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Computer Modeling of the Transient RF Discharge in Nitrogen

—— A Continuum Model with the Energy Equation ——

Nobuyasu SATO*, Tomonori KAMIBAYASHI**, and Hiroaki TAGASHIRA**

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Abstract.

A continuum model is used for simulating the development of the transient RF discharge between parallel plates in nitrogen under a plasma processing condition. Non-equilibrium characteristics of the electron swarm are taken into account using ionization and excitation coefficients obtained by solving the electron energy equation simultaneously with the continuity equation for electrons. Significant characteristics of the transient RF discharge such as the temporal variations of the gap voltage, the discharge power and the discharge current are calcluated by numerically solving the continuity equations for electrons and ions using the F. C. T. SHASTA algorithm together with Poisson's equation and a RF circuit equation. The spatio-temporal evolutions of the electron and ion densities, the photon emission of the 2nd positive band and the space charge field are also calculated. The validity of the present model is discussed by comparing these calculated data with experimental observations and with data obtained by a Monte Carlo technique.

1. Introduction.

For modeling the RF discharge used for the plasma processing, there are mainly two kinds of techniques. One is based on the Monte Carlo technique and the other is called the continuum model. The Monte Carlo method proposed by Kushner (1983, 1986) is one of the most fundamental method for dealing with the RF discharge but consumes lots of computing time. On the other hand, with the continuum model, calculations can be carried out without any computer time restrictions as far as electron and ion motions are concerned. However, a complication with the continuum model is

* Faculty of Education, Iwate University, Ueda, Morioka 020.
** Faculty of Engineering, Hokkaido University.
This study has been carried out mainly at the Department of Electrical Engineering in Hokkaido University.

that the non-equilibrium characteristic of the electron swarm caused by the electrode boundaries and by the time varying electric fields need to be appropriately taken into account. In the previous reports (Kamibayashi, 1987; Sato, 1988(a)), this has been done by using the modified Friedland equation (Friedland, 1974; Sato, 1985) for obtaining non-equilibrium values of the ionization coefficient. Precise investigations with this method has revealed, however, that the non-equilibrium characteristic of the electron swarm can be represented only for the case of the steady state situation. Graves (1986, 1987) has proposed a continum model for a 'steady' RF discharge in which the spatial non-equilibrium values of the ionisation coefficient have been obtained by solving the enthalpy equation for electrons.

In the present simulation, this method is applied for modeling the 'transient' RF discharge. Continuity equations for electrons, ions and excited molecules are solved simultaneously with the electron energy equation which is derived from the enthalpy equation with an assumption of the Maxwellian electron energy distribution function. The situation for the present simulation is as follows: parallel plane electrodes with a gap length of 1 *cm*, an electrode radius of 5 *cm*, a sample gas pressure of 2 *Torr* and a radio frequency of 10 *MHz*.

Significant characteristics of the transient RF discharge such as the temporal variations of the gap voltage, the discharge current and the discharge power, and the spatio-temporal evolutions of the electron and ion densities, the space charge field and the photon emission from excited molecules are calculated and discussed by comparing with the experimental observations (Haydon, 1978; Kemp, 1987). The validity of the electron energy equation for representing the non-equilibrium characteristic of the electron swarm for the case of the transient discharge is also discussed using data obtained by the Monte Carlo simulation in nitrogen (Sato, 1988(b)).

2. Calculation.

2. 1 Continuity equations.

For the geometry of the present electrode system, continuity equations for electrons, ions and excited molecules may be represented in the one dimensional form as follows:

$$\frac{\partial N_e}{\partial t}+\frac{\partial N_e W_e}{\partial x}=\gamma_i+\frac{\partial^2}{\partial x^2}(D_e N_e)-\alpha_r N_e N_p \quad (1)$$

$$\frac{\partial N_p}{\partial t}+\frac{\partial N_p W_p}{\partial x}=\gamma_i+\frac{\partial^2}{\partial x^2}(D_p N_p)-\alpha_r N_e N_p \quad (2)$$

$$\frac{\partial N_{ex}}{\partial t}=\gamma_{ex}-\frac{1}{\tau}N_{ex} \quad (3)$$

In these equations, the subscripts e, p and ex refer respectively electrons, ions and excited molecules. W and D are the drift velocity and the diffusion coefficient respectively. $\gamma_{i,\ ex}$ is the rate of the ionization or the excitation, α_r is the electron-ion recombination rate and τ is the life time of the excited molecule including quenching effects.

Assuming the Maxwellian energy distribution for electrons, the energy balance equation of electrons is represented as

$$\frac{\partial\varepsilon}{\partial t}\left(\frac{3}{5}N_e h_e\right)+\frac{\partial q_e}{\partial x}+J_e\cdot eE+\gamma_i H_i+\gamma_{ex}H_{ex}=0, \tag{4}$$

where

$$J_e=W_eN_e-\frac{\partial}{\partial x}(D_eN_e)$$

and

$$q_e=J_eh_e-K_e(N_e,T_e)\frac{\partial T_e}{\partial x}.$$

In Eq.(4), h_e is the electron enthalpy, e is the electron charge and E is the electric field. $H_{i,ex}$ is the energy loss due to the ionization or excitation collision. K_e and T_e are the electron thermal conductivity and the electron temperature. Using the relations

$$h_e=\frac{5}{2}\kappa T_e,\ \ K_e=\frac{5}{2}\kappa D_eN_e \text{ and } \varepsilon=\frac{3}{2}\kappa N_eT_e,$$

Eq.(4) is rewritten as

$$\frac{\partial\varepsilon}{\partial t}-\frac{5}{3}\left[\frac{\partial}{\partial x}(W_e\varepsilon)-\frac{\partial^2}{\partial x^2}(D_e\varepsilon)\right]=\left[N_eW_e-\frac{\partial}{\partial x}(D_eN_e)\right]eE-\gamma_{ex}H_{ex}-\gamma_iH_i \tag{5}$$

The electron collision rate $\gamma_{i,ex}$ may be represented as

$$\gamma_{i,ex}=N_ek_{i,ex}Exp(-1.5E_{i,ex}N_e/\varepsilon)$$

where $k_{i,ex}$ and $E_{i,ex}$ are respectively the collision frequency and the activation energy for the ionization or excitation process. These equations are solved numerically using F.C.T. SHASTA algorithm (Boris, 1973; Book, 1975; Morrow, 1985).

2. 2 Swarm parameters.

The swarm parameters used for the continuity equations such as the drift velocity and the diffusion coefficient of electrons and ions are represented by appropriate functions of E/p using many published data as follows:

$W_e=3.0\text{x}10^5\ E/p\ (cm/sec)$ for $E/p<255\ (V/cm\ Torr)$,

$W_e=4.82\text{x}10^6(E/p)^{0.5}$ for $E/p>255$,

$W_p=1.24\text{x}10^3(E/p)^{0.5}\ (cm/sec)$,

$D_e/\mu_e=(0.036E/p+0.04)\ (V)$ and $D_p/\mu_p=0.025\ (V)$.

The values of $H_{i,ex}$, $k_{i,ex}$ and $E_{i,ex}$ are estimated from the electron collision cross section data. As shown in Fig.1, the electron collision frequency curves reduced from the cross

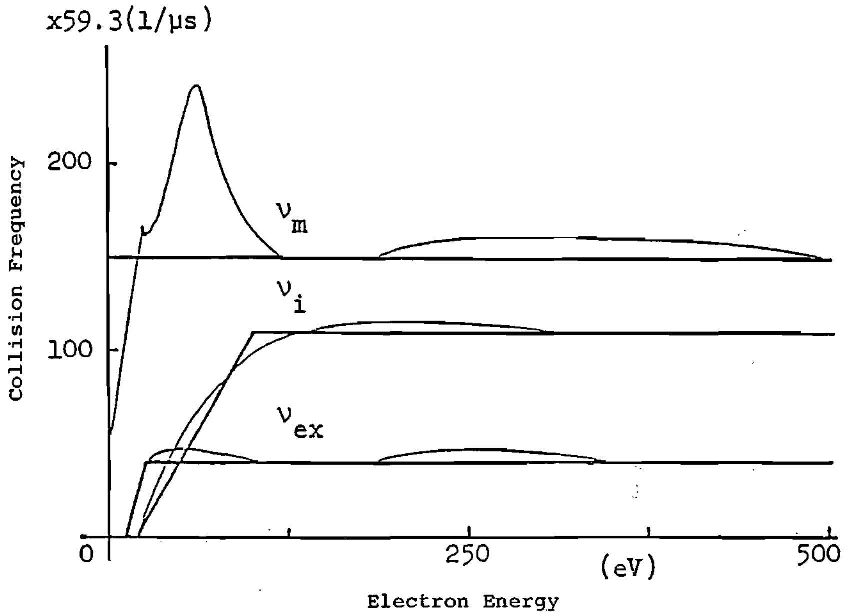


Fig. 1 Electron collision frequency in nitrogen.

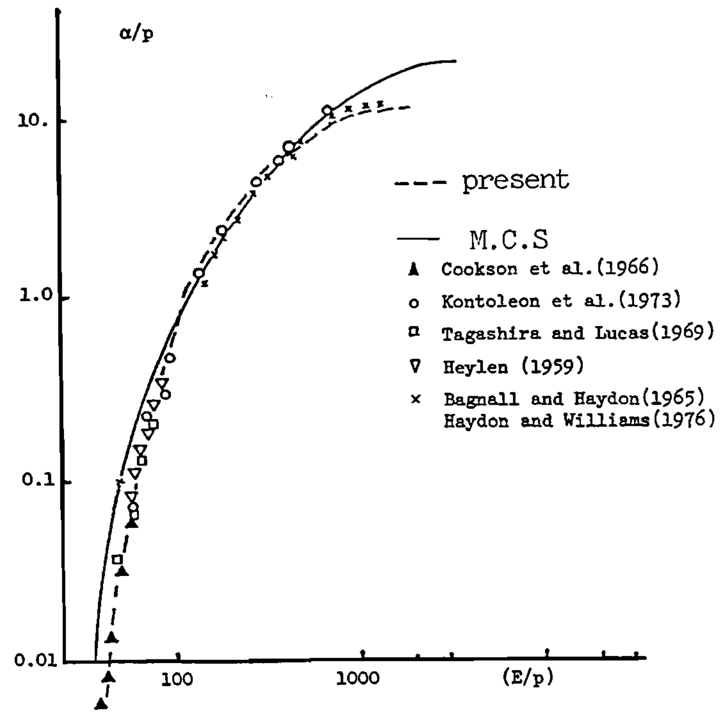


Fig. 2 Ionization coefficient in nitrogen.

section may be approximately represented by linear lines. The value of the collision loss energy $H_{i,ex}$ corresponds to the threshold energy of the ionization or excitation. The collision frequency $k_{i,ex}$ and the activation energy $E_{i,ex}$ are taken from the value of the horizontal line and from the value of the energy where the line becomes horizontal, respectively.

In order to examine the validity of the energy equation with these parameters, the ionization coefficients under steady state conditions are calculated using Eqs. (1) and (5). As shown in Fig. 2, the calculated ionization coefficient is in good agreement with the experimental data in a wide range of E/p.

2. 3 Boundary condititions.

The electrodes are assumed to be a complete sink for both electrons and ions. However, the secondary electron emissions from the cathodic electrode due to the photon irradiation (γ_p effect) and the ion impact (γ_i effect) on the electrode surface are taken into account. At the cathodic electrode,

$N_e(t)=N_0+N_{\gamma p}(t)+N_{\gamma i}(t)$ for electrons,

$N_p(t)=0$ for ions and

$\varepsilon(t)=\varepsilon_0$ for the electron energy,

where N_0 is the initial electron density supplied by a ultra violet irradiation. $N_{\gamma p}$ and $N_{\gamma i}$ are the electron densities released from the electrode due to the γ_p and γ_i effect respectively. ε_0 is an average energy of electrons released from the electrode. At the anodic electrode,

$N_e(t)=0$ and $N_p(t)=0$.

2. 4 RF circuit.

For generating the RF transient discharge, a particular circuit, as shown in Fig. 3, which includes a RF potential source and the plane electrodes is set to a resonant condition with the potential source at a frequency of 10 *MHz*. With this resonant circuit,

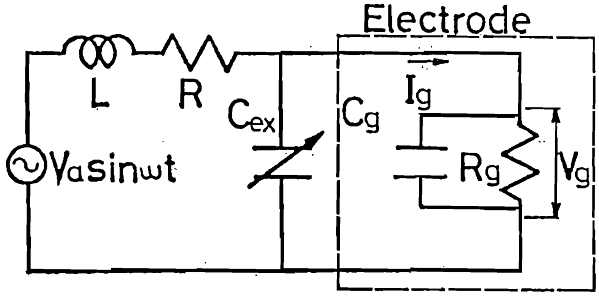


Fig. 3 RF circuit and electrodes.

the supplied gap voltage is raised to the breakdown voltage and then rapidly collapses within a short time interval after the discharge has started. This provides a transient discharge without any succeeding intensive steady RF discharge. The temporal variation of the gap voltage V_g is calculated by numerically solving the equation

$$\frac{d^2V_g}{dt^2}+\frac{R}{L}\frac{dV_g}{dt}+\frac{V_g}{LC}=\frac{V_a}{LC}SIN(\omega t)-\frac{R}{LC}I_g-\frac{1}{C}\frac{d}{dt}I_g$$

using Runge Kutta Nystrom method. The discharge current I_g in the circuit due to the motion of electrons and ions between the electrodes is calcuated using the current equation modified to include the electron diffusion (Sato, 1980; Morrow, 1985),

$$I(t)=\frac{\pi d^2 e}{V_g}\int_0^d[N_eW_e+N_pW_p+\frac{\partial}{\partial x}(D_eN_e)]E_s dx.$$

3. Results and discussions.

Fig. 4(a) shows the temporal variations of the discharge current I_g (true current plus displacement current), the gap voltage V_g and the discharge power P. The variation of the maximum electric field E_{max}/p within the gap space is also shown in Fig. 4(b). After the application of the source potential V_a, the envelope of the peak gap voltage V_g increases with a time constant $2L/R$. During this process, the phase difference between I_g and V_g is 90°, so that no discharge power is consumed in the gap space. This indicates a low conductivity situation of the gap space. However, the electron and ion densities increase gradually due to the ionization process, which eventually leads to

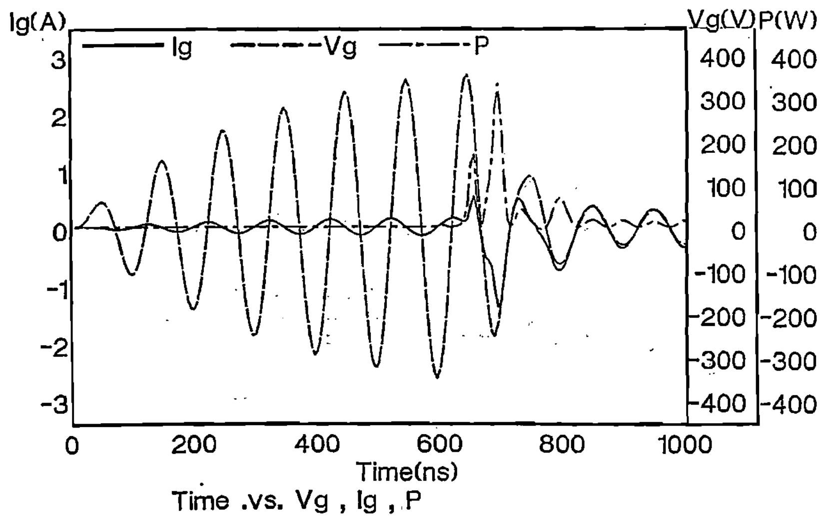
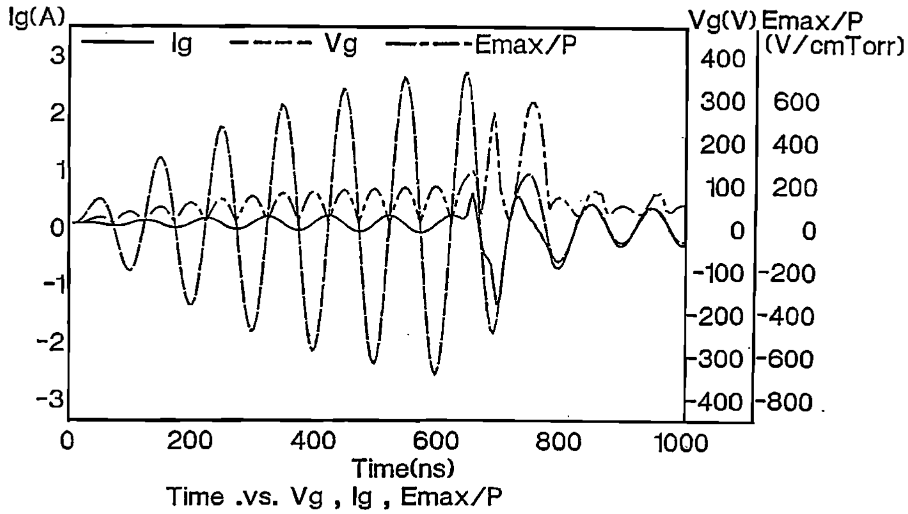


Fig. 4 Development of the transient RF discharge in nitrogen. $V_a=45(V)$, $p=2(Torr)$ and $f=10\ MHz$.
(a) V_g, I_g and P vs Time.



(b) V_g, I_g and E_{max}/p vs *Time*.

the transient discharge. During the transient part of the discharge, the discharge current I_g increases sharply, while the gap voltage V_g collapses to approximately the value of the source potential. The phase difference between I_g and V_g becomes zero, which gives rise to a maximum peak of the discharge power P. The value of the E_{max}/p also reaches a maximum which implies the formation of the cathode fall due to the space charge accumulation. After the transient diseharge, the peak values of V_g and I_g decrease to constant low values by maintaining a zero phase difference. This indicates a high conductivity condition of the gap space due to the high density space charge accumulation.

For Calculations with various values of the source potential V_a, the general features of the RF discharge development are basically the same as one another. These calculated temporal variations of V_g and I_g are qualitatively in good agreement with the experimental observation by Haydon and Plumb (1978).

Figs. 5(a) and (b) show the spatio-temporal evolutions of the electron and ion densities in the transient part of the discharge development. Electrons can move along the direction of the RF electric field, while ions do not move significantly but increase due to the ionization process, which results in the appearance of a high density positive net charge distribution in the neighbourhood of the cathodic electrode, as shown in Fig. 5(c). This gives rise to the formation of the intense field region called the cathode fall, as shown in Fig. 5(d), which can provide high energy electrons in the gap space.

Fig. 5(e), (f) and (g) show respectively the variations of the photon emission of the nitrogen 2nd positive band, the electron energy and the ionization coefficient. In the present model, the values of the ionization coefficient is determined by the electron energy. Before the initiation of the transient discharge, the electron energy is high

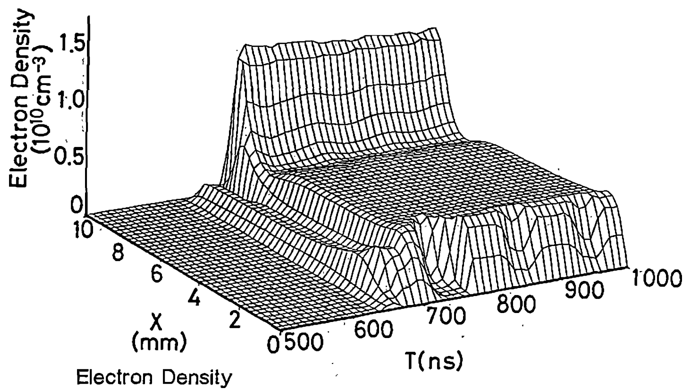
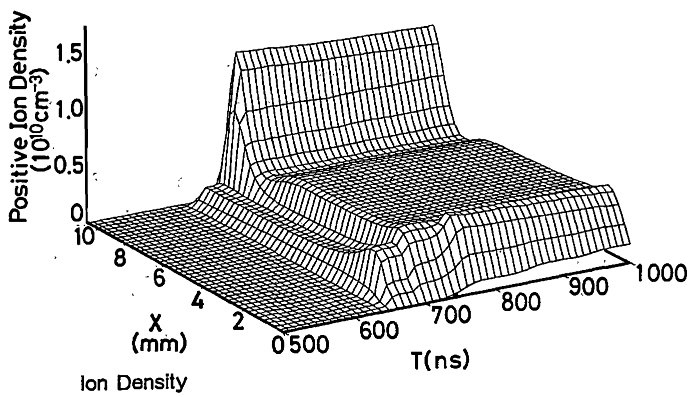
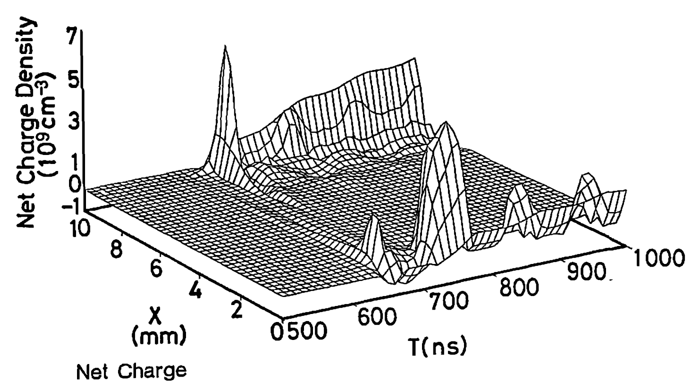


Fig. 5 Spatio-temporal evolutions of the space charge, electric field and photon emission. V_a=45 (*V*), p=2 (*Torr*) and f=10 *MHz*.

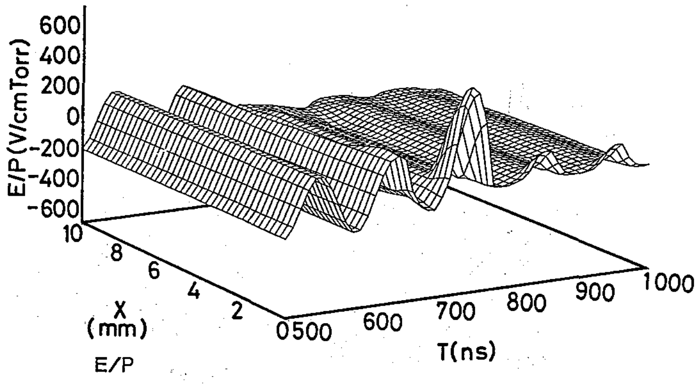
(a) Electron density.



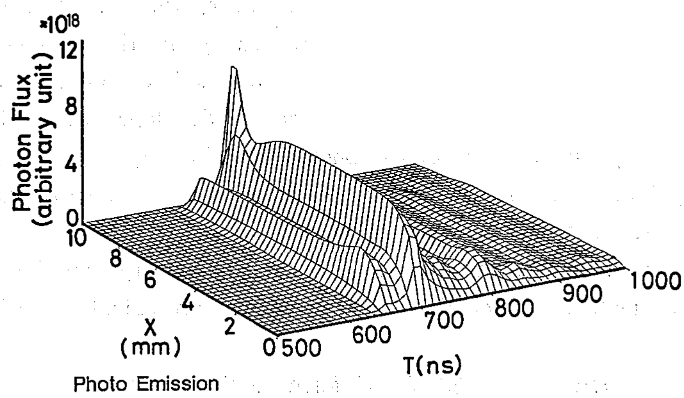
(b) Positive ion density.



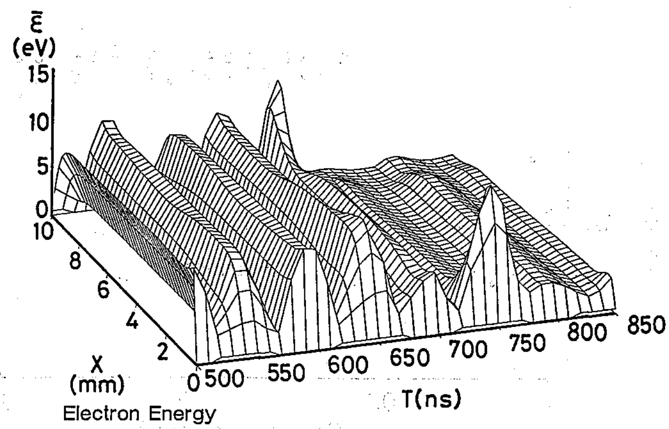
(c) Net charge density.



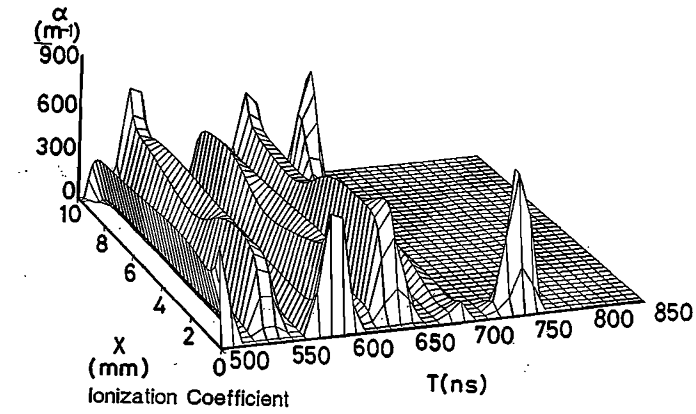
(d) Electric field.



(e) Photon emission.



(f) Electron energy.



(g) Ionization coefficient.

enough to take place the ionization process. However, when the cathode fall is formed, the electron energy is not so high as that expected by the field strength.

The intensity of the photon emission from the excited molecule has an intensive peak only during the transient part of the discharge development. Although this main feature of the temporal variation of the photon emission agrees with the experimental observation by Kemp (1987), the spatial distribution of the photon emission across the gap space is different from the observation.

In order to examine the cause of these discrepancies, the spatial variation of the ionization coefficients under idealized field conditions are calculated using Eqs. (1) and

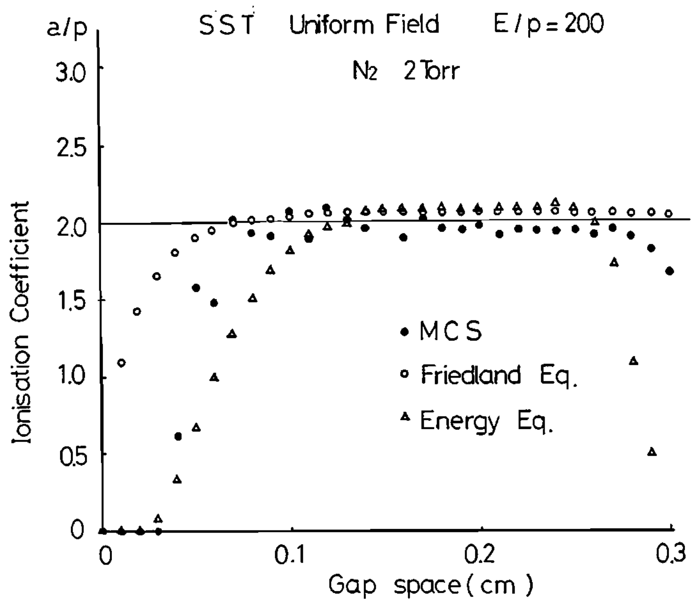
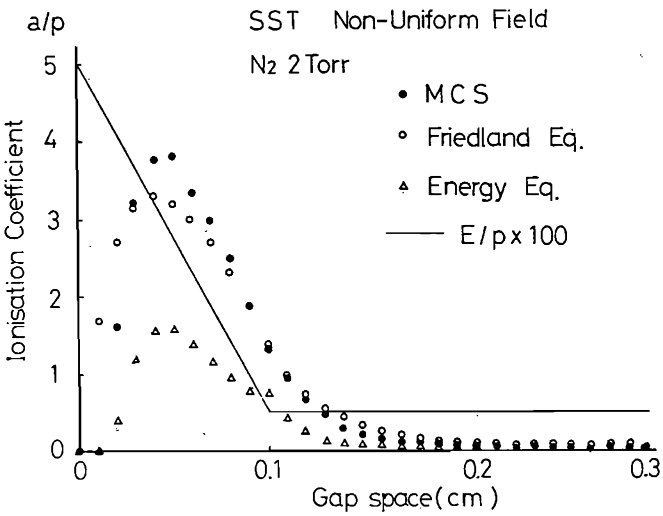
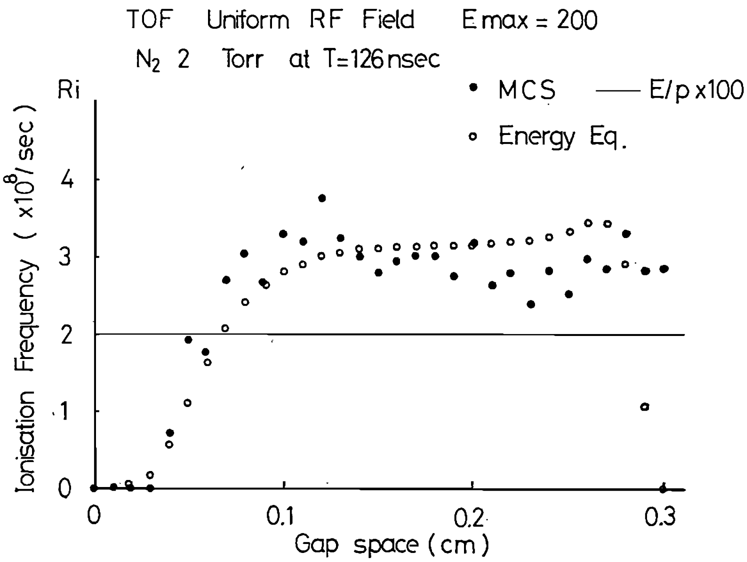


Fig. 6 Comparison of the ionization coefficient with Monte-Carlo data in idealized field.
(a) Uniform DC field.



(b) Non-uniform DC field.



(c) Uniform RF field.

(5) and is compared with data obtained by a Monte Carlo technique (Sato, 1988(b)).

As shown in Fig. 6(a), for the case of the uniform DC field, the energy equation method can approximately reproduce the non-equilibrium characteristic of the ionization coefficient in the neighbourhood of the cathode.

For the case of a non-uniform DC field, which corresponds to the cathode fall region in the glow discharge, the values of the ionization coefficient obtained by the energy equation are much smaller than the Monte Carlo data. The Monte Carlo data show an overshooting characteristic in the region where the electric field decreases sharply, which indicates that the electron energy distribution is different from the Maxwellian distribution function.

For the case of an RF field, Fig. 6(c) shows the time of flight sampling data of the Monte Carlo calculation at the peak phase position of the applied RF field. A significant observation is that the spatial variation of the ionisation frequency shows a overshooting characteristic even though the electric field is uniform. The energy equation method can not represent such a non-equilibrium characteristic of the electron swarm. These facts suggest some limitations for applying the energy equation to the transient RF discharge.

4. Conclusion.

The present investigation has revealed the validity as well as the limitations for applying the electron energy equation to the continuum model of the transient RF discharge. The continuum model combined with the electron energy equation can represent the developments of the discharge current and discharge power which may be regarded as integrated quantities of the electron swarm over the gap space. However, this model can not reproduce the spatially resolved experimental observations. Since the fundamental assumption of this model is that the electron energy distribution would be a Maxwellian distribution, phenomena caused by the distortion of the energy distribution such as the overshooting characteristic in the spatial variation of the ionization coefficient can not be predicted with the present model.

For improving the continuum model, further studies need to be developed by taking the non-equilibrium characteristic of the electron swarm into account appropriately.

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