A Novel Approach to Simulate the Potential at the Center Axis of Poisson's Equation in Cylindrical Co-Ordinates for Plasma Immersion Ion Implantation Processes

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ABSTRACT

A novel and practical method is developed to resolve the three dimensional Poisson's and Laplace's equation at the center axis in cylindrical coordinates. The method employs the rectangular xyz co-ordinates to solve the potential ϕ along the center axis. The new approach is tested by comparing the potential distribution of a biased cylindrical duct simulated by two dimensional l'Hospital rule. The capability of the method to model non-symmetry field structure is verified by simulating the potential distribution inside the cylindrical duct with only a three quarter of the wall biased with a positive voltage.

Keywords: Poisson's equation, center axis, numerical iteration, cylindrical co-ordinate, non-symmetry field.

1 INTRODUCTION

Plasma immersion ion implantation (PIII) has attracted the attention of materials scientists, physicists, and engineers as an alternative surface modification technique [1]. It emulates conventional beam-line ion implantation in that the implantation time is independent of the sample size and large industrial components of an irregular shape can be treated relatively easily due to its non-line-of-sight characteristic [2-4]. However, owing to the complex nature of a plasma and the plasma-sample interactions, the processing conditions for different types of samples are different and sometimes difficult to identify. An empirical approach is the most straightforward but can be tedious and time consuming. Theoretical simulation eliminates the guesswork and when conducted iteratively with experiments, can pinpoint the correct plasma and processing conditions much more efficiently [5].

PIII can be classified as an electrostatic process as the pulsing frequency is not fast enough to create electromagnetic radiation. The potential ϕ in the volume of the chamber can be described by Poisson's equation: ${}^2\phi = -\rho / \varepsilon_o$, where ρ is the charge density and ε_o is the dielectric constant. The equation can be solved by the finite difference method. To simulate implantation into a three-dimensional structure such as a commercial gear like a bearing or bore, we choose to work in cylindrical coordinates. When working in cylindrical coordinates, attention must be paid to the center axis r = 0, since Poisson's equation is undefined:

$$\frac{f^2\phi}{fr^2} + \frac{1}{r}\frac{f\phi}{fr} + \frac{1}{r^2}\frac{f^2\phi}{f\theta^2} + \frac{f^2\phi}{fz^2} = -\frac{\rho}{\varepsilon_o} \qquad (1)$$

In this article, we present a new and practical approach to approximate the potential by using rectangular coordinates at the center axis. We test the method by simulating the potential distribution inside a cylindrical duct using a grounded plate, i.e., zero potential covers one end of the duct and 50 volts are applied to the wall of the duct. The other end of the duct is connected to the grounded cylindrical chamber. The accuracy of the new method is assessed by comparing the potential distribution to 2D simulation. In two-dimensional (r-z) coordinates, the center axis can be solved by l'Hospital's rule. The potential distribution generated by a non-symmetrical field will be presented.

2 MODELING AND SIMULATION RESULTS

We use an empty cylindrical duct without any plasma, i.e., ρ = 0.0, to test the 3D simulation at the center axis (r = 0) of the cylindrical coordinate of the method. Without any space charges, Poisson's equation becomes Laplace's equation. The radius of the duct is 0.2 meter and the length is 0.5 meter. A grounded plate with zero potential covers one end of the duct. A voltage of 50V is applied to the wall of the hole. The other end of the duct is connected to a grounded cylindrical chamber. The length of the chamber is 0.5 meter and radius is 0.4 meter.

The potential inside the duct and chamber can be simulated by solving the 2D Laplace's equation since the geometry has a cylindrical symmetry [5,6]. Therefore, the 3D method can be verified.

2.1 2D l'Hospital's Rule Approach

In 2D geometry, Laplace's equation is of the form,

$$ {}^2\phi = \frac{f^2\phi}{fr^2} + \frac{1}{r}\frac{f\phi}{fr} + \frac{f^2\phi}{fz^2} = 0 \qquad (2) $$

At the center axis $r = 0$, we can use l'Hospital's rule [6] and Laplace's equation becomes,

$$ {}^2\phi = 2\frac{f^2\phi}{fr^2} + \frac{f^2\phi}{fz^2} = 0 \qquad (3) $$

We can write down the finite difference approximation of Eq. (3) as,

$$ {}^2\phi \cong 2\frac{\phi_{i+1,k} - 2\phi_{i,k} + \phi_{i-1,k}}{(\Delta r)^2} + \frac{\phi_{i,k+1} - 2\phi_{i,k} + \phi_{i,k-1}}{(\Delta z)^2} = 0 \qquad (4) $$

The potential is obtained by an iterative method [6]. The potential contour line of the cross section cylindrical duct is shown in Fig. 1. We use a relative error of < $1.0\text{x}10^{-4}$ to obtain the plot [6]. It is observed that the first derivative of the potential, $f\phi / fr$ along the center axis is zero, and the potential radically decrease outward into the chamber as shown in Fig. 1.

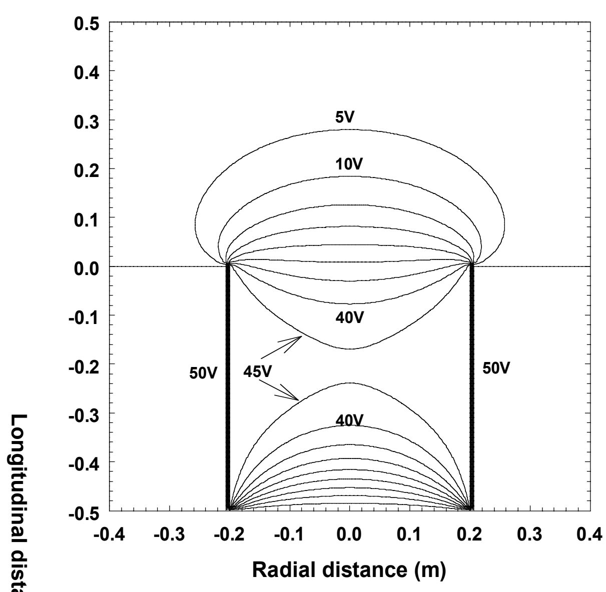

Fig. 1: Potential contour line of the cross section of the cylindrical duct with the potential at the center axis solved by l'Hospital's rule.

2.2 3D Rectangular Approach

In 3D geometry, Laplace's equation in cylindrical coordinates is written as,

$$ {}^2\phi = \frac{f^2\phi}{fr^2} + \frac{1}{r}\frac{f\phi}{fr} + \frac{1}{r^2}\frac{f^2\phi}{f\theta^2} + \frac{f^2\phi}{fz^2} = 0 \qquad (5) $$

At $r = 0$, we can use Laplace's equation in xyz coordinates instead,

$$ {}^2\phi = \frac{f^2\phi}{fx^2} + \frac{f^2\phi}{fy^2} + \frac{f^2\phi}{fz^2} = 0 \qquad (6) $$

The finite difference approximation of Eq. (6) becomes,

$$ {}^2\phi \cong \frac{\phi_{i+1,j,k} - 2\phi_{i,j,k} + \phi_{i-1,j,k}}{(\Delta x)^2} + \frac{\phi_{i,j+1,k} - 2\phi_{i,j,k} + \phi_{i,j-1,k}}{(\Delta y)^2} + \frac{\phi_{i,j,k+1} - 2\phi_{i,j,k} + \phi_{i,j,k-1}}{(\Delta z)^2} = 0 \qquad (7) $$

In xyz coordinates, we need to insert four adjacent points / nodes of potential into Eq. (7) to derive the potential at the center axis along the x-y (r-θ) plane, i.e., $\phi_{i-1,j,k}$, $\phi_{i+1,j,k}$, $\phi_{i,j+1,k}$, and $\phi_{i,j-1,k}$. At the same time, Laplace's equation of the rest of the plane is solved in cylindrical coordinates by Eq. (5). The center point is surrounded by a circle of points depending on Δθ, for example, 72 points for $\Delta\theta = 5°$. Hence, 72/4 = 18 sets of points can be chosen in Eq. (7), for example, $\phi_{i-1,j,k} = \phi_{r,\theta=0,z}$, $\phi_{i+1,j,k} = \phi_{r,\theta=180,z}$, $\phi_{i,j+1,k} = \phi_{r,\theta=90,z}$, $\phi_{i,j-1,k} = \phi_{r,\theta=270,z}$ with $\Delta x = \Delta y = \Delta r$. To take into equal weight among all sets of points, an average is made. The potential is also obtained by an iterative method [6]. The potential contour line of the cylindrical duct cross section is shown in Fig. 2. In this iteration, we use a lower upper relative error boundary of < $5.0\text{x}10^{-5}$. The potential contour line profile is more or less the same as in Fig. 1. The rectangular coordinates treatment at the center axis is thus acceptable. The accuracy can be improved by further lowering the upper relative error boundary.

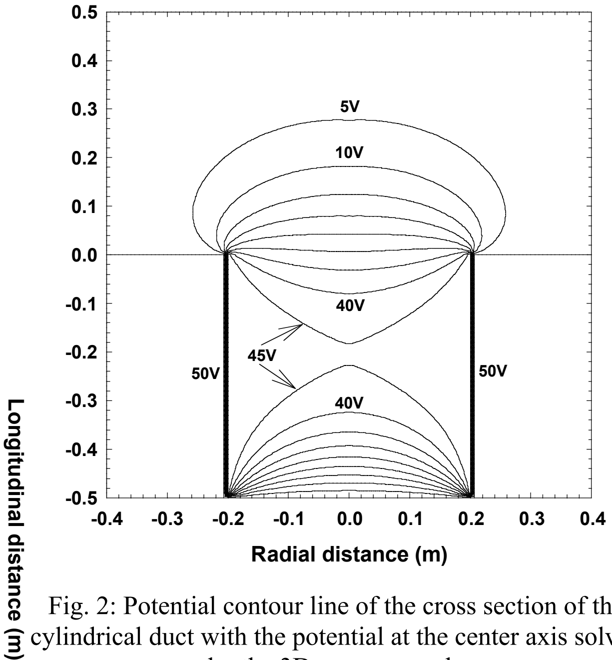

Fig. 2: Potential contour line of the cross section of the cylindrical duct with the potential at the center axis solved by the 3D xyz approach.

2.3 Asymmetrical Potential Field Structure

The xyz method is applied to generate the asymmetrical potential field structure. A quarter of the duct wall from 0º to 90º degree is set to 0V, while the rest of the duct wall is biased to 50V. The potential contour line of the cross section of the asymmetrical field duct along the (r-z) plane is depicted in Fig. 3a. The plane is oriented at θ = 45°/225°. The potential contour lines increase smoothly from the duct wall with 0V to the wall biased at 50V. There is no discontinuity along the center axis. The potential contour line of the cross section along the (r-θ)/(x-y) plane is displayed in Fig. 3b. The saw-tooth structure at the circular boundary of the duct wall is due to a deficiency in the plotting program. The plotting pixel is rectangular. The plane is chosen at half-height of the duct. It is also observed that the potential extends smoothly from the right hand corner with 0V to the rest of the plane through the center axis. It shows that the xyz treatment can accurately and successfully simulate the potential distribution at the center axis.

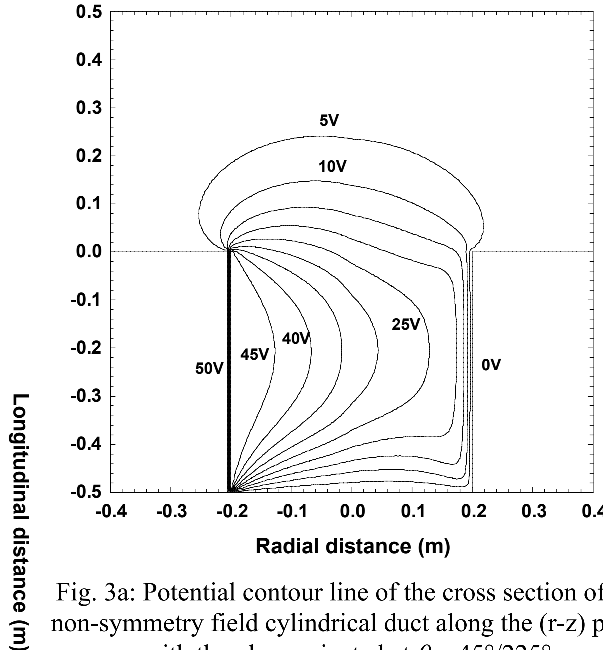

Fig. 3a: Potential contour line of the cross section of the non-symmetry field cylindrical duct along the (r-z) plane with the plane oriented at θ = 45°/225°.

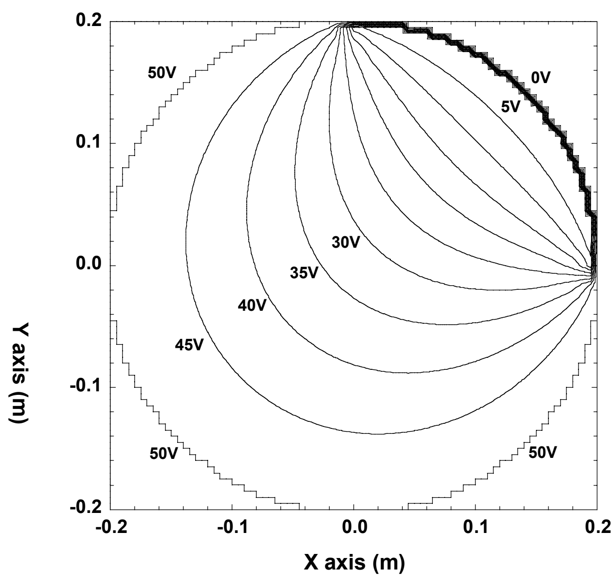

Figure 3b: the potential contour line of the cross section of the non-symmetry field cylindrical duct along the (r-θ)/(x-y) plane is plotted. The plane is chosen at half-height of the duct. The saw-tooth structure at the circular boundary of the duct wall is due to the de-efficient of the plotting program.

3 CONCLUSION

We have developed a novel method to solve the 3D Poisson's and Laplace's equations at the center axis in cylindrical coordinates. The novel method treats the center axis by rectangular xyz coordinates and averages the surrounding set of points to estimate the center potential.

The accuracy of the method is assessed by comparing the potential contour lines of a biased cylindrical duct with the potential contour lines solved by the 2D l'Hospital rules. The capability of the novel method to model asymmetrical field distribution is also verified. A quarter of the duct wall is set different from the rest of the wall generating a asymmetrical potential distribution inside the duct space. The method is shown to successfully simulate the asymmetrical potential field strength inside the cylindrical duct and can be applied to simulate plasma immersion ion implantation into industrial bearings [4].

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