

Modelling of microwave plasma used for thick highly boron doped diamond deposition

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A 1D-model is used to simulate H_2/CH_4 plasmas at high power density conditions for MW diamond deposition. Profiles of temperatures and species density have been estimated for different microwave power densities (MWPD) to highlight the mechanisms occurring in the plasma volume. Furthermore, the numerical results are compared to spectroscopic measurements in order to validate the model developed for high MWPD conditions. Finally, a kinetic scheme for boron containing species is suggested and the results have been brought closer to experimental doping efficiency measurements.

I. Introduction

Wide band gap semiconductors are the best materials for switching devices, and among them, diamond is the most promising candidate. The essential step to make unipolar power devices entirely made in diamond consists in elaborating a thick single boron-doped diamond crystal presenting high purity and high quality bulk. The achievement relies on the ability in mastering the $H_2-CH_4-B_2H_6$ plasma responsible for boron doped diamond in microwave plasma assisted chemical vapor deposition (MPACVD). High thickness (around $100\mu m$) associated with a high level of doping (10^{20} boron atoms/cm³) and a pure microstructural diamond single crystal calls for very energetic plasma, *ie* high pressure ($>100hPa$) and high microwave power ($>2000W$).

The purpose of this work is to understand the mechanisms involved in high power density ($50-200 W.cm^{-3}$) H_2-CH_4 plasma containing 0 to 10000 ppm of B_2H_6 . Reaching this goal requires the development of species and energy transport model reliable for high power density conditions. This model has been used to determine electron and gas temperatures, species concentrations occurring in H_2/CH_4 plasma and to analyze the influence of boron containing species.

In particular our objective is (1) to identify governing phenomena in H_2-CH_4 plasma and validate the model at high power density and (2) to highlight the chemical kinetics scheme for diborane dissociation in these conditions and the key species for incorporation of boron into diamond.

II. H_2/CH_4 Model

The calculations are based on a 1D-model previously developed in the Laboratory [1, 2] providing axial profiles of temperatures and concentrations. The thermal non equilibrium is described by taking into account two energy modes (translation-vibration-rotation mode of heavy species and translation mode of electrons) where electrons are described by a bi-Maxwellian distribution. The thermochemical model describes the kinetic scheme of hydrogen, carbon and boron containing species which represents 33 species and around 150 reactions. The investigation of the plasma transport requires one to derive the conservation equations for species density, total energy and electron energy modes. According to the experimental conditions of the investigated reactors, the convective fluxes are neglected regarding diffusion fluxes.

The solution of the equations system involves the knowledge of the axial profile of the microwave power density. This parameter can be estimated using optical emission spectroscopy measurements coupled with an energy balance of the plasma [1]. In the frame of actinometry measurements (see Derkaoui communication in this conference), few pourcents of Ar (3%) was introduced in the feeding gas. For all experimental conditions, the axial profile of the 750 nm argon line intensity was recorded with a spatial resolution of 1 mm.

First calculations were carried out with H_2/CH_4 kinetic model for high MWPD conditions. Figure 1 presents the axial profile of gas temperature and H density for three different MWPD conditions. The comparison of the profiles shape confirms the plasma volume may be considered as constant. Indeed, the

total pressure in the reactor chamber was adjusted in order to keep it constant in order to maintain as much as possible constant the ratio of the power coupled to the plasma over the total density.

We can highlight that the higher the power density, the smaller the thermal boundary layer. This decrease is attributed on the one hand to the location where the microwave energy is mainly absorbed and on the other hand to the reduction of the thermal diffusivity at high power density.

The net H-atom production is mainly carried out by the thermal dissociation of molecular hydrogen at high power density. Two processes are responsible for the production of H atoms: $\text{H}_2 + \text{H}_2 \rightarrow 2\text{H} + \text{H}_2$, and $\text{H}_2 + \text{H} \rightarrow 3\text{H}$, which dominates under conditions of high H-atom density. Diffusion towards locations of lower H-atom density ensures an efficient transport of H-atom through the surface boundary layer, where they recombine.

The 1D-model developed for high power density conditions has been validated by comparison with experimental profiles of H atom density that have been obtained by actinometry technique and TALIF measurements.

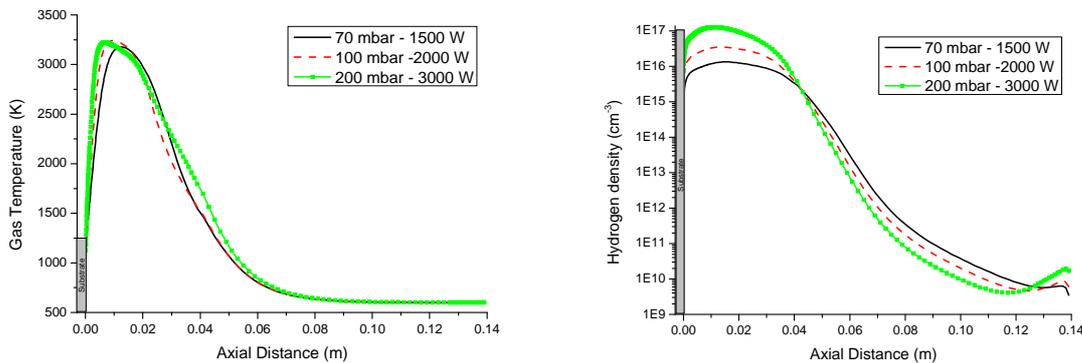


Fig. 1: Profile of gas temperature (left) and H density (right) according 3 experimental conditions for (95/5)% of $\text{H}_2\text{-CH}_4$ plasma

III. $\text{H}_2/\text{CH}_4/\text{B}_2\text{H}_6$ Model

Issaoui *et al.* [3] have surprisingly observed that increasing the MWPD strongly decreases the boron doping efficiency by almost two orders of magnitude. This phenomenon can be explained either by the improvement of production of active boron doping species in the plasma, or by the decrease of the sticking coefficient of boron onto the diamond surface. The model of the chemical kinetic scheme for boron containing species allows to identify the key mechanisms occurring in the plasma volume that can lead to increase the doping efficiency. This model is a simple one including main boron containing species and reactions.

References

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3. Issaoui, R., et al., *Growth of thick heavily boron-doped diamond single crystals: Effect of microwave power density*. Appl Phys Lett, 2010. **97**.