Plasma sheath physics and dose uniformity in enhanced glow discharge plasma immersion ion implantation and deposition

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(Received 13 March 2009; accepted 8 June 2009; published online 14 July 2009)

Based on the multiple-grid particle-in-cell code, an advanced simulation model is established to study the sheath physics and dose uniformity along the sample stage in order to provide the theoretical basis for further improvement of enhanced glow discharge plasma immersion ion implantation and deposition. At \( t = 7.0\) \( \mu \text{s} \), the expansion of the sheath in the horizontal direction is hindered by the dielectric cage. The electron focusing effect is demonstrated by this model. Most of the ions at the inside wall of the cage are implanted into the edge of the sample stage and a relatively uniform ion fluence distribution with a large peak is observed at the end. Compared to the results obtained from the previous model, a higher implant fluence and larger area of uniformity are disclosed. © 2009 American Institute of Physics. [DOI: 10.1063/1.3160309]

I. INTRODUCTION

Plasma immersion ion implantation (PIII) has been widely applied to the surface modification of various materials to improve the surface physical, chemical, electrical, optical, and magnetic properties. However, the process requires external plasma sources such as radio frequency plasma source. In enhanced glow discharge plasma immersion ion implantation and deposition (EGD-PIII&D), the external plasma sources are not required and the plasma with a density reaching \( 10^9 \) to \( 10^{10} \) \( \text{cm}^{-3} \) is produced by self-glow discharge. An electron-focusing electric field is formed between the small pointed hollow anode and large tabular cathode inside a dielectric cage when a negative voltage pulse is applied to the sample stage. Consequently, the electrons including secondary electrons are all focused to the region near the hollow anode. A higher ionization rate of the gas through the hollow anode can be achieved. The ions with high density are accelerated and implanted into the sample by the negative voltage similar to that in typical PIII, but more effective ion implantation can be achieved. Furthermore, ionization of some solid materials with poor electrical conductivity and some semiconducting materials that are difficult to ionize in typical plasma sources can be enhanced by this method.

The glow discharge characteristics and distribution of the plasma electron density have been investigated experimentally. A two-dimensional (2D) numerical simulation model has been developed based on the multiple-grid particle-in-cell (PIC) system to investigate the sheath physics in EGD-PIII&D. A malformed sheath and an implant fluence distribution with a sharp decline near the edge of the sample stage are obtained. However, the results are in contrast to previous simulation results for PIII. It is suspected that the dielectric cage used as a gas container where glow discharge is generated plays a key role in the expansion of the plasma sheath and implant fluence distribution. In this paper, we report an advanced numerical simulation model to investigate the temporal evolution of the sheath and fluence uniformity.

II. SIMULATION

Compared to the previously reported experimental configuration, the one used in this work is slightly modified. The sample stage radius is reduced from 120 to 90 mm and covered completely by the dielectric cage with a radius of 130 mm. The schematic of our EGD-PIII&D model is illustrated in Fig. 1. A 2D cylindrical coordinate in the \( r-z \) plane is
adopted in this simulation. According to the cylindrical symmetry of the model, the simulated region is set as the \( r-z \) plane with area of 0.18 \( \times \) 0.42 \( \text{m}^2 \). The multiple-grid system has two cell confinements. The region within \( r \leq 0.13 \text{ m} \) and \( z \leq 0.33 \text{ m} \) is divided into cells with size of 1 \( \times \) 1 \( \text{mm}^2 \). This region contains the dielectric cage, sample stage, and rod. The rest of the region is divided into cells with size of 2 \( \times \) 2 \( \text{mm}^2 \). The simulation results with sufficient accuracy are guaranteed and the computing time can be shortened as much as possible by the multiple-grid PIC code.\(^9,10\)

To simplify the calculation, the following assumptions are made:

1. In theory, when a PIC particle passes through the \( z \)-axis (Fig. 1) from right to left, there would be another particle passing through the same boundary from left to right with the same energy and momentum. Hence, the \( z \)-axis (where \( r=0 \)) can be assumed to be the left boundary and the PIC particles passing through the left boundary will be reflected back into the simulation region with a reverse velocity along the \( r \) direction of \( V_r \).
2. Plasma generation is not considered in our simulation, and the Ar plasma with a density of \( 1.0 \times 10^{10} \text{ cm}^{-3} \) is distributed uniformly within the dielectric cage. The PIC particles are utilized to represent the ions and their locations are updated by Newton’s equations of motion.
3. Due to the low working pressure inside the cage of around 0.5 mTorr, collisions between the Ar ions and background gas can be ignored. The Ar ions are accelerated only by the focusing electric field.
4. Although secondary electrons make a contribution to improve the rate of ionization, they are not considered in our calculation as they do not contribute to the ion implant fluence.
5. No ions are assumed to penetrate into the dielectric cage. They only accumulate on the inside surface of the cage and the charges can be neutralized by incoming ions or electrons. Hence, the surface potential of the cage is determined by the accumulated surface charges and surrounding space potential.
6. The electrons are considered to be in thermal equilibrium and described by the Boltzmann distribution. The electrons’ temperature is 8 eV.
7. When a PIC particle passes through the top, right, and bottom boundaries, it is considered to be lost.

A negative voltage pulse of \(-10 \text{ kV} \) at 50 Hz is applied to the sample stage. The evolution of the space potential, ion density, and electron density are simulated for a pulse duration of 51 \( \mu \text{s} \) with a rise time of 1 \( \mu \text{s} \). The fall time is not considered. The dielectric constant of the cage is 7.5 and the bottom boundaries are set with mirror symmetry with \( d\phi / dr = 0 \) (left and right) and \( d\phi / dz = 0 \) (top and bottom). \( \phi \) is the space potential.

The potential of each node is estimated by iterating the finite difference equations of Laplace’s formula, Poisson’s formula, and Gauss’ law via the successive over relation. The methods of calculating the potential inside the cage at the boundaries of the cage and outside the cage have been described previously.\(^6,17\)

III. RESULTS AND DISCUSSION

The temporal evolution of the potential contour lines is shown in Fig. 2. In the initial implantation stage, the potential contour lines expand evenly along the vertical and horizontal direction according to the shape of the sample stage. At \( t=7.0 \mu \text{s} \), the plasma sheath in the horizontal direction hits the cage wall, and the potential configuration is divided into two parts by the boundary of the cage. However, the implantation process is not affected and continues normally. Because there is no plasma outside of the cage, the potential contours are almost invariable at the later stage of implantation. It is also shown that the plasma sheath keeps on expanding until the end of the pulse.

Figure 3 depicts the ion density distribution at different times. At \( t=40 \mu \text{s} \), two regions of centralized plasma can be clearly observed. One is adjacent to the bias substrate and the other is in the vicinity of the hollow anode. It is similar to previous simulation and investigation of the plasma distribution.\(^2,4\) Expansion of the sheath is relatively slow because of the bigger chamber compared to previous simulation. As a result of the sheath expansion, more ions in the sheath are implanted into the sample stage and so the density of the remnant plasma is quite small. Furthermore, loss of the ions located at the top inside edge of the cage is more seriously and most of them are considered to be accelerated and injected into the edge of the sample stage. The temporal evolution of the electron density is exhibited in Fig. 4. Once the negative voltage pulse is applied to the sample stage, the plasma sheath is formed almost at the same time. Electrons are expelled to the hollow anode under the focusing electric field formed by the small-pointed anode and large tabular cathode. The phenomenon of electron focusing can be observed clearly in Figs. 4(c) and 4(d).
The ion implant fluences along the sample stage after different time intervals are displayed in Fig. 5. A large peak is observed near the edge of the sample stage and the implant fluence along the rest of the sample stage is correspondingly uniform. Despite the obstacle put forth by the cage to the sheath expansion in the horizontal direction, the sheath covers part of the region at the top inside edge of the cage. Hence, the edge of the sample stage receives more ions originating from the top inside edge of the cage. In the later stage of the implantation, since the plasma is not generated in our simulation, the implant fluence varies slightly between 40 and 51 μs.

**IV. CONCLUSION**

The sheath physics and dose uniformity of EGD-PIII&D are investigated using a numerical model utilizing the multiple-grid PIC code. The sheath is reflected after it reaches the cage wall at $t = 7\, \mu s$. The electron focusing effect is clearly demonstrated by this model. The new model is not believed to affect the self-glow discharge of the system. The ions near the inside wall of the cage are implanted into the edge of the stage, and so an ion implant fluence distribution with a sharp peak at the edge of the dielectric cage is achieved. In comparison with the previous model, the implantation fluence increases by almost 40%, and a larger area of radius $\leq 7.0\, \text{cm}$ receives a uniform implant fluence distribution. Both are significant and important improvements for EGD-PIII&D.

**ACKNOWLEDGMENTS**

The work was financially supported by Hong Kong Research Grants Council (RGC) General Research Funds (GRF) No. CityU 112306 and CityU 112307 and National Science Foundation of China No. 10775103.