Sheath Structure in Oxygen Plasma for Different Presheath Plasma Density

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Abstract

Zinc oxide films are used as transparent conductive electrode for preparing organic light-emitting devices. In plasma-enhanced vapor deposition oxygen plasma is formed which then react with zinc atoms forming zinc oxide plasma, which is then deposited to the substrate. Hence, the proper understanding of the oxygen plasma-wall interaction is of crucial importance because of its application in plasma depositions. We have studied the sheath structure in oxygen plasma formed in front of an absorbing material wall for different density at the presheath side. We have used a kinetic trajectory simulation model to simulate the oxygen plasma. It has been observed that the sheath structure is highly affected by the plasma density at the presheath side. Hence, the densities of particles reaching the wall can be controlled by adjusting the presheath plasma density which is the key to thin film deposition.

Keywords: plasma, sheath, presheath, quasineutrality, Bohm criterion

Introduction

Whenever plasma comes in contact with a material surface, such as an electrode or a wall, the surface typically becomes negatively charged due to absorption of fast moving electrons. The negatively charged surface repels electrons but attracts ions which are thus pulled towards the surface. This gives rise to a positive space charge region near the surface, characterized by charge separation resulting in a strong electric field. This positive space charge region, known as sheath, separates the negatively charged wall from the quasi-neutral presheath plasma. The sheath structure is responsible for the flow of particles and energy towards the wall, and for release of impurities from the latter, and may also affect the bulk-plasma behavior. It plays an important role in determining the overall plasma properties. The potential falls off rapidly as we move towards the wall, so that the electric field is relatively strong and the motion of the plasma particles is dominated by the electric (rather than magnetic) forces. The energy distribution of energetic particles striking a wall is of crucial importance, for many applications in plasma processing. [1-5]

In this present work we have studied the sheath structure for oxygen plasma in front of an absorbing wall with different presheath plasma densities. The study of the oxygen plasma sheath is important because of its applications in the plasma deposition. Zinc oxide films have been studied experimentally for application to low-cost transparent electrodes in solar cells such as amorphous silicon or copper indium dieseline. Zinc oxide films are usually prepared by methods such as high temperature chemical vapor deposition, plasma-enhanced chemical vapor deposition and sputtering. Compared to high temperature chemical vapor deposition, plasma-enhanced chemical vapor deposition is an attractive process for film growth due to its lower substrate temperature requirement [6]. In plasma-enhanced vapor deposition oxygen plasma is formed which then react with zinc atoms forming zinc oxide plasma, which is then deposited to the substrate. The plasma deposition can be controlled by the sheath structure [7]. Here we have used the Kinetic Trajectory Simulation model [8] to obtain the solution of a non-neutral, time-independent, collisionless plasma sheath. We have studied a space charge sheath adjacent to an absorbing wall with presheath plasma on the other side, which we assumed to be described by a two-fluid solution.

We assume the electron and ion velocity distribution functions at the sheath edge to be cut-off Maxwellian in such a way that the most important requirements of the presheath-sheath transition are satisfied, i.e. quasineutrality, the sheath-edge singularity condition; continuity of the first three moments of each species, and the kinetic Bohm criterion [8, 9].

The Plasma Sheath Model

We have considered the plasma problem to be $1d1v$, which indicates the fact that our model is one-dimensional both in configuration and in velocity space (shown schematically in Fig. 1). The relevant coordinates are x and v; both defined normal to the boundaries. The magnetic field B is normal to the wall and assumed to be "infinitely" strong, so that the $1d1v$ approximation is appropriate. The direction of inhomogeneity is the x direction, i.e., the macroscopic field variables are assumed to be functions of x only. The simulation region considered is bounded by two parallel planes located at $x = 0$ and $x = L$, and the plasma is assumed to consist of electrons and one species of singly charged ions. The two boundaries are specified as follows. The right hand boundary ($x = L$) is the sheath entrance (or sheath edge or injection plane), separating the non-neutral, collisionless sheath region ($x < L$) from the quasineutral, collisional presheath region ($x > L$), whereas the left-hand boundary ($x = 0$) represents an absorbing wall.

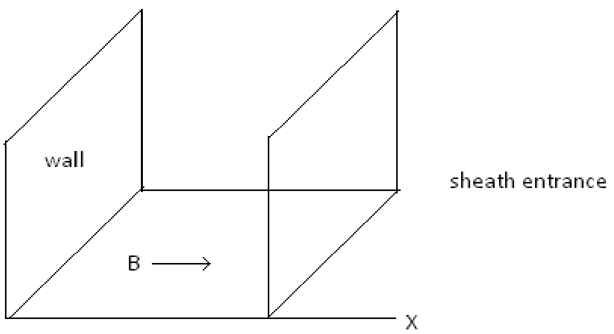


Fig. 1: *1d1v* plasma sheath model

The boundary potentials $\phi(x=0)$ and $\phi(x=L)$ and the boundary injection distribution functions $f^s(L,v)$ are assumed to be known/given. In this work, we restrict ourselves to the potential distribution $\phi(x)$ which decreases monotonically from $\phi(L)=0$ to $\phi(0)=\phi_0 \le 0$.

Basic concepts of Kinetic Trajectory Simulation (KTS)

KTS is an iterative method for numerically calculating self-consistent time independent kinetic plasma states in some given bounded spatial region. KTS method is one of the best methods to study the plasma sheath as it is more accurate than the fluid approximation, on which all the parameters are taken as average. In KTS model the distribution function of the particle species involved are calculated by using the related kinetic equations following the collisionless trajectory of the particle species in the phase space.

For collisionless cases the kinetic equation takes the well known form of "Vlasov equation"

$$\frac{\mathrm{d}f^s}{\mathrm{dt}} \equiv \frac{\partial f^s}{\partial t} + \vec{v}.\frac{\partial f^s}{\partial \vec{x}} + \vec{a}.\frac{\partial f^s}{\partial \vec{v}} = 0 \qquad (1)$$

or,

$$f^s = constant \qquad (2)$$

This means that the velocity distribution function is constant for an observer moving along a collisionless trajectory. Hence, the distribution function at every point along the trajectory can be obtained if it's value at one point (i.e., at the boundary) is given.

We assume that the plasma particles (electrons and ions) enter the simulation region from the right-hand boundary, that the left-hand boundary does not emit any particles, and that both boundaries are perfectly absorbing. At the left-hand boundary, the distribution functions satisfy the boundary conditions,

$$f^s(x=0, v \ge 0) = 0 \qquad (3)$$

At the right-hand boundary

$$f^e(x=L, v<0) = A^e \exp\left[-\left(\frac{v}{v_{tf}^e}\right)^2\right] \qquad (4)$$

and

$$f^i(x=L, v<0) = A^i \exp\left[-\left(\frac{v - v_{mL}^i}{v_{tf}^i}\right)^2\right]\Theta\left(v_{cL}^i - v\right) \qquad (5)$$

where

$v_{tf}^s = \sqrt{\frac{2k_B T_f^s}{m^s}}$ is the species s thermal velocity, v_{mL}^i is the ion "Maxwellian-maximum" velocity at $x = L$, and v_{cL}^i (with $v_{cL}^i < 0$) is the ion cut-off velocity at $x = L$. Here T_f^e and T_f^i are the formal electron and ion temperatures.

Numerical Parameters

We choose the plasma parameters at the presheath by satisfying quasi-neutrality condition, the sheath-edge singularity condition, continuity of the first three moments of each species, and the kinetic Bohm criterion [4, 5]. We specifically consider the following parameters at the presheath side of the sheath-presheath boundary: plasma density n_{ps} =

$0.5x10^{18}$ m^{-3}, $0.7x10^{18}$ m^{-3}, $1.0x10^{18}$ m^{-3}, $1.2x10^{18}$ m^{-3}, $1.5x10^{18}$ m^{-3}; electron temperature = 10^5 K, ion temperature 10^3 K. The resulting dimensional sheath parameters at the sheath side of the sheath-presheath boundary are then obtained from the coupling scheme [4, 5]. We choose the sheath to be of width $10\lambda_D^e$, where $\lambda_D^e = \sqrt{\varepsilon_0 kT / e^2 n_{L-}^e}$ is the Debye length at the sheath entrance associated with the injected electrons.

The discrete ion injection velocities are discretized uniformly with 200 grid points, such that the ion injection velocity grid step is considerably less than the ion thermal velocity. The region between $x = 0$ to L is discretized uniformly with 41 grid points.

We define the system to have reached convergence if the maximum difference in potential values before and after iteration equals 10^{-7} V or less.

Results and Discussion

Fig. 2 shows the typical potential profile in the sheath region. In this and in subsequent plots the distance is normalized in terms of the electron Debye length at the entrance. It is observed that the potential decreases as we move towards the wall from the sheath entrance. The potential decreases slowly at first but the gradient is large closer to the wall. Hence the major drop in the potential occurs just in the vicinity of the wall.

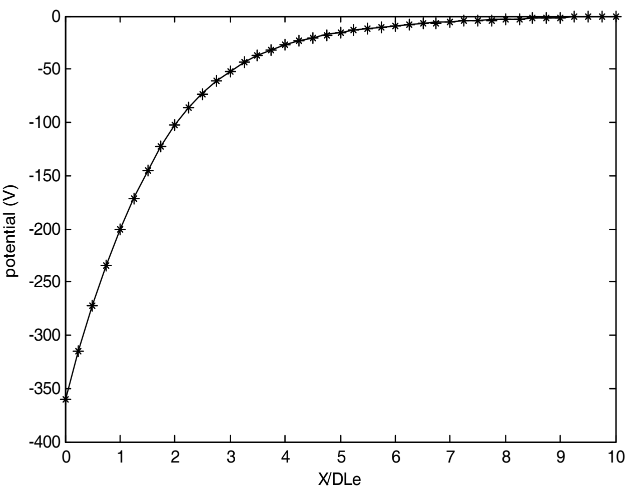


Fig. 2: Typical Self-consistent potential profile versus the distance from the wall

A typical electron and ion density profile is shown in Fig. 3. Both electron and ion density decreases from the sheath entrance towards the wall. The electron density decreases much faster and (in this particular case when the presheath plasma density is $1.2x10^{18}$ m^{-3}) the ion density at the wall is about 44 times more than that of electrons. This is due to repulsion of electrons by the negative wall. The electron and ion densities reaching the wall decrease linearly with the decrease in plasma density at the sheath entrance (Fig. 4).

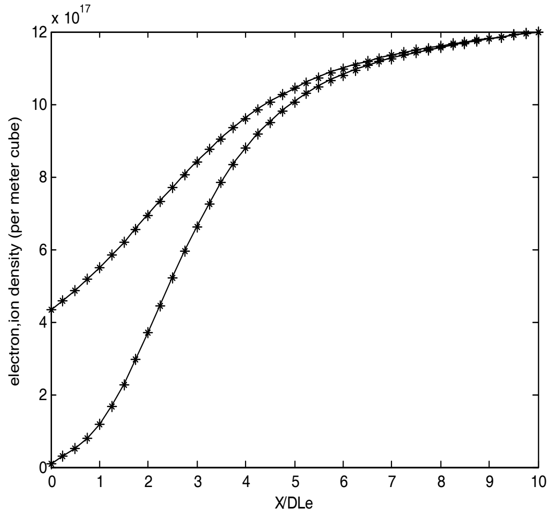
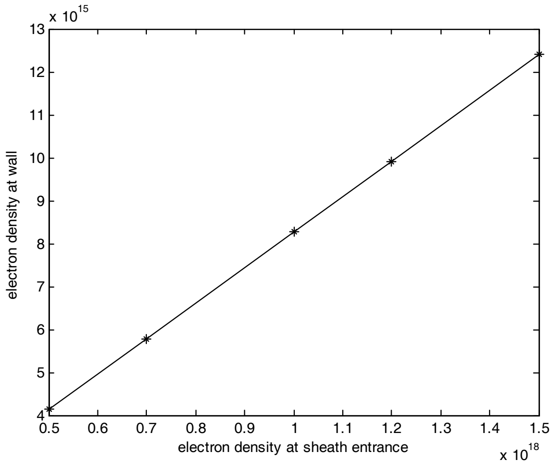


Fig. 3: Typical Self-consistent ion and electron density distribution



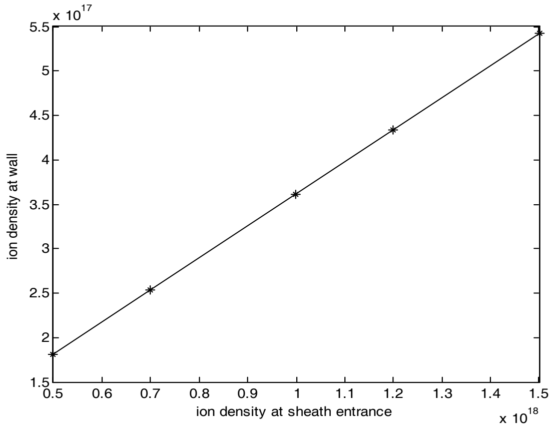


Fig. 4: Electron and ion densities reaching the wall versus the plasma density at the sheath entrance

The typical variations of electron and ion kinetic energy in the sheath region are shown in Fig. 5. The electron energy decreases whereas the ion energy increases linearly as we move towards the wall. Typically it is found that an electron having 6.9×10^{-18} J of energy at the sheath entrance has just over 5.0×10^{-18} J of energy as it reaches the wall. Opposite to that an ion starting at the sheath entrance with 45 J has 406 J of energy when it reaches the wall.

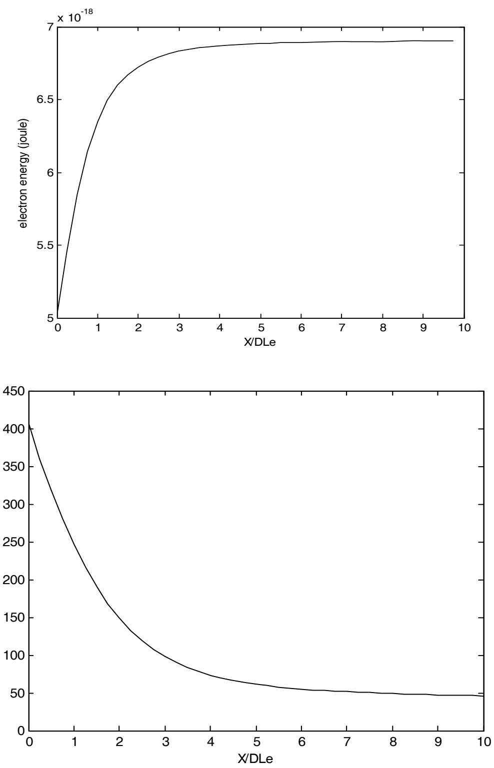


Fig. 5: Typical electron and ion energy versus the distance from the wall

Conclusion

The kinetic model has been used for the accurate study and prediction of oxygen plasma sheath structure for different presheath plasma density. It has been observed that the ion and electron densities decrease monotonically from the sheath entrance towards the wall in all cases. The electron density decreases much faster than that of ions and hence the total charge density increases towards the wall. The ion and the electron density at the wall are minimum with the charge density reaching maximum. The electric field is always negative in the sheath region and its magnitude increases towards the wall. The ion density at the wall exceeds the electron density by one order of magnitude. It is due to the fact that a part of electrons are repelled by high value of negative wall potential and in order to conserve the flux a small number of ions are attracted by thus repelled electrons. This shows that the sheath structure is highly influenced by the plasma density at the presheath. Hence, the densities of particles reaching the wall can be controlled by adjusting the presheath plasma density which is the key to thin film deposition. The work developed here provides a suitable basis for an important study in future, the main purpose being to arrive at more realistic plasma-wall transition description, accordingly understand the energy distribution of energetic particles striking a material wall which is of crucial importance, for many applications in plasma processing.

As a continuation of this work the following features may be considered in future: higher dimensional analysis, collisional sheath consideration, structure of the substrate, etc.

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