Detailed model of diamond crystal growth by MPCVD

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Microwave plasma activated chemical vapor deposition (MPCVD) of single crystal diamond (SCD) is one of the prospect techniques for enhancement of growth rate and uniformity in comparison with high pressure high power technology. Strong local increase of gas temperature up to ~3000C above the substrate provides a heating of the substrate up to ~1000C, while reactive radicals – products of CH_4 dissociation in plasma, interact with the substrate and provide lateral growth of the material on the extended area. However, the localization of heat source and radicals concentration in microwave plasma volume causes one of the key problems in diamond MPCVD technology – a significant non-uniformity of crystal growth over the larger area with diameters up to 100 mm. The complex task of improvement of diamond growth process performance typically requires an enhancement of the radial uniformity of the electric field, gas temperature, plasma density, CH_3 and H profiles near the substrate, which is based on an optimization of growth chamber details such as cavity, plasma domain and substrate holder. A combination of experimental measurements with accurate numerical modeling may help to reduce costs and increase efficiency of SCD development. However, most numerical models are not fully consistent due to absence of chemical kinetics of various radicals interactions [1] and lack of self-consistent simulations of substrate with crystal heating [2].

In this study we present CH_4/H_2 microwave plasma modeling results with consideration of complex model of microwave plasma chemistry with detailed resolution of substrate holder. Advanced electrons kinetics has been implemented in the present model to increase accuracy of plasma properties, gas temperature and radicals concentration calculations. Elementary processes of electron impact excitation of rotational, vibrational, electronic states and ionization of H, H_2, C_mH_n were considered, electron energy distribution functions are calculated as a function of electric field. Concentrations and fluxes to the substrate of major contributors to diamond growth are calculated based on chemical model of C_mH_n ($2 \geq m, n \geq 0$) species interactions in microwave plasma, which considers 14 components and 86 volumetric reactions [4]. Surface chemistry model of diamond growth is described by the major processes of surface passivation by H, species recombination and carbon containing radicals deposition including the deposition of carbon radicals with sp2 and sp3 hybridization [4]. Numerical model validation is completed for the typical experimental conditions of pressure 150 Torr and power 1500 W [2, 3]. Plasma behavior in chamber volume, SCD growth rates and uniformity are demonstrated and discussed for wide ranges of neutral gas pressure 50 – 500 Torr and loaded microwave power 500 – 3000 W at 2.45 GHz considering Bristol reactor design.

References

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