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ABSTRACT

Plasma immersion ion implantation (also known as plasma source ion implantation) is a process in which a target is immersed in a plasma and a series of large negative voltage pulses are applied to it to extract ions from the plasma and implant them into the target. A general one dimensional model is developed to study this process in different coordinate systems for the case in which the pressure of the neutral gas is large enough that the ion motion in the sheath can be assumed to be highly collisional.

I. INTRODUCTION

In plasma immersion ion implantation, a target immersed in a plasma is pulsed repetitively with large negative voltages. When the pulse is applied, electrons are repelled from the target on the time scale of the inverse electron plasma frequency, creating a uniform ion sheath. The ions, on a longer time scale, are attracted and implanted into the surface of the target. As the ions are implanted, the ion density in the sheath drops. This causes the sheath-plasma edge to recede and uncover more ions to increase the ion density in the sheath and sustain the potential drop across the sheath. The velocity of the moving sheath edge depends upon, among other factors, the pressure of the background neutral gas. Here we develop a general one dimensional model to study this process in different geometries for the case in which the pressure of the neutral gas is high enough that the ion motion in the sheath can be assumed to be highly collisional. We obtain analytic expressions for normal ion velocity distribution $f(v_x)$, sheath motion $s(t)$, ion flux at the target $J(t)$ and other parameters of interest. We apply this general model to the planar and spherical targets and compare the analytic results with those obtained by simulation. The following analysis was inspired by the work of Lieberman[2], and Scheuer, Emmert, and Conrad *et al.*[3-6]

II. ASSUMPTIONS

At time $t=0^+$, the potential at the target drops to $-V_0$. This negative potential forces the electrons away from the target forming an ion sheath. The sheath-plasma edge, r_s, moves far enough away, as shown in Figure 1(a), so that the potential drop across the sheath equals V_0. The ion density in the sheath, n_s, is still the same as that in the plasma, n_0. At this point, the ions in the sheath, starting at essentially zero velocity, are accelerated by the resultant electric field. However, before traveling far, the ions collide with the neutral particles and scatter or lose their energy. Since the ions suffer many collisions before reaching the target, located at $r = r_a$, the time-varying ion density at any point in the sheath is assumed to change more slowly than the ion transit time through the sheath. The assumptions for this model are:

(1) The electron motion is instantaneous (inertialess).

(2) Charge exchange is the dominant ion-neutral collision mechanism.

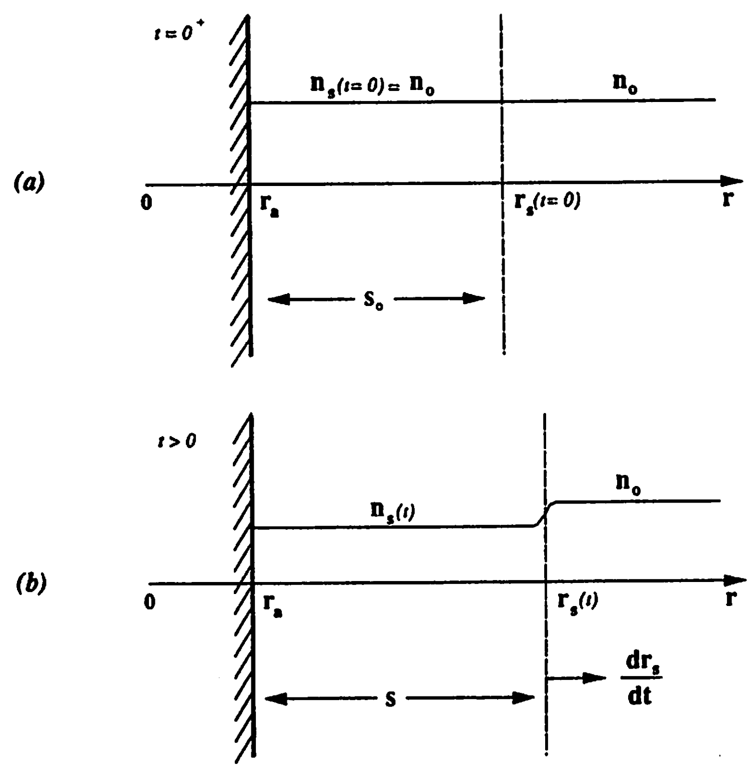

Figure 1. The ion charge density in the sheath and the sheath edge at time $t = 0^+$, and $t > 0$.

(3) The ion motion is highly collisional, hence $s \gg \lambda_i$ where $s = r_s - r_a$ is the sheath thickness, and λ_i is the ion-neutral mean free path.

(4) The applied voltage V_0 is much larger than the electron temperature T_e, hence $s \gg \lambda_D$ where λ_D is the Debye length. The plasma potential is also chosen as the reference potential, $\phi_{plasma} = 0$.

(5) The ion charge density in the sheath is uniform in space but varying slowly in time, as seen in Figure 1(b). This is seen experimentally in DC glow discharges[7] and is also seen in simulation (see Section V). Further, we assume this charge density to be constant during the ion transit time in the sheath.

(6) In order to sustain a constant potential drop across the sheath, the ion loss at the target (the implanted ion current) is compensated by the uncovering of ions at the moving plasma sheath edge.

(7) Ions, having undergone many collisions with the neutrals in the plasma, enter the sheath at the neutral temperature (room temperature).

III. ONE DIMENSIONAL ANALYSIS

Assuming constant ion charge density in the sheath region, $n_i = n_s$ (with $n_e = 0$), one can apply Gauss' law:

$$\nabla \cdot \mathbf{E} = \frac{e}{\varepsilon_0} n_s \tag{1}$$

with a boundary condition $E_r(r_s) \approx 0$ to get $E_r(r)$ (r is a general one dimensional coordinate). Having found the electric field in the sheath, the electric potential can be obtained from $\nabla\phi = -\mathbf{E}$. The boundary condition at the target states that $\phi(r_a) = -V_0$ when the pulse is applied.

Now let us assume an ion, after suffering a charge-exchange collision with a neutral, starts from rest at $r = r_0$ as seen in figure 2. This ion is accelerated by $E_r(r)$ according to the one dimensional equation of motion:

$$\ddot{r} = \frac{e}{M} E_r(r) \tag{2}$$

This acceleration occurs in planar, cylindrical and spherical coordinates since we assume that the total ion velocity has dropped to near zero after the charge-exchange collision; hence conservation of angular momentum forces the other velocity components to remain zero after the collision.

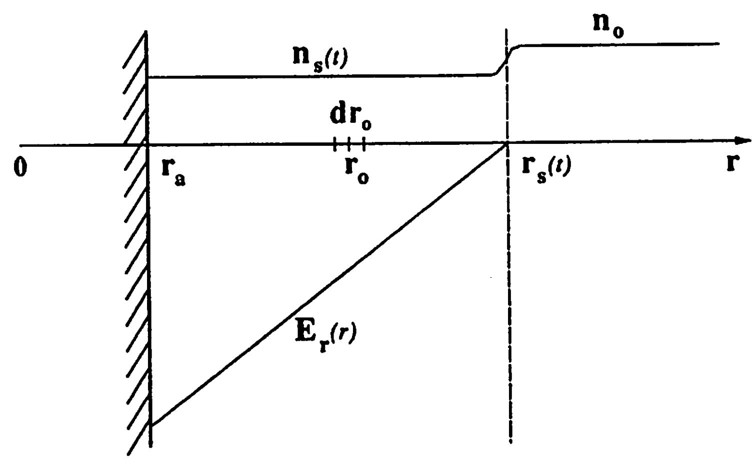

Figure 2. An ion is assumed to be accelerated from rest at $r = r_0$ after a charge-exchange collision. The electric field shown is typical in the planar coordinates.

Equation (2) can be integrated with the following substitutions:

$$\dot{r} = u_r$$

$$\ddot{r} = \frac{du_r}{dt} = \frac{du_r}{dr} u_r$$

This gives:

$$\frac{du_r}{dr} u_r = \frac{e}{M} E_r(r)$$

or,

$$u_r^2(r, r_0) = 2\frac{e}{M} \int E_r(r) dr + c_1 \tag{3}$$

where c_1 can be determined using the initial condition $u_r = 0$ at $r = r_0$. The velocity of the ion at the target, $r = r_a$, starting at r_0 is then:

$$u_a = u_r(r_a, r_0) \tag{4}$$

assuming the ion does not collide with a neutral again before reaching the target.

We now can get an expression for $f(u_a)$, the normal ion velocity distribution, by applying the condition for conservation of particles:

$$f(u_a) du_a = \exp\left(-\frac{r_0 - r_a}{\lambda_i}\right) n_s A(r_0) dr_0$$

where $A(r_0)$ is the cross-sectional area at r_0, λ_i is the ion-neutral mean free path and dr_0 is as shown in Figure 2. The exponential factor, containing the neutral pressure dependence, is the probability of an ion, starting from rest at r_0, striking the target without suffering a charge exchange collision. Thus, we have:

$$f(u_a) = c_2 \exp\left(-\frac{r_0 - r_a}{\lambda_i}\right) n_s A(r_0) \frac{dr_0}{du_a} \tag{5}$$

where dr_0/du_a is calculated from (4) and c_2 is determined by normalization.

Having calculated the ion velocity distribution, one can compute the average ion velocity at the target from:

$$\overline{u_a} = \int u_a f(u_a) du_a \tag{6}$$

The average ion current density at the target is then given by $J_a = \overline{e n_a u_a}$ which is:

$$J_a = e n_s \overline{u_a} \tag{7}$$

where the bar denotes average value over the velocity distribution and the ion density at the target, n_a, is assumed to be the same as in the sheath.

Noting that $\int_S \mathbf{J} \cdot \mathbf{ds} + \frac{\partial}{\partial t} \int_V \rho dV = 0$ guarantees conservation of charge, the sheath motion can be calculated from:

$$J_a A(r_a) = -\frac{\partial}{\partial t}(e n_s V(r_s, r_a)) + \frac{\partial}{\partial t}(e n_0 V(r_s)) \tag{8}$$

where $V(r_s, r_a)$ is the volume of the sheath region and $\partial V(r_s)$ is the volume of the shell at r_s uncovered by the moving sheath edge over the interval ∂t. The first term in the right hand side of (8) is the rate of change of the total ion charge in the sheath. This rate of change is zero if there is no charge accumulation in the sheath region, i.e. the ion density in the sheath, n_s, decreases at the same rate that the volume of the sheath region increases. The second term in the right hand side of (8) is the rate at which the ions in the plasma are uncovered by the moving sheath edge as shown in Figure 1(b). This is the rate at which the ions are introduced into the sheath region which must be the same as the ion loss at target if there is no charge accumulation in the sheath.

Equation (8) can be integrated for $r_s(t)$. This could then be used to determine the time dependence of such parameters as J_a and $\overline{u_a}$. $J_a(t)$ represents the rate of ions implanted into the target per unit time, which is an important parameter in the ion implantation process.

IV. PLANAR COORDINATE SYSTEM

For simplicity in this case one can assume that the target is located at the origin, $r_a = 0$, hence $r_s = s$. In one dimensional planar geometry (1) becomes:

$$\frac{\partial E}{\partial x} = \frac{e n_s}{\varepsilon_0}$$

Integrating this from the sheath edge to some arbitrary position in the sheath, x, and assuming that $E(s) = 0$, we have:

$$E(x) = \frac{e n_s}{\varepsilon_0}(x - s)$$

The electric potential with respect to the plasma potential is then:

$$\phi(x) = \frac{e n_s}{\varepsilon_0}\left(s x - \frac{x^2}{2} - \frac{s^2}{2}\right)$$

Applying the boundary condition, $\phi(0) = -V_0$, we obtain:

$$n_s = \frac{2\varepsilon_0 V_0}{e s^2} \tag{9}$$

Thus, the equation of motion for an ion starting from rest at $x = x_0$ after a charge transfer collision in the sheath is:

$$\frac{d^2 x}{dt^2} = \frac{eE(x)}{M} = \frac{2eV_0}{Ms^2}(x - s)$$

where s, the sheath thickness, is assumed to vary slowly compared with the ion transit time. Integrating this using (3), we find:

$$u^2 = \frac{u_m^2}{s^2}[(x^2 - x_0^2) - 2s(x - x_0)]$$

where $u_m^2 = 2eV_0/M$ is the maximum ion velocity at the target. The ion velocity at the target is then given by:

$$u_a^2 = \frac{u_m^2}{s^2}(2sx_0 - x_0^2) \tag{10}$$

Equation (5) in this case becomes:

$$f(u_a) = c_3 e^{-x_0/\lambda_i} n_s A(x_0) \frac{dx_0}{du_a}$$

Solving (10) for x_0 and differentiating x_0 with respect to u_a:

$$f(u_a) = \frac{c_3 u_a}{(1 - u_a^2/u_m^2)^{1/2}} \exp\left(\frac{s}{\lambda_i}\left((1 - u_a^2/u_m^2)^{1/2} - 1\right)\right)$$

The parameter c_3 is determined by normalization to be:

$$c_3 = \frac{s}{\lambda_i u_m^2 (1 - e^{-s/\lambda_i})}$$

The complete expression for $f(u)$ is therefore:

$$f(u_a) = \frac{s u_a}{\lambda_i u_m^2 (1 - e^{-s/\lambda_i})(1 - u_a^2/u_m^2)^{1/2}} \exp\left(\frac{s}{\lambda_i}\left((1 - u_a^2/u_m^2)^{1/2} - 1\right)\right) \qquad (11)$$

Assuming $s \gg \lambda_i$, the average ion velocity at the target can be found using (6) to be:

$$\overline{u}_a = \left(\frac{e V_0 \pi \lambda_i}{M s}\right)^{1/2} \qquad (12)$$

Inserting (12) and (9) into (7), we get:

$$J_a = \varepsilon_0 \left(\frac{4\pi e \lambda_i}{M}\right)^{1/2} \frac{V_0^{3/2}}{s^{5/2}} \qquad (13)$$

The current density given by (13) has the same dependence on s and λ_i as the equation obtained by Lieberman[8], but is greater by roughly a factor of three. Lieberman uses $\mu = 2e\lambda_i/\pi M u$ for the mobility of the ions in the sheath; this mobility is valid for the case in which ions are moving in a constant uniform applied electric field[9]. The electric field in the sheath is not constant, hence the expression for the average mobility has a different coefficient.

In planar geometry, the term $n_s V(r_s, r_a)$ in Equation (8) is time-invariant, hence:

$$J_a = e n_0 \frac{ds}{dt}$$

Thus the sheath velocity is:

$$\frac{ds}{dt}=\frac{\varepsilon_0}{e n_0}\left(\frac{4\pi e\lambda_i}{M}\right)^{1/2}\frac{V_0^{3/2}}{s^{5/2}}$$

or,

$$\frac{ds}{dt}=u_0\frac{s_0^{5/2}}{s^{5/2}} \tag{14}$$

where $s_0=(2\varepsilon_0 V_0/e n_0)^{1/2}$ is the initial sheath thickness, and $u_0=(eV_0\pi\lambda_i/Ms_0)^{1/2}$ is a characteristic ion velocity in the sheath. Integrating (14), we find:

$$s(t)=s_0(1+\omega_0 t)^{2/7} \tag{15}$$

where $\omega_0=(7u_0/2s_0)$ is a characteristic frequency for the ions in the sheath.

Putting (15) into (9), (12) and (7), we obtain:

$$n_s(t)=\frac{n_0}{(1+\omega_0 t)^{4/7}} \tag{16}$$

$$\overline{u}_a(t)=\frac{u_0}{(1+\omega_0 t)^{1/7}} \tag{17}$$

$$J_a(t)=\frac{e n_0 u_0}{(1+\omega_0 t)^{5/7}} \tag{18}$$

One can also insert (15) into (11) to obtain the velocity distribution of ions as a function of time.

V. COMPARISONS WITH SIMULATION

We use the code PDP1[10-11] to simulate a one dimensional planar bounded plasma system. The Particle-in-Cell method, covered in detail by Birdsall and Langdon (1985)[12], is implemented in PDP1 to solve for the particle and field parameters self-consistently. The code also uses a Monte Carlo scheme to model the collisions of charged and neutral particles (charge-exchange and scattering ion-neutral collisions and elastic, excitation and ionization electron-neutral collisions) with laboratory cross-sections used to determine $\nu(E)$. In order to compare the analytic results, Equations (11), (17) and (18), with the simulation, we need only consider ion-neutral charge-exchange collisions.

At time $t = 0$, a pulse with a fall time of 1μsec and magnitude 500 V is applied to the left electrode, and the potential at the electrode is kept at this constant value thereafter. Initially the space between the two electrodes is filled with a uniform plasma. The neutral gas used for these runs is argon and the other common parameters are: length = 30 cm, area = 100 cm^2, $n_0 = 10^7$ cm^{-3}, V_0 = -500 V, fall time = 1 μsec, and T_e = 1 eV.

Figure 3 shows the ion and electron number densities at time $t = 1\mu$sec, when the pulse is fully applied and a later time $t = 7\mu$sec for the neutral pressure of p = 50 mTorr. These density profiles tend to justify our assumption of uniform ion density in the sheath.

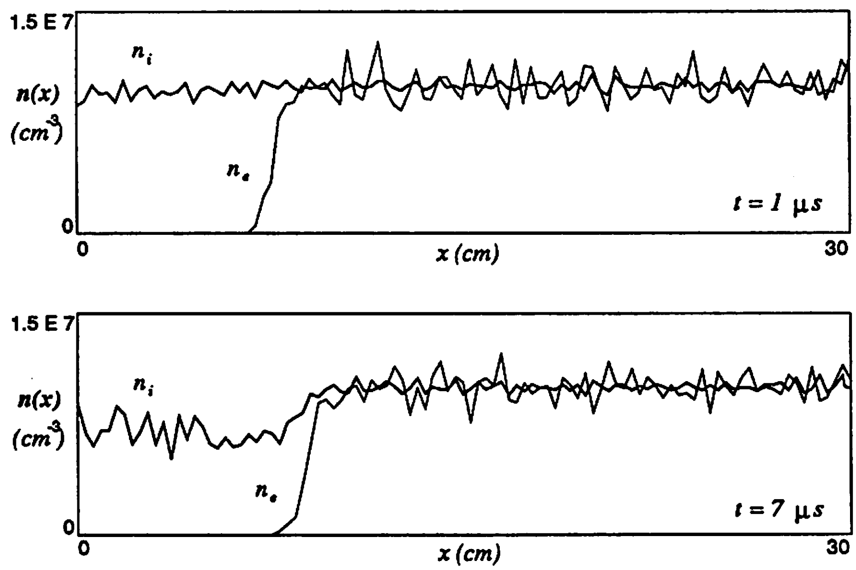

Figure 3. At $t = 1\mu$sec, the potential at the left electrode is V_0, the sheath edge has moved to its initial position and the ion density in the sheath appears to be roughly the same as that in the plasma. At $t = 7\mu$sec, the sheath edge has moved further away from the electrode and the ion density in the sheath has a nearly uniform profile.

As previously described, one can put (15) into (11) to get the instantaneous velocity distribution of ions. Doing so, we compare the result with the simulation at the following pressures: p = 20, 50, and 100 mTorr, as seen in Figure 4.

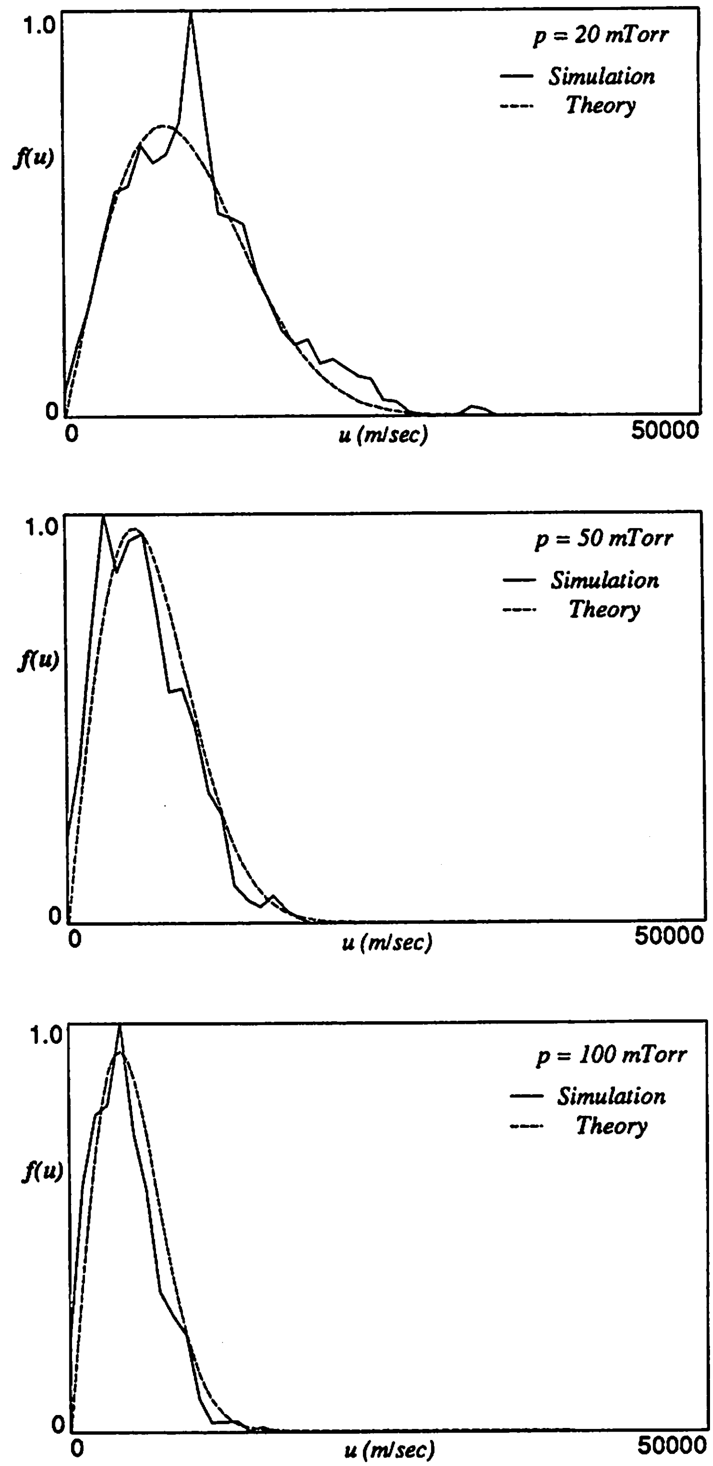

Figure 4. Ion velocity distribution at the target. Note that the maximum ion velocity at the target, $u_m = (2eV_0/M)^{1/2}$, is roughly 50000 m/sec for this applied voltage.

Figure 5 displays a comparison of Equation (17), average ion velocity at the target as a function of time, with simulation for the neutral pressures of 20 and 30 mTorr.

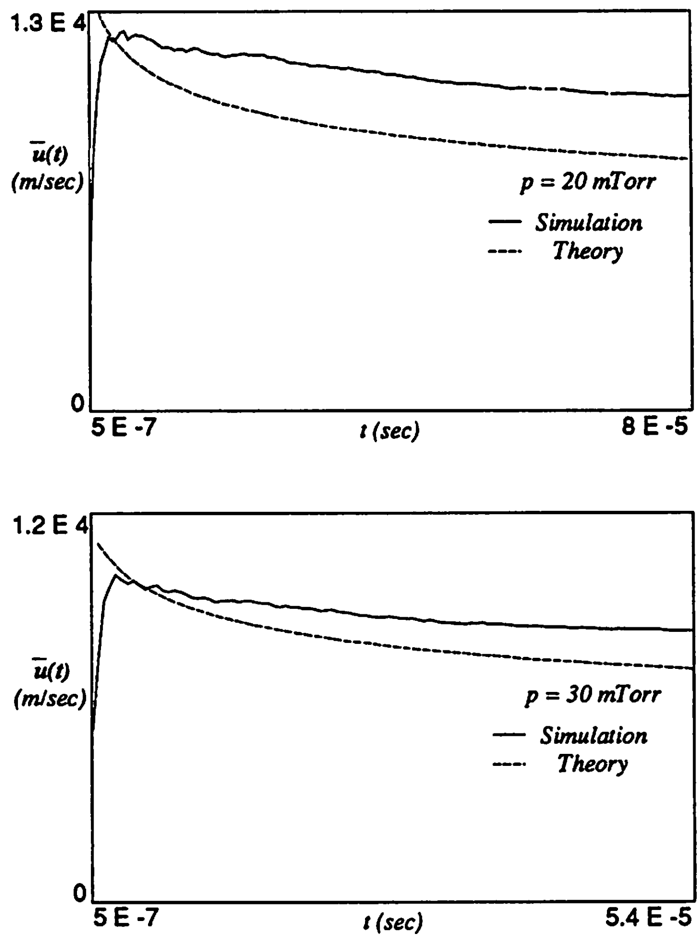

Figure 5. The time response of average ion velocity at the target.

Equation (18), the ion flux at the target as a function of time, is compared in Figure 6 with simulation for the neutral pressures of 50 and 100 mTorr. Although the ion flux compares well with the simulation, the analytic average ion velocity appears to be somewhat smaller than the one obtained by simulation. The discrepancy may come from the constant profile assumed for the ion density in the sheath. The ion density seen in the simulation is not quite uniform, being slightly lower at the target.

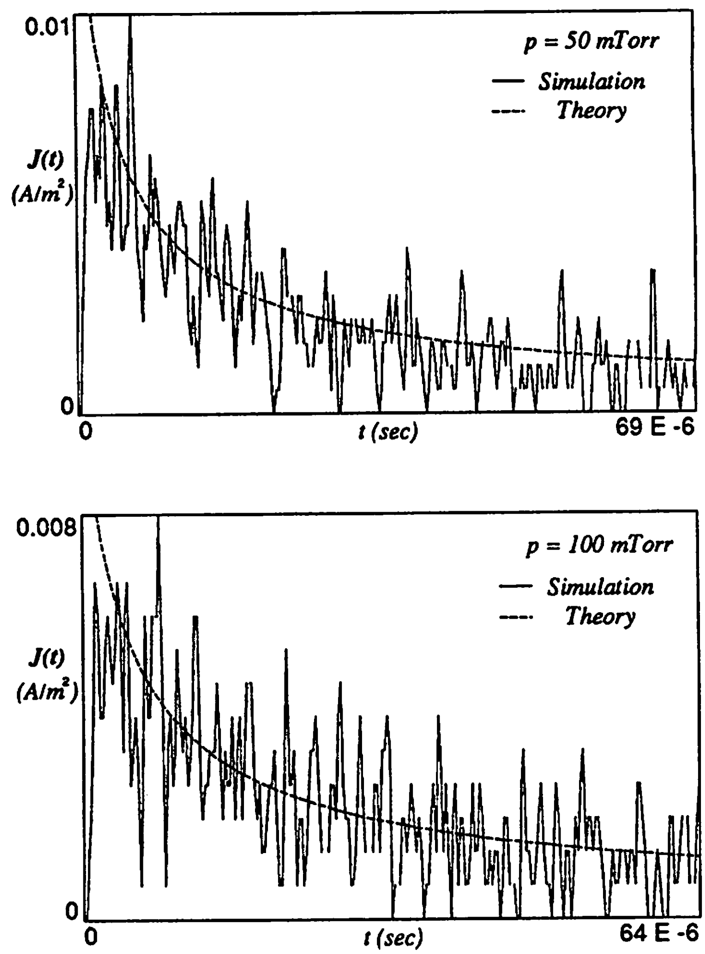

Figure 6. The time response of average ion velocity at the target.

VI. SPHERICAL COORDINATE SYSTEM

In this geometry, we assume the target to be a sphere of radius r_a, hence (1) becomes:

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 E_r) = \frac{e n_s}{\varepsilon_0}$$

One can integrate this from the sheath edge, r_s, to some r in the sheath to obtain:

$$E_r(r) = \frac{e n_s}{3\varepsilon_0}\left(r - \frac{r_s^3}{r^2}\right)$$

provided $E_r(r_s) = 0$. The electric potential with respect to the plasma potential is then:

$$\phi(r) = -\frac{e n_s}{3\varepsilon_0}\left(\frac{r^2}{2} + \frac{r_s^3}{r} - \frac{3}{2} r_s^2\right)$$

Applying the boundary condition, $\phi(0) = -V_0$, we get:

$$n_s = \frac{6 V_0 \varepsilon_0 r_a}{e R^3} \tag{19}$$

where

$$R^3 = r_a^3 + 2r_s^3 - 3r_s^2 r_a$$

At time $t=0$, the density in the sheath is assumed to be the same as in the bulk plasma. Hence, the initial position of the sheath edge can be found from (19) to be:

$$r_{s_0} \approx (3 r_a V_0 \varepsilon_0 / e n_0)^{1/3} + r_a/2$$

This expression is the same as that derived by Conrad[13] plus a correction term, $r_a/2$, for the case in which r_s is comparable to r_a.

We will carry on the analysis assuming $r_s \gg r_a$, where the electric field can be approximated by:

$$E_r(r) \approx -\frac{e n_s}{3\varepsilon_0}\left(\frac{r_s^3}{r^2}\right)$$

and R^3 reduces to:

$$R^3 \approx 2r_s^3 \tag{20}$$

Equation (2) in this case becomes:

$$\ddot{r} = -\left(\frac{e^2 n_s}{3\varepsilon_0 M}\right)\frac{r_s^3}{r^2}$$

Integrating this, using (3), we get:

$$u^2 = r_a u_m^2\left(\frac{1}{r} - \frac{1}{r_0}\right)$$

where $u_m^2 = (2e V_0/M)(2r_s^3/R^3)$ is the maximum ion velocity at the target modified by a scaling factor due to the geometry. The ion velocity at the target is then:

$$u_a^2 = r_a u_m^2\left(\frac{1}{r_a} - \frac{1}{r_0}\right) \tag{21}$$

Equation (5) in this coordinate system becomes:

$$f(u_a) = c_4 \exp\left(-\frac{r_0 - r_a}{\lambda_i}\right) r_0^2 \frac{dr_0}{du_a}$$

Solving for r_0 in (21) and differentiating it with respect to u_a:

$$f(u_a) = c_4 \frac{u_a/u_m}{(1-(u_a/u_m)^2)^4} \exp\left(-\frac{r_a}{\lambda_i} \frac{(u_a/u_m)^2}{1-(u_a/u_m)^2}\right)$$

The constant c_4 is determined by normalization to be:

$$c_4 = \frac{2r_a^3}{u_m(\lambda_i r_a^2 + 2\lambda_i^2 r_a + 2\lambda_i^3)}$$

For $r_a \gg \lambda_i$:

$$c_4 \approx \frac{2r_a}{u_m \lambda_i}$$

Putting this value into the expression for $f(u)$:

$$f(u_a) = \frac{2r_a}{u_m \lambda_i} \frac{u_a/u_m}{(1-(u_a/u_m)^2)^4} \exp\left(-\frac{r_a}{\lambda_i} \frac{(u_a/u_m)^2}{1-(u_a/u_m)^2}\right) \tag{22}$$

The average ion velocity at the target, given by (6), is then:

$$\overline{u_a} = \left(\frac{r_s^3}{R^3}\right)^{1/2} \left(\frac{eV_0 \pi \lambda_i}{M r_a}\right)^{1/2} \tag{23}$$

Inserting (23) and (19) into (7):

$$J_a = \varepsilon_0 \left(\frac{36\pi e r_a \lambda_i}{M}\right)^{1/2} \frac{V_0^{3/2}}{r_s^3} \left(\frac{r_s^3}{R^3}\right)^{3/2} \tag{24}$$

Using Equation (8) to determine the motion of sheath edge in this geometry and noting that the term $n_s V(r_s, r_a)$ is time-invariant for $r_s \gg r_a$, we have:

$$4\pi r_a^2 J_a = 4\pi r_s^2 e n_0 \frac{dr_s}{dt}$$

which, assuming $r_s \gg r_a$ and using (20) can also be written as:

$$\frac{dr_s}{dt} = \frac{u_0 r_a^2 r_{s_0}^3}{r_s^5} \tag{25}$$

where $r_{s_0}^3 = (3V_0\varepsilon_0 r_a/en_0)$ is the initial position of the sheath edge, and $u_0 = (eV_0\pi\lambda_i/2Mr_a)^{1/2}$ is a characteristic ion velocity in the sheath. Equation (25) can be integrated to find r_s as a function of time to be:

$$r_s = r_{s_0}(1+\omega_0 t)^{1/6} \tag{26}$$

where $\omega_0 = 6u_0 r_a^2/r_{s_0}^3$ is a characteristic ion frequency in the sheath.

One can put (26) into (19), (23) and (7) to obtain:

$$n_s(t) = \frac{n_0}{(1+\omega_0 t)^{1/2}} \tag{27}$$

$$\overline{u}_a(t) = u_0 \tag{28}$$

$$J_a(t) = \frac{en_0u_0}{(1+\omega_0 t)^{1/2}} \tag{29}$$

Even when r_s is comparable to r_a, Equations (26)-(29) may be used to approximate the sheath dynamics. One can also obtain the velocity distribution of ions as a function of time by inserting (26) into (22).

VII. COMPARISONS WITH SIMULATION

The code PDS1[14] is used in this case to simulate a one dimensional spherical bounded plasma system. This code is the same as PDP1 with the basic difference that the field parameters and equations of motion are solved in the spherical coordinates. This code also uses a Monte Carlo scheme to model the collisions of charged and neutral particles, and again we need only consider ion-neutral collisions to compare the analytic results with the simulation. In this case we will compare Equation (11) with the simulation running with argon as the background neutral gas and the following parameters: r_a = 1 cm, p = 50 mTorr, $n_0 = 10^7$ cm^{-3}, V_0 = -10000 V, fall time = 1 μsec, and T_e = 1 eV.

For these parameters, the ion-neutral mean free path, initial position of the sheath edge, average ion velocity, and the characteristic ion frequency and period in the sheath are calculated to be respectively: $\lambda_i = 0.164$ cm, $r_{s_0} = 11.8$ cm, $u_0 = 7.86 \cdot 10^4$ m/s, $\omega_0 = 2.87 \cdot 10^4$ Hz, and $T = \omega_0^{-1} = 3.5 \cdot 10^{-5}$ sec.

Figure 7 shows a reasonable agreement between theory and simulation for the distribution function.

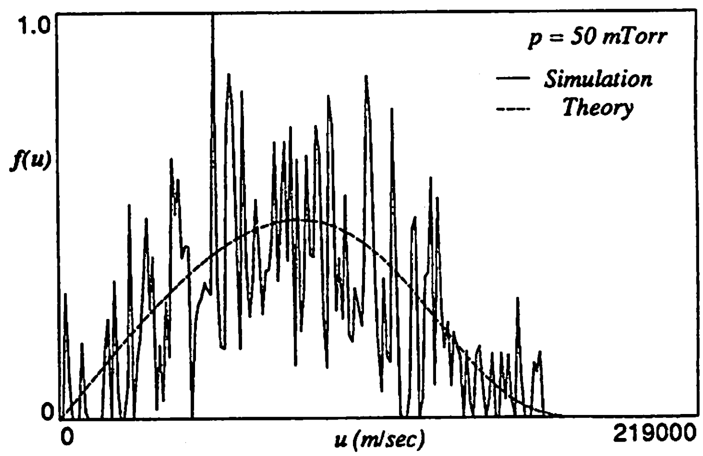

Figure 7. Ion velocity distribution at the target.

Equation (28), average ion velocity at the target as a function of time, is compared in Figure 8 with simulation. The simulation also suggests that the average ion bombardment energy at the spherical target, with $r_s \gg r_a$, is time-invariant in contrast to the time-variant result obtained for the planar target (Equation 17; Figure 5).

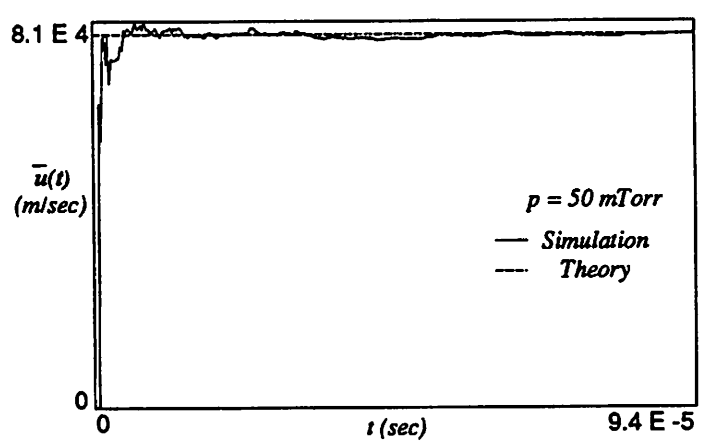

Figure 8. Average ion velocity at the target as a function of time.

The ion charge accumulation in the target is obtained by integrating, Equation (29), the ion current density into the target, over a time interval. This analytic result was calculated, compared with simulation, and shown to be smaller by roughly a factor of two. The disagreement may be a result of the assumption of a constant profile for the ion charge density in the sheath. The observed ion charge density from simulation is not quite uniform, being slightly higher at the target, unlike what was seen for the planar target.

VIII. SUMMARY

A one dimensional collisional model has been developed to study plasma immersion ion implantation in the high pressure regime. The model describes the sheath expansion as a function of time, ion velocity distribution at the target, and the ion flux at the target as a function of time. The problem is solved in both planar and spherical coordinate systems and the analytic results compare well with those obtained by simulation.

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