

# Simulation of Inductively Coupled Plasma of Ar/C<sub>2</sub>H<sub>2</sub>/CH<sub>4</sub>/H<sub>2</sub> gas mixture in PECVD reactor and calculating the reactor efficiency

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**Abstract** - Inductively Coupled Plasma based CVD technique plays an important role in thin film deposition and formation of carbon nanostructures at a temperature below 600°C (1). ICP involves generation of plasma by applying radio frequency-based power (2). During the formation of plasma, various losses occur in the system which is difficult to measure in experimental conditions precisely. Simulation model helps in mimicking actual experimental condition for calculating these losses and ultimately the overall efficiency of the PECVD system. COMSOL Multiphysics can be used as a tool to measure the losses and by careful manipulation of various parameters, the optimized set of parameters can be adjusted for more economical and safer plasma generation for thin films and carbon Nanostructure synthesis.

**Key Words:** Inductively Coupled Plasma, COMSOL Multiphysics, Thin film deposition, carbon Nanostructures

## 1. INTRODUCTION

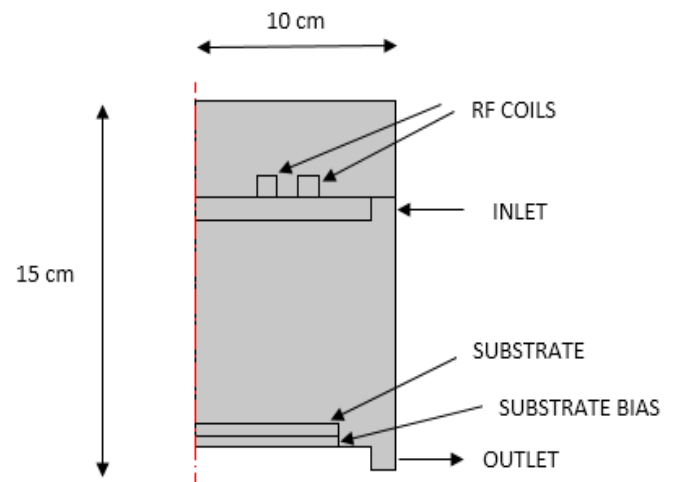
Carbon Vapor Deposition methods have been the major source for the thin film depositions at Nanoscale and formation of carbon structure at Industrial level because of their ability to produce these structures at 500 to 1100° C, which makes it suitable for working with delicate substrates. Typically, Radiofrequency plasma conditions are suitable for breaking gases into radicals and ions for deposition purpose. A commercial PECVD reactor comprises of a spiral antenna having number of turns on top of the chamber and consists of a generator operating at Radiofrequency of 13.56 MHz providing power ranging from 1200 to 1500 W (3). Practically it is inconvenient to study the PECVD system at every time and measure various working parameters of it, so situational models are important in analyzing the system at each step. COMSOL Multiphysics 5.2a is an elemental analysis tool or solver which provides conventional physics-based systems available at one platform using solution of partial differential equations. It can be incorporated to design the same practical PECVD system and analyze various parameters with simple GUI. As practically it is impossible and dangerous to measure losses in a PECVD unit, here COMSOL is handy in calculating various system parameters along with various losses in the system. By calculating various losses in a PECVD system, the overall efficiency of PECVD can be easily calculated using COMSOL, which is practically not possible in the experimental system.

## 2. MODEL

COMSOL Multiphysics 5.2a is used to model a two-dimensional PECVD model of plasma of complex Ar/CH<sub>4</sub>/C<sub>2</sub>H<sub>2</sub>/H<sub>2</sub> gas mixtures at low-pressure of 20mTorr and low temperature of 300K to simulate a practical PECVD system and calculate the various losses in the system and ultimately calculate the overall efficiency of PECVD system.

### 2.1 Geometry

For analysis purpose of a 3D plasma chamber, a 2D axis-symmetric geometry is considered.



**Fig- 1.** 2D Axis Symmetric Model of 3D PECVD System

The plasma reactor chamber consists of a metal cylinder of radius 10 cm and height 15 cm as shown in Fig-1. A substrate platform of radius 7 cm is placed 8 cm below the chamber top. A four-turn spiral antenna (inductive coil) named Coil 1 is located at the top of the chamber and is connected to a 13.56 MHz generator providing power of 1200 W. This RF coil is the main source for ICP plasma source. The antenna configuration with only four coil turns was chosen intentionally to generate low-temperature plasmas with non-uniform density along the radial direction.

The model incorporates Inductively coupled Plasma module under plasma physics of COMSOL. This interface couples the Drift-Diffusion, Heavy Species Transport, and magnetic field interfaces into an integrated Multiphysics interface.

### 2.2 Reactions and Materials

**Table -1:** Reactions considered for the Simulation Model

Electron Impact reactions				
S No	Reaction	Type	Thresh old(eV)	Ref.
1	e+Ar=>e+Ar	Elastic	0	4
2	e+Ar=>e+Ar <sup>s</sup>	Excitation	11.5	4
3	e+Ar <sup>s</sup> =>e+Ar	Super elastic	-11.5	4
4	e+Ar=>2e+Ar <sup>+</sup>	Ionization	15.8	4
5	e+Ar <sup>s</sup> =>2e+Ar <sup>+</sup>	Ionization	4.24	4
6	Ar <sup>s</sup> +Ar <sup>s</sup> =>e+Ar+Ar <sup>+</sup>	Penning Ionization	-	4
7	Ar <sup>s</sup> +Ar=>Ar+Ar	Metastable quenching	-	4
Plasma chamber Wall Surface reaction				
No	Reaction	Sticking Coefficient	Ref.	
8	Ar <sup>s</sup> =>Ar	1	5	
9	Ar <sup>s</sup> +=>Ar	1	5	
Reactions				
No	Reaction	Rate Coefficients (m <sup>3</sup> /(s.mol))	Ref.	
10	Ar <sup>++</sup> +C <sub>2</sub> H <sub>2</sub> =>C <sub>2</sub> H <sub>2</sub> <sup>++</sup> +Ar	25.29 x10 <sup>7</sup>	6,7	
11	Ar <sup>++</sup> +H <sub>2</sub> =>Ar+H <sub>2</sub> <sup>+</sup>	0.448 x10 <sup>8</sup>	6,7	
12	C <sub>2</sub> H <sub>2</sub> <sup>++</sup> +H <sub>2</sub> =>C <sub>2</sub> H <sub>3</sub> <sup>++</sup> +H	0.1656 x10 <sup>6</sup>	6,7	
13	H <sub>2</sub> <sup>++</sup> +H=>H <sup>++</sup> +H <sub>2</sub>	1.062 x10 <sup>7</sup>	6,7	
14	C <sub>2</sub> H <sub>2</sub> <sup>++</sup> +H=>C <sub>2</sub> H <sup>++</sup> +H <sub>2</sub>	0.713 x10 <sup>8</sup>	6,7	
15	C <sub>2</sub> H <sub>3</sub> <sup>++</sup> +H=>C <sub>2</sub> H <sub>2</sub> <sup>++</sup> +H <sub>2</sub>	1.126 x10 <sup>6</sup>	6,7	
16	C <sub>2</sub> H <sup>++</sup> +H <sub>2</sub> =>C <sub>2</sub> H <sub>2</sub> <sup>++</sup> +H	0.182 x10 <sup>8</sup>	6,7	
17	C <sub>2</sub> H <sub>2</sub> <sup>++</sup> +H=>C <sub>2</sub> H <sub>2</sub> <sup>++</sup> +H <sub>2</sub>	0.713x10 <sup>8</sup>	6,7	
18	H <sup>++</sup> +CH <sub>4</sub> =>CH <sub>3</sub> <sup>++</sup> +H <sub>2</sub>	0.385x10 <sup>8</sup>	8	
19	H <sub>2</sub> <sup>++</sup> +CH <sub>4</sub> =>CH <sub>3</sub> <sup>++</sup> +H <sub>2</sub> +H	0.379x10 <sup>8</sup>	8	
20	CH <sub>3</sub> <sup>++</sup> +H=>CH <sub>2</sub> <sup>++</sup> +H <sub>2</sub>	1.55x10 <sup>7</sup>	8	
21	CH <sub>2</sub> <sup>++</sup> +H=>CH <sup>++</sup> +H <sub>2</sub>	0.165x10 <sup>8</sup>	8	
22	CH <sup>++</sup> +H=>C <sup>++</sup> +H <sub>2</sub>	1.242x10 <sup>7</sup>	8	

**Table -1:** Materials used for the simulation model

Medium	Electrical conductivity	Relative Permittivity	Relative Permeability
RF coils (Coil 1)	6*10 <sup>7</sup> S/m	1	1
Dielectrics /Insulator	0	1	4.2

**2.3 Losses in PECVD system**



**Fig- 2** Flow of losses in PECVD

When a time-varying electric current is applied to the RF coils at 13.56 MHz and 1200 W power source, it produces a time-varying magnetic field in the plasma chamber filled with gases. As per Lenz's law, a time-varying electric current flows inside the chamber gases in opposite direction to oppose the magnetic field. This electric current in the gas chamber ionizes the Argon gas to form the plasma by transformer action.

The losses due to transformer action involve ohmic losses in the coils of PECVD and Iron losses which include Hysteresis and eddy current loss (9). The eddy current loss can be neglected as the coils are laminated cores. The constant Hysteresis loss is calculated as

$$W_h = K_h B_{max}^{1.6} fV \text{ (watts)}$$

where,  $K_h$  = Steinmetz hysteresis constant,  $V$  = volume of the core in m<sup>3</sup>,  $f$ =13.56 MHz, Total volume of Coil= 30.4 x 10<sup>-6</sup> m<sup>3</sup>, Maximum Flux Density= 0.01 T and  $K_h$  = 100

$$\text{Total Hysteresis loss} = 2 \times W_h = 26.82 \text{ W}$$

Due to ionization of gases, the formation of plasma takes place breaking constituent gases in various Ions, radicals, and neutrals. It involves electron-impact reaction, various inter-species reactions, and reactions with plasma wall as specified in Table 1.

During plasma formation mainly two types of losses take place namely Capacitive power deposition loss and Collisional Power Loss. Another loss is volumetric losses due to the electric and magnetic field which is of the order of 10<sup>-14</sup> and can be neglected.

The overall efficiency of a PECVD unit can be calculated using the formula

$$\text{Efficiency, } \eta = 1 - \frac{\text{Total losses (Energy)}}{\text{Input (Energy)}}$$

### 3. RESULTS

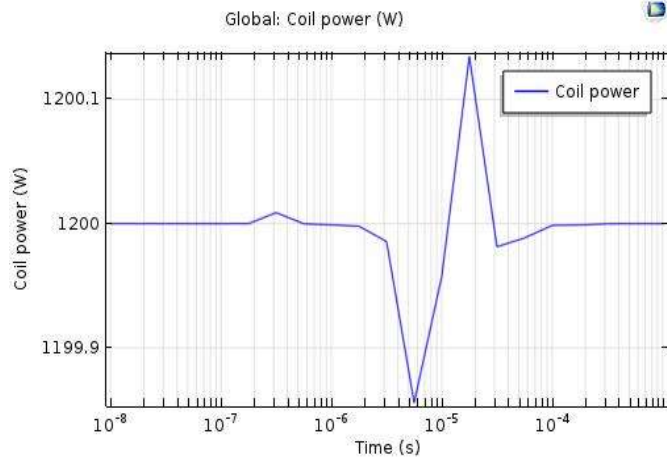


Fig- 3 Coil Power

Initially, the power dissipated is all dissipated in the coil (~1200 W). After about 1 microsecond, the plasma ignition begins and as the neutral gas atoms split into electrons and ions, the electrons begin to absorb more and more power. At this time a countercurrent start flowing in the coil as per Lenz's law. Over a period of 2 microseconds, the system restores again by increasing its power intake up to 1300 W for few microseconds. The plasma goes from absorbing no power to absorbing around 1300 W and restored back to 1200W as shown in Fig- 3

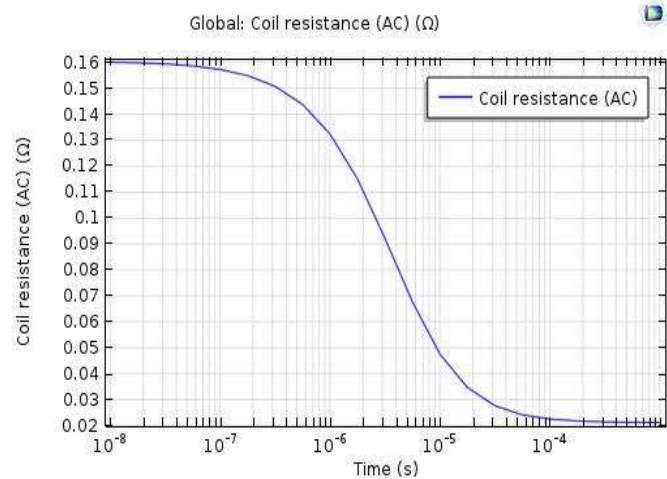


Fig- 4 Coil Resistance

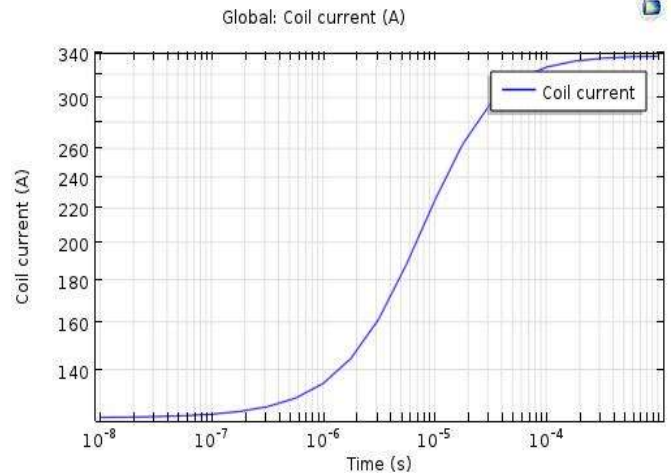


Fig- 5 Coil Current

The resistance of the coil decreases by a little less than a factor of 8 from 0.16 to 0.02 when the plasma is on as shown in Fig- 4. There is a substantial opposing current induced back into the coil from the plasma. The coil current increases from 135 A to 350 A after few microseconds when plasma is generated as shown in Fig- 5. The electric potential applied across the coil needs to increase in order to maintain the same total current

Using the coil current and coil resistance plot data the ohmic (I<sup>2</sup>R) loss plot is shown in Fig- 6

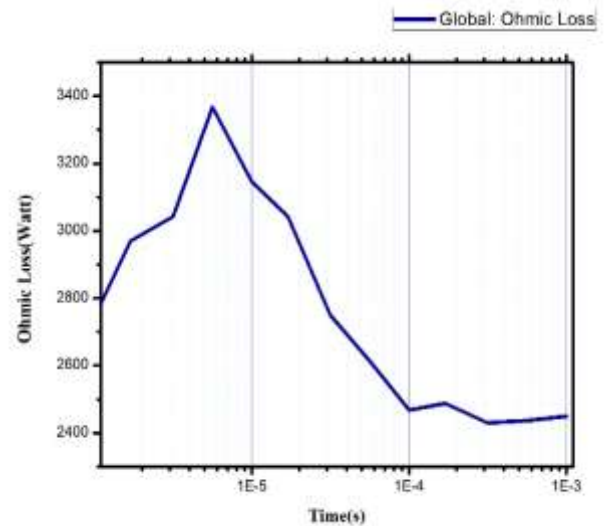
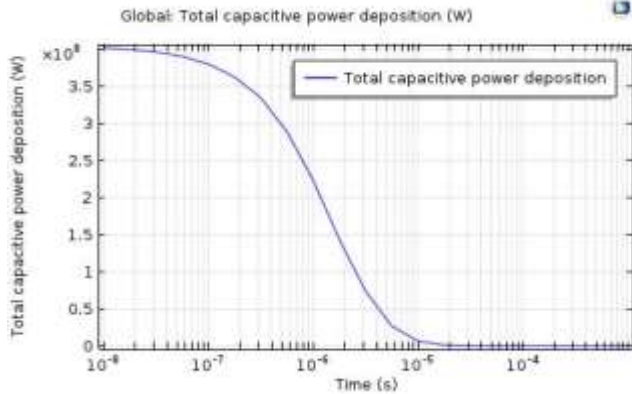


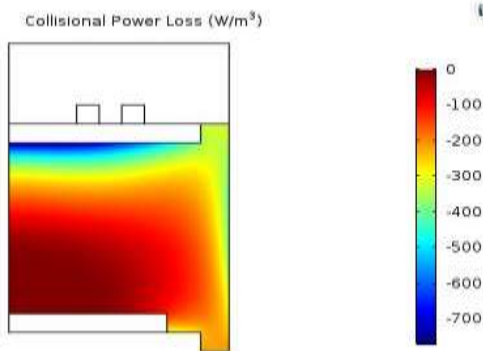
Fig- 6 Ohmic Loss

Using Trapezoidal rule in the curve of Fig.6 the ohmic loss is calculated to be 57.7 W.

Fig- 7 shows the energy loss due to capacitive power deposition and it gradually reduces to zero just after plasma starts to build up at microseconds and is calculated to be 2.2W.



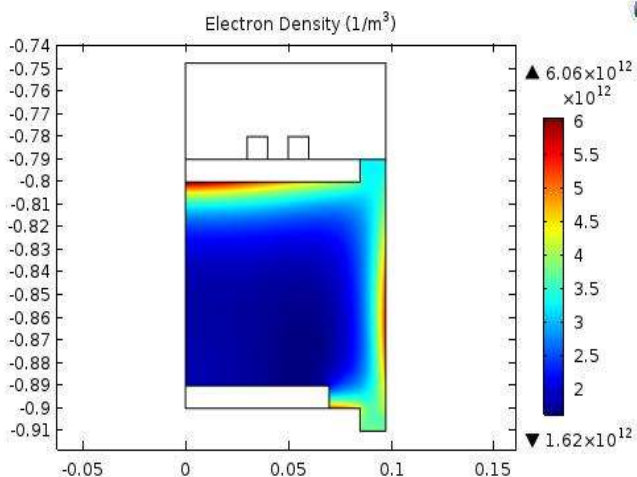
**Fig- 7** Capacitive Power Deposition



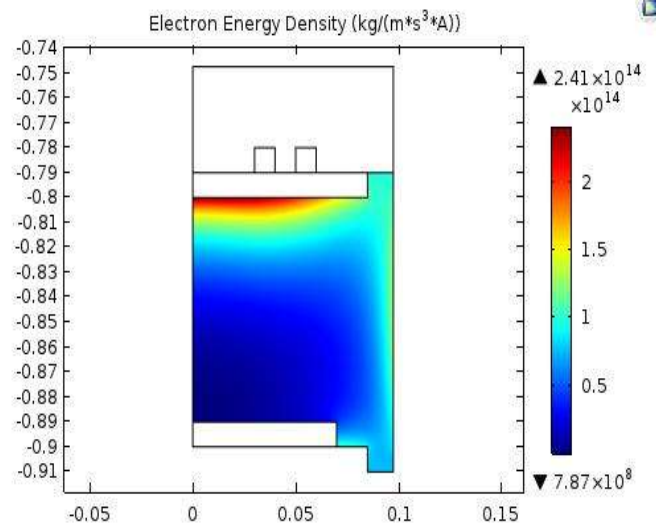
**Fig- 8** Collision Power Loss

The per unit volume Collisional Power Loss is shown in Fig-8 and is maximum near the coil and Plasma chamber interface with a value of  $733 \text{ W/m}^3$ . So, for total volume, it is calculated to be  $2.47 \text{ W}$ .

The initial electron density was considered to be  $10^{12} / \text{m}^3$ . After plasma generation finally, the maximum electron density reaches up to a value of  $6.06 \times 10^{12} / \text{m}^3$  around the walls of plasma chamber due to various electron impact reactions as shown in Fig-9.

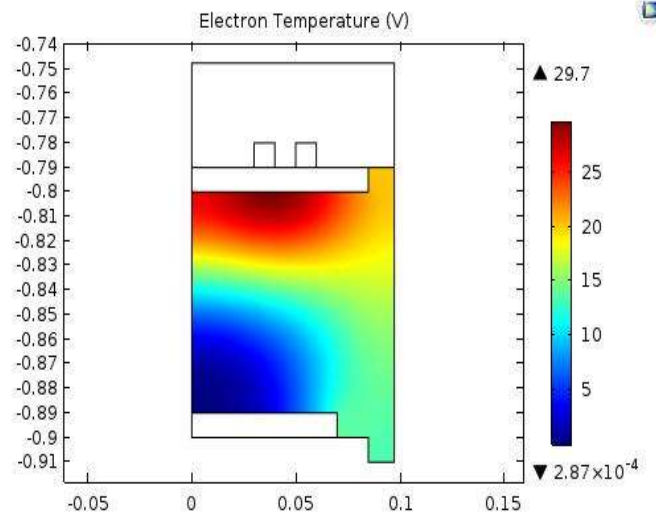


**Fig- 9** Electron Density



**Fig- 10** Electron Energy Density

Fig- 10 shows the electron energy density inside the chamber reached up to a value of  $2.41 \times 10^{14}$ .



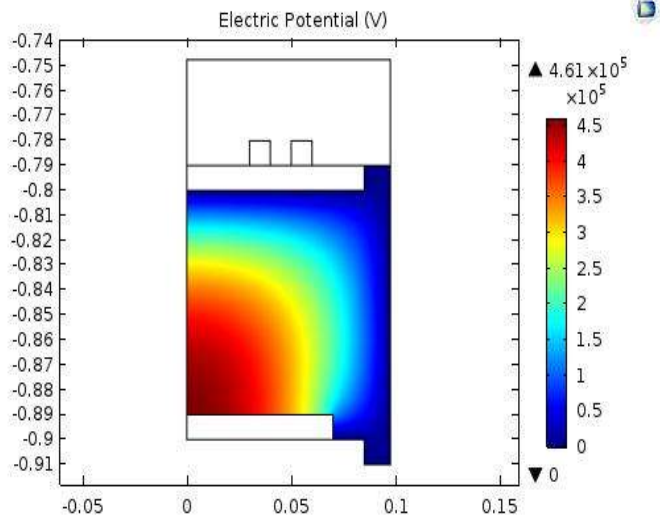
**Fig- 11** Electron Temperature

The plasma generation in the chamber causes an increase in the electron temperature up to a maximum value of  $29.7$  (in the unit of volts) which is equivalent to  $11000 \text{ K}$  which is shown in Fig- 11.

The electric potential generated inside the chamber due to plasma action is found to be  $4.81 \times 10^5$  and is maximum in the center of the chamber.

Total loss in the system is calculated to be  $89.19 \text{ W}$  giving an overall efficiency of  $92.51 \%$ . Which mainly comprises ohmic loss in the coil and collisional power loss in the plasma chamber.





**Fig- 12** Electric Potential

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#### 4. CONCLUSION

This paper presents the simulation results of low-pressure Inductively coupled RF plasmas in Ar/CH<sub>4</sub>/C<sub>2</sub>H<sub>2</sub>/H<sub>2</sub>. The calculation is performed by COMSOL Multiphysics. It is found that total losses in our PECVD unit are 89.19 W and the efficiency is calculated to be 92.51 % and mainly depends upon the type of material taken for coils, the operating parameters of coils. Also, the losses due to plasma formation depend upon the operating conditions of plasma chamber as initial electron density, temperature, pressure of chamber types of constituent gases.☐

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