Self consistent simulation of dust formation and dynamic in non-equilibrium RF Ar-acetylene plasma

G. Tetard[1], A. Michau[1], S. Prasanna[1], P. Brault[2] , K. Hassouni[1(*)]

[1] *LSPM, CNRS-UPR3407, Université Sorbonne-Paris-Nord, 99 Avenue J. B. Clément 93430 Villetaneuse, France.*

[2] *GREMI, CNRS-UMR XXX, Université d'Orléans*
(*) *khaled.hassouni@lspm.cnrs.fr*

Dust particle formation and dusty plasmas dynamics in electrical discharges are of great interest in many research or technological fields ranging from astrophysics to fusion sciences and including microelectronics processes and material processing [1]. In this paper, we present a computational investigation of dust formation and dusty plasma effects in capacitively coupled Ar/C_2H_2 RF discharges. More specifically, we developed a fully coupled dusty plasma model that describes the coupled effects of (i) discharge dynamics, (ii) complex chemical kinetics that results in molecular growth and dust-particle nucleation, and (iii) aerosol dynamics that govern the space-time evolution of dust-particle size distribution and plasma characteristics. The discharge dynamics is described using a drift-diffusion model taking into account flow effect that may be of a critical importance in the investigated plasmas [1]. Molecular growth routes through neutral radicals, negative ions or positive ions were considered in the chemistry and reactive flow models [2]. The impact of molecular growth kinetics on the discharge dynamics was fully taken into account by a proper consideration of the major heavy ions involved in the discharge equilibrium. The molecular growth kinetics is considered up to a largest molecular edifice (LME) with a prescribed maximum number of carbon atoms. The growth rate of this LME determines the nucleation rate in the model. The aerosol dynamics were described assuming a bimodal size-distribution with a nucleation mode and a core mode. This assumption proved to give accurate description as far as the evolution of the core distribution is concerned [3]. The aerosol dynamics model takes into account nucleation as determined by the molecular growth model, particle growth due to the deposition of radicals or ions inferred either form the plasma model or from the molecular growth model, and coagulation effects within the nucleation mode or between the nucleation and the growth modes. The enhancement of coagulation kinetics due charge fluctuation is also taken into account for the nucleation mode that may exhibits significant population of neutral or positively charged particles.

Simulations were carried out for several feed gas composition, i.e., C_2H_2% in Ar/C_2H_2 mixture. Results showed that, depending on the discharge conditions, the molecular growth is governed by either neutral or positively charged polyynes chemistries initiated by acetylene and C_2H radical. They also show that dust-nucleation competes with surface deposition on the electrodes, and strongly depends flow velocity [3]. In particular, dust particle formation kinetics significantly depends on the nature of the interaction between radicalar species or ions and electrodes. As for dust-particle formation, results showed that nucleation takes place continuously in the discharge gap. It is more enhanced in the bulk of the discharge when the positive ion molecular growth route is dominant, while it takes place in the whole discharge gap when the radical route is predominant. Eventualy, results showed that when increasing the amount of acetylene in the feed gas, the discharge transitions from (i) a low dust-particle density plasma with a small Havnes number, a fairly large particle diameter and almost no dusty plasma effect to (ii) a high density dust-particle density plasma with a large Havnes number, i.e., larger than 10, a fairly small particle diameter, i.e., <10 nm, and a strong dusty-plasma effect. They also show a counter-intuitive effect where larger dust-particle density significantly enhance positive ion density and therefore particle nucleation kinetics. This shows a self-promoting effect under large acetylene concentration in the feed gas, i.e., 50%, where larger dust particles density favours particle nucleation

Acknowledgement: This work was supported by the French 'Agence Nationale de la Recherche' and EUROFUSION. One of the author (KH) acknowledges the support of the Institut Universitaire de France.

[1] R. L. Merlino and J. A. Goree., Physics Today 57, 7, 32 (2004), doi: 10.1063/1.1784300.

[2] A. Michau et al., Plasma Sources Sciences and Technol. 25, 1 (2016) 015019.

[3] G. Tetard et al. Plasma Processes and Polymers, 19, 5 (2022), 2100204

[4] G. Tetard et al J. Phys D (2024)