Self-Consistent Simulation of Microwave PACVD Reactors for Diamond Growth

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Abstract

Recent Microwave Plasma-Assisted Chemical Vapor Deposition (PACVD) experiments at higher pressures have reported faster diamond growth rates and higher quality samples.[1] This transition necessitates the development of numerical models that can accurately capture the underlying physics in this new pressure regime. A flexible-geometry, multi-physics, self-consistent simulation of hydrogen-based plasmas for microwave PACVD reactors is being developed.

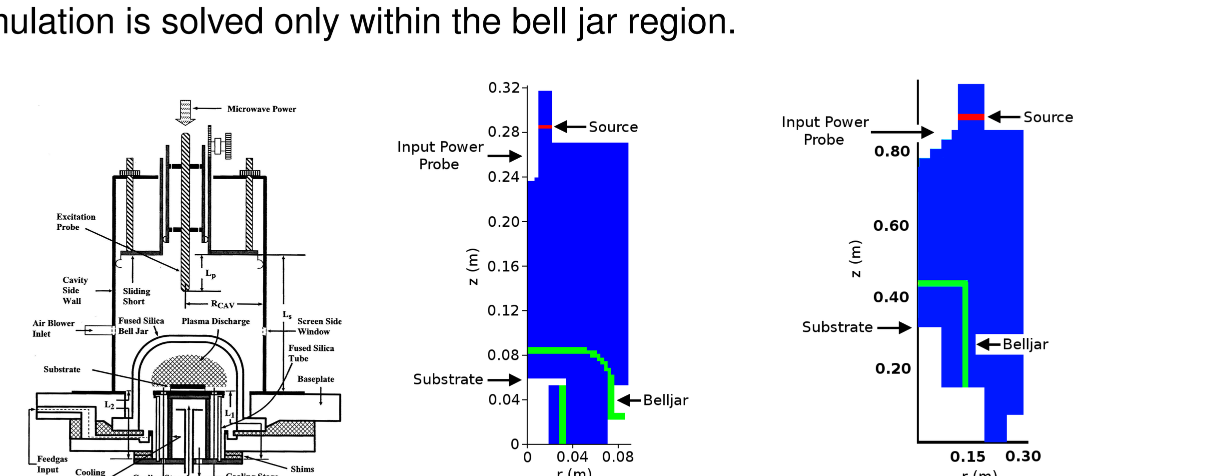
Motivation

- Higher pressures for Microwave PACVD reactors result in:[1]
  1. Faster growth rates
  2. Better quality diamond
- Development of multi-physics simulations at higher pressures will:
  - Aid in development of new reactors
  - Help understand underlying mechanisms
- As a first step, a geometry-flexible, **moderate pressure**, fluid based, multi-physics simulation is being developed
- To demonstrate flexibility, two reactor geometries used:
  1. f = 915 MHz, (Université Paris Nord)
  2. f = 2.45 GHz, (Michigan State University)

Problem Statement

Geometry

Labeled schematics for both reactors are provided in Figure 1.[2, 3] The electromagnetic simulation comprises of the entire reactor cavity, while the plasma simulation is solved only within the bell jar region.



(a) Side view (b) Simulation domain (MSU) (c) Simulation domain (U. Paris Nord)

Figure 1: *(a) Complete side view of MSU Microwave PACVD reactor and (b) half-space numerical analog, and (c) Université Paris Nord reactor.*

Electromagnetics

- Microwave energy introduced into the reactor cavity via a waveguide (*see Source*)
- Energy absorbed by the high frequency oscillations of electrons within plasma (*above the substrate*)
- Glass bell jar confines plasma and hydrocarbon gas
- Reactor cavity is designed to support a (TM_{01i}) modes; i = 3,4
- A Finite-Difference Frequency Domain (FDFD) model was chosen over the standard Finite-Difference Time Domain (FDTD) for two reasons:
  - Computational efficiency
  - Inherent steady-state solution
- Electron Energy Distribution Function (EEDF) included as frequency-domain complex electrical conductivity,

$$\vec{J}_e = \sigma \vec{E} \tag{1a}$$

$$\sigma = \frac{q_e^2 n_e}{m_e}\left(\frac{\nu_{eff} - j\omega}{\nu_{eff}^2 + \omega^2}\right) \tag{1b}$$

- Absorbed power calculated: $\mathcal{P}_abs = \vec{J}_e \cdot \vec{E}$

Plasma

Hydrogen ions and electrons included: H_2, H, H(n=2), H(n=3), H^+, H^{2+}, H^{3+}, H^-, and e^-.[2] The continuity equations and energy balance equations govern the plasma physics:

$$\nabla\left(\rho \frac{M_s}{M} D_s \nabla x_s\right) + W_s = 0 \tag{2}$$

$$\nabla\left(\lambda_v \nabla T_v + \lambda_{e^-} \nabla T_{e^-} + \lambda_g \nabla T_g - \rho \sum_s D_s h_s \nabla x_s\right) + \mathcal{P} - Q_{rad} = 0 \tag{3}$$

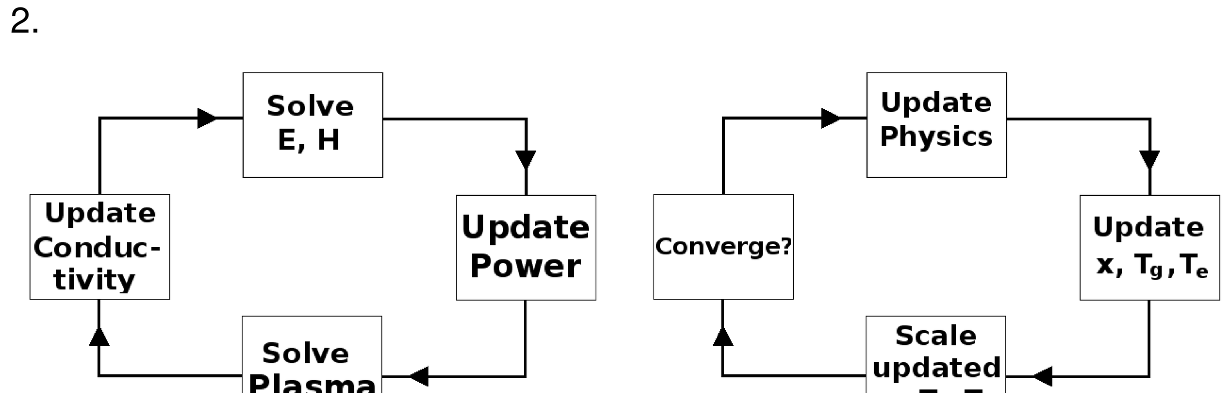
where $\mathbf{x}_s$ is the molar fraction of species s. These equations are coupled and non-linear in nature. A Gauss-Seidel iterative solver is used to converge toward a solution.

Boundary Conditions

The gas temperature is initially set to 1200 K at the substrate surface, and 600 K at the wall of the quartz dome.[2] The azimuthal symmetry of the problem forces the $\hat{r}$ components to have zero value at the $r = 0$ axis, while zeroed Neumann conditions are applied to $\hat{z}$ fields.

Solution Process

An *initial guess* conductivity is required to start the simulation (ensuring non-trivial absorbed power). An overview of the solution process is provided in Figure 2.



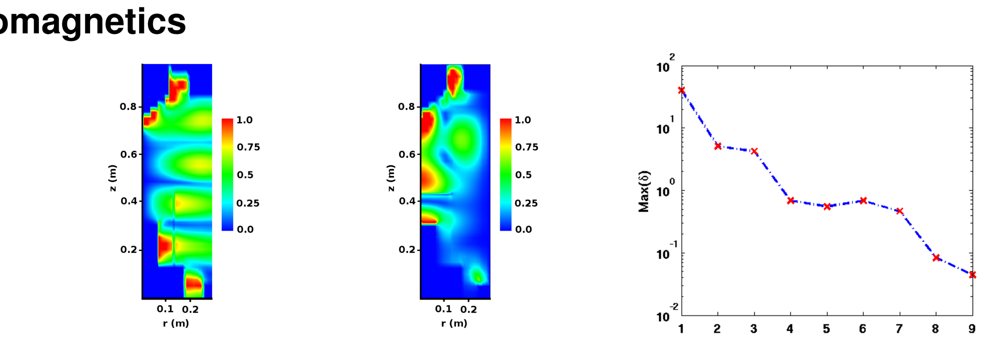
(a) Global (b) Plasma

Figure 2: *Solution process for (a) complete system and (b) plasma convergence.*

Results

Université Paris Nord Reactor (3000 Watts, 40 Torr)

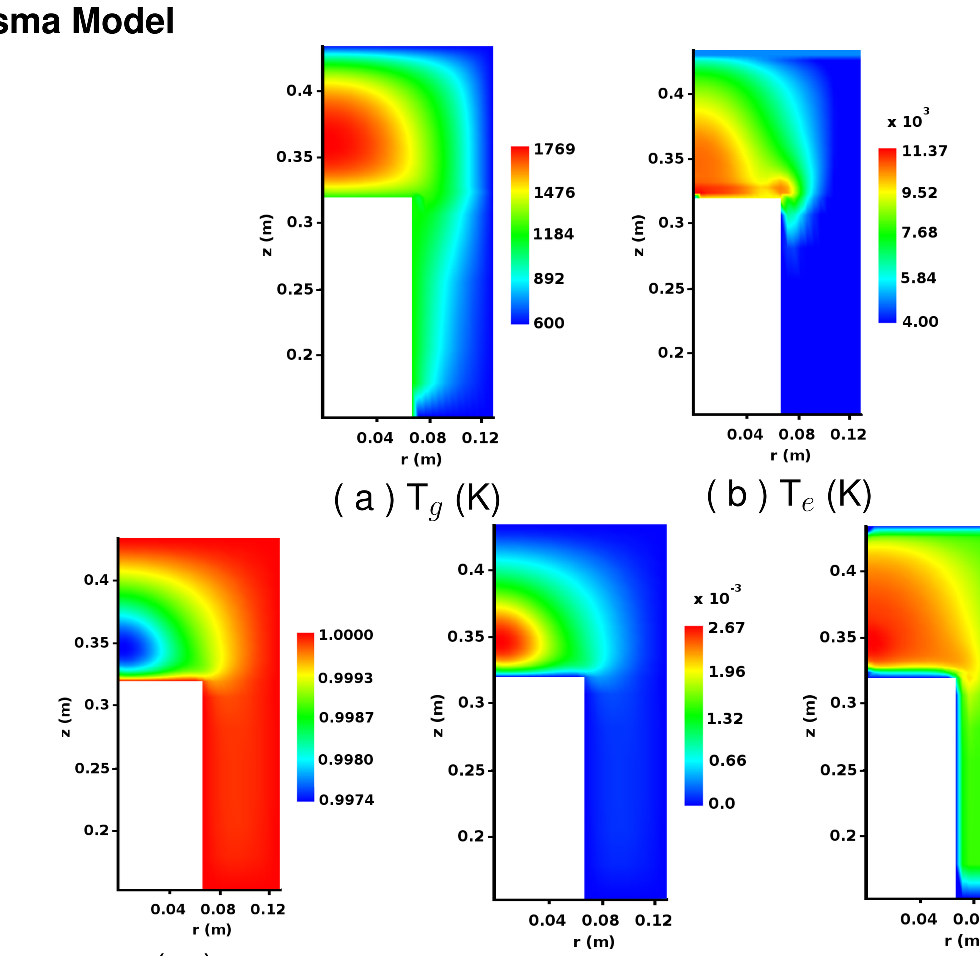
Electromagnetics



(a) $|\vec{E}_r|(n.u.)$ (b) $|\vec{E}_z|(n.u.)$ (c) $ErrorConvergence$

Figure 3: *(a) $\hat{r}$ and (b) $\hat{z}$ electric field components during plasma ignition, and (c) total solution error versus iteration number.*

Plasma Model

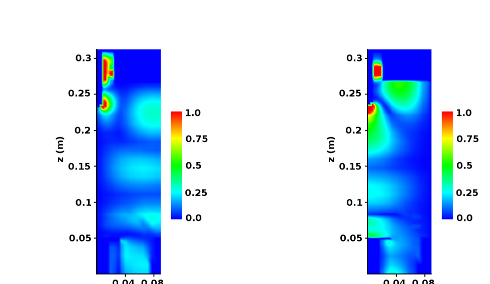


(a) T_g (K) (b) T_e (K) (c) x_{H_2} (d) x_H (e) x_{e^-}

Figure 4: *Université Paris Nord reactor (a) gas temperature (T_g), (b) electron temperature (T_e), (c) electron density (n_e), (d) H_2 molar fraction (x_{H_2}), (e) H molar fraction (x_H), and (f) electron molar fraction (x_{e^-}) with a total $\mathcal{P}$ of 3000 Watts and pressure of 40 Torr.*

MSU Reactor (400 Watts, 40 Torr)

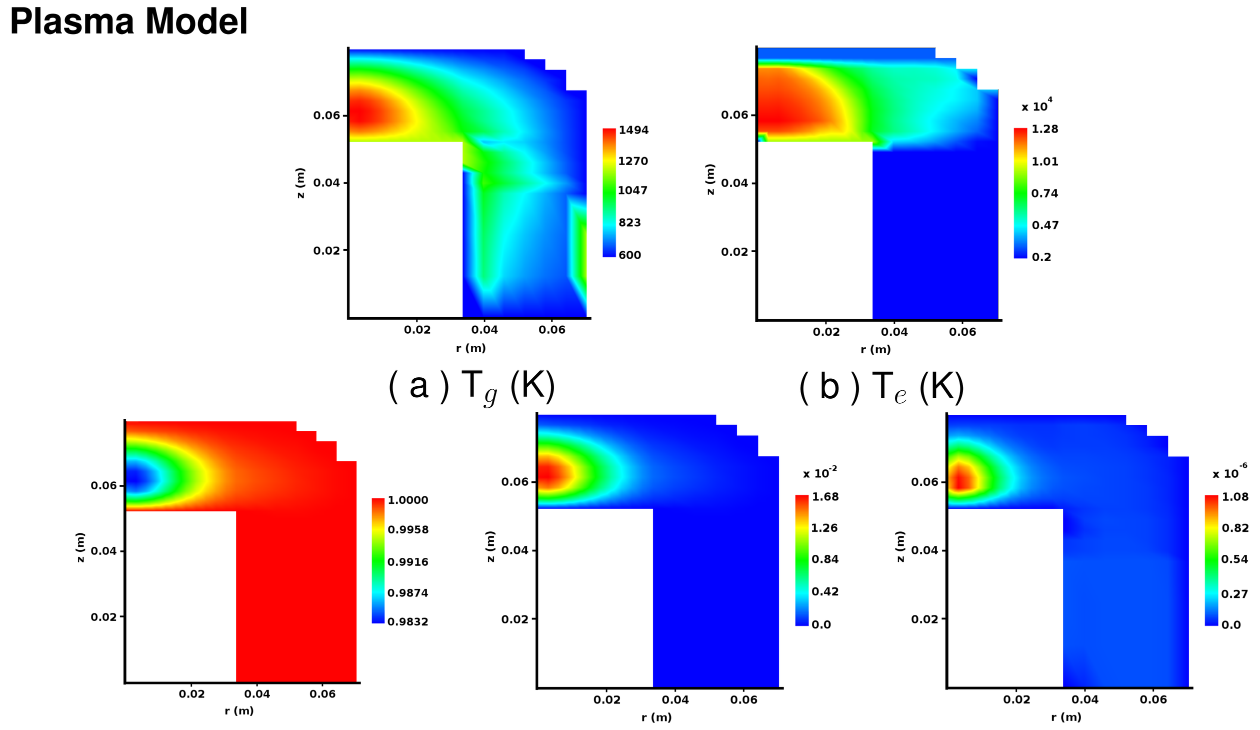
Electromagnetics



(a) $\vec{E}_r(V/m)$ (b) $\vec{E}_z(V/m)$

Figure 5: *(a) $\hat{r}$ and (b) $\hat{z}$ electric field components during plasma ignition.*

Plasma Model



(a) T_g (K) (b) T_e (K) (c) x_{H_2} (d) x_H (e) x_{e^-}

Figure 6: *MSU reactor (a) gas temperature (T_g), (b) electron temperature (T_e), (c) electron density (n_e), (d) H_2 molar fraction (x_{H_2}), (e) H molar fraction (x_H), and (f) electron molar fraction (x_{e^-}) with a total $\mathcal{P}$ of 400 Watts and pressure of 40 Torr.*

Conclusions

- Moderate pressure, multi-physics Microwave PACVD diamond reactor simulation is under development
- Flexibility with respect to geometry observed
- Future work:
  - Improve stability, efficiency
  - Higher pressures (convection, time-dependent)
  - Thermal processes
    - Substrate, bell jar temperature profiles
    - Internal substrate cooling
    - Heat capacity of samples, substrate
  - Model diamond deposition process
    - Deposition rate profile
    - Update diamond sample height

References

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[3] Stanley Shengxi Zuo, *Microwave Plasma-Assisted CVD Polycrystalline Diamond Films Deposition at Higher Pressure Conditions*, PhD Dissertation, 2009.