2D Fluid Approaches of a DC Normal Glow Discharge: Current Densities

Abstract. In this manuscript, both electric and energy behavior of a 2D spatial distributions in the Cartesian geometry of electron, ion and total longitudinal current densities as well as both ionization and energy sources terms of a DC glow discharge in the normal mode and in low gas pressure are presented for the first time in the literature. The model used in this work is the second order fluid model (continuity and momentum transfer equations and energy equation for electrons). The set of equations are coupled in a self-consistent way with Poisson’s equation. The results obtained in the stationary state are in good agreement with those given by literature.

Introduction DC glow discharges are widely used in the microelectronics industry as a source of reactive species for plasma etching or deposition (see e.g. Refs. [1-3]). A better understanding of these discharges and the ability to predict their properties for different operating conditions are a prerequisite for a better control of the process. Modeling of the discharges helps towards an understanding of their physical details and assists in optimizing their applications. In this manuscript, the model is based on the local average energy approximation. The all physic average sizes depend on the local average energy of electron or ion. This approach was adapted by Schmitt et al. [4], Belenguer and Bouf [5], Oh et al. [6] and Bouchikhi et al. [7-9] in a one-dimensional geometry, who use the first three moments of the Boltzmann equation and suppose that the distribution function is Maxwellian for electrons. The simplification assumes in the moments of the Boltzmann equation was as follows:

1) The drift energy is negligible compared to the thermal energy.
2) The kinetic pressure tensor is diagonal and isotropy.
3) The average collision frequency depends on the local average energy.
4) The term (\( \frac{\partial}{\partial t} \)) in the movement quantity transfer equation is negligible compared with source term (in which intervene the frequency of exchange movement quantity \( V_m \)).
5) An ionization coefficient is calculated with a Maxwellian distribution.
6) The secondary electron emission from the cathode is caused by the impact of positive ions.

These assumptions also are used in the work of Bouchikhi et al. [10, 11] in a two-dimensional geometry. The authors have studied the DC glow discharge in the Subnormal mode [10] and in the normal mode [11]; we have presented the 2D spatial distributions of electron and ion densities, both longitudinal and transversal electric field as well as electron temperature.

There are many problems for numerical simulation of current density in a 2D geometry. Therefore, this manuscript is concerned to represent the 2D spatial distributions of electron, ion and total longitudinal current densities, as well as, both ionization and energy sources terms. Since, it is rare to find such distributions in literature. On the other hand, these distributions are necessary to numerical simulations then for optimizing the reactor of plasma.

The outline of the manuscript is as follows. The model is briefly introduced and the initial boundary conditions, as well as numerical technique are described. The results obtained are shown, discussed and validated. Finally, concluding remarks are presented.

Discharge model Under the continuum assumptions, which were cited previously, the set of governing equations are as follows:

Continuity equations for electron and ion:

\[ \frac{\partial n_e}{\partial t} + \nabla \cdot (n_e \mathbf{V}_e) = S, \]

\[ \frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{V}_i) = S, \]

Momentum transfer equations \([12, 13]\) for the electrons and positive ions are:

\[ \mathbf{F}_e = -\mu_e n_e \mathbf{E} - \nabla D_e n_e, \]

\[ \mathbf{F}_i = \mu_i n_i \mathbf{E} - \nabla D_i n_i, \]

\[ S = K_n \frac{n_e}{T_e} \exp(-E_e / K_b T_e), \]

The relation between the electric field and the space charge in the inter-electrode space is given by Poisson’s equation:

\[ \nabla E = \frac{1}{\varepsilon_0} (n_i - n_e). \]

The electric field \( \mathbf{E} \) is related to the potential by the following relation:

\[ E = -\nabla V. \]

The EINSTEIN’S relation is:

\[ D_e = \frac{\mu_e K_b T_e}{|e|}. \]

The equations for the electron energies are \([10, 11]\):

\[ \frac{\partial n_e E_e}{\partial t} + \frac{5}{3} \nabla \cdot \mathbf{F}_e = S_e, \]

\[ \mathbf{F}_e = -\mu_e n_e E_e \mathbf{E} - \nabla D_e e E_e. \]
The initial distributions of the electron and ion densities are set as a Gaussian form \[ n(x, y) = n_0 \exp(-x^2 / \sigma^2) \] given by the following relation:

\[
\begin{align*}
E_x &= \frac{\partial V}{\partial x} = \frac{\partial V}{\partial y} = 0, \\
E_y &= -\frac{\partial V}{\partial y} = 0.
\end{align*}
\]

The boundary conditions are set as follows:
- The electron density is equal to zero at the anode.
- The electron and ion densities are taken as zero at the dielectric walls.
- The electric potential is in accordance with the Neumann condition \( \frac{\partial V}{\partial y} = 0 \) at the dielectric walls.
- The secondary electron emission coefficient at the cathode is taken to be 0.046. The electron temperature at the cathode is 0.5 (eV).
- The inter-electrodes spacing is \( L = 3.525 \) cm. The electron radius is \( \varepsilon = 5.08 \) cm. Neutral species density is \( N = 2.83 \times 10^{16} \) cm\(^{-3} \); gas temperature is 323 (K); ion diffusivity is \( D_i = 10^2 \) cm\(^{-2} \) s\(^{-1} \); both electron and ion mobility are \( \mu_e = 2 \times 10^5 \) cm\(^2\) V\(^{-1}\) s\(^{-1} \) and \( \mu_i = 2 \times 10^3 \) cm\(^2\) V\(^{-1}\) s\(^{-1} \); ionization rate prefactor is \( K_i = 2.5 \times 10^{-6} \) cm\(^3\) s\(^{-1} \); ionization rate activation energy is \( E_i = 24 \) (eV) and ionization enthalpy loss is \( H_i = 15.578 \) (eV).

**Initial and boundary conditions**

The transport coefficients for an argon gas have been taken from Lin et al. [14–16]. The inter-electrodes spacing is \( L = 3.525 \) cm. The electron radius is \( \varepsilon = 5.08 \) cm. Neutral species density is \( N = 2.83 \times 10^{16} \) cm\(^{-3} \); gas temperature is 323 (K); ion diffusivity is \( D_i = 10^2 \) cm\(^{-2} \) s\(^{-1} \); both electron and ion mobility are \( \mu_e = 2 \times 10^5 \) cm\(^2\) V\(^{-1}\) s\(^{-1} \) and \( \mu_i = 2 \times 10^3 \) cm\(^2\) V\(^{-1}\) s\(^{-1} \); ionization rate prefactor is \( K_i = 2.5 \times 10^{-6} \) cm\(^3\) s\(^{-1} \); ionization rate activation energy is \( E_i = 24 \) (eV) and ionization enthalpy loss is \( H_i = 15.578 \) (eV).

**Numerical technique**

The spatial discretization scheme used for the transport equations is the Scharfetter-Gummel [19] exponential scheme. This discretization is carried out in the Cartesian geometry. The transport equations of charged particles (electrons and ions) and Poisson's equation of them are solved using an implicit technique with a typical integration time step of the order of \( 10^{-6} \) s. Then, the resolutions of the equations set are solved by Thomas algorithm combined with the iterative relaxation method. The calculations were carried out on a Pentium 4 (3 GHz) personal computer. It took typically 24 hours and 30 minutes of run time to reach the converged solution for one set of discharge conditions.

**Results and discussion**

In this section, the results are given for the DC normal glow discharge in low pressure argon gas between plane-parallel electrodes. Two-dimensional distributions of the longitudinal current densities and both ionization and energy sources terms are presented to illustrate the discharge behavior.

Figs. 1, 2 and 3 represent the 2D spatial distributions and the contour plots of the longitudinal current densities of electron and ion and total in the stationary state of the normal glow discharge, respectively.

I observe that the distributions of the longitudinal current densities of electron, ion and total are more important at the symmetry axis of the electrodes (corresponding for \( y = 0 \) (cm) of the electrode width). I notice, that the current densities of electron, ion and total decrease linear towards dielectric walls because of the boundary conditions that are imposed. The electron current density (see Figure 1) in the anodic region is larger than the current density in the cathode region; it is of order -1.8 \times 10^{-3} mAcm\(^{-2} \) in the anodic region at the symmetric axis of the electrodes. The longitudinal electron current density cannot be null in the cathode sheath because of the secondary electron emission efficiency process that is presence, which has caused by bombardment positive ions cathode surface from the ionized gas.

I also notice that the longitudinal ion current density (see Fig. 2) in the cathode region is larger than the current density in the anodic region due to the ionization process of ions positive towards electrode cathode. It is about 1.8 \times 10^{-3} mAcm\(^{-2} \) in the cathode region at the symmetric axis of the electrodes. I observe there are accumulations of charged particle species of both ions in the anodic sheath region and of electrons in the cathode sheath. I notice that the longitudinal electron current density in the anodic sheath has the same value just like ion species in the cathode sheath, which has an almost symmetric behavior between the current densities of ion and electron species. Consequently, the longitudinal total current density (see Fig. 3) is almost constant in the inter-electrodes spacing (it has an average value which is 1.8 \times 10^{-3} mAcm\(^{-2} \) at the symmetric axis of the electrodes) and decreases on the dielectric walls' direction.

Fig. 4 illustrates the 2D spatial distributions and the contour plots of the ionization source term in the stationary state. It depends exponentially on electron temperature but varies linearly with electron density. The ionization source term is characterized in the discharge by two peak values; the first one in the sheath cathode and the second one in the negative glow. These two values with abscissas are \( S = 1.3762 \times 10^{13} \) cm\(^{-3}\) s\(^{-1} \) for XL=0.7931 and \( S = 5.0773 \times 10^{13} \) cm\(^{-3}\) s\(^{-1} \) for XL=0.6724 at the symmetric axis of the electrodes. The electron temperature influences directly on the ionization source term in both regions; the cathode sheath, and dielectric walls because of the electron density that is less significant. Fig. 5 represents the 2D spatial distributions and the contour plots of the energy source term in the stationary state. It is composed of three terms in the 2D geometry. Two terms are due to the heating, the first one of these two terms is generated by longitudinal electric field with longitudinal electron flux, and the second one is generated by transversal electric field with transversal electron flux. The third term is due to the cooling effect of electron species, it is generated by ionization process. I notice that the energy source term has a symmetric value because of the physical phenomena's equilibrium which is in progress (cooling and heating). The heating effect due to the transversal electric field is perceptible on the dielectric walls.
Fig. 1. Presentation in 2D and in contour plots of the longitudinal current density of electron in the stationary state.

Contour plots of the longitudinal electron current density (mA/cm²)

Fig. 2. Presentation in 2D and in contour plots of the longitudinal current density of ion in the stationary state.

Contour plots of the longitudinal ion current density (mA/cm²)

Fig. 3. Presentation in 2D and in contour plots of the longitudinal total current density in the stationary state.

Contour plots of the longitudinal total current density (mA/cm²)
Contour plots of the energy source term (cm$^{-3}$s$^{-1}$eV)

Fig. 4. Presentation in 2D and in contour plots of the energy source term in the stationary state

Contour plots of the ionization source term (cm$^{-3}$s$^{-1}$)

Fig. 5. Presentation in 2D and in contour plots of the ionization source term in the stationary state

Validity of the model

I investigated this discharge of the same conditions of both charged particles transports and geometry parameters as Lin et al. To validate my results; I compared those issues on the symmetric axis of the electrodes with those given by Lin et al.

I observe that the longitudinal current densities of electron, ion and total are in good agreement with those obtained by Lin et al.

Concluding remarks

In this article, a two-dimensional spatial distributions of the longitudinal current densities of electron, ion and total, and both ionization and energy sources terms have been presented in the stationary state of a DC normal glow discharge. Monatomic argon gas in low pressure has been utilized in this study. The discharge is maintained by a secondary electron emission coefficient at the cathode. The model used in this work is based on the first three moments of the Boltzmann’s equation and the Poisson’s equation. The simulation results obtained were validated by using a comparative study with those of Lin et al.
Nomenclature
\( n_e, n_i \) Electron and ion densities
\( \Phi_e, \Phi_i \) Electron and ion fluxes
S Net source term
\( \mu_e, \mu_i \) Electron mobility, Ion mobility
\( D_e, D_i \) Electron diffusivity, Ion diffusivity
K_i Ionization rate prefactor
E_i Ionization rate activation energy
\( T_e \) Electron temperature
N Gas density
KB Boltzmann’s constant
\( \varepsilon_0 \) Permittivity of free space
e Particle charge
\( \Phi_e \) Electron energy flux
\( H_i \) Energy loss per ionizing collision

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