First results of the "MERMOSE" campaign : influence of aircraft engine thrust on physical and chemical properties of soot particles. A study from the macroscale down to the atomic scale by HRTEM, XPS and NEXAFS

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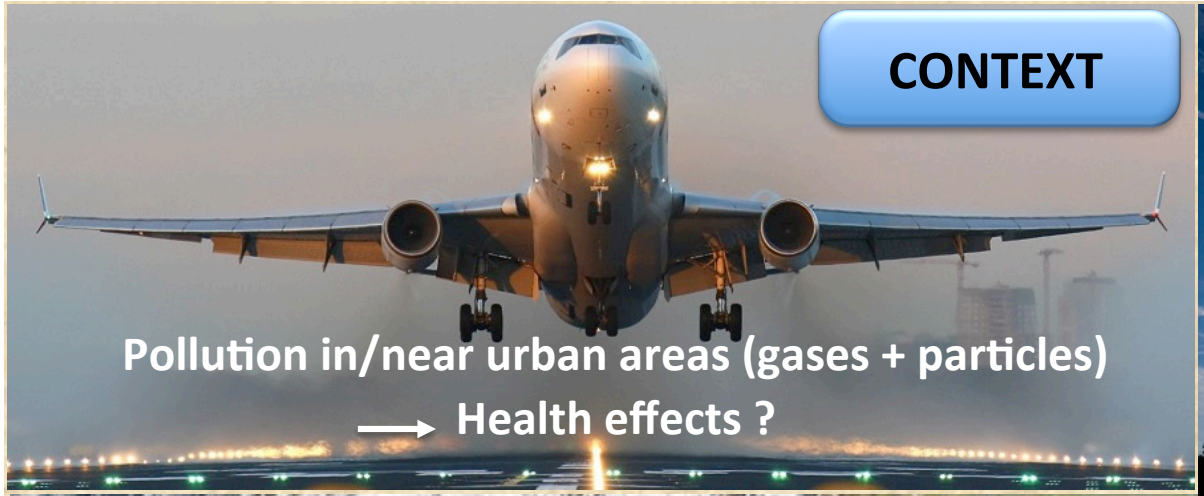
Canadian Light Source Centre canadien de rayonnement synchrotron

IRSN Institut de radioprotection et de sûreté nucléaire

ONERA The French Aerospace Lab

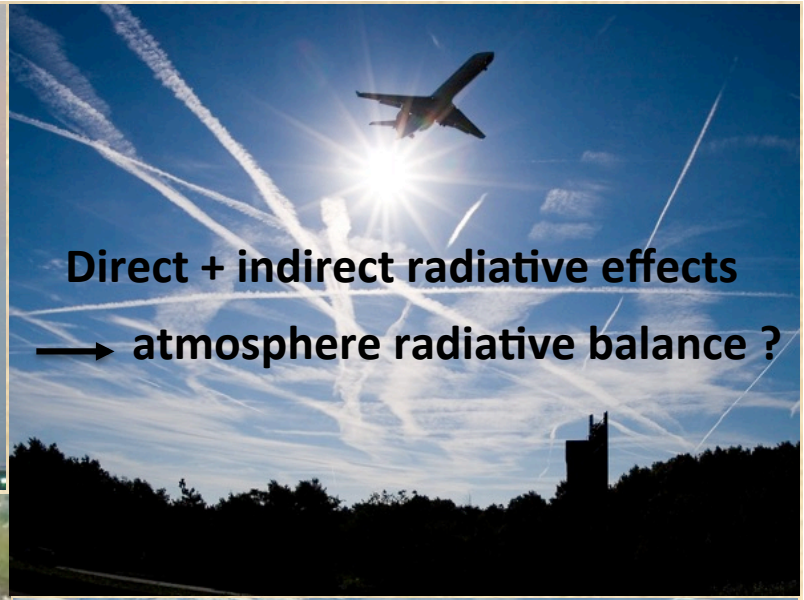
SAFRAN Snecma

CONTEXT



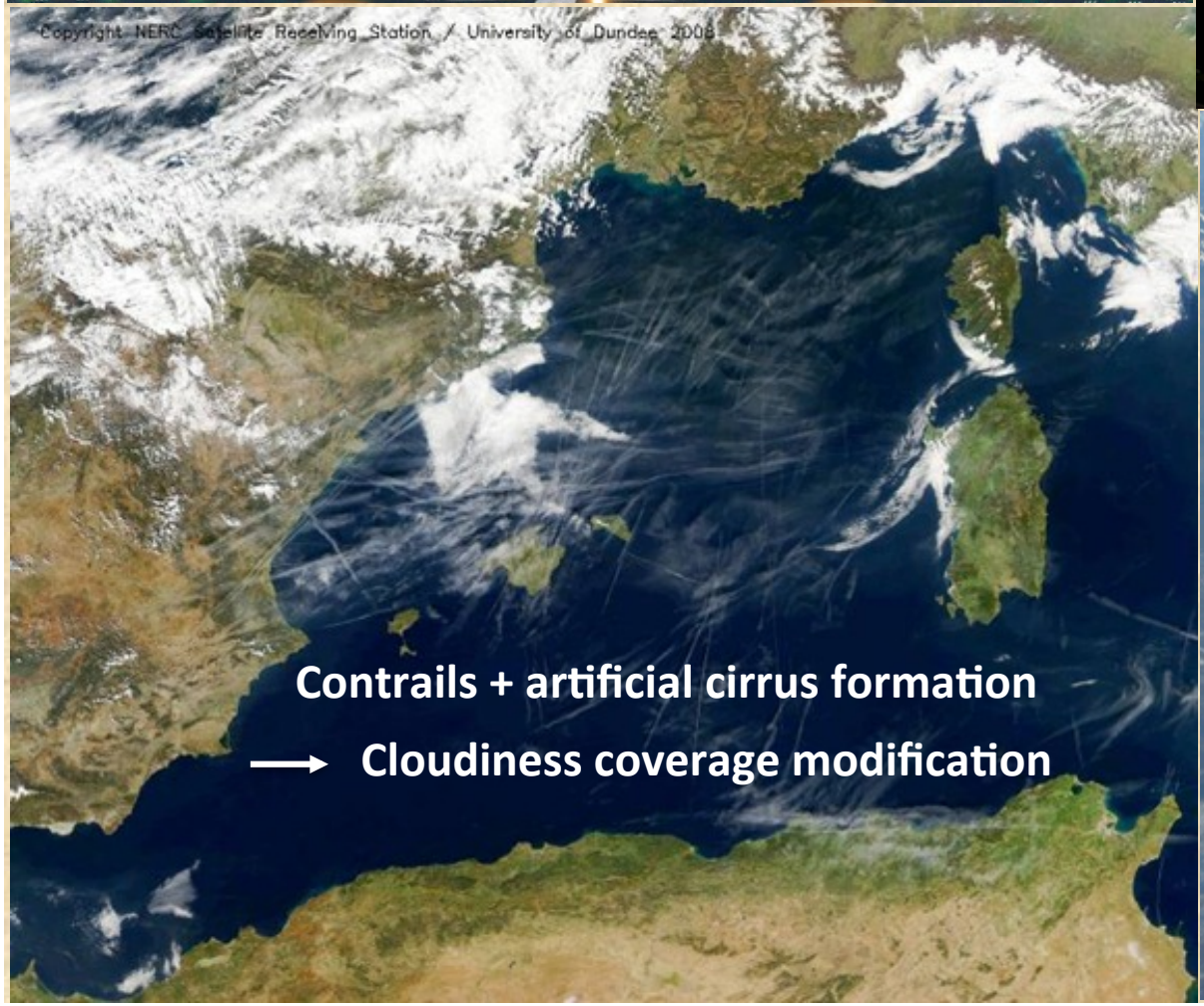
Pollution in/near urban areas (gases + particles)

→ Health effects ?



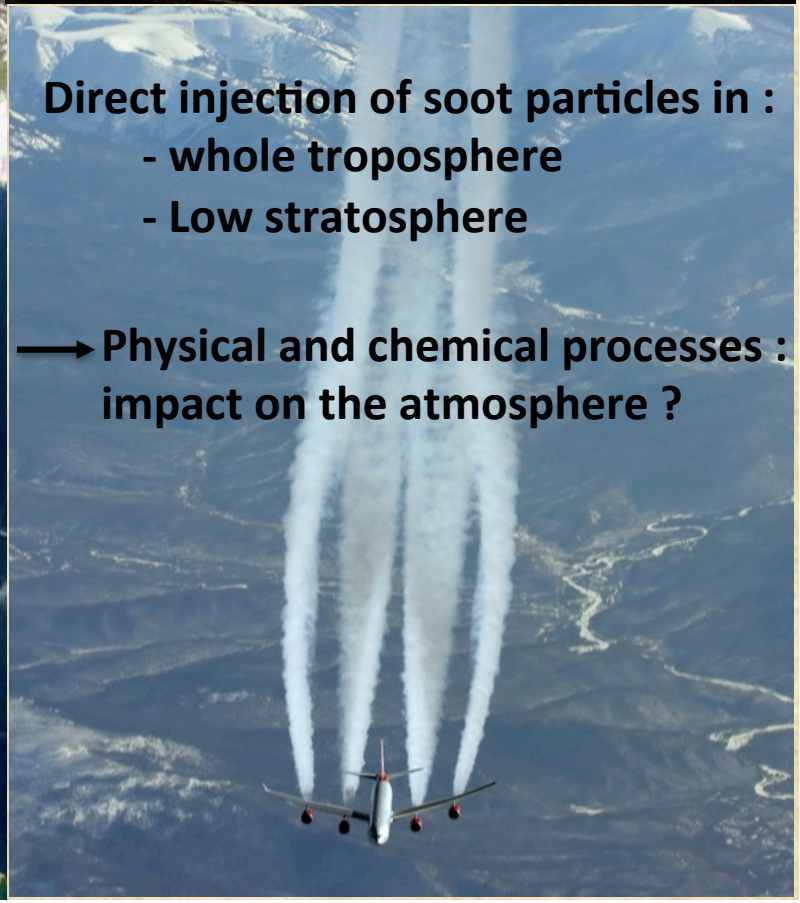
Direct + indirect radiative effects

→ atmosphere radiative balance ?



Contrails + artificial cirrus formation

→ Cloudiness coverage modification

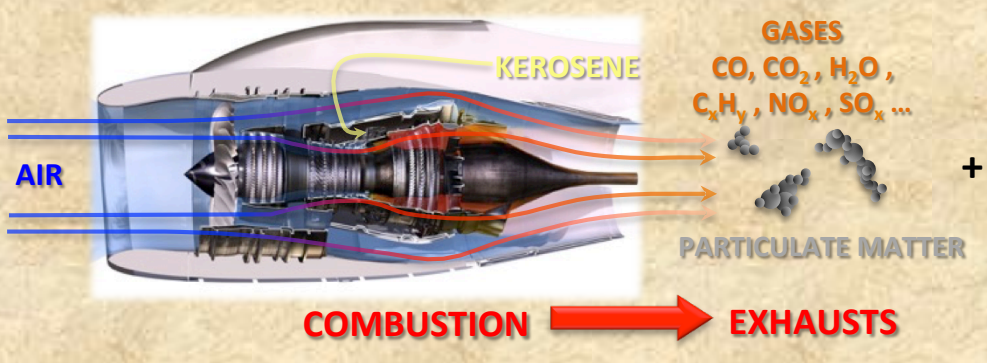


Direct injection of soot particles in :

- whole troposphere
- Low stratosphere

→ Physical and chemical processes : impact on the atmosphere ?

« MERMOSE » project : measurement and study of the reactivity of aircraft engine emissions



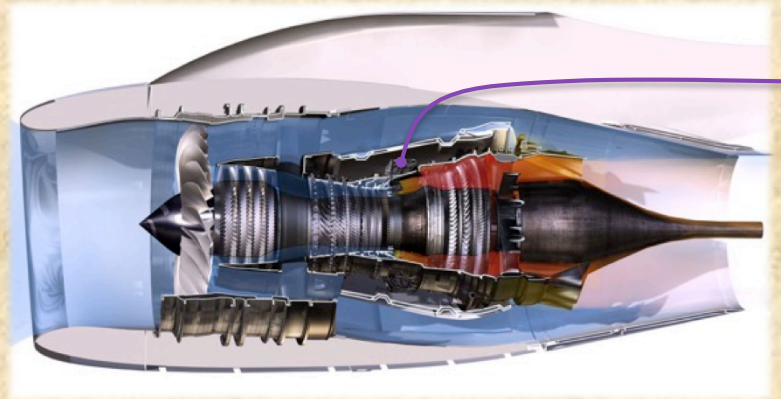
+ poster N° 33 (F.-X. Ouf *et al.*)

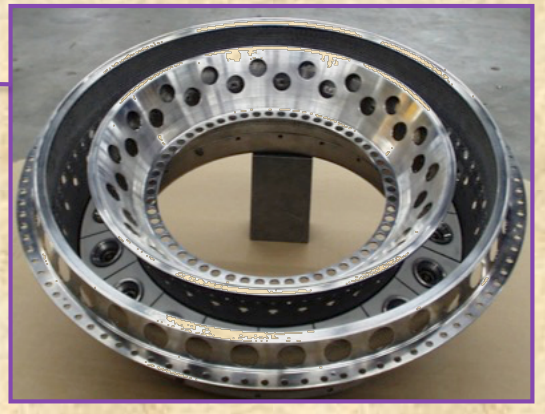
1. Test bench facilities

- Characterisation of particles and gases emitted by a modern turbofan engine (SaM146-1S17 ; PowerJet)

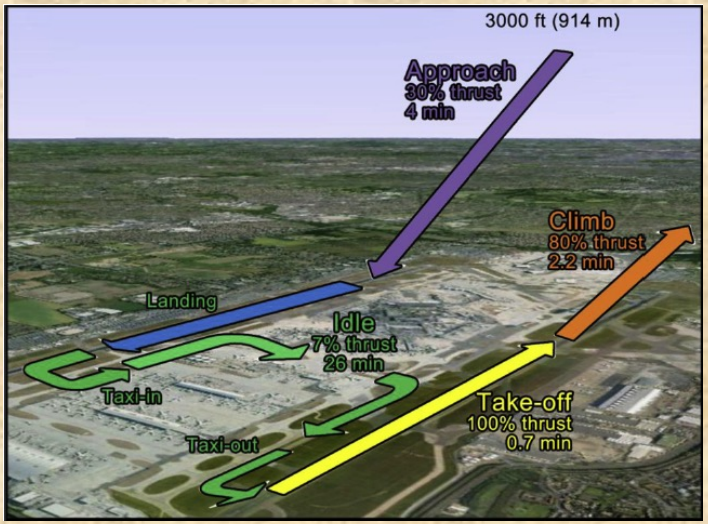
2. Laboratory investigations

- Characterisation of soot particles and their impact on ice crystal formation
- Look for aircraft soot surrogates





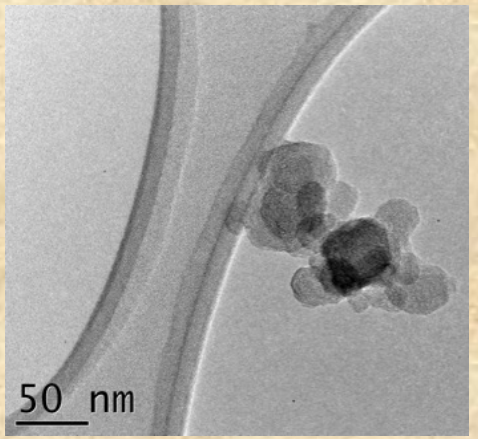
- Engine certified by Snecma in June 2010
- Turbo-fan with an optimised single annular combustor
- 15400 to 17800 lb of thrust
- Fan diameter : 1.22 m
- Engine length : 2.20 m
- Fuel : Jet A1



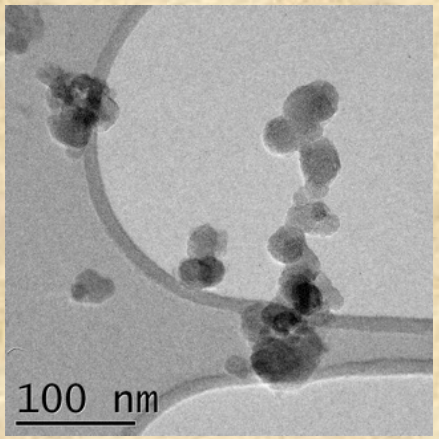
Engine thrust : 30, 70, 85 , 100 % F_{00} (take-off)

SOOT AGGREGATES MORPHOLOGY

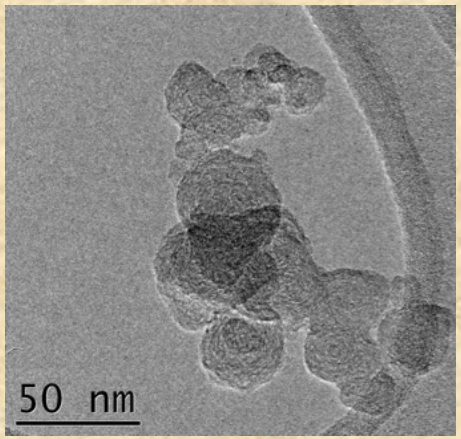
30%



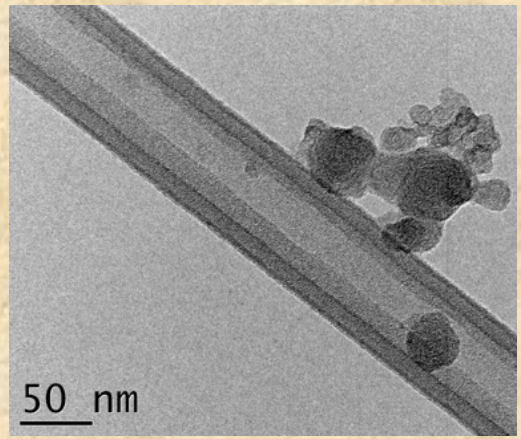
70%



85%



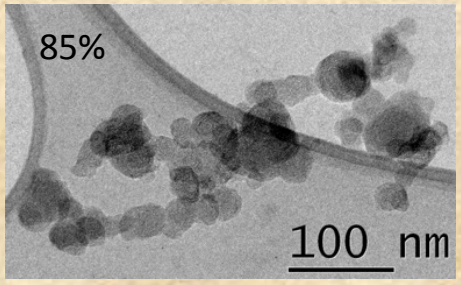
100%

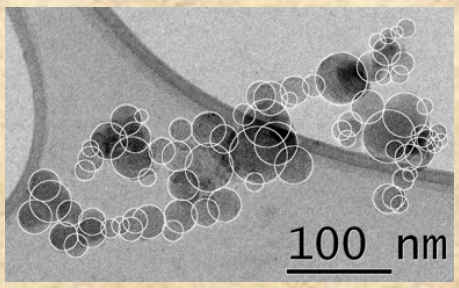


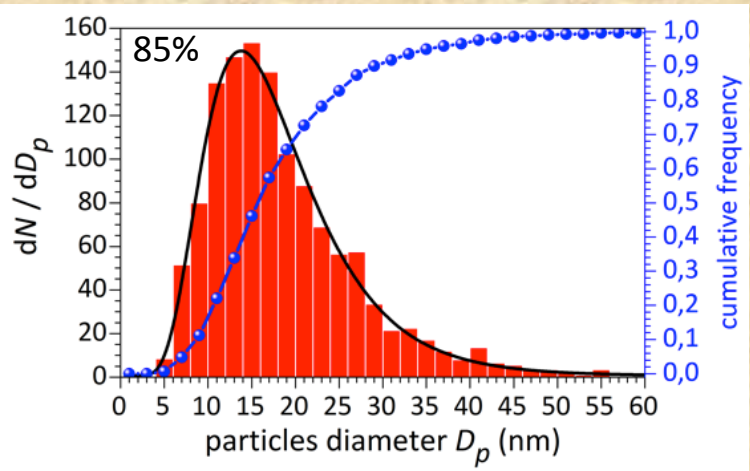
- Irregular and compact : $1.7 \leq Df \leq 1.9$
- Composed of aggregated primary particles
- Morphology : no evolution with engine power

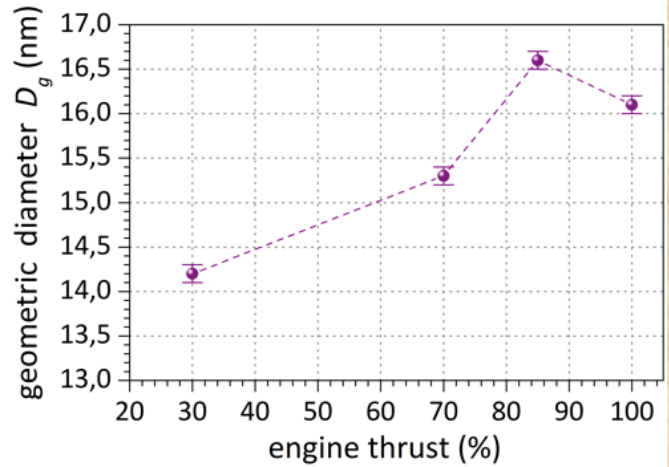
SOOT PRIMARY PARTICLES DIAMETER

- **size distribution**





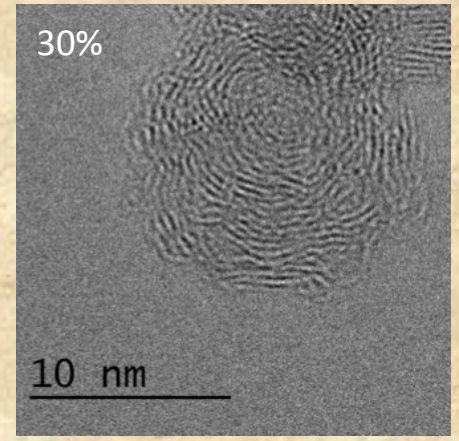


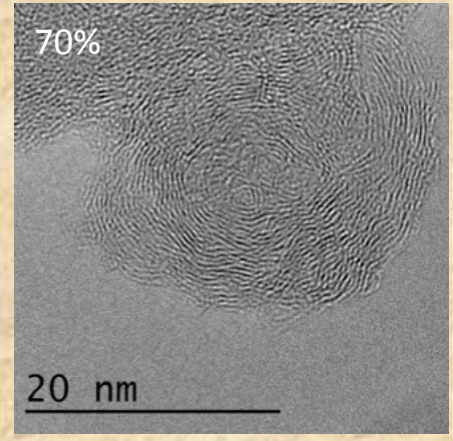


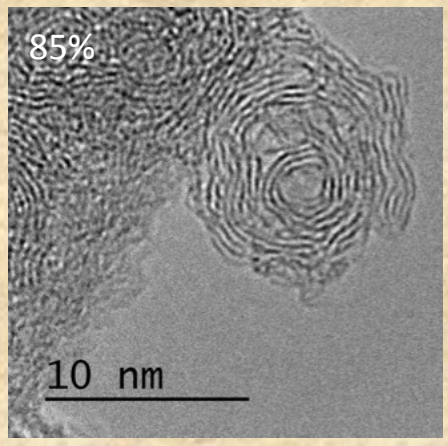
	30%	70%	85%	100%
N	1865	1298	2496	2555
distribution	lognormal	lognormal	lognormal	lognormal
mode (nm)	12.0 ± 0.1	13.0 ± 0.2	13.8 ± 0.2	13.7 ± 0.2
d_g (nm)	14.2 ± 0.1	15.2 ± 0.1	16.6 ± 0.1	16.1 ± 0.1
σ_g	1.51 ± 0.01	1.49 ± 0.01	1.54 ± 0.01	1.50 ± 0.01

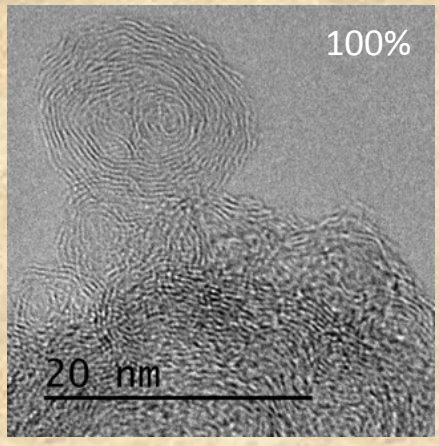
Particles' diameter tends to increase with engine thrust

- **turbostratic texture**

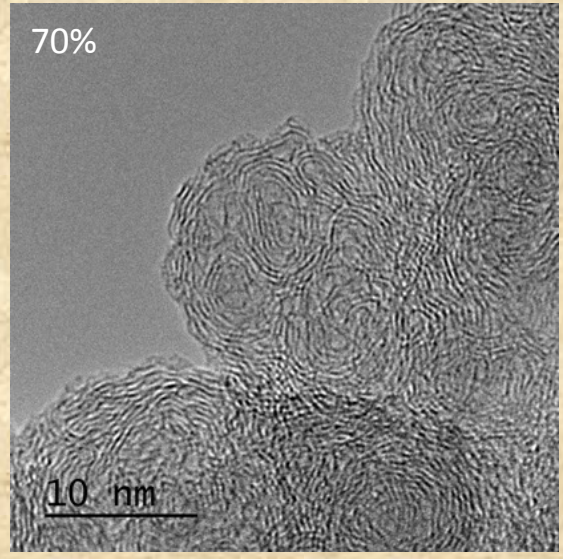


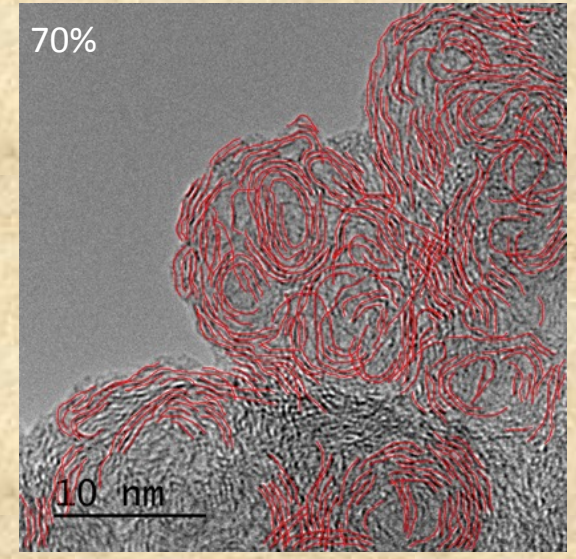


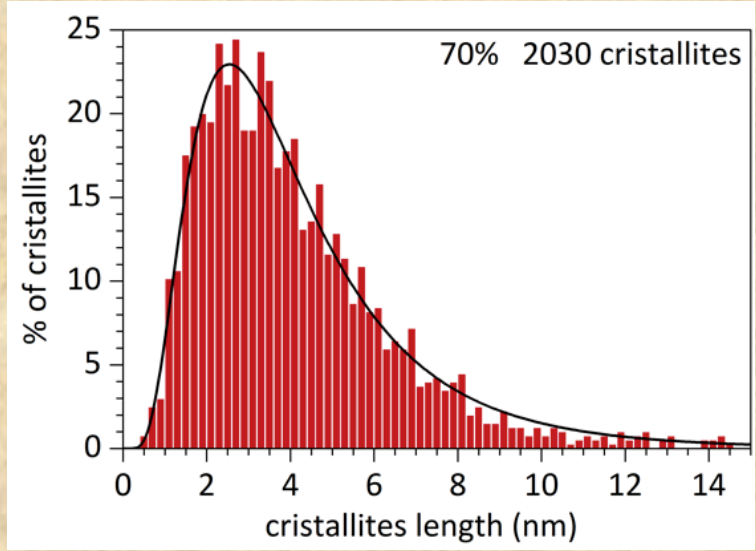




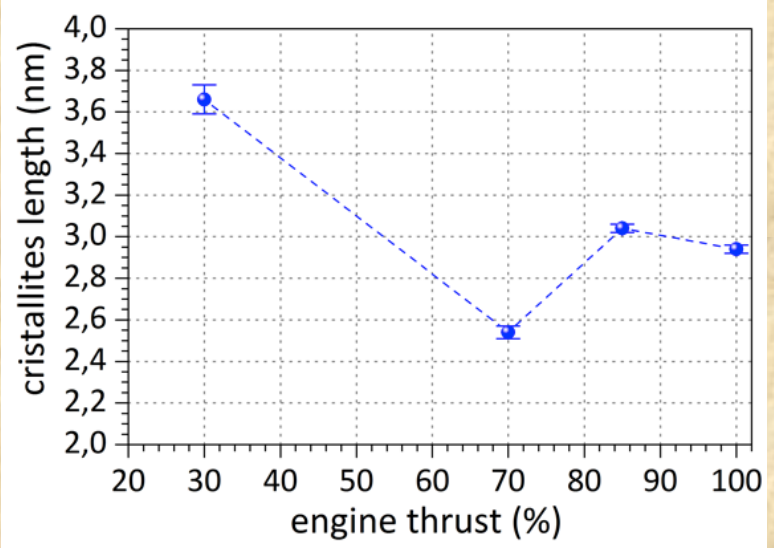
CARBONACEOUS CRISTALLITES LENGTH





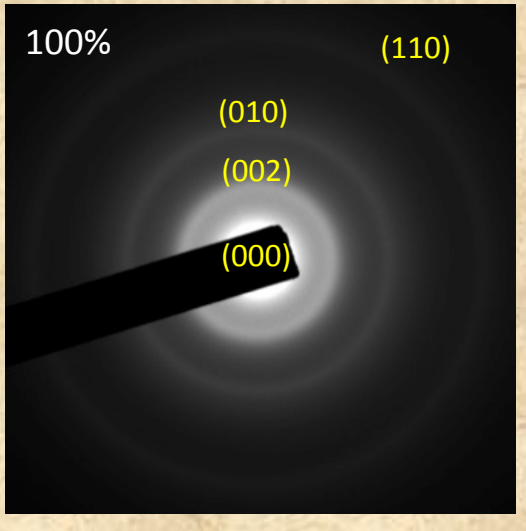


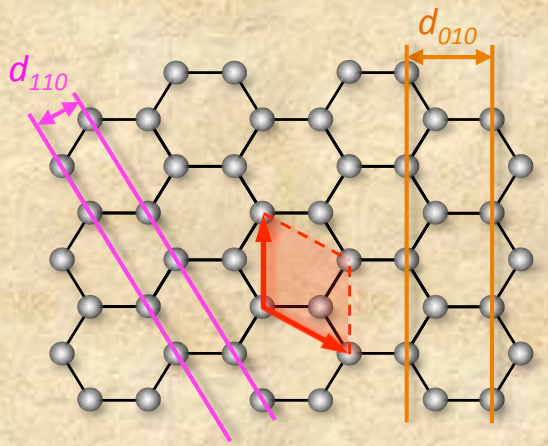
	30%	70%	85%	100%
N	2221	2030	2130	2128
distribution	lognormal	lognormal	lognormal	lognormal
mode (nm)	3.66 ± 0.07	2.54 ± 0.03	3.04 ± 0.05	2.94 ± 0.04
L_g (nm)	4.97 ± 0.09	3.59 ± 0.04	4.27 ± 0.07	4.10 ± 0.05
σ_g	1.74 ± 0.03	1.80 ± 0.02	1.79 ± 0.02	1.78 ± 0.02

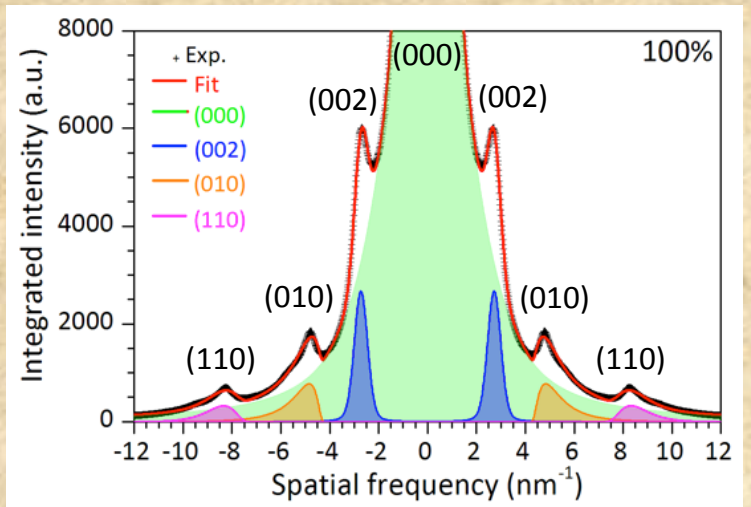


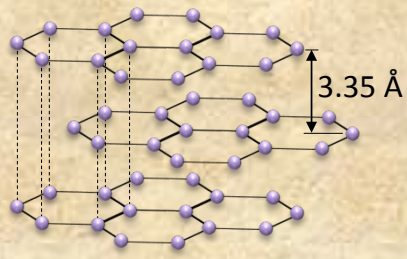
Cristallites' length tends to decrease with increasing engine thrust

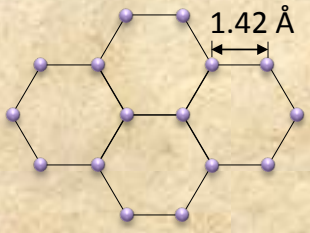
CARBON BONDING LENGTH





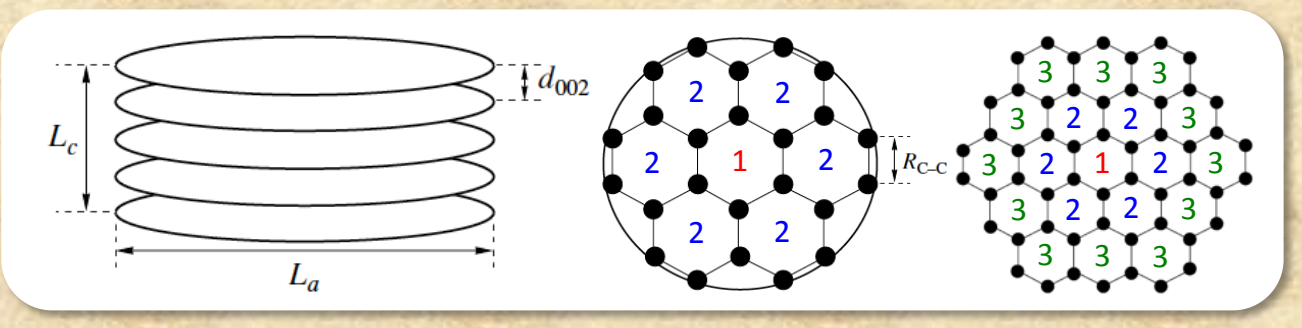






	Graphite	30%	70%	85%	100%
d_{002} (Å)	3.35	3.63	3.65	3.68	3.63
d_{010} (Å)	2.13	2.07	2.06	2.07	2.09
d_{110} (Å)	1.23	1.20	1.20	1.20	1.21
$L_{C\text{-}C}$ (Å)	1.42	1.39	1.38	1.39	1.40
		-2.2%	-2.7%	-2.4%	-1.4%

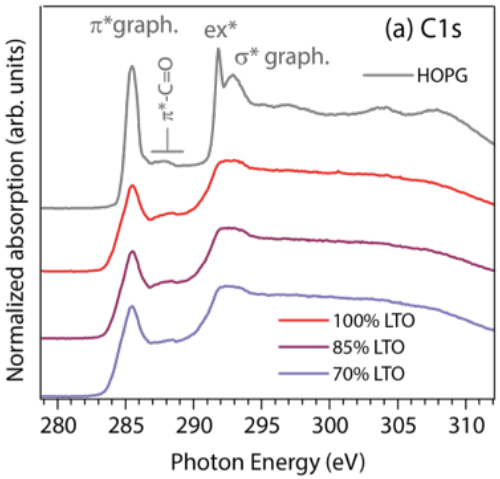
- $L_{C\text{-}C}$: from 1.33Å (ethylene), 1.39Å (benzene) to 1.54Å (diamond)

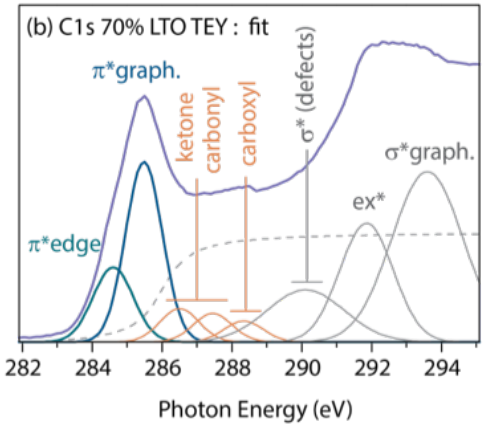


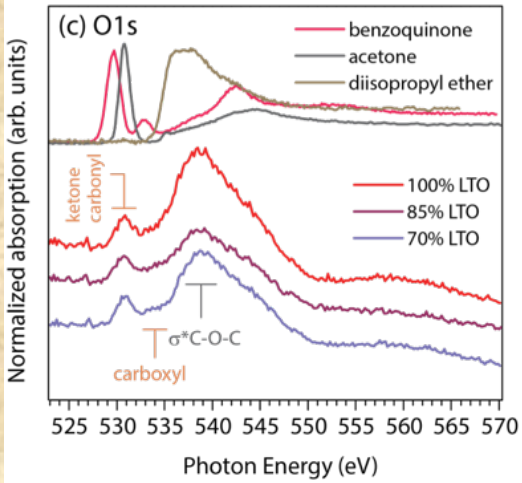
p	N	m	χ	$R_{C\text{-}C}$, nm	L_a, nm
1	6	6	2	0.13040	0.23
2	24	12	1.6	0.13630	0.71
3	54	18	1.5	0.13827	1.20
4	96	24	1.4545	0.13925	1.69
5	150	30	1.42857	0.13984	2.18
6	216	36	1.41176	0.14023	2.67
8	384	48	1.39130	0.14073	3.66

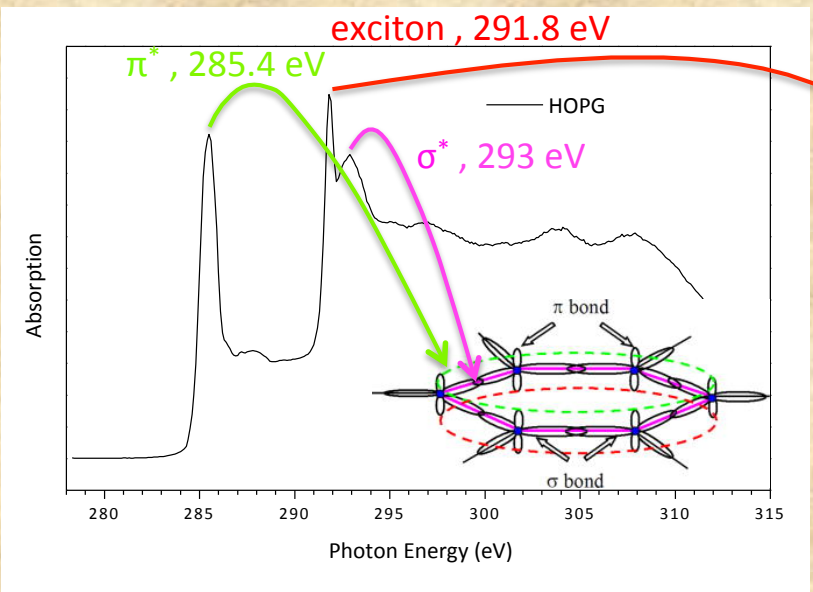
E.A. Belenkov, Inorganic Materials **37**(9) (2001) 928-934

NEXAFS (Total Electron Yield : bulk signal)









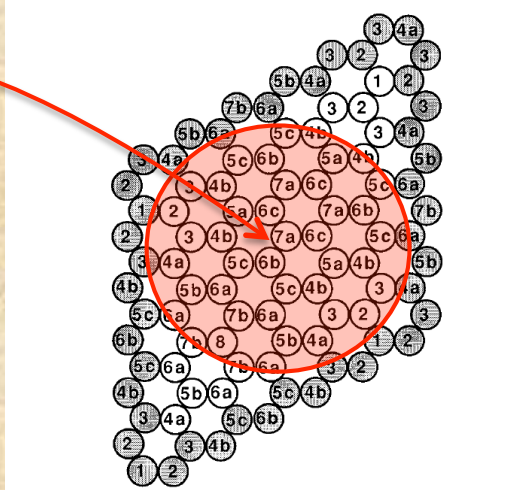
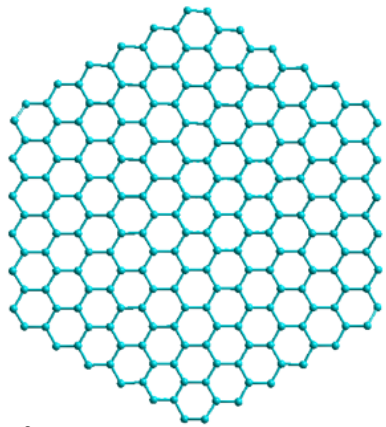


FIG. 1. Supercell used in the calculations. The core-excited atom is at location 1, and the higher numbers indicate the distance from a core-hole site.

Engine thrust	70%	85%	100%
$\pi^*_{edge} / \pi^*_{graph}$	45%	45%	47%



28 Å : C_{edge} / $C_{graph.}$ = 44 %

HRTEM : 25 ≤ L (Å) ≤ 36

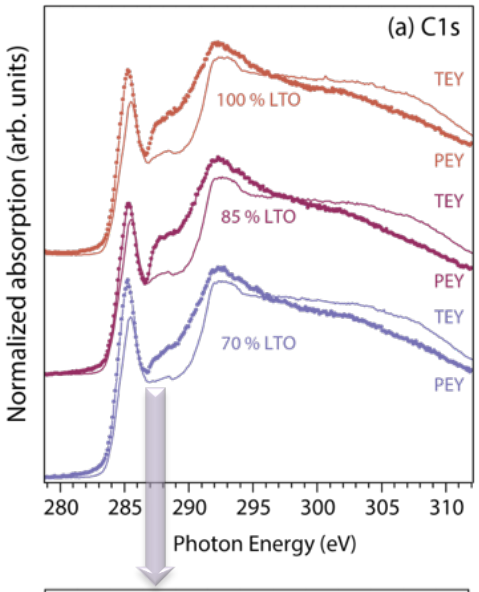
☞ Belenkov :

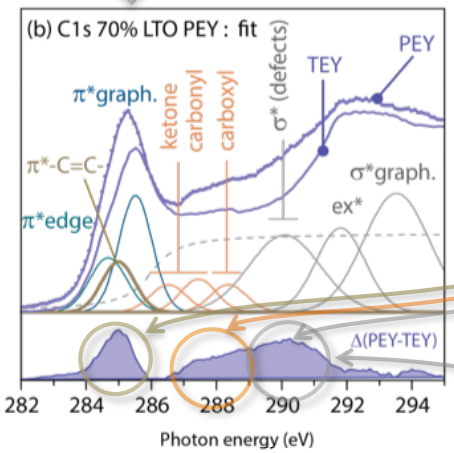
p = 6 ; L_a = 27 Å ; $R_{c\text{-}c}$ = 1.402 Å

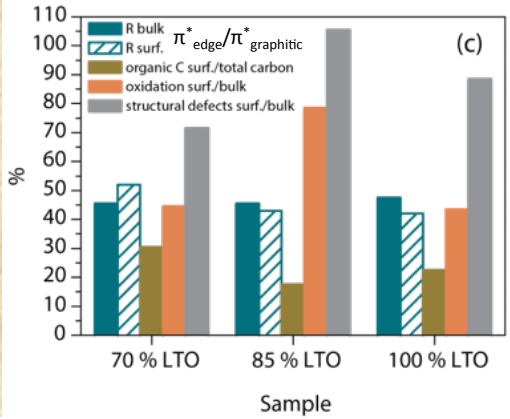
OXYGEN SPECIATION (qualitative)

- Ketones, carbonyls
- Carboxyls
- Ethers (linear or cyclic)

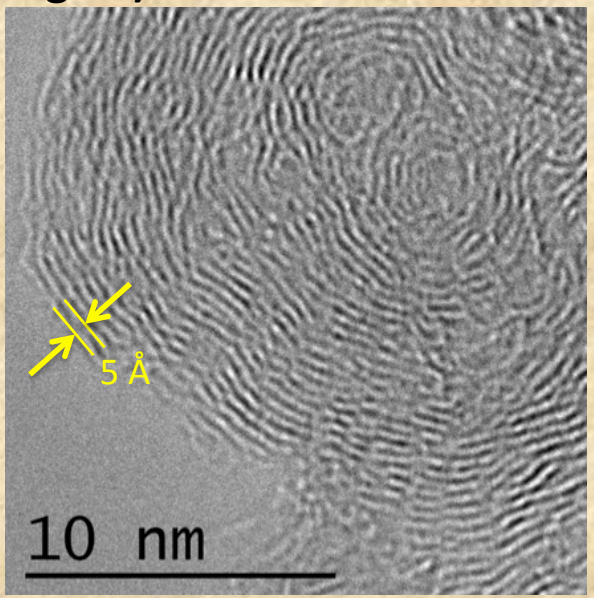
NEXAFS (Partial Electron Yield : surface signal)





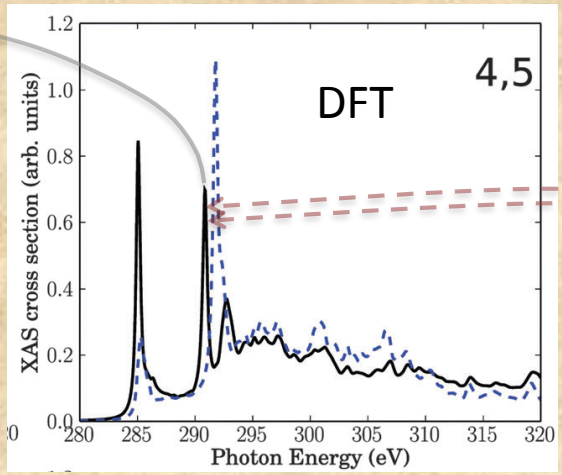


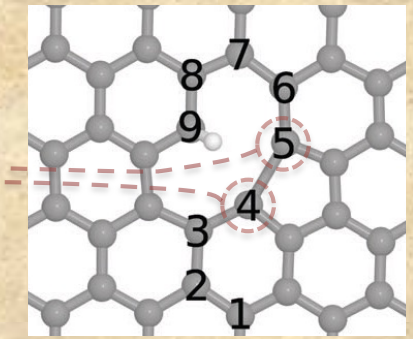
NEXAFS with the PEY method :
Probes 6 Å, ≈ 2-3 outermost layers
➔ Soot particles surface



- -C=C- functionalities of small aliphatic chains are observed
- More oxydation (between 40 and 80 % with respect to the bulk signal)
- Resonance at the surface assigned to C-C distances 4% shorter than in graphene (in agreement with TEM) ➔ more structural defects at the surface

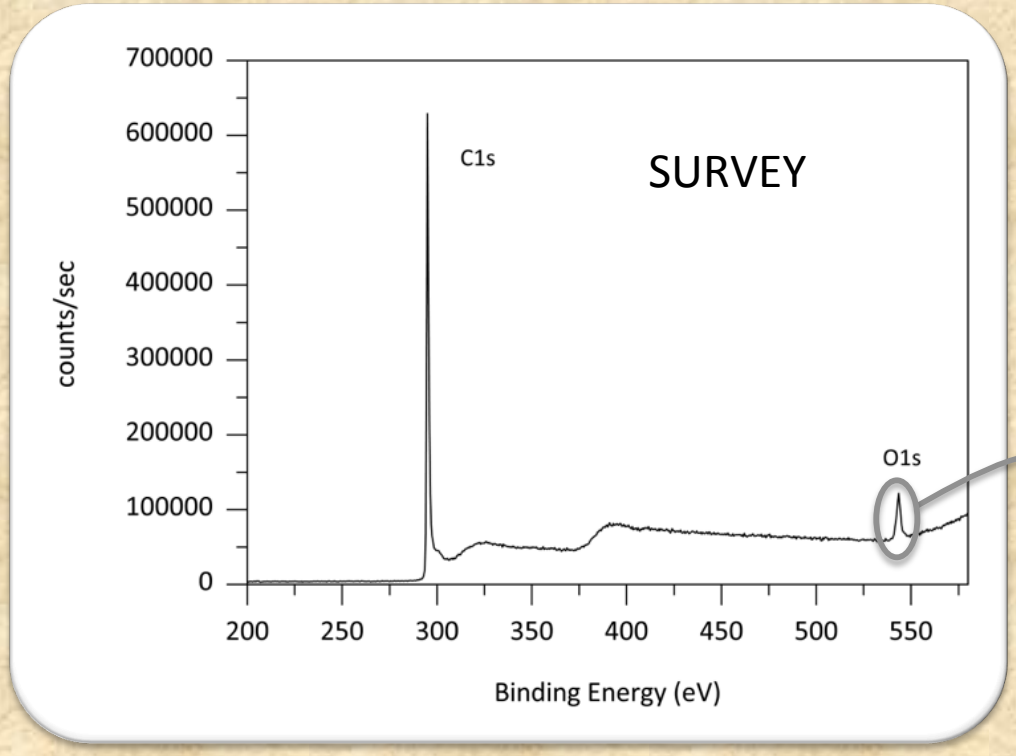
DIFFERENCES BETWEEN THE BULK AND SURFACE' SIGNALS

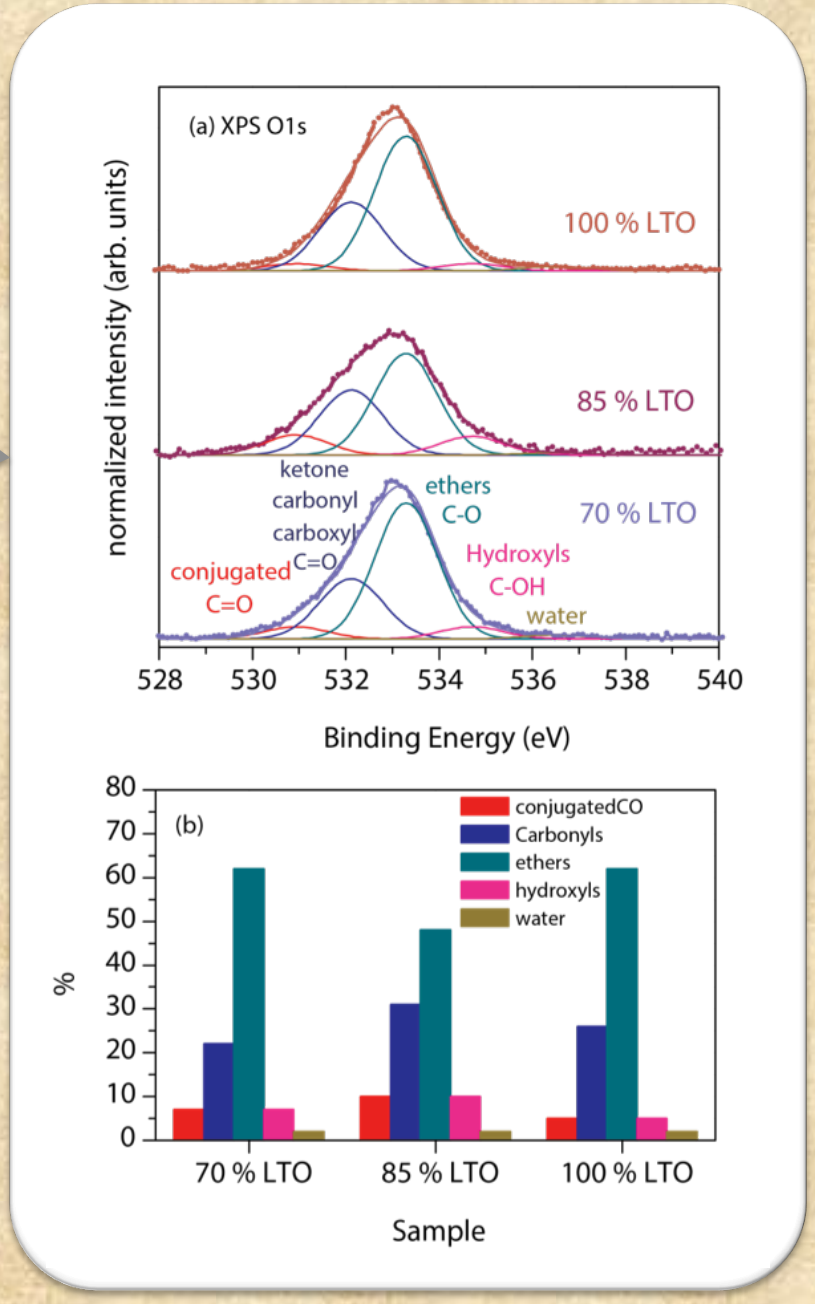




Ehlert *et al*. PCCP **16** (2014) 14086

O1s XPS : oxygen concentration and oxygen speciation at the surface

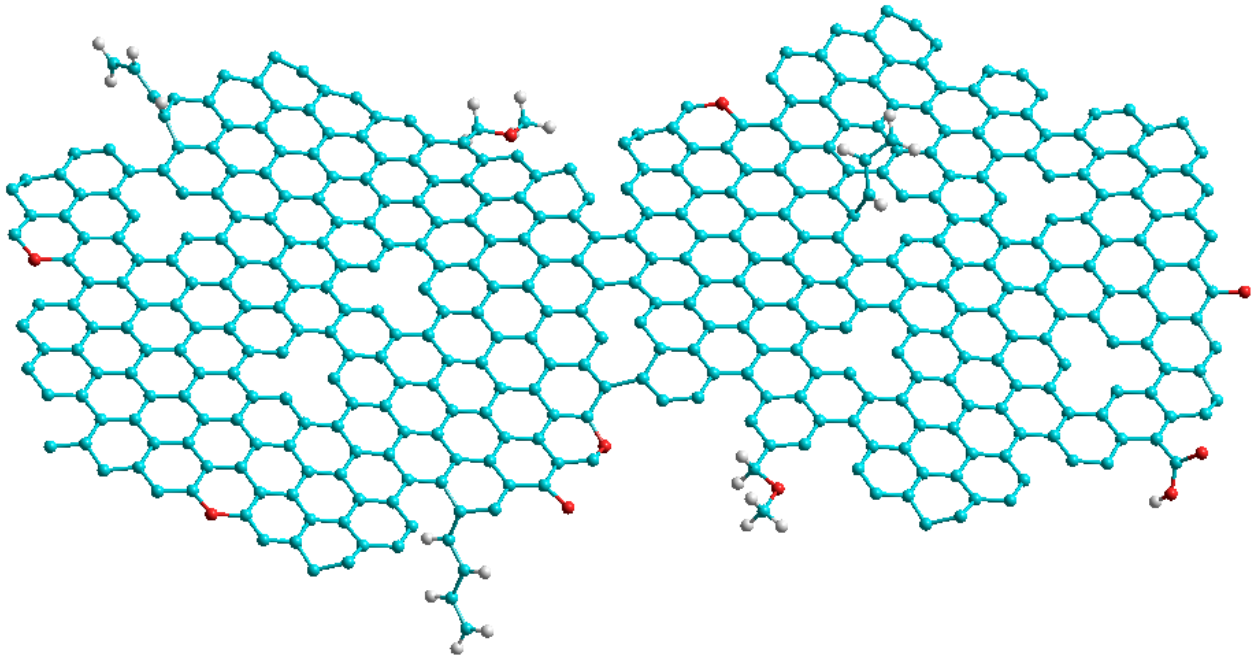




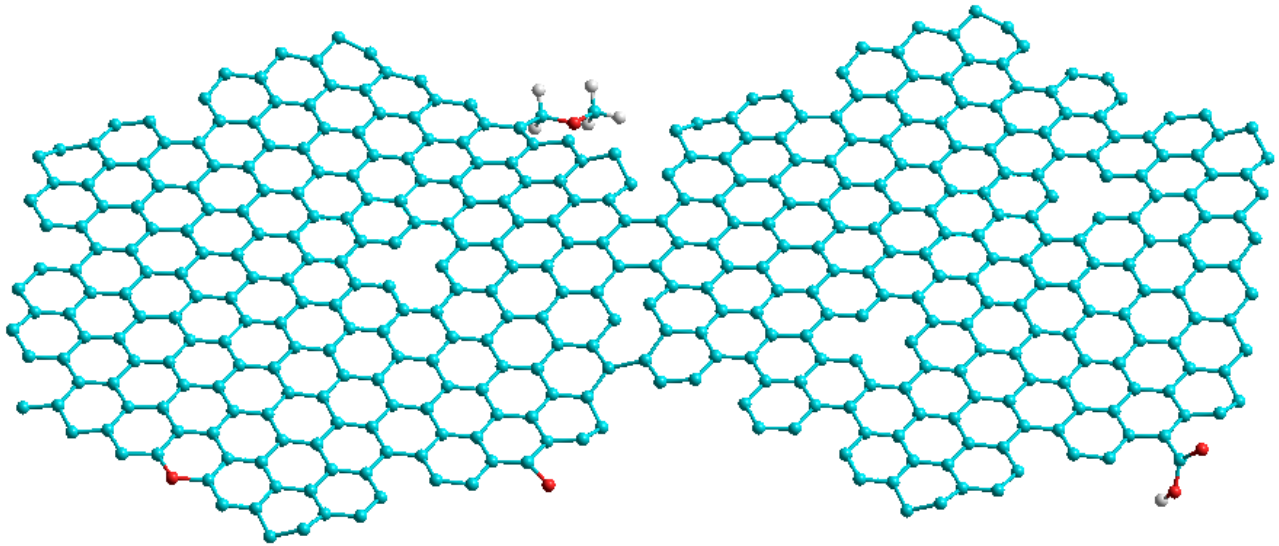
	O/C (Surface)	O/C (Volume)
100%	3,5 %	2,4 %
85%	1,7 %	1 %
70%	2,3 %	1,8 %

A SKETCH OF SURFACE AND BULK CRISTALLITES

SURFACE



VOLUME

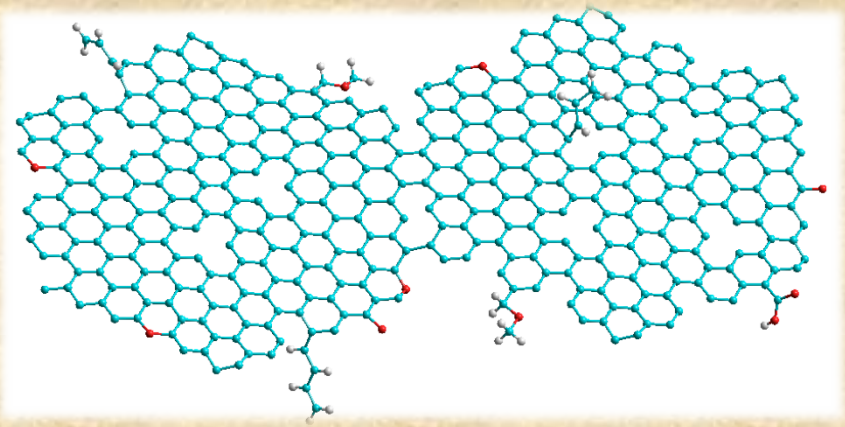


SUMMARY - CONCLUSION

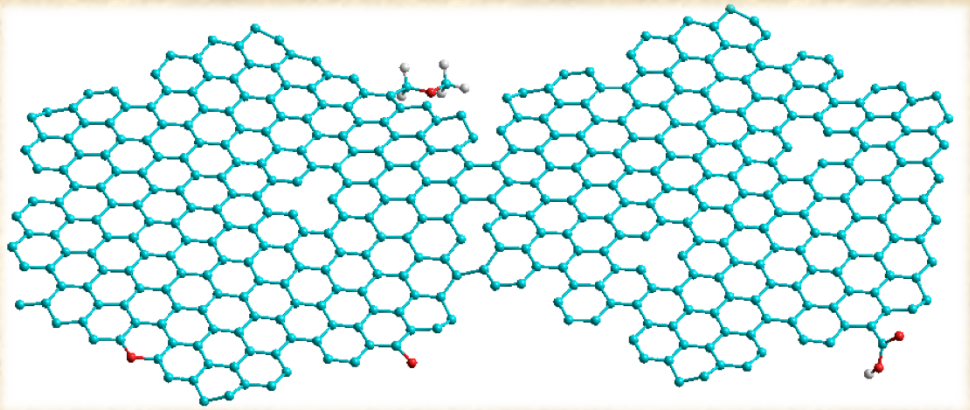
Sampling and characterization of soot particles emitted from a full SaM146-1S17 turbofan engine :

- Submicrometric aggregates
- Aggregates' morphology does not evolve with engine thrust
- Nanometric primary particles having diameters < 20 nm that increase with engine thrust
- Cristallites size < 4 nm that decreases when engine thrust increases
- C-C bonds < C-C graphite
- Structural defects more pronounced at the particles' surface compared to the bulk
- Outermost cristallites more oxidized than in the « bulk » (surface : O/C ≤ 3.5 % - bulk : O/C ≤ 2.4 %)
- Presence of aliphatic chains (likely linking cristallites)
- Oxygen speciation : ketone, carbonyl, carboxyl, ether (linear and cyclic)
- Our sketch of carbonaceous cristallites constituting the soot primary particles :

SURFACE



VOLUME



Thank you for your attention !
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