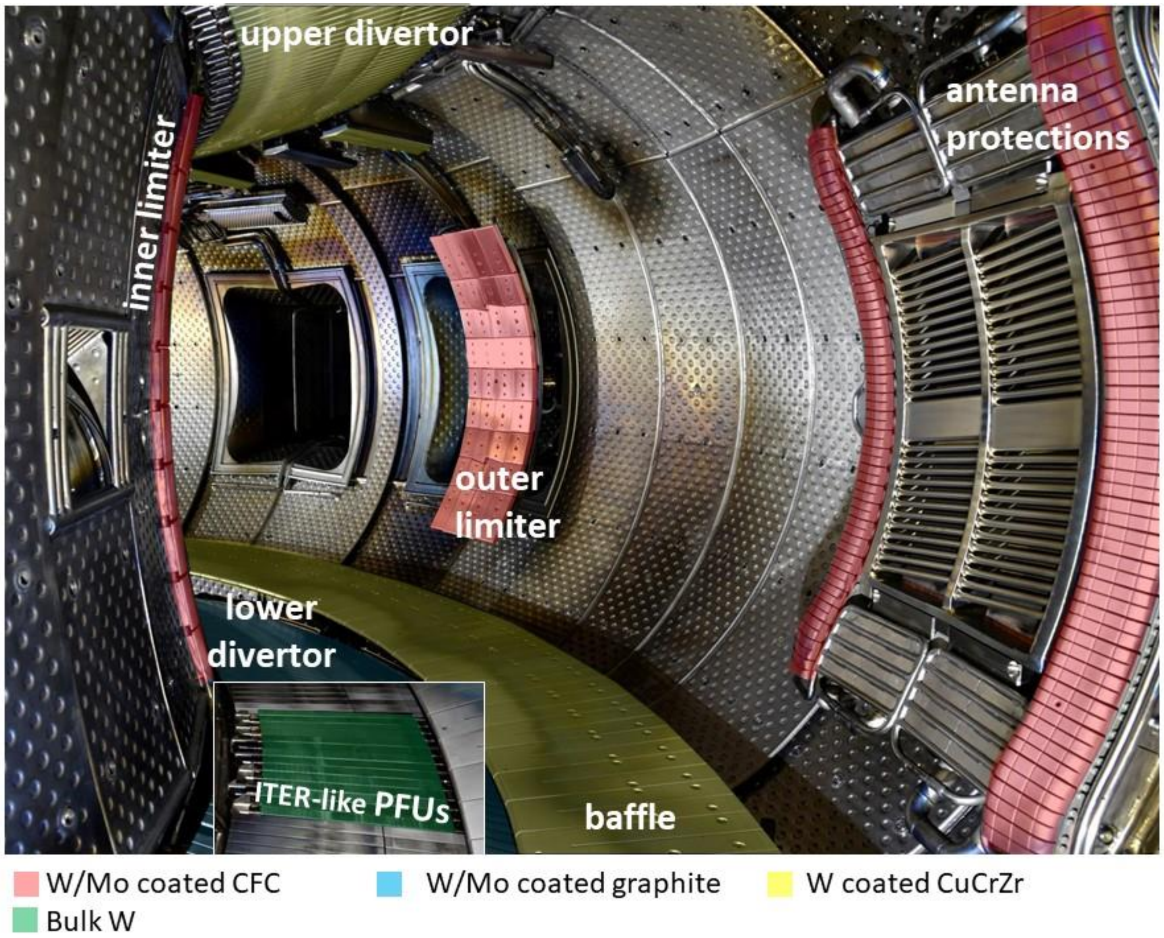
Dust production mechanisms

A. Michau and K. Hassouni

LSPM, Laboratoire des Sciences des Procédés et des Matériaux
Université Paris 13, Sorbonne Paris Cité, CNRS (UPR 3407)
93430 Villetaneuse, France

19/10/2022

Example : W in West

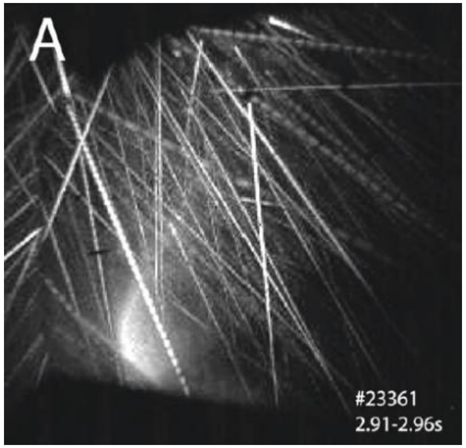


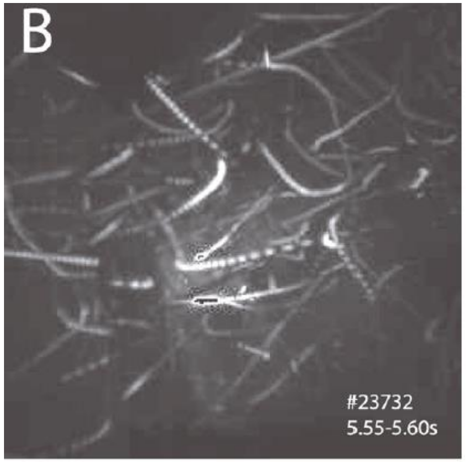
The C3 campaign averaged net erosion rate is roughly ~0.1 nm s^{-1}, in the same range as what was found in AUG

=> What happened to this removed material ?

Observation of dust particles

In-situ visualisation of **micrometric particles** in ASDEX Upgrade





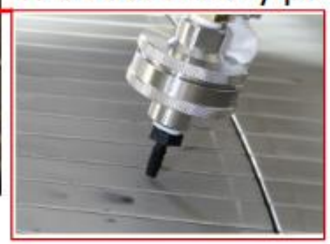
Rode et al. Phys. Scr. 2009 014024

But smallest particles cannot be seen

Ex situ obervation of NPs

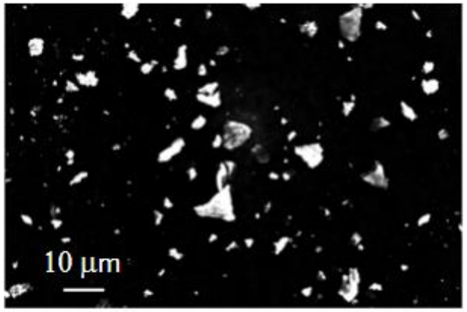
Examples from C. Arnas (PIIM) M. Diez and E. Bernard (IRFM) in WEST

Filter holder connected to a vacuum dry pump



Inertial plasma-facing units (PFUs): graphite tiles with W coating of 15 μm

Part of dust produced during plasmas of 2020:
77 min of D plasmas (L mode) + 3 boronizations



Various shapes, sizes and chemical compositions (can contain all materials present inside the tokamak: W, Mo, Cu, Fe, Cr, Ag + O, B, N ...)

This can be carried out only between two campaigns : many plasma ignitions/disruptions

direct interpretation is difficult !

Simulation can help !

Observed dust microparticles

S. Peillon, et al. Nuclear Materials and Energy 24 (2020) 100781

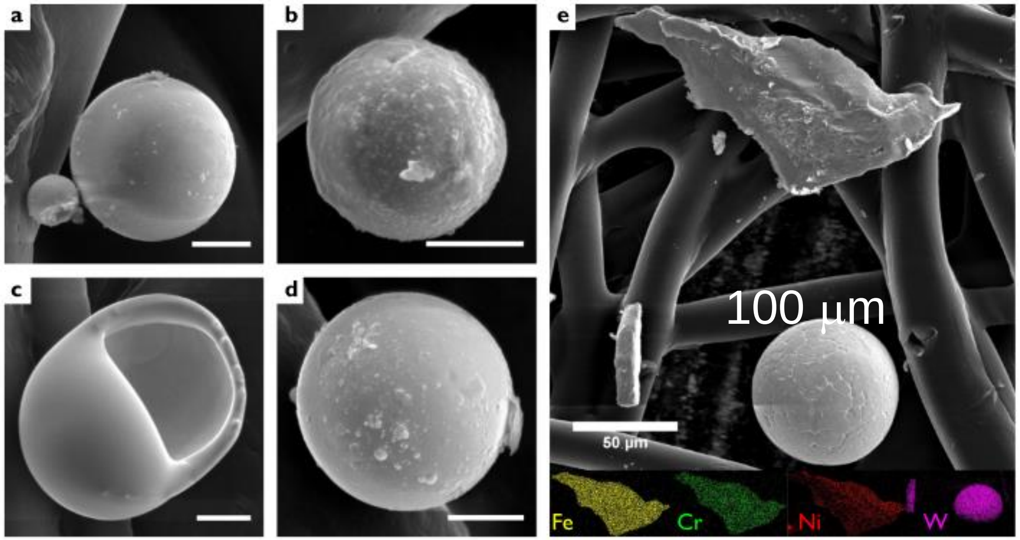
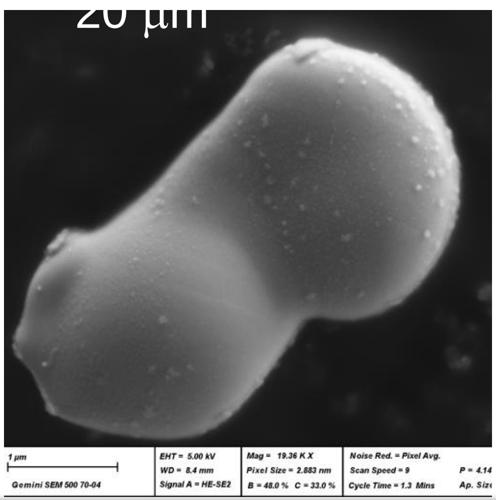


Fig. 2. a to **d** SEM micrographs of particles collected with the Duster Box inside the WEST tokamak (scale bars are 5 µm). **e** SEM and EDS analysis of stainless steel and tungsten particles deposited on a sampling filter.

- Spherical and regular shape : droplet ejected from molten metal (divertor) after an anomalous event (disruption/elm (?))
- Size depends on the event release of energy on the surface but maybe also on the local conditions that can be responsible for evaporation before solidification

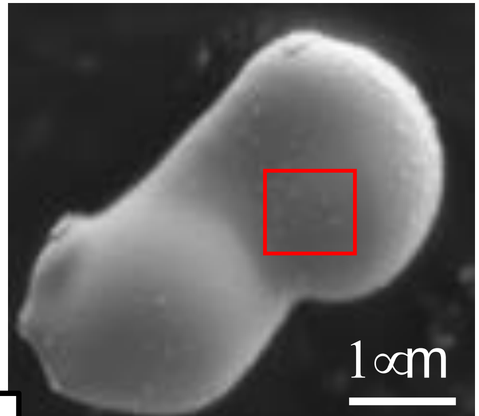


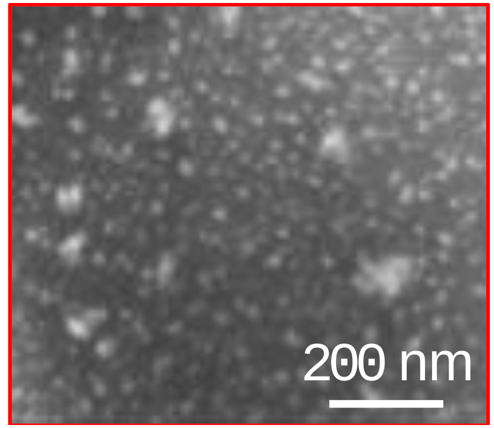
Different sizes of spherical micrometric particles observed

From C. Arnas (to be published)
West C4 2019

Observed dust nanoparticles

From C. Arnas
(to be
published)
West C4 2019

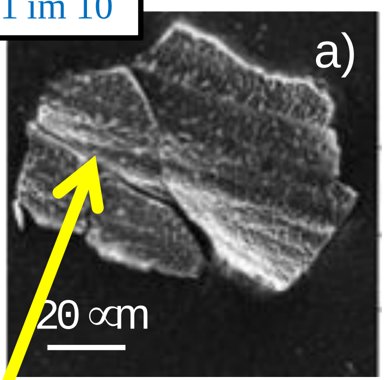


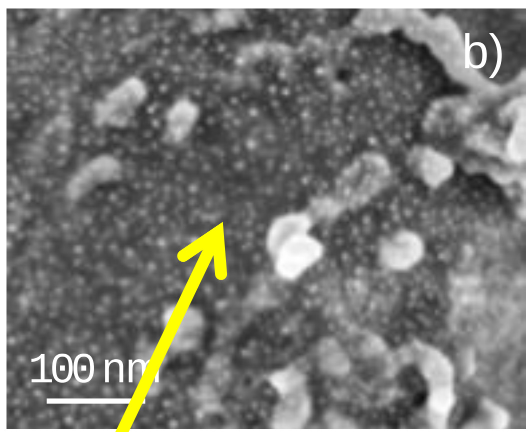


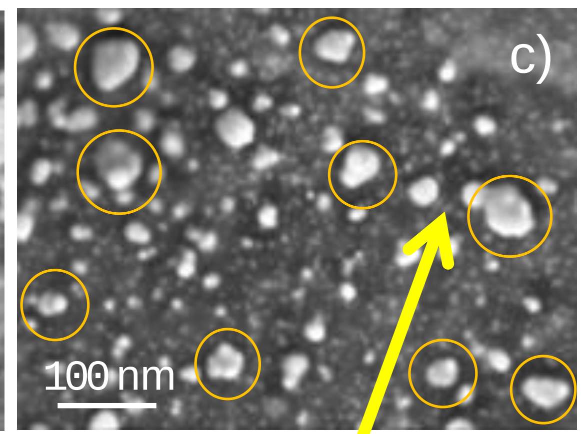
Small NPs (5 nm) are observed

C5 2020 : ITER-like -

MEB 3 nov2021 im 10







Flake boronised

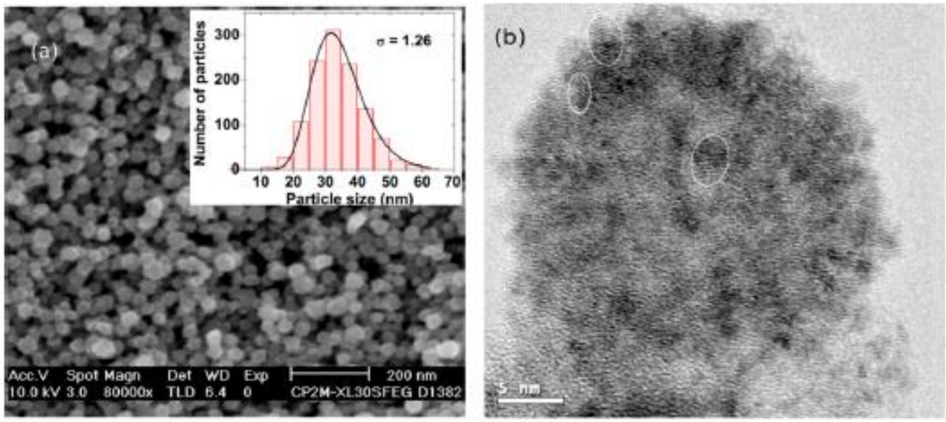
Small Nps 5nm observed on the surface

coagulation

Observation in laboratory plasma

Production of NPs by sputtering under soft plasma conditions

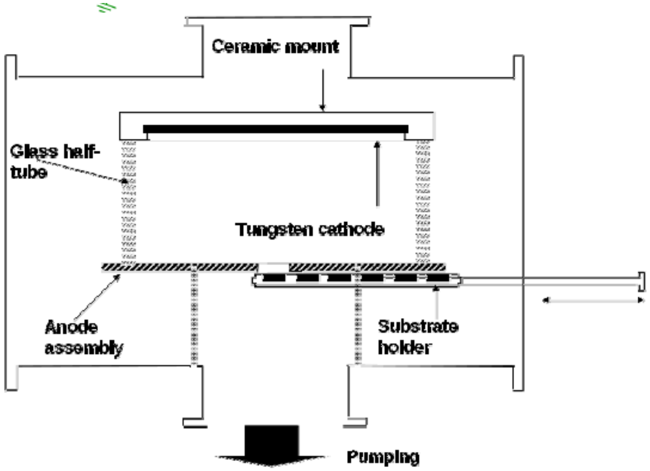
Kumar et al PoP 20 (2017)



Lognormal distribution
averaged diameter 30 nm
Agglomerate of 5nm Nps

Magnetron discharge

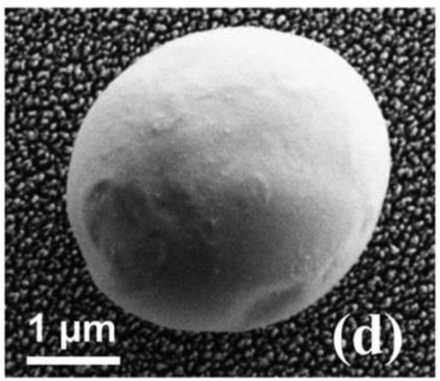
W sputtering



Different NPs production routes in laboratory plasmas

ARC

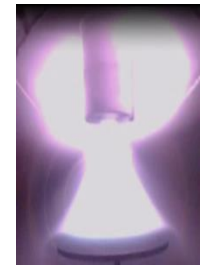
10^6 W/cm^2

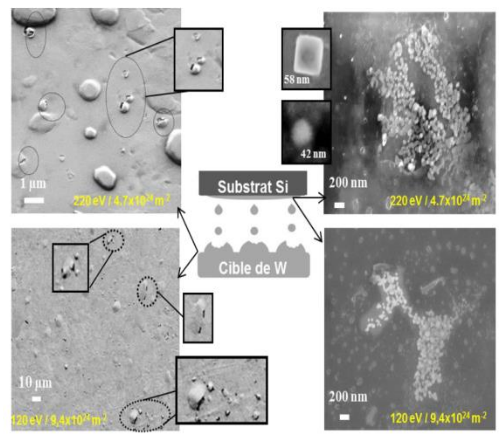


Solidified droplets
+ large NPs population

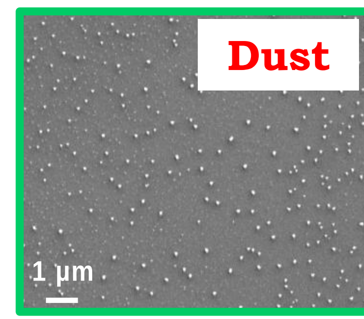
Glow discharges with high z species

Soft conditions





Blister burst => Nps



Nucleation of NPs

K. Ouaras et al. JNM 2016
K. Ouaras et al PoP 2017

Interpretation

Nps are observed with and without droplets

⇒ Nucleation in a ‘vapor cloud’ around the droplet after disruption

⇒ Nucleation of Nps deposited on boronised flakes without droplet (formation without disruption)

In which conditions are they observed ?

- **Disruptions**
- **Case of plasmas with high sputtering rate and moderate temperature that favour the molecular growth**

Large quantities of Nps can be produced

Whatever their fate they could contribute to determine the nature of impureties and may therefore affect the plasma characteristics

Investigated scenari for Nps production

- **Standard plasma conditions** (**mechanism 1**) :

  especially (semi)-detached plasmas with high Z radiative species

  – **Enhanced Sputtering** followed by nucleation in the vapour

- **Anomalous events** (**mechanism 2**) :

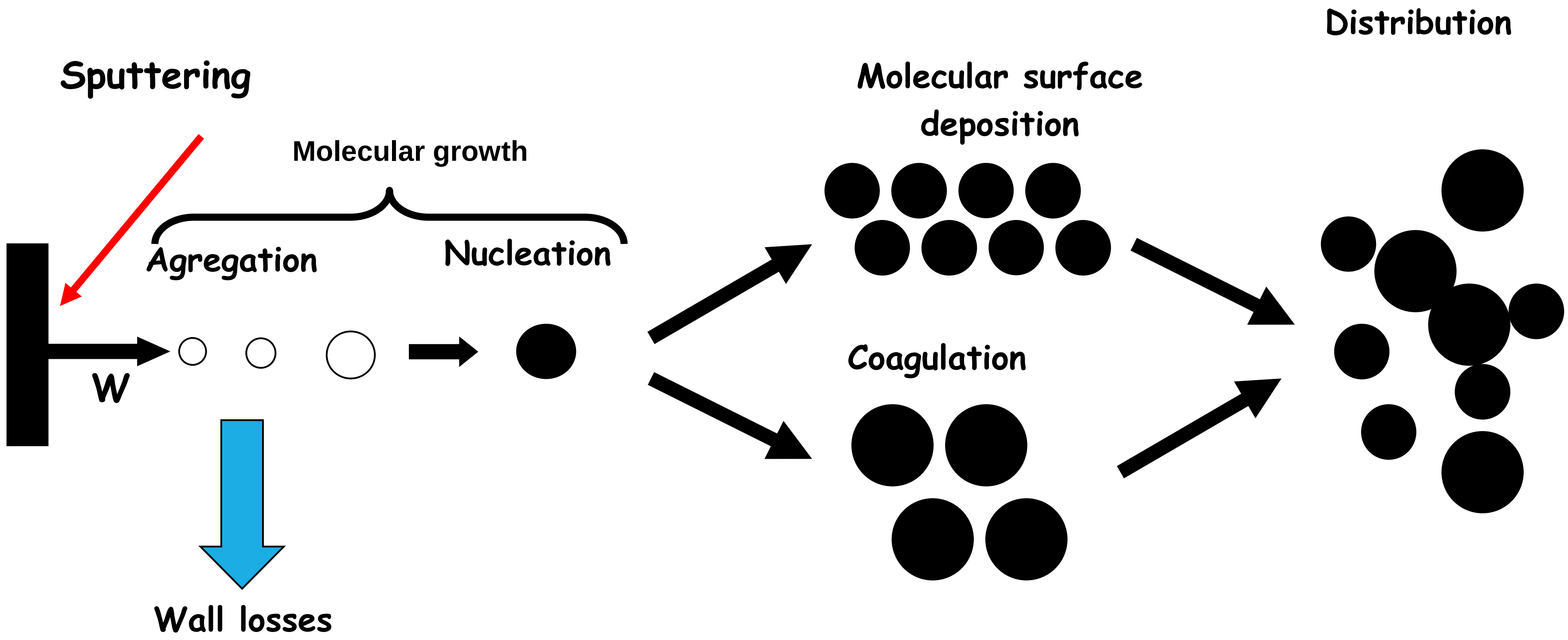
  melting and vaporisation

  – produce droplets => micrometric particle (not considered)

  – May produce Nps by nucleation in a supersaturated vapour (CNT ?)

Mechanism 1:What do we already have

'Standard Plasma conditions'



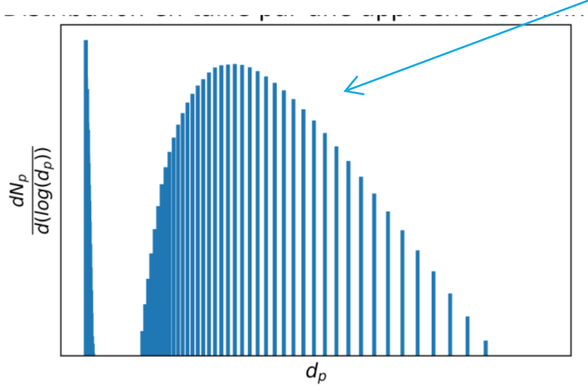
Molecular growth model

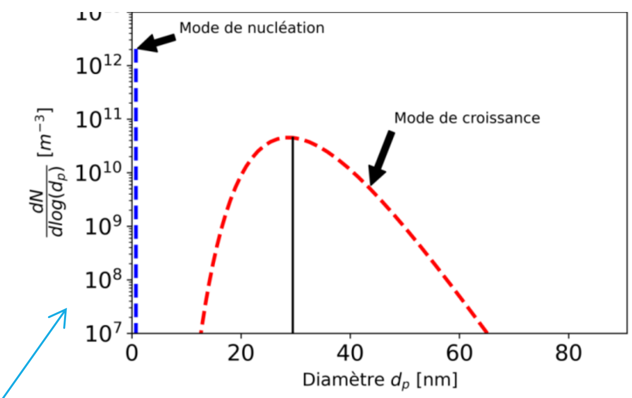
Aerosol Model

Aerosol model

- Need to solve for the particle charge (depend on plasma condition and size)

- Existing: Sectional model
  - Precise but CPU expensive -> **preliminary analysis**



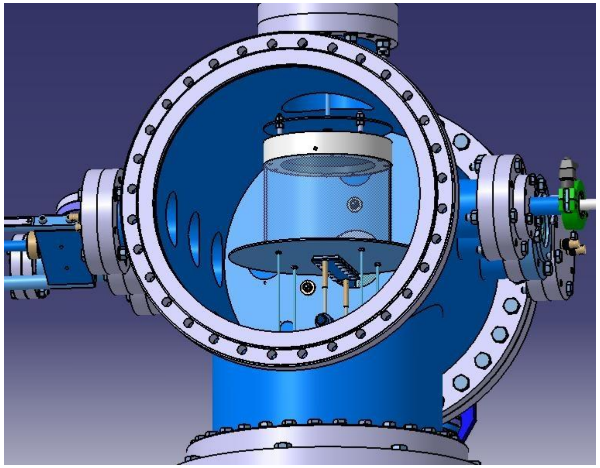


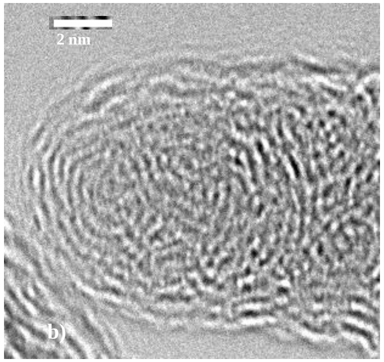
- Multi-modal moment model can be easily used in integrated plasma modeling

  ➔ **perform extensive studies**

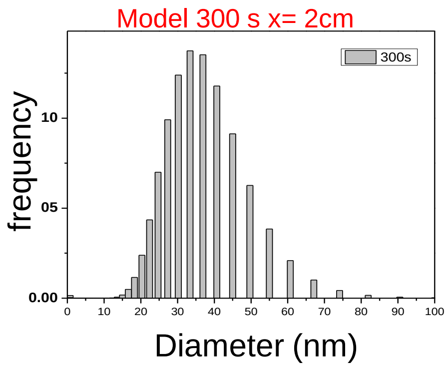
Prediction of the size distribution

Argon DC Discharge - graphite Cathode

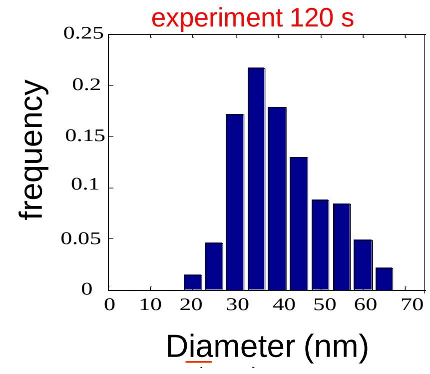




Particle density 10^8 cm^{-3} close to measurements



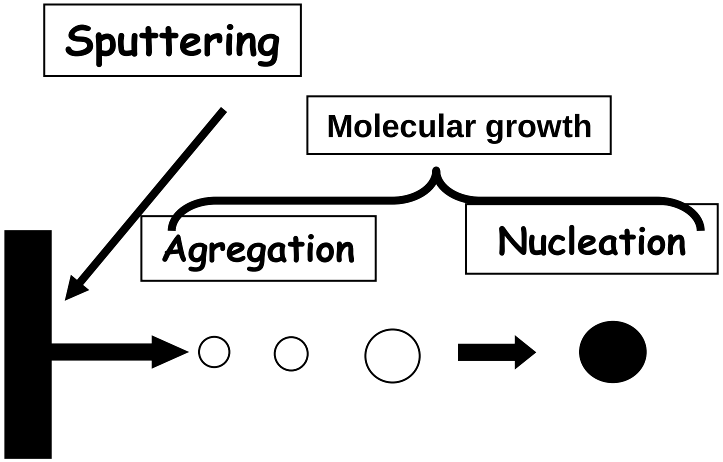
d=34 nm



d=35 nm

- **Conditions**
  - **A 14 cm gap**
  - **voltage V_d ~ - 600 V**
  - **Current = 80 mA**
  - **Pressure = 0.6 mbar**
  - **Discharge Duration 5 mn**
  - **Volume ~1 L**

Molecular growth model



Issue :

W is ionised in the plasma

➔ **We need molecular growth model for W/Be system**

$W_n^{m+} + W^{p+}$ ➔ $W_{n+1}^{(m+p)+}$ almost not known

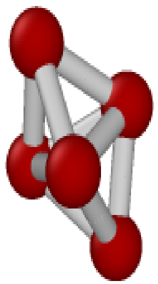
Scenario 1 : Research methology

- Determine the stable neutral and charged W_n structure using eitheir MD with prescribed interaction potential or DFT
- Determine the interaction potentials for W^{p+}/W_n & W_n^{p+}/W systems
- Determine the coagulation cross sections by MD simulation using these potentials

Stable neutral and charged W_n structure

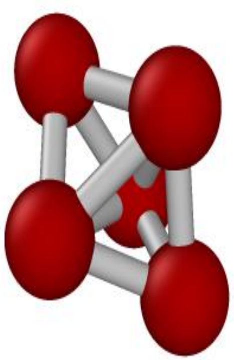
First comparison between MD and DFT : the case of W_5

MD-simulated annealing : heating up to 3000K and cooling to 0 K



EAM potential

E= 5,77 eV/atom



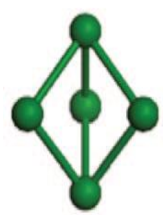
Tersoff potential

E= 4,99 eV/atom

DFT (article Jiguang Du et al, 2009), method: Gradient corrected DFT

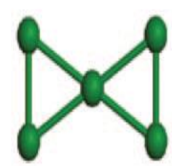
W_5-*a* (C_{2v})

E= 4,61 eV/atom



W_5-*b* (D_{3h})

E= 4,39 eV/atom



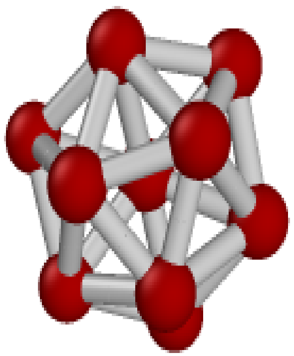
W_5-*c* (D_{2h})

E= 4,05 eV/atom

UNIVERSITÉ PARIS 13

Stable neutral and charged W_n structure
First comparison between MD and DFT : the case of W_{10}

MD-simulated annealing : heating up to 3000K and cooling to 0 K



EAM potential

E= 6,57 eV/atom

DFT (article Jiguang Du et al, 2009), method: Gradient corrected DFT

W_{10}-*a* (C_{3v})

E= 5,44 eV/atom

W_{10}-*b* (D_{2h})

E= 5,42 eV/atom

W_{10}-*c* (D_{4d})

E= 5,42 eV/atom

Evaluation the impact of XC functionals and basis sets on the stable state optimization

Different XC functions

W_2			
Exchange correlation function	Basis set	Bond energy (eV/atom)	Bond length (Å)
B3LYP	LANL2DZ	-4.55 (-4.54[1,2])	2.039 (2.039[1,2])
B3PW91	LANL2DZ	-4.93 (-4.93[1])	2.031 (2.031[1])
LSDA	LANL2DZ	-6.46 (-6.48[1])	2.036 (2.037[1])
B3P86	LANL2DZ	-5.01	2.028 (2.029[2,3])

- Different exchange-correlation functions involve obtaining structures with different energies and bond lengths

Gaussian

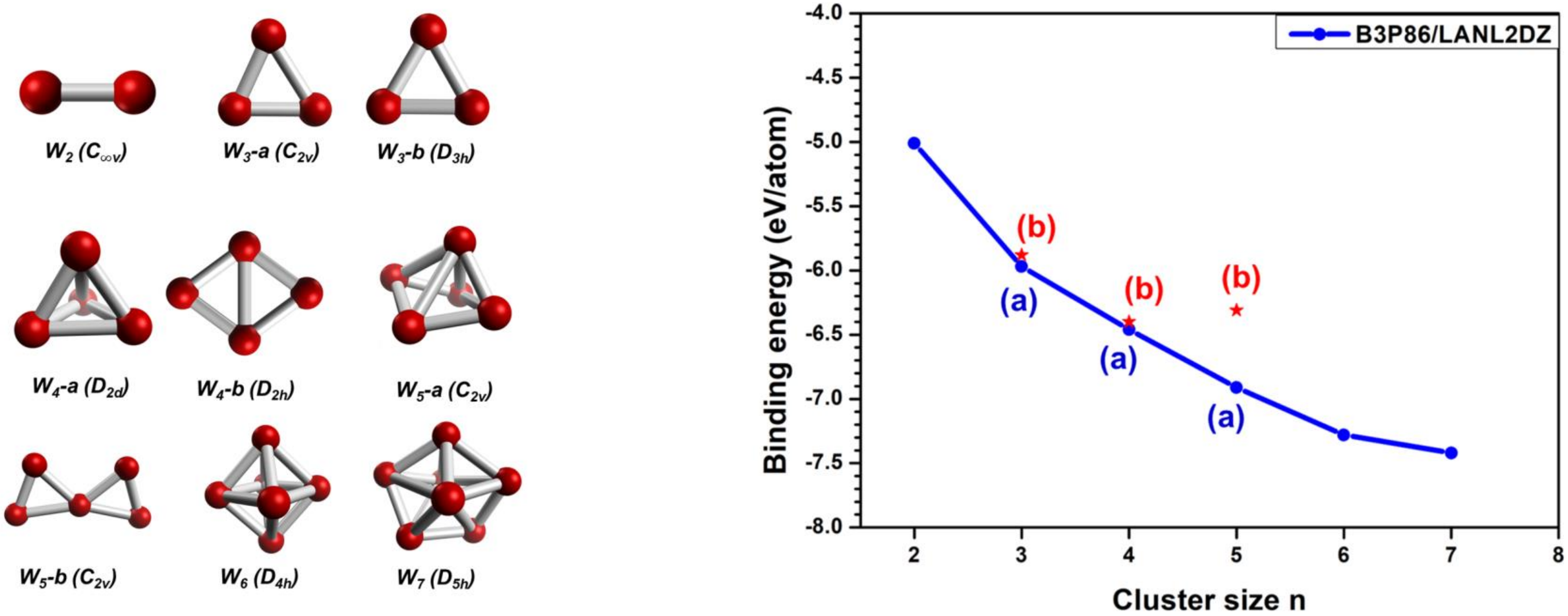
Different basis set

W_2			
Exchange correlation function	Basis set	Bond energy (eV/atom)	Bond length (Å)
B3LYP	LANL2DZ	−4.55	2.039
B3LYP	LANL08	−4.53	2.031
B3LYP	LANL2TZ	−4.53	2.036

- The DFT basis set used does not affect the energies and bond lengths of the optimized structures

stable neutral and charged W_n structure

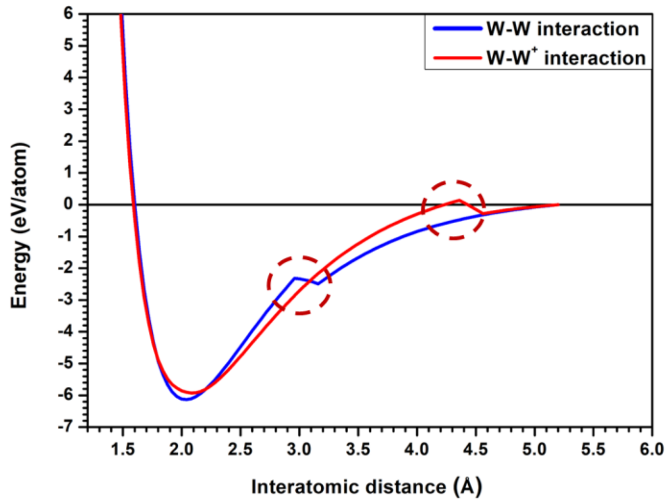
Stable structures of small tungsten clusters



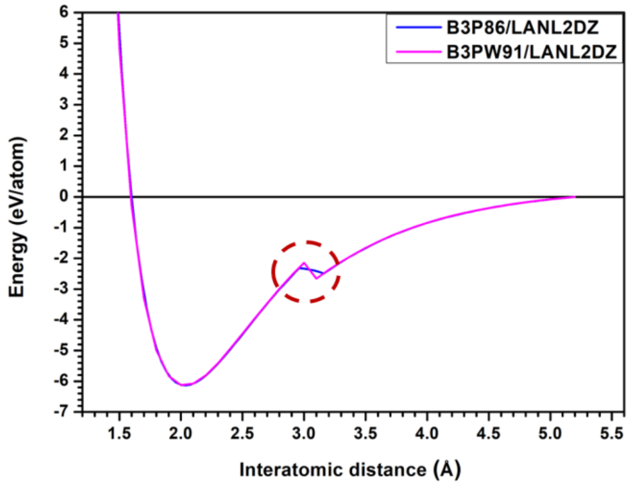
Interaction potential

Interaction potential for W-W and W-W⁺ systems

➢ We estimate the W-W interaction energy as a function of W-W distance



There are jumps in the potential energy surface

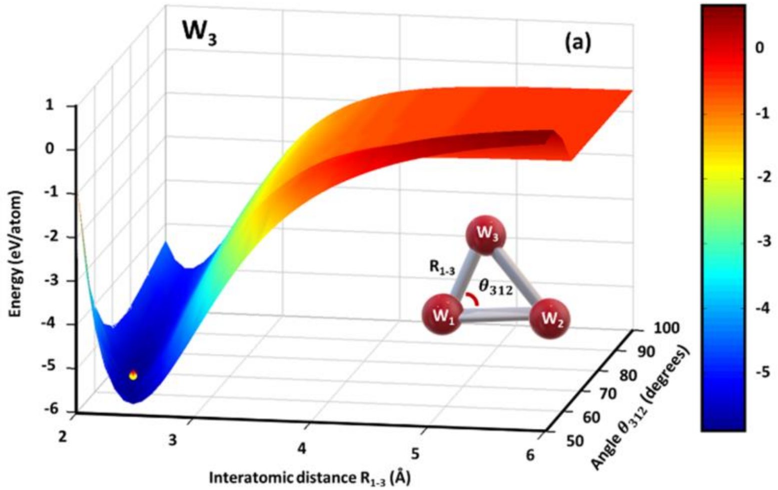


➢ Origin of this jump ? Any idea ?

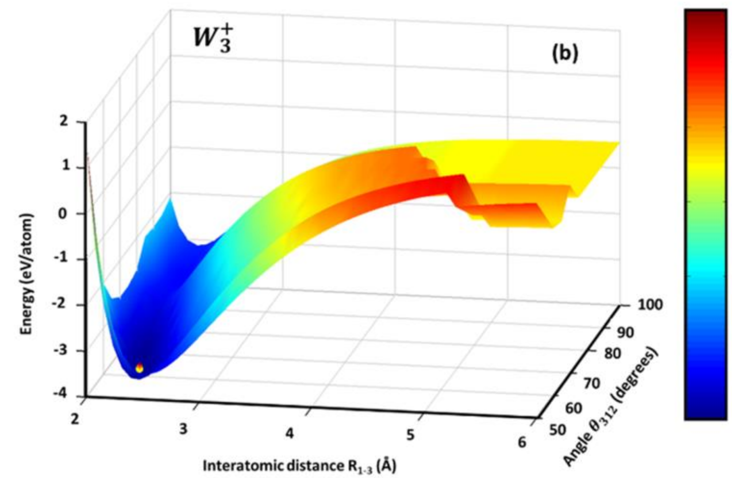
Interaction potential

Interaction potential for W-W_2 and W^+-W_2 systems

- Potential energy surface scan using the B3P86/LANL2DZ method by varying the distances $R_{1\text{-}2}$ and $R_{1\text{-}3}$ in a similar way and the angle formed by the bonds 1-2 and 1-3



The neutral trimer energy is minimal for $R_{1\text{-}2} = R_{1\text{-}3}$ = 2.240 Å and θ_{213} = 65°



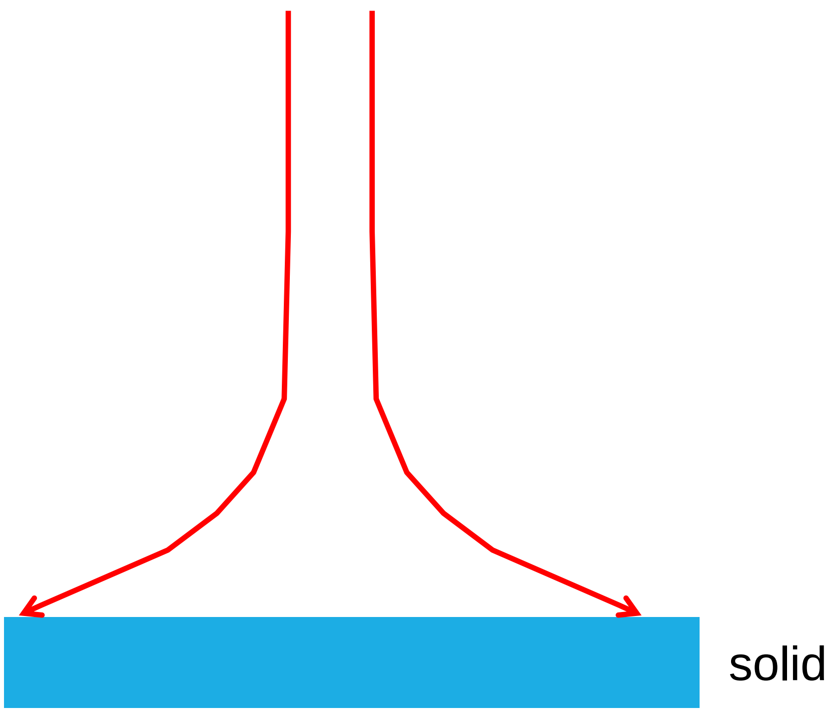
The charged trimer energy is minimal for $R_{1\text{-}2} = R_{1\text{-}3}$ $R_{2\text{-}3}$ = 2.320 Å and θ_{213} = 60°

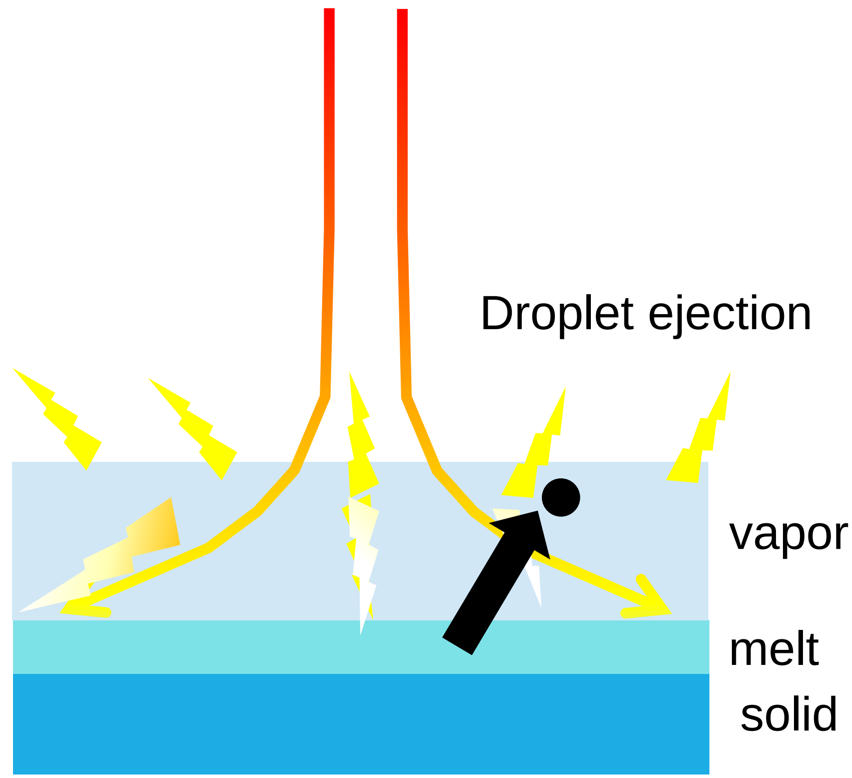
Scenario 2 : anomalous events

$e^- + D^+ + T^+ + He^+$

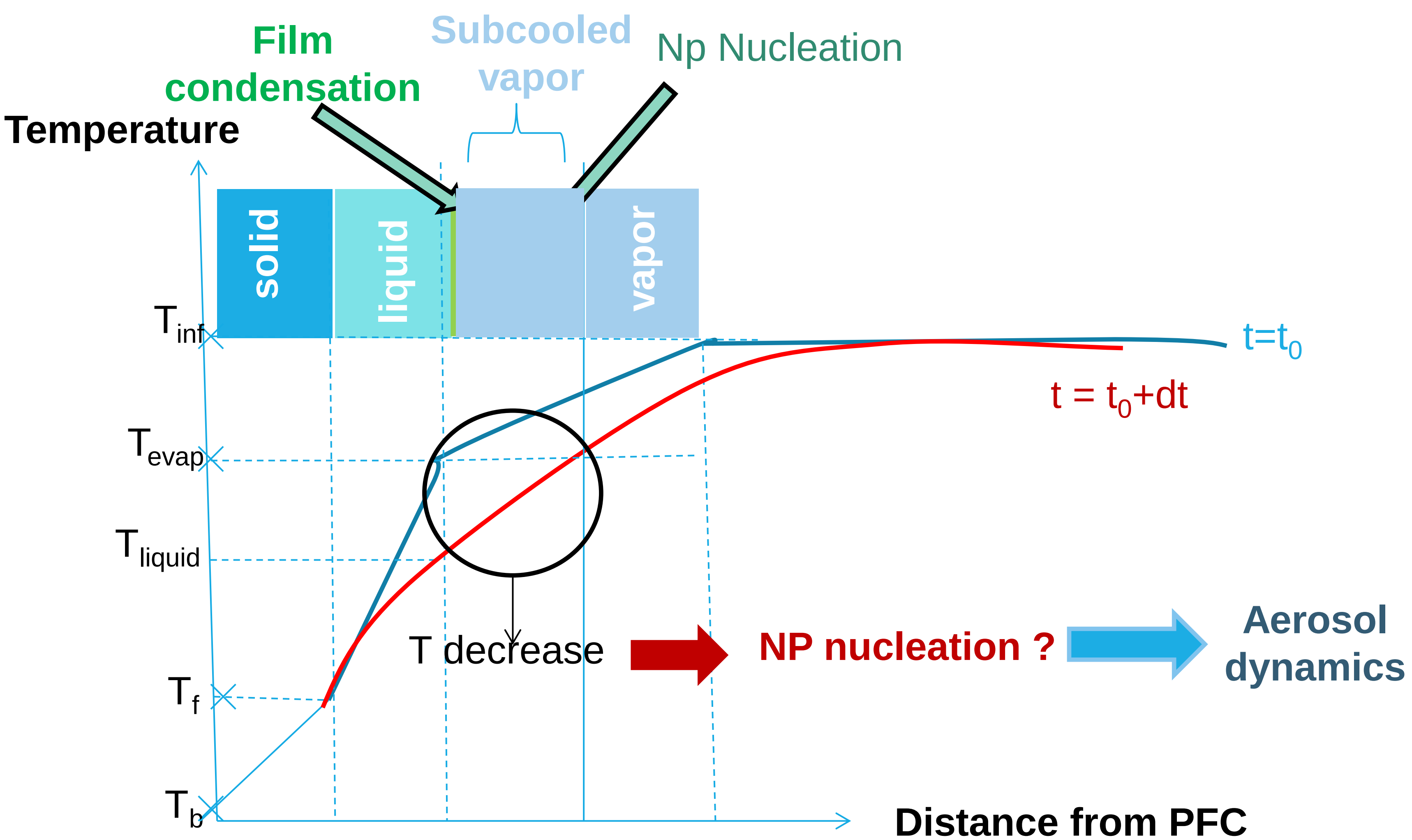
$\langle T \rangle$ = 1-50 keV ; $n=10^{12}$-10^{13} cm^{-3} ;

ε_d=0,1-1MJ/cm^{-2} ; $\tau_d \approx 1$ ms





Temperature evolution after disruption



Scenario 2: studies planned

To determine if nucleation is possible, we are developping **simple model** that solves for the **coupled phenomena** of :

- heat transfer near the wall
- melting/vaporization
- Screening/cooling of the vapour
- nucleation
- Aerosol dynamics

(first three items) → Simple models

detailed model
⇩
simple model

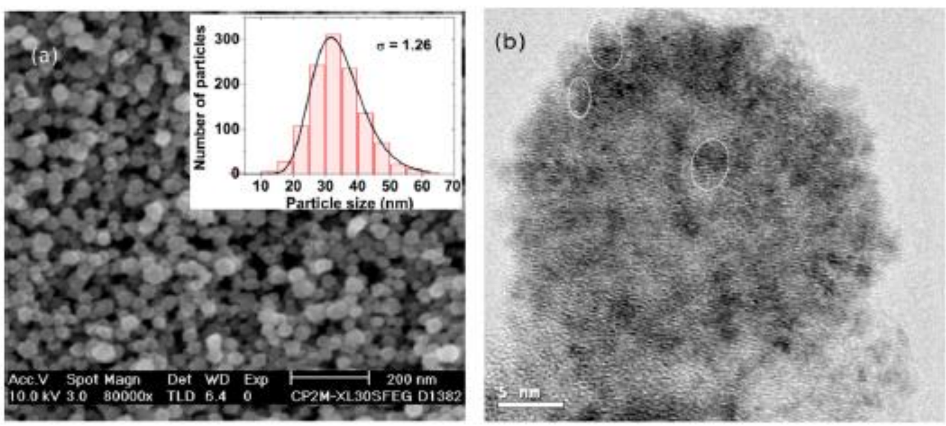
Thank you for your attention

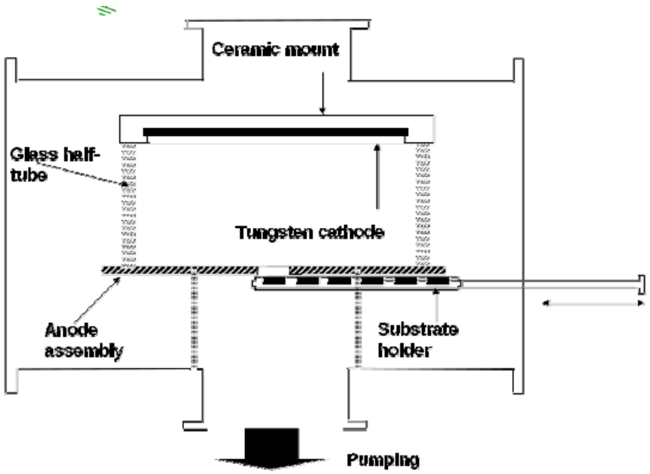
Possible validation of 'soft conditions'

Kumar et al PoP 20 (2017)

Magnetron discharge

W sputtering

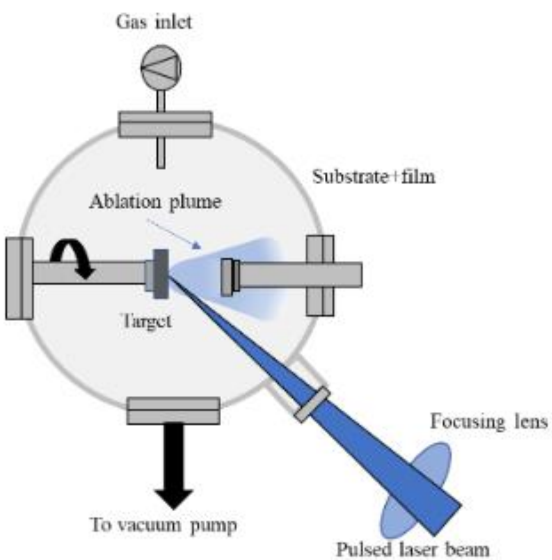


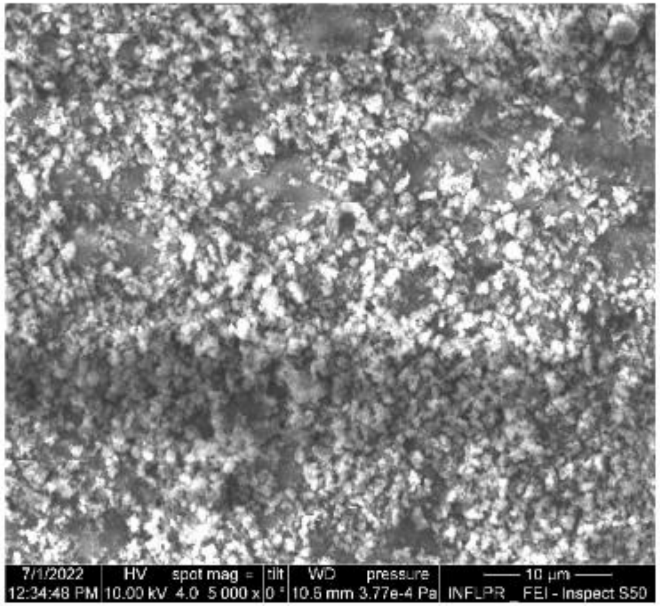


Lognormal distribution
averaged diameter 30 nm
Agglomerate of 5nm Nps

Possible validation of high heat flux conditions

Be nanoparticles obtained by Pulsed Laser Ablation in Gas Phase (PLA-Gas)





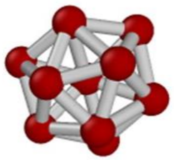
Images of a Be particle deposit obtained after cumulated PLA experiments in various gases (H_2, He, Ne, Ar) at various pressure values (in the range 10^{-2}-7 mbar)

A. Palla - Papavalu , A. Bercea, C. Porosnicu, B. Butoi, et al. INFLPR

Determination of the most stable structures ⇔ targets during the collisions involved in the molecular growth

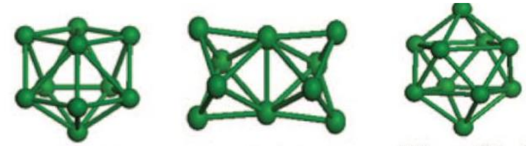
Use of classical MD is questionable

EAM



E= -6,57 eV/atoms

≠



W_{10}-*a* (C_{3v}) E= 5,44 eV/atoms

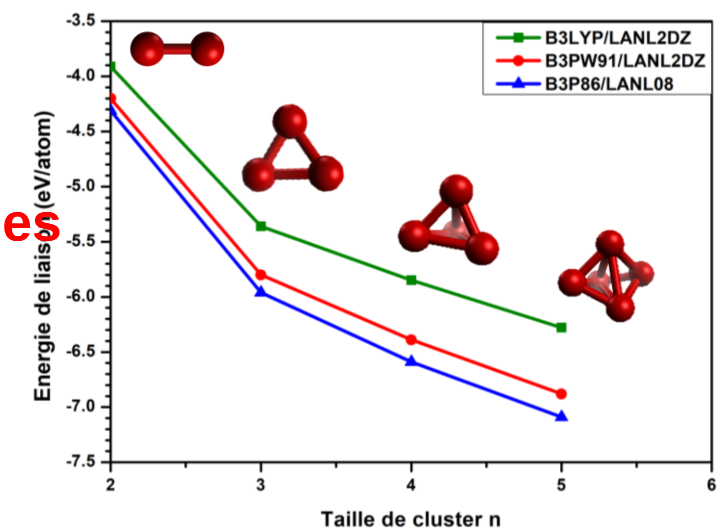
W_{10}-*b* (D_{2h}) E= 5,42 eV/atoms

W_{10}-*c* (D_{4d}) E= 5,42 eV/atoms

W_{10} structure obtained by classical MD (EAM)

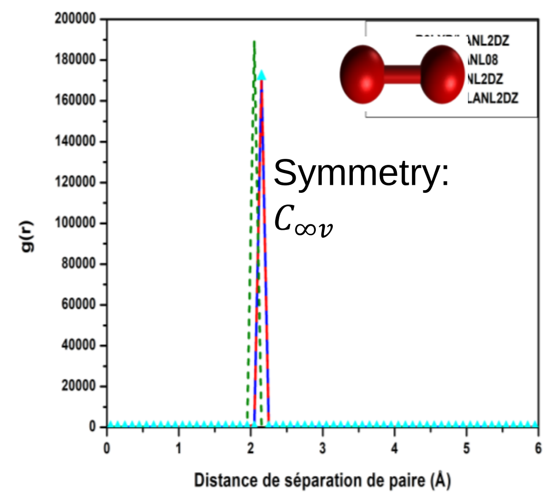
structures obtained by DFT

We make use of DFT and TD-DFT approaches With PPC



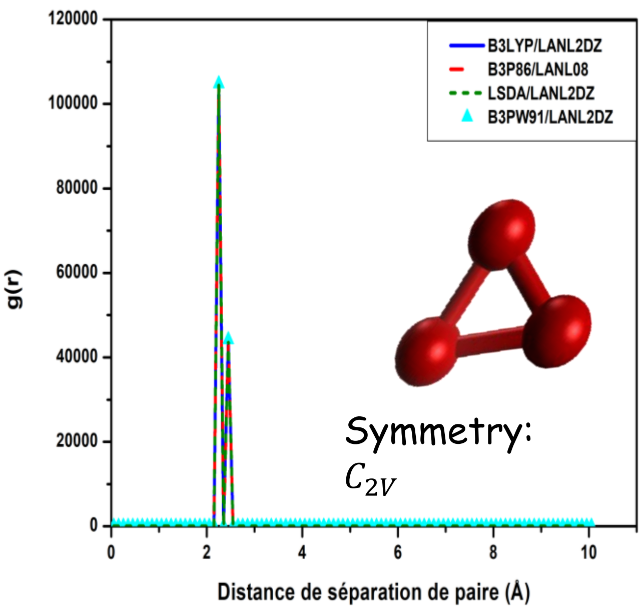
Step 1 : Evaluate basis sets and XC functionals evaluation through stable state optimization. The case of W_2

XC functionals	Basis set	Bond energy (eV/atom) – this work	Bond length (Å) this work	Bond energy (eV/atom) Xue-Ling et al (2009)	Bond length (Å) Xue-Ling et al (2009)
B3LYP	LANL2DZ	-3.91	2.182	4.54	2.039
B3PW91	LANL2DZ	-4.20	2.171	4.936	2.031
B3P86	LANL08	-4.31	2.165		
LSDA	LANL2DZ	-6.51	2.036	6.48	2.06



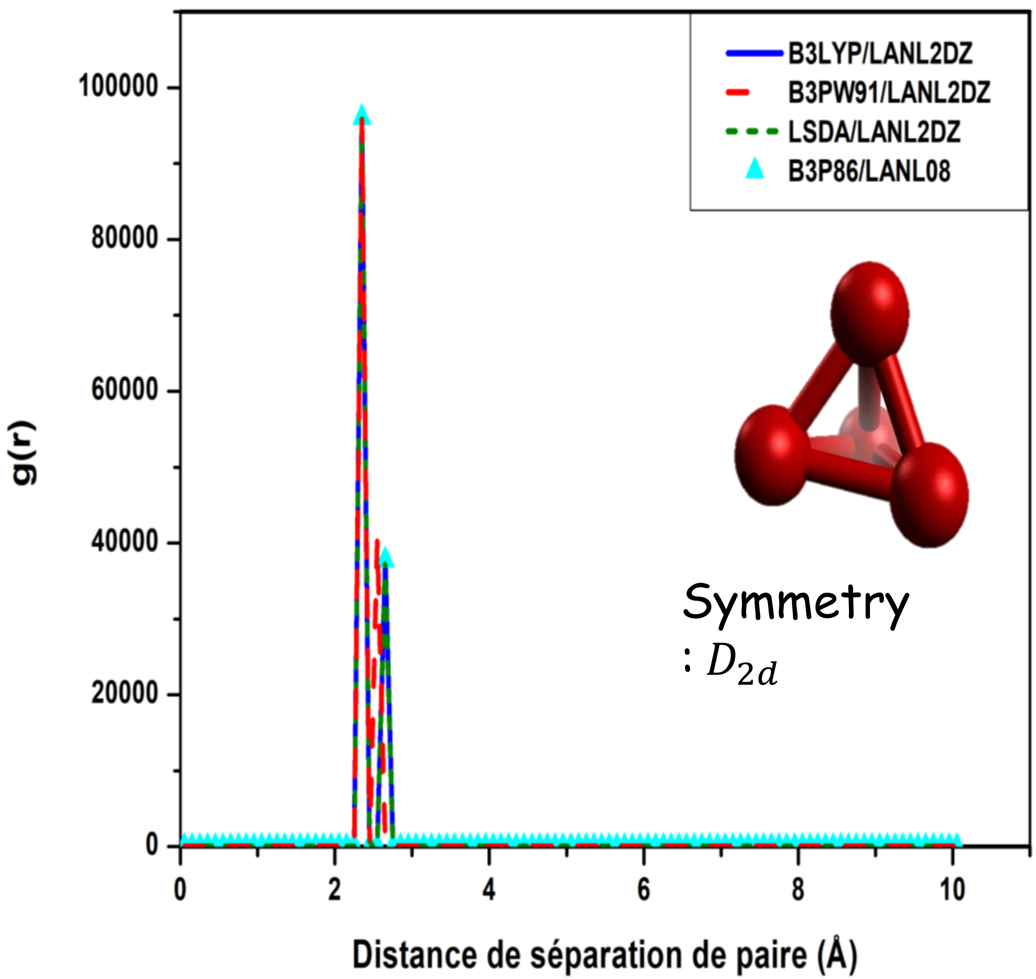
Step 1 : Evaluate basis sets and XC functionals evaluation through stable state optimization. The case of W_3

XC functionals	Basis set	Bond energy (eV/atom)	Bond length (Å)
B3LYP	LANL2 DZ	-5.36	R_{12}=2.253 R_{13}= 2.254 R_{23}= 2.454
B3PW91	LANL2 DZ	-5.80	R_{12}=2.241 R_{13}= 2.242 R_{23}= 2.441
B3P86	LANL08	-5.96	R_{12}=R_{13}= 2.232 R_{23}= 2.422
LSDA	LANL2 DZ	-7.52	R_{12}=R_{13}= 2.244 R_{23}= 2.428



Step 1 : Evaluate basis sets and XC functionals evaluation through stable state optimization. The case of W_4

XC functionnals	Basis set	Bond energy (eV/atom)
B3LYP	LANL2DZ	-5.85
B3PW91	LANL2DZ	-6.39
B3P86	LANL08	-6.59
LSDA	LANL2DZ	-8.16



Research methodology

- DFT approach makes use of :
  - A given basis set over which the wavefunction is expanded.
  - A prescribed form of exchange/correlation functionnal

➔ First step :determine the 'best' functional and basis set. Performed on stable state determination

➔ Second step determine the whole PES W_n-W^+/W_n^+-W

➔ Third step : perform Molecular dynamic simulation

Step 1 : Evaluate basis sets and XC functionals evaluation through stable state optimization. The case of W_5

Functionals	Basis sets	Bond energy (eV/atom)
B3LYP	LANL2DZ	-6.28
B3PW91	LANL2DZ	-6.88
B3P86	LANL08	-7.09