của hỗn hợp SiH4-Xe. Trong bài báo này, chúng tôi đã tính toán bằng chương trình Bolsig+ các hệ số vận chuyển electron liên quan đến E/N (tỷ lệ của trường điện E với mật độ số trung tính N) trong phạm vi 10-1000 Td (Townsend) cho hỗn hợp SiH4-Xe 10%, 30%, 50%, 70% và 90%. Các hệ số đó là độ linh động, hàm phân phối năng lượng electron (EEDF), hệ số khuếch tán, hệ số ion hóa.

Từ khóa: Hỗn hợp khí SiH_4 –Xe, Silic đa tinh thể, Hệ số chuyển động electron, Phương trình xấp xỉ bậc hai Boltzmann, Phần mềm Bolsig+.

I. INTRODUCTION

Low-temperature polycrystalline silicon has been used for thin-film transistors in liquid crystal displays for reason it has higher mobility than conventional amorphous silicon. Poly-Si layer must be manufactured at or below 300°C in order to eliminate thermal expansion/stress in thin multilayer structure on a very large substrate. Currently, poly-Si film has been obtained by recrystallizing the amorphous silicon layer with excimer laser irradiation. Silane (SiH_4) has been widely studied for polycrystalline and amorphous silicon deposition by plasma enhanced chemical vapor deposition (PECVD) [1]. A high-density plasma having low electron temperature can be achieved by this microwave plasma excitation system, especially when xenon gas is used.

Polycrystalline silicon (poly-Si) films are very important for silicon-gate metal oxide semiconductor (MOS) integrated circuits, charge-coupled devices, solar cells, thin-film transistors (TFT), and various other applications in semiconductor processing [2].

Changing the RF or gas mixture ratio is expected to help increase the deposition rate of the thin film. The properties of the thin films would also be improved with different dilution gases. Zhang and Zhang controlled the generation of HSRS to improve the photo-induced degradation of hydrogenated amorphous silicon

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(a-Si:H) films using a mixture of SiH_4 with H_2, He, and Ar [3]. Study the deposition of a hydrogenated silicon (Si:H) film using SiH_4-Xe Dielectric Barrier Discharge using PECVD [4]. In this study, the electron transport coefficients of SiH_4-He mixtures are obtained by using the Bolsig+ program [5].

II. ANALYSIS

Bolsig+ is considered a more generic and easier-to-use tool as compared to other BE solving methods. A wide variety of fundamental processes in gas–discharging plasma can be assessed and estimated using BE, which typically includes the process of electron–atom collisions, elastic collisions, electron-impacted atom excitation, the transition of collisions between the surrounding atoms, and the ion-atom collisions resulting from the elastic collision [6]. Bolsig+ program, which was developed by G.J. M. Hagelaar and L.C. Pitchford [7]. Therefore, these coefficients are important data for fluid models of gas discharges. The electron transport coefficients and EEDF can be obtained by solving Boltzmann [7]. The Bolsig+ freeware [7] is a useful tool to calculate the electron transport coefficients and it has been successfully applied for many gases and their mixtures such as He and Ar [8], N_2 and SF_6 [9], SiH_4 and C_2H_4 [10]. The validity of output results depends on the accuracy of the electron collision cross section set of using gases. Therefore, the electron collision cross section sets were chosen from [11] for SiH_4 and from [12] for Xe.

The electron collision cross section sets were chosen from [11] for SiH_4 and from [12] for Xe. The electron collision cross section sets for the Xe atom and SiH_4 molecule are shown in Figure 1 and 2. Information on electron collision cross sections for these molecules is also listed in Table 1 for the Xe atom and Table 2 for the SiH_4 molecule. The set of electron collision cross sections for the SiH_4 molecule consists of one elastic cross section , seven excitation cross section. The set of electron collision cross sections for the Xe molecule consists of cross sections for one attachment cross section and one momentum transfer cross section, five excitation cross section , one ionization cross section .

III. RESULTS AND DISCUSSION

In the present work, electron energy distribution function, the electron mobility, diffusion coefficients, ,mean energy and ionization cefficient and total collision frequency have been calculated with varying reduced electric field E/N at several concentrations of SiH_4–Xe gas mixture, above the excitation temperature of 300 K.

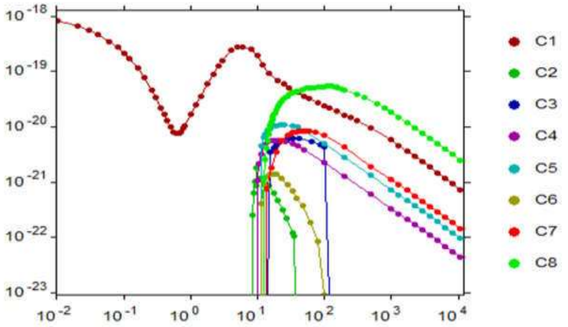

Figure 1. Electron collision cross section set for Xe atom.

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

Denoted	Electron collision cross section	Threshold energy (eV)
C1	Elastic	
C2	Excitation	8.31
C3	Excitation	8.44
C4	Excitation	9.69
C5	Excitation	10.0
C6	Excitation	11.0
C7	Excitation	11.7
C8	Excitation	12.12

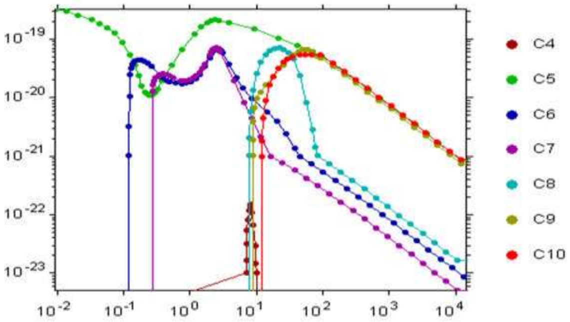

Figure 2. Electron collision cross section set for SiH_4 molecule.

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

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

In this study, the coefficients for the fluid model, which include energy mobility, energy diffusion coefficient, and ionization cefficient in SiH_4 – Xe mixtures with several concentrations, were calculated using Bolsig+ freeware. Figure 3-7. The EEDF for 1 Td, 10 Td, and 100 Td in a 10% SiH_4 – 90% Xe mixture was calculated and shown in Figure 3. The mobility and diffusion coefficient of electrons, related to the concentration of SiH_4 – Xe mixtures, are given in Figure 4 and 5 as functions of E/N. Figure 6 gives the ionization coefficient of the SiH_4 molecule by the concentration of the SiH_4 molecule in the SiH_4 – Xe mixture as functions of E/N. We calculated for different ionization degrees and shown in Figure 7. It is clear to see that the electron-electron collisions in the fluid model for SiH_4 – Xe mixture affect the ionization coefficients. It is clear to see that the ionization coefficient depends not only on E/N or the mean energy, but also on the ionization degree.

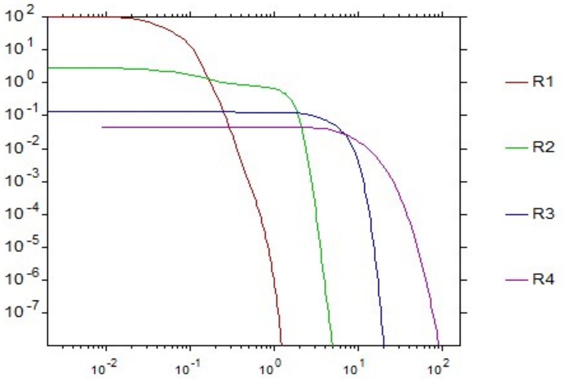

Figure 3. EEDF for 10% SiH_4- 90% Xe mixtures at 1 Td (R1 curve), 10 Td (R2 curve) and 100 Td (R3 curve) and 1000Td (R4 curve).

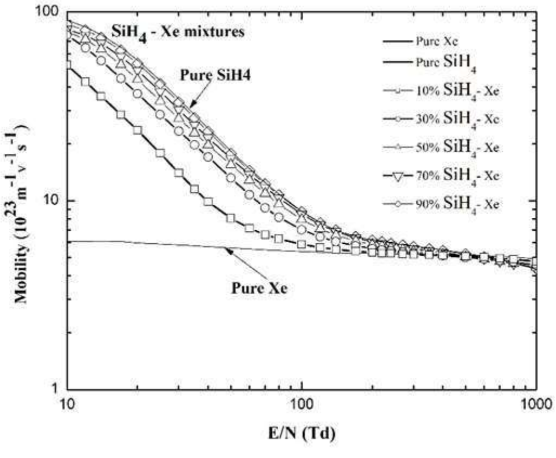

Figure 4. The mobility E/N in the SiH_4-Xe mixtures.

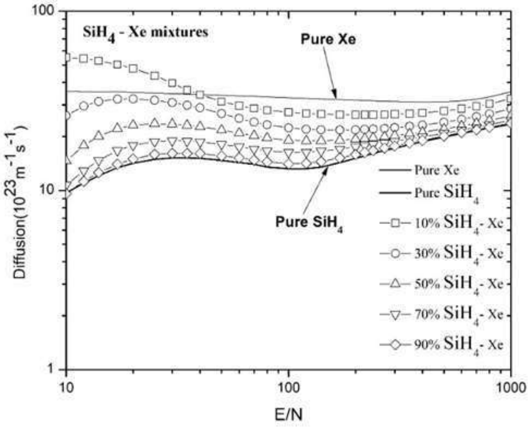

Figure 5. Diffusion coefficient in the SiH_4-Xe mixtures.

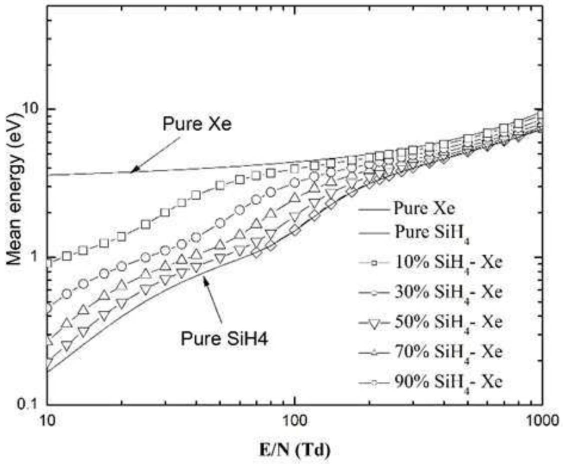

Figure 6. Mean energy in the SiH_4-Xe mixtures.

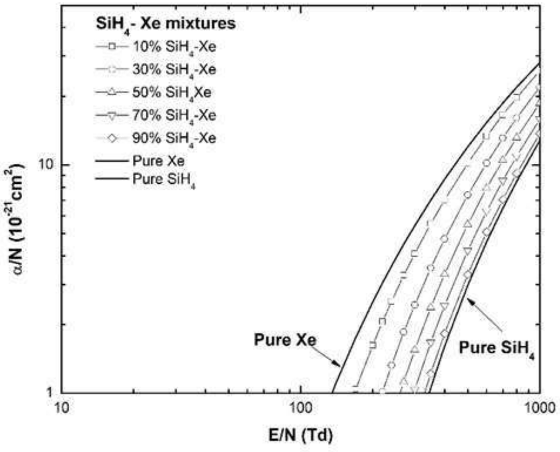

Figure 7. Ionization coefficient in the SiH_4-Xe mixtures.

IV. CONCLUSIONS

The electron mobility coefficients, including energy mobility, diffusion coefficient, and ionization coefficient, were calculated for SiH_4 – Xe mixtures using Bolsig+ freeware. These results are based on reliable electron collision cross-section sets for SiH_4 and Xe molecules. Therefore, these calculated plasma properties are useful data for various applications using SiH_4 – Xe mixtures, especially in dielectric barrier discharge and plasma-enhanced chemical vapor deposition.

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