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EFFECT OF PLASMA DISCHARGE PARAMETERS ON CONTROL OF SILICON NITRIDE THIN FILMS DEPOSITION

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Abstract- This research is dedicated to the comprehensive two-dimensional (2D) simulation of radiofrequency (RF) plasma discharge, specifically under the conditions of low temperature and low pressure. The investigation delves deep into the intricate transport phenomena taking place during the deposition processes involved in creating silicon nitride thin films. A series of simulations is employed to analyze the impact of pressure, voltage, and excitation frequency on crucial plasma discharge characteristics, such as electron density, electron temperature, and ionic flux. The primary goal is to discern optimal values for these parameters that contribute to an enhanced deposition process. The outcomes of the study highlight that the most advantageous conditions involve a pressure set at 0.7 Torr, a voltage of 100 V, and a frequency of 100 MHz. Employing these optimal parameters not only facilitates an increased deposition rate of silicon nitride thin films but also ensures the preservation of surface quality. The significance of these findings lies in their potential to optimize the deposition process and enhance the quality of the resulting thin films in low-temperature, low-pressure RF plasma discharge scenarios.

Keywords: 2D Simulation, RF Plasma Discharge CCP, Reactor, Silicon Films, Deposition Rate.

1. INTRODUCTION

Silicon nitride has garnered significant attention owing to its favorable physical attributes. With excellent high temperature resistance, high hardness, resistance to degradation, chemical inertness, superb thermal shock resistance, low internal stress, low coefficient of friction, and high dielectric strength, it proves to be well-suited for diverse applications including engine components, cutting tools, and micro-electronic devices [1, 2]. The capacitive coupled plasma reactor (CCP) is widely used for etching and deposition of silicon nitride materials [3,4]. The CCP reactor integrates various processes during deposition, including the generation of electrical charges, fluid flow, and chemical reactions on the surface [5]. These processes are mathematically described by a set of nonlinear and dispersive differential equations [6, 7].

In tackling this system of equations, 2D simulations prove especially valuable as they enable the examination of plasma discharge evolution on the radial (r) and axial (z) [8, 9]. Numerous studies have leveraged this approach, including the works [10-12]. To improve the performance of RF deposition we must study the effect of physicochemical parameters on the evolution of the plasma discharge characteristics [13-16] and on the rate of deposition [17, 18], whose goal is to reduce the production costs and increase process throughput and substrate size.

T. Novikova, et al. [17] demonstrated that, in a CCP reactor with RF discharge of hydrogen, adjusting the excitation frequency and pressure serves as a means to enhance the deposition rate. M. Bavafa, et al. [18] highlighted the substantial impact of pressure variation on the uniformity of the deposited layer. Additionally, T. Lafleur, et al. [19] observed that an increase in frequency leads to a higher deposition rate of hydrogenated silicon without compromising film properties. Furthermore, S. Sharma, et al. [20] established that manipulating the applied voltage and control frequency offers an independent means to control ion density and energy in a low-pressure CCP device, with potential benefits for plasma processing applications.

Our aim is to explore the optimal values for pressure, voltage, frequency, and ionic flux in a silicon nitride RF plasma discharge. This investigation seeks to achieve a more uniform deposition of silicon thin films without compromising surface integrity. We adopt a 2D hybrid macroscopic-microscopic model that describes the characteristics of the silicon nitride plasma in different regions of the discharge. The source terms are formulated by considering the most reactive chemical reactions that take place during the process. The differential equations associated with the numerical model are resolved using the finite element method. We show the results of of RF plasma discharge of silicon nitride simulation, for sinusoidal voltage amplitude V_0 in the range 100 to 160V, a pressure p in the range 0.3 to 0.7 Torr and a frequency f_{RF} in the range 13.56 to 100 MHz. By systematically altering these parameters, we conducted a comprehensive examination and comparison of the two-dimensional evolution of discharge characteristics.

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Our investigation extended to a final computation time, ensuring stability in the system. This allowed us to analyze how changes in these key parameters influence the overall behavior of the discharge over an extended period, providing valuable insights into the stability and dynamics of the system. This study is structured as follows: Section 2 provides an in-depth explanation of the deposition model, utilizing a capacitive coupled plasma reactor. In Section 3, the results of the 2D evolution are presented, highlighting the electron density, temperature and ionic flux, and the comprehensive discussion on how pressure, voltage, and frequency influence both the plasma discharge and ion flux. The study concludes with final remarks in Section 4.

2. SIMULATION MODEL

2.1. Plasma Equations

Within this section, our focus lies in examining the dynamic evolution of key features in the silicon nitride plasma discharge in CCP reactor. We systematically manipulate the pressure, voltage, and frequency variables to explore their influence on electron density, temperature and ionic flux of the RF plasma discharge. The overarching objective is to elucidate and discuss the intricate interplay of these parameters, shedding light on the discharge mechanism as it varies with each parameter. Through this analysis, we aim to gain insights that will facilitate the enhancement of the discharge rate in the CCP reactor while preserving the integrity of the surface.

The formalism used in this work is based on the density transport equations for charged species as Equations (1) and (2), the energy and momentum transport equations for electrons as Equations (3)-(6) coupled with the Poisson Equation (7) [21]. In these equations, the densities and energy are expressed macroscopically, while the source terms are calculated from the distribution function and the corresponding cross sections as Equations (8)-(10). In our 2D simulations of low-temperature cold plasma, we have employed a physical framework grounded in Equations (1)-(7). This scheme assumes variations in density and energy r along and z directions, incorporating the assumptions outlined in [20, 22].

$$\frac{\partial n_e}{\partial t} + \nabla\Gamma_e = S \quad (1)$$

$$\frac{\partial n_i}{\partial t} + \nabla\Gamma_i = S \quad (2)$$

$$\frac{\partial n_\varepsilon}{\partial t} + \nabla\Gamma_\varepsilon + E\Gamma_e = S_\varepsilon \quad (3)$$

$$\Gamma_e = -n_e\mu_e E - \nabla\left(n_e D_e\right) \quad (4)$$

$$\Gamma_i = -n_i\mu_i E - \nabla\left(n_i D_i\right) \quad (5)$$

$$\Gamma_\varepsilon = -n_\varepsilon\mu_\varepsilon E - \nabla\left(n_\varepsilon D_\varepsilon\right) \quad (6)$$

$$\nabla E = \frac{e}{\varepsilon_0}\left(n_i - n_e\right) \quad (7)$$

The set of equations employed has been specifically formulated for a two-dimensional resolution using the finite element method, applied on a compact domain. This system encompasses comprehensive boundary and initial conditions chosen to guarantee the existence and uniqueness of the solution. The finite element method, employed in this context, enables a robust and accurate resolution of the system within the specified domain, ensuring the reliability and stability of the solution throughout the simulation [23], where, $\mu_i = \frac{Z_i}{m_i v_{iN}}$, $D_e = \frac{k_B T_e}{m_e v_{eN}}$, $D_i = \frac{k_B T_i}{m_i v_{iN}}$ $n_\varepsilon = n_e\varepsilon$ and $D_\varepsilon = n_e D_e$.

The computation of the source terms of Equations (8)-(10) in the fluid model relies on the utilization of the electron energy distribution function $f_0(\varepsilon)$ and the cross sections $\sigma_r(\varepsilon)$ [5]. These cross sections account for the most reactive collisions as detailed in our previous work [3]. This comprehensive approach ensures a thorough consideration of the dynamic interactions within the system, incorporating essential collision mechanisms of plasma discharge.

$$S = \sum x_r k_r N_n n_e \quad (8)$$

$$S_\varepsilon = \sum x_r k_r N_n n_\varepsilon \quad (9)$$

$$k_r = \sqrt{\frac{2e}{m_e}} \int \varepsilon\sigma_r\left(\varepsilon\right) f_0\left(\varepsilon\right) d\varepsilon \quad (10)$$

The simulation integrates cross sections data for SiH_4 NH_3 collisions obtained from the Hayashi database [24]. This database provides crucial information about the collision characteristics between these molecules, contributing to the accuracy of the simulation results. In this study, we focus on specific chemical species [3], acknowledging their significant role in plasma chemistry and their pronounced impact on the deposition process [13, 14]. The inclusion of these species in our analysis is crucial for capturing the intricacies of the chemical interactions that govern the deposition dynamics within the plasma system.

2.2. Boundary Conditions

For Poisson's Equation (7), the boundary condition involves specifying the electrical potential values on the electrodes [16, 17].

- At the cathode: $V_0 = 0$, anode: $V_{rf} = V_0 \sin(2\pi f_{RF} t)$

$$\Gamma_e = \frac{v_{th} n_e}{2} - \gamma\Gamma_i \quad (11)$$

$$\Gamma_i = \mu_i n_i \nabla V \quad (12)$$

where, $v_{th} = \sqrt{\frac{8 k_B T_e}{\pi m_e}}$.

$$\Gamma_\varepsilon = \frac{5 n_\varepsilon v_{th}}{6} - \gamma\varepsilon_i\Gamma_i \quad (13)$$

These conditions are essential in governing the behavior of charged particles within the system and are integral to achieving accurate simulation results.

2.3. Geometry Reactor

The two-dimensional numerical model used in this study simulates the operation of the RF discharge inside a capacitive coupled plasma (CCP) reactor under a wide range of physical and numerical conditions. The model serves as a tool for determining the key dimensions and operational parameters that influence the discharge. To increase computational efficiency, a rectangular geometry (*r* and *z*) of an axisymmetric nature is adopted, in which only one half of the reactor is explicitly modeled.

Figure 1 illustrates the geometry of the computational domain. The inter-electrode distance is set at approximately d=2.7×10^{-2} m. To improve convergence over a wide range of parameter values, a refined triangular mesh is used at the edges of the computational domain. This geometric configuration optimizes the simulation process, enabling a complete understanding of landfill behavior while minimizing computational requirements.

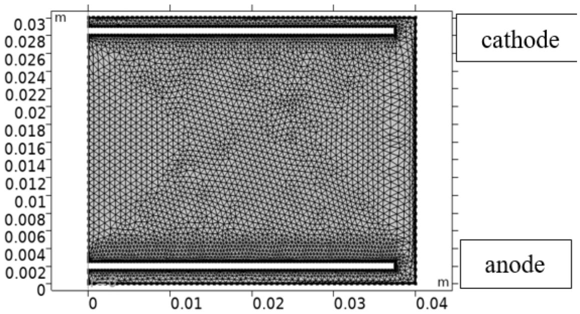


Figure 1. The structure of the computational domain

5. SIMULATION RESULTS

In large area plasma sources, the most difficult problem is to maintain deposition uniformity on the substrate surface; this is directly dependent on the distribution of fundamental plasma characteristics and ion flux. The (CCP) reactor is animated by a sinusoidal voltage with a frequency f_{RF} at a temperature of 500K. The deposition precursor utilized in this simulation consists of a mixture of silane (SiH_4) diluted with ammonia (NH_3). The RF voltage is applied to the anode at a pressure p and an inter-electrode distance d. In this section, we unveil the outcomes of the numerical simulation illustrating the RF plasma discharge characteristics during the deposition of silicon nitride. The reactor's operation is propelled by a sinusoidal voltage with an amplitude V_0 in the range 100 to 160V, pressure p in the range 0.3 to 0.7 Torr and frequency f_{RF} in the range 13.56 to 100 MHz.

Figures 2-4 represent the influence of the pressure on the density, electronic temperature and ion flux. Figure 2 shows the two-dimensional evolution of the electron density, varying the pressure from 0.3 to 0.7 Torr. Looking at this figure, we notice that the electron density shows a high concentration in the plasma region in contrast to the sheath region (as already presented in the one-dimensional evolution [13]). Moreover, the maximum density is 1.89×10^{15} cm^{-3} for 0.3 Torr pressure, 3.99×10^{15} m^{-3} for 0.5 Torr and 4.8×10^{15} m^{-3} for 0.7 Torr pressure. We can notice that the increase of the pressure influences more strongly the collision frequency between the species and consequently increases the electronic density.

Figure 3 shows that the electronic temperature exhibits a strong gradient at the anode. Comparison of the electronic temperature evolution, in the pressure range 0.3 to 0.7 Torr, does not reveal a large difference, moreover, the maximum temperatures at the surface for the three pressures are close 14.7 eV, 15.3 eV and 15.1 eV, respectively. This general trend is in agreement with the experimental results reported in [17, 18].

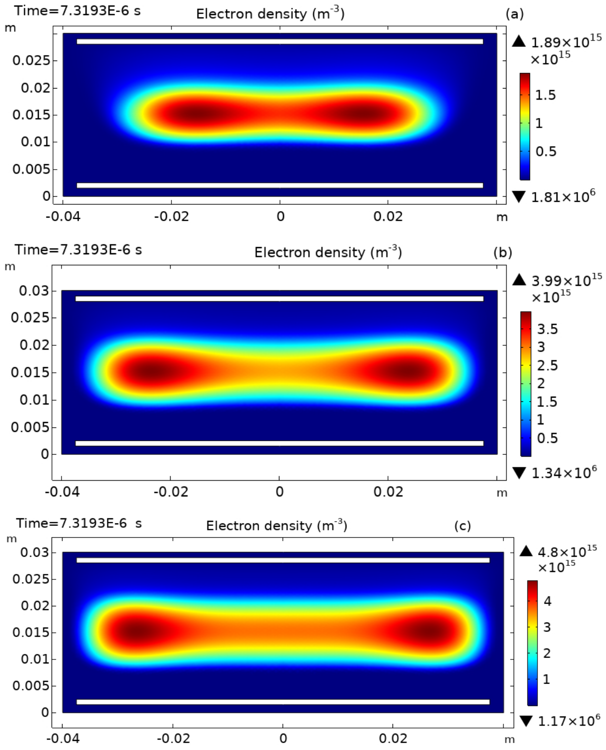


Figure 2. 2D Evolution of electron density (m^{-3}) in CCP reactor for pressures (a) 0.3 Torr, (b) 0.5 Torr and (c) 0.7 Torr

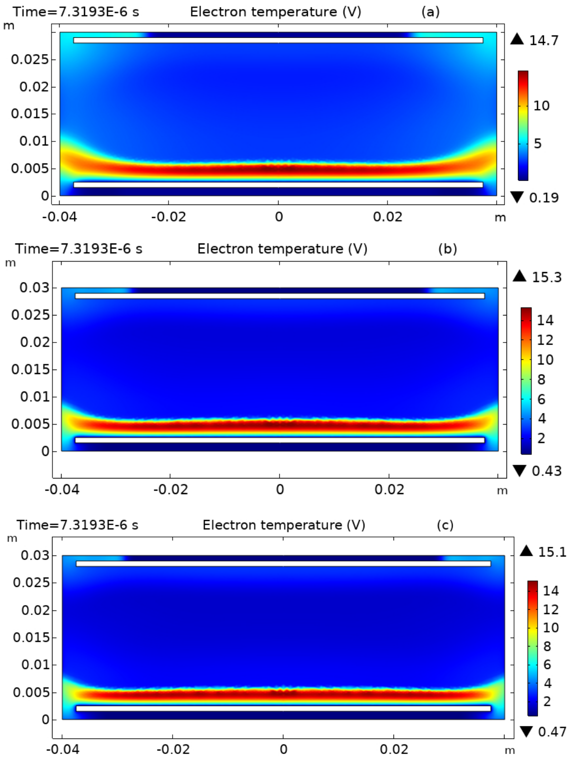


Figure 3. 2D Evolution of electron temperature (eV) in CCP reactor for pressures of, a) 0.3 Torr, b) 0.5 Torr, c) 0.7 Torr

Figure 4 illustrates that in the anodic region the ion flux registers zero due to the absence of collisions among particles. As the system transitions into the plasma mass phase, there is a noticeable race in the ion flux, attributed to the heightened ionization of the gas during this stage. Upon reaching the cathodic region, the ion flux attains its maximum (absolute value). We note that the ion flux rises slowly when the pressure increases from 0.3 to 0.7 Torr. We conclude that the variation of the pressure influences the evolution of the ion flux.

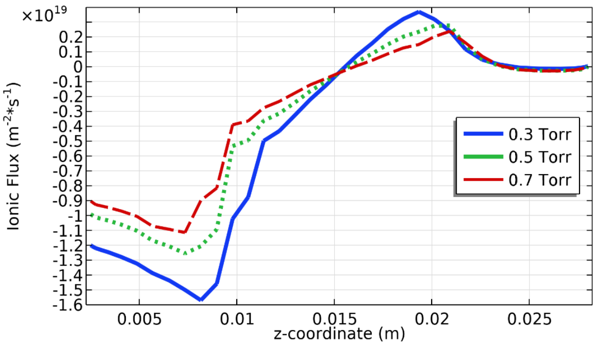
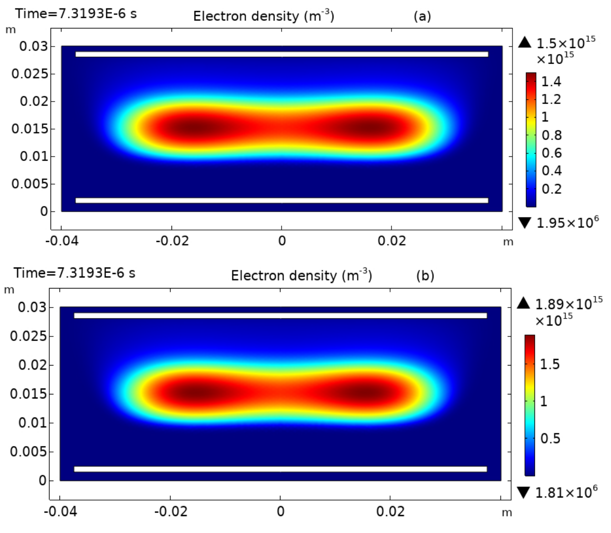


Figure.4. Evolution of ion flux (m^{-2}s^{-1}) in CCP reactor pressures of 0.3 Torr, 0.5 Torr and 0.7 Torr

We now vary the initial voltage of the discharge in a range between 100 and 160 V and keeping the pressure and frequency constant (0.3 Torr and 13.56 MHz, respectively). Figures 5-7 show the evolution of the density, the electron temperature and the ionic flux respectively. Figure 5 shows that the maximum densities of the discharge by applying the voltages 100 V, 130 V and 160 V are 1.5×10^{15} m^{-3}, 1.89×10^{15} m^{-3} and 2.41×10^{15} m^{-3} respectively. We can see that the electron density increases with increasing voltage, which improves the deposition rate. Also, the maximum surface temperature, Figure 6, increases remarkably 9.63 eV, 14.7 eV and 20 eV, respectively. However, such an increase in temperature increases the reactivity of the particles which can lead to the deterioration of the surface.



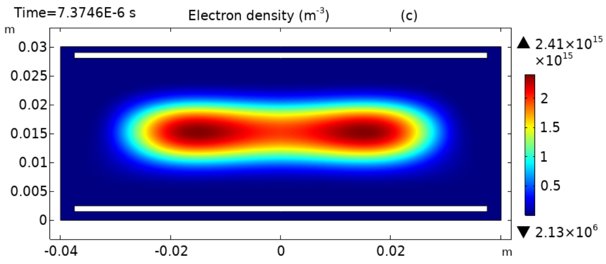


Figure 5. 2D Evolution of electron density (m^{-3}) in CCP reactor for voltages of a) 100 V, b) 130 V, c) 160 V

Ion flux is shown in Figure 7 for voltages of 100 V, 130 V and 160 V. An increase in anode voltage is accompanied by a corresponding increase in ionic flux (absolute value), showing a beneficial trend for thin-film deposition quality. This observation underlines the positive impact of higher voltages on ionic flux enhancement, thus contributing to improved thin film deposition quality. Figures 8-10 represent the influence of the excitation frequency on the density, electronic temperature and ion flux.

Figure 8 shows that the largest increase in the maximum density is a value of 2.58×10^{16} m^{-3} corresponds to the frequency 100 MHz. In addition, it can be seen that a change in frequency from 13.56 MHz to 50 MHz resulted in an increase in the density value from 1.89×10^{15} m^{-3} to 1.43×10^{16} m^{-3}. Figure 9 shows a strong decrease in temperature presented by a value of 4 eV at the surface for the frequency 100 MHz. Concerning the frequencies 13.56 MHz and 50 MHz, respectively we notice a decrease from 14.7 eV to 15 eV (as a maximum value). Therefore, when the frequency rises to 100 MHz the temperature at the surface decreases significantly.

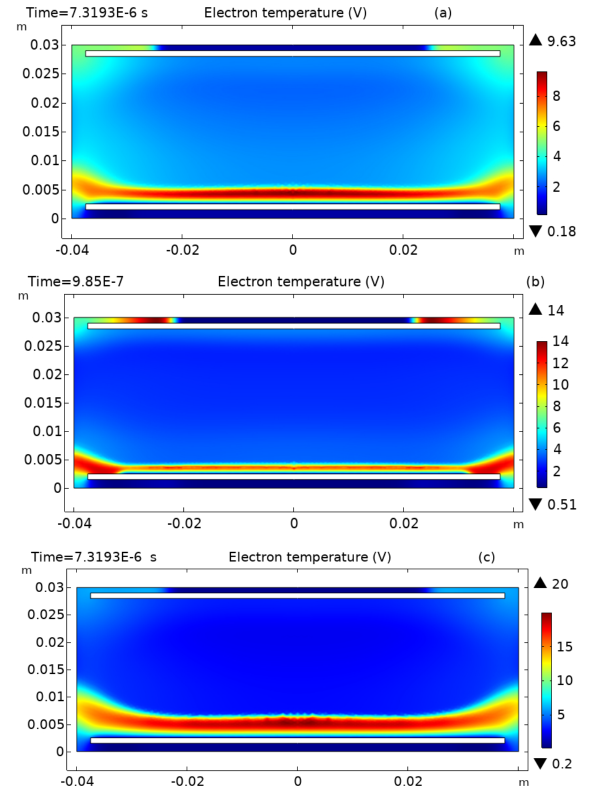


Figure 6. 2D Evolution of electron temperature (eV) in CCP reactor for voltages of a) 100 V, b) 130 V, c) 160 V

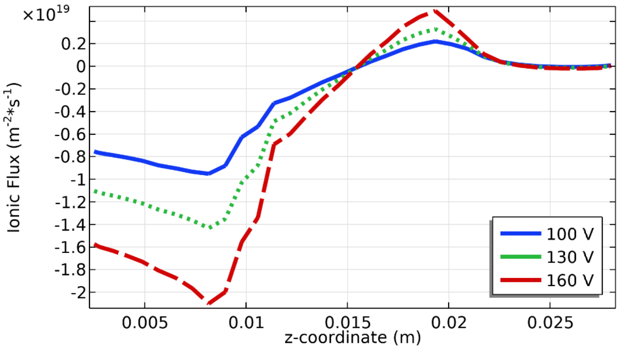


Figure 7. Evolution of ion flux ($m^{-2}s^{-1}$) in CCP reactor for voltages of; a) 100 V, b) 130 V, c) 160 V

Regarding the variation of ionic flux compared to the frequency, shown in Figure 10, we find that the ionic flux at the electrodes is improved by the increase of the frequency. Indeed, the ionic flux at the anode is important more and more as the frequency increases, it rises to 0.5×10^{20} $m^{-2}s^{-1}$ at the frequency of 100 MHz. At the cathode region, the flux increases (in absolute value) with the increase of the frequency, it rises to 1.6×10^{20} $m^{-2}s^{-1}$ at the frequency of 100 MHz.

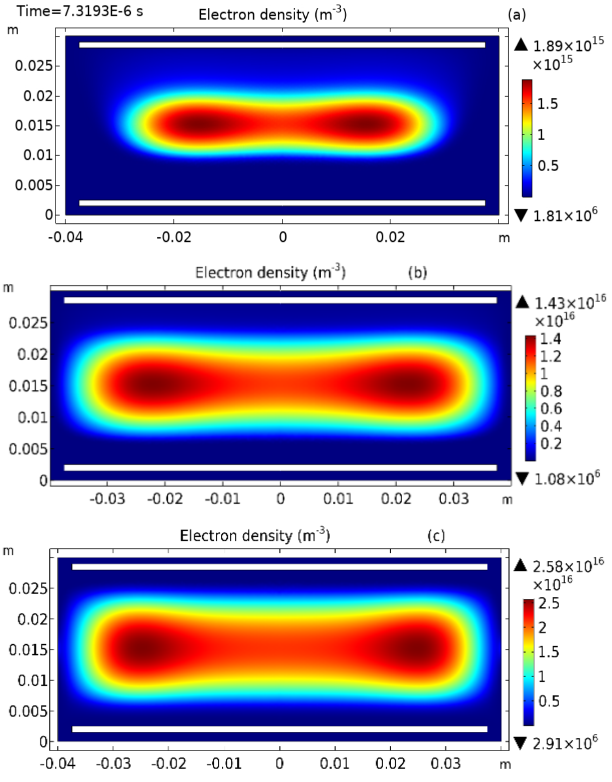
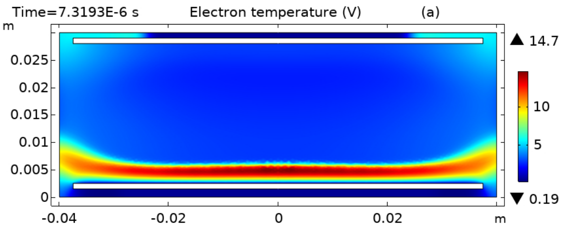


Figure 8. 2D Evolution of electron density (m^{-3}) in CCP reactor for frequencies of a) 13.56 MHz, b) 50 MHz, c) 100 MHz



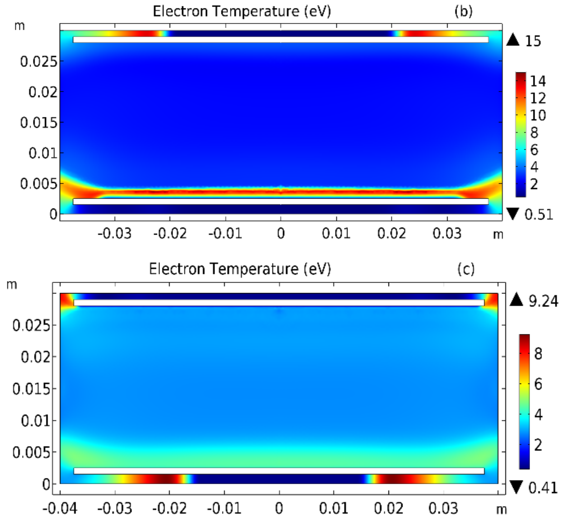


Figure 9. 2D Evolution of electron temperature (eV) in CCP reactor for frequencies of a) 13.56 MHz, b) 50 MHz, c) 100 MHz

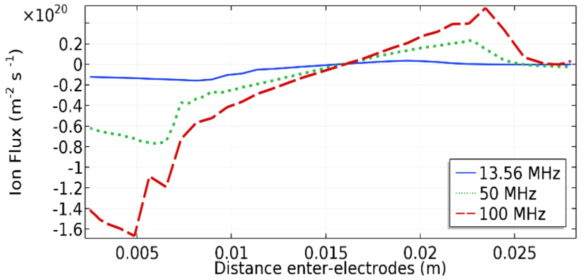


Figure 10. Evolution of ion flux ($m^{-2}s^{-1}$) in CCP reactor for frequencies of a) 13.56 MHz, b) 50 MHz, c) 100 MHz

4. CONCLUSIONS

In this work, we present the results of RF plasma discharge in a CCP reactor considering two-dimensional simulation. We considered a wide range of physical parameters in order to run our 2D model and select the optimal values by varying the pressure, breakdown voltage and excitation frequency. The results are presented at a computational time when saturation was reached. To summarize the results of this work we find that:

- First, an elevation in pressure leads to a rise in electron density with a small variation in temperature and ionic flux when varying the pressure 0.3 Torr and 0.7 Torr.
- Secondly, the variation of the voltage between 100 V and 160 V does not really influence the electron density, however, the increase of the voltage implies a notable growth in the electron temperature at the surface.
- In the third observation, elevating the frequency from 13.56 MHz to 100 MHz is associated with a growth in electron density and a concurrent decrease in surface temperature.

Upon comprehensive analysis of the results and taking into account the criteria of achieving high electron density and low electron temperature, it becomes apparent that the optimal values for this two-dimensional manipulation in equilibrium are 0.7 Torr for pressure, 100 V for voltage, and 100 MHz for frequency. These identified values prove advantageous for enhancing the deposition rate without compromising surface integrity, thus facilitating improved deposition of silicon nitride thin films.

NOMENCLATURES

1. Acronyms

CCP	Capacitive Coupled Plasma
RF	Radiofrequency

2. Symbols / Parameters

D_e : Electron diffusivity
D_i : Ion diffusivity
D_ε : Energy diffusivity
E : Electric field
f_{RF} : Frequency
f_0 : Maxwellian electron energy distribution
K_B : Boltzmann's constant (1.381×10^{-23} J/K)
K_r : Kinetic coefficient
m_e : Electron mass (9.11×10^{-31} kg)
m_i : Masse of the species
N_n : Total density of neutral
n_e , n_i : Electron and ion density
p : Pressure
V_0 : Sinusoidal voltage amplitude
V_{rf} : Electrical potential
T_e : Electron Temperature
S : Term source
γ : Acceleration of a particle
ρ : Density
ε : Energy
μ_e : Electron mobility
μ_i : Ion mobility
μ_ε : Energy mobility
$\sigma_r(\varepsilon)$: Cross section
Γ : Particle flux
Γ_e : Electron flux
Γ_i : Ion flux
Γ_ε : Energy flux
v_{th} : Thermal velocity of electron
v_{eN} , v_{iN} : Collision frequency

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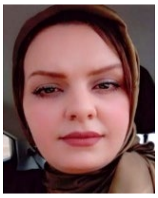

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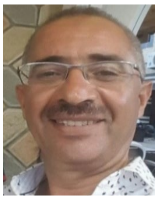
Scientific Memberships: Organization of the 6th International Conference on Materials and Environmental Science (ICMES 2023)



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Doctorate: Physics, Department of Physics, Faculty of Sciences, Mohamed I University, Oujda, Morocco, 1996
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Scientific Publications: 8 Papers, 2 Theses