MONTE CARLO SIMULATION OF ELECTRON SWARM UNDER
HIGH FREQUENCY FIELDS

H. Tagashira, K. Kitamori, M. Shimozuma and Y. Sakai

§ Department of Electrical Engineering, Hokkaido University, Japan 060
§§ College of Medical Technology, Hokkaido University, Sapporo, Japan 060
§§§ Department of Industrial Engineering, Hokkaido Institute of Technology, Sapporo, Japan 061-24

ABSTRACT

The behaviour of electron swarm in high frequency fields (13.56 MHz) in SiH₄ and CH₄ is studied by a Monte Carlo method. The results show that the electron energy distribution and mean energy fluctuate appreciably during one cycle of the applied field and that the DC and AC energy distributions differ even under an equivalent condition. The longitudinal diffusion coefficient is found to keep an almost constant value even within one cycle.

1. INTRODUCTION

Recently, weakly ionized high frequency plasmas of monosilane (SiH₄) and other gases are often used in plasma processing of semiconductors and other purposes. The electron component in the plasmas serves as a generating agent of important dissociated, excited and ionized species as well as electron itself for maintaining plasma. However, knowledge on the properties of electrons in high frequency plasmas appears scarce, and particularly so in such an important gas as monosilane. The present article reports the results of a Monte Carlo simulation of the behaviour of electrons in monosilane, methane(CH₄) and monosilane and nitrogen mixtures at 13.56 MHz and 135.6 MHz for comparison in weakly ionized plasmas.

2. METHOD OF SIMULATION

A free flight time (FFT) technique is used. This technique utilizes the following formula to generate the free flight time t of an electron, which is being traced, between two successive collisions.

\[ \tau = \exp\left\{ -\int_0^\tau v(v) \, dt \right\} \]

(1)

Here, \( \tau \) is a random number between 0 and 1 and \( v = v(t) \) is the speed of the electron at time t. \( v \) is the electron collision frequency and is represented by

\[ v = qNv \]
where \( N \) is the gas number density and \( q \equiv q(v) \) is a total electron collision cross section:

\[
q \equiv q_m + q_v + q_d + q_{ex} + q_i
\]  \hspace{1cm} (2)

Here, the subscripts \( m, v, d, ex \) and \( i \) respectively refer to momentum transfer, vibration, dissociation, excitation and ionization.

When a collision is judged to occur, the kind of collision is determined by arranging equation (2) as

\[
1 = \frac{q_m}{q} + \frac{q_v}{q} + \frac{q_d}{q} + \frac{q_{ex}}{q} + \frac{q_i}{q}
\]  \hspace{1cm} (3)

and by comparing a newly generated random number \( \xi \) with the value of the successive sum of the right hand side terms of equation (3). The threshold energy is subtracted from the energy of the electron at the collision, then the speed of the electron just after the collision is determined. The direction of the electron just after the collision is specified by generating another random number assuming isotropy in scattering. When ionization occurs, the difference of the electron energy at the collision and the ionization threshold is distributed to the two electrons after the collision at a ratio of 0.8 to 0.2.

With the procedure described above and a simple Newtonian kinetics, the motion of an electron is now traced as a function of time. All of the electrons (the initial ones and the progenies) are traced (reference(1)). The sampling of the swarm parameters are done exactly following the definition of the parameters (reference(2)).

3. COLLISION CROSS SECTIONS

The electron collision cross sections used in the present article are shown in figures 1 and 2 respectively for monosilane and methane. The Townsend first ionization coefficient and electron drift velocity calculated from the cross sections agree well with experiment, particularly in a middle range of \( E/p_0 \). The cross sections for nitrogen are taken from reference(3).

4. RESULTS AND DISCUSSION

Figure 3 compares the electron energy distribution in \( \text{SiH}_4 \) for DC with that for AC (13.56 MHz). It is noted that for DC, \( E/p_0 \) is taken equal to 30 \( \text{V cm}^{-1}\text{Torr}^{-1} \) and an equivalent field strength of \( \sqrt{2} \) \( \times \) 30 \( \text{V cm}^{-1}\text{Torr}^{-1} \) at peak is assumed for AC. The AC distribution in figure 3 is the average distribution over a cycle. It is seen that unlike a prediction based on a two-term approximation (references(4), and (5)), the AC distribution clearly differs from that for DC, the AC distribution being shifted towards the origin in this case. As will be also shown later in figures 8 and 9 for \( \text{SiH}_4 \) and \( \text{CH}_4 \) mixtures, and for nitrogen, respectively, it appears that the DC electron energy distribution generally differ from each other.

Figure 4 shows the energy distributions in \( \text{SiH}_4 \) at the peak of
the field and at the instant at which the field crosses zero. It is seen that the distributions at these two typical instants differ considerably. The energy distribution at the zero crossing moment is shifted appreciably towards the origin, and abounds with electrons with very low energy and lacks electrons with medium and high energy. Particularly, the electrons with energies higher than about 8 eV are almost missing. From figure 1, one can see that this is due to inelastic collision processes.

Figure 5 shows the variation of the mean electron energy $\bar{e}$, the average electron speed $W_V$ (electron drift velocity for the pulsed Townsend experiment, see reference (6)) and the ionization frequency $R_i$ as a function of time. The peak value of $E/p_0$ is taken equal to 65 Vcm$^{-1}$Torr$^{-1}$ and 25% nitrogen is mixed with the rest (75%) of SiH$_4$. It is seen that $\bar{e}$ fluctuates with the double frequency and the variation is not purely sinusoidal. Moreover, the amplitude of variation is very large and some phase shift exists in reference to the variation of $E/p_0$.

The average velocity $W_V$ fluctuates almost in phase with the external field, but the shape is far from sinusoidal. The sharp transient just after the $E/p_0$ changes the sign is due to the fact that at the instant at which the field is low, low energy electrons abounds and these electrons start to move quickly when the field changes its sign because of the deep Ramsauer minimum of the momentum transfer cross section as seen in figure 1.

The ionization frequency $R_i$ is seen to appear at the peak of the field since at this peak $E/p_0$ value, the tail of the electron energy distribution just reaches the ionization threshold of SiH$_4$. Therefore, electrons are injected in the plasma in a series of pulses under such a condition.
The variation of the mean electron energy $\bar{E}$ and the average speed $\langle v \rangle$ at 135.6 MHz in CH$_4$ is shown in figure 6. It is seen that the variation of $\bar{E}$ is of double frequency, but the amplitude of the variation is far smaller than at 13.56 MHz, though not shown here. The fluctuation of $\bar{E}$ in CH$_4$ at 13.56 MHz is found similar to that in SiH$_4$. At 135.6 MHz, the difference between DC and equivalent AC energy distribution is found smaller than that at 13.56 MHz. Figure 7 shows the variation of the second order moment along the field $M_x$ and parallel to the field $M_y$ is shown. It is seen that despite the sharp variation of $\langle v \rangle$, $M_x$ and $M_y$ increase almost linearly with time, thus suggesting that the longitudinal and transverse diffusion coefficients, respectively defined by a half of the time derivative of $M_x$ and a fourth of the time derivative of $M_y$, may be defined as constants even under AC electric field.

Figure 8 shows the DC and equivalent AC electron energy distributions in the 25% CH$_4$ and 75% SiH$_4$ gas mixture. The difference between the DC and AC distribution is clear, and the AC distribution is shifted towards the origin. In figure 9, a similar comparison is made with nitrogen. The AC distribution again is shifted towards the origin here. There is an important difference, however, between figure 8 and 9. In the case of the CH$_4$ and SiH$_4$ mixture of figure 8, the AC distribution has larger values at the tail, whereas with figure 9, the DC distribution has larger values at the tail.

This means that with the CH$_4$ and SiH$_4$ mixture, the AC distribution crosses the DC one at two points i.e. at about 2.5 eV and 7.5 eV, while with N$_2$ the AC distribution crosses the DC distribution only once, at about 2.5 eV. This is naturally due to the difference of the cross sections. However, these two cases suggest that too easy a judgment that the AC distribution
always has larger values at the high energy tail should not generally hold.
Another thing that may be pointed out with figure 9 is that with nitrogen which has very large vibrational cross section, the electrons lose the energy for vibrational excitation particularly when the varying field assumes low values which suit vibrational excitation, therefore making a large difference between the AC and DC distribution; the field is constant with the latter and if its value is above a certain level, vibrational excitation would not occur in a preferable way.

5. CONCLUSIONS

A Monte Carlo simulation of the electron swarm under an AC electric field of 13.56 MHz has been performed for SiH₄ and other gases. The results show that, unlike a previous prediction, the electron energy distributions under a DC and an equivalent AC field generally differ, and that the energy distribution "breathes" rather deeply during one cycle of the field. The electron mean energy varies with double frequency, generally in non-sinusoidally and with a phase shift in reference to the field. The average electron velocity are found to vary almost in phase with the field, but the shape of the variation is far from sinusoidal. It is found that despite the alternating field, the longitudinal and transverse diffusion coefficients have almost constant values. The shift towards the origin is seen in all the equivalent AC energy distributions in reference to the DC distributions. With SiH₄ and CH₄, an AC distribution crosses the equivalent DC distribution at two energies and the AC distribution has higher values at the high energy tail, while with nitrogen the number of crossing is one and the AC distribution has lower values at the high energy tail. It is also shown that electrons are injected in a series of pulses in plasma at certain E/p₀ values since ionization occurs appreciably only at the peak of the applied electric field. It is shown that at 135.6 MHz, the variation of the
mean electron energy is far smaller than that at 13.56 MHz and the difference between the DC electron energy distribution and the equivalent AC distribution is also far smaller than that at 13.56 MHz.

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REFERENCES