Theoretical investigation of sheath expansion and implant fluence uniformity in enhanced glow discharge plasma immersion ion implantation

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In enhanced glow discharge plasma immersion ion implantation that involves a small-pointed anode and large area tabular cathode, the high negative substrate bias acts as the plasma producer and supplies the implantation voltage. An electric field is created to focus the electrons and the electron-focusing field in turn enhances the glow discharge process. The sheath physics is theoretically investigated using numerical simulation based on the multiple-grid particle-in-cell code. Electron focusing is corroborated and the plasma sheath has enough expansion when $t=40\,\mu s$ so that a uniform distribution of the incident ion fluence is attained. © 2008 American Institute of Physics. [DOI: 10.1063/1.2977962]

A plasma source ion implantation and deposition method, enhanced glow discharge plasma immersion ion implantation and deposition (EGD-PIII&D), which does not require external plasma sources has been proposed recently.1–3 In this technique, the plasma is produced by self-glow discharge as a result of the high negative voltage bias. The small-area, pointed-shape hollow anode and large area tabular cathode form an electron-focusing electric field. Using a special electric field design, the electrons from either the plasma or target (secondary electrons) can be focused to a special hollow anode and the special electron-focusing field in turn enhances the glow discharge process to achieve more effective ion implantation into the substrate. In our previous work, the glow discharge region is simulated by the finite element method.4 The calculated equipotential patterns in the implantation chamber disclose three different regions, which are in qualitative agreement with pictures of the light intensity captured by a camera. The effects of different distances between the anode and cathode on the glow discharge characteristics and the influence of the plasma electron density are evaluated.5 The results disclose that the electron density is quite uniform approaching the negatively biased substrate when the implantation chamber is large and the depth profile of the implanted ions exhibits a typical Gaussian distribution.3 However, the physics of the glow discharge enhanced mechanism as well as the dynamics of the sheath in EGD-PIII&D are unclear. In general, the expansion of the sheath into the plasma determines the ion fluence implanted into the target.6 Consequently, it is important to understand the fundamental phenomenon in this process. In this work, in order to study the sheath physics in EGD-PIII&D, two-dimensional (2D) numerical simulation is developed and performed based on the multiple-grid particle-in-cell (PIC) code implantation.7,8 The issues investigated here include the potential distribution, density profiles of the plasma ions and electrons, as well as incident ion fluence distribution.

The experimental setup of the system has been described elsewhere.4 The system consists of a gas tube (grounded hollow anode), dielectric cage, sample stage, and supporting rod. It is placed inside a bigger vacuum chamber. The gas tube, dielectric cage, metal sample stage, and supporting rod are aligned along the $r=0$ axis and the system possesses cylindrical symmetry. A 2D cylindrical coordinate system in the $r-z$ plane is thus adopted in the simulation. The simulated
The region covers the \( r-z \) plane with area of \( 0.18 \times 0.42 \text{ m}^2 = 7.56 \times 10^{-2} \text{ m}^2 \). The top \( z \), bottom \( z \), and \( r=0.18 \text{ m} \) boundaries are far away from the bigger chamber walls and mirror symmetries are applied when iterating the potential, i.e., for top and bottom \( z \) boundaries \( d\phi/dz=0 \) and for the \( r=0.18 \text{ m} \) boundary \( d\phi/dr=0 \), where \( \phi \) is the space potential.\(^9\) At \( r=0 \), Poisson’s equation in cylindrical coordinate is singular and l’Hospital rule is applied to remove the singularity.\(^9\) The multiple-grid PIC method is employed to simulate the ion motion and ion sheath evolution.\(^7,8\) The multiple-grid system has two cell confinements. The region within \( r\leq0.13 \text{ m} \), \( z\geq0.09 \text{ m} \), and \( z\leq0.33 \text{ m} \) is divided into cells with size of \( 1 \times 1 \text{ mm}^2 \). The inside volume of the dielectric cage and sample stage are well contained in this region. The rest of the region is divided into cells with size of \( 2 \times 2 \text{ mm}^2 \). 42 786 nodes are used in the simulation. A negative voltage pulse of \(-10 \text{ kV} \) is applied to the sample stage and the Ar plasma is generated within the dielectric cage. The surface potential of the cage will vary with the accumulated surface charges and surrounding space potential due to the dielectric cage.\(^9\) Therefore, a much larger volume is simulated in this system. The model of handling dielectric objects in PIII has been described elsewhere.\(^10\) It is assumed that no charges can penetrate into the dielectric volume and Laplace’s equation is used to solve the potential. The plasma is generated inside the cage and Poisson’s equation is used to solve the potential. Outside the cage, the volume is free of plasma since argon gas is only supplied to the cage and therefore, Laplace’s equation is also used to solve the potential. At the dielectric boundaries, the generalized Gauss’ law is adopted to solve the potential. The dielectric constant is 7.5. The aim of this work is to investigate the ion sheath motion and ion fluence distribution along the sample. Hence, plasma generation is not considered here for simplicity. A uniform \( \text{Ar}^+ \) plasma of density of \( 1.0 \times 10^{15} \text{ m}^{-3} \) is initially distributed inside the cage. The \( \text{Ar}^+ \) ion motion is simulated by PIC particles. 12 \( \times 12 \) PIC particles are equally placed in each cell inside the cage volume. A total of 2 570 400 PIC particles are inserted at the beginning of the simulation. Collisions between the \( \text{Ar}^+ \) ions and neutral \( \text{Ar} \) atoms are not considered because the working pressure is relatively low at 0.5 mTorr.\(^11\) The electrons are described by the Boltzmann distribution at a temperature of 8 eV. The plasma potential is set to zero. 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 (SOR).\(^8,10,12,13\) The iteration does not stop unless the relative error of each node is less than \( 10^{-6} \). To expedite the convergence, a SOR factor of 0.95 is used. The iteration does not converge when the factor is greater than or equal to 1.0. The location of the PIC particles is updated by Newton’s equation of motion. A time step of 4.15 ns is used in the simulation such that any PIC particle cannot travel a distance larger than a cell length of 1 mm at full kinetic energy of 10 keV. Only the interior surface of the dielectric cage facing the plasma is charged by the plasma. However, at equilibrium, the positive ion flux is balanced by the negative electron flux and surface charging of the dielectric wall can be ignored. This balance will be destroyed when an ion sheath is formed at the dielectric wall pushing the electrons away and the wall will be charged positively by the ion flux. The accumulated surface charges are considered in the simu-
lation unless the electron density calculated using the Boltzmann distribution is less than one-tenth of the plasma density and the electron flux is too little to counterbalance the ion flux. It shows that the surface potential of the dielectric wall has to be less than −60 V. The voltage of the sample stage drops linearly to −10 kV in 1 μs. The simulation ceases at 51 μs.

Figure 1 displays the time-dependent potential configuration and plasma sheath. At first glance, the contours exhibit a concave geometry. The potential configuration can be divided into two parts by the boundary of the glass chamber. Since there is no plasma outside of the glass chamber, the contours are almost invariable. The plasma sheath inside expands as time elapses. It is noted that the sheath shape is not very conformal to the sample geometry. The difference between the sheath configuration at \( t=40 \mu s \) and \( t=50 \mu s \) is negligible. It can thus be inferred that the plasma sheath has attained enough expansion in the case of \( t=40 \mu s \).

Figure 2 depicts the ion and electron distributions at different times. The plasma sheath forms when a negative potential is applied to the target holder, as shown in Fig. 2(I). The width of the sheath is larger at the target substrate because of the large negative bias. At \( t=20 \mu s \), the configuration of the plasma exhibits two central zones. One is adjacent to the bias substrate and the other is in the vicinity of the hollow anode. It is in good agreement with our previous investigation of the plasma distribution.\(^5\) Subsequently, at \( t=40 \mu s \), the plasma in the upper half of the implanter chamber contracts. It indicates expansion of the ion sheath. All the ions in the sheath are implanted into the substrate and at the end, there is only a small plasma density in the anode region. The electron density configuration is similar to that of the ion density basically. However, it is important to note that the electrons are focused in the hollow anode. In Fig. 2(II) of the electron density configuration, the density of electron is still very high at the hollow anode although there are remnants of the plasma in the glass chamber. The thermal plasma electrons concentrate at the hollow anode because its zero potential is relatively higher than other parts of the glass chamber. It corroborates our previous findings that the electric field formed by the small-pointed anode and large tabular cathode can focus the electrons. The electrons concentrating on the anode can play an important role in producing and sustaining the plasma.\(^4\)

The ion implantation fluence distribution along the sample stage after different time intervals of \( t=1, 20, 40, \) and 51 μs are exhibited in Fig. 3. At 1 μs, the fluence distribution is quite uniform. It can be observed that the uniform section gets smaller as the process continues because as the ion sheath expands, the ion sheath is not conformal to the sample surface. The ion fluence distribution between \( t=20 \mu s \) and \( t=40 \mu s \) varies slightly and most of the ions are implanted into the sample in the initial 20 μs. After 20 μs, the ion density is greater reduced since no plasma is generated. A small number of ions is implanted at an inner area of radius \( \leq 3 \) cm between \( t=40 \mu s \) and \( t=51 \mu s \) because the ion sheath is very nonconformal and far away from the sample stage. The results are in good agreement with the configuration of the plasma potential and ions sheath evolution.

To recapitulate, numerical investigation utilizing the multiple-grid PIC code is developed to investigate the sheath physics in EGD-PIII&D. The sheath configuration shows that the plasma sheath has attained enough expansion in the case of \( t=40 \mu s \). The thermal plasma electrons concentrate at the hollow anode at the later pulse time. The uniform distribution of the incident ion implantation fluence stems from the configuration of plasma potential and ion sheath evolution.

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