Effects of Tube Length and Radius for Inner Surface Plasma Immersion Ion Implantation Using an Auxiliary Electrode

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Abstract—Plasma immersion ion implantation of the inner surface of a finite-length small cylindrical tube with a coaxial, grounded auxiliary electrode is modeled using a two-dimensional particle-in-cell model. Various ratios of tube lengths against tube diameters are simulated. It is found that a peak in total accumulated dose is observed near the ends of the tube. Provided that it is long enough, the ions that come from the outside of the tube cannot pass through the middle-plane. That is, the tube can be divided conceptually into an “end” and a “middle” region, while the middle remains empty and all the flux goes to the end. In other words, a one-dimensional model can be applied to the “middle” region. The simulation results including the enhanced ion dose agrees with our experimental data.

Index Terms—Inner surface, ion implantation, particle-in-cell, plasma application.

I. INTRODUCTION

INNER surface modification of many industrial components, such as dies, bushings, pipes, etc. using plasma immersion ion implantation (PIII) is of practical importance and has attracted the attention of physicists and materials scientists [1]–[4]. One drawback of PIII of inner surfaces is low ion impact energy [5], [6]. It has been shown that by inserting a zero potential conductive auxiliary electrode along the axis of the implanted cylindrical tube, the average ion impact energy can be raised [7]. It has also been determined that the normalized auxiliary radius should range from 0.1–0.3 in order to maximize the dose and produce a larger number of ions with high impact energy [8].

In this article, we use a two-dimensional particle-in-cell (PIC) model [9] to investigate realistic cases in two dimensions, such as the important and practical situation when the cylindrical tube is of a finite length. The results acquired for different bore radii and tube lengths are reported. Our results reveal that the ions from outside of the tube are always implanted into a small region near the end thereby giving rise to nonuniform dose distribution along the interior surface. In a short tube, some of the ions pass through the midplane and arrive at the other end of the tube. However, if it is long enough, the ions from the outside of the bore cannot pass through the midplane. Hence, the tube can be divided conceptually into an “end” and a “middle” region, while the middle remains empty and all the flux goes to the end. In other words, simulation in the middle section can be simplified to be one-dimensional (1-D). The enhanced ion dose and other simulation results agree with our experimental data [10].

II. KINETIC MODEL AND NUMERICAL SIMULATION

Two basic assumptions are made for the ions. First, the condition is noncollisional. That is, the ion mean free path is greater than the sheath thickness, and it is valid in typical low pressure PIII applications. Second, the ions acquire directed motion only by the electric field. The electrons are assumed to be in thermal equilibrium, so that the electron density \( n_e \) is given by the Boltzmann’s relationship

\[
    n_e = n_o \exp \left( \frac{e \phi}{kT_e} \right) \tag{1}
\]

where \( n_o \) is the initial ion density, \( k \) is the Boltzmann’s constant, and \( T_e \) is the electron temperature. Thus, we only need to follow the ion dynamics. Poisson’s equation relates the potential \( \phi \) to the electron density \( n_e \) and ion density \( n_i \)

\[
    \nabla^2 \phi = -\frac{e}{\varepsilon_o} (n_i - n_e) \tag{2}
\]

where \( \varepsilon_o \) is the permittivity in free space and \( e \) is the electron charge. The ions are governed by Newton’s equations of motion [11]

\[
    \Delta \vec{p} = \vec{V}_i \Delta t - \frac{q}{2M} \nabla \phi (\Delta t)^2 \tag{3a}
\]

\[
    \vec{V}_b = \vec{V}_b - \frac{q}{M} \nabla \phi \Delta t \tag{3b}
\]

where \( q \) is the ion charge, \( M \) is the ion mass, \( \vec{V}_a \) and \( \vec{V}_b \) are the velocities before and after the time step \( \Delta t \). The plasma quantities can be made dimensionless in cylindrical coordinates by normalization

\[
    \rho = \frac{r}{D}, \quad L = \frac{z}{D}, \quad T = t \omega_f, \quad \Psi = \frac{\phi}{\phi_f}
\]

\[
    N = \frac{n_i}{n_o}, \quad VL = \frac{\nu_f^2}{v_{max}}, \quad \text{and} \quad V\rho = \frac{\nu_f^2}{v_{max}}
\]

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where \( r \) and \( z \) are the radial and longitudinal distances, \( \phi_p \) is the peak voltage of the pulse, \( \mathbf{v}_r^0 \) and \( \mathbf{v}_z^0 \) are the ion velocity components along the radial and longitudinal direction, \( D = \sqrt{-\frac{4\pi e\phi_p}{c\eta_0}} \) is the ion-matrix overlap length, \( \omega_{\text{p}} = \sqrt{n_0 e^2\varepsilon_0 M} \) is the ion plasma frequency, \( \eta_{\text{max}} = \sqrt{2\omega_{\text{p}}/D} \) is the velocity the ion would have if it fell through a potential drop \( \phi_p \), and \( M \) is the ion mass. For instance, \( M = 28 \times 1.67264 \times 10^{-27} \text{ kg} \) (nitrogen molecule, single positive charge), \( n_0 = 1 \times 10^9 \text{ cm}^{-3} \), and \( \phi_p = -50000 \text{ V} \), we obtain \( D = 10.5 \text{ cm} \), \( \omega_{\text{p}} = 7.8079 \times 10^6 \text{ s}^{-1} \), \( T_{\text{pi}} = \frac{1}{\omega_{\text{pi}}} = 0.127 \mu\text{s} \), and \( \eta_{\text{max}} = 5.8489 \times 10^7 \text{ cm s}^{-1} \).

The vertical cross section of the cylindrical bore and auxiliary electrode is depicted in Fig. 1. The central gray bar symmetrically divides the tube into two equal halves. The midplane of the tube is another symmetry plane and only a quarter of the vertical cross section is thus required in our simulation. We assume that the top and right boundaries of the simulation regions are connected by a neutral plasma. Therefore, at these boundaries \( \Psi = 0.0 \). At the tube surface \( \Psi = 1.0 \) and on the surface of the auxiliary electrode \( \Psi = 0.0 \). At the bottom boundary \( \partial \Psi / \partial L = 0.0 \). The rise time of the applied voltage is set to zero and initially, and the ions are evenly distributed in the simulation region. We adopt the finite difference method to solve the equations [11]. After the position and velocity of each ion at a particle time step are derived, they will be weighted to the four corners of the mesh containing the ion. Provided the sheath is far away, the potential \( \Psi \approx 0.0 \) and the density of electron \( n_e \approx n_0 \) according to (1). The electrical acceleration will be weak and the heavy ions will not move at all. The densities of the electrons and ions will remain constant in the bulk plasma. When the ion hits the bore surface, it will be removed. The simulation model does not include the recombination process of the electrons and ions. We do not also include any generation mechanism of ion-electron pairs like secondary electron bombardment. The dose and impact angle surrounding the bombardment area will be automatically accumulated. If the ion crosses the bottom boundary, it is assumed that another ion from the other side with reverse longitudinal ion velocity will cross the boundary refilling the lost ion.

### III. RESULTS AND DISCUSSIONS

The auxiliary electrode radius is set to be equal to 0.1 D (in our case 1.05 cm), and the bore lengths and inner radii of the tube are varied. A total of four different cases are investigated: total tube length \( = 2 \) and \( 8 \) times \( D \) (half bore length \( = 1 \) and \( 4 \) times \( D \), i.e., 10.5 and 42 cm) and inner radii \( = 0.5 \) (5.25 cm) and 1.0 D (10.5 cm). The thickness of the tube is zero. As shown in Fig. 1, a single grid line represents the tube. However, the electric field has different values inside the tube and outside of it. Thus, a double-valued electric field can be set inside and outside the tube even though the ion density is displayed as a single average value. We use zero rise time for the applied potential \( |\phi_p| = 30 \text{ kV} \) and \( T_e = 5 \text{ eV} \).

The other simulation parameters are: grid spacing \( = 0.02D \) (0.21 cm) and time step \( = 0.002T_{\text{pi}} \) (2.54 \times 10^{-4} \mu\text{s} \), where \( T_{\text{pi}} = 1/\omega_{\text{pi}} \). The area of one cell \( 4.0 \times 10^{-1}D^2 \), i.e., \( 0.0441 \text{ cm}^{-2} \). The maximum simulation area is \( 6 \times 3D^2 \) and a total of 45,000 cells are considered. Each cell contains \( 1 \times 10^9 \times 0.0441 = 4.41 \times 10^6 \text{ cm}^{-3} \) nitrogen molecules. One hundred particles (ions) are initially uniformly placed in each cell. Therefore, each particle represents \( 4.41 \times 10^5 \text{ cm}^{-3} \) of nitrogen molecules in our example. The simulation lasted for \( 40T_{\text{pi}} = 5.08 \mu\text{s} \). We will continue the discussion of the result in a more general approach and not refer to any particular case. The normalized parameters are adopted.

#### A. Potential

The temporal evolution of the potential contour lines is displayed in Fig. 2 for \( t = 20, 80, 200, \) and \( 400T_{\text{pi}} \). The potential contour lines of bore radius equal to 1.0 D and bore length (half) equal to 1.0 and 4.0 D are depicted in Fig. 2(a) and (b). Fig. 2(c) and (d) illustrate the case when the bore radius is 0.5 D. Comparing Fig. 2(a) and (c) to Fig. 2(b) and (d), the potential contour lines pack more closely in the bore with inner radius \( = 0.5 \). The evolution of the potential sheath of the top region above 3.0(3.5) D of the long bore is identical to that of the short bore with bore radius equal to 1.0(0.5) D. In a deeper region of the long bore shown in Fig. 2(b) and (d), the potential sheath is vertical implying that there is only a radial electric field in this region.

#### B. Ion Density

The temporal evolution of the ion density is exhibited in Fig. 3. As shown in Fig. 3(a) and (b), the ions are bunched together near the inner surface of the tube (with radius = 1.0 D) at around 0.5 D from the top. However, when the tube radius is reduced to 0.5 D, the ion accumulation begins earlier and the location moves to around 0.15 D from the top.
Fig. 2. Temporal evolution of the normalized potential for (a) radius = 1D, half-length = 1D and (b) radius = 1D, half-length = 4D.
Fig. 2. (Continued.) Temporal evolution of the normalized potential for (c) radius = 0.5D, half-length = 1D and (d) radius = 0.5D, half-length = 4D.
Fig. 3. Temporal evolution of the normalized ion density for (a) radius = 1D, half-length = 1D and (b) radius = 1D, half-length = 4D.
Fig. 3. (Continued.) Temporal evolution of the normalized ion density for (c) radius = 0.5D, half-length = 1D and (d) radius = 0.5D, half-length = 4D.
Fig. 4. Evolution of the total incident dose along the inner surface of the bore for (a) radius = 1D, half-length = 1D and (b) radius = 1D, half-length = 4D.

C. Total Dose

The local incident doses along the inner surface of the tube are displayed in Fig. 4. The two cases of bore radius equal to 1.0 are shown in Fig. 4(a) and (b). The other two cases of bore radius equal to 0.5 are exhibited in Fig. 4(c) and (d).

as depicted in Fig. 3(c) and (d). At \( t = 40 \), the inside of the tube is observed to be empty. The density oscillations observed along the longitudinal axis and above the top of the tube are due to the sheath edge lying along a row or column and jumping from grid lines to grid lines.
Initially, the inner surface of the bore is evenly implanted except a small peak at the top of the bore where the electric field is concentrated. After some time, the deeper region of the bore is not implanted. The total dose reaches 5000 as shown in Fig. 4(a) and (b) (bore radius = 1.0 D), but only 2000 as shown in Fig. 4(c) and (d) (bore radius = 0.5 D). Only a small region of the inner surface continues to get implanted at later time as illustrated by the instantaneous dose (D) and impact...
Fig. 5. Evolution of the instant dose (0.5T accumulation) along the inner surface of the bore for (a) radius = 1D, half-length = 1D and (b) radius = 1D, half-length = 4D.

angle (E). The total dose peaks at 0.5 D from the top of the bore for a bore radius of 1.0 D as shown in Fig. 4(a) and (b). When the bore radius is 0.5 D, the peak is located at 0.15 D from the top of the tube as shown in Fig. 4(c) and (d).

D. Instantaneous Dose

The instantaneous incident dose along the inner surface of the tube using an accumulation of $0.5T_{pe}$ is depicted in Fig. 5. When the bore radius is 1.0 at $t$ is $2.0T_{pe}$, around 700 ions
Fig. 5. (Continued.) Evolution of the instant dose (0.5T accumulation) along the inner surface of the bore for (c) radius = 0.5D, half-length = 1D and (d) radius = 0.5D, half-length = 4D.

(100 ions per cell) are implanted evenly along the inner surface except at the top of the bore as shown in Fig. 5(a) and (b). However, after the ions present initially inside the bore have been exhausted, outside ions with an impact angle less than 180 degree [see instant impacted angle (E)] are implanted into a small region 0.5 D from the top of the bore. No ions arrive
at the rest of the surface when the bore length (half) is longer than 1.0 D. Therefore, a peak of accumulated implanted dose is observed at this area exhibited in Fig. 4(a) and (b).

Fig. 6. Evolution of the instant impact angle (average of 0.5T) along the inner surface of the bore for (a) radius = 1D, half-length = 1D and (b) radius = 1D, half-length = 4D.

Fig. 5(c) and (d) depict the case of bore radius equal to 0.5 D. When the bore is narrower, the ions inside the bore are exhausted sooner and outside ions are implanted into an area.
Fig. 6. (Continued.) Evolution of the instant impact angle (average of 0.5T) along the inner surface of the bore for (c) radius = 0.5D, half-length = 1D and (d) radius = 0.5D, half-length = 4D.

0.15 D from the top of the bore as shown in Fig. 5(c) and (d). In both cases, it can be observed that the ions implanted into the inner surface decrease with time. In fact, as shown in Fig. 5(c) and (d), no ions arrive at \( t = 40T_{\text{r}} \). Therefore, the total accrued dose into the inner surface of the bore will not increase anymore.
E. Impact Angle

The impact angle of the ions along the inner surface of the bore using an average of $0.5T_p^*$ is depicted in Fig. 6. The impact angle $\theta$ is defined in Fig. 1. If there is no ion impact, the impact angle will be set to zero. As shown in Fig. 6(a) and (b) with bore radius of 1.0 D and $t$ equal to $2.0T_p^*$, most of the implanted ions incident at a normal angle except near the top region. Some of the ions come from outside of the tube and can pass through the midplane of the bore to be implanted into the other side. However, the chance becomes smaller if the tube length is larger or narrower. As displayed in Fig. 6(a), at a later time, the impact angle can be larger than 180$^\circ$. These ions must come from the other side of the bore with velocity pointing upward and at $t = 4.0T_p^*$, these ions arrive at the top of the bore. Fig. 6(b)–(d) does not reveal any impact angle greater than 180$^\circ$ and no ions have passed through the midplane.

IV. CONCLUSION

For the practical case when the bore length is finite, our results show that after all the ions present initially in the bore have been exhausted, outside ions are influenced by the auxiliary electrode and implanted into a small area near the top of the bore. A local region with a maximum total dose thus results. When the bore radius is 1.0/0.5 D, the peak is located at 0.5/0.15 D from the top of the bore. If the bore is short, some of the ions can pass through the midplane of the bore and land on the other side. We have observed that some of the ions can indeed pass through the midplane of the bore and get implanted into the top of bore. The impact angle of these ions points upwards. However, as the bore gets longer, the chance of these outside ions passing through diminishes. They will thus not add to the accrued dose in the deeper region of the bore. Provided that the bore is long enough, we can conceptually divide the inner bore surface into a middle region and an end region covering the rest of the bore. According to our results, the boundary between the “middle” and “end” regions can be demarcated at 1.0/0.05 D from the top of the bore for a bore radius of 1.0/0.5 D. Implantation into the middle region can thus be simplified and simulated by a 1-D model [8]. For example, we can use the 1-D normalized PIC equations

\begin{align}
\frac{\partial^2 \psi}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \psi}{\partial \rho} &= N_e - N_I \tag{4a} \\
\Delta \rho &= \frac{V_p \Delta T}{\sqrt{2}} + \frac{1}{8} \frac{\partial \psi}{\partial \rho} (\Delta T)^2 \tag{4b} \\
\Delta V_p &= \frac{1}{\sqrt{8}} \frac{\partial \psi}{\partial \rho} \Delta T. \tag{4c}
\end{align}

The simulation results are in good agreement with our experimental results reported elsewhere.

REFERENCES


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