Particle-in-cell numerical simulation of non-uniform plasma immersion ion implantation

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Abstract

Plasma immersion ion implantation (PIII) is attracting more attention as a surface processing technique. During PIII, the plasma is not frequently uniform due to hardware limitations, although numerical simulation of PIII processes is usually based on a uniform plasma environment. This may lead to incorrect and incomplete understanding of the PIII process and dynamics. In this work, numerical simulation is conducted using the particle-in-cell (PIC) model to consider the effects of non-uniform plasma in the vacuum chamber. The plasma source that is installed on top of the chamber produces down-stream plasmas with density diminishing from top to bottom. The simulation results demonstrate that the non-uniform plasma gives rise to an evidently different plasma sheath configuration and consequently different implantation dynamics compared to the uniform plasma case. The incident dose on the top surface is not uniform and the dose peak appears at a certain distance away from the target edge initially and gradually moves towards the central zone as time elapses. In comparison with uniform plasma implantation, the dose non-uniformity is more severe in the non-uniform plasma case although the plasma is uniform horizontally. This is due to the different focusing effects of the plasma sheath that depends on the plasma distribution.

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1. Introduction

Plasma immersion ion implantation (PIII) is a cost effective and efficient technique to enhance surface properties [1,2]. This technique also enables more effective surface treatment of industrial components with irregular shapes. Therefore, the technique has been utilized to improve the wear resistance, corrosion resistance, biocompatibility, and other properties of materials and components [3–6]. In order to understand and predict PIII processes, numerical simulation is frequently performed using different models [7–10]. In general, a uniform plasma is assumed in the PIC model simulation [11–14]. However, in practice, the plasma is frequently not uniform due to the hardware limitations and plasma diffusion [15,16]. Thus, it is also important to consider the effects of plasma non-uniformity during numerical simulation. In this work, we investigate the effects of non-uniform plasma.

The plasma source is located on top of the chamber and produces down-stream plasmas with continuously diminishing densities vertically from top to bottom. The expansion dynamics of the plasma sheath, incident dose distribution, impact angle of incoming ions are investigated using a particle-in-cell (PIC) model to disclose the effects of the non-uniform plasma.

2. Model

During PIII, the electrons near the target are expelled away when the target is biased to a high negative potential. Subsequently, a plasma sheath forms and the ions in the sheath are accelerated towards and implanted into the exposed conductive surface. In the simulation, the ions are assumed to be non-collisional and cold (low pressure PIII conditions) and accelerated only by the electric field. The electrons are in thermal equilibrium and the electron density is given by the Boltzmann relationship:

\[ n_e = n_i \exp \left( \frac{e\Phi}{kT_e} \right) \]
where $n_{ij}$ is the initial ion density in the cell of $(i, j)$, $k$ is the Boltzmann constant, $T_e$ is the electron temperature, and $e$ is the electron charge. Poisson equation relates the potential $\phi$ to the electron density $n_e$ and ion density $n_i$ as follows:

$$\nabla^2 \phi = -\frac{e}{\varepsilon_0} (n_e - n_i),$$

where $\varepsilon_0$ is the permittivity in free space and $e$ is the electron charge. The ions are accelerated by the electric field and their motion is described by Newton’s equations of motion. The ion trajectories are determined by the following equations:

$$\ddot{r}_i = \frac{F}{M} = -\frac{q}{M} \nabla \phi,$$

$$\ddot{r}_i(t + 1) = \ddot{r}_i(t) - \frac{q}{M} \frac{\partial \phi}{\partial r} \Delta t,$$

$$\ddot{z}_i(t + 1) = \ddot{z}_i(t) - \frac{q}{M} \frac{\partial \phi}{\partial z} \Delta t,$$

$$\Delta \dot{r} = \ddot{r}_i(t) \Delta t - \frac{q}{2M} \frac{\partial \phi}{\partial r} (\Delta r)^2,$$

$$\Delta \dot{z} = \ddot{z}_i(t) \Delta t - \frac{q}{2M} \frac{\partial \phi}{\partial z} (\Delta z)^2,$$

where $F$ is the force exerted on the particle by the electric field, $M$ is the particle mass, $q$ is the ion charge, $\ddot{r}_i(t)$ is the acceleration at time $t$, and $\ddot{r}_i(t + 1)$, $\ddot{z}_i(t)$, and $\ddot{z}_i(t + 1)$ are the initial and final velocities of the particle. Eq. (2) can be solved by the finite difference method [8,17].

In the numerical simulation, the plasma quantities and the space size are normalized as follows:

$$\rho = \frac{r}{D}, L = \frac{z}{D}, T = t \omega_{pi}, \psi = \frac{\phi}{\phi_p}, N = \frac{n_i}{n_0}, V^L = \frac{v_i}{v_{max}},$$

where $D = \sqrt{-4\varepsilon_0 \phi_p/(cm_0)}$ is the ion-matrix overlap length, $n_0 = \frac{1}{m \times n} \sum_{i=0}^{m} \sum_{j=0}^{n} n_{i,j}$ is the initial integral average ion density in the simulation space $(m \times n)$, $\omega_{pi} = \sqrt{n_0 e^2/(n_0 M)}$ is the ion plasma frequency, and $v_{max} = \sqrt{-2e \phi_p/M}$ is the maximum velocity accelerated by the potential drop $\phi_p$. The dimension of the simulation region is $2D \times 1.5D$. The radius of the target is 0.5D, thickness is 0.06D, and height of the target holder is 0.6D. Numerical simulation is conducted for both the uniform and non-uniform plasma distributions.
non-uniform plasmas for comparison. Initially, the plasma density in the chamber is $N=1$ for the uniform plasma case whereas the density is 1 only at the horizontal plane along the top surface of the target holder for the non-uniform plasma case, as shown in Fig. 1.

3. Results and discussion

The plasma distributions around the target holder for the uniform and non-uniform plasmas at $1T$, $5T$, $10T$ and $20T$ are displayed in Fig. 1. The semi-spherical plasma sheath forms quickly around the target holder right from the beginning (e.g. $1T$). The focusing effects of the plasma sheath can be observed and the expansion of the plasma sheath is different in different cases. In the presence of a non-uniform plasma, the plasma sheath expands very rapidly and the ions are depleted quickly beneath the target holder. In contrast the expansion of plasma sheath above the top surface is slower due to gradually increasing plasma density as experimentally investigated by M. Keidar, et al. [18]. It is well consistent with that higher plasma density leads to a thinner sheath and a smaller expansion velocity [19].

The top surface is more interested since the samples are frequently laid on here in practice. Fig. 2 depicts the incident ion dose after different time intervals ($t=1T$, $t=5T$, $t=10T$, and $t=20T$). The amount and distribution of the incident dose are different under different plasma conditions. The dose is not evenly distributed on the top surface in both the uniform and non-uniform plasma cases. A dose peak is clearly observed and it moves towards the center of the top surface if the negative pulse is maintained. A central high-dose zone whose edge is characterized by the dose peak is formed. The dose peak moves towards the central zone on the top surface, as observed by other authors [9]. In contrast, in the non-uniform plasma case, the non-uniformity of incident dose within the zone with high dose is more severe. Moreover, the top surface receives much more ions due to higher plasma density above the target holder. It is also seen that the zone with a high incident dose is larger in the non-uniform plasma case. Different focusing effects of the plasma sheath are responsible for the differences. The higher plasma density above the top surface confines the rapid expansion of plasma sheath, and consequently, the focusing effect of sheath becomes weaker. Thus, the dose peak is a little further away from the target holder.
the center of the top surface compared to that in the uniform plasma case as shown in Fig. 2. In addition, the weaker focusing effects also induce less ions to enter the central zone and the dose non-uniformity within the central zone with high dose is more severe. On the other hand, focusing is more evident for a uniform plasma, and so the variations in the incident dose within the central zone with high dose become smaller as time elapses.

The ion impact angle along the top surface is exhibited in Fig. 3. The difference in the incident angles is small between the two cases. In the central zone, the ions are implanted with a larger impact angle (nearly 90°) and the angle rapidly decreases away from the target center, as displayed by Kwok and Chu [9]. The distribution of ion impact angle along the top surface is similar to that of small square target simulated by two-dimensional fluid modeling [20]. Near the edge, the angle is less than 20°. As a result, the edge section of top surface receives a smaller ion dose. Many ions fly just above edge zone and are implanted into the surface at a distance away from the edge where a dose peak is apparently observed. Generally, the impact angle is larger for the non-uniform plasma case suggesting weaker focusing of the plasma sheath.

4. Conclusion

Numerical simulation using a two-dimensional particle-in-cell model is conducted to investigate the effects of non-uniform plasma in plasma immersion ion implantation. Under the non-uniform plasma condition, a higher plasma density above the top surface confines the expansion of the plasma sheath and reduces the focusing effects of the plasma sheath. Hence, the top surface receives a much higher ion dose and dose non-uniformity is more severe. A larger zone with a high dose is also observed and the zone shrinks with time in the presence of a non-uniform plasma. This is due to the different sheath focusing effects induced by the different plasma conditions and must be considered in practice.

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