

Study of Gas Phase Chemistry in Chemical Vapor Deposition Reactors for Diamond Growth

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Abstract: Chemical vapor deposition (CVD) is used for diamond synthesis with applications spanning electronics and quantum sensing. CH₄ diluted in H₂ is typically used as feedstock. We have recently applied *ab-initio* quantum chemistry methods to develop a comprehensive quantitative model of the surface kinetics of diamond growth [1]. This model requires as input data the concentrations of active species involved in the growth, namely, CH₃, C₂H₂, H₂ molecules, H atoms, and, in the case of phosphorous doping of diamond, phosphorous-containing species near the substrate surface. Now we are developing an in-house computer code for self-consistent simulations of microwave and hot filament CVD reactors. A gas phase model describing chemical kinetics in a PH₃/CH₄/H₂ mixture has been developed and fluxes of species, which can contribute to the diamond growth and its phosphorus doping have been analyzed.

1. Introduction

Advancing chemistry vapor deposition (CVD) technology requires better understanding of plasma physics and chemistry of material growth. A reliable model of CVD reactor that provides data on fluxes of gas-phase material precursors can potentially guide experimental decisions about proper gas pressure, power, temperature, flow rate, etc. The goal of this work is to develop such a model to do self-consistent simulations of microwave resonant cavity reactors for the diamond growth.

2. Methods

Our self-consistent model includes modules for neutral chemistry and gas flow, electromagnetics, and weakly-ionized nonequilibrium plasma physics and chemistry. The latter is based on non-Maxwellian electron energy distribution function and approximate calculation of vibrational energy balance. It accounts for electron and neutral gas heating. The modules are coupled together using global iterations. Because this problem is quite complex numerically and there is a strong interdependency between the mentioned modules, these modules were initially validated separately for simpler problems.

3. Results and Discussion

For a validation, we solve for electromagnetic field in an empty cavity, consider pyrolysis of PH₃/CH₄/H₂ mixture, solve for viscous gas flow through a pipe, and calculate electron energy distribution function by BOLSIG+ [2] and compare it with previous simulations [3].

As an example of self-consistent simulations, figure 1 shows the distribution of the electric field in a plasma in a cylindrical chamber.

We will give a detailed presentation of our model and will report on our on-going efforts to validate it and compare our simulation results with experiments.

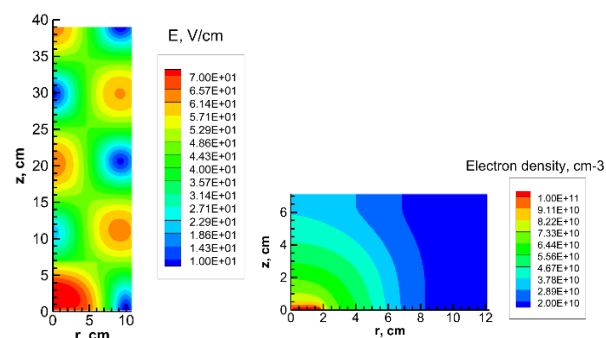


Figure 1. Calculated electric field in a cylindrical cavity of height 39.2 cm and radius 12 cm, with plasma generated near the lowest antinode of the field. The gas pressure is 38 Torr and the absorbed power is 800 W.

4. Conclusion

Synthesis of diamond often requires finding optimal plasma conditions for material growth. We are developing a computational tool to help to guide experiments on the diamond growth. The tool will be used for understanding complicated chemistry involved and plasma instabilities. Separate modules of the model work and the next step will be running self-consistent simulations for diamond co-doping studies.

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References

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