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NUMERICAL SIMULATION OF THE FLUID FLOW IN THE MULTI-HOT-FILAMENT CHEMICAL VAPOR DEPOSITION - MHFCVD

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ABSTRACT

Multi hot-filament chemical vapor deposition (MHFCVD) is a common method employed for diamond deposition. In this method a mixture of hydrocarbon in excess of hydrogen is thermally activated by a hot filament. Due to the filament-substrate proximity, large temperature variation across the substrate is possible. In this work the role of fluid flow and heat transfer in the MHFCVD was investigated. The equations of conservation of mass, momentum, and energy were solved numerically to calculate the temperature distribution and fluid flow fields, using the commercial software CFX. The calculation takes into account two different sets up configurations. The influence of heat transfer and convective transport is reported.

1. INTRODUCTION

Diamond is a unique material due to its many interesting properties like high hardness, low friction coefficient, high thermal conductivity, transparent upon UV until IR radiation, high refraction index and biological compatibility [1-3]. The attractive and unique proprieties combined with acceptable deposition rates have led to the applications of diamond films in small areas of drills, dies and some bearing surfaces [2,3]. Diamond films have now been grown using a variety of deposition techniques for a wide range of applications conditions.

Multi-hot-filament chemical vapor deposition (MHFCVD) is one of these techniques that have been used extensively to deposit diamond films. MHFCVD is a process whereby a solid material is deposited from a vapor by a chemical reaction occurring on or in the vicinity of a normally heated substrate surface. By varying the experimental conditions-substrate material, substrate temperature, composition of the reaction gas mixture, total pressure gas flows, etc. – materials with different properties can be grown [4]. Basically in a typical CVD reactor a mixture of the gases is introduced (inlet gas), cross the activation source (filament) where the reaction take place and produce the precursor species, that are transported to the surface of the growth an then react to form the diamond. In this process, we must emphasize the importance of the hydrogen presence. The activation source must be able to supply enough hydrogen to produce the hyper saturation of the hydrogen in the region of the growth, which is responsible for the stabilization of the surface diamond and for the etching of graphite. In fact, the H is the direct responsible for the growth in a meta stable phase.

A schematic diagram of the MHFCVD reactor used in this work is shown in Fig.1. In this MHFCVD processes, the flow of gases plays an important role in controlling the rate and uniformity of deposition, because it governs the supply of reactants to the substrate for reactions that may be limited by mass transport.

In order to obtain a deeper insight of the gas flow in the MHFCVD reactor, the heat transfer has been numerically modeled in two different sets up reactor, Fig.1 and Fig.2. The configurations are planned in such way that the convective flow either aids or opposes the transport of various species to the substrate.

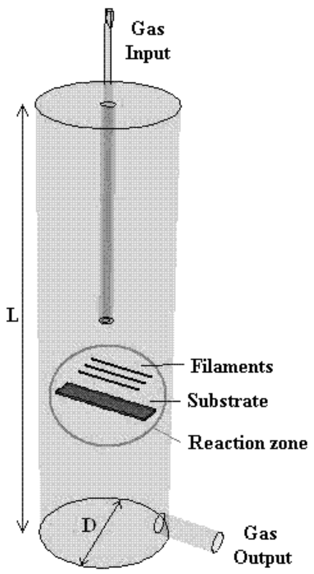

Figure 1 – Config. 1.

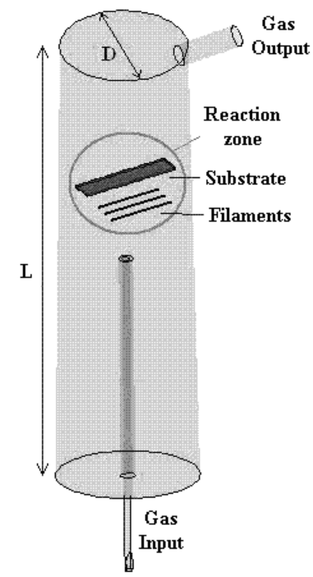

Figure 2 – Config. 2.

2. MATHEMATICAL MODEL

The mathematical model can be described by the governing partial differential equations, i.e., the equations of conservation of momentum, mass, and heat. The convective effect is done by Boussinesq approximation. A 3D reactor model was solved together with other physical input necessary to define the system adequately. The numerical results have

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been obtained by finite volume method, with an unstructured mesh grid (10^6 elements).

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad \textbf{(1)}$$

Momentum equation:

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = \nabla \cdot \mu \left[(\nabla \vec{v}) + (\nabla \vec{v})^T \right] + $$
$$+ \nabla \left[\left(\mu' - \frac{2}{3} \mu \nabla \cdot \vec{v} \right) \right] - \nabla p + \rho \vec{g} \quad \textbf{(2)}$$

Energy equation:

$$\frac{\partial T}{\partial t} + \nabla \cdot (T \vec{v}) = \lambda (\nabla^2 T) \quad \textbf{(3)}$$

where: ρ is the density of the fluid, $\vec{v}$ the velocity vector, Cp the specific heat, T the temperature, λ thermal diffusion coefficient, t the time, p the pressure, $\vec{g}$ the external force and μ the viscosity coefficient.

The following assumptions are made for the model formulation: (1) the flow of the gas mixture in the reactor is laminar. This is a realistic assumption, since flow in CVD reactor is normally slow and laminar to insure uniform film growth. (2) Binary diffusion coefficients are used in the hydrogen carrier gas mixture. This assumption is valid, because the more conventional techniques frequently utilizes CH_4 as a carbon-bearing feedstock and dilute this gas with large amounts of H_2 to achieve inlet gas mixtures containing less than 1 mol % CH_4. (3) No chemical reaction takes place in this model. The calculations were performed with the geometry shown in Figs. 1 and 2. In the calculation multi filaments of the diameter 0.25 mm was held 7 mm above the substrate. The distance between the filaments is of 3 mm. The temperature of the substrate and filament were maintained at 1000 K and 2500 K respectively. The reference pressure was 4.0×10^3 Pa (30 Torr) and the walls were maintained at the temperature 328 K. The gas flow rate is around 1.7×10^{-6} m/s (100 sccm). The simulation was performed using CFX [5], a commercial code that employs finite volume. The multi-filament reactor is used to growth diamond films over a large area and an inhomogeneous growth and low growth rate are the two problems related to the physical parameters of the gas during MHFCVD. Our calculations shows a close look near the filament and substrate for the configurations 1 and 2 and identify the presence of a vortex between the substrate and filament.

3. RESULTS AND DISCUSSION

When a mixture of hydrogen and methane comes near the hot filament, the temperature and consequently its composition changes. Temperature, pressure and flow composition are very important factors responsible for the amount of various species formed near the filament. In the Figs. 3 and 4 we show the distribution temperature near de filament and substrate for configuration 1 and 2 respectively.

The Figs 3 and 4 shows no major difference in the temperature distribution. In the configuration 1 the natural convective flow opposes the transport of various species towards the substrate and in the configurations 2 aids the transport. This may suggest that the gas flow has an insignificant influence on the temperature distribution. In addition, our calculation shows that on substrate the temperate is uniform, which may not be correct, because in the presence of filaments, temperature gradients across the substrate may appears due to the proximity of the filament to the substrate [4]. Our calculations do not able to the mesh used over on the substrate.

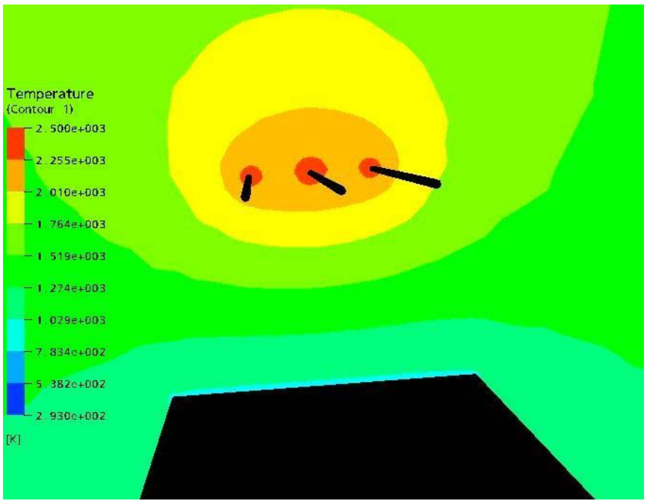

Figure 3 - Configuration 1 - Temperature distribution.

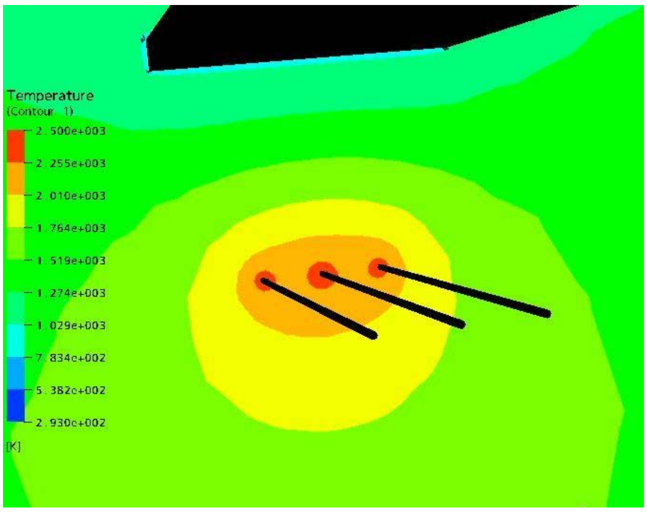

Figure 4 - Configuration 2 - Temperature distribution.

The Figs. 5 and 6 show the fluid flow for both configurations 1 and 2 respectively. The important major difference in the Figs is the presence of two vortexes between the filament and substrate. The presence of the vortexes do not avoid etching of graphite once the vortexes velocity is too small and besides characteristic diffusion lengths, the distance a species will diffuse before being consumed chemically, were estimated for hot-filament CVD conditions by [8] and the characteristic diffusion lengths for H is 10 mm , which agree with our assumption that the vortexes do not affect the etching of graphite. In the Fig. 6 the vortex formation does not appear and the convection may be the cause of it.

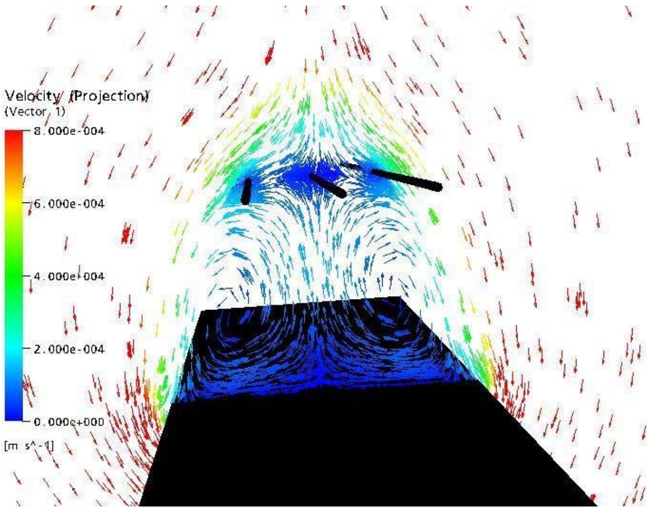

Figure 5 - Configuration 1 - Velocity vector field.

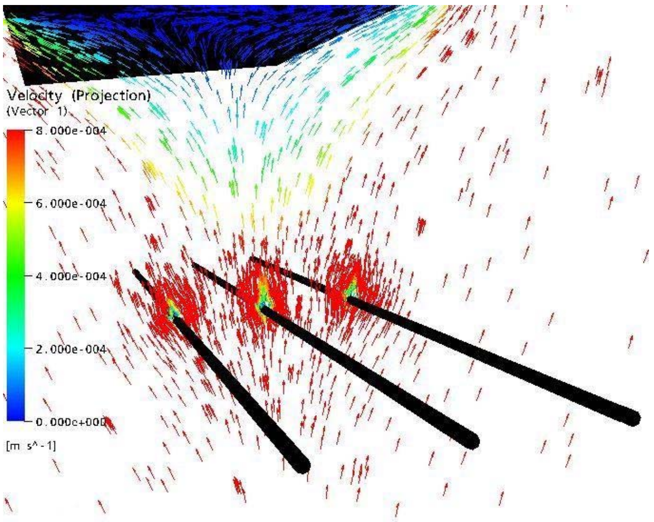

Figure 6 - Configuration 2 - Velocity vector field.

We do not have experimental results for a multi-filament reactor but the reference [6,7] reported, for a single straight hot-filament reactor, HFCVD, that the convective transport is not the dominant mechanism of species transport from the filament to the substrate surface. The Fig. 7 shows a comparison of a calculated temperature and two experimental results. In this case the calculations are made for a single straight hot-filament reactor. It is observed that the computed values are in a good agreement with the experimental observations [4,7].

The importance of the two main transport mechanisms, i.e. convective and diffusive mass transport, can be examined with the help of a dimensionless number, the Peclet number for mass transport. The references [7,8] reported low values of Peclet number in their hot filament systems. The Peclet number and the experimental results observed, as mentioned previously in the references above, indicate that convection is not an important factor in the design of hot filament reactor.

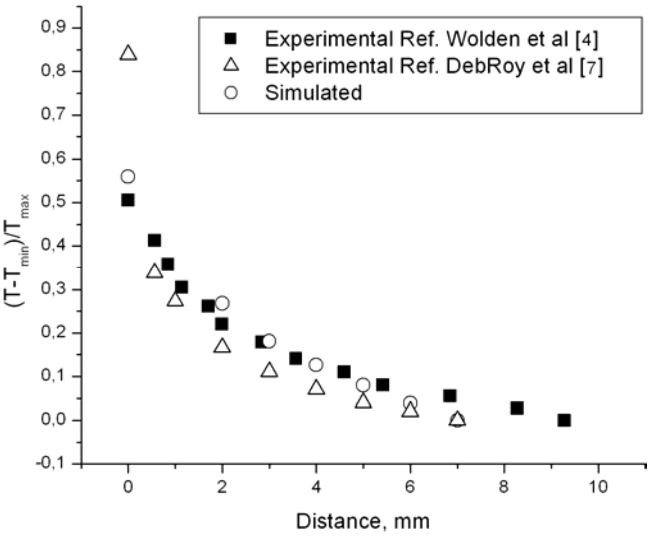

Figure 7 - Temperature profile between filament and substrate for a single straight hot-filament reactor, comparison of simulated temperature with experimental results.

4. CONCLUSIONS

The multi filament reactor is used to growth diamond films over a large area. Song et al [9] reported that the inhomogeneous growth and low rate are the main two problems with HFCVD deposition of diamond films over a large area. During the deposition, molecules of gas that contained carbon (CH_4) and hydrogen (H_2) are excited by heating of hot filaments. The excited molecules (H and CH_3) are transferred over and condensed on the substrate surface and combined to form sp^2 and sp^3 carbon hybridization states. The characteristic diffusion length of CH_3 is between 0.07-2mm, in this case the CH_3 may be consumed chemically between the filament and substrate and the vortexes may play some role in the recombination of CH_3. From the simulation is possible o obtain the profile temperature and compare with experimental results with a good agreement. This paper also shows that the CFX software is a powerful tool to simulate complex geometries.

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