Coupling of ToF-SIMS and AFM for the identification of the chemical species involved in the nucleation process of soot particles in flame combustion

J. Elias[1], A. Faccinetto[1], X. Mercier[1], N. Nuns[2], S. Godey[3], D. Deresmes[3] and T. Mélin[3]

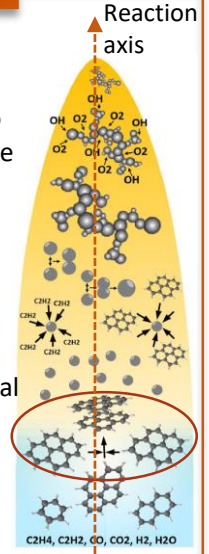
[1] Univ. Lille, CNRS, UMR 8522 - PC2A - Physicochimie des Processus de Combustion et de l'Atmosphère, F-59000 Lille, France

[2] Univ. Lille, CNRS, M. E. Chevreul Institut, F-59000 Lille, France

[3] Univ. Lille, CNRS, UMR 8520 - IEMN - Institut d'Électronique de Microélectronique et de Nanotechnologie, F-59000 Lille, France

Introduction

The soot nucleation process, corresponding to the transformation of gaseous molecular precursors into condensed phase soot particles, is the less understood step of the soot formation process in flame combustion. The hypothesis of a nucleation process driven by the dimerization of small polycyclic aromatic hydrocarbons (PAHs), has been used in models but experimental evidences are still lacking.
In this work, ToF-SIMS and AFM are coupled with the aim of characterizing the species involved in the soot nucleation process.



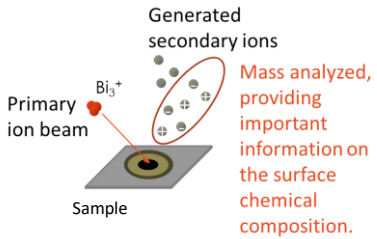
(Kholghy et al., *Carbon 100,* 2016)

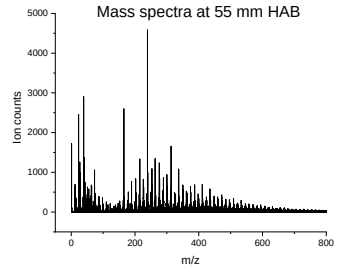
Sampling

- **Laminar methane diffusion flame** stabilized at atmospheric pressure.
- Samples extracted from the centreline of the flame at different heights above the burner (HAB) using a quartz microprobe and deposited on titanium wafers.

ToF-SIMS

Time-of-Flight Secondary Ion Mass Spectrometry

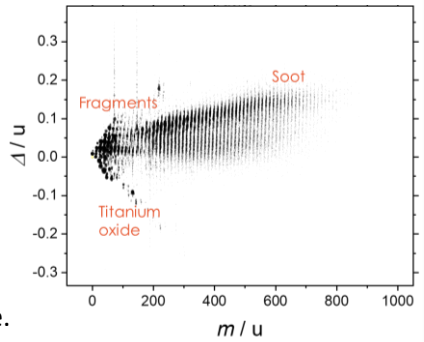




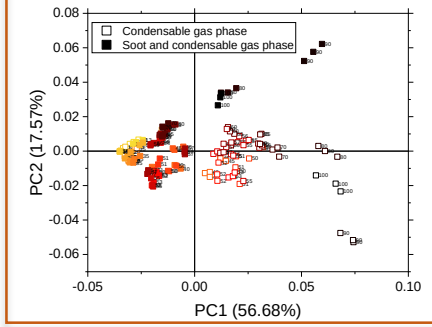
Results

Mass defect plot $\Delta = m/z - m$

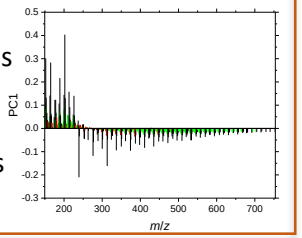
➡ Assignement of a molecular formula to the selected *m/z*.



Principal Component Analysis:
PCA is used to classify the data and explain the variance of the database.

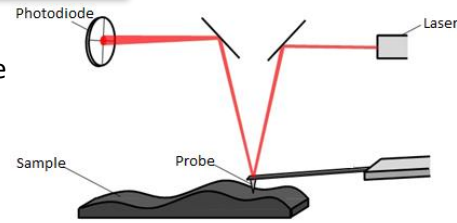


- Different behavior in the nucleation zone of the flame.
- PC1<0 : high mass PAHs
- PC1>0 : low mass PAHs

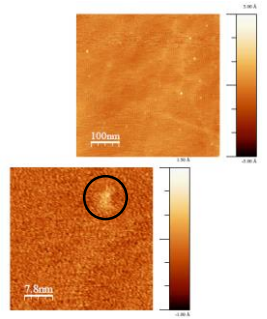


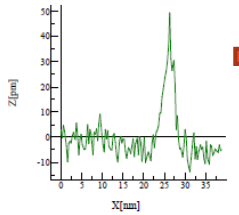
AFM

Atomic Force Microscopy delivers direct molecular imaging of the surface at the atomic scale and gives access to the electronic properties of the molecular species.

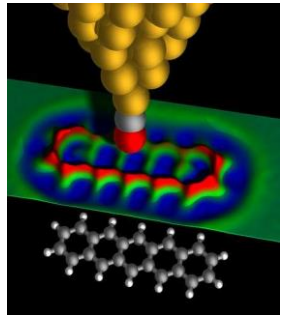


Preliminary results





➡ Soft spherical structures on a 55 mm HAB sample having a 2-4 nm diameter and a 0.3 Å height, consistent with the size of nascent soot nanoparticles.

Perspectives

In future work, we will use a functionalized CO tip, which probes the molecules with a sub-Å oscillation amplitude at low temperature, to resolve isomeric structures that are detected at the same *m/z*, for a complete characterization of the species involved in the soot nucleation process.