Self-consistent simulation of microwave assisted hydrogen methane plasmas

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Abstract: Self-consitent simulations of microwave assisted hydrogen methane plasmas have been performed for wide range of operating conditions. The simulations clearly indicate that the properties of the plasma change substantially with addition of small amounts of methane. In general, self-consistent simulations would be important to correctly predict the coupling between plasma and microwave.

Keywords: MW plasma, self-consitent simulations, CVD diamond

1. Introduction

MW assisted hydrogen-methane plasmas have been used extensively for growth of carbon materials such as CVD diamond, graphene and carbon nano-tubes. Graphene is usually grown at low pressures (>25 mbar) where as CVD diamond can be grown at relatively high pressures. Microwave radiation energizes the few free electrons to very high temperature, which collide with heavy species resulting in a self-sustaining plasma. In a conventional resonating MW cavity, the plasma occurs close to one of the available anti-nodes in the reactor and the substrate is placed closed to this anti-node enabling growth of diamond or graphene. The quality of the deposit depends on the coupling between microwave and the plasma which again depends on various factors such as MW power, pressure, concentration of the precursor gases etc. Understanding the coupling between the microwave and the plasma is critical for design and optimization of efficient MW reactors. In this article, we discuss the effects of concentration of methane in a hydrogen plasma for carbon material processing in a MW assisted plasma reactors which have been used for growing CVD diamonds and graphene at LSPM [1]

2. Discussion

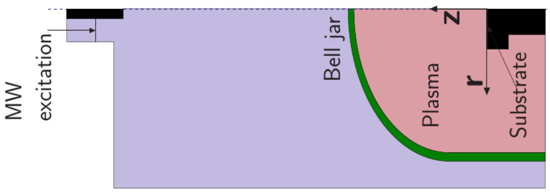

Fig. 1 Schematic of MW plasma reactor used for the present studies.

Self-consistent simulations [2] have been performed for different conditions. The model mainly comprises of two modules namely the plasma and the maxwell module which are solved iteratively. The plasma module solves for the complex chemistry and energy equations using finite volume method while the MW module treats the maxwells equations.

The reactor (Fig 1.) considered for the present study are characterized by having two anti-nodes, one close to the substrate and the other close to the top of the quartz window. At normal operating conditions, the plasma is formed close to the substrate which is desirable. However as the MW power is increased, the plasma can become unstable as two plasma zones can be formed.

We have observed that the addition of methane into the reactor affects the general plasma characteristics. Fig 2. shows the effect of concentration of methane on the plasma at pressure of 25 mbar and MW power 750 W. It can be seen that double plasma formation can take place at relatively lower power when compared to that of pure hydrogen plasma. Infact, addition of methane lowers the threshold microwave power density.

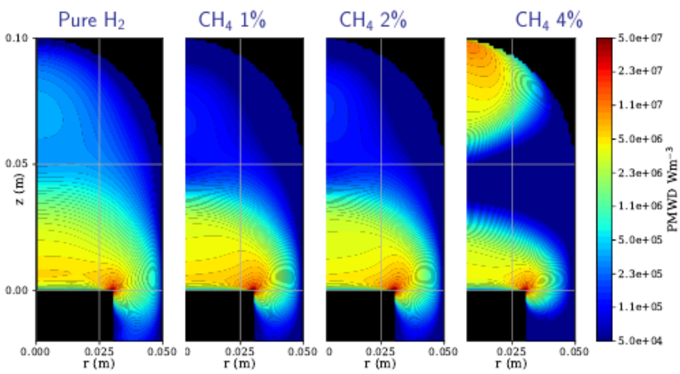

Fig. 2 Effect of methane on the MW-plasma coupling at pressure 25 mbar and 750 W.

The threshold MW power density (PMWD) at which the plasma becomes unstable have been measured experimentally for various concentration of methane in a MW bell jar reactor. This is achieved by visualizing the plasma emissive value at different conditions. The threshold power as a function of methane concentration has been tabulated in Table 1.

Table 1. Threshold MW power as a function of MW power at 25 mbar.

	MW power (W)	
% CH4	Numerical	Experiments
0	960	950
2	920	900
10	750	860
15	650	810
20	600	760

Both numerical simulations and experiments clearly indicate that addition of methane lowers the threshold MW power. The difference between the experiments and numerical simulations is due to the uncertainty of the MW power losses in the experiments.

Similar results have been observed numerically for different pressures. The present results are important because the effective range of operation of the MW reactor depends on the precursor gas concentration and pressure. The present observation can be explained by the dominant ions present in the reactor. The dominant ions in the reactor is a function of methane concentration and pressure. With the addition of methane, hydrocarbon ions become the dominant ion which are much heavier when compared to hydrogen ions (H+ or H3+). The properties of the plasma are thus altered due to the lower mobility of hydrocarbon ions. In general, a hydrocarbon plasma achieves much higher temperature resulting in increase in plasma volume. This accelerates the formation of secondary plasma.

Fig 3. shows the gas temperature and atomic hydrogen concentration at a pressure of 200 mbar and power 2500 W. The results are in agreement with experimental observations. It is seen that the addition of methane increases the temperature of the reactor. As a result the the dissociation of hydrogen increases with addition of methane.

The results clearly demonstrate the importance of self-consistent simulations as even dilute quantities of methane can have substantial effect on the microwave-plasma coupling. The properties of the plasma strongly is dictated by the precursor gas and pressure.

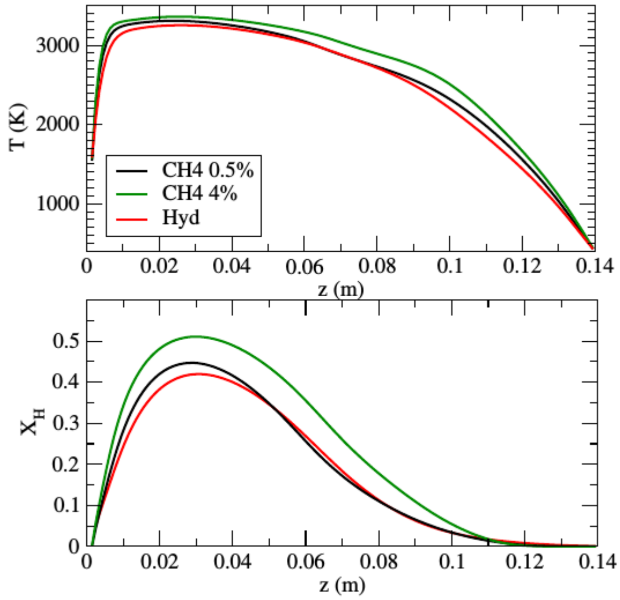

Fig. 3 Effect of methane on the gas temperature and atomic hydrogen at pressure 200 mbar and 2500 W.

3. References

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