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Behavior of the floating potential in an electronegative sheath as a function of electronegativity and negative ion temperature

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Abstract. Through a simple one-dimensional collisionless plasma sheath model, behavior of the floating potential in an electronegative plasma sheath is studied. Specially, the floating potential behavior as a function of the plasma electronegativity for various negative ion temperatures has been studied. It has been observed that negative ion temperature strongly affects the variation of floating potential.

1. Introduction

As it has been known, the plasma sheath formation is important for the understanding of the fundamental plasma properties, such as the number of particles reaching the surface and their impact energy [1], and is especially important for near-wall processes, such as plasma processing [2]. The theoretical study of the interface, which exists between plasma and a metallic surface, is important because it has several applications in plasma technology where the plasma is confined to a finite volume or flows around a rigid body. Despite efforts by numerous researchers [3–7], this problem has not been well understood and some surprising effects have been observed [8].

The low-pressure electronegative plasma, in which electron attachment allows a significant number of negative ions to exist, has been extensively used in processes of drying, etching, thin-film deposition and semiconductor manufacturing industry. The density ratio of negative ion, n_{-p}, to electron density, n_{-e}, in the bulk plasma can vary in a very wide range from 10^{-3} to 10^{3} depending on the operation conditions and gas compositions, and it generally reaches $10^{2} \sim 10^{3}$ in strongly electronegative and low-density plasma produced by radio-frequency (RF) capacitively coupled discharge. Due to the prominent roles of the electronegative plasma nowadays, many experimental and theoretical investigators have made a lot of investigations [9–10].

As it was mentioned, electronegative plasmas are of special interest because of their wide use in industry in which many electronegative gases such as O_2, H_2, CF_4 *etc*., are used [11–13]. On the other hand, electropositive plasma generally includes only positive ions as ion components, but electronegative plasma includes both positive and negative ions. The presence of three-component plasma containing electrons, positive and negative ions, influences the floating potential and in this

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way modifies the fluxes of charged species to the substrate and the other related matters [14].

In diagnosis techniques, such as the use of Langmuir probes or mass spectrometry, the number of particles reaching the probe also depends essentially on the structure of the interface. Therefore, the main characteristics of this interface, such as floating potential, sheath thickness *etc*., are governed by the structure of the sheath [15].

In order to apply these electronegative gases to plasma processing, the influence of negative ions on plasma parameters should be investigated. In this case, the behavior of the floating potential and the sheath thickness corresponding to the multivaluation of the Bohm potential was studied by Shindo et al. [16].

In this paper, simple classic equations of the steady plasma sheath that includes the presence of negative ions in the plasma are used to investigate the effects of the electronegativity of the plasma and the negative ion temperature on the floating potential. The floating potential is a quantity of interest because it is the potential of a metallic plane surface left isolated in the plasma by which many parameters of the plasma sheath, such as sheath thickness, ion impact energy *etc*., can be analyzed [17].

This work is somewhat similar to an earlier investigation done by Li et al. [9]. It seems that they show some similarities, but also important differences. In that investigation, the floating potential within the sheath has been determined by Poisson's equation and an adaptive step size Runge–Kutta scheme has been used to solve the equation, but here the floating potential will be obtained in the absence of a net current through the surface in the presence of negative ions in the plasma sheath. In addition, in the earlier paper, the floating potentials as a function of electronegativity converges to constant values (at high electronegativity and fixed negative ion temperature) that decrease with decreasing of the negative ion temperature. However in the present paper it will be shown that this potential, unlike in the mentioned paper, behaves as a decreasing function of electronegativity at a fixed negative ion temperature and the floating potential increases with a decrease in negative ion temperature.

2. The sheath model

Consider the steady, collisionless and planar plasma, as depicted in Fig. 1. In this model, the plasma consists of positive ions, negative ions and electrons; their densities at the plasma edge (interface between plasma and pre-sheath) are n_{+p}, n_{-p} and n_{ep} and at the sheath edge ($x = 0$) (interface between pre-sheath and sheath) are n_{+s}, n_{-s} and n_{es}, respectively. The corresponding temperatures will be T_i, T_{i-} and T_e, respectively.

From the model, floating potential is defined as the electric potential reached by an isolated metal inside the plasma. First, expressions for the current densities collected at the metallic plane due to each type of particles (positive and negative ions and electrons) have been obtained by using the plasma fluid theory. By equating the positive and negative charges of current densities at the metallic plane and solving the resulted equations, we can obtain information about the floating potential and its dependence on the plasma parameters, such as the electronegativity of the plasma and negative ion temperature.

We apply the case of a plane metallic surface placed in a weakly ionized and neutral plasma in which the difference between the positive ion and the total negative

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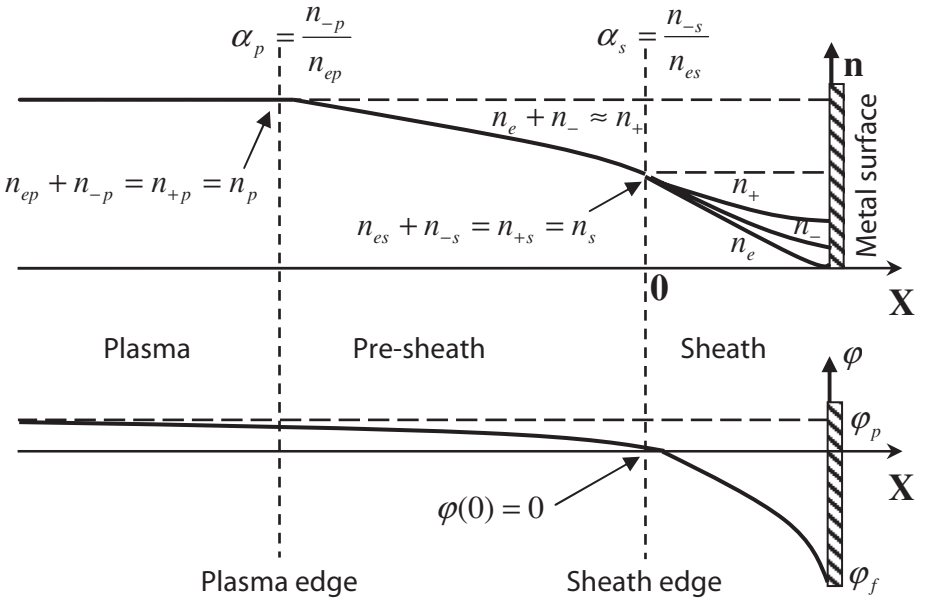


Figure 1. Schematic diagram of the considered problem.

densities is neglected,

$$n_p = n_{+p} = n_{-p} + n_{ep}, \tag{2.1}$$

where n_p is the plasma density at the plasma edge. The ratio of negative ions to electrons in the plasma has been defined as the plasma electronegativity,

$$\alpha_p = n_{-p}/n_{ep}. \tag{2.2}$$

In addition, at the sheath edge, we will consider the quasi-neutrality condition, $n_s = n_{+s} = n_{-s} + n_{es}$ and define the ratio of negative ions to electrons at the sheath edge as the sheath edge electronegativity,

$$\alpha_s = n_{-s}/n_{es}. \tag{2.3}$$

As it has been known, the potentials in the pre-sheath regions repel the colder negative ions, thus reducing α_s at the sheath edge as compared to α_p at the plasma, thus increasing the importance of the electrons in the sheath region. Considering α_p as the known quantity for an electronegative plasma, α_s must be determined numerically from [2]

$$\alpha_p = \alpha_s \exp\left[\frac{(1+\alpha_s)(\gamma-1)}{2(1+\lambda\alpha_s)}\right], \tag{2.4}$$

where $\gamma = \frac{T_e}{T_-}$ is the temperature ratio of electrons to negative ions. Also, we know that α_p is, in turn, determined from a diffusion solution within the plasma region in terms of $\alpha_p = n_{-p}/n_{ep}$, the value at the center of the plasma.

If $e\varphi_f \gg k_B T_e > k_B T_-$, then most of the negatively charged particles will not have enough energy to reach the metallic surface and, if we do not consider collisions for these particles, they will come back to the plasma with the same energy. Under this consideration, the negatively charged particle densities in the sheath region can be

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described by the Boltzmann relationships [15]:

$$n_e(x) = n_{es}\exp\left(\frac{e\varphi(x)}{T_e}\right), n_-(x) = n_{-s}\exp\left(\frac{e\varphi(x)}{T_-}\right). \tag{2.5}$$

The electron flux to the surface is equal to

$$j_e = j_{es}\exp\left(-\frac{e\varphi_f}{T_e}\right), \tag{2.6}$$

where $\varphi_f = (\varphi_w - \varphi_s) < 0$ is the potential drop in the sheath (φ_w is the wall potential and φ_s is the sheath edge potential); and the chaotic flux at the sheath edge is

$$j_{es} = n_{es}\sqrt{T_e/2\pi m}, \tag{2.7}$$

where m is the electron mass, and φ_f is the potential drop in the sheath region or floating potential. Near the surface, electrons are repelled because of the Boltzmann distribution (5).

The size of the near-wall collisionless sheath is governed by the local Debye radius (r_D), and is thin with respect to ion mean free path, λ_i [7]. The separation into plasma and sheath is, to some extent, a matter of convention because at a distance of order λ_i from the plasma boundary, the charge separation and the field strength smoothly increases toward the surface. This region is often referred to as the pre-sheath. The directed ion velocity, u_i, continuously increases toward the wall up to the ion sound speed, c_s, at some point near the wall (sheath edge). For $r_D < \lambda_i$, the quasi-neutral approximation ($n_s = n_{+s} = n_{-s} + n_{es}$) becomes invalid near this point, the electric field diverges, the transition to the sheath occurs and n_e decreases rapidly toward the wall. This point is usually adopted as the location of the sheath edge and is normally derived from the Bohm criteria [2, 7], which for $T_i \ll T_e$ and ions of mass M has the following simple form:

$$u_{is} \equiv u_B = \sqrt{T_e/M}. \tag{2.8}$$

Therefore, the positive ion flux in the sheath (and to the surface) is equal to

$$j_i = n_s u_{is} = n_s\sqrt{T_e/M}. \tag{2.9}$$

Here, we have used the continuity of ion flux (assuming no ionization in the sheath), $n(x)u(x) = n_s u_{is}$. When the metallic plane is isolated, the net current density collected by it is zero ($j_i - j_e = 0$), therefore

$$j_i = j_e. \tag{2.10}$$

It can be finally found that the floating potential of the electropositive plasma in the near-wall sheath becomes [7]

$$\varphi_f = \frac{T_e}{2e}Ln\left(\frac{\beta}{2\pi}\right), \quad \beta = \frac{M}{m}. \tag{2.11}$$

The generalization of the Bohm criterion for an electronegative plasma [18] is

$$u_{i\,\mathrm{New}} = \sqrt{\frac{T}{M}\left(\frac{1+\alpha_s}{1+\gamma\alpha_s}\right)}. \tag{2.12}$$

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Corresponding to the absence of a net current through the surface in the presence of negative ions in the plasma sheath, we must have

$$j_{i\,\mathrm{New}} = j_{ei\,\mathrm{New}} + j_{-}. \tag{2.13}$$

By substituting (1), (3), (5), (6), (9) and (12) into (13), we find

$$n_{es\,\mathrm{New}}(1+\alpha_s)\sqrt{\frac{T_e}{M}}\sqrt{\left(\frac{1+\alpha_s}{1+\gamma\alpha_s}\right)} = n_{es\,\mathrm{New}}\sqrt{T_e/2\pi m}\exp\left(-\frac{e\varphi_{f\,\mathrm{New}}}{T_e}\right) + \alpha_s n_{es\,\mathrm{New}}\sqrt{T_e/\gamma 2\pi M}\exp\left(-\frac{\gamma e\varphi_{f\,\mathrm{New}}}{T_e}\right). \tag{2.14}$$

After some simplifications

$$\sqrt{T_e/2\pi m}\exp\left(-\frac{e\varphi_f}{T_e}\right) = \sqrt{\frac{1+\gamma\alpha_s}{(1+\alpha_s)^3}}\left[\sqrt{T_e/2\pi m}\exp\left(-\frac{e\varphi_{f\,\mathrm{New}}}{T_e}\right) + \alpha_s\sqrt{T_e/\gamma 2\pi M}\exp\left(-\frac{\gamma e\varphi_{f\,\mathrm{New}}}{T_e}\right)\right], \tag{2.15}$$

we will find the final equation

$$\exp\left(-\frac{e\varphi_f}{T_e}\right) = \sqrt{\frac{1+\gamma\alpha_s}{(1+\alpha_s)^3}}\left[\exp\left(-\frac{e\varphi_{f\,\mathrm{New}}}{T_e}\right) + \alpha_s\sqrt{1/\gamma\beta}\exp\left(-\frac{\gamma e\varphi_{f\,\mathrm{New}}}{T_e}\right)\right], \tag{2.16}$$

that can be reduced to

$$aY^{\gamma} + bY - c = 0, \tag{2.17}$$

where

$$a = \sqrt{1/\gamma\beta}\sqrt{\frac{1+\gamma\alpha_s}{(1+\alpha_s)^3}(\alpha_s)^2}, \quad b = \sqrt{\frac{1+\gamma\alpha_s}{(1+\alpha_s)^3}}, \quad c = \exp\left(-\frac{e\varphi_f}{T_e}\right) = \sqrt{2\pi/\beta},$$
$$Y = \exp\left(-\frac{e\varphi_{f\,\mathrm{New}}}{T_e}\right).$$

As it can be seen, degree of (17) would be defined by the negative ion temperature (γ) and could be solved numerically. The exact value of the new floating potential ($\varphi_{f\,\mathrm{New}}$) can be obtained as a function of Y

$$\varphi_{f\,\mathrm{New}} = \frac{T_e}{e}(-Ln\,[Y]). \tag{2.18}$$

Also, we could define

$$\delta = \frac{\varphi_{f\,\mathrm{New}}}{\varphi_f} = -2\frac{Ln\,[Y]}{Ln\left[\dfrac{\beta}{2\pi}\right]}, \tag{2.19}$$

as the normalized new floating potential in the presence of negative ions to the floating potential of plasma sheath in their absence. In the calculations of this work, the electron temperature has been chosen $T_e = 0.1$ eV.

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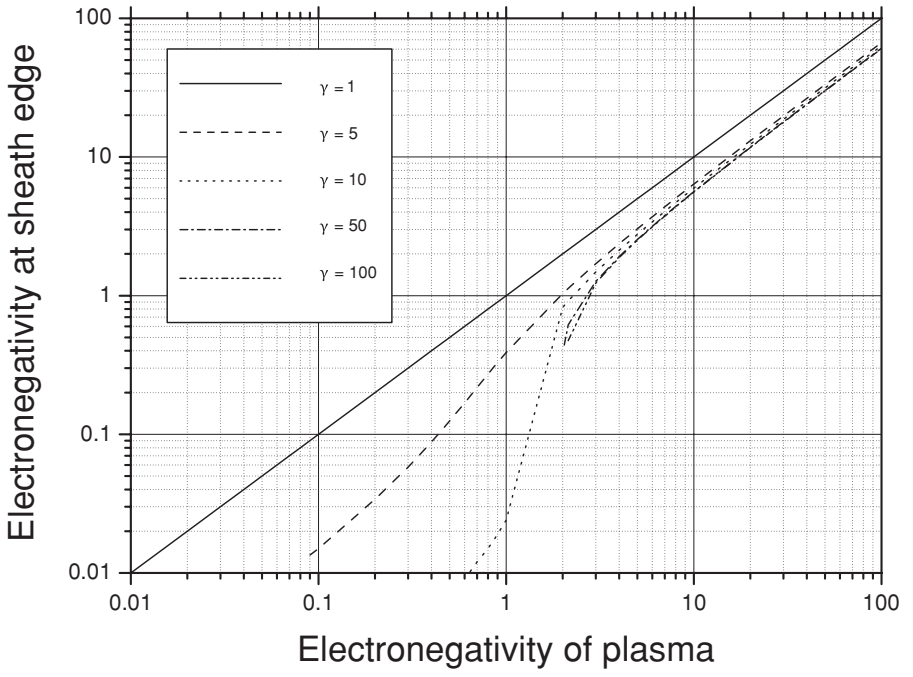


Figure 2. Electronegativity at the sheath edge, α_s, as a function of electronegativity at the plasma edge, α_p, for various values of the negative ion temperature.

3. Results and discussion

In order to study the influence of the composition of three-component electronegative plasma and negative ion temperature on the floating potential of a metallic wall in vicinity of a plasma, various relative concentrations of negative ions (electronegativity) and negative ion temperatures were introduced. In the model, plasma electronegativity has been varied from $\alpha_p = 0.01$ to 100, and the negative ion temperature ratio has been changed from $\gamma = 1$ to 100

The numerical solution of (4) has been shown in Fig. 2. As it shows, the behavior of the electronegativity at the sheath edge, α_s, as a function of the electronegativity at the plasma edge, α_p, strongly depends on the negative ion temperatures. For example, α_s depicts an intense jump from zero value near $\alpha_p = 2$ for $\gamma = 50$ and 100. Another notable matter is that the variation of α_s with α_p is completely linear with the same slope, for $\alpha_p > 3$ and is independent of the negative ion temperature.

Figure 3 depicts the normalized new floating potential of the plasma sheath as a function of the plasma electronegativity, α_p, of the oxygen plasma ($\beta = 29\,165$) for various values of the negative ion temperature. As it could be expected, the new floating potential behaves differently on the basis of the negative ion temperature. For $\gamma = 1$, the normalized floating potential, δ, is a decreasing function of α_p from $\alpha_p = 0.01$ to $\alpha_p = 100$ and is not more than unity. For $\gamma = 5$ and 10, δ behaves non-monotonically. This behavior might be related to the multivaluation of the Bohm criterion in electronegative plasmas, which is the one causing the non-monotonic behavior of the floating potential [16]. As it can be seen, δ increases continuously up to $\alpha_p \sim 1$ and 2, respectively, and then, decreases. For $\gamma = 50$ and 100, when

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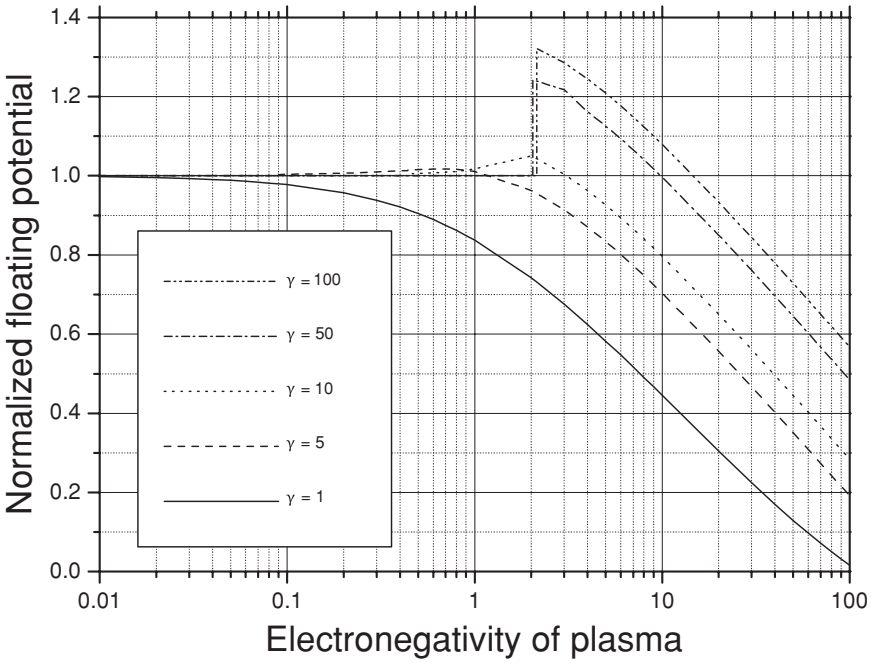


Figure 3. The normalized new floating potential of the plasma sheath as a function of the plasma electronegativity, α_p, for various values of the negative ion temperatures.

$\alpha_p < 2$, normalized floating potential does not change ($\varphi_{f\,\mathrm{New}} = \varphi_f$) because of the absence of negative ions at the sheath edge according to Fig. 2, while around $\alpha_p = 2$, it suddenly jumps to a value that is higher than 1 ($\varphi_{f\,\mathrm{New}} > \varphi_f$) and then decreases with the plasma electronegativity.

In addition, Fig. 3 shows the effects of the negative ion temperature on floating potential. Clearly, it could be seen that at a fixed plasma electronegativity, the floating potential increases as negative ion temperature decreases.

Now more specifically a comparison of Fig. 3 with the result of Li et al.'s paper in [9] is done. In Fig. 2(b) of the mentioned paper, the floating potential as a function of electronegativity converges to constant values as a function of electronegativity at a fixed negative ion temperature and high electronegativity that decreases with decreasing of the negative ion temperature, but in Fig. 3 of the present paper it will be shown that this potential, unlike the mentioned paper, behaves as a decreasing function of the electronegativity (at a fixed negative ion temperature) and the floating potential increases as negative ion temperature decreases.

4. Conclusion

Based on the steady and collisionless plasma assumption, the sheath floating potential of negative ions containing oxygen plasma has been studied. A practical model of the sheath floating potential is proposed, which allows almost all of the net space charge to be contained within the sheath. The floating potential shows different behaviors with respect to the plasma electronegativity that strongly depends on the temperature of negative ions.

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For $\gamma = 5$ and 10, the normalized floating potential behavior is continuously non-monotonical, but for $\gamma = 50$ and 100, corresponding to the absence of negative ion at the sheath edge for approximately $\alpha_p < 2$, it jumps to the value which is higher than unity and starts to show decreasing behavior as a function of plasma electronegativity. Finally, when the negative ion temperature decreases, the floating potential increases.

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