



HAL
open science

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

Jessy Elias, Xavier Mercier, Alessandro Faccinetto, Nicolas Nuns, S. Godey, D. Deresmes, Thierry Melin

► To cite this version:

Jessy Elias, Xavier Mercier, Alessandro Faccinetto, Nicolas Nuns, S. Godey, et al.. Coupling of ToF-SIMS and AFM for the identification of the chemical species involved in the nucleation process of soot particles in flame combustion. European Aerosol Conference – EAC 2020, Aug 2020, Aachen, Germany. pp.457. hal-03008218

HAL Id: hal-03008218

<https://hal.science/hal-03008218v1>

Submitted on 16 Nov 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

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. Elias¹, A. Faccinetto¹, X. Mercier¹, N. Nuns², S. Godey³, D. Deresmes³ and T. Mélin³

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

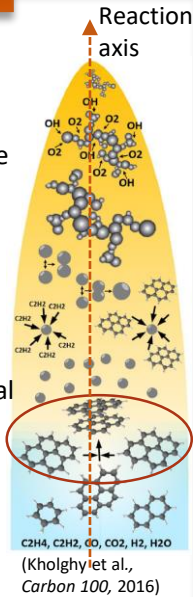
² Univ. Lille, CNRS, M. E. Chevreul Institut, F-59000 Lille, France

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



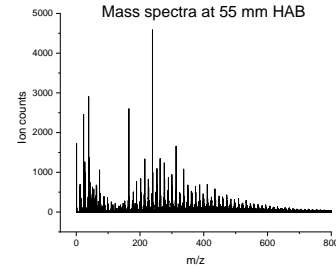
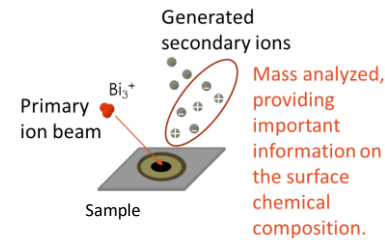
Introduction

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.



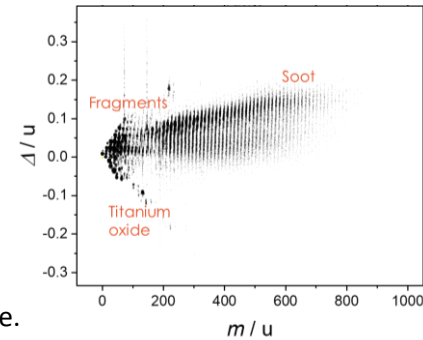
ToF-SIMS

Time-of-Flight Secondary Ion Mass Spectrometry



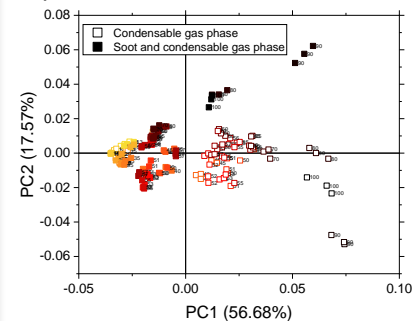
Results

Mass defect plot $\Delta = m/z - m$
 ➔ Assignment of a molecular formula to the selected m/z .

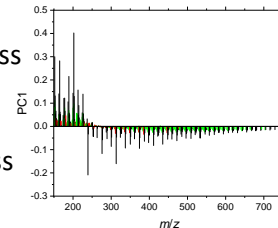


Principal Component Analysis:

PCA is used to classify the data and explain the variance of the database.

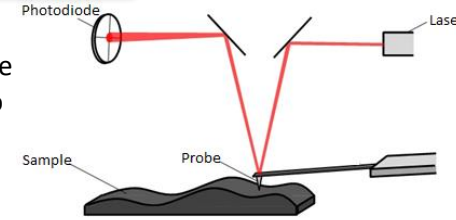


- Different behavior in the nucleation zone of the flame.
- PC1 < 0 : high mass PAHs
- PC1 > 0 : low mass PAHs

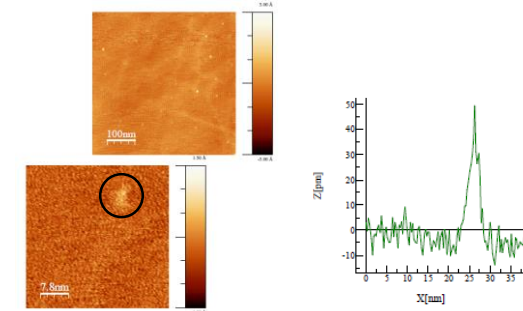


AFM

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.



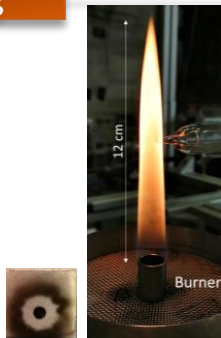
Preliminary results



➔ 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.

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.



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.

