Two-dimensional particle-in-cell plasma immersion ion implantation simulation of gear/windmill geometry in cylindrical co-ordinates along the \((r-\theta)\) plane

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Abstract

Plasma immersion ion implantation (PIII) into gear/windmill structures is simulated by the particle-in-cell (PIC) method in cylindrical co-ordinates. In cylindrical co-ordinates, the gear/windmill geometry becomes a periodic regular structure. An equal number of particles are placed inside the cell with the same angular and radial distance. The ion density represented by each particle is obtained and varies according to the radial distance of the particle. PIII simulation of a rectangular trench is carried out and compared with the cylindrical gear/windmill. The evolution and distribution of the potential and ion density contour lines are the same for these two geometries. The incident doses of a gear (windmill) will be larger than that of the trench. It is due to the space compression in cylindrical co-ordinates along the decreasing radial direction. The incident doses will thus be underestimated when treating a gear tooth using a rectangular trench.

Keywords: Plasma processing and deposition; Ion implantation; Numerical simulation; Particle-in-cell simulation

1. Introduction

Plasma immersion ion implantation (PIII) circumvents the line-of-sight restrictions of conventional beamline ion implantation [1–5] and is therefore an excellent method to treat large and irregular industrial targets like ball bearings [6–8], inner surface of bores [9,10], and gears. The gear crack propagation trajectories in a moving tooth [11], influence of tooth friction in gear dynamic [12], load distribution [13], gear distortion, changes of residual stresses, and hardness during quenching [14] have been numerically investigated by the finite element method (FEM) in a rectangular co-ordinate system. A gear can be treated as a modified ‘windmill’ geometry. A gear/windmill structure can be treated as an irregular geometry in rectangular co-ordinates. However, in cylindrical co-ordinates, it is a regular periodic structure. In this work, we numerically investigate plasma immersion ion implantation of a single tooth sector of a gear/windmill by the particle-in-cell (PIC) method in two-dimensional cylindrical co-ordinates along the \((r, \theta)\) plane [15]. The incident doses along the outer gear circumference, sidewall, and bottom circumference are compared with the simulated results of the PIII process of the trench. The structure of a trench is similar to a sector of a gear except that it is presented in rectangular co-ordinates. PIII of a trench has been numerically investigated by PIC [16]. The dimension settings of the trench are made comparable to the gear/windmill. The potential and density contour lines are derived at different voltage pulse durations. The incident doses along the top, side, and bottom circumference are also generated at different pulse durations. Our results show that the incident doses into a gear/windmill are greater than that into the trench. It is due to the space compression in cylindrical co-ordinates along the decreasing radial direction.

2. Numerical simulation

The simulated region of a gear (windmill) tooth is depicted in Fig. 1a. The base and outer radii \(r_1\) and \(r_2\) are equal to 0.5 and 0.7 m. Therefore, the sidewall is of height 2.0 m; that is, the distance between the \(r\) boundary and the base line is \(= 1.5\) m. The thickness of the tooth is presented in degrees of the sector, and that
of the tooth and base sectors is equal to 18°. The entire simulated region is within a sector of \( r = 2.0 \) m and \( \theta = 36^\circ \). However, the area covered by the gear is not used. The base surface is set at the center of the simulated region partitioning the tooth into two halves. The left and right boundaries are periodical; that is, particles crossing those boundaries will come back to the simulated region from the opposite boundary. The simulated region is filled with cylindrical cells divided equally along the \( r \) and \( \theta \) direction. In this paper, \( dr = 0.02 \) m and \( d\theta = 1^\circ \). However, the cell at a longer \( r \) has a greater area since the circumference is larger. One-hundred particles are equally placed in each cell. The spaces between the adjacent particles are \( dr/10 = 0.002 \) and \( d\theta/10 = 0.1^\circ \). The particle density is equal to

\[
n_o \times \frac{d\theta}{10 \times 360} \times \pi \left( \left( \frac{r + dr}{20} \right)^2 - \left( \frac{r - dr}{20} \right)^2 \right)
\]

\[
= n_o \times \frac{d\theta}{10 \times 360} \times \pi \times \frac{dr}{20} \times r
\]

where \( n_o \) is the ion density and \( r \) is the particle position along the \( r \) direction. Therefore, the particle at a greater \( r \) position will represent more ions. A total of 252,000 ions are used in the simulation.

The simulation settings of the trench are made comparable to the gear as depicted in Fig. 1b. The base line is located at \( y = 0 \). The maximum \( y \) value is 1.5 m; that is, the distance between the \( y \) boundary and base line = 1.5. The sidewall is of height 0.2 m. The circumference of the top surface of the gear is not equal to its base line, although the degrees are the same. The circumference of the top surface = 0.22 m and the base line = 0.16 m. In the trench settings, we have compromised and equalized the length of the top surface = baseline = 0.18 m giving a total length along the \( x \) simulated region to be 0.36. We will discuss the effects on the incident doses by compromising the top and baseline surfaces later in this article. The size of the dividing cell is \( dx = 0.01 \) and \( dy = 0.02 \) m. The baseline of the trench is made the center of the simulated region and the top surface is partitioned into two halves. The left and right boundaries are periodical. One-hundred particles are placed in each cell giving a total of 252,000 particles. Each particle represents the same amount of ions as \( \left( n_o \times \frac{dx}{10} \times \frac{dy}{10} \right) \).

The electron temperature is equal to 2 eV and follows Boltzmann’s distribution. The ions are assumed to be cold and collisionless at low pressure. The plasma density is set as \( 1 \times 10^{14} \) m\(^{-3} \). The plasma consists of singly charged nitrogen ions. They will only be driven by the electric field created by the high negative voltage pulses applied to both targets, i.e. trench and gear. The applied voltage is \(-20 \) kV. The potential of the simulated region is governed by Poisson’s equation. The potential at each node, and therefore Poisson’s equation, is estimated by the finite difference method [17]. The nodes within the simulated region will iterate until the potential of each node has relaxed and converged to within a relative error of \( 1 \times 10^{-4} \). The particle movement is handled by Newton’s equations. After the particle position has been updated at the time step, the
The potential contour lines of the sector of the gear (windmill) and trench at pulse durations of 1, 5, 10 and 20 μs are plotted in Fig. 2a,b. At 1 μs, the potential contours have bent inwards following the concave structure of both targets. As the ions are being removed and land onto the target surfaces, the ion sheath as well as potential lines evolve into a smooth circumference around the gear geometry and straight line in the trench co-ordinate.

### 3. Numerical results

The potential contour lines of the sector of the gear (windmill) and trench at pulse durations of 1, 5, 10 and 20 μs are plotted in Fig. 2a,b. At 1 μs, the potential contours have bent inwards following the concave structure of both targets. As the ions are being removed and land onto the target surfaces, the ion sheath as well as potential lines evolve into a smooth circumference around the gear geometry and straight line in the trench co-ordinate.
The ion density contour lines at pulse durations of 1, 5, 10 and 20 μs are plotted in Fig. 3a,b. After the first few microseconds, the ions inside the ‘volcano area’ of both structures are attracted and removed. The ions leaving the ion sheath will be accelerated by the strong electric field established between the ion sheath and target surfaces. The amount of ions is too small to fill up the empty spaces, and therefore, at 20 μs, the ion density near the surfaces of the targets is too small to be reflected in the contour plot showing a zero value in those areas. The $2 \times 10^{13} \text{ m}^{-3}$ ion density contour line at 0.6 and 0.7 m from the base line is at 10 and 20 μs in both figures. It shows that the propagating speed of the ion sheath is similar in both geometries.

The incident doses of the left-handed top surface, left-handed sidewall and bottom surface of both geometries are plotted in Figs. 4–6. The incident doses are calculated by accumulating the incident particle densities divided by the cell width. The cell width for the sidewall is 0.02 m. In the trench geometry, the cell width of the top and bottom surfaces is 0.01 m. However, as mentioned before, in the gear geometry, the circumference of half of the top surface = 0.11 m and the base line = 0.16 m. Therefore, the cell width of the top surface is 0.012 m and of the bottom base line is 0.0088 m. The cell bears the same distance of 1.0°. In principle, the incident dose of the top surface of a gear should be less than that on the top surface of a trench since it is divided by a larger length. On the opposite, the incident dose of the bottom surface should be larger than that of the base surface of a trench since it is divided by a smaller value. However, we will shortly see that they are not the dominating factor when comparing doses between these geometries.

The incident dose of the top surface always exceeds that of the sidewall and bottom surfaces. It is because the same number of ‘projected ions’ is shared by the sidewall and bottom surfaces. There is an increase of the incident doses at the corner at the beginning of the implantation process due to the focusing of the electric field near the corner. The small increase becomes the background at a longer implantation time. The ions
obtain enough momentum at later time and will equally distribute along the surfaces. The curvature of the bottom surface also reaches a background level at longer pulse durations as shown in Fig. 6. The sidewall shows a distinct ladder distribution of incident doses with the highest dose at the top open area. The ladder distribution is retained at longer pulse durations reflecting that it is always harder for the ions to land on the bottom area of the sidewall. The maximum dose of the sidewall is greater than that of the bottom surface, but it is outnumbered at longer times of 10 and 20 μs. At a longer implantation time, the momentum of the ions is so high that it is hard for the electric field to pull them to the sidewall.

It is observed that the incident doses of the gear geometry are higher than the trench co-ordinates. The difference becomes more obvious at larger pulse durations. The implantation ions originate from the uncovering process of the ion sheath because when expanding, the ion sheath uncovers more ions. The ion flux will indeed depend on the covered area of the ion sheath. In the trench geometry, the ion sheath area will more or less maintain the same amount of area and the ion flux will not exceed certain values. However, in the case of a gear geometry, as the ion sheath expands in the increasing r direction, the ion sheath area will uncover more and more ions. We can think of it as a focusing effect of ions from a large ion sheath area into a smaller target surface. Therefore, the incident dose difference in the gear geometry becomes more obvious at a larger pulse duration.

4. Conclusion

We have simulated plasma immersion ion implantation into a gear (windmill) geometry by the particle-in-cell method. The simulation is carried out in cylindrical co-ordinates in which the gear (windmill) becomes a periodic regular structure. The angular and radial distance of each cell is the same and an equal number of particles is placed inside the cell. The ion density represented by each particle is different according to its radial distance. Plasma immersion ion implantation into a rectangular trench is simulated to compare with that into a cylindrical gear. It is found that the evolution and distribution of the potential and ion density contour lines are the same between these two geometries. The non-uniform incident doses along the top and bottom surfaces will reach background values at larger implantation time since the ions will gain larger momentum. The incident doses of the sidewall always show a ladder shape with a maximum at the top open area because it is harder for the ions to land on the bottom area of the sidewall. In cylindrical co-ordinates (r, θ), the circumference will increase as r increases. Therefore, the ion sheath will uncover more ions at longer implantation time (larger r). The extra ions will compress and focus into the smaller target surface area. The incident doses of a gear (windmill) will be larger than that of the trench. The incident doses will thus be underestimated when treating a gear’s tooth by a rectangular trench.

Acknowledgments

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References