2D Fluid Approaches of DC Magnetron Discharge

C. Costin[1], L. Marques[2], G. Popa[1], G. Gousset

Laboratoire de Physique des Gaz et des Plasmas, Universite Paris Sud XI, Bat. 210, 91405 Orsay Cedex, France

[1]Faculty of Physics, Al. I. Cuza University, 11 Carol I Blvd., 700506 Iasi, Romania

[2]Departamento de Fisica, Universidade do Minho, 4710-057 Braga, Portugal

Abstract

A two dimensional (r,z) time-dependent fluid model was developed and used to describe a DC planar magnetron discharge with cylindrical symmetry. The transport description of the charged species uses the corresponding first three moments of Boltzmann equation: continuity, momentum transfer and mean energy transfer (the latter one only for electrons), coupled with Poisson equation. An original way is proposed to treat the transport equations. Electron and ion momentum transport equations are reduced to the classical drift-diffusion expression of the fluxes since the presence of the magnetic field is introduced as an additional part in the electron flux, while for ions an effective electric field was considered. Thus, both continuity and mean energy transfer equations are solved in a classical manner. Numerical simulations were performed considering Argon as buffer gas, with a neutral pressure varying between 5 and 30 mtorr, a gas temperature from 300 to 350 K and cathode voltages lying from -200 up to -600 V. Results obtained for densities of the charged particle, fluxes and plasma potential are in good agreement with previous works.

Keywords: Magnetron discharge, Numerical modelling, Fluid model

Introduction

Magnetron discharge stands out from other low pressure electrical discharges through the presence of **a** strongly non-homogenous magnetic field in front of the cathode (target). This field is created by a pair of magnets co-axially disposed under the cathode plate (fig. 1). As a consequence of the geometric arrangement a balanced or unbalanced structure of field lines emerges **[1].** A strong axial electric field, E_z, is present in the magnetic field region due to the cathode fall. The simultaneous action of these two fields leads to a high density confined plasma, permitting thus a low voltage operating discharge (hundreds volts) at very low pressure, typically about 10 mTorr. Larmour radius for ions is of the order of centimeters while, the thickness of the cathode fall does not exceed a few millimeters. Thus, the ions might be considered as being not affected by the magnetic field but accelerated directly to the cathode where by impact on the surface they are able to generate secondary electrons and to sputter particles which can typically be used for surface deposition of a wafer placed in front of the target.

Magnetron discharges were and still are extensively studied experimentally, analytically or numerically for better understanding of both physical and chemical processes involved in their multiple applications. Working in pure rare gases [2-5,9] or reactive mixtures [5-8], in DC [7-9], RF [5,6] or pulsed regimes [2-4], magnetron discharges are mainly and widely used as sputter/deposition sources.

During the last years, many numerical models were proposed to properly describe these discharges and to speed up the computing time. Particle-in-cell/Monte Carlo collision (PIC-MCC) is a very common technique applied for 2D [10-12] or 3D [13] simulations. It is easy to implement, without a priori physical approximations except the classical nature of particle trajectories, being very useful for non-equilibrium processes, but it requires a very large computational time. Hybrid model combines particle and continuum models, achieving more reasonable computing times. In some works [1,14] fast electrons, such as secondary emitted electrons at the cathode which are accelerated in the cathode fall (mainly giving the ionisation rate), are treated by Monte Carlo model while for slow electrons and ions, which are the dominant particle population, the fluid equations are used. Other authors [15] combine a particle simulation of neutral atoms and ions with a fluid description of electrons. This time such a model is applied for stationary plasma thrusters (SPT), devices related with magnetron discharges through the presence of a magnetic field. In the kinetic model [16,17] a microscopic description of the plasma is carried out. The distribution functions of the particles are calculated by solving Boltzmann equation and macroscopic plasma parameters can be obtained by integrating over distribution functions. The kinetic model is often combined with a collisional radiative one [18,19], the latter requiring to solve rate balance equations for excited species.

Despite numerous paper devoted to the modelling of this type of discharge, those using the fluid approach are very rare and rather one-dimensional treatment of fluid equations is mentioned [20,21]. This is manly due to the difficulty to treat the effect of the inhomogeneous magnetic field on the electrons. The problem is typically 3D but it can be spatially reduced to 2D in the particular case of cylindrical symmetry. For numerical simulations fluid model has an advantage upon the computing time but it looses its validity with decreasing of the gas pressure when the mean free path of charged particles strongly exceeds the characteristic length of the discharge. Although magnetron discharges work at low pressures (1 to tens mtorr), the presence of the magnetic field reduces the effective distance covered by electrons between two collisions, which is equivalent to an increase of the pressure, thus fulfilling the hydrodynamic hypothesis. As an alternative point of view, the set of fluid equations considered in this work should be regarded as a pure macroscopic representation of the electron Boltzmann equation whose solution concerns mainly the calculation of the electron density and mean energy. Such quantity plays a crucial role in defining a spatial dependence for the electron distribution function, when adopting the *local mean energy approximation* as in this work. We must pay attention that, due to the large electron density the Boltzmann equation stay available to describe the electron kinetics and, consequently, we can suppose that is effective also for the moments of its. Even if the fluid model deals with mean values and macroscopic quantities, valuable information of the discharge can be provided.

This paper presents an original approach of two dimensional *(r,z)* time-dependent fluid model used to describe the transport of two charged species, electrons and positive ions, in a cylindrical symmetry DC planar magnetron reactor. The transport of the charged species is described by the corresponding first three moments of Boltzmann equation: continuity, momentum transfer and mean energy transfer equation (the latter only for electrons), coupled with Poisson equation. Due to the strong coupling of the fluid equations in presence of the magnetic field, some assumptions are required in order to simplify the numerical procedure. Thus, all transport equations are treated in the same manner, using classical drift-diffusion expression for fluxes. This condition is achieved by introducing the influence of the magnetic field as an additional part in the electron flux and considering an effective electric field for ions. Boundary conditions are settled for the fluxes of the charged particles and for electric potential at the walls.

Computations were performed for a planar magnetron device, schematically drawn in fig. 2. The Argon was chosen as working gas. Due to the cylindrical symmetry of the system only a bi-dimensional picture is plotted. The cathode is a metallic disc with r_{cath} = 16.5 mm radius, grounded metallic walls playing the role of the anode ($R_{max} = Z_{max}$= 26.95 mm). Neutral gas pressure varies between 5 and 30 mtorr, while its temperature lies between 300 and 350 K. The applied DC voltage on the cathode ranges from -200 to -600 V. Magnetic field structure is unbalanced, as shown in fig. 2. For a convenient visualization, the length of the plotted vectors is proportional to the logarithm of magnetic field strength, ln *B,* measured and numerically fitted as presented in [22]. In the region where the field lines are parallel to the cathode ($r \approx 9.5$ mm), magnetic field strength decreases from about 750 Gauss at $z = 0$ to 20 Gauss at $z \approx 15$ mm. Several plasma parameters such as plasma potential, densities of the charged particles and ion flux at the cathode yield from the model and they are discussed as representative results.

Model equations

A two-component fluid model was considered in order to describe the magnetron discharge. Basic fluid equations were written for electrons (1a-1c) and ions (1a,1b). They consist on the first three moments of Boltzmann equation, continuity (1a), momentum transfer (1b) and mean energy transfer (1c):

$$\frac{\partial n_s}{\partial t} + \nabla \cdot \vec{\Gamma_s} = S \tag{1a}$$

$$m_s n_s \left[\frac{\partial \vec{v_s}}{\partial t} + \left(\vec{v_s} \cdot \nabla \right) \vec{v_s} \right] = q_s n_s \left(\vec{E} + \vec{v_s} \times \vec{B} \right) - \nabla \vec{\vec{P_s}} - m_s n_s f_{ms} \vec{v_s} \left(1 + \frac{n_e f_{iz}}{n_s f_{ms}} \right) \tag{1b}$$

$$\frac{\partial (n_s \varepsilon_s)}{\partial t} + \nabla \cdot (\vec{\Gamma_{\varepsilon s}}) = -\vec{\Gamma_s} \cdot \vec{E} - \theta_s n_s , \tag{1c}$$

where s is the type of particle ($s = e$ - for electron and i- for ion, respectively), n_s - the density, m_s - the mass, v_s - the velocity of the fluid particle, f_{iz} - the ionisation frequency by electron-neutral impact, f_{ms} - the total momentum transfer frequency for s species - neutral collisions, $\vec{E}$ - the electric field intensity, $\vec{B}$ - the magnetic field strength, $\vec{\vec{P}}_s$ - the pressure tensor, q_s - the particle charge, t - the time, ε_S - the mean energy (in eV), θ_S - the energy loss rate by collisions with s -neutral; $\vec{\Gamma}_S = n_S \vec{v}_S$ is the flux of particles and $\vec{\Gamma}_{\varepsilon S} = n_S \langle \varepsilon_S \vec{v}_S \rangle$ - the energy flux. Considering that both electrons and ions are created only by electron-neutral ionization collisions, the source term in the continuity equation is $S = f_{iz} n_e$. Magnetic field, $\vec{B}$, considered in the calculations takes into account only the stationary magnetic field produced by the magnets behind the cathode, excluding the one generated by movement of the charged species. In particular, the azimuthal drift current in the plasma ring in front of the target can be in the order of few Amperes [23]. The magnetic field generated by such currents can be estimated of about few percents of the static field when the latter one has hundreds Gauss strength. The electric field and plasma potential are given by Poisson equation

$$\Delta V = -\frac{e}{\varepsilon_0}(n_i - n_e) \tag{2}$$

$$\vec{E} = -\nabla V\,. \tag{3}$$

All equations are developed in cylindrical coordinates (r, φ, z). Due to axial symmetry of the magnetron, the electric and magnetic fields have no azimuthal components, but the presence of the $\vec{E}\times\vec{B}$ drift generates a flux component, $\Gamma_{s\varphi}$, under φ direction. However, disregarding the possible drift current instabilities, this component can be expressed as a function of Γ_{sr} and Γ_{sz}, permitting thus to reduce the problem to a bi-dimensional one, (r,z).

Electron transport treatment

Starting from the momentum transfer equation (1b), the electron flux can be expressed in the form

$$\vec{\Gamma}_e = \vec{\Gamma}_e^0 + \vec{\Gamma}_e^1 \tag{4}$$

with $\vec{\Gamma}_e^0$ the classical drift-diffusion flux and $\vec{\Gamma}_e^1$ a contribution of the magnetic field. To obtain (4) some simplifying assumptions were made in equation (1b): i) the inertial term $m_e n_e\left[\partial\vec{v}_e/\partial t + (\vec{v}_e\cdot\nabla)\vec{v}_e\right]$ was neglected due to small mass of the electron; *ii)* the ionisation frequency f_{iz} was also neglected with respect to the total electron-neutral momentum transfer frequency, f_{me} *iii)* considering isotropic electron distribution function, the pressure tensor becomes a scalar, $P_e = n_e kT_e$. Thus, the momentum transfer equation can be written as

$$n_e\overrightarrow{\mathrm{v}_e} = -\frac{e}{m_e f_{me}} n_e\vec{E} - \nabla\left(\frac{kT_e}{m_e f_{me}} n_e\right) - \frac{e}{m_e f_{me}} n_e\overrightarrow{\mathrm{v}_e}\times\vec{B}\,, \tag{5}$$

where $\mu_e = e/(m_e f_{me})_c$ and $D_e = kT_e/(m_e f_{me})$ are electron mobility and diffusion coefficient, respectively. The two electron flux components are then

$$\overrightarrow{\Gamma_e^0} = -\mu_e n_e\vec{E} - \nabla(D_e n_e) \tag{6a}$$

and

$$\overrightarrow{\Gamma_e^1} = -n_e\overrightarrow{\mathrm{v}_e}\times\overrightarrow{\Omega_e}/f_{me} = -\overrightarrow{\Gamma_e}\times\overrightarrow{\Omega_e}/f_{me}\,, \tag{6b}$$

where $\vec{\Omega}_e = e\vec{B}_e/m_e$ is related to electron cyclotron giro-frequency. Due to the cylindrical symmetry $\vec{\Gamma}_e^0$ has only two components, $\vec{\Gamma}_{er}^0$ and $\vec{\Gamma}_{ez}^0$, while $\vec{\Gamma}_e^1$ has also the azimuthal one induced by the magnetic field

$$\begin{pmatrix}\Gamma_{er}^1\\ \Gamma_{e\varphi}^1\\ \Gamma_{ez}^1\end{pmatrix} = \frac{1}{f_{me}^2+\Omega_e^2}\begin{pmatrix}-\Omega_{ez}^2 & \Omega_{er}\Omega_{ez}\\ f_{me}\Omega_{ez} & -f_{me}\Omega_{er}\\ \Omega_{er}\Omega_{ez} & -\Omega_{er}^2\end{pmatrix}\begin{pmatrix}\Gamma_{er}^0\\ \Gamma_{ez}^0\end{pmatrix}. \tag{7a}$$

The azimuthal flux component $\Gamma_{s\varphi}$ can be deduced from the combination of the eqs. (4) and (7a) as a function of Γ_{er} and Γ_{ez},

$$\Gamma_{e\varphi} = \frac{1}{f_{me}}\left(\Gamma_{er}\Omega_{ez} - \Gamma_{ez}\Omega_{er}\right). \tag{7b}$$

The reduced electron transport parameters, D_eN and μ_eN, depend on electron energy distribution function (EEDF), $f(\vec{r},u)$, where $u = m_e v^2/2e$ is the electron kinetic energy in eV. Under the classical two terms approximation of EEDF they can be written [24] as

$$D_e(\vec{r})N = \frac{1}{3}\sqrt{\frac{2e}{m_e}}\int_0^\infty \frac{u}{\sigma_{me}(u)} f_0(\vec{r},u)du \tag{8a}$$

$$\mu_e(\vec{r})N = -\frac{1}{3}\sqrt{\frac{2e}{m_e}}\int_0^\infty \frac{u}{\sigma_{me}(u)} \frac{df_0(\vec{r},u)}{du}du, \tag{8b}$$

where σ_{me} is the total electron-neutral momentum transfer collision cross section, N is the gas density and $f_o(\vec{r},u)$ is the isotropic part of $f(\vec{r},u)$, satisfying the normalization condition

$$\int_0^\infty f_0(\vec{r},u)u^{1/2}du = 1.$$

The energy flux is written in the same manner as the particle flux, with corresponding reduced transport coefficients, $D_{\varepsilon e}N$ and $\mu_{\varepsilon e}N$ [24]

$$D_{\varepsilon e}(\vec{r})N = \frac{1}{\varepsilon_e(\vec{r})}\frac{1}{3}\sqrt{\frac{2e}{m_e}}\int_0^\infty \frac{u^2}{\sigma_{me}(u)} f_0(\vec{r},u)du \tag{8c}$$

$$\mu_{\varepsilon e}(\vec{r})N = -\frac{1}{\varepsilon_e(\vec{r})}\frac{1}{3}\sqrt{\frac{2e}{m_e}}\int_0^\infty \frac{u^2}{\sigma_{me}(u)} \frac{df_0(\vec{r},u)}{du}du. \tag{8d}$$

The spatial map of electron transport parameters can be obtained adopting the local mean energy approximation [24], which consists in introducing the spatial dependence of EEDF via the electron mean energy profile, $\varepsilon_e(\vec{r})$, The profile $\varepsilon_e(\vec{r})$ of the electron mean energy is obtained as solution of electron mean energy transfer equation (lc). Due to the high density ($n_0 \sim 10^{10}$ cm^{-3}) of the magnetron plasma a maxwellian EEDF was considered instead of calculating the solution of electron Boltzman equation,

$$f_0(\vec{r},u) = f_0[\varepsilon_e(\vec{r}),u] \equiv \frac{2}{\sqrt{\pi}}\left[\frac{2\varepsilon_e(\vec{r})}{3}\right]^{-\frac{3}{2}} e^{-\frac{3u}{2\varepsilon_e(\vec{r})}}. \tag{9}$$

In the equation (lc), electron energy loss rate in elastic and inelastic (excitation, ionisation) collisions is calculated according to the same reference [24]

$$\theta_e(\vec{r}) = N\frac{2m_e}{M_n}\sqrt{\frac{2e}{m_e}}\int_0^\infty \sigma_{e-n}^{el}(u) f_0(\vec{r},u)u^2du + \sum_k^{inel} W_k f_{ke}(\vec{r}), \tag{10}$$

where M_n is the mass neutral atoms, σ_{e-n}^{el} is elastic cross section of the electron-neutral collision, W_k the energetic threshold for the k - inelastic process characterized by f_{ke} collision frequency. All collision frequencies are calculated with

$$f_{ke}(\vec{r}) = N\sqrt{\frac{2e}{m_e}}\int_0^\infty \sigma_{ke}(u) f_0(\vec{r},u)\, u\, du\,, \tag{11}$$

using collision cross sections given by [25]. Elastic, excitation and ionization collisions with ground state neutrals are considered.

Ion transport treatment

In the ion momentum transfer equation, the inertial term cannot be neglected due to the ion heavier mass. Magnetic field influence was not considered because ion cyclotron giro-radius is larger than the linear dimension of the examined region. In front of the cathode, where the magnetic field is important, ion Larmour radius is higher than 7 cm, while the linear dimension of the examined region is 2.7 cm. Under such assumptions, ion momentum transfer equation becomes

$$n_i\overrightarrow{\mathrm{v}_i} = \frac{e}{m_i f_{mi}} n_i \vec{E} - \nabla\left(\frac{kT_i}{m_i f_{mi}} n_i\right) - \frac{n_e f_{iz}}{n_i f_{mi}} n_i \overrightarrow{\mathrm{v}_i} - \frac{1}{f_{mi}} n_i \left[\frac{\partial \overrightarrow{\mathrm{v}_i}}{\partial t} + \left(\overrightarrow{\mathrm{v}_i}\cdot\nabla\right)\overrightarrow{\mathrm{v}_i}\right], \tag{12}$$

where the ion pressure was also considered as scalar, $P_i = n_i kT_i$, by the reason of isotropic ion distribution function assumed. For convenience the ion flux is written in a drift-diffusion form, by introducing an effective electric field, $\vec{E}^{eff}$, [26] as that

$$\overrightarrow{\Gamma_i} = n_i\overrightarrow{\mathrm{v}_i} \equiv \mu_i n_i \overrightarrow{E^{eff}} - \nabla(D_i n_i)\,. \tag{13}$$

Identifying these two expressions, (12) and (13), for the ion flux and performing some simple calculations [27], an equation for the space-time evolution of $\vec{E}^{eff}$ is yielded

$$\frac{\partial \overrightarrow{E^{eff}}}{\partial t} = f_{mi}\left(\vec{E} - \overrightarrow{E^{eff}}\right) - f_{iz}\frac{n_e}{n_i}\frac{\overrightarrow{\mathrm{v}_i}}{\mu_i} - \frac{1}{\mu_i}\left(\overrightarrow{\mathrm{v}_i}\cdot\nabla\right)\overrightarrow{\mathrm{v}_i}\,. \tag{14}$$

Argon ions reduced diffusion coefficient is deduced from Einstein relation

$$D_i N = \mu_i N \frac{kT_i}{e}\,, \tag{15}$$

where ion reduced mobility depends on the reduced effective electric field, $\mu_i N = f(\vec{E}^{eff}/N)$. The data adopted for this dependence are given in [28] for E/N in the range of 0 - 2 x 10^3 Td and were extrapolated up to 10^5 Td according to [29]. Argon ions were supposed to be thermalised at gas temperature, $T_i = T_{Ar}$. The ion momentum transfer frequency, f_{mi}, was calculated through the expression for classical mobility

$$f_{mi} = N\frac{e}{m_i(\mu_i N)}\,. \tag{16}$$

Boundary conditions

Fluid equations as well as Poisson equation can be solved only if boundary conditions are specified. For charged particles, these conditions are imposed upon fluxes. All parallel fluxes with respect to any surface are zero, $\Gamma_s^{\parallel} = 0$, $s = e,\ i$. In the absence of the magnetic field, the normal electron flux to the anode surface must verify $\Gamma_e^{0\perp} = \frac{1}{2} n_e \langle v_e \rangle$ [24], where $\langle v_e \rangle$ is the mean electron velocity obtained by integrating over EEDF. At the cathode, in the same conditions, normal flux has two components: one is coming from the discharge, $\frac{1}{2} n_e \langle v_e \rangle$, while the other one is due to the secondary electrons emitted by ion impact, $-\gamma_i \Gamma_i^{\perp}$, where γ_i, is the coefficient for secondary electron emission. Due to the very low electron density in the cathode fall, being 3 to 4 orders of magnitude lower than the one in the anode sheath, the inner flux is negligible with respect of the flux of the secondary electron emitted, permitting thus to write $\Gamma_e^{0\perp} = -\gamma_i \Gamma_i^{\perp}$. Taking into account the magnetic field, total normal flux is $\vec{\Gamma}_e^{\perp} = \vec{\Gamma}_e^{0\perp} + \vec{\Gamma}_e^{1\perp}$, with $\vec{\Gamma}_e^{1\perp}$ given by (7a) and $\Gamma_e^{\parallel}$ zero.

Because the secondary emission coefficient has a strong influence on the properties of the magnetron discharge, some remarks have to be done. Due to the presence of a strong magnetic field close to the cathode surface, the secondary electron trajectory is turned around the field lines, enabling electrons to interact with the target, which reflects or recaptures them. The last process diminishes the effective value of the coefficient for total secondary electron emission without magnetic field, γ_i, so that the magnetron discharge "sees" only a fraction of it, $\gamma_{net} = \gamma_i(1-p)$ [30]. As the probability of the recapture, *p,* depends on both orientation and magnitude of the magnetic field strength on the cathode surface, from fig. 2 it can be concluded that γ_{net} depends on the radial position, $\gamma_{net}(r) = \gamma_i(1-p(r))$. Also, it must be mentioned that secondary electrons can collide with gas neutrals or they can interact with the cathode. Once a collision takes place, the electron can no longer return to the surface. Thus, the probability of the recapture depends of the electrons mean free path and, implicitly, of the gas pressure [30]. Even if γ_{net} depends of the position, according to [30] a constant coefficient γ_d can be calculated for the whole cathode surface, as being the effective coefficient "seen" by the discharge. In our case it is not necessary to introduce an effective coefficient because it appears explicitly from the calculus, thus it can also be estimated. Assuming $\Gamma_e^{0\perp} = -\gamma_i \Gamma_i^{\perp}$, the total normal electron flux at the cathode becomes

$$\Gamma_e^{\perp} = -\gamma_i \Gamma_i^{\perp}\left(1 - \frac{\Omega_{er}^2}{f_{me}^2 + \Omega_e^2}\right) = -\gamma_{net}\Gamma_i^{\perp}, \tag{17}$$

with

$$\gamma_{net} = \gamma_i\left(1 - \frac{\Omega_{er}^2}{f_{me}^2 + \Omega_e^2}\right). \tag{18}$$

Expression (18) clearly shows the dependence of γ_{net} on the gas pressure, through f_{me}, on the magnetic field, by $\Omega_{e,cr}$ and implicitly on the position.

According to [31], below 500 eV, γ_i can be considered independent of the ion energy for clean metal surfaces, with typical values in the range of 0.05—0.1. For the Ar-Cu couple, ref. [32] reports a mean value for γ_i, at about 0.01 versus reduced electric field, *E/p,* in the range of hundreds of $\mathrm{Vcm^{-1}torr^{-1}}$. In this paper it was chosen for γ_i an intermediate value between the two references, $\gamma_i = 0.02$. The boundary conditions for the equivalent flux are available for electron energy transport by changing $\langle v_e \rangle$ to $\langle \varepsilon_e v_e \rangle$ and taking a mean energy, $\varepsilon_0 = 1$ eV, for secondary electrons emitted at the cathode surface, even if in the literature are given energy values between 2-6 eV [33]. For all surfaces, normal ion flux is given by, $\Gamma_i^{\perp} = \frac{1}{4} n_i v_{thi} + \delta \mu_i n_i E_{eff}^{\perp}$ where v_{thi} is ion thermal velocity; $\delta=1$ if $E_{eff}^{\perp}$ is directed to the surface and $\delta=0$ otherwise. For Poisson equation, the boundary conditions include the fact that the anode is grounded ($V_{anode} = 0$) and that a negative voltage, $V_{cathode}$, is applied to the cathode. For symmetry reasons at the reactor axis $\partial V/\partial r = 0$ and for particle density $\partial n_s/\partial r = 0$, $s = e,i$.

Numerical solution

As was already mentioned above, due to cylindrical symmetry of the magnetron, a bi-dimensional (r,z) treatment is complete for a proper description of the discharge. Even if an electronic azimuthal flux exists, it can be expressed in (r,z) co-ordinates system as shown in eq. (7b). For the charged particles, continuity type equations,

$$\frac{\partial n_s}{\partial t} + \left[\frac{1}{r}\frac{\partial}{\partial r}(r\Gamma_{sr}) + \frac{\partial}{\partial z}(\Gamma_{sz})\right] = S, \quad s = e,i, \tag{19}$$

have to be solved. The transport equation for electron energy has the same form, by changing particle density with electron mean energy density and correctly expressing the source term S_ε. In the equations (19) the fluxes of the charged species must be introduced in order to obtain the particle densities. If the expression of the global flux for electrons (5) and ions (12) are used, it will result a complicated system to be solved. Two conditions are imposed to simplify the problem: i) the fluxes are expressed under the forms (4) and (13) and *ii)* only the drift-diffusion component of the flux is kept in the left side terms of the equations (19). The last condition does not affect ions equation because in the expression (13) the flux has already a classical drift-diffusion form. Under these assumptions, equations (19) are developed as

$$\frac{n_e^{t+\Delta t} - n_e^t}{\Delta t} + \left[\frac{1}{r}\frac{\partial}{\partial r}(r\Gamma_{er}^0) + \frac{\partial}{\partial z}(\Gamma_{ez}^0)\right]^{t+\Delta t} = S^t - \left[\frac{1}{r}\frac{\partial}{\partial r}(r\Gamma_{er}^1) + \frac{\partial}{\partial z}(\Gamma_{ez}^1)\right]^t, \tag{20a}$$

$$\frac{n_i^{t+\Delta t} - n_i^t}{\Delta t} + \left[\frac{1}{r}\frac{\partial}{\partial r}(r\Gamma_{ir}) + \frac{\partial}{\partial z}(\Gamma_{iz})\right]^{t+\Delta t} = S^t, \tag{20b}$$

which gives a semi-implicit temporal discretization scheme, where Δt is the time step. The spatial discretization method is based on the finite difference scheme. The equations (20a,b) are multiplied by *rdrdz* and are integrated over a grid cell, permitting thus to avoid the singularity problem of the divergence for $r = 0$. The drift-diffusion fluxes for electrons and ions are discretized using the Scharfetter-Gummel exponential scheme [34]. The equations (20a,b) can then be solved to obtain particle densities and the drift-diffusion fluxes. After that, $\vec{\Gamma}_e^{1\perp}$ is deduced from eq. (7a) and the total electron flux is obtained. Plasma potential is calculated from the Poisson equation for every time step. All equations are numerically solved using a band matrix method [35], including the boundary conditions.

The time step value is constrained by the convergence of the numerical methods used to solve the system of equations mentioned above. First of all, Courant-Friedrichs-Lewy (CFL) stability criterion [36,37] must be accomplished. This condition imposes to a particle to cover at the most dimension of one cell per time step. Also, for the stability of the space charge and electric field, the time step must be upper limited by Maxwell relaxation time [37].

Results

Simulation results in Argon are presented here for a pressure p = 20 mtorr, neutral temperature T_{Ar} = 350 K and a polarization of the cathode of -550 V. Spatial distribution of the potential in the reactor is plotted in fig. 3. In the largest part of the discharge, plasma potential is slowly positive. The cathode fall thickness is about 5 mm on the magnetron axis while in the highest confinement zone it does not exceed 3.8 mm. This zone corresponds to the region where vectors $\vec{E}$ and $\vec{B}$ are perpendicular to each other. As the electric field is axially dominant in the cathode fall, the magnetic field must be radial and, according to fig. 2, this occurs in front of the cathode at about 9.5 mm radius. Confinement zone is visible in fig. 3, being characterized by a higher local potential but more evident is fig. 4 where electron and ion densities are yielded. Representation is bi-dimensional (r,z), but rotating the picture around z-axis, according to the cylindrical symmetry, it is clearly shown that the negative glow in magnetron is a torus. Maximum density both for electrons and ions reaches 2.5 x 10^{10} cm $^{-3}$ at r = 9.5 mm, z = 5 mm. The electron density decreases significantly in the anode sheath and cathode fall with respect of the volume, the white zone in fig. 4a corresponding to a density smaller than 2.4 x 10^{8} cm $^{-3}$. Plasma potential and charged particle densities are in very good shape agreement with previous results from hybrid model [1,14], the latter ones having the same spatial profile above-mentioned. Comparable results are given also by PIC simulation [11-13], even if they were performed for a different geometry. In fig. 5 is given the axial ion particle flux in the cathode fall. While ion energy at the target does not depend of the radial position r, particle flux is a measure of the sputtering profile of the cathode. It must be mentioned that unlike figs. 2-4 this picture is plotted in a reduced region in front of the cathode, r_{max}= 16.5 mm, z_{max} = 10 mm, there where ion flux is really interesting. Positive/negative values of the ion flux denote the orientation from/toward the cathode of the flux vector. Plotting data were not limited to the cathode fall (z<5 mm) in order to put in evidence also the positive diffusive flux due to the ion density gradient.

Concluding remarks

An original treatment of fluid equations is proposed in this paper. Separating the electron flux in two parts and treating the influence of the magnetic field as an additional term in the flux expression seems to be a valid and convenient approach. Calculated results are in good shape agreement with previous one obtained by PIC or hybrid schemes. Even more, if this approach works for a term containing a vector product, $\vec{v}_e \times \vec{B}$, that creates a strong coupling between the flux components, Γ_{er}, $\Gamma_{e\varphi}$, Γ_{ez}, it is expected so much the more to work for the other neglected terms in eq. (1b). Thus, we can consider the electron inertial term, pressure anisotropy or the contribution of the finite fraction f_{iz}/f_{me} to the total electron flux. Each term can be introduced following the same procedure presented in this paper, the advantage being an easy way for linearizing and solving eq. (la,c) by keeping in the left side term only a drift-diffusive flux form. Such approaches, which solve time-dependent fluid equations, can be used for RF magnetron discharges without modifications except for the applied potential at the cathode.

Acknowledgements

One of the authors (C Costin) would like to thank French Government for his PhD fellowship at *Laboratoire de Physique des Gaz el des Plasmas.* We are also grateful to T Minea for very helpful discussions. This work was partly supported by CNCSIS Romania, grant A/1344/40213/2003.

References

[1] Shidoji E, Ando E and Makabe T (2001) *Plasma Sources Sci. Technol.* 8 621

[2] Kouznetsov V, Macak K, Schneider J M, Helmersson U and Petrov I (1999) *Surf. Coat. Technol.* 122 290

[3] Gudmundsson J T, Alami J and Helmersson U (2001) *Appl. Phys. Lett.* 78 3427

[4] Ehiasarian A P, New R, Munz W-D, Hultman L, Helmersson U and Kouznetsov V (2002) *Vacuum* 65 147

[5] Bruckner W, Kaltofen R, Thomas J, Hecker M, Uhlemann M, Oswald S, Etefant D and Schneider C M (2003), *J. Appl. Phys.* 94 4853

[6] Lee J, Kim J H and Im S (2003) *Appl. Phys. Lett.* 83 2689

[7] Snyders R, Wautelet M, Gouttebaron R, Dauchot J P and Hecq M (2003) *Surface. Coat. Technol.* 174 1282

[8] Debal F, Wautelet M, Bretagne J, Dauchot J P and Hecq M (2000) *Plasma Sources Sci. Technol.* 9 152

[9] Mihaila I, Popa G, Anita V, Costin C, Sirghi L and Turcu I (2002) *Le Vide - Science, Technique et Applications* 57 (304) 316 (in French)

[10] Minea T M, Bretagne J, Gousset G, Magne L, Pagnon D and Touzeau M (1999) *Surf. Coat. Technol.* 116 558

Minea T M, Bretagne J and Gousset G (1999) *IEEE Trans. Plasma Sci.* 27 94

[11] Shon C H and Lee J K (2002) *Appl. Surf. Sci.* 192 258

[12] Kondo S and Nanbu K (2001) J. *Vac. Sci. Technol.* A 19 830

Kondo S and Nanbu K (2001) *J. Vac. Sci. Technol.* A 19 838

[13] Nanbu K, Segawa S and Kondo S (1996) *Vacuum* 47 1013

Nanbu K and Kondo S (1997) *Jpn. J. Appl. Phys.* 36 (7B) 4808

[14] Shidoji E, Ohtake H, Nakano N and Makabe T (1999) *Jap. J. Appl. Phys.* 38 2131

Shidoji E, Nakano N and Makabe T (1999) *Thin Solid Films* 351 37

Shidoji E, Ness K and Makabe T (2001) *Vaccum* 60 299

Shidoji E and Makabe T (2003) *Thin Solid Films* 442 27

[15] Hagelaar GJM, Bareilles J, Garrigues L and Boeuf J-P (2002) *J. Appl. Phys.* 91 5592

Garrigues L, Bareilles J, Boeuf J-P and Boyd I D (2002) *J. Appl. Phys,* 91 9521

Hagelaar GJM, Bareilles J, Garrigues L and Boeuf J-P (2003) *J. Appl. Phys.* 93 67

[16] Porokhova I A, Golubovskii Yu B, Bretagne J, Tichy M and Benkhe J F (2001) *Phys. Rev.E* 63 56408

Porokhova I A, Golubovskii Yu B, Holik M, Kudrna P, Tichy M, Wilke C and Behnke J F (2003) *Phys. Rev. E* 68 16401

[17] White R D, Robson R E and Ness K F (2001) *J. Phys. D* 34 2205

[18] Trennepohl Jr W, Bretagne J, Gousset G, Pagnon D and Touzeau M (1996) *Plasma Sources Sci. Technol.* 5 607

[19] Debal F, Bretagne J, Dauchot J P, Hecq M and Wautelet M (2001) *Plasma Sources Sci. echnol.* 10 30

[20] Cramer N F (1997) *J. Phys. D* 30 2573

[21] Bradley J W and Lister G (1997) *Plasma Sources Sci. Technol. 6* 524

Bradley J W (1998) *Plasma Sources Sci. Technol.* 7 572

[22] Minea T (1999) *PhD Thesis* Université Paris-Sud XI Orsay France 14 (in French)

[23] Rossnagel S M and Kaufman H R (1987) *J. Vac. Sci. Technol.* A 5 88

[24] Alves L L, Gousset G and Ferreira C M (1997) *Phys. Rev. E* 55 890

Alves L L, Gousset G and Vallee S (2003) *IEEE Trans. Plasma Sci.* 31 572

[25] Bretagne J, Callede G, Legentil M and Puech V (1986) *J. Phys. D: Appl. Phys.* 19 761

[26] Richards A D, Thompson B E and Sawin H H (1987) *Appl. Phys. Lett.* 50 492

[27] Salabas A, Gousset G and Alves L L (2002) *Plasma Sources Sci. Technol.* 11 448

[28] Ellis H W, Pai R Y, McDaniel E W, Mason E A and Viehland L A (1976) *Atomic Data Nuclear Data Tables* 17 177

[29] Phelps A V (1991) *J. Phys. Chem. Ref. Data* 20 557

[30] Buyle G, De Bosscher W, Depla D, Eufinger K, Haemers J and De Gryse R (2003) *Vacuum* 70 29

[31] Phelps A V and Petrovic Z Lj (1999) *Plasma Sources Sci. Technol.* 8 R21

[32] Auday G, Guillot P, Galy J and Brunet H (1998) *J. Appl. Phys.* 83 5917

[33] Chapman B (1980) *Glow discharge processes* New York: Wiley pp 91

[34] Scharfetter D L and Gummel H K (1969) *IEEE Trans. Electron Devices,* ED-16 64 *y*

[35] Press W H, Teukolsky S A, Vetterling W T and Flannery B P (1992) *Numerical Recipes in Fortran. The Art of Scientific Computing,* Second Edition, Cambridge University Press.

[36] Courant R, Friedrichs K O and Lewy H (March 1967) *IBM J. Res. Develop.* 215

[37] Barnes M S, Colter T J and Elta M E (1987) *J. Appl. Phys.* 61 81