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Numerical Simulation of a Microwave Argon PACVD Plasma Reactor at Low Pressure

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Abstract: ***Discharge characteristics of argon microwave plasma were investigated by using fluid simulation of a MPACVD (Microwave Plasma Assisted Chemical Vapor Deposition) reactor based on finite elements method at low pressure (25-250) Pa. The microwave power was 2.45 GHz TM mode transmitted through the resonant cavity. Microwave power and pressure were considered simulation parameters and argon was used for working gas. A self-consistent fluid model was developed in Comsol Multiphysics Plasma Module for studying the discharge phenomena. The 2D plasma fluid model gives a complete description of spatial-and time evolution of the discharge characteristics such us: electron density and electron temperature. Simulation results show a strong effect of input parameters on the species densities distribution in the plasma.***

Keywords: Finite element method, COMSOL MWP module, microwave plasma, plasma fluid model

1. Introduction

The MPACVD processes involve many complex and highly coupled phenomena. Thus, the numerical simulation is an indispensable tool to understand the plasma behavior inside the reactor, and to improve the knowledge of deposition or etching **[1, 2, 3]**.

We choose the plasma fluid model to characterize the plasma due to his flexibility and speed of computations **[4, 5]**. Plasma fluid model allows us to estimate the time-variation of electron density and electron temperature. These quantities are crucial to characterize the plasma and its applications in syntheses or surface treatment **[6]**.

In this present work, we applied the finite element method for numerical simulation of a pure argon discharge characteristics in a MPACVD reactor using COMSOL Multiphysics software. The main objective of this work is to understand the diverse transfer phenomena related to species existing in this type of discharge in order to control these phenomena and predict the physicochemical properties of the microwave discharge.

The paper is organized as follow, equations solved with the fluid plasma model are considered in section 2 while section 3 shows the plasma chemistry. Section 4 is devoted to describe the geometry modeled. In section 5, the numerical results and discussion are presented. Finally, we kept section 6 for a conclusion.

2. Model Description

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy.

Convection of electrons due to fluid motion is neglected **[6, 7]**:

- Electron density equation:

$$\frac{\partial n_e}{\partial t} + \nabla.\mathbf{\Gamma_e} = R_e - (\mathbf{u}.\nabla)n_e \tag{1}$$

$$\mathbf{\Gamma_e} = -(\boldsymbol{\mu_e}.\mathbf{E})n_e - \mathbf{D_e}.\nabla n_e \tag{2}$$

- Mean electron energy equation:

$$\frac{\partial n_\varepsilon}{\partial t} + \nabla.\mathbf{\Gamma_\varepsilon} + \mathbf{E}.\mathbf{\Gamma_e} = R_\varepsilon \tag{3}$$

$$\mathbf{\Gamma_\varepsilon} = -(\boldsymbol{\mu}_\varepsilon.\mathbf{E})n_\varepsilon - \mathbf{D}_\varepsilon.\nabla n_\varepsilon \tag{4}$$

- Poisson's equation:

$$\mathbf{E} = -\nabla V \tag{5}$$

Where n_e denotes the electron density $(1/m^3)$, R_e is the source term (electron rate expression) in unit $(1/(m^3.s))$, $\mathbf{u}$ is the electronic speed vector (m/s), $\mathbf{\Gamma_e}$ is the electron flux $(1/(m^2.s))$, μ_e is the electron mobility $(m^2/(V.s))$, $\mathbf{E}$ is the electric field (V/m), D_e is the electron diffusivity (m^2/s), n_ε denotes the electron energy density (V/m^3), R_ε is the energy loss/gain due to inelastic collisions $(V/\ (m^3.s))$, $\mathbf{\Gamma_\varepsilon}$ is the electron energy flux $(1/\ (m^2.s))$, μ_ε is the electron energy mobility $(m^2/(V.s))$, D_ε is the electron energy diffusivity (m^2/s) and V is the electric potential (Volt).

The following relationships hold **[7, 8]** for Maxwellian electron energy distribution function:

$$D_e = \mu_e T_e \tag{6}$$

$$D_\varepsilon = \mu_\varepsilon T_e \tag{7}$$

$$\mu_\varepsilon = \left(\frac{5}{3}\right)\mu_e \tag{8}$$

T_e is the electron temperature (eV) depending on the mean electron energy, it is defined as:

$$\tilde{\varepsilon} = \frac{n_\varepsilon}{n_e} \tag{9}$$

$$T_e = \left(\frac{2}{3}\right)\tilde{\varepsilon} \tag{10}$$

The source coefficients in the above equations are determined by the plasma chemistry using rate coefficients. Suppose that there are *M* reactions which contribute to the growth or decay of electron density and *P* inelastic electron-neutral collisions. In general *P* >> *M*. In the case of rate coefficients, the electron source term is given by:

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e \quad (11)$$

Where x_j denotes the mole fraction of the target species for reaction j, k_j is the rate coefficient for reaction j (m^3/s) and N_n is the total neutral number density ($1/m^3$).

The energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_\varepsilon = \sum_{j=1}^{M} x_j k_j N_n n_e \Delta\varepsilon_j \quad (12)$$

Where $\Delta\varepsilon_j$ is the energy loss from reaction j (eV).

The rate coefficients k_k may be computed from cross section data by the following integral [5]:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon \quad (13)$$

Where $\gamma = \left(\frac{2q}{m_e}\right)^{1/2}$ in unit $(C/kg)^{1/2}$, m_e is the mass of the electron (kg), ε is the energy (eV), σ_k is the collision cross section, and $f(\varepsilon)$ is the electron energy distribution function (EEDF). In this case a Maxwellian EEDF is assumed.

The boundary conditions of the present model on the walls of metal reactor are:

$$n_e = 0\ m^{-3} \quad ; \quad V = 0\ Volt \quad ; \quad T_e = 0\ eV \quad (14)$$

$$\mathbf{n} \times \mathbf{E} = 0 \quad (15)$$

3. Plasma Chemistry

The chemical mechanism for the plasma consists of only 3 species and 7 reactions **[7]**:

- Elastic reaction:
  e + Ar => e + Ar $(\Delta\varepsilon = 0eV)$
- Excitation reaction:
  e + Ar => e + Ars $(\Delta\varepsilon = 11{,}5eV)$
- Superelastic reaction:
  e + Ars => e + Ar $(\Delta\varepsilon = -11{,}5eV)$
- Ionization reaction:
  e + Ar => 2e + Ar+ $(\Delta\varepsilon = 15{,}8eV)$
  e + Ars => 2e + Ar+ $(\Delta\varepsilon = 4{,}24eV)$
- Penning ionization:
  Ars + Ars => e + Ar + Ar+
- Metastable quenching:
  Ars + Ar => Ar + Ar

Stepwise ionization can play an important role in sustaining low pressure argon discharges. Excited argon atoms are consumed via superelastic collisions with electrons, quenching with neutral argon atoms, ionization or Penning ionization where two metastable argon atoms react to form a neutral argon atom, an argon ion and an electron. The latest reaction is responsible for heating of the argon gas. The 11.5eV of energy which was consumed in creating the electronically excited argon atom is returns to the gas as thermal energy when the excited metastable quenches. In addition to volumetric reactions, the following surface reactions are implemented:

Ars => Ar and Ar+ => Ar

When a metastable argon atom makes contact with the wall, it will revert to the ground state argon atom with some probability (the sticking coefficient).

4. Geometry Modeled

The plasma is maintained by an electromagnetic wave (2.45GHz) that propagates into a cylindrical waveguide in TM mode. Here we are interested on the interaction of the electromagnetic wave with the argon gas inside the microwave cavity reactor. The MPACVD reactor was simulated in 2D space geometry as shown in Figure 1.

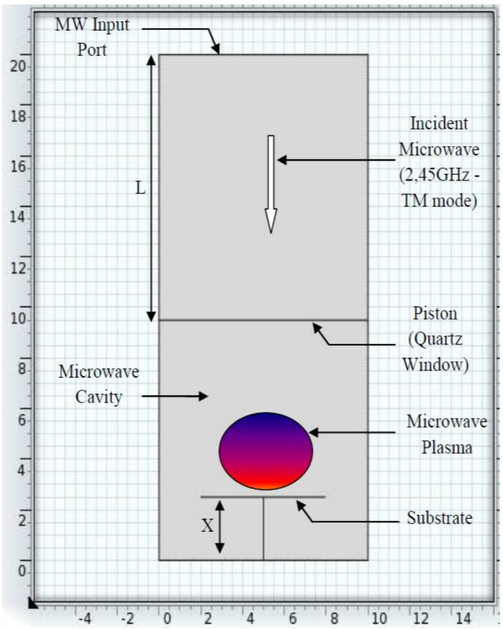

Figure 1: The diagram of 2D geometry modeled

5. Numerical Results and Discussions

The simulation results shown in this section were all performed in the geometry presented in the Figure 1. The pressure of the simulated Ar gas was in the range (25-250) Pa.

5.1 Impact of Piston and Substrate Positions

The spatial distribution of electron density for different values of parameters X (substrate position) and L (piston position) is studied. It is necessary to adjust simultaneously the parameters X and L, in order to maintain the plasma volume and to control its location. The best frequency response of power output is obtained for X=25mm and L=105mm. In this case the coupling is up to 2.45 GHz **[9]**. Figure 2 shows the form and location of plasma discharge obtained in these conditions at an input power of 1kW and gas pressure of 3mTorr.

The electric field cartography in the plane of the substrate holder is also calculated and presented in Figure 3. It is shown that electric field is consistent and azimuthally directed parallel to the cylinder axis. So it's a TM mode.

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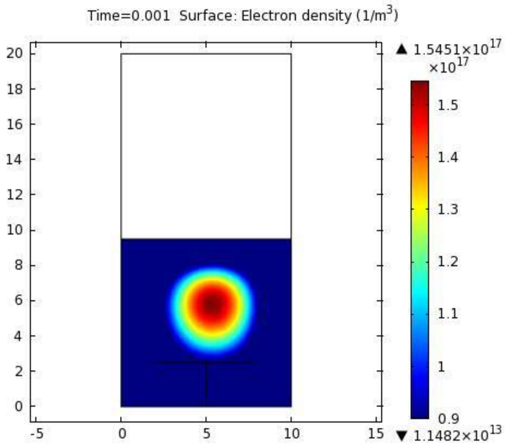

Figure 2: Spatial distribution of the electron density after 0,001s for 1kW input power at 3mTorr

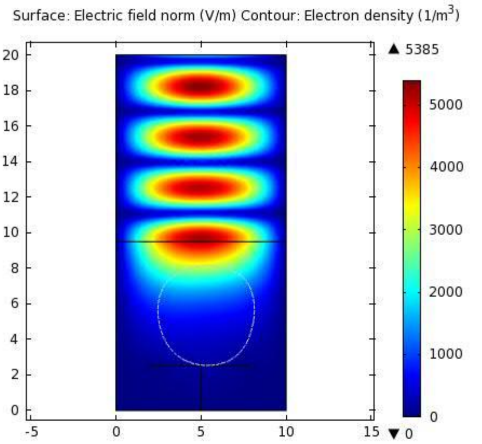

Figure 3: Simulated electric field norm distribution after 0,001s with 3mTorr argon pressure for 1kW input microwave power

5.2 Impact of Microwave Power and Gas Pressure on Electron Density

The MWP module developed in this study provides the effect of the input parameters such as microwave power and gas pressure on the plasma discharge characteristics. The electron density in argon plasma discharge is plotted as a function of the incident microwave power, as shown in Figure 4. Results indicate that, at a given gas pressure, electron density increases linearly with microwave power. For example, at a pressure of 1.95Torr, the electron density increases from 7.84x10^{17} m^{-3} to 2.76x10^{18} m^{-3} when the incident power increases from 400W to 1600W.

We can also note that, at given incident power, electron density increases with increase of gas pressure to 2.25Torr. If the pressure is further increased (beyond 2.5Torr), the electron density decreases. This behavior is better presented in Figure 5, representing plasma density as function of gas pressure for several microwave powers.

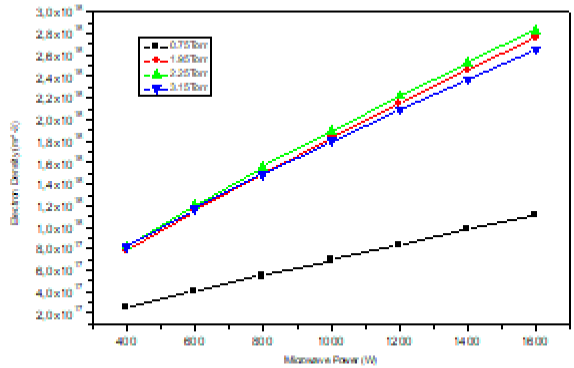

Figure 4: Dependence of electron density on microwave power for different argon pressure at 19mm above the substrate

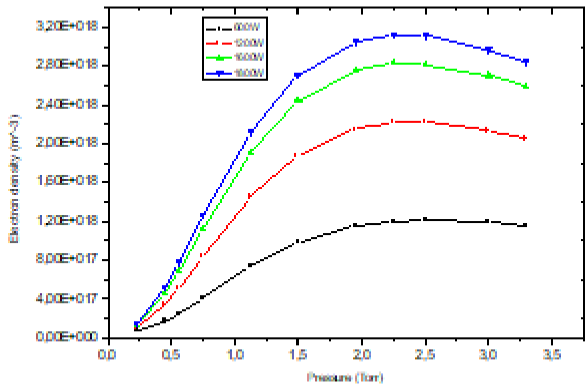

Figure 5: Dependence of electron density on argon pressure for different incident power at 19mm above the substrate

It is clearly seen that, keeping the positions of substrate and piston constant, we should adjust simultaneously the pressure and the incident power, in order to maintain the plasma discharge volume and to control its location inside the cavity.

5.3 Impact of Microwave Power and Gas Pressure on Electron Temperature

The evolution of the electron temperature as function of incident microwave power for several pressures of argon gas is shown in Figure 6.

The numerical results show that electron temperature decreases by increasing incident power. While, the electron temperature decreases with the pressure at a constant incident power. This can be understood since increasing of gas pressure causes augmentation of collision frequency for electrons with neutrals. Therefore electrons more easily transfer their energy to neutral particles and reduce their kinetic energy **[10, 11]**.

On the other hand, the electron temperature decrease by increasing of the microwave power is due to the presence of an ionizing mechanism by step in argon plasma discharge which becomes significant when electron density exceeds $10^{17} m^{-3}$ and it may play a lead role above $10^{18} m^{-3}$ **[9, 12]**.

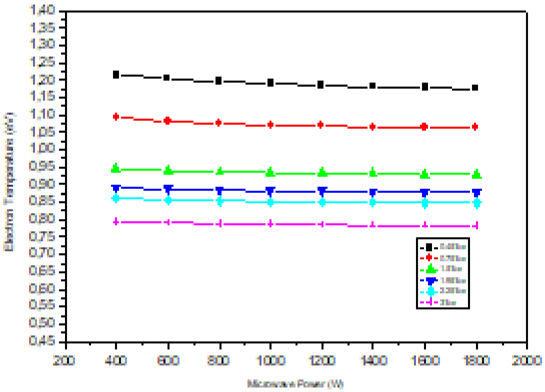

Figure 6: Dependence of electron density on argon pressure for different incident power at 19mm above the substrate

6. Conclusion

In this paper, a fluid plasma model for simulating argon microwave plasma characteristics was performed. The simulation results were obtained at low pressures by solving the electron density equation, mean electron energy equation and Poisson's equation. The governing equations are solved in two-dimensional geometry using the finite element method. The effect of substrate and piston positions is clearly illustrated in order to maintain the plasma volume and to control its location. Numerical results have allowed us to study the effect of operating input parameters, especially gas pressure and microwave incident power on the characteristics of the plasma discharge such as: electron density, electron temperature and plasma volume. The calculated simulation results showed a good satisfactory agreement with experimental and numerical results.

References

[1] D. Benyoucef, Modélisation Particulaire et Multidimensional des Décharges Hors Equilibre à Basse Pression Excités par Champs Electromagnétiques", Ph.D. dissertation, Dept Elect. Eng, Toulouse III – Paul Sabatier Univ, 2011.
[2] J. van Dijk, G. M. W. Kroesen, A. Bogaerts, "Plasma Modelling and Numerical Simulation", *J. Phys. D: Appl. Phys*. 42, (14pp): 190301, 2009.
[3] M. El Bojaddaini, H. Chatei, M. Atounti, M. El Haim, I. Driouch, M. El Hammouti, "Numerical Simulation of Hydrogen Microwave Plasma Discharge Using a Fluid Model Approach", *Applied Mathematical Sciences*, Vol. 6, no. 121:6003-6019,2012.
[4] M. El Haim, "Modélisation Numérique et Caractérisation des Décharges Micro-ondes : Application aux Réacteurs MPACVD", Ph.D. dissertation, Mohammed 1st Univ, Oujda, Morocco, 2015.
[5] O. C. Zienkiewicz, R. L. Taylor, *"the Finite Element Method, Butterworth Heinemann",* 5th Edition, 2000.
[6] G. J, M. Haagelaar, L. C. Pitchford, "Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models", Plasma sources Sci. Technol. 14: 722-733, 2005.
[7] V. E. Golant, A. P. Zhilinsky, I. E. Sakharov, "Fundamentals of Plasma Physics", (Wiley, New York), 1980.
[8] S. Pancheshnyi, S. Biagi, M. C. Bordage, et al., "The LXCat Project: Electron Scattering Cross Sections and Swarm Parameters for Low Temperature Plasma Modeling", *Chemical Physics* 398:148-153, 2012.
[9] L. Latrasse, "Conception, Caractérisation et Applications des Plasmas Micro-onde en Configuration Matricielles", Ph.D. dissertation, Université Joseph Fourier, 2006.
[10] W. Tan, T. A. Grotjohn, "Modeling the Electromagnetic Field and Plasma Discharge in Microwave Plasma Diamond deposition Reactor", *Diamond and Related Materials* 4, 1145-1154, 1995.
[11] M. Moisan and J. Pelletier, "Physique des Plasmas Collisionnels : Application aux Décharges Hautes Fréquences", pp 217-9, *Grenoble : EDP Sciences*, 2006.

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