

Ion flux's pressure dependence in an asymmetric capacitively coupled rf discharge in NF_3

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Abstract: Starting from an analytical macroscopic/phenomenological model yielding the self-bias voltage as a function of the absorbed radio-frequency (rf) power of an asymmetric capacitively coupled discharge in NF_3 this paper studies the dependence of the ion flux onto the powered electrode on the gas pressure. An essential feature of the model is the assumption that the ions' drift velocity in the sheath near the powered electrode is proportional to E^α , where $\mathbf{E} = -\nabla U$ (U being the self-bias potential), and α is a coefficient depending on the gas pressure and cross section of elastic ion-neutral collisions. The model also considers the role of γ -electrons, stochastic heating as well as the contribution of the active electron current to the global discharge power balance. Numerically solving the model's basic equations one can extract the magnitude of the ion flux (at three different gas pressures) in a technological etching device (Alcatel GIR 220) by using easily measurable quantities, notably the self-bias voltage and absorbed rf power.

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1 Introduction

In a capacitive discharge, with a driving frequency ω much less than the electron plasma frequency ω_{pe} nearly all of the applied rf voltage is dropped across the space charge sheaths

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near the electrodes. The rectification of time-varying sheath potentials in such discharges results in dc potentials and especially when the powered electrode approximately equals the amplitude of the applied discharge voltage. Ions crossing the powered electrode sheath cannot follow the high-frequency field. They gain energy practically equal to the dc sheath potential and, hence, strike the electrode surface (wafer) at tens to hundreds of electronvolts. Recently, we [1] advanced a diagnostic method for determining the ion flux Γ_i onto the powered electrode by using two measurable quantities (the self-bias voltage U_0 and the total rf power P absorbed by the discharge) in an asymmetric capacitively coupled α -discharge. The physical ground of the method has been extended [2] to γ -capacitive discharges taking into account the influence of the γ -processes and the contribution of the active electron current to the discharge energetics. Here, we also include the stochastic electron heating in the power balance.

2 Analytical description of a space-charge sheath

For simplicity, we consider a one-dimensional model of the sheath at the smaller active electrode of a strongly asymmetric capacitively coupled discharge. We assume that the ions' drift velocity inside the sheath is [2]

$$v_i = aE^\alpha \quad (\mathbf{E} = -\nabla U), \quad (1)$$

where a is a coefficient depending on the gas pressure and cross section for elastic ion–neutral collisions, and U being the self-bias potential. The exponent α depends on the elastic ion–neutral collision mechanism as well as on the dependence of the interaction cross section on the ion velocity itself. If the dominant interaction mechanism is the induction of a dipole moment due to the ion electric field, then the cross section is proportional to v_i^{-1} , the ion–neutral collision frequency is constant and hence $\alpha = 1$. When the ion interaction with the parent gas is governed by the charge exchange process, the cross section, and correspondingly the ion mean free path do not depend on the ion's velocity [3], and $\alpha = 1/2$. Available experimental data suggest that we usually have a situation lying somewhere between these two cases, where the cross section for elastic ion–neutral interaction falls off with velocity, however not so rapidly as v_i^{-1} . It seems reasonable, in the absence of more elaborate data, to accept $\alpha = 3/4$ notwithstanding that it does not follow from any particular model.

The spatial alteration of the electric field in the sheath space-charge region is governed by the equations

$$n_i \mathbf{v}_i = \mathbf{\Gamma}_i, \quad (2)$$

$$\nabla \cdot \mathbf{E} = \frac{en_i}{\varepsilon_0}. \quad (3)$$

The solutions to Eqs. (1)–(3) for a plain geometry (axis x perpendicular to the powered electrode) are

$$v_i(x) = a^{1/(1+\alpha)} [e\Gamma_i(1+\alpha)/\varepsilon_0]^{\alpha/(1+\alpha)} x^{\alpha/(1+\alpha)}, \quad (4)$$

$$E(x) = [e\Gamma_i(1+\alpha)/(a\varepsilon_0)]^{1/(1+\alpha)} x^{1/(1+\alpha)}, \quad (5)$$

$$U(x) = -\frac{1+\alpha}{2+\alpha} [e\Gamma_i(1+\alpha)/(a\varepsilon_0)]^{1/(1+\alpha)} x^{(2+\alpha)/(1+\alpha)}. \quad (6)$$

The appropriate boundary conditions are

$$U(d) = -U_0 \quad \text{and} \quad v_i(\text{plasma-sheath edge}) = \sqrt{kT_e/M} \equiv v_B,$$

where d is the width of the space-charge layer, U_0 is the potential difference in the sheath; the potential of the quasi-neutral plasma is taken to be zero whilst that of the electrode is $-U_0$. The first boundary condition determines, via the solution (6), d as a function of the sheath voltage U_0 and the ion flux Γ_i specified by the plasma bulk processes. The second boundary condition states that the ions enter the collisionless sheath at Bohm's speed v_B [4].

The power P which the source of high-frequency voltage introduces into the plasma can be split into two parts [1]:

- (i) P_{sheath} – the power that sustains a constant potential difference between the plasma bulk and powered electrode and ensures energy for ion bombardment of the vessel's walls (as well as power for accelerating γ -electrons).
- (ii) P_{plasma} – the power expended for sustaining the bulk plasma in the discharge, i.e. the power which heats the electron fluid.

We assume that P_{plasma} consists of Ohm's power P_{Ohm}^c , delivered from the capacitive current passing through the space-charge sheath onto the bulk resistance of the quasi-neutral plasma, and the Ohm's power P_{Ohm}^a of the active current (conductivity current) crossing the sheath. The P_{Ohm}^c is given by

$$P_{\text{Ohm}}^c = J_c^2 \text{Re}(Z_{\text{plasma}}), \quad (7)$$

where J_c is the effective value of the capacitive current density and $\text{Re}(Z_{\text{plasma}})$, measured in $\Omega \text{ m}^2$, is the active resistance of a column of quasi-neutral plasma with unit cross section area. Bearing in mind that the plasma resistance is inversely proportional to its (plasma) density and the ion flux Γ_i is proportional to n_i , we can write down

$$\text{Re}(Z_{\text{plasma}}) = b/\Gamma_i, \quad (8)$$

where b is a coefficient of proportionality independent of Γ_i , U_0 and P_{plasma} . The determination of b demands a specification of the discharge geometry and mechanism of ion drift to the walls. Using the above expression for Z_{plasma} together with Eq. (6) and the definition of capacitive current, finally we get

$$P_{\text{Ohm}}^c = \frac{\omega^2 b}{2} (1+\alpha)^2 U_0^{2/(2+\alpha)} \Gamma_i^{-\alpha/(2+\alpha)} (e/a)^{2/(2+\alpha)} [\varepsilon_0/(2+\alpha)]^{(2+2\alpha)/(2+\alpha)}. \quad (9)$$

In calculating the active Ohm's power P_{Ohm}^a we use an expression which is well known from probe theory for the electron current to the repelling electrode [5]

$$j_e = j_{e0} \exp[eu(t)/kT_e], \quad (10)$$

where j_{e0} is the random electron current density and $u(t) = -U_0(1 + \sin \omega t)$. It is easy to show [2] that under the condition $eU_0 \gg kT_e$

$$P_{\text{Ohm}}^a = \text{Re}(Z_{\text{plasma}}) \langle j_e^2 \rangle = b e^2 \Gamma_i \sqrt{\pi e U_0 / k T_e}, \tag{11}$$

where the angular brackets mean a time averaging over one field period.

Now we can make a balance of the total power delivered to the discharge. Let θ be the energy supplied to an electron–ion pair during its existence in the region of quasi-neutral plasma. It is a sum of the ionization energy eU_i ; kinetic energy $\frac{1}{2}kT_e$ of an ion leaving the quasi-neutral plasma (for detail, see section 9.4.2 in [5]); averaged electron kinetic energy $\frac{3}{2}kT_e$; energy of an electron in the ambipolar electric field $\sim kT_e$ (the factor in front of kT_e depends on the logarithm of the ion–electron mass ratio, as well as on the θ/kT_e ratio), and the total energy of all inelastic collisions which suffers an electron during its presence in the plasma. The total power per unit area, expended in quasi-neutral plasma, is $\theta\Gamma_i$, and equals the sum of those powers which are supplied via the previously mentioned mechanisms

$$\theta\Gamma_i = P_{\text{Ohm}}^c + P_{\text{Ohm}}^a. \tag{12}$$

The replacement of P_{Ohm}^c and P_{Ohm}^a with their expressions given by Eqs. (9) and (11), respectively, yields the following relationship between Γ_i and U_0 :

$$\Gamma_i = A \left(1 - \beta\sqrt{U_0}\right)^{-(2+\alpha)/(2+2\alpha)} U_0^{1/(1+\alpha)}, \tag{13}$$

where

$$A = \left(b\omega^2/2\theta\right)^{(2+\alpha)/(2+2\alpha)} (e/a)^{1/(1+\alpha)} \varepsilon_0 (1 + \alpha)^{(2+\alpha)/(1+\alpha)} (2 + \alpha)^{-1} \tag{14}$$

and

$$\beta = \frac{e^2 b}{\theta} \sqrt{\frac{\pi e}{k T_e}}. \tag{15}$$

The full power released into discharge is

$$\begin{aligned} P &\equiv P_{\text{sheath}} + P_{\text{plasma}} = \Gamma_i (eU_0 + \theta) \\ &= A (eU_0 + \theta) U_0^{1/(1+\alpha)} \left(1 - \beta\sqrt{U_0}\right)^{-(2+\alpha)/(2+2\alpha)}. \end{aligned} \tag{16}$$

Following the method described in [1], from at least three experimental points of the $U_0(P)$ dependence we determine those coefficients B , C and D which best fit the function

$$P = (BU_0 + C) U_0^{1/(1+\alpha)} \left(1 - D\sqrt{U_0}\right)^{-(2+\alpha)/(2+2\alpha)}. \tag{17}$$

After obtaining the coefficients B , C , and D , comparing Eqs. (17) and (16) we have $Ae = B$, $A\theta = C$, $\beta = D$, and

$$P_{\text{sheath}} = \frac{B}{\left(1 - D\sqrt{U_0}\right)^\delta} U_0^{(2+\alpha)/(1+\alpha)}, \tag{18}$$

$$P_{\text{plasma}} = \frac{C}{(1 - D\sqrt{U_0})^\delta} U_0^{1/(1+\alpha)}, \quad (19)$$

where $\delta = (2 + \alpha)/(2 + 2\alpha)$. Note that from the expression for P_{sheath} alone one finds

$$\Gamma_i = \frac{B}{e(1 - D\sqrt{U_0})^\delta} U_0^{1/(1+\alpha)}. \quad (20)$$

This expression has a great practical significance since Γ_i is the basic quantity qualitatively characterizing the wafer/surface plasma treatment. Moreover, having calculated the coefficients B and C , we can obtain the value of another important gas-discharge parameter, notably $\theta (= eC/B)$.

The contribution of secondary and photo electrons, collectively named γ -electrons, to the total flux is $\gamma\Gamma_i$, where γ , of order 0.01–0.02, is the coefficient of secondary ion–electron emission. This finally yields that now

$$\Gamma_i = A \left(1 - \beta\sqrt{U_0} - \eta U_0\right)^{-(2+\alpha)/(2+2\alpha)} U_0^{1/(1+\alpha)}, \quad (21)$$

where $\eta = \gamma/U_i$ (U_i is the ionization potential) and, accordingly, Eq. (17) modifies to

$$P = (BU_0 + C) U_0^{1/(1+\alpha)} \left(1 - D\sqrt{U_0} - HU_0\right)^{-(2+\alpha)/(2+2\alpha)}, \quad (22)$$

where H is a coefficient of determination, and you need four experimental points in the $U_0(P)$, which is the self-loading as a function of the supplied power. The ion flux correspondingly is

$$\Gamma_i = \frac{B}{e(1 - D\sqrt{U_0} - HU_0)^\delta} U_0^{1/(1+\alpha)}. \quad (23)$$

In order to take into account the influence of the stochastic electron heating on the power balance, we assume that the bulk electrons are elastically reflected from the border of the sheath space charge. We assume that the border oscillates in time as $d(1 - \sin \omega t)$ with a velocity amplitude $v_0 = \omega d$. One can show that the time average gain of electron energy during electron's collisions with sinusoidally oscillating plasma–sheath border is

$$\langle \Delta E_{\text{kin}} \rangle = 2mv_0^2. \quad (24)$$

Thus the power of stochastic heating of the electron fluid is

$$P_{\text{stoch}} = \Gamma_e m \omega^2 d^2, \quad (25)$$

where $\Gamma_e = n_e \sqrt{kT_e/2\pi m}$ is the random electron flux falling onto reflecting surface. The electron number density at the quasi-neutral plasma–sheath interface equals the ion number density

$$n_i \equiv \Gamma_i/v_B = \Gamma_i \sqrt{M/kT_e}. \quad (26)$$

Then one finds that

$$P_{\text{stoch}} = (2 + \alpha)^{(2+2\alpha)/(2+\alpha)} (1 + \alpha)^{-2} \sqrt{mM/2\pi} \\ \times (\varepsilon_0 a/e)^{2/(2+\alpha)} \Gamma_i^{\alpha/(2+\alpha)} \omega^2 U_0^{(2+2\alpha)/(2+\alpha)}. \quad (27)$$

Thus the total power balance equation finally becomes

$$P = P_{\text{Ohm}}^c + P_{\text{Ohm}}^a + P_{\text{stoch}} + e\Gamma_i U_0. \quad (28)$$

From this equation, by applying an appropriate numerical procedure, one can get the ion flux Γ_i at given P and U_0 .

3 Experimental results and discussion

The experimental measurements were performed using an Alcatel GIR 220 technological equipment for reactive ion etching. The operating frequency is 13.56 MHz and the supplied power varies from 20 to 300 W. The measurements were carried out with the NF_3 at three different pressures of 1.1, 2.0, and 6.3 Pa, respectively. We note that the NF_3 is a ‘difficult’ molecular gas in the sense that it is easily dissociable. Unfortunately we were unable to evaluate and take into account that dissociation in our model. In order to do this, it is necessary to apply a more elaborated, kinetic, approach in the discharge modelling. Such a consideration is however beyond the scope of the present paper. Thus, we cannot now estimate the error introduced by neglecting that phenomenon.

We present here results obtained under the assumption that all the mechanisms of getting energy into the plasma occur. By applying an appropriate numerical code (similar to the general linear least squares [6]), from measured absorbed-power–self-bias-voltage data one can derive the total power P released into discharge and the ion flux Γ_i onto powered electrode as functions of the self bias U_0 . One can obtain, of course, also the magnitudes of P_{plasma} and P_{sheath} , as well as other important gas-discharge characteristics, namely the energy θ required for sustaining an electron–ion pair in the discharge.

The power P_{plasma} expended for sustaining the bulk NF_3 plasma and for electrons’ stochastic heating at pressure of 1.1 Pa at low absorbed powers is larger than that for providing a constant potential difference between the plasma bulk and the powered electrode (P_{sheath}) as well as for accelerating the γ -electrons. However the magnitude of P_{plasma} decreases with increasing the absorbed power P ; at low powers P_{plasma} is around 70% of P , while at the highest power density of 1.75 W cm^{-2} (i.e. power of 300 W) it is 30%. In the case of the highest pressure $p = 6.3 \text{ Pa}$ P_{plasma} is 95% of P decreasing to 58% at the highest total power. At 2.0 Pa at low powers P_{plasma} is 85% diminishing to 38% at 300 W. Theoretically calculated dependences of P_{plasma} and P_{sheath} on the supplied rf power density for the NF_3 discharge at the three gas pressures are shown in Figs. 1 and 2. Figures 3 and 4 represent the theoretically obtained dependences of both the self bias U_0 and ion current density $e\Gamma_i$ on the absorbed full power density P . The main conclusion

which can be drawn from all the figures is that the gas pressure of 1.1 Pa is optimal for processing purposes – at such a pressure one can extract the highest ion flux. We finish our discussion with reporting the values of the parameter θ . At 1.1 Pa we get for θ ($= eC/B$) 433 eV. As is logically to expect, with increasing the pressure the magnitude of θ should increase – the obtained values are correspondingly 648 eV at 2.0 Pa, and 1007 eV at 6.3 Pa.

Irrespective of the reasonable values for the ion current density extracted from the experimental data, the model should be improved by considering the dissociation which turns out to be an important phenomenon for molecular gases used in industry. That study is in progress and will be reported elsewhere.

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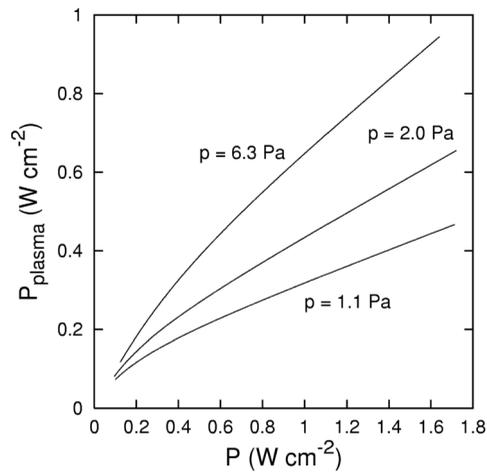


Fig. 1 Theoretically calculated dependences of P_{plasma} on the supplied rf power density P in a NF_3 capacitive discharge at gas pressures of 1.1, 2.0, and 6.3 Pa, respectively.

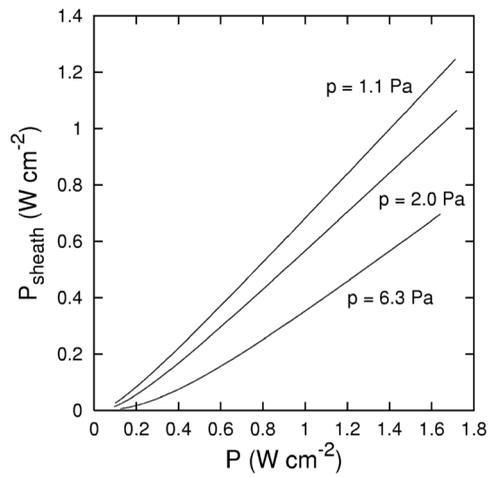


Fig. 2 Theoretically calculated dependences of P_{sheath} on the supplied rf power density P in a NF_3 capacitive discharge at the same gas pressures as in Fig. 1.

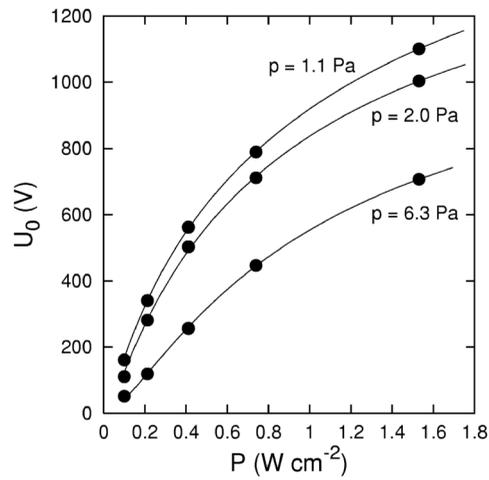


Fig. 3 Theoretically found dependences of the self-bias voltage U_0 on the absorbed power density P in a NF_3 capacitively coupled rf discharge at gas pressures of 1.1, 2.0, and 6.3 Pa, respectively, compared with the corresponding 5 experimentally measured P - U_0 points.

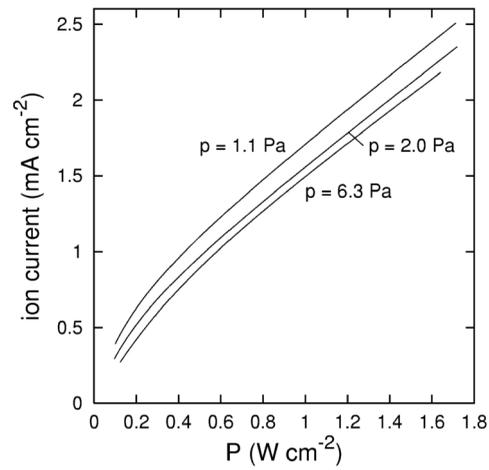


Fig. 4 Theoretically found dependences of the ion current density $e\Gamma_i$ in the space-charge sheath adjacent to the powered electrode on the absorbed total power density P in a NF_3 discharge at the same conditions as in Fig. 3.