Tahar ALILI[1], Abdelaziz BOUCHIKHI[2], Mohamed RIZOUGA[1]

[1] University of Sciences and Technology of Oran, USTO-MB, 31000, Algeria
[2] University of Saïda, Faculty of technology, Department of electrical engineering, Saïda 20000, Algeria

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Neon Spatio-Temporal Distributions in a DC Glow Discharge

Abstract. *In this presents work the neon spatio-temporal distributions of electron and ion densities, the potential and electric field, the mean electron energy and the metastable atom density are discussed for the first time in the literature. A 1D DC glow discharges behavior has been described with fluid model. It's about the first three moments of the Boltzmann's equation coupled with the Poisson's equation with a self-consistent way. The term source is dominated by both ionization processes, it's about of electron-impact ionization of ground state atoms and chemo-ionization processes. Our model is validated theoretical and experimental.*

Streszczenie. *W artykule analizowany jest przestrzenno czasowy rozkład jonów i elektronów przy wyładowaniu DC w obecccności atomów neonu. Analizowane są też pole elektryczne, średnia energia elektronu, gęstość atomów neonu.* ***Czasowo-przestrzenny rozkład neonu przy wyładowaniu DC***

Keywords: Glow discharge ; Fluid model; Metastable atom density; BOLSIG+
Słowa kluczowe: wyładowanie DC, model cieczowy, równanie Bolzmanna

Introduction

Glow discharges are becoming widely accepted as sources for analytical techniques, like atomic absorption spectrometry (AAS), optical emission spectrometry (OES), and mass spectrometry (MS). The AAS is designed to an spectro-analytical procedure for the quantitative determination of chemical elements using the absorption of optical radiation by free atoms in the gaseous state. The principle of OES is involved in applying electrical energy in the form of spark generated between an electrodes and a meta sample, whereby the vaporized atoms are brought to a high energy state within a so-called " discharge plasma". The MS is an analytical technique that ionizes chemical species and sorts the ions based on their mass to charge ratio. In simpler terms, a mass spectrum measures the masses within a sample. Mass spectrometry is used in many different fields and is applied to pure samples as well as complex mixtures. To acquire better results in theses fields of application, a good understanding of the glow discharge is desirable. One way to attempt this is by mathematical modeling [1-7].

In this work, an investigation is made concerning the role of neon metastable atoms in the discharge. In section 2, the model discharge is described, it contains the initial and boundary condition as well as the numerical procedure. In section 3, the results are discussed for neon discharge. Finally, the conclusion of the work is given in section 4.

Discharge Modeling

Our discharge modeling is based on the first three moments of the Boltzmann transport equations. The Continuity equations and momentum transfer equations of electrons, positively charged ions and metastable atom. The energy equation is given only for electrons and the Poisson equation is the determination of the electric potential [2,5,6]. The kinetic scheme, including the processes in our discharge are mentioned in the Table 1.
Then, the model in the case of the one-dimensional Cartesian geometry considered the corresponding basic system of partial differential equation reads:

(1) $$\frac{\partial n_e}{\partial t} + \frac{\partial \varphi_e}{\partial x} = n_e n_o K_o^{io} + n_m n_m K^{ci} ,$$

(2) $$\frac{\partial n_+}{\partial t} + \frac{\partial \varphi_+}{\partial x} = n_e n_o K_o^{io} + n_m n_m K^{ci} ,$$

(3) $$\frac{\partial n_m}{\partial t} + \frac{\partial \varphi_m}{\partial x} = n_e n_o K_o^{m} - 2 n_m n_m K^{ci} - \frac{n_m}{\tau_m} ,$$

(4) $$\frac{\partial \varepsilon_e n_e}{\partial t} + \frac{\partial \varphi_{e\varepsilon}}{\partial x} = -e\varphi_e E + \varepsilon^{ci} n_m n_m K^{ci} - n_e P^{ec} - n_e(\varepsilon^m n_o K_o^m + \varepsilon^{io} n_o K_o^{io}) ,$$

(5) $$\frac{\partial^2 V}{\partial x^2} = -\frac{e}{\varepsilon_o}(n_+ - n_e)$$

With $\varepsilon^m = 16.6$ eV, $\varepsilon^{io} = 21.56$ eV and $\varepsilon^{ci} = 2\varepsilon^m - \varepsilon^{io}$. $\tau_m = 14.73$ s [13] and $E = -\partial V / \partial x$.

Momentum transfer equations for electrons, ions, metastable atoms and electron energy are:

(6) $$\varphi_e = -n_e \mu_e E - \frac{\partial D_e n_e}{\partial x} ,$$

(7) $$\varphi_+ = n_+ \mu_+ E - \frac{\partial D_+ n_+}{\partial x} ,$$

(8) $$\varphi_m = -D_m \frac{\partial n_m}{\partial x} ,$$

(9) $$\varphi_{e\varepsilon} = -n_e E \mu_{e\varepsilon} - \frac{\partial n_e D_{e\varepsilon}}{\partial x}$$

With $D_m = 150$ cm^{2}s^{-1}torr [14]. The ion mobility is calculated from their drift velocity: $w_+ = (11.27E/n)/(1+0.01288E/n)^{0.5}$ [15] where E/N is in Td. The ion diffusivity is calculated according to the Einstein's relation [4]. The coefficients for electrons in neon as dependences on the mean electron energy are obtained from BOLSIG+ software.

Initial and boundary conditions

The discharge is established between two parallel plate electrodes and the radius of the electrode is assumed to be much greater than the electrode gap and the distributions of the physical properties are almost uniform along the radial direction. The powered electrode which initiates the discharge at $x = 0$ cm, is considered as the cathode ($V_{cathode} = -V_{DC}$). The grounded electrode has been taken at $x = 1$ cm, is considered as the anode ($V_{anode} = 0$).

Table 1. Kinetic scheme of processes

Processes	Name of Processes	Rates coefficients		Ref
		Symbol	Value	
$Ne + e^- \rightarrow Ne + e^-$	Elastic Collision	P^{ec}	Calculated (eVs^{-1})	[8-9]
$Ne + e^- \rightarrow Ne^+ + 2e^-$	Ionization	K_o^{io}	BOLSIG+ (cm^3s^{-1})	[10-11]
$Ne + e^- \rightarrow Ne_m^* + e^-$	Excitation	K_o^m	BOLSIG+ (cm^3s^{-1})	[10-11]
$Ne_m^* + Ne_m^* \rightarrow Ne^+ + e^- + Ne$	Chemo-ionization	K^{ci}	$3.6x10^{-10}$ (cm^3s^{-1})	[12]

In time $t = 0$, the electron, ion and metastable atom densities are assumed constant and equal to 10^3 cm^{-3} . A mean electron energy has been taken 1 eV.
Assuming a predominant field-driven flux close to the cathode the relation $\partial D_+ n_+ / \partial x = 0$ has been employed for the positive ion density $\forall t$ >0, while vanishing metastable atom density, i.e., $n_m = 0$ has been prescribed at the cathode. At the anode, the electron density and the metastable atoms are assumed to be zero. The electron flux parting the cathode is computed by the expression
$\varphi_e(x = 0, t) = -\gamma\varphi_+(x = 0, t)hg \ \forall t$ >0, the mean electron energy is assumed to be 5 eV at the cathode and the gas temperature is equal to 310 K in the discharge.

Numerical procedure

For the transport equations of the electron, ion and electron energy a finite difference method has been used. For This technique the exponential approximation has been taken into account [1-7]. The Poisson and metastable atom equations are also discretized spatially with the finite difference method. The discretization of the terms of the time with the finite difference method on the right position has been employed . Therefore, each discretized equation is represented by a tridiagonal matrix, which are resolved by Thomas's technique.

Results and discussion of neon discharge

In this paragraph, we will survey the spatio-temporal development of the abnormal glow discharge in the presence of metastable atom density. The applied potential at the cathode is -300 V. The constant value for the secondary electron yield is 0.26 [16]. The gas pressure is 3 Torrs. The neutral species density is determined from the gas pressure and temperature with the ideal gas law. The time step Δt=10ps and a uniform subdivision of the space interval in 250 elements, have been used.

Fig. 1 represents the temporal evolution of the potential (a), the densities of electrons (b), ions (c) and metastable atoms (d), electric field (e) and the mean electron energy (f). We observe that the discharge is characterized by three zones: the first one occupied the time simulation between 10^{-11} and 10^{-5} s, the second one occupied the time simulation between 10^{-5} and $2.5x10^{-5}$ s, the final zone occupied the time simulation between $2.5x10^{-5}$ and 4 $x10^{-5}$ s.

For the first zone, we remark that the electrons, ions numbers and metastable atom densities are approximately indistinguishable. Consequently, the net space charge density is negligible. The electric potential is characterized the Laplace form because of the net space charge density that is present. Hence, the electric field is quasi constant. The mean electron energy is also constant, because the electric field is present.

In the second zone, we observe a pseudo appearance of the cathodic region, this is typified by an importance of ion number density and less significant to the electron number density. This is explained to the accelerate electron species that spread a great deal faster than ion species and move rapidly from the cathodic region. Therefore the quantities (n_e-n_+) is significant which influence the potential as a chute. Consequentially, the electric field is important. The latter acquires an important energy of electron species.

We observe, that the metastable atom density is significant. This discharge is maintained by secondary emission processes as well as the presence of metastable atom density. Before t=$2.5x10^{-5}$ s we observe a pseudo appearance of negative glow, where it is characterized by the same electron and ion densities. Therefore the net space charge density is negligible and hence the electric potential and electric field are constants. Consequentially, the metastable density is increased.

In the final zone, we observe three different regions' the anode and cathode regions and the plasma region. The anode region is typified by ion number density, that is less imperative compared to the electron number density. In this zone we observe the convergence of all physical properties of the discharge at the time 4 $x10^{-5}$ s.

Conclusion

In order to study the effect of metastable atom density, a second order fluid electric model has been developed in the case of a DC low-pressure Neon glow discharges. The Poisson equation for the potential and electric field is coupled to the first three moments of the Boltzmann's conservation equations neglecting inertia of the charged particles. In the framework of the local energy approximation, the basic data used in this work are determined from BOLSIG+ software. The role of metastable atom density in the discharge is clear for investigation into side of plasma glow discharge for many pure gases and gas mixtures. We note that the glow discharge is maintained by secondary electron emission and the presence of metastable atom density in this case of discharge.

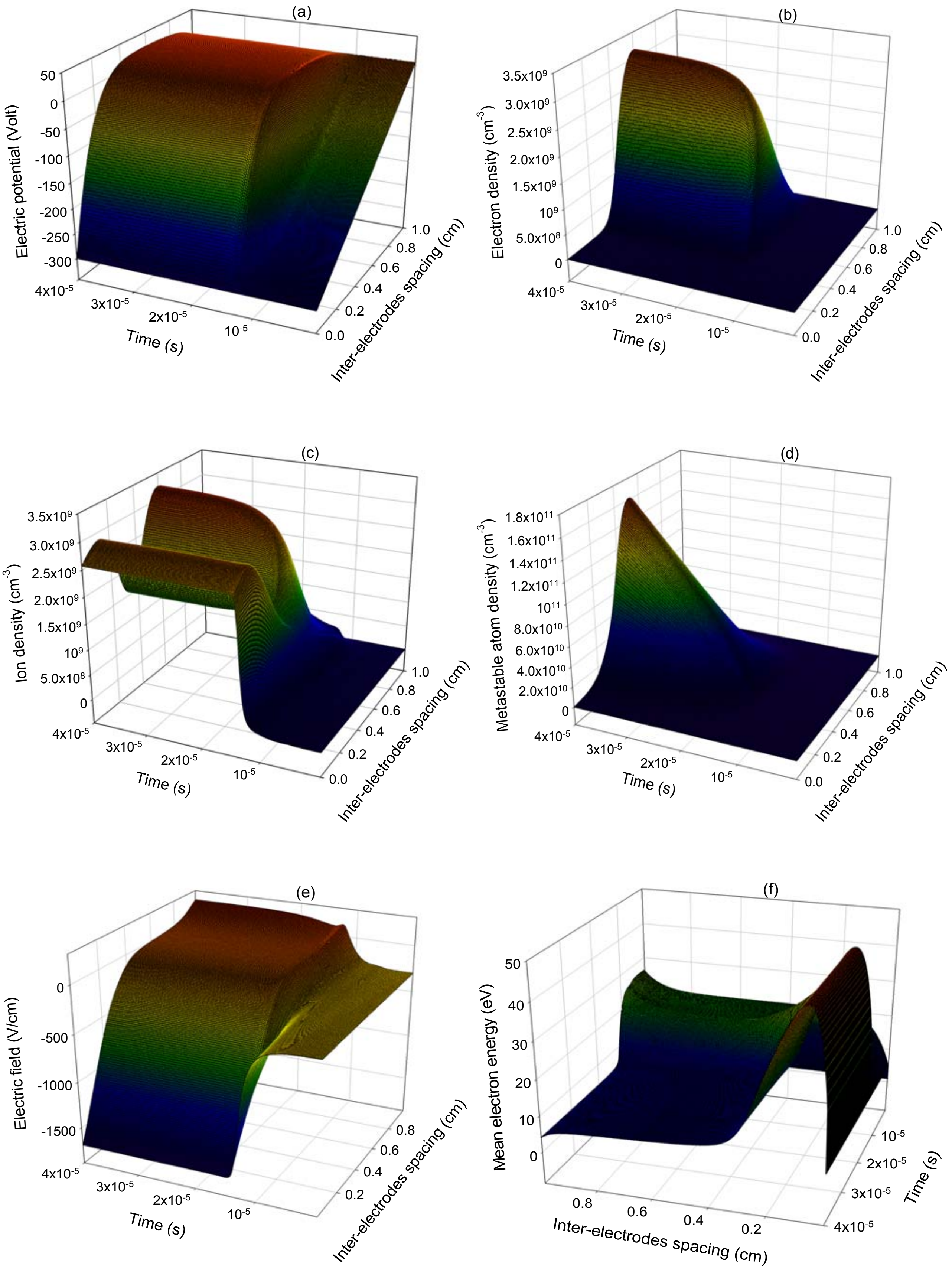

Fig. 1. Neon spatio-temporal distributions of electric potential (a), electrons volume number (b), ions volume number (c), metastable atom density (d), electric field (e) and mean electron energy (f) at 300 V

Nomenclature

n_e, n_+, n_m - Electron, ion and metastable atom densities

φ_e , φ_+ , φ_m - Electron, ion and metastable atom fluxes

n_o - Constant background gas density

K_o^m - Rate coefficient of electron-impact excitation of ground state atoms

ε^m - Energy loss of excited atoms

K_o^{io} - Rate coefficient of electron-impact ionization of ground state atoms

ε^{io} - Energy loss of ionized atoms

K^{ci} - Rate coefficient of chemo-ionization processes

ε^{ci} - Energy gain of chemo-ionization processes

τ_m - Metastable lifetime

P^{ec} - Energy loss per electron due to elastic collision of electrons with the background gas

ε_e - Mean electron energy

$\varphi_{e\varepsilon}$ - Electron energy flux

V - Electrostatic potential

E - Electric field strength

ε_o , e - Permittivity of free space and elementary charge

μ_e , μ_+ - Electron mobility, Ion mobility

D_e , D_+ , D_m - Electron diffusivity, Ion diffusivity and metastable atom diffusivity

$\mu_{e\varepsilon}$, $D_{e\varepsilon}$ - Mobility and diffusivity of electron energy transport.

***Authors**:*

Tahar Alili: University of Sciences and Technology of Oran, USTO-MB, 31000, Algeria.

Abdelaziz Bouchikhi: University of Saïda, Faculty of technology, Department of electrical engineering, Saïda 20000, Algeria.

Mohamed Rizouga: University of Sciences and Technology of Oran, USTO-MB, 31000, Algeria.

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