DC magnetron discharge fluid model using a new numerical scheme

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Numerical modelling of an electrical discharge by fluid model can be accomplished through different procedures and approaches. A 2D time-dependent one was applied in order to describe a cylindrical symmetry Argon DC planar magnetron discharge. All transport equations, which means continuity and momentum transfer equations for electrons and ions and electron mean energy transport equation are solved in the same manner, using corrected classical drift-diffusion expressions for fluxes. For the validity of this last approach, the presence of magnetic field has been introduced as a correction in the electronic flux expression, while for ions an effective electric field has been considered. Plasma potential is given by Poisson equation.

1. Introduction

Having a widely spread for applications, like thin films deposition and material sputtering, magnetron discharges were and still are studied experimentally, analytically or numerically, for a better understanding.
For numerical simulations, the fluid model has an advantage upon the computing time, but it looses his validity with pressure decreasing, when the mean free path of charged particles exceeds the characteristic length of the discharge. Although magnetron discharges work at low pressures (1 to tens mtorr), the fluid model can be applied due to the presence of magnetic field that reduces the effective distance covered by electrons between two collisions, thus hydrodynamic hypothesis being fulfilled.
A 2D time-dependent fluid model was applied in order to describe a cylindrical symmetry Argon DC planar magnetron discharge.

2. Model equations

The first three moments of Boltzmann equation, continuity, momentum transfer and mean energy transfer equations (eq. 1-3), are considered for electrons. For ions, only the first two of them were taken into account (eq. 1,2).

$$\frac{\partial n_s}{\partial t}+\nabla\cdot(n_s\vec{v}_s)=f_{iz}n_e \qquad (1)$$

$$m_s n_s\left[\frac{\partial \vec{v}_s}{\partial t}+\left(\vec{v}_s\cdot\nabla\right)\vec{v}_s\right]=q_s n_s(\vec{E}+\vec{v}_s\times\vec{B})-\nabla P_s$$

$$-m_s n_s f_{ms}\vec{v}_s\left(1+\frac{n_e f_{iz}}{n_s f_{ms}}\right) \qquad (2)$$

$$\frac{\partial(n_e\varepsilon_e)}{\partial t}+\nabla\cdot(n_e\varepsilon_e\vec{v}_e)=-\vec{\Gamma}_e\cdot\vec{E}-\theta_e n_e, \qquad (3)$$

where $s = e$ (i) for electrons (ions), n_s is s - type particle density, m_s - mass, v_s - mean velocity, f_{iz} - ionisation frequency, f_{ms} - total momentum transfer frequency between s - type particles and neutrals, $\boldsymbol{E}$ - electric field intensity, $\boldsymbol{B}$ - magnetic field induction, P_s - pressure tensor, q_s- electrical charge ($-e$ for electrons, $+e$ for ions), t - time, ε_e - electron mean energy (eV), θ_e - electron energy loss term in e-neutral collisions. The inertial term $m_e n_e[\partial\vec{v}_e/\partial t+(\vec{v}_e\cdot\nabla)\vec{v}_e]$, from the momentum transfer equation for electrons (eq. 2), was neglected due to their small mass; also, into a first approximation, the ionisation frequency, f_{iz}, was neglected with respect to the total momentum frequency, f_{me}. Under these circumstances, electronic flux can be written as a sum, $\vec{\Gamma}_e=\vec{\Gamma}_{0e}+\vec{\Gamma}_{1e}$, of a flux given by Fick law, $\vec{\Gamma}_{0e}=-\mu_e n_e\vec{E}-\nabla(D_e n_e)$, μ_e, D_e being electron mobility and, respectively, diffusion coefficient and the contribution of magnetic field, $\vec{\Gamma}_{1e}=-n_e\vec{v}_e\times\vec{\Omega}/f_{me}$, considered as a correction for the classical flux, $\vec{\Omega}=e\vec{B}/m_e$ being the cyclotron pulsation. The energy flux is written in the same manner, the transport coefficients, $\mu_{\varepsilon e}$, $D_{\varepsilon e}$, being those specific for energy transport [1]. Both electronic and ionic pressure are considered as scalars, $P_s=n_s kT_s$. For ions, the term $(\vec{v}_i\cdot\nabla)\vec{v}_i$ and the magnetic field influence were neglected, the others being important. For the purpose of writing ionic flux by means of the Fick law, an effective electric field, $\boldsymbol{E}_{eff}$, must be introduced [1].
Electron transport parameters and the energy loss term, depending of mean energy, were calculated according with [1,2] using a Maxwellian electron distribution function. Ion transport parameters were taken constant, corresponding to the gas temperature [3].
Poisson equation is included to obtain plasma potential and electric field.
Boundary conditions for charged particle fluxes and potential must be imposed. All parallel fluxes with respect of any surface are zero. Normal electronic flux to the surface must verify $\Gamma_e^{\perp}=n_e\langle v_e\rangle/2$ [1]. At the cathode surface, two different cases were considered: the flux is given only by secondary emission, characterized by γ coefficient, $\Gamma_e^{\perp}=-\gamma\Gamma_i^{\perp}$, or the drift-diffusion component is also taken into account,

$\Gamma_e^{\perp}=n_e\langle v_e\rangle/2-\gamma\Gamma_i^{\perp}$. The same boundary conditions are available for electron energy transport by changing $\langle v_e\rangle$ with $\langle \varepsilon_e v_e\rangle$ and taking an energy of 1 eV for secondary electrons emitted at the cathode. Normal ion flux is given by $\Gamma_i^{\perp}=n_i v_{thi}/4+\delta\mu_i n_i E_{eff}^{\perp}$, where v_{thi} is ionic thermal velocity, and δ is 1 if $E_{eff}^{\perp}$ is directed to the surface, 0 if contrarily.

3. Numerical solution

Space grid was chosen bi-dimensional (r,z) due to the magnetron reactor cylindrical symmetry. Fluxes expressed by Fick law are discretized using the Scharfetter-Gummel exponential scheme [4]. Electronic flux given by eq. (2) is introduced in continuity eq. (1), which, together with eq. (3), are integrated using a semi-implicit algorithm. The classical drift-diffusion flux $\overrightarrow{\Gamma_{0e}}$ is kept in the left side term of the equation, while the flux correction $\overrightarrow{\Gamma_{1e}}$ is introduced on the right side of the equation, as a source term, calculated at the beginning of every time step. The ion flux having a drift-diffusion expression, ions continuity equation, as well as Poisson equation, can be integrated using an implicit method. All equations are discretized and linearized using a finite difference scheme and they are numerically solved by direct band matrix method [5], taking into account the boundary conditions.

4. Results and conclusions

The model was applied for a cylindrical symmetry Argon DC planar magnetron discharge, with a metallic cathode (r_{cath} = 16.5 mm) and metallic walls as grounded anode ($R_{max} = Z_{max}$ = 26.95 mm). For a –200 up to –500 V voltage applied on the cathode, neutrals pressure varies between 5-30 mtorr, for a 300-350 K temperature. Magnetic field map in front of the cathode is obtained according to [6]. To illustrate one of the results, spatial discharge potential distribution is given in *fig. 1* for p_{Ar} = 20 mtorr, T_{Ar} = 350 K, V_{cath} = -200 V.

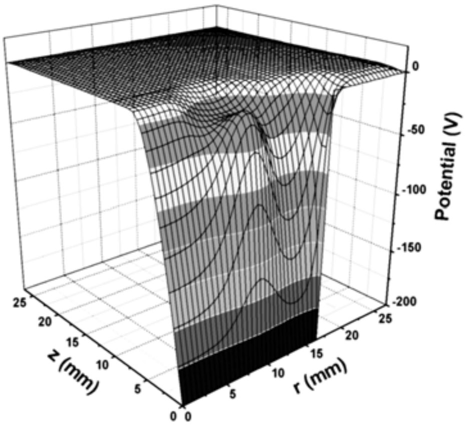

Fig. 1. Potential distribution (p_{Ar} = 20 mtorr, T_{Ar} = 350 K, V_{cath} = -200 V)

The secondary emission coefficient, γ, was set to 0.2. Treating the presence of magnetic field as a flux correction for electrons seems to be a valid approach. Much more, any other neglected term in eq. (2) can be introduced in the same manner, the advantage being an easy way for linearizing and solving eq. (1) and (3) by taking into account in the left side term only a drift-diffusive form flux. Finally, according to *fig. 2*, the term f_{iz}/f_{me} exceeds 5% for electron energy higher than 10 eV, then it will be considered in electron momentum transfer equation afterwards.

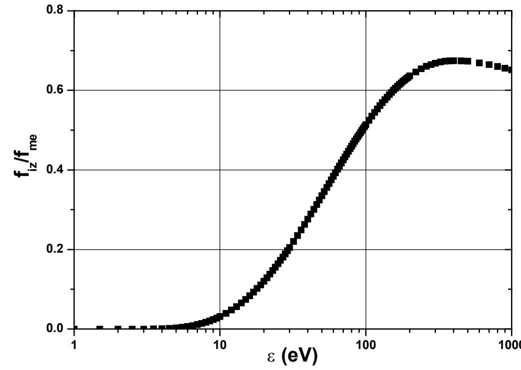

Fig. 2. The ratio between ionisation frequency and total momentum transfer frequency e-Argon neutrals

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6. References

[1] A. Salabas, G. Gousset, L.L. Alves, *Plasma Sources Sci. Technol.* **11**, pp 448 (2002)
[2] L. L. Alves, G. Gousset and C. M. Ferreira, *Phys. Rev. E* **55** (1), pp 890 (1997)
[3] A. V. Phelps, *J. Appl. Phys.* **76** (2), pp 747 (1994)
[4] D. L. Scharfetter and H. K. Gummel, *IEEE Trans. Electron Devices,* **ED-16,** pp64 (1969)
[5] W. H. Press, S. A. Teukolsky, W. T. Vetterling, B.P. Flannery, *Numerical Recipes in Fortran. The Art of Scientific Computing*, Second Edition, Cambridge University Press (1992)
[6] Tiberiu Minea, *Thèse*, Université Paris-Sud XI, France (1999)