Hybrid particle-in-cell (PIC) ions and Boltzmann electron distribution simulation of direct-current plasma immersion ion implantation into three-dimensional objects

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Received 11 October 2009, in final form 26 January 2010
Published 19 February 2010
Online at stacks.iop.org/JPhysD/43/095203

Abstract
A hybrid protocol including particle-in-cell (PIC) ions and Boltzmann electron distribution is developed to simulate plasma immersion ion implantation (PIII) into an S-shaped bar inside a grounded cylindrical cage consisting of a mesh. A multiple-grid system with three cell confinements is adopted to achieve sufficient accuracy and acceptable computational time. The simulation results reveal that the implantation fluence distribution along the major curvature is more uniform than that obtained by conventional PIII.

1. Introduction

A good way to modify the surface of a large object is plasma immersion ion implantation (PIII) [1, 2]. During the process, the object is placed in a vacuum chamber and exposed to a radio frequency sustained gas plasma. Negative high voltage pulses of several tens of kilovolts are applied to the target. Electrons in the vicinity of the negatively biased sample are repelled and an ion sheath is established. Positive ions are then accelerated towards and implanted into the target. Depending on the pulse duration and pulsing frequency, the processing time can last from minutes to hours. Since the target is immersed in the plasma, the target is surrounded by an ion sheath when negative voltage pulses are applied and to achieve deep implantation. An over-propagated ion sheath also causes instability to plasma generation if the necessary electrons required to sustain the discharge are depleted. To reduce the thickness of the ion sheath, the pulse duration can be shortened but it will take a longer time to obtain the required ion fluence. If the pulsing frequency is increased to compensate for the shorter pulse duration, the load on the power modulator is increased. An alternative is to increase the ion density, but a higher plasma density is equivalent to increasing the conductivity in space. Electrical arcing is more likely to happen, in particular, for targets with sharp corners. If the plasma density is raised by increasing the background gas pressure, collisions will reduce the net implantation energy.

In 2000, we proposed direct-current (dc) PIII that can restrict the expansion of ion sheath [4]. In this low-pressure steady-state dc mode, a grounded conducting grid divides the chamber into two parts. In the lower part, a strong electric field is formed between the negatively biased wafer stage and the boundaries created by the grid and the lower part of the chamber walls. The upper part confines the plasma since the grounded grid stops the expansion of the ion sheath towards the lower part. In this way, a continuous low-pressure discharge can be maintained in the volume above the target.

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the grid. Positive ions from the plasma diffuse into the lower part through the grid and are subsequently implanted into the sample. Since the ion sheath is stopped by the grounded conducting grid, the pulse duration can be increased to over 100 µs without encountering adverse effects such as non-uniform ion distribution and excessive plasma damage to samples such as polymeric materials, which typically plague conventional PIII. The processing time is also significantly reduced. The methodology was experimentally conducted by Fu et al [5] on a large flat target such as a 300 mm diameter silicon wafer. The concept has recently been extended to three-dimensional (3D) samples and experimentally verified by implanting NiTi S-shaped rods used for surgical correction of scoliosis [6]. In this modified setup that is suitable for treating 3D targets, a grounded Al housing and stainless steel mesh are used to surround the sample stage and the rods. It has been shown that a TiN barrier is formed on the bar and this quasi-dc PIII process can improve the efficacy of the process [6].

In this paper, we provide the numerical evidence by using a hybrid model including particle-in-cell (PIC) ions and Boltzmann electrons [7, 8]. The simulation is conducted in 3D rectangular coordinates. To reduce the number of nodes but retain the resolution at the critical region, the multiple-grid PIC method [8–11] is employed.

2. Multiple-grid PIC simulation

A detailed description of the experimental setup can be found elsewhere [12]. An S-shaped rod is placed in the middle of the chamber on a cylindrical stainless steel sample stage. The sample stage is shielded by a grounded aluminium cylindrical cage capped with an Al cover with a central hole. The rod is surrounded by a cage made of stainless steel fine mesh and a flat solid Al dish is inserted on top of the cage. The S-shaped rod and the sample stage are completely shielded from the plasma. The plasma can only diffuse into the cage through the fine mesh. The chamber was pumped down to a base pressure of $9 \times 10^{-5}$ Torr. During the implantation, 20 sccm nitrogen gas was fed into the chamber and the pressure increased to $8.8 \times 10^{-4}$ Torr. Under such a low working pressure, the ions–ions and the ions–neutrals collisions were ignored. Two simulations were conducted to model the implantation uniformity along the S-shaped rod using the meshed cage and without the cage (normal PIII conditions). Based on a previous probe measurement [13], a nitrogen plasma density of $3 \times 10^{15}$ m$^{-3}$ is used in the simulations using N$_2^+$ which is the dominant ion under such conditions. The electrons are in thermal equilibrium at a temperature of 2.5 eV [13]. A voltage of $-35$ kV is applied to the rod via the sample stage and the simulations cease at 15 µs with a zero rise time.

A volume of $0.3$(x-axis) $\times$ $0.3$(y-axis) $\times$ $0.6$(z-axis) = 0.054 m$^3$ is modelled. A parallelepiped sample stage of length 0.15 m, width 0.15 m and height 0.08 m is located at the centre of the bottom of the simulation region. The S-shaped rod with a radius of 3 mm is made up of two arcs and placed on top of the sample stage at the centre. The bottom arc consists of a 30$^\circ$ partial circle with a radius of 0.3 m. The virtual centre of this circle is at $-0.11$ m, 0.15 m and 0.23 m. The top arc is also a 30$^\circ$ partial circle with a radius of 0.1 m. The virtual centre of this smaller circle is at 0.237 m, 0.15 m and 0.43 m. Both arcs are parallel to the x–z plane at $y = 0.15$ m. The convex side of the top arc faces the negative x direction and the bottom arc faces the positive x direction as illustrated in Figure 1. (a) Schematic of the simulation setup showing the three multiple-grid regions, the sample stage, the S-shaped bar, the cylindrical can and the cylindrical mesh; the sample stage is a parallelepiped. (b) The nodes created at the rod surfaces and part of the nodes representing the meshed cage boundaries.
Figure 2. Potential and ion density contours plotted in the x–z plane with \( y = 0.15 \) m with the potential contours having an interval of 5 kV and the ion density contours having an interval of \( 1.0 \times 10^{15} \) m\(^{-3} \). (a) and (c) depict the potential and density contours when the bar is surrounded by the meshed cage. (b) and (d) depict the potential and density contours when the bar is opened in space.

Figure 3. Potential and ion density contours plotted in the y–z plane with \( x = 0.15 \) m with the potential contours having an interval of –5 kV and the ion density contours having a line interval of \( 1.0 \times 10^{15} \) m\(^{-3} \). (a) and (c) depict the potential and density contours when the bar is surrounded by the meshed cage. (b) and (d) depict the potential and density contours when the bar is opened in space.

To achieve sufficient accuracy and acceptable computation time, a multiple-grid system with three cell confinements is adopted. The finest cell of size 2.5 mm \( \times \) 2.5 mm \( \times \) 2.5 mm divides region 1 between \( x = 0.1 \) m and \( x = 0.2 \) m; \( y = 0.1 \) m and \( y = 0.2 \) m; and \( z = 0.08 \) m and \( z = 0.485 \). This region contains the entire S-shaped rod of height 0.4 m and part of the sample stage. The cell of size 5.0 mm \( \times \) 5.0 mm \( \times \) 5.0 mm divides a bigger region 2 between \( x = 0.05 \) m and 0.25 m; \( y = 0.05 \) m and 0.25 m; and \( z = 0.0 \) m and 0.58 m. This region encloses the previous region. The cage consists of a fine mesh and the sample stage. The largest cell of size 10.0 mm \( \times \) 10.0 mm \( \times \) 10.0 mm divides the rest of the simulation region 3. The three regions are illustrated in figure 1(a) and 467 120 nodes are created. Extra nodes are created along the S-shaped rod surface adding the total number of nodes to 468 785 [15]. The nodes created at the rod surface and part of the nodes representing the meshed cage boundaries are shown in figure 1(b). To maintain a smooth transition for the PIC ions from outside the meshed cage into the cage region, zig-zag boundaries of the cage are adopted and no extra nodes are created for the cage. Virtual nodes are created at boundaries between multiple grids to solving Poisson’s equation [15] and the final nodes amount to 508 262. The PIC particles are uniformly distributed over the regions giving a density of 1 per 15.625 mm\(^3\), i.e. one PIC particle inserted in the finest cell of size 2.5 mm \( \times \) 2.5 mm \( \times \) 2.5 mm. Although the quality of the ion number density was low, it did
not affect the accuracy of the simulation because the space potential and electric field were dominated by an external source. Eight PIC particles are inserted into the cell of size 5.0 mm $\times$ 5.0 mm $\times$ 5.0 mm, and 64 PIC particles are inserted into the cell of size 10.0 mm $\times$ 10.0 mm $\times$ 10.0 mm. Two simulations are conducted without and with the meshed cage. The PIC particles are not inserted inside the meshed cage volume and below the Al top cover volume. A total of 2 274 256 PIC particles are initially inserted into the case with the meshed cage and a total of 2 764 184 PIC particles are inserted into the case without the meshed cage. The locations of the PIC particles are updated by Newton’s equation with a time step of $2.55 \times 10^{-9}$ s such that they cannot move more than 2.5 mm with a full kinetic energy of 35 keV.

3. Results and discussion

The potentials of the nodes outside the meshed cage are solved and iterated by finite difference using the finite difference Poisson’s equation assuming Boltzmann electron distribution, temperature equal to 2.5 eV and plasma potential of 50 V through successive over relaxation (SOR) [8, 14]. The iteration does not terminate unless the relative error of each node is less than $1 \times 10^{-6}$. A SOR factor of 0.95 is used in the iteration. When the negative pulse is turned on, the electrons inside the meshed cage and below the Al top cover are repelled and absorbed by the grounded wall or mesh. Therefore, in this region, the finite difference Poisson’s equation is replaced by Laplace’s equation. However, when the meshed cage is removed, all the nodes are iterated using the finite difference Poisson’s equation.

The potential and ion density contour lines after simulating for 15 $\mu$s are plotted in figures 2 and 3. The potential contours have a line interval of 5000 V and the ion density contours have a line interval of $1.0 \times 10^{15}$ m$^{-3}$. In figures 2 and 3, the ion density contours show discontinuity gaps in the inner region around the S-shaped bar because the PIC particle density is not sufficiently high. However, a strong electric field is developed in this region as a result of the $-35$ kV bias and the ion density is not a dominant factor in the potential distribution. The ion trajectories and ion fluence distribution along the S-shaped bar are not affected by a low PIC particle density.

In figure 2, the contours are plotted in the $x-z$ plane with $y = 0.15$ m. The S-shaped bar curvature is clearly shown. Figures 2(a) and (c) display the potential and ion density contours when the S-shaped bar is implanted in the presence of the cylindrical mesh. Because of the blockage, the ion sheath does not develop outside the mesh area and the potential and ion density contours are confined inside the cylindrical mesh. Figures 2(b) and (d) depict the potential and ion density contours when the S-shaped bar is implanted without the cylindrical mesh (conventional PIII). The ion sheath expands and develops according to the curvature of the S-shaped bar and the ion sheath reaches the right-hand side boundary.

Figure 3 plots the contours in the $y-z$ plane with $x = 0.15$ m. The S-shaped bar cuts through this plane only at a few points. Figures 3(a) and (c) show the potential...
and ion density contours when the S-shaped bar is implanted with the cylindrical mesh. Again, the ion sheath does not develop outside the mesh area because of the cylindrical mesh blockage. Figures 3(b) and (d) show the potential and ion density contours when the S-shaped bar uses the conventional PIII setup. In this case, the ion sheath expands and develops evenly on the left- and right-hand sides of the bar because the S-shaped bar is symmetrical in this plane.

The accumulated ion doses along the S-shaped bar, i.e. the z-axis, after 15 $\mu$s are displayed in figure 4. The S-shaped bar is divided into small sectors of $dz = 2.5$ mm for a total of 160 sectors. Each sector is divided equally into four arcs as viewed from the top. The first arc faces the $-x$ and $+y$ directions, the second arc faces the $+x$ and $+y$ directions, the third arc faces the $-x$ and $-y$ directions and the fourth arc faces the $+x$ and $-y$ directions. Any PIC particles falling within each tiny arc are accumulated. The ion dose distributions along the S-shaped bar implanted inside the cylindrical mesh (new approach) are shown in figures 4(a.i) to (a.iv), whereas the ion dose distributions along the S-shaped bar implanted in open space (conventional PIII) are exhibited in figures 4(b.i) to (b.iv). As shown in figure 4(b), the distributions of the ion fluences are non-uniform along the length of the S-shaped bar. The ion fluences are higher at the top and gradually decrease to the bottom. This is typical of conventional PIII and the situation becomes worse for a longer implantation time when the ion sheath propagates into the wider open space [3]. Owing to the disturbance of the top arc, the ion fluences show two peaks at the top above $z = 0.3$ m. A small peak is observed at the bottom in the $-x$ direction arising from the extra focusing effect at the junction between the bar and the supporting stage.

When the bar is implanted inside the cylindrical cage (new approach), more uniform ion fluence distributions are achieved. As shown in figure 4(a), uniform distributions are observed along the major bottom curvature below $z = 0.3$ m. The total ion fluences are reduced because the ion flux is controlled by ion diffusion into the mesh which in turn depends on the plasma potential. The double peaks at the top region above $z = 0.3$ m are altered but not reduced. The mesh diameter is too big to smooth out the unbalanced electric field from the top arc. The ion fluences along the $-x$ direction are less than those along the $+x$ direction. They can be made more uniform by mechanically rotating the bar inside the cylindrical mesh.

4. Conclusions

In summary, a hybrid method utilizing PIC ions and Boltzmann electrons has been developed to simulate nitrogen PIII in an S-shaped bar inside a grounded cylindrical cage made of a mesh. The results show that the ion fluence distributions along the major curvature of the bar are more uniform than those without the cage (conventional PIII method). The simulation results corroborate the experimental data and provide the numerical evidence for further development of the quasi-3D dc PIII technique.

References