Theoretical investigation of plasma immersion ion implantation of cylindrical bore using hollow cathode plasma discharge

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A B S T R A C T

Plasma immersion ion implantation of the internal surface of a cylindrical bore with a small diameter is difficult. The use of radio-frequency hollow cathode discharge as the internal plasma source for ion implantation is proposed. The implantation dynamics and plasma sheath expansion are investigated numerically using the particle-in-cell model. The inner diameter of the tube in our simulation is 20 mm and the external diameter of the hollow cathode is 12 mm. Three electric field zones are observed due to the existence of the electrode with ground potential in the tube. The ions undergo acceleration in the region close to the hollow cathode, maintain their velocity in the zone without the electric field due to overlapping of the plasma sheath, and decelerate in the region near the open end of the tube. Most of the ions are implanted into the surface away from the open plane of the hollow cathode. This is attributed to the special configuration of vertical electric field. The simulation results have demonstrated that plasma immersion ion implantation using a hollow cathode can be effectively applied to the treatment of the inner wall of a cylindrical bore, especially the ones with a small diameter.

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1. Introduction

Since the advent of plasma immersion ion implantation (PIII) in the 1980s for the surface modification of metals [1–3], it has been applied to samples with convex and concave surfaces. A tube or bore is an example of a concave surface and has many industrial applications. However, PIII of the interior of cylindrical bores, especially ones that have small diameters, is technically difficult. Owing to overlapping of the converging plasma sheaths from opposite surfaces inside a small hollow bore, the maximum ion impact energy is only 36.8% of the maximum potential drop. The ion impact energy decreases with the square of the radius of the bore [4]. In order to improve the impact energy of ions implanted into the inner wall, Zeng et al. inserted a grounded conductive auxiliary electrode along the axis of the cylindrical bore to be plasma implanted [5]. They also suggested that the normalized auxiliary electrode radius should range from 0.10 to 0.30 in order to maximize the dose and produce a larger number of ions with higher impact energy [6]. Although this technique can substantially improve the bombardment energy of the incident ions, there are remaining problems associated with the uniformity of the plasma density and depletion of plasmas inside the bore. The plasma can rapidly extinguish on a time scale of less than 1 µs under some conditions and the use of longer pulses is not possible. An internal grid-enhanced radio-frequency discharge was utilized by Liu et al. [7]. By introducing a coaxial RF plasma antenna covered with a conductive anode mesh (ground potential), more uniform ion implantation as well as deposition onto the inner surface can be accomplished. However, it is still difficult to treat hollow tubes with small diameters as the mesh serving as the anode limits the diameter of the tube. In addition, the space is needed to capacitively couple the radio frequency (RF) discharge. Here, we propose a new technique to overcome the problem. A hollow cathode discharge sustained by RF is utilized to implant the inner wall. Our results show that it is possible to treat tubes as small as 20 mm in diameter. In this work, in order to fathom the process, numerical simulation using the particle-in-cell model is performed.

2. Theoretical modeling

In the simulation, the ions are assumed to be non-collisional and cold and they acquire directed motion only by the electric field. In the hollow vacuum cathode chamber, the electrons are assumed to be in thermal equilibrium, so that the electron density $n_e$ is given by the Boltzmann relationship:

$$n_e = n_{ij} \exp \left( \frac{e \Phi}{kT_e} \right),$$

where $n_{ij}$ is the initial ion density in the cell of $(i, j)$, $k$ is Boltzmann constant, $T_e$ is the electron temperature, and $e$ is the electron charge.
Poisson’s equation is used to relate the potential \( \phi \) to the electron density \( n_e \) and ion density \( n_i \) as follows:

\[
\nabla^2 \phi = -\frac{e}{\varepsilon_0} (n_i - n_e),
\]

where \( \varepsilon_0 \) is the permittivity in free space and \( e \) is the electron charge.

Outside the hollow vacuum chamber, the potential is solved using the difference method for electrostatic field. The ions are accelerated by the electric field and their motion is described by Newton’s equations of motion [8]. The simulation region is demarcated by dotted lines as shown in Fig. 1. The simulation region is 1.5 cm × 30 cm, and the tube length and inner radius are 25 cm and 1.0 cm, respectively. The inner radius of the hollow cathode is 0.4 cm and the thickness is 0.2 cm. Initially, the nitrogen plasma density in the hollow vacuum charmer is \( 1 \times 10^{11}/cm^3 \) (singly charged nitrogen molecule with an energy of 2 eV) [9,10]. The plasma density is zero outside the hollow cathode in the bore. At the tube wall, a zero rise-time pulse with negative potential, \( \phi_p = -20 \text{ kV} \) is applied. The potential at the hollow cathode wall is zero. The top and right-hand side boundaries of the simulation regions are the chamber walls. \( \partial \psi / \partial r = 0.0 \) at the left symmetry boundary and \( \partial \psi / \partial L = 0.0 \) at the bottom symmetry boundary are applied in the simulation.

3. Results and discussion

The electric potential around the negatively biased tube is shown in Fig. 2. The simulated space may be divided into three zones. Zone I near the hollow cathode is featured by ion acceleration. As shown in Fig. 2b, ion acceleration occurs in a narrow space less than 2 cm. Most of the ions fly upwards due to the parallel potential lines and directly enter Zone II. Zone II has no electric field resulting in no ion acceleration due to overlap of the plasma sheath inside a small cylindrical bore [4]. The ions in this zone maintain their initial velocity before they reach Zone III as shown in Fig. 2c. Zone III is near the vacuum chamber (ground potential) in which the electric field is opposite to that in Zone I and so the ions are retarded.

In order to disclose the dynamics of the implanted ions, some marked ions on the horizontal surface at the outlet of the hollow cathode source are chosen. The trajectories of different ions are relatively complex as revealed in Fig. 3. Ion #1 near the center flies upwards directly due to the vertical electric field. After acceleration in Zone I, it flies through Zone II at a high velocity and then enters Zone

Fig. 1. Schematic of plasma immersion ion implantation of a cylindrical bore using hollow cathode discharge. The simulation region is demarcated by dotted lines.

Fig. 2. Contour of the electric potential around the hollow cathode and tube: (a) entire distribution, (b) distribution near the open end of the tube, and (c) distribution near the open end of the hollow cathode.
where it is decelerated and rebounded at near Point A as a result of the opposite electric field. It returns into Zone I where it is decelerated and accelerated again. Finally, it flies out of Zone I and is implanted into the inner wall on the opposite side. The track “BC” shown in Fig. 3 is produced not by this ion but by that on the left symmetric to ion #1 (vertical axis being the symmetrical axis). Ion #2 has a similar trajectory as ion #1. It is accelerated in Zone I and then enters Zone III. However, after slowing down in Zone III, it does not return to Zone I but rather is implanted into the opposite wall. Interestingly, ion #5 finally goes out of the tube after several oscillations. Only ions #3 and #4 are directly accelerated and implanted to the right wall. It should
be noted that all the ions but ion #1 have curved trajectories initially when flying towards the central zone. This can be attributed to the focusing effects of the plasma sheath at the open end of the hollow cathode as shown in Fig. 2.

Fig. 4 depicts the time-dependent ion velocity of the implanted ions. The abrupt change in the velocity indicates ions passing the vertical axis (symmetrical plane) and flying into the opposite side. The end of each curve shows that the marked ions are implanted into the surface. As shown in Fig. 4a, ion #1 possesses the longest flight time while ion #4 has the shortest one as indicated by the longest track of ion #1 disclosed in Fig. 3. The potential distribution in Fig. 2 is consistent with the time-dependent velocity of the ions in Fig. 4. The time when the velocity of ions is constant indicates that the ions fly into Zone II in which there is no gradient in the electric potential. Ion #3 possesses the highest implantation velocity (radial velocity) since it is accelerated in both Zone I and Zone III. At the open end of the tube, the radial electric field is higher due to the focusing effect at the corner as shown in Fig. 2c. Fig. 5 demonstrates the distribution of incident ion fluence along the tube axis. The ions are mainly implanted into the zone from \( L = 10 \text{ cm} \) to \( L = 25 \text{ cm} \). The ion fluence peaks near \( L = 13 \text{ mm} \) and gradually diminishes at the tube open end. It is consistent with the contour of the electric potential. Most of the ions are initially accelerated by the vertical component of the electric field near the opening of the hollow cathode. This leads to ions flying towards the open end of the tube. The ions are also accelerated simultaneously by the horizontal component of the electric field. Thus, they have a curve trajectory when moving towards the sidewall of the tube. It should be noted that rebounding is more evident for some ions which fly downwards and are implanted near the open end of the hollow cathode. Therefore, the second fluence peak is observed at \( L = 7.5 \text{ cm} \) as demonstrated by Fig. 5. This rebounding occurs before \( t = 100T \) since the value of the second fluence peak does not increase further with time. These trajectories are determined by the time-dependent configuration of the plasma sheath near the open end of the hollow cathode. In the beginning, the equivalent potential line is more or less horizontal thereby making more ions flying directly into Zone III and then rebound back. On a longer time scale, the edge of the plasma sheath curves in the hollow cathode giving rise to more ions directly implanted without entering Zone III. The distribution of the ion fluence may also be reflected by the contour of the ion density in the tube as shown in Fig. 6. Initially at time such as \( 50T \), there are no ions in Zone II less than \( 12 \text{ cm} \) since the average vertical component of the electric field is large. Afterwards, at \( t = 100T \), for instance, there is very little change due to the inward expansion of the plasma sheath leading to ion rebounding. Later on more ions are implanted in the zone from \( L = 8 \text{ cm} \) to \( L = 13 \text{ cm} \) due to the curved plasma sheath in the hollow cathode.

4. Conclusion

The dynamics of plasma immersion ion implantation of the internal surface of a cylindrical bore using hollow cathode discharge is investigated using the particle-in-cell model. The simulation results demonstrate the efficacy of this technique. Some ions may pass through three zones that include the acceleration zone, zone without electric field, and deceleration zone. This leads to complicated trajectories of the ions before they are implanted into the wall of the cylindrical bore. Most of the ions only obtain a small part of the energy and are implanted at a shallow depth. The implant fluence peaks near the open end of the tube. With a longer pulse duration, a second fluence peak appears due to the rebounding effect resulting from the reverse electric field near the open end of the tube. The distribution of the incident ions is consistent with that of contour of the ion density in the simulation zone.

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