Plasma, heating and kinetics in diamond CVD

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Abstract: In this contribution, we report modeling of a microwave-driven sub-atmospheric pressure hydrogen-methane plasma chemical vapor deposition of diamond. The model includes self-consistent simulation of electromagnetic, heat transfer, plasma chemistry and growth kinetics. Findings demonstrate that the interplay between gas temperature and CH_3 radical distribution play key role in uniform diamond wafer-scale growth.

1. Introduction

Microwave plasma assisted chemical vapor deposition (MPCVD) has been the technological backbone of producing lab-grown diamond. Recent progress in MPCVD homo- and heteroepitaxy, allowing for large-area and high-quality diamond crystal growth, opens many big opportunities in future high-power and quantum electronics. At the same time, growth uniformity remains a fundamental issue for reliable production of high quality wafers at scale [1].

Here, we conduct self-consistent plasma, heat and kinetics modeling to obtain physico-chemical insights in attaining growth uniformity through macroscopic reactor design optimizations and tuning.

2. Methods

In this work, a conventional industry-grade MPACVD reactor operated at 2.45 GHz frequency under typical process conditions is modelled: H_2 mixture with 5% CH_4, absorbed power 1-5 kW and pressure 150-300 Torr. Our model includes self-consistent electromagnetic simulation, heat transfer, plasma chemistry, and growth kinetics in order to calculate diamond growth profile as a function of process time.

3. Results and Discussion

It is demonstrated that conventional 2.45 GHz reactors may not be suitable for large area growth due to limited skin depth. Such limitation results in non-uniform plasma density, gas temperature and, thus, reactive species flux distribution. In Fig.1, it is seen that the CH_3 (main building block in diamond epitaxy) flux behaves differently when attempting to grow on a conventional size substrate of 5 mm as compared to the length scale beyond 20 mm (important size benchmark in microelectronics.) Depending on the flux direction and distribution, either lateral area outgrowth [2] or loss (due to growth nonuniformity) can be induced.

This indicates a key challenge for MPACVD reactor development – increase plasma region dimensions through the optimization of the reactor design and recipe tuning. It will be discussed that increasing the process cavity dimensions to operate at 915 MHz could help increase the flatness of CH_3 flux thereby resulting in improved uniformity of diamond growth.

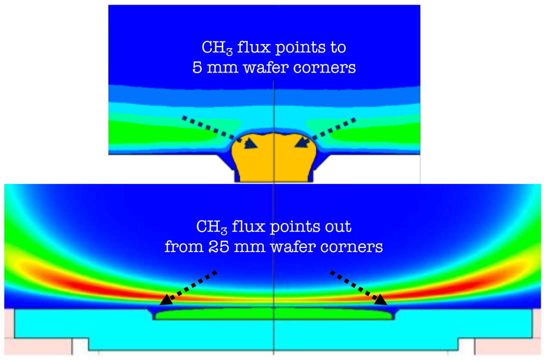

Fig. 1. Comparison between 5 mm versus 25 mm diamond growth in a 2.45 GHz reactor highlighting the interplay between the growth rate uniformity and methyl radial distribution.

4. Conclusion

Investigation of CH_3 radial formation activated by hydrogen-plasma and corresponding means of its flux shaping was conducted. Our results bridge the gap between the input reactor parametrization/optimization and the resulting growth uniformity of laterally large diamond wafers during MPACVD homoepitaxy. In particular, by self-consistently modelling RF mode structure of the input power, plasma properties, gas heating and plasma chemistry we can directly visualize gaseous temperature and CH_3 distributions as functions of the reactor inputs and predict the degree of lateral growth uniformity.

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References
[1] Baryshev and Muehle, IEEE Trans. Plasma Sci. **52**, 1082-1103 (2024).
[2] Bai et al., Front. Carbon **3**, 1367715 (2024).