ELECTRON TRANSPORT COEFFICIENTS AND RATE COEFFICIENTS IN C_2H_4-N_2 MIXTURE FOR FLUID MODEL

CÁC HỆ SỐ CHUYỂN ĐỘNG CỦA ELECTRON VÀ HỆ SỐ TỶ LỆ TRONG HỖN HỢP KHÍ C_2H_4-N_2 CHO MÔ HÌNH CHẤT LỎNG

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Ngày nhận bài: 20/5/2018, Ngày chận bài: đăng: 04/6/2018, Phản biện: TS. Phạm Mạnh Hải

Abstract:

Fluid models of C_2H_4-N_2 mixture play vital role in various industrial applications. The plasma properties, which include energy mobility, energy diffusion coefficient and rate coefficients in various concentrations of C_2H_4 in C_2H_4-N_2 mixture, were calculated using Bolsig+ freeware based on reliable electron collision cross section sets for C_2H_4 and N_2 molecules. The electron energy distribution function in case of no electron-electron collision and case of electron-electron collision with different ionization degrees were also discussed.

Keywords:

Bolsig, electron collision cross sections, Boltzmann equation, fluid model, plasma properties.

Tóm tắt:

Các mô hình chất lỏng của hỗn hợp khí C_2H_4-N_2 đóng vai trò quan trọng trong các ứng dụng công nghiệp khác nhau. Các tính chất plasma bao gồm tính biến động năng lượng, hệ số khuếch tán năng lượng và hệ số tỷ lệ theo các mật độ khác nhau của khí C_2H_4 trong hỗn hợp khí C_2H_4-N_2 được tính toán bằng phần mềm Bolsig+ dựa trên các bộ tiết diện va chạm electron tin cậy của các phân tử C_2H_4 và N_2. Hàm phân bố năng lượng của electron trong trường hợp không có va chạm electron-electron và trường hợp có va chạm electron-electron với các mức độ ion hoá khác nhau cũng được thảo luận.

Từ khóa:

Bolsig, các bộ tiết diện va chạm electron, phương trình Boltzmann, mô hình chất lỏng, tính chất plasma.

1. INTRODUCTION

Fluid models of gas discharge describe the transport of electron, ions and other reactive particle species in gaseous molecules. The electron transport coefficients and rate coefficient mainly depend on the electron energy distribution function (EEDF). Therefore, these coefficients are important data for fluid models of gas discharges. The electron transport coefficients and EEDF can be obtained by solving Boltzmann equation. G.J.M. Hagelaar and L.C. Pitchford [1] have analysed the relationship between the electron transport coefficient which calculated by solving Boltzmann equation (BE) with common fluid equations. They have also developed Bolsig+ freeware to calculate the electron transport coefficients and rate coefficients that are input data for fluid models.

The use of C_2H_4-N_2 mixtures has been significant in the process of laboratory dielectric barrier discharge and plasma-enhanced chemical vapor deposition [2-5]. Well-organized simulation methods are necessary to provide plasma properties that often difficult to obtain from experiments. However, there is no report of plasma properties for C_2H_4-N_2 mixtures. Therefore, in this study, the coefficients for fluid model, which includes energy mobility, energy diffusion coefficient and ionization rate coefficient in C_2H_4-N_2 mixtures, were calculated using Bolsig+ freeware. These coefficients are important input data for numerical simulation of gas discharge [1, 6, 7].

In this study, the EEDF of this mixture were also disccused in both case of no electron-electron collisions and case of electron-electron collisions with different ionization degrees

2. ANALYSIS

Bolsig+ freeware, which developed by G. J. M. Hagelaar and L. C. Pitchford [1] to generate data for fluid discharge modeling. These results include mobility, mean energy, rate coefficients, energy loss coefficients [1]. This software based on solving the Boltzmann equation [1]. In ionized gases, the Boltzmann equation for an ensemble of electrons is given as:

$$\frac{\partial f}{\partial t} + v \cdot \Delta f - \frac{e}{m} E \cdot \nabla_v f = C[f] \qquad (1)$$

Where f is the electron distribution in six-dimensional phase space, v are the velocity coordinates, e is the elementary charge, m is the electron mass, E is the electric field, ∇_v is the velocity-gradient operator and C represents the rate of change in f due to collisions. After solving this equation, transport coefficients of electrons are calculated as following:

Mean energy:

$$\bar{\varepsilon} = \int_0^\infty \varepsilon^{3/2} F_0 d\varepsilon \qquad (2)$$

Energy mobility:

$$\mu_\varepsilon N = -\frac{\gamma}{3}\int_0^\infty \frac{\varepsilon}{\sigma}\frac{\partial F_0}{\partial \varepsilon} d\varepsilon \qquad (3)$$

Energy diffusion coefficient:

$$D_\varepsilon N = \frac{\gamma}{3}\int_0^\infty \frac{\varepsilon}{\sigma} F_0 d\varepsilon \qquad (4)$$

Rate coefficient:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k F_0 d\varepsilon$$ (for each collision process) (5)

Here, F_0 is isotropic part of the EEDF and normalized by:

$$\int_0^\infty \varepsilon^{1/2} F_0 d\varepsilon = 1 \qquad (6)$$

N is the concentration of atoms, σ 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, σ_k is the effective momentum transfer cross section accounting for pobssible anisotropy of the elastic scattering.

The Bolsig+ freeware [1] is a good simulation tool for understanding of gas discharge. It is sucessfully used for many gases and their mixtures such as Ar and N_2 [1], Xe and Ne [8], SiH_4 and H_2[9].

As shown in above equations, the electron collision cross section sets for C_2H_4 and N_2 molecules are required as input data. The validity of output results depend on accuracy of electron collision cross section set of using gases. Therefore, the electron collision cross section sets were therefore chosen from [10] for C_2H_4 and from [11] for N_2. The reliability of these sets have been proven in [10] for C_2H_4 and in [11] for N_2 molecules.

3. RESULTS AND DISCUSSION

The electron collision cross section sets for C_2H_4 and N_2 molecules were shown in Figs. 1 and 2. Information of electron collision cross sections for these molecules were also listed in Table 1 for C_2H_4 molecule and Table 2 for N_2 molecule. The coefficients for fluid model, which include energy mobility, energy diffusion coefficient and ionization rate coefficient in C_2H_4-N_2 mixtures with several concentrations, were calculated using Bolsig+ freeware and shown in Figs. 3-6. The mobility and diffusion coefficient of electrons, related to the concentration of C_2H_4-N_2 mixtures, are given in Figs. 3 and 4 as functions of E/N. The mobility decreases with increasing E/N while the diffusion coefficient increases with increasing E/N. The mobility and diffusion coefficient in C_2H_4-N_2 mixtures are suggested to be between with those in pure C_2H_4 and N_2 molecules. The mobility and diffusion coefficient in C_2H_4-N_2 mixtures decreases with increasing percentage of C_2H_4 in mixture.

Fig. 5 gives the ionization rate coefficient of C_2H_4 molecule by the concentration of C_2H_4 molecule in C_2H_4-N_2 mixture as functions of E/N. The rate of ionization coefficient of C_2H_4 molecule increases with increasing E/N and decreases with increasing percentage of C_2H_4 molecule in the mixture.

In this study, the influence of electron-electron collisions in C_2H_4-N_2 mixture was analyzed. For example, the EEDF in 50%C_2H_4-50%N_2 mixtures at 1, 10 and 100 Td, were calculated and shown in Fig.6. The EEDF for 10 Td in 50%C_2H_4-50%N_2 mixture, taking into account electron-electron collisions, were calculated for different ionization degrees and shown in Fig. 7. It is clearly to see that the electron-electron collisions in fluid model for C_2H_4-N_2 mixture affect to ionization rate coefficients. It is clearly to see that the ionization rate coefficient depends not only on E/N or the mean energy, but also on the ionization degree.

Table 1. Information of electron collision cross sections for C_2H_4 molecule

Denoted	Electron collision cross section	Threshold energy
C1	Attachment	
C2	Momentum transfer	
C3	Excitation	0.12 eV
C4	Excitation	0.18 eV
C5	Excitation	0.37 eV
C6	Excitation	4.4 eV
C7	Excitation	7.7 eV
C8	Ionization	10.6 eV

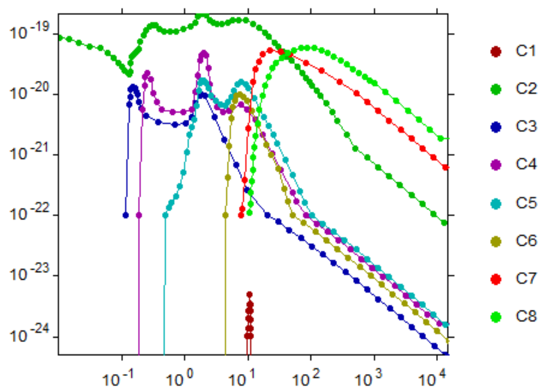

Figure 1. Electron collision cross section set for C_2H_4 molecule

Table 2. Information of electron collision cross sections for N_2 molecule

Denoted	Electron collision cross section	Threshold energy
C9	Momentum transfer	
C10	Excitation	0.02 eV
C11	Excitation	0.29 eV
C12	Excitation	0.29 eV
C13	Excitation	0.59 eV
C14	Excitation	0.88 eV
C15	Excitation	1.17 eV
C16	Excitation	1.47 eV
C17	Excitation	1.76 eV
C18	Excitation	2.06 eV
C19	Excitation	2.35 eV
C20	Excitation	6.17 eV
C21	Excitation	7.00 eV
C22	Excitation	7.35 eV
C23	Excitation	7.36 eV
C24	Excitation	7.80 eV
C25	Excitation	8.16 eV
C26	Excitation	8.40 eV
C27	Excitation	8.55 eV
C28	Excitation	8.89 eV
C29	Excitation	11.03 eV
C30	Excitation	11.87 eV
C31	Excitation	12.25 eV
C32	Excitation	13.00 eV
C33	Ionization	15.60 eV

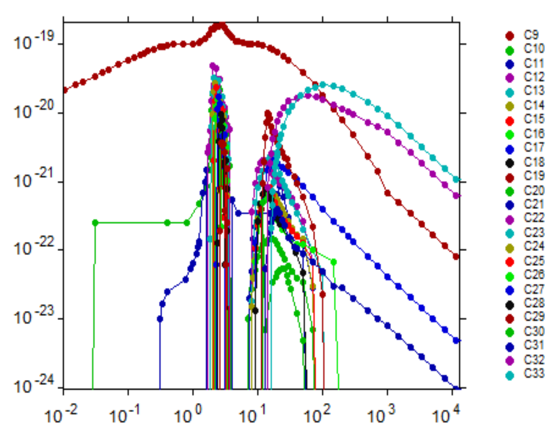

Figure 2. Electron collision cross section set for N_2 molecule

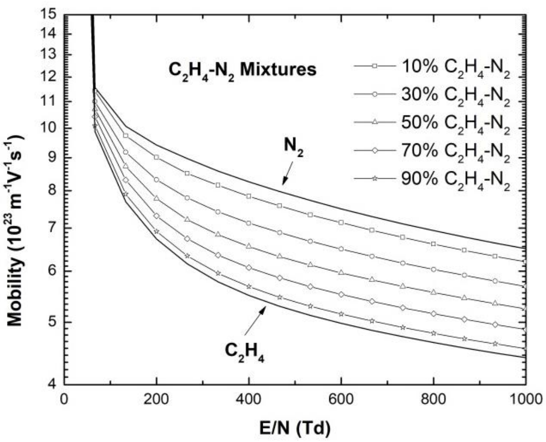

Figure 3. Energy mobility in C_2H_4-N_2 mixtures

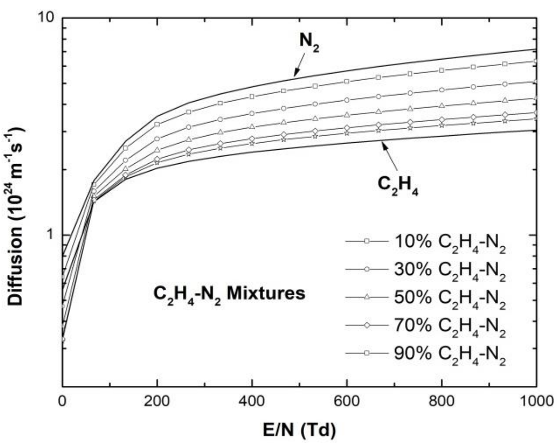

Figure 4. Energy diffusion coefficient in C_2H_4-N_2 mixtures

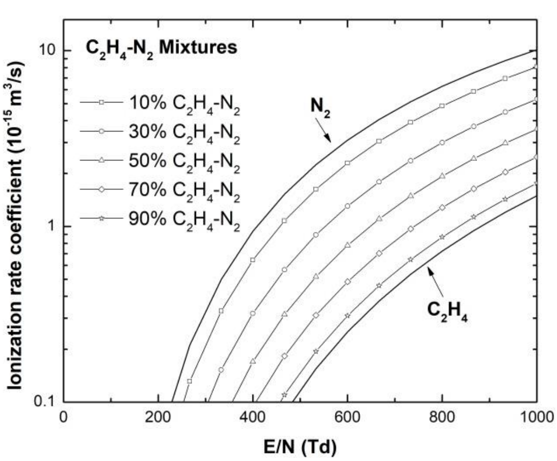

Figure 5. Ionization rate coefficient in C_2H_4-N_2 mixture

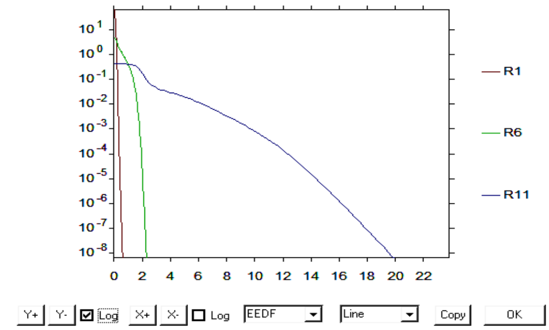

Figure 6. EEDF for C_2H_4-N_2 mixtures at 1 Td (R1 curve), 10 Td (R6 curve) and 100 Td (R11 curve)

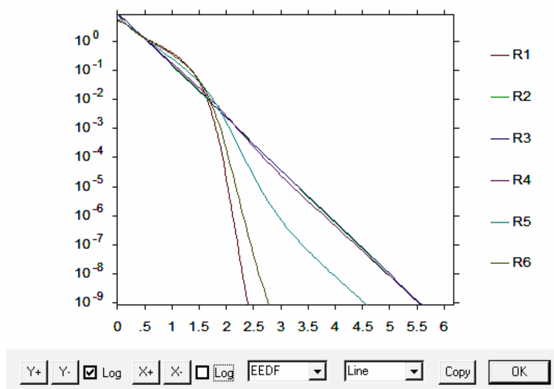

Figure 7. EEDF for 10 Td in C_2H_4-N_2 mixture, taking into account electron-electron collisions, for different ionization degrees. R1 curve shows EEDF without e-e collision. R2, R3, R4, R5 and R6 curves show EEDF for, ionization degree is 10^{-2}, 10^{-3}, 10^{-3},10^{-4},10^{-5} and 10^{-6}, respectively

4. CONCLUSIONS

The plasma properties, which include energy mobility, energy diffusion coefficient, and ionization rate coefficient, were calculated for C_2H_4-N_2 mixtures using Bolsig+ freeware. These results based on reliable electron collision cross section sets for C_2H_4 and N_2 molecules. Therefore, these calculated plasma properties are useful data for various applications using C_2H_4-N_2 mixture, especially in dielectric barrier discharge and plasma-enhanced chemical vapor deposition.

ACKNOWLEDGEMENTS

This research was supported by Center for Research and Applications in Science and Technology, Hung Yen University of Technology and Education, under grant number UTEHY.T014.P1718.28.

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