Simulation of CVD Diamond growth in Hot Filament Reactor by Direct Simulation Monte Carlo

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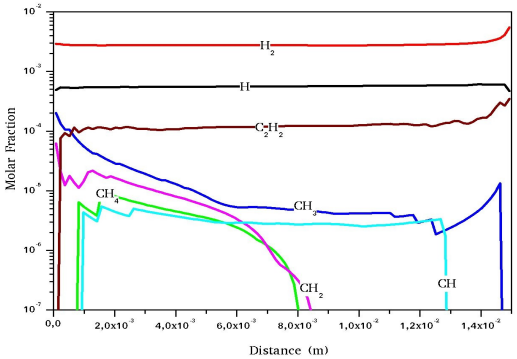
Several techniques are used to obtain diamond films. However, the most used is the Chemical Vapor Deposition (CVD). Although widely used, the knowledge of mechanisms is limited due to its complexity, however, macroscopic simulations have contributed to a significant improvement and a better understanding of the mechanisms involved in CVD. Therefore, we developed a simulation model of the chemical reactions present in the CVD process for homogeneous and heterogeneous phase based on DSMC (Direct Simulation Monte Carlo) technique initially proposed by Bird [1].

The Figure 1 shows the molar fraction versus filament/substrate distance. The initial conditions was 30% of H, 69,5% of H_2 and 0,5% of CH_4, 2500 K for filament temperature and 30 Torr for reactor's pressure. The results are in excellent agreement with those obtained by Coltrin et al. [2].

Figure 2 shows the results for the initial conditions of gas phase proposed by Coltrin versus simulation time. Solid lines represent data obtained by our CODE and the squares are the data obtained from the CHEMKIN package. The consumption of CH_4 during the CVD process is essential, because it allows the formation of precursor species such as CH_3 for the formation of the diamond. It is verified that the CH_4 consumption decrease but, due to the continuous inlet flux the CH_4 continue to survive during the entire simulation. However we note that the data obtained from CHEMKIN does not represents the reality for a HFCVD reactor because the CH_4 decreases and desappear few seconds after the growth process has been started, doesn't considering the inlet CH_4 continuously in the process to allow the film growth with several hours duration.



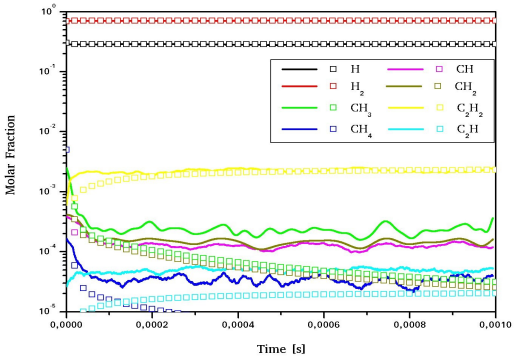


Figure 1 – Distance from filament to substrate Figure 2 – Data from CHEMKIN and CODE

Keywords: CVD Diamond, Simulation, DSMC, Monte Carlo,

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[1] G. A. Bird. *"The Physics of Fluids"*, v. 13, n. 11, p. 2676-2681, 1970.
[2] Coltrin, M. E. Dandy, D. S. Journal of Applied Physics 74, 5803-5820, 1993.
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