Numerical analysis of monoenergetic electrons energy effect on dynamic potential profile of plasma sheath

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Abstract. The dynamic behavior of the electric potential distribution of a plasma sheath region in the presence of monoenergetic electrons with two different values of energy, larger (fast electrons) and smaller (slow electrons) than the cathode potential energy, is examined numerically by the finite difference method. Exploring and comparing the plots of numerical computation results shows that the time evolution of the non-monotonic potential distribution heavily depends on the energy of monoenergetic electrons.

1. Introduction

The study of sheath formation at the boundary of the plasma is of great practical importance. In plasma immersion ion implantation (PIII) (Mändl et al. 1997; Sheridan et al. 1998; Zeng et al. 1999; Qi et al. 2000; Bilek 2001; Yukimura 2001; Mukherjee et al. 2002; Kwok et al. 2003; Lacoste and Pelletier 2003; Masamune and Yukimura 2003; Ma et al. 2003; Rauschenbach and Mändl 2003; Tian et al. 2004, 2005, 2009; Meige et al. 2005; Sakudo et al. 2006; Ghomi et al. 2007, 2009; Huang et al. 2007; Li and Wang 2007; Mukherjee et al. 2007; Ghomi and Ghasemkhani 2009; Lejars et al. 2010; Li et al. 2010, 2012; Zhu et al. 2011), a plasmacontaining species to be implanted into a substrate is generated by an external plasma source or by the negative bias applied to the substrate (Conrad et al. 1987; Meige et al. 2005). After the negative bias is applied, electrons are repelled away from the surface leaving heavy ions forming an ion matrix sheath. These positive ions will subsequently be accelerated by the electric field inside the ion sheath and implanted to the substrate surface (Lieberman and Lichtenberg 1994; Chu et al. 1996).

When a low-pressure gas discharge is confined in a solid vessel, there is the possibility of particle emission from the walls. In particular, when the wall is bombarded from the plasma by ions, electrons, metastables, neutrals, and photons, it can readily release energetic (non-Maxwellian) electrons. The nature of the space charged region that may form at the boundary of the plasma can be modified significantly by the presence of this group of electrons. Although these electrons may be generated by secondary emission from the confining structure, the exact nature of the source is not important for this analysis, provided that they are approximately energetic (Ingram and Braithwaite 1990; Demidov et al. 2005; Gyergyek et al. 2010).

In plasma with non-Maxwellian electrons, a nonmonotonic distribution of the potential can be formed inside the ion sheath with the potential larger than the biased electrode potential. It is supposed that the initial conditions of a sheath formation transient process determine the type of the steady-state potential distribution being formed. However, the steady-state model is not able to predict what kind of solution, monotonic or non-monotonic, is realized in the experiment. It is understood that in order to answer this question, a time-dependent model should be developed (Gurovich et al. 2006).

A collisionless and time-dependent sheath model has been used to examine how the non-monotonic potential distribution can be formed inside the sheath due to the presence of non-Maxwellian electrons in the plasma. The appearance of a non-monotonic profile of the potential in front of cathode depends on the density of the energetic electrons and time. In addition, it was found that this dependency on the fast electrons density is stronger than dependency on time (Sharifian and Shokri 2007). To the best of our knowledge, no analysis has been done on the effect of the energetic electrons energy on the ion sheath dynamics.

Present work will examine the effect of energy of these energetic electrons on the ion sheath potential distribution dynamics. Here the applied dynamic model is exactly the same as the one used in our previous paper (Sharifian and Shokri 2007) and shares the same simplification: the density of two groups of energetic electrons has been assumed to be constant inside the sheath (Gurovich et al. 2006).

This work has been organized in four sections, including the Introduction as Sec 1. In Sec. 2, we present the equations that model the ion sheath dynamics in the presence of energetic electrons. Numerical results of the model are studied in Sec. 3. Finally, in Sec. 4, conclusions are presented.



Figure 1. Two groups of energetic electrons. (a) Fast, and (b) slow.

2. The sheath model

We assume a planar collisionless plasma sheath in front of an electrode having high negative potential, $|eU_0| \ge T_e$. The one-dimensional space in front of the cathode at the initial time is covered with a neutral plasma in which the difference between the ion (n_i) and the total electron densities $(n_e^{\text{(tot)}} = n_e + n_b)$ is neglected, $n_e^{\text{(tot)}} = n_i = n_o$; in addition, we neglect the electric field in this region. The plasma consists of cold ions, Maxwellian (plasma) electrons, and assumed non-Maxwellian (energetic) electrons.

In contrast to the plasma electrons, the energetic electrons will penetrate into the ion sheath and even reach the surface of the cathode (Schott 1987).

The sheath evolutions are simulated by using cold, collisionless two-fluid theory of plasma along with the Poisson equation (Sheridan and Alport 1994; Ghomi et al. 2006). The potential distribution is defined by the Poisson equation,

$$\nabla^2 \phi = -\frac{e}{\varepsilon_0} \left(n_i - n_e^{(\text{tot})} \right) = -\frac{e}{\varepsilon_0} (n_i - n_e - n_b).$$
(1)

The plasma electron density n_e can be calculated using the Boltzman relation,

$$n_e = n_o(1 - \alpha) \exp(e\phi/T_e), \qquad (2)$$

where n_i is the ion density, ϕ is the potential, e is the electron charge, T_e is the electron temperature, ε_0 is the free space permittivity, and α describes the relative number density of energetic electrons, $\alpha = n_b/n_o$.

Density of energetic electrons inside the sheath is assumed to be determined by their energy function distribution $f_b(w)$ at the sheath entrance,

$$f_b(w) = n_b \delta(w - w_b), \tag{3}$$

where w_b is the energetic electrons energy.

Here the effect of two groups of energetic electrons on the ion sheath dynamics has been studied. The first group (fast electrons) has energy being very large than the potential energy of the biased electrode (several times) and will contribute once in any point inside the sheath (Fig. 1(a)). The second group (slow electrons) has energy equal to the potential energy of the biased electrode and contributes once in any point inside the sheath before the formation of the non-monotonic potential distribution, but after the appearance of the nonmonotonic potential distribution it contributes twice inside the section of the sheath region, i.e., on away from the plasma boundary to the electrode and on the inverse path of their trajectory after reflection from the extreme point of the potential distribution with potential higher than the electrode potential. These slow electrons are absent behind the extreme point (Fig. 1(b)).

Therefore, the two-fluid equations and the Poisson equation along with (1) and (2) are written as follows:

$$\frac{\partial n_i}{\partial t} + \frac{\partial}{\partial x}(n_i v_i) = 0, \tag{4}$$

$$\frac{\partial v_i}{\partial t} + v_i \frac{\partial v_i}{\partial x} = -\frac{e}{m} \frac{\partial \phi}{\partial x},\tag{5}$$

$$\frac{\partial^2 \phi}{\partial x^2} = -\frac{e}{\varepsilon_0} [n_i - n_o(1 - \alpha) \exp(e\phi/T_e) - \alpha n_o], \quad (6)$$

where m is the mass of ion and v is the ion velocity. These equations can be made dimensionless by using the following variables (Sheridan and Alport 1994):

$$\tau = t\omega_{pi}, \quad X = x/\lambda_D, \quad \varphi = e\phi/T_e, \quad n = n_i/n_o,$$
$$U = v_i/v_{is}, \tag{7}$$

where $\omega_{pi} = (n_o e^2 / m \epsilon_0)^{1/2}$ is the ion plasma frequency, $\lambda_D = (\epsilon_0 T_e / n_o e^2)^{1/2}$ is the Debye length, and $v_{is} = (T_e / m)^{1/2}$ is the ion-acoustic velocity. Consequently, the dimensionless forms of (4)–(6) become

$$\frac{\partial n}{\partial \tau} + \frac{\partial (nU)}{\partial X} = 0, \tag{8}$$

$$\frac{\partial U}{\partial \tau} + U \frac{\partial U}{\partial X} = -\frac{\partial \varphi}{\partial X},\tag{9}$$

$$\frac{\partial^2 \varphi}{\partial X^2} = -[n - (1 - \alpha) \exp(\varphi) - \alpha].$$
(10)

In the above equations, the quasi-neutrality condition of the background plasma, $n_e^{(tot)} - n_i = 0$, has been applied. Furthermore, we changed the nonlinear Poisson equation (10) to a linear equation and used the iteration (Emmert and Henry 1992) and the finite difference relaxation method to solve this equation. Boundary conditions are $\varphi = \varphi_t$ on the substrate, and $\varphi = 0$ in the plasma. Furthermore, n = 1 and U =0 is used at the simulation region-plasma boundary. Moreover, since everywhere is plasma at the initial time, we used n = 1 and U = 0 as the initial condition for the simulation of the problem.

These equations, initial conditions, and boundary conditions precisely specify the time-evolution of the onedimensional sheath. The size of the simulation region is 100 times than that of λ_D . This size was specifically chosen, so extended, in order to cover the sheath region during the time of interest in this dynamic simulation. Therefore, the simulation region size does not affect the natural ion dynamics. The plasma is N₂⁺ with a density of 2.0×10^{12} cm⁻³ and plasma electron temperature of 2 eV (Gurovich et al. 2006). At time $\tau = 0$, the target bias



Figure 2. Schematics diagram of the considered problem.

was switched to $\varphi = -100$ with zero rise time ($r_t = 0$). For solving the equations of this model, we use a grid spacing of $\Delta x = 0.5$, and a time step of $\Delta \tau = 0.0125$. The simulation was run to a final time of $\tau = 10$, which is much longer than the duration of the ion-matrix phase of the simulation.

3. Results and discussion

In the present work, the effect of the energetic electrons energy on the ion dynamics in the sheath near the negative biased electrode has been simulated. The simulation region with qualitative energetic electrons inside the sheath region is illustrated schematically in Fig. 2.

Figure 3 depicts the normalized potential profile inside the simulation region in the absence ($\alpha = 0.0$) and presence of fast and slow energetic electrons ($\alpha = 0.4$) at normalized times, $\tau = 8$ (Fig. 3(a)) and $\tau = 10$ (Fig. 3(b)) as a function of position.

Figure 3(a) shows the monotonic potential distribution in the absence and presence of fast and slow energetic electrons up to normalized time $\tau = 8$. Also, it can be seen that the temporal evolution of the potential distribution up to normalized time $\tau = 8$ in the presence of fast energetic electrons is the same as slow electrons, but is different from their absence. For example, the value of the sheath length in the presence of energetic electrons is approximately two times the sheath length in their absence at $\tau = 8$.

It can be seen in Figure 3(b) that after the appearance of the non-monotonic potential distribution $(\tau > 8)$, temporal evolution of the potential distribution heavily depends on the energy of energetic electrons. Non-monotonic potential peak in the presence of slow electrons is about two times than that of fast electrons. Also, distance of the point with the potential peak for the slow electrons case compared with the fast electrons case keeps more away from the cathode. In other words, the sheath thickness of slow electrons is the largest of all cases.



Figure 3. The normalized potential distribution inside the simulation region in the absence of energetic ($\alpha = 0.0$) and presence of fast and slow energetic electrons ($\alpha = 0.4$) at normalized times (a) $\tau = 8$, and (b) $\tau = 10$.

4. Conclusion

We have presented particular results of our detailed onedimensional numerical study of the effect of the energetic electrons energy on sheath dynamics near the cathode in the presence of energetic electrons with energy of several times than the electrode potential energy (fast case) and with electrons energy equal to the electrode potential energy (slow case).

The potential profile evolution as a function of distance inside the sheath region between the plasma and the biased electrode was found. It was found that before the appearance of the non-monotonic potential distribution, the dynamic behavior of the potential profile for both fast and slow cases is similar.

But after the appearance of the non-monotonic potential, as it has been expected physically, the sheath dynamics strongly depends on the energetic electrons energy which could be listed as follows:

- The value of maximum potential in the slow electrons case is more than the fast electrons case (about two times). Furthermore, the point with maximum potential in the slow electrons case keeps more away from the cathode compared to the fast electrons case.
- 2. The sheath thickness of the slow electrons case is the largest of all cases.

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