Including Convective Flows in a Self-Consistent Hydrogen-Based Microwave PACVD Reactor Model

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Motivation

- Higher pressures for Microwave PACVD reactors result in:
  1. Faster growth rates
  2. Better quality diamond
- Development of multi-physics simulations at higher pressures will:
  - Help understand underlying mechanisms
  - Aid in development of new reactors

Governing Equations

Electromagnetics (FDFD)

\[ \nabla \times \left( \frac{1}{\varepsilon} \nabla \times \mathbf{E} \right) = \mathbf{B} \]

Conductivity

\[ \sigma = \frac{q^2 \rho_n}{m_e} \left( \frac{v_{\text{ej}}}{v_{\text{ej}} + \omega} \right) \]

Solution Process

- Electromagnetics: Direct (sparse)
- Plasma (Scalar): Gauss-Seidel Line Relaxation
- Plasma (Flows): Implicit direct solver [2]

Validation

Electron Density

Figure 3: Simulated (red) and experimentally measured (black) electron density versus pressure at constant power of 600 Watts. Experimental data from Gro\textit{t}john et. al., 2000.

Geometry

Figure 1: (a) Schematic of MSU Microwave PACVD reactor, (b) discretized mesh, (c) electromagnetics and (d) plasma simulation domains.

High Pressure Results

Electromagnetic Module

Figure 4: (a) \( |\mathbf{H}_\|| \) (A/m), (b) \( |\mathbf{E}_\|| \) (V/m) and (c) \( |\mathbf{E}_\times| \) (V/m) solutions when operating at 250 Torr and 3 kW. The same scale is used in both electric field plots.

Plasma Flow Module

Figure 5: MSU reactor (a) gas temperature, (b) H molar fraction, (c) electron density, and (d) vector gas flow for \( P_{\text{abs}} \) of 3 kW and pressure of 250 Torr.

Conclusions

- Self-consistent multi-physics Microwave PACVD diamond reactor simulation accurate at higher pressures
  - Convective forces significant above 150 Torr
  - Influence primarily in mole fractions
- Future work:
  - Substrate temperature
  - Hydrocarbons

References