



Nonuniform plasma diffusion and multi-pulse effect in plasma-based ion implantation



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ABSTRACT

The nonuniform plasma caused by plasma diffusion and the incomplete plasma recovery during short pulse-off time have great influences on the sheath dynamics and the implantation efficiency in plasma-based ion implantation (PBII). In this paper, a magnetized plasma diffusion fluid model is established to describe the plasma diffusion in PBII process. Together with a magnetized sheath fluid model, the full pulse period including sheath dynamics during pulse-on time and plasma recovery during pulse-off time can be described, and the models are verified to be accurate by comparing with experimentally measured electron density profiles. The influence of process parameters on sheath dynamics, the influence of incomplete plasma recovery under multi-pulse bias on implantation efficiency are investigated by solving the presented models with considering plasma diffusion. It is found that the variations of process parameters which accelerate the plasma diffusion reduce the steady-state sheath thickness and increase the ion implantation current, and vice versa. Change the pulse frequency from 1 kHz to 100 kHz under typical PBII process parameters significantly increases the average ion implantation current density, and the limiting factor which affects the implantation efficiency is converted from duty cycle to plasma diffusion. Increasing the plasma density and decreasing the transverse magnetic field are the effective methods to improve the implantation efficiency as well. The results reported here help to provide a theoretical guidance for the parameters optimization in PBII process.

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1. Introduction

Plasma-based ion implantation (PBII) is an effective surface modification technique developed by Conrad in 1987 [1], which can eliminate the line-of-sight restriction of conventional ion beam implantation and has been demonstrated to be very effective in improving the wear and corrosion resistance for metals and alloys [2,3]. Since the ion acceleration occurs mainly in the sheath during PBII process, the sheath dynamics is extremely important and has been investigated by analytical theories and computer simulations in the past [4–6]. In addition, to suppress secondary electrons emission [7], enhance ion implantation uniformity and increase plasma density [8], an external magnetic field can be introduced into PBII and the process has been studied experimentally [9] and numerically [10,11].

In these pioneering researches, a uniform plasma distribution is normally assumed during the simulation, although in practice the plasma around the target is expected to be nonuniform due to plasma diffusion [12,13]. In addition, these aforementioned

researches only considered a single pulse, under the assumption that plasma has enough time between pulses to flow back into the sheath region, where the ions are drained and implanted into the target during pulse-on time. However, the off time between pulses is generally not long enough for complete plasma recovery, especially for the magnetized plasma. For the components with irregular shape, such as inner surface of tube [14] or PBII batching [15], the sheath overlap caused by incomplete plasma recovery could result in the depletion of ion implantation dose and the deterioration of modification uniformity. Moreover, the recovery process determined by plasma diffusion is influenced by process parameters, and appropriate pulse parameters such as pulse length and duty cycle should be adopted under different process parameters. Some numerical studies using particle-in-cell (PIC) method [16,17] and fluid model [18] have demonstrated that the plasma dynamics parameters, such as sheath expansion and ion implantation current must be affected during the next pulse-on time if the plasma recovers incompletely. Chung et al. [19] experimentally investigated the plasma recovery during pulse-off time in PBII and compared the results with a fluid model [20]. However, the primary reason for plasma recovery, namely the plasma diffusion is ignored in their model. Moreover, these existing models for

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plasma recovery were studied in the absence of magnetic field, and no systematic studies have been reported about the effects of plasma diffusion and multi-pulse bias in PBII.

In this paper, a magnetized plasma diffusion fluid model is built up using the equations of ion continuity and ion motion, and adopting a variable diffusion coefficient of the ion. The validity of the presented models is identified by comparing with measured electron density profiles. The influences of plasma diffusion and incomplete plasma recovery under multi-pulse bias in PBII are studied using the presented models. The results reported here help to provide a theoretical guidance for the parameters optimization in PBII process.

2. Magnetized plasma diffusion fluid model

2.1. Model description

Under the low working pressure in PBII, the ions collide with neutrals at an effective ion velocity $|\mathbf{u}_i|$, namely the ion drift velocity rather than the ion thermal velocity u_{th} . The ion mobility μ_i depends on the ion drift velocity $|\mathbf{u}_i|$ and can be written as [21]:

$$\mu_i = \frac{2q\lambda_i}{\pi M |\mathbf{u}_i|} \quad (1)$$

where q is the ion charge, $\lambda_i = 1/(n_g \sigma_m)$ is the ion mean-free path, n_g is the neutral gas density, σ_m is the ion-neutral momentum transfer cross-section, and M is the mass of the ion. Under a magnetic field, the mobility of ions traversed the magnetic field can be derived as [21]:

$$\mu_{\perp i} = \frac{\mu_i}{1 + (\omega_c \tau_m)^2} \quad (2)$$

where $\omega_c = qB/M$ is the ion rotation frequency, B is the magnetic field strength, $\tau_m = 1/\nu_m$, $\nu_m = |\mathbf{u}_i|/\lambda_i$ is the ion-neutral momentum transfer frequency. For the plasma diffusion perpendicular to the magnetic field, adopting an experimentally verified diffusion coefficient $D_{\perp a} \approx \mu_{\perp i} T_e$ [22], which can be written as:

$$D_{\perp a} \approx \mu_{\perp i} T_e = \frac{2qT_e \lambda_i}{\pi M} \frac{|\mathbf{u}_i|}{|\mathbf{u}_i|^2 + (\omega_c \lambda_i)^2} \quad (3)$$

where T_e is the electron temperature in V, and the corresponding electric field is [22]:

$$\mathbf{E} = -T_e \frac{\nabla n_i}{n_i} \quad (4)$$

where n_i is the ion density. Substituting the ion flux $\Gamma = -D_{\perp a} \nabla n_i$ into the ion continuity equation:

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (\Gamma) = K_{iz} n_g n_e \quad (5)$$

then (5) becomes:

$$\frac{\partial n_i}{\partial t} - \frac{2qT_e \lambda_i}{\pi M} \nabla \cdot \left(\frac{|\mathbf{u}_i|}{|\mathbf{u}_i|^2 + (\omega_c \lambda_i)^2} \nabla n_i \right) = K_{iz} n_g n_e \quad (6)$$

where t is time, K_{iz} is the ionization rate coefficient of electron-neutral collision and $n_e = n_i$ is the electron density. Together with the ion motion equation:

$$\frac{\partial \mathbf{u}_i}{\partial t} = -\mathbf{u}_i \cdot \nabla \mathbf{u}_i + \frac{q}{M} (\mathbf{E} + \mathbf{u}_i \times \mathbf{B}) - \frac{qT_i}{M} \frac{\nabla n_i}{n_i} - \frac{F_c}{M} \quad (7)$$

where T_i is the ion temperature, and F_c is the collisional drag force, which can be written as [23]:

$$F_c = \frac{\pi}{2} M \nu_m \mathbf{u}_i \quad (8)$$

and substituting (4) and (8) into the ion motion (7) then:

$$\frac{\partial \mathbf{u}_i}{\partial t} = -\mathbf{u}_i \cdot \nabla \mathbf{u}_i - \frac{q(T_e + T_i)}{M} \frac{\nabla n_i}{n_i} + \frac{q}{M} \mathbf{u}_i \times \mathbf{B} - \frac{\pi}{2} \nu_m \mathbf{u}_i \quad (9)$$

During pulse-off time, the electrons flood back into the sheath region on a time scale of about the inverse electron plasma frequency and neutralize the net charge in this region, therefore the electric field is vanished and the ions in the sheath are not further accelerated toward the target. When all the energetic ions reach the target surface, a floating sheath will be formed on it. The electric force dominates the magnetic Lorentz force as one approaching the plasma boundary [24], therefore the ion flux near the target surface can be written as $\Gamma = -D_a \nabla n_i$, where $D_a \approx \mu_i T_e$ is the plasma ambipolar diffusion coefficient in the absence of magnetic field. Ignoring the floating sheath thickness, the ion velocity on the target surface is the Bohm velocity:

$$u_B = -D_a \frac{\nabla n_i}{n_i} \Big|_{\text{target}} \quad (10)$$

then the boundary condition of ion density on the target surface can be derived from (10) as:

$$\nabla n_i \Big|_{\text{target}} = -\frac{\pi}{2} \frac{n_i}{\lambda_i} \quad (11)$$

Therefore, the initial nonuniform plasma before applying the negative pulsed bias onto the target and the plasma recovery during pulse-off time can be described by solving the nonlinear Eqs. (6) and (9):

$$\begin{aligned} \frac{\partial n_i}{\partial t} - \frac{2qT_e \lambda_i}{\pi M} \nabla \cdot \left(\frac{|\mathbf{u}_i|}{|\mathbf{u}_i|^2 + (\omega_c \lambda_i)^2} \nabla n_i \right) &= K_{iz} n_g n_e \\ \frac{\partial \mathbf{u}_i}{\partial t} = -\mathbf{u}_i \cdot \nabla \mathbf{u}_i - \frac{q(T_e + T_i)}{M} \frac{\nabla n_i}{n_i} + \frac{q}{M} \mathbf{u}_i \times \mathbf{B} - \frac{\pi}{2} \nu_m \mathbf{u}_i \end{aligned} \quad (12)$$

with the boundary condition of Eq. (11). For describing the plasma diffusion outside the sheath region during pulse-on time, the boundary condition on the sheath boundary is:

$$\nabla n_i \Big|_{\text{sb}} = -\frac{\pi}{2} \frac{n_i}{\lambda_i} \quad (13)$$

and the sheath boundary is defined where the ion velocity is the Bohm velocity u_B .

However, the Eq. (12) are not appropriate to describe the sheath dynamics and the ion implantation process in the sheath region during pulse-on time, for which a well-established sheath fluid model is used, which composed of the equations of ion continuity and ion motion, Poisson's equation, and Boltzmann's relationship of electrons,

$$\begin{aligned} \frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{u}_i) &= 0 \\ \frac{\partial \mathbf{u}_i}{\partial t} + (\mathbf{u}_i \cdot \nabla) \mathbf{u}_i &= \frac{q}{M} (-\nabla \varphi + \mathbf{u}_i \times \mathbf{B}) - \frac{\pi}{2} \nu_m \mathbf{u}_i \\ \nabla^2 \varphi &= -\frac{q}{\varepsilon_0} \left(n_i - n_0 \exp\left(\frac{\varphi}{T_e}\right) \right) \end{aligned} \quad (14)$$

where φ is the plasma potential, ε_0 is the permittivity of free space. The boundary condition for Eq. (14) is:

$$\varphi \Big|_{\text{target}} = \varphi_p \quad (15)$$

where φ_p is the negative bias on the target.

In summary, the full pulse period including the sheath dynamics during pulse-on time and the plasma recovery during pulse-off time can be modeled and calculated repeatedly by these models. The initial nonuniform plasma before applying the negative pulsed bias onto the target, the plasma diffusion outside the sheath region during pulse-on time and the plasma recovery during pulse-off time can be described by solving the Eq. (12) with the boundary condition of Eqs. (11) or (13). The sheath dynamics and the ion implantation process in the sheath region during pulse-on time

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