Computational study of a glow discharge device

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Abstract. The glow discharge is the basis of conventional techniques used to improve the tribological properties of materials, such as the generation of thin films using ionic beams and the sputtering process for the treatment of surfaces. This work focuses on the numerical study of the glow discharge in a system composed of a cylindrical quartz chamber containing argon gas, whose length and radius are 20 cm and 2.5 cm, respectively. Said chamber is limited by two copper electrodes whose potentials are 0 V (Anode) and -500 V (Cathode), respectively. In order to analyze this time-independent discharge, the generation of secondary electrons allowing the discharge to be self-sustained as well as the manifestation of fixed regions, among others, numerical modeling is carried out by using the Plasma Module of COMSOL Multiphysics software. The presented results in this paper can be useful to understand, design and build new technologies focused on the area of treatment of surfaces.

1. Introduction

There is a wide variety of surface modification processes assisted with glow discharge based techniques to produce surfaces or coatings that improve the properties as Microhardness, resistance friction wear and corrosion [1,2]. This discharge is important because is both self-sustained and continuous, having a cold cathode that emits secondary electrons induced by ions beams allowing a current range of 1 mA - 100 mA [3,4].

This work focuses on the study numerical of the glow discharge features, such as the generation of secondary electrons, the manifestation of fixed regions with a particular glow for each gas, the presence of constant voltage value between the electrodes [5]. In this discharge, the secondary electrons cause a layer of large positive space charge at the cathode with a strong electric field. Said region is known as cathode fall. In order to understand this discharge, in this work the usual configuration of a long glass cylinder with the positive anode at one end and a negative cathode at the other is considered. It is worth mentioning that although it is not necessarily the configuration used in the processing applications, it has the advantage of symmetry so has been widely studied. In the present paper, this system is modeled by using the plasma module of the software COMSOL Multiphysics, a powerful tool to model low-temperature plasmas[6]. The obtained results, allow to understand, design and build new technologies focused on material modification processes.
2. Theoretical formulation and physical scheme.

2.1. Physical model and electron transport theory

The traditional scheme for the generation of a glow discharge is shown in Figure 1. This consists of a cylindrical quartz chamber, containing argon gas under a pressure of 0.0375 Torr, whose length and radius are 20 cm and 2.5 cm, respectively. Said chamber is limited by two copper electrodes whose potentials are -500 V (Cathode) and 0 V (Anode), respectively. Due to the complexity of coupling the electrostatic field to the transport equations of both the electrons and heavy species, the Plasma Module of COMSOL Multiphysics is used, which, provides the interface that allows put together these quantities and facilitates the simulation of Direct Current discharges (DC discharges). The first approach used by said software is to model the plasma as a fluid, which is a valid approximation to describe very collisional plasmas, as in the present case where the mean free path for the electron is much smaller than the cavity length.

![Figure 1. Physical scheme for the glow discharge generation.](image)

Equation (1) and Equation (2) describe the evolution of both the electron density and electron energy density, respectively.

\[
\frac{\partial n_e}{\partial t} + \nabla \cdot \tilde{\Gamma}_e = R_e \tag{1}
\]

\[
\frac{\partial n_e}{\partial t} + \nabla \cdot \tilde{\Gamma}_e + \vec{E} \cdot \tilde{\Gamma}_e = R_e \tag{2}
\]

Where \(n_e\) is the electron density, \(\tilde{\Gamma}_e\) the total flow of electrons, \(\vec{\mu}_e\) the mobility of electrons, \(\vec{D}_e\) the electron diffusivity, \(R_e\) is the speed of creation or annihilation of electrons, \(\tilde{\Gamma}_e\) the total flow electron energy, which is defined in a similar way that the total flow of electrons, and \(R_e\) the energy change due to the inelastic collisions between the electrons and the neutral atoms [6].

2.2. Heavy species transport theory

In order to describe the flow of \(k (=1,2,\ldots,Q)\) heavy species and \(j (=1,\ldots,N)\) reactions, the Equation (3) is used for the first \(Q-1\) species,

\[
\rho \frac{\partial w_k}{\partial t} + (\vec{u} \cdot \nabla) w_k = \nabla \cdot \tilde{j}_k + R_k \tag{3}
\]

Where \(j_k\) is the diffusive flux vector, \(R_k\) is the rate expression for species \(k\), \(\rho\) is the density of the mixture, \(w_k\) is the mass fraction of the \(k\)th species; and \(\tilde{j}_k = \rho w_k \tilde{V}_k\), \(\tilde{V}_k\) is the diffusive flux vector for species \(k\). Its definition depends on the chosen diffusion model. In the present work the averaged mixing model is used [6, 7].
2.3. Boundary conditions
The Glow discharge is self-sustaining by the secondary electrons emission which arise from the ions impact. The secondary emission flux for electrons is defined by the Equation (4).

\[ \hat{n} \cdot \vec{\Gamma}_{e,s} = \sum_{k=1}^{N} \gamma_k (\vec{\Gamma}_k \cdot \hat{n}), \]  
(4)

Where \( \hat{n} \) is the vector perpendicular to cathode (or anode) surface, \( \gamma_k \) the secondary emission coefficient, and \( \vec{\Gamma}_k \) is the ions flow o in the surface. The average energy of the electrons emitted from the cathode (or anode) is given by the Equation (5), where \( \Delta \varepsilon_k \) is the ionization energy, and \( \Psi \) is the work function of the cathode (or anode) [8, 9]. For the present case \( \Psi = 4.7 \) eV, the work function for copper.

\[ \tilde{\varepsilon}_k = \Delta \varepsilon_k - 2\Psi. \]  
(5)

On the dielectric surface (cylindrical quartz chamber), due to the difference in the fluxes between the electrons and the ions the charge is accumulated. This process is described by the Equation (6).

\[ \frac{\partial \rho_s}{\partial t} = \hat{n} \cdot \vec{j}_i + \hat{n} \cdot \vec{j}_e, \]  
(6)

Where \( \vec{j}_i \) and \( \vec{j}_e \) are the total ion current and the total electron current at the the cylindrical surface, respectively, and \( \hat{n} \) is the outgoing unit vector to the chamber surface. The Equation (7) presents the surface charge density, \( \sigma_s \), which is used as boundary condition [6].

\[ \sigma_s = -\hat{n} \cdot \vec{D}. \]  
(7)

2.4. Physical parameters of the glow discharge
Table 1 shows the typical values of the physical parameters in a glow discharge [10, 11]. These values will be taken as reference to validate the scope of our simulation results [12].

| Physical parameter                        | Typical values                      |
|------------------------------------------|-------------------------------------|
| Current                                  | \( 10^{-4} \) A - 0.5 A             |
| Electron temperature in the positive column | 1 eV - 3 eV                      |
| Voltage between electrodes               | 100 V - 1000 V                     |
| Gas pressure                             | 0.03 Torr - 30 Torr                 |
| Concentration of ions and electrons in the positive column | \( 10^{13} \) m\(^{-3}\) - \( 10^{16} \) m\(^{-3}\) |

3. Results and discussions
Figure 2 shows the flow of secondary electrons on the cathode surface as a function of the time. For the interval \( 10^{-8} \) s to \( 10^{-7} \) s, said flow is zero because the effects of cascades are negligible, leading to the discharge Townsend regime or dark regime; which is characterized by a low current, approximately \( 10^{-7} \) A. In the interval \( 10^{-7} \leq t < 10^{-4} \) s the secondary emission flow increases exponentially, generating the discharge regions. For times greater than \( 10^{-4} \) s the secondary electron emission flow in the cathode keep constant, showing one of the main characteristics of the discharge, i.e. it’s self-sustaining by the secondary electrons. The Figure 3 show the dependence of the discharge current on the axial position whose values is approximately
−3.95 × 10⁻⁴ A. This current value show good agreement with the order of magnitude reported in the literature (see Table 1).

Figure 2. Secondary electron emission flow in the cathode.

Figure 3. Discharge current as a function of the axial position.

The ion concentration as a function of the axial position is show in Figure 4. It can be noted that the ion concentration is greater than the electron concentration at the cathode z=0, (see Figures 4). These electrons are emitted with an energy of about 7 eV (see Figure 5), which is not enough to generate either ionization or excitation in the argon gas, which require energies of 15.8 eV and 11.5 eV, respectively. However a region near the cathode, known as the Aston dark space, is formed. Said region is characterized by having a low energy value, 7 eV in this case.

Next to the Aston dark space, there is a zone where an exponential increase in these concentrations is present, which is known as the dark cathode space or crooks (See Figure 4.

Figure 4. Ion concentration: (a) Depending on the length, (b) Azimuthal profile.

Next to the Aston dark space, there is a zone where an exponential increase in these concentrations is present, which is known as the dark cathode space or crooks (See Figure 4.
and Figure 6). There occurs the higher ionization rate of the discharge, which leads to an increase in the density of the space charge and causing an abrupt change in the potential, which goes from -500 V up to -20 V, forming the region of the cathodic fall (see Figure 7). Next to the area of the cathodic fall is a segment larger than the previous one, wherein the potential is low. Said region is composed of negative luminescence, the dark space of Faraday and the positive column, whose potential is approximately constant (see Figure 7).

![Graph of Electron Temperature](image1)

**Figure 5.** Electron temperature: (a) Depending on the length, (b) Azimuthal profile.

![Graph of Concentration Electrons](image2)

**Figure 6.** Concentration electrons: (a) Depending on the length, (b) Azimuthal profile.

Figure 4 and Figure 6 also show the positive column, which is determined by the local processes of both formation and losses of charged particles as well as the electric current. The loss of charged particles in the positive column is due to internal collisions and its recombination with the surface, which is balanced due to the ionization rate in a steady-state regime, where the equality of the electrons and ions concentration $0.3 \times 10^{15} \text{ m}^{-2}$ is reached (See Figure 4
and Figure 6). The ionization rate depends on both the electron temperature, $2.3 \text{ eV}$, and the electric field (See Figure 5). Therefore, the change of electrical potential in this region is low compared to the cathode layer (Figure 7).

![Figure 7](image-url)

**Figure 7.** Electrical potential: (a) Depending on the length, (b) Azimuthal profile.

At the opposite end of the positive column region, the anode repels the ions and attracts the electrons from this, creating a negative spatial charge near the anode which leads to an increase of the electric potential (see Figure 7). The reduction of the concentration of electrons in this area explains the dark space of the anode (see Figure 6).

4. Conclusions
A glow discharge in a cylindrical chamber containing argon under a pressure of 0.0375 Torr was simulated by using the Plasma Module of COMSOL Multiphysics. Several parameters of said discharge were obtained, such as their independence of the time, the generation of secondary electrons as a result of the ions collisions with the cathode, which allows the discharge to be self-sustained in the range of 1 mA - 100 mA, and the manifestation of fixed regions where a particular glow originates, among others. The obtained results show agreement with those reported in the literature, which can be useful for designing experiments dedicated to the material processing using plasmas.

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