Ann. Rep. Fac. Educ., Iwate Univ., Vol. 49 No. 1 (1989. 10), 69~78

Electron Swarm Parameters in SiH_4/H_2.

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(Received June 30, 1989)

Abstract.

A Monte Carlo technique is used for investigating electron swarm motion in the presence of elastic, excitation, ionization and attachment collisions through a SiH_4(20%)/H_2(80%) mixture under uniform field conditions. It has been shown that mixing a fraction of SiH_4 into the hydrogen gas gives rise to drastic changes in the electron energy distribution function. This fact indicates that the swarm parameters in the mixture can not be reduced by combining each of the swarm parameters obtained individually in SiH_4 and H_2 assuming a linear relationship of the values to their partial pressure ratios. The swarm parameters for drift velocity (v_d), mean energy (ε), ionization (α/p), excitation (α_{ex}/p), dissociation (α_d/p) and attachment (η/p) coefficients are evaluated directly by using the electron energy distribution functions obtained by the simulation in the E/p range of 10–2000 *V/cmTorr*.

1. Introduction.

Low pressure glow discharges in SiH_4 and SiH_4/H_2 mixtures have been investigated in relation to the fabrication of amorphous silicone films. For the theoretical analysis of the discharge processes such as modeling of the discharge development, precise data on the electron swarm parameters need to be investigated. However, no data in silane-hydrogen mixtures have been published so far, although the electron transport through a background of the silane gas has been studied by Ohmori (1986) using Boltzmann equation analysis and in hydrogen the swarm parameters have been reported by a number of previous workers (Folkard, 1971 ; Kontoleon, 1973 ; Saelee, 1977).

When the swarm parameters for each of the component gases in the mixture are known, values of the parameters in the mixture used to be evaluated by assuming a linear relationship between these values and the partial pressure ratios of the mixed component gases. This method may be only valid when the electron collision cross sections of the component gases are so similar to each other that the electron energy distribution is not so much modified by mixing these gases.

For the case of SiH_4/H_2 mixtures, this assumption is not realistic since the electron colli-

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sion cross sections of silane are about one order of magnitude larger than those of hydrogen. Therefore the swarm parameters in the mixture should be obtained directly from a set of collision cross sections compiled with the cross section data of hydrogen and silane by taking into account the partial pressure ratio of the mixture.

In the present paper, a Monte Carlo simulation of electron swarm motion in the mixture of $SiH_4(20\%)/H_2(80\%)$ in a steady state condition is carried out under various values of the uniform field strength. The calculation method used here is basically the same as that proposed by Itoh and Musha(1960) and developed by Sakai et al (1972). At the first step of the calculation, the electron energy distribution functions for various values of E/p are obtained and then used for evaluating the swarm parameters such as the drift velocity, mean energy and ionization, excitation, dissociation and attachment coefficients. Simulation results in the mixture are discussed by comparing with data obtained in the silane or hydrogen single gas.

2. Computational method.

2.1 Tracking of electron motion.

An electron is released at the cathode, $x=0$, with an energy so that the initial electrons can have a uniform energy distribution in the energy range from 0 to $\Delta\varepsilon$ $(=h\nu-\phi)$ eV. $h\nu$ and ϕ are respectively the energy of the external irradiation light on the cathode surface and the work function of the cathode electrode. The initial electron is also assigned a direction of motion θ, an angle to the electric field direction. After a flight of a length Δl, which is less than one-tenth of the elctron mean free path, the electron velocity v, energy ε and direction of motion θ are determined from the momentum and energy conservation laws as follows:

$$\varepsilon' = \frac{1}{2}mv'^2 = \frac{1}{2}mv^2 + eE\Delta x$$

$$m'v'\cos\theta' = mv\cos\theta + eE\Delta t$$

$$m'v'\sin\theta' = mv\sin\theta$$

$$\Delta x = \Delta l\cos\theta$$

$$v' = \sqrt{\frac{2e}{m}E\Delta l\cos\theta + v^2}$$

$$\cos\theta' = \pm\frac{1}{v'}\sqrt{\frac{2e}{m}E\Delta l\cos\theta + v^2\cos^2\theta}$$

$$\Delta t = \frac{m}{eE}\left[\pm\sqrt{\frac{2e}{m}E\Delta l\cos\theta + v^2\cos^2\theta} - v\cos\theta\right]$$

where ε', v' and θ' represent the situation of the electron motion after a flight of Δl. The electron motion is tracked in this way to the first collision. The collision event is ascertained

at every path length by comparing a uniform random number with the collision probability represented as

$$P_{\Delta l}=Nq_T(v)\Delta l$$

where N is the number density of the sample gas and q_T is the total collision cross section of the mixture.

Types of collision such as elastic and inelastic collisions are also determined by comparing the ratios of the cross sections q_{el}(elastic), q_{ex}(excitation), q_i(ionization), q_a(attachment) to the total cross section q_T with a random number ξ as follows :

$\xi \leqq q_{el}/q_T$; elastic collision,

$q_{el}/q_T \leqq \xi < [q_{el}+q_{ex}]/q_T$; excitation collision,

$[q_{el}+q_{ex}]/q_T \leqq \xi < [q_{el}+q_{ex}+q_a]/q_T$; attachment collision,

$[q_T-q_i]/q_T < \xi$; ionization collision,

When a collision event takes place, energy loses are calculated, which depends on the type of the collision. For the elastic collision the momentum transfer energy loss is subtracted and for the excitation collision the excitation threshold energy is subtracted. When the ionization collision occurs, the incident electron energy is reduced by the ionization threshold energy and the remainder is delivered to the newly born electron and to the parent electron with a ratio using a random number. Then the new direction of electron motion is determined by assuming spherical symmetry of the collision scattering. The progeny electron is also tracked in the same way as for the parent electron. This process is continued until the electron has passed through the gap space and absorbed into the anode or cathode. At both the cathode and anode surface, it is assumed that 50% of electrons reached the electrode may be reflected back to the gap space.

2 . 2 Cross sections and sampling method.

In order to save computing time, a set of simplified cross sections of the mixture is used for the calculation ; the excitation cross sections are combined into a single one and the energy dependence of the cross sections is approximated so that the collision frequencies reduced from the cross section data can be represented with linear lines as shown in figures 1 and 2. The cross section data of hydrogen and silane are taken respectively from the data compiled by Taniguchi (1979) and by Ohmori (1986). The set of the cross sections for SiH_4 (20%)/H_2(20%) are obtained by adjusting each of the cross section in silane and in hydrogen according to the partial pressure.

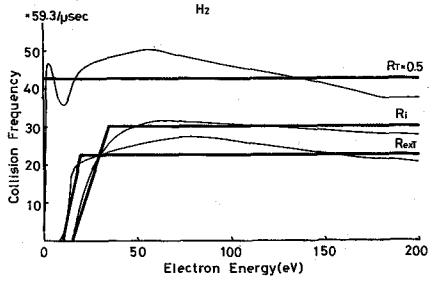

Figure 1. Electron collision frequencies in hydrogen.
R_T, R_i, and R_{exT} are respectively the total momentum transfer, ionization and total excitation collision frequencies.

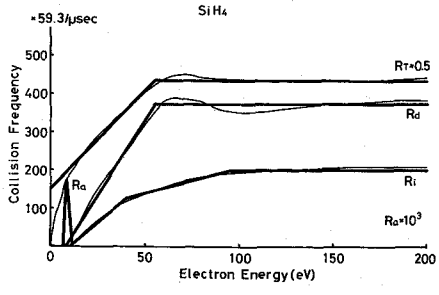

Figure 2. Electron collision frequencies in SiH_4.
R_T, R_i, R_d, and R_a are respectively the total momentum transfer, ionization, dissociation and attachment collision frequencies.

At the end of the simulation process, average values for the electron energy ε, velocity v and the other inelastic collision frequencies are obtained using the steady state Townsend (SST) sampling method for a series of fixed spatial intervals Δx_s in the gap space.

The drift velocity v_d and electron mean energy $\bar{\varepsilon}$ are calculated using formulae,

$$v_d(x) = \sum_{j=1}^{N} v_j \cos\theta_j \Delta t_j / \sum_{j=1}^{N} \Delta t_j \quad \text{and} \quad \bar{\varepsilon}(x) = \sum_{j=1}^{N} \varepsilon_j \Delta t_j / \sum_{j=1}^{N} \Delta t_j,$$

where Δt_j is the staying time of the jth electron in the region Δx_s and N is the total number of electrons which pass though the region Δx_s.

The electron energy distribution function $f(\varepsilon)$ is obtained with formula,

$$f(\varepsilon, x) = \sum_{j=1}^{N} \delta_j(\varepsilon, x) \Delta t_j / \sum_{j=1}^{N} \Delta t_j$$

where $\delta_j(\varepsilon)$ is unity when the jth electron is sampled in the energy range $\varepsilon \sim \varepsilon + \Delta\varepsilon$.

The ionizatin, excitation, dissociation and attachment frequencies are obtained with formula,

$$R_k(x) = \sum_{j=1}^{N} V_1 \varepsilon_j^{1/2} q_k(\varepsilon_j) \Delta t_j / \sum_{j=1}^{N} \Delta t_j,$$

where the subscript k corresponds to the type of collisions and V_1 is the electron velocity at 1 eV.

3. Results and discussions.

Figure 3 shows the electron energy distribution function in the mixture at $E/p=200$ $V/cmTorr$ in comparison with those in hydrogen and in silane. In hydrogen, the high energy tail of the distribution function is significant. This results from small values of both the elastic and inelastic collision cross sections of hydrogen. For the case of the silane gas, it should be noticed that the cross sections of silane are about one order of magnitude larger than those of hydrogen, therefore a number of high energy electrons in silane decreases sharply with increasing electron energy. When the silane gas is mixed with the hydrogen gas, the high energy tail of the distribution function of the mixture can give rise to dramatic changes of the swarm parameters associated with the silane molecules.

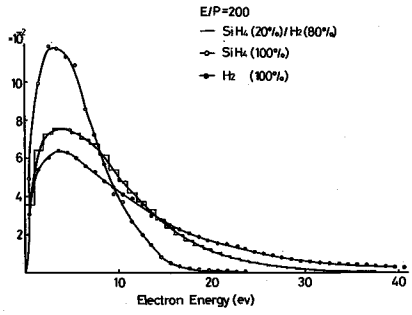

Figure 3. Electron energy distribution functions in H_2, SiH_4 and SiH_4/H_2 at E/p=200 V/cmTorr.

In order to obtain steady state values of the swarm parameters, the non-equilibrium region for the electron swarm in the gap space needs to be ascertained. Figure 4 shows the spatial variations of the ionization, excitation and attachment coefficients and the electron mean energy calculated at $E/p=200$ $V/cmTorr$ at a pressure of 0.25 $Torr$. In front of the cathode surface, the non-eqilibrium characteristic of the electron swarm is observed in the spatial range of $x=0\sim0.5$ cm. The non-equilibrim region is also observed in front of the anode surface, which is narrower than that of the cathode. Consequently the equilibrium values of the swarm parameters are obtained by taking the values in the spatial range around mid gap.

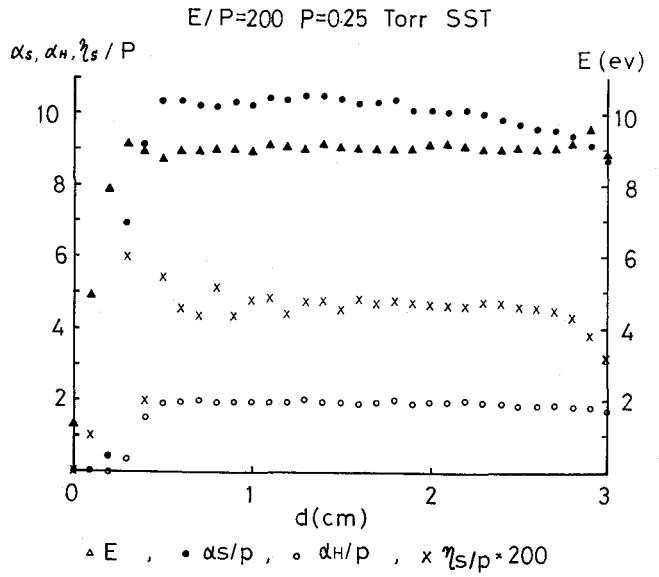

Figure 4.
Spatial variations of the swarm parameters (SST sampling) in SiH_4/H_2 at $E/p=200\,V/cmTorr$ at a pressure of 0.25 Torr.

Figure 5 shows the ionization coefficients of silane and hydrogen molecules in the mixture. The ionization coefficients in the single gas of silane and hydrogen are also shown in this figure. A significant observation is that in the high E/P range the ionization coefficient

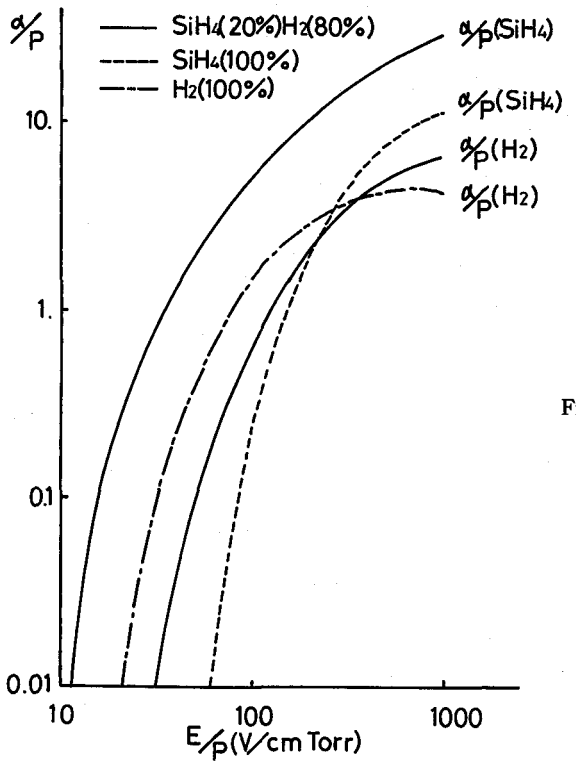

Figure 5. Comparison of the ionization coefficients in SiH_4/H_2 with the ionization coefficients in the H_2 and SiH_4 single gases.

α_S/p of the silane molecule in the mixture is 3～10 times larger than that in the silane single gas and that the curve α_S/p versus E/p is extended to the low E/p region. This results from the appearance of the high energy tail in the electron energy distribution due to mixing of the hydrogen gas. On the other hand, the ionization coefficient α_H/p of the hydrogen molecule in the mixture decreases more sharply than that in the hydrogen single gas with decreasing E/p. This is caused by the reduction of high energy electrons in the low E/p range due to mixing of the silane gas. These facts indicate that the ionization coefficient in the mixture can not be obtained by combining α_S/p and α_H/p in each single gas of silane and hydrogen according to their partial pressures of the mixture.

Figure 6 shows the attachment frequency R_a/p of the silane molecule in the mixture in comparison with that in the silane single gas. Although the values of the attachment frequencies are 2～3 order of magnitude smaller than the ionization frequencies as shown in this figure, the attachment process plays an important role for the plasma development in SiH_4 and SiH_4/H_2 mixtures (Sato, 1989). As shown in figure 2, the attachment cross section has a resonant type characteristic with a low energy threshold. This indicates that the value of the attachment frequency is mainly determined by a number of low energy electrons in the

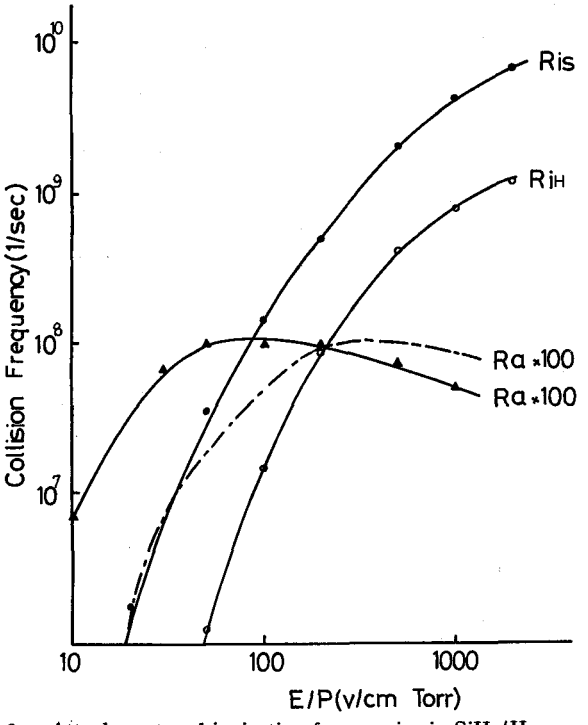

Figure 6. Attachment and ionization frequencies in SiH_4/H_2.
R_{iS} and R_{iH} are respectively the ionization frequencies of the silane and hydrogen molecules. R_a is the attachment frequency of the silane molecule. Dashed line is R_a in the silane single gas.

energy range around the threshold energy. Therefore the variation of the electron energy distribution in the low energy range results in a drastic change for the E/p dependence of the attachment frequency. The curve R_a/p versus E/p of the mixture shifts from that of the silane single gas to the low E/p region. This is explained by the fact that in the silane single gas the number of electrons in the energy range around 7 eV decreases more sharply than that in the mixture with decreasing E/p.

Figure 7 shows the dissociation frequencies of the silane and hydrogen molecules in the mixture calculated by using the electron energy distribution function of the mixture with the cross sections R_d and $b^3\,\Sigma_u^+$ shown in figures 2 and 8, respectively. Also shown is the excitation frequency of the hydrogen molecule to the state $a^3\,\Sigma_g^+$ which can emit photons observable from actual discharge plasmas of the mixture. The dissociation frequency R_d/p of the silane molecule in the mixture is about five times larger than that in the silane single gas in the high E/p region and the curve R_d/p versus E/p of the mixture is extended to the low E/p region. It may be a valuable information for the development of the plasma processing technique to know that in the silane-hydrogen mixture the dissociation event can take place more frequently than in silane even in a low electric field condition.

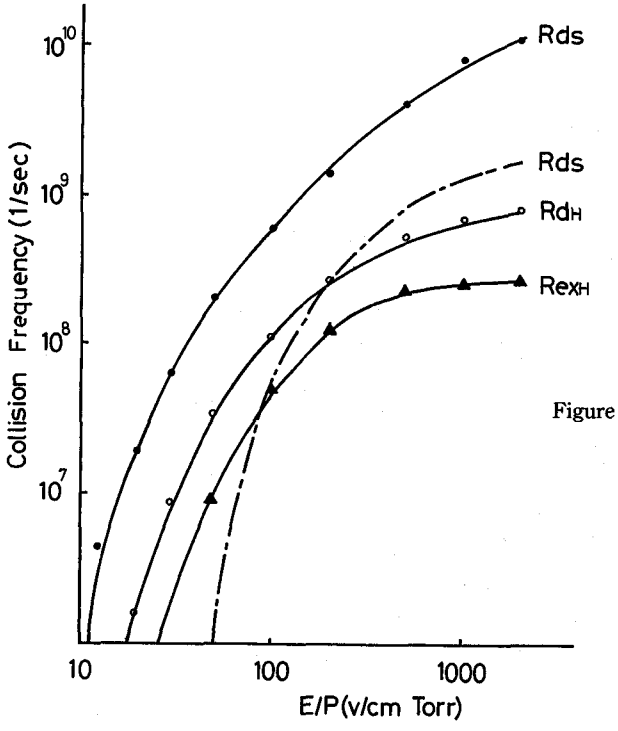

Figure 7. Dissociation and excitation frequencies in SiH_4/H_2. R_{ds} and R_{dH} are respectively the dissociation frequencies of the silane and hydrogen molecules. Dashed line is R_{ds} in the silane single gas.

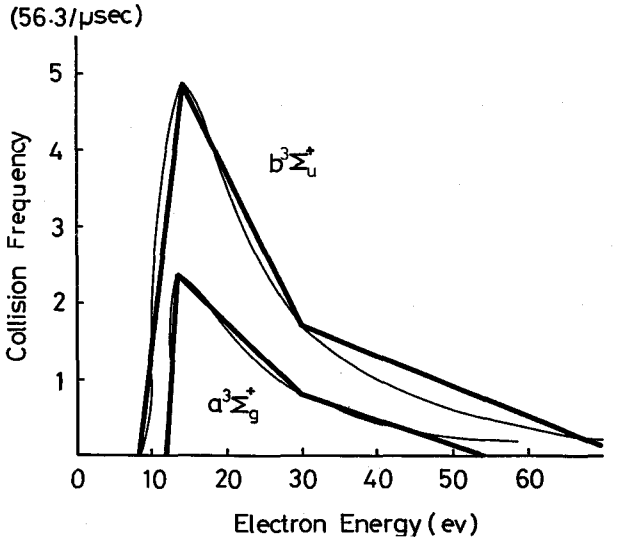

Figure 8. Excitation collision frequencies of the hydrogen molecule to the $a^3\Sigma_g^+$ and $b^3\Sigma_u^+$ states.

As described above, the drastic change of the swarm parameter in the mixture should be explained by the variation of the electron energy distribution. As shown in figure 9, however, the electron mean energy in the mixture is only ~2 times larger than that in the silane single gas within the whole E/p range presented here, while the values of the swarm parameters change about one order of magnitude from those in the silane single gas. This indicates that not only the value of electron mean energy but also the variation of the high energy tail in the electron energy distribution function are responsible for the drastic variations of the swarm parameters by mixing SiH_4 into H_2.

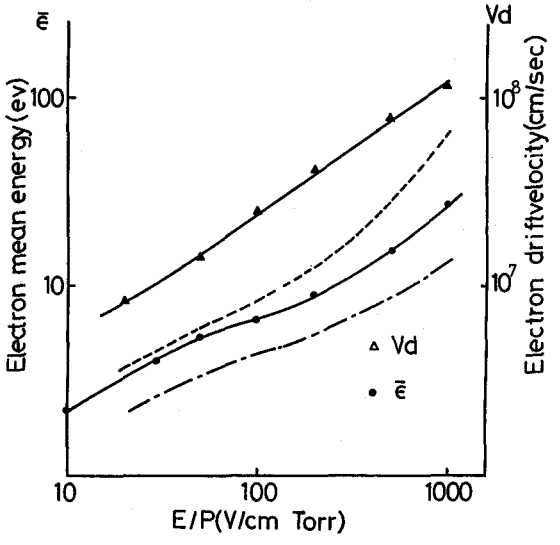

Figure 9. Electron mean energy and drift velocity in the mixture.
····· mean energy in hydrogen,
— · — mean energy in silane.

4. Conclusion.

The swarm parameters in a silane-hydrogen mixture have been evaluated by using the Monte Carlo technique and discussed in comparison with the swarm parameters in silane or in hydrogen. Mixing of a small amount of the silane gas into the hydrogen gas gives rise to drastic changes in the electron energy distribution because the electron collision cross section of the silane gas is about one order of magnitude larger than those of the hydrogen gas. This results in significant variations of the swarm parameters in the mixture. In this study, for saving computing times, the simplified sets of the cross sections have been used for the simulation, which may bring ambiguity on the value of the obtained swarm parameters. Despite this, the values of the swarm parameters as well as their E/p dependence presented here may be a valuable information for the investigation of the plasma processing technique.

Further simulation analyses need to be carried out by using a set of precise cross section data with various values of mixing ratios.

Acknowledgment.

The authors wish to acknowledge valuable discussions with Dr. K. Kitamori of Hokkaido Institute of Technology. They also wish to thank Dr. Y. Ohmori of Hokkaido Polytechnic College for giving us information on the cross section data.

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