

SELF-CONSISTENT PARTICLE SIMULATION OF RADIO FREQUENCY
CF₄ DISCHARGE: EFFECTS OF SECONDARY ELECTRON EMISSION
COEFFICIENT AND GAP DISTANCE BETWEEN ELECTRODES
CF₄ RF プラズマの粒子シミュレーション: 二次電子放出係数および電極間距離の影響

Kazuki DENPOH and Kenichi NANBU*

伝宝 一樹, 南部 健一*

Central Research Laboratory, Tokyo Electron Limited

650 Mitsuzawa, Hosaka-cho, Nirasaki 407-01

**Institute of Fluid Science, Tohoku University*

2-1-1 Katahira, Aoba-ku, Sendai 980-77

東京エレクトロン(株) 総合研究所, 407-01 韮崎市穂坂町三ツ沢 650

*東北大学流体科学研究所, 980-77 仙台市青葉区片平 2-1-1

Abstract

The radio frequency CF₄ discharge between parallel electrodes is simulated by the use of the Particle-in-Cell/Monte Carlo method to examine the effects of secondary electron emission by ion impact and gap distance between electrodes on the discharge structure and reactions.

1. Introduction

In recent ULSI techniques, the dimensions of microelectronics devices have been decreasing according to endless circuit integration. Under such circumstances, severe plasma control for dry etching is required to obtain best etching characteristics. Consequently, theoretical understanding of plasma phenomena has become important for optimization of reactor design and operating conditions.

In the previous paper[1], we were successful in self-consistent simulation of radio frequency CF₄ discharge between parallel electrodes by using the Particle-in-Cell/Monte Carlo(PIC/MC) method[2]. The simulation have clarified the discharge structure, sustaining mechanism, and important reactions.

The aim of the present work is to examine the effects of secondary electron emission coefficient by ion impact and gap distance between electrodes on the discharge structure and reactions in order to obtain fundamental knowledge on plasma control.

2. Description of the model

The region simulated, as illustrated in Fig. 1, is the inside of a cylinder between parallel electrodes with radius R . The electrodes are separated by distance D . The voltage V applied to the electrode at $z = 0$ is $V = V_{rf} \sin \omega t$, where $\omega (= 2\pi f)$ is the angular frequency and t is time. The electrode at $z = D$ is grounded ($V = 0$). The charged species taken into account in the present work are electron, five positive ions (CF₃⁺, CF₂⁺, CF⁺, C⁺, F⁺), and two negative ions (CF₃⁻, F⁻). The motions and collisions of these particles are simulated self-consistently by the use of the PIC/MC

method[2]. The electric field is determined by solving the Poisson equation with a sampled space charge distribution. The leap-frog scheme is used to solve the equation of motion. Electrons are absorbed and ions are neutralized on the electrodes. Secondary electron emission by ion impact is also considered on the electrodes. At the cylindrical boundary $r = R$ the charged particles are specularly reflected.

The collisions implemented into our simulation are electron-CF₄ collision, ion-CF₄ collision, and positive-negative ion recombination. A set of cross-section data compiled by Itoh *et al.*[3] is employed for electron-CF₄ collision(Fig. 2). The ion-CF₄ collision is simulated by the use of the collision model developed for elastic and endothermic reactions[1]. The positive-negative ion recombination are handled by our method[4] with rate constant of $5.5 \times 10^{-13} \text{ m}^3/\text{s}$ [5].

3. Results and discussion

The simulation is performed for the three cases in Table 1, where p is the gas pressure and γ is the secondary electron emission coefficient.

Figures 3-5 show the electric field at four times in a rf-period, time-averaged electron and ion(CF₃⁺, F⁻, CF₃⁻) densities, and representative reaction rates(R_i : ionization, R_a : electron attachment, R_d : electron detachment, R_r : positive negative ion recombination, $R_{\text{CF}_3^+}$: CF₄-CF₃⁺ reactive collision) obtained for the three cases, respectively. Also the ratios of ion densities to electron density in the center of bulk is tabulated in Table 2. The results for CASE-2 were already demonstrated in the previous work[1].

Firstly, let us discuss the effect of γ by comparing Figs. 3 and 4. The increase of γ leads to a slight increase of electric field, an appreciable increase of reaction rates and densities of electron and ions, and therefore decrease of sheath thickness. Roughly, there can be seen no essential differences in the discharge structure between the two. As shown in Table 2, however, the most prominent is that secondary electrons make the fractions of CF⁺, C⁺, and F⁺ much larger, which means high energy impact in electron-CF₄ collision.

Next, let us compare Figs. 4 and 5 to discuss the influence of the gap distance between electrodes. The decrease of the electrode-spacing affects the discharge structure. For the narrow gap ($D=10$), the electric field penetrates into the bulk and oscillates electrons in that portion. This results in much larger ionization rate. Due to increased loss to the electrodes, however, the electron density in the bulk is as same as that for $D = 25.4$ mm. Furthermore, the maxima of ion densities shift from the sheath edge to the bulk center. The rates for electron detachment from negative ions and CF₄-CF₃⁺ reactive collisions for $D = 10$ mm are larger in comparison with those for $D = 25.4$ mm because ions can have much energy in the stronger electric field for the narrow gap case.

Table 1 Simulation conditions.

CASE	D (mm)	γ	p (mTorr)	V_{rf} (V)	f (MHz)
1	25.4	0.0	200	200	13.56
2	25.4	0.1	200	200	13.56
3	10.0	0.1	200	200	13.56

Table 2 Ratios of ion densities to electron density.

SPECIES	CASE-1	CASE-2	CASE-3
CF_3^+	34	31	76
CF_2^+	0.16	0.17	2.1
CF^+	0.04	0.07	1.5
C^+	0.006	0.05	0.67
F^+	0.006	0.04	0.71
F^-	21	19	50
CF_3^-	12	11	30
Electron	1.0	1.0	1.0

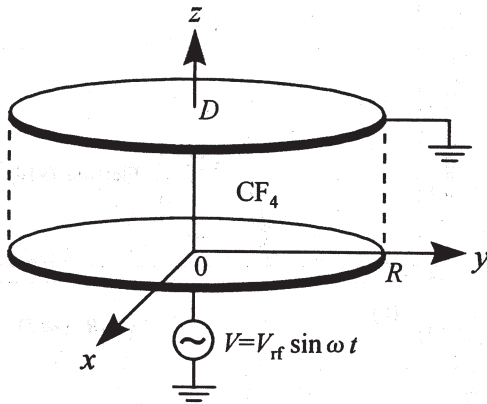


Fig. 1 Computational domain.

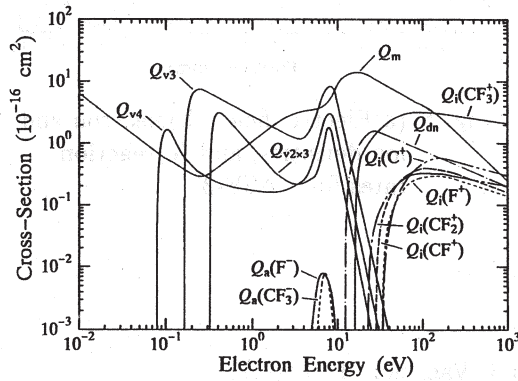


Fig. 2 Electron impact cross-sections for CF_4 .

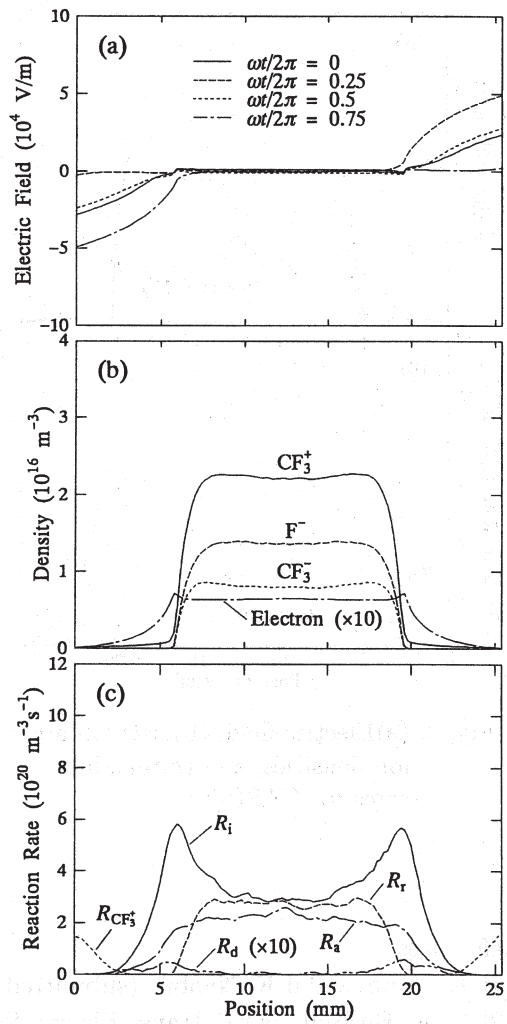


Fig. 3 (a)Electric field, (b)electron and ion densities, and (c)reaction rates for CASE-1.

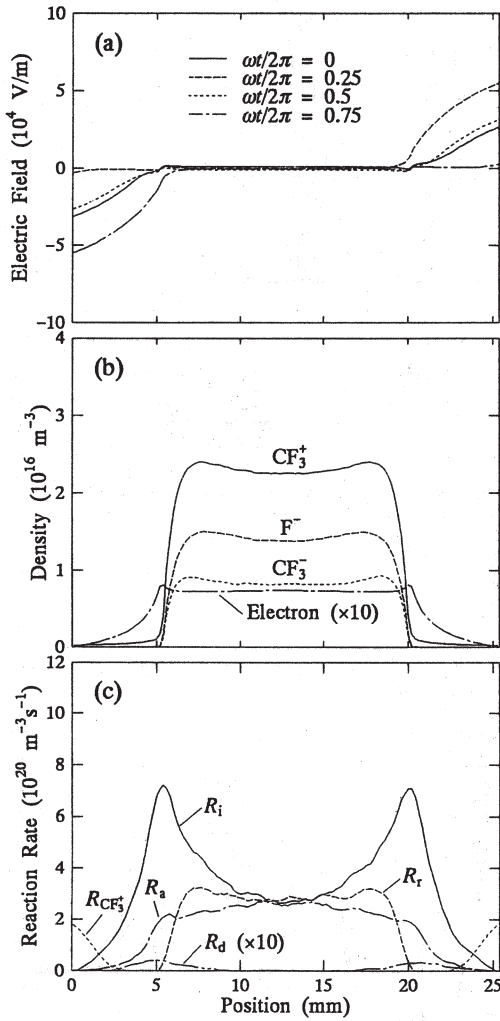


Fig. 4 (a)Electric field, (b)electron and ion densities, and (c)reaction rates for CASE-2.

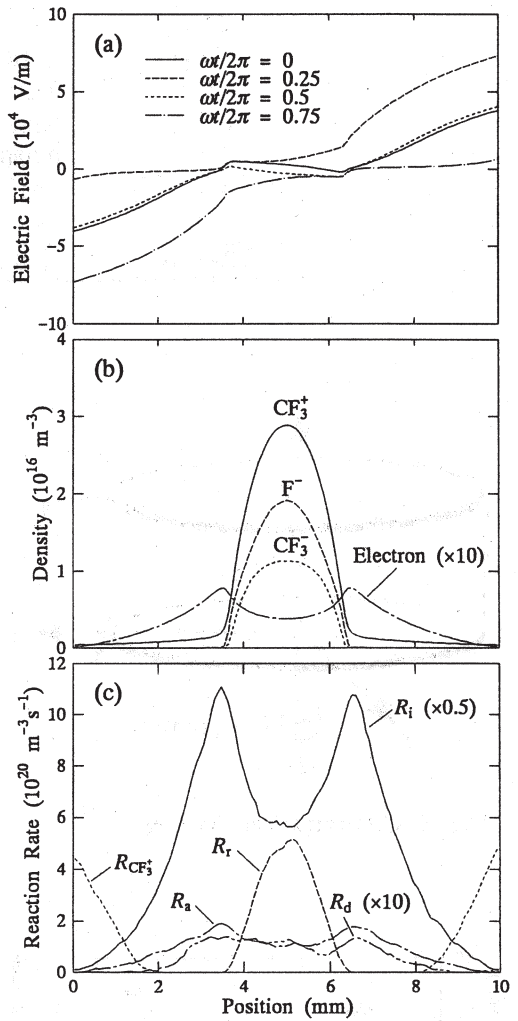


Fig. 5 (a)Electric field, (b)electron and ion densities, and (c)reaction rates for CASE-3.

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