Synthesis of diamond films by microwave plasmas:

modelling/experimental coupling approach

***Laboratoire des Sciences des Procédés et des Matériaux* – UPR CNRS 3407**

Research team: ***Diamond and Carbon Materials***

Supervisor: ***Audrey Valentin*** (+33 (0)1 49 40 34 18, audrey.valentin@lspm.cnrs.fr)

Thesis supervisor: ***Fabien Bénédic*** (+33 (0)1 49 40 34 23, fabien.benedic@lspm.cnrs.fr)

The growth by PECVD (Plasma-Enhanced Chemical Vapor Deposition) process of diamond films with a very low density of crystalline defects, well-defined crystalline orientations and high microstructural quality, over the widest possible surface, is a major challenge for the emergence of high-performance applications. The optimization of the characteristics of diamond films synthesized by PECVD is based on the knowledge and control of growth mechanisms according to operating conditions (working pressure, gas composition, microwave power, substrate temperature, etc.). This requires both experimental studies and the development of numerical tools capable of making the link between experimental conditions, plasma composition, interactions between active species with the surface of the substrate and film, the growth rate of the different crystalline faces and the morphology/final texture of the deposited film. For these studies, the laboratory has for several years had plasma models [1], a macroscopic geometric growth model [2] and, more recently, a kinetic Monte-Carlo model that links the first two numerical tools [3].

In this context, the proposed thesis topic will focus on the study and the control of the growth of nano-, poly- and mono-crystalline diamond films by microwave-assisted CVD plasmas through an approach coupling crystal growth experiments and plasma diagnostics and the use of the modeling tools described above, more particularly the kinetic Monte Carlo code that should be improved, in order to master growth mechanisms to produce diamond films with properties suitable for different applications.

This thesis topic is part of the ANR TRAMPOLINE project (2023-2026) which focuses more particularly on the spatial location of nitrogen-vacancy (NV) colored centers in diamond crystals for applications in the field of quantum technologies.

The candidate should have a strong interest in experimental sciences and numerical modeling, as well as good knowledge in various scientific fields (materials structure and physics, thin films, process engineering, plasma processes, plasma diagnostics...).

This thesis from university Sorbonne Paris Nord will take place from October 2023 at the LSPM within the research operation "Diamond and Carbon Materials" of the axis "Plasma Processes, Nanostructures and Thin Films" (PPANAM).

References

[1] K. Hassouni, O. Leroy, S. Farhat, A. Gicquel, Modeling of H_2 and H_2/CH_4 Moderate-Pressure Microwave Plasma Used for Diamond Deposition, Plasma Chemistry and Plasma Processing. **18** (1998) 325–362. https://doi.org/10.1023/A:1021845402202.

[2] F. Silva, J. Achard, X. Bonnin, A. Michau, A. Tallaire, O. Brinza, A. Gicquel, 3D crystal growth model for understanding the role of plasma pre-treatment on CVD diamond crystal shape, Physica Status Solidi (a). **203** (2006) 3049–3055. https://doi.org/10.1002/pssa.200671101.

[3] A. Valentin, O. Brinza, S. Farhat, J. Achard, F. Bénédic, 3D kinetic Monte-Carlo simulations of diamond growth on (1 0 0) surfaces, Diamond and Related Materials, **123** (2022) 108865. 10.1016/j.diamond.2022.108865.