Post doc Offer:

Self-consistent modeling of dusty plasma to study formation of nano-diamonds in a MW-plasma reactor

Abstract :

This proposal concerns numerical studies on high quality nanodiamonds formation in miwrowave assisted plasma. the proposed work consist of understanding the mechanisms that governs nanoparticles (NPs) formation and growth to improve the process using numerical simulations.

Context:

The unique properties of nanodiamonds finds application in wide range of areas such as drug delivery, biomarkers, tribological applications and quantum technologies. Nanodiamonds with defects such as N-vacancy (NV centers) have immense potential towards development of quantum technologies. However, producing high quality nanodiamonds with high purity, high crystallinity, photostability and size control remains challenging. Recently, PEMA group at LSPM have demonstrated production of large number of diamond particles with high crystallinity and small sizes (50 to 200 nm) by tuning the operating conditions of the MW assisted plasma reactor used originally for growth of CVD diamond. Nonetheless, despite the encouraging results obtained so far, many applications requires diamond NP's with narrow size distributions and a tight control of the average size in the nanometer range. Therefore the process needs to be optimized to obtain high quality nanodiamonds with size control. For this purpose, it is necessary to understand how the different gas phase elementary processes, transport phenomena and plasma-surface interaction involved in the deposition plasma affect the nucleation of nano-diamonds. It is in particular necessary to understand the different pathways for the formation of nano-diamonds and other allotropes of carbon as high quality of nano-diamond with size control is desirable. This understanding of nanodiamond formation will guide in production of NV-centers using Nitrogen doping.

Nanodiamonds growth takes place in MW hydrogen-methane plasmas which are complex media containing electrons, neutral and charged molecular species, large clusters which could possibly nucleate into solid carbon nanostructures such as nanodiamonds, graphene, fullerene and amorphous carbon. These plasmas remain poorly understood and are governed by diverse phenomena occurring on wide scales ranging between the molecular size, particle sizes to the size of the plasma i.e. gas phase collisional processes, plasma-surface interaction processes, aerosol dynamics, interaction between microwave and the dusty plasma etc. The ultimate objective of the modelling group is to build a predictive multi-dimensional self-consistent fluid model with interaction between MW-plasma and particles.

Work description

The post-doc will mainly focus on understanding the different phenomena that govern the nanoparticle formation and plasma evolution through modelling and comparison with experiments. The objective of the modelling work is to accompany the experimental team to optimize the process of NPs fabrication and control. The candidate will be involved in the development of the chemistry scheme resulting in the NP nucleation and particle growth. For this purpose, a simple 0D/1D plasma model [1] coupled with aerosol model that follow particle transport and growth will be used to predict the formation of carbon NPs in the plasma. Extensive studies will be performed to understand the phenomena that govern the NPs formation and size and quality which are poorly understood and is critical in the development of several carbonated NPs processes and is expected to produce publications interesting for large audience.

Opportunities

First Although the candidate will be working with the modelling group, he/she will carry out extensive interaction with the experimental group that produces (nano)diamond in MW plasmas.

The results of this study will also be used to describe a reduced scheme for particle nucleation and growth that could be implemented by the group in the in-house 2 dimensional self-consistent model constructed for MW assisted plasmas for H2-methane plasmas [2, 3].

The candidate will also have the opportunity to interact with the molecular dynamics team of the lab who are involved in calculating collision cross-sections.

Requirements

1) The candidate should have a background in fluid dynamics / heat transfer and chemistry. Knowledge of aerosol dynamics is a plus.
2) The candidate is expected to have fair programming skills, preferably Fortran.
3) The candidate should be capable of carrying out research independently and be able to regularly present his/her results to other collaborating groups.

Duration of postdoc

The duration of postdoc is for a period of 1 year with a Gross salary of around 2600 € (2100 € net) based on the experience.

Location

LSPM UPR3407 Villetaneuse
Medelling Group : K. Hassouni, S. Prasanna and A. Michau

Point of contact

Interested candidates can send their Cvs to -
Swaminathan Prasanna
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[1] K. Hassouni, F. Mohasseb, F. Bénédic *et al.*, "Formation of soot particles in Ar/H2/CH4 microwave discharges during nanocrystalline diamond deposition: A modeling approach," *Pure and applied chemistry,* vol. 78, no. 6, pp. 1127-1146, 2006.

[2] S. Prasanna, A. Michau, C. Rond *et al.*, "Self-consistent simulation studies on effect of methane concentration on microwave assisted H2-CH4 plasma at low pressure," *Plasma Sources Science and Technology,* vol. 26, no. 9, pp. 097001, 2017.

[3] S. Prasanna, C. Rond, A. Michau *et al.*, "Effect of buoyancy on power deposition in microwave cavity hydrogen plasma source," *Plasma Sources Science and Technology,* vol. 25, no. 4, pp. 045017, 2016.