

Project code: ENR-MAT.01.IAP

Report on the project DUST-FORM “NanoDust in Metallic Tokamak”

Reporting after a quarter of the project duration
January 2022- September 2022

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Project rationale

Premises

Incidence of particles in fusion reactors, sizes ~200 nm-10 μm is a common fact;

- Particles are detrimental to reactor operation (core plasma cooling and fuel trapping);

- Particle types: droplets, aggregates, individual particles with various shapes;

- Source of particles – i) wall erosion under high heat fluxes (melting, evaporation) in particular during anomalous events, ii) sputtering;

- Particles under 200 nm, mostly neglected in previous researches, but present (WEST results, laboratory experiments);

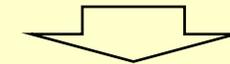
One expect the particle production decreasing in the detached/semi-detached divertor regime (small heat and charged species flows to the walls);

BUT

- Seeding with high-Z gases (e.g. N_2 , Ne, Ar, Kr) required for detached regime might lead to enhanced sputtering due to their higher mass;
- Detached regime (lower temperature, larger density) might enhance the clustering and particle nucleation and their lifetime;

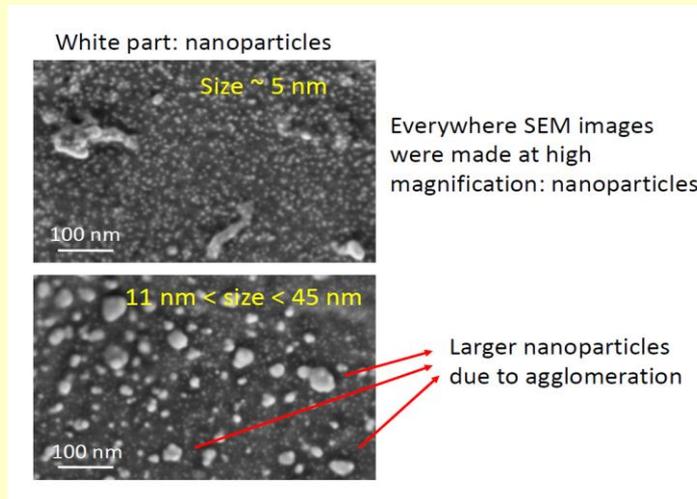


Production of nanometric particles may increase!



Research questions:

- Is nanometric particles production enhanced?
- How such nanoparticles influences the edge plasma?



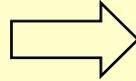
Particles collected from WEST (image from Cecile Arnas, PIIM)

Research questions and project structure

Research questions:

Is nanometric particles production enhanced (laboratory experiments)?

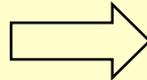
- search for enhanced sputtering in laboratory experiments - magnetron sputtering (for W);
- search for particle production during lasers high energy deposition on surface (for Be);
- collect particles in WEST;



WP3 : Experimental investigation of W and Be dust particles production through plasma-surface and laser-surface interaction; Particles collections in tokamak. (INFLPR -*Gheorghe Dinescu* - responsible for WP, IRFM).

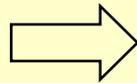
How such nanoparticles nucleate, growth and evolve in plasmas?

- consider physical phenomena as melting, evaporation, nucleation from vapors, growth, and transport



WP2 : Modelling of dust particle production kinetics through plasma/surface interaction under edge plasma conditions. (LSPM -*Khaled Hassouni*- responsible for WP, IRFM, PIIM);

How such nanoparticles influences the edge plasma?



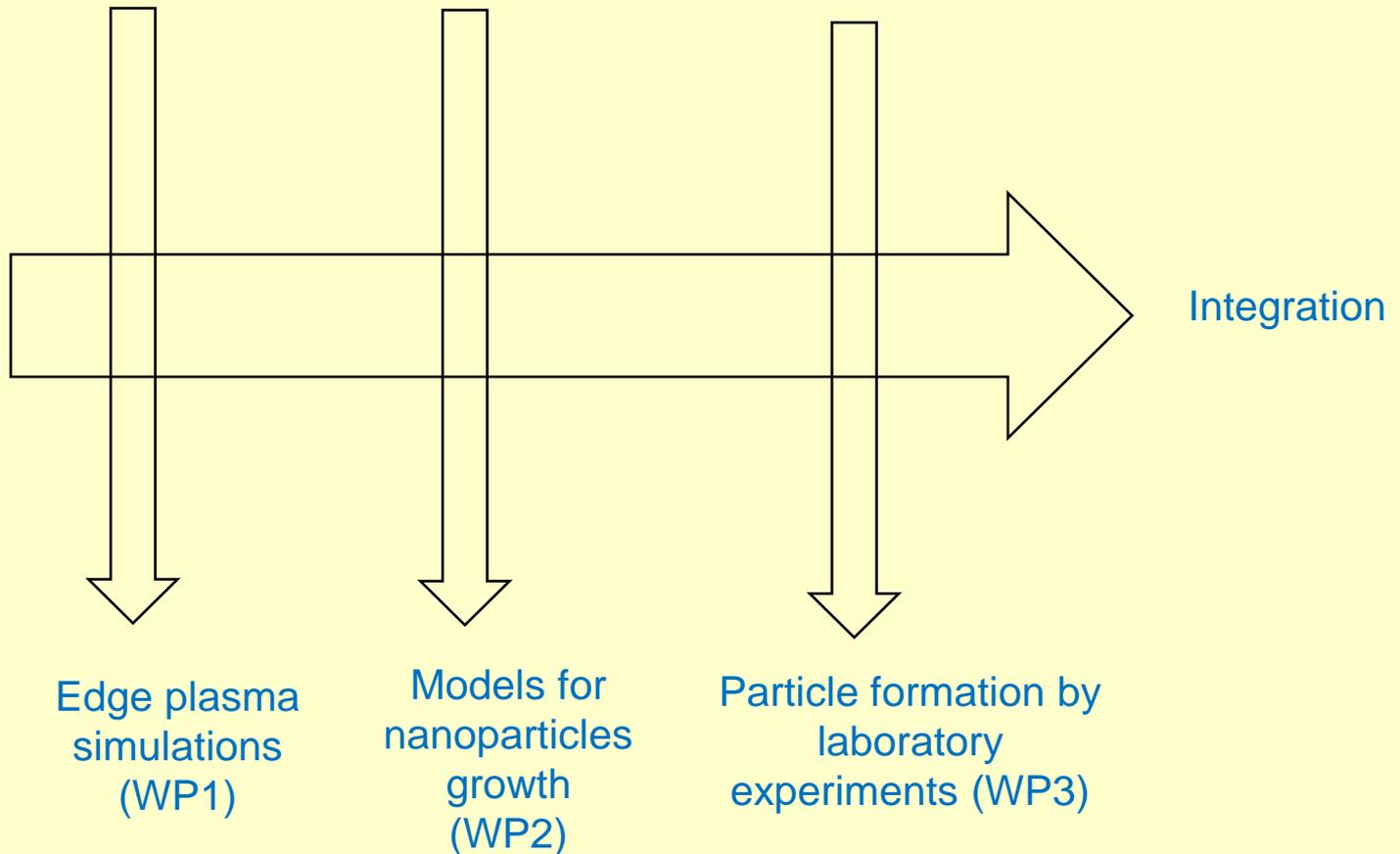
WP1 - Edge plasma integrated simulation with impurity and dust transport (IRFM - *Nicolas Fedorzack* responsible of the WP, PIIM, LSPM)

Research tools:

- **edge plasma simulation:** codes SOLEDGE3X- EIRENE, Te, ne, n_w in WEST and ITER) ERO2, DUMBO - creation, transport, survival time of particles in detached/semidetached plasma;
- **particles formation:** models for nucleation from vapors, growth and transport;
- **experimental:** Magnetron Sputtering Gas Aggregation, Laser Ablation, Be facility, dust collecting tools.

Project challenges

1. Advance with the research as deep as possible along the research directions
2. Integrate the works across the research directions to increase the fusion relevance



Presentation outline

Handling challenge 1: Advances along the research directions

Using discharge sputtering and laser deposition of energy at substrates as tools to study W and Be particle formation

- Formation of W nanoparticles via Magnetron Sputtering Gas Aggregation (MSGGA);
- Formation of W and Be nanoparticles by deposition of energy onto W, Be surfaces by a laser beam (PLA-W, PLA-Be)
- Dust collection in Tokamak.

Physical models for nucleation and growth

- Models for nucleation of particles from a W gas;
- Results of calculations for binding energy of W clusters ;

Edge-plasma simulation codes with impurity and dust transport

Models for edge plasma description

Results from WEST

Handling challenge 2: Advances in integration across the research directions

Selection of relevant parameters for integration of works

- Screening for the relevant parameters
- Conceive models suitable for verification both with the experiments and the codes

Concluding remarks and further work

Investigation of W and Be particle formation by discharge sputtering and laser deposition of energy at substrates

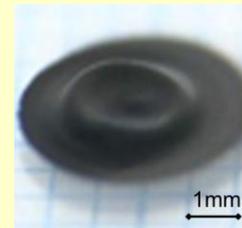
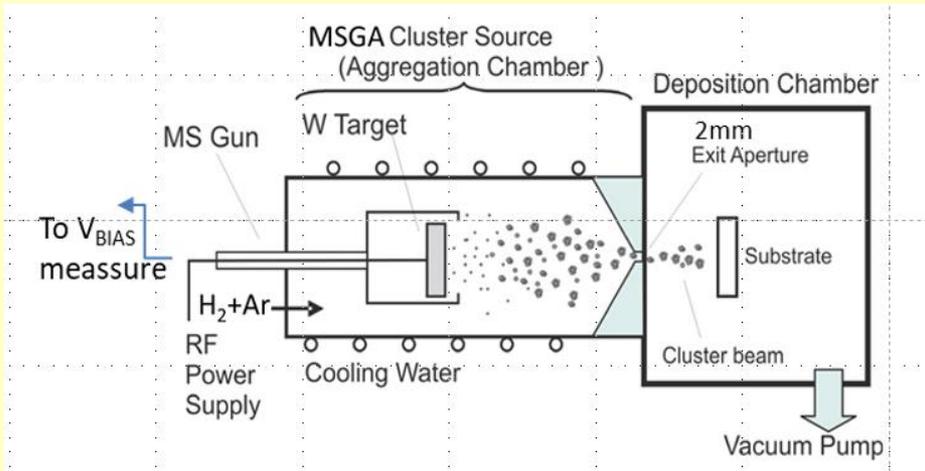
Producing W nanoparticles from sputtered W material

Producing W and Be nanoparticles from a laser plasma

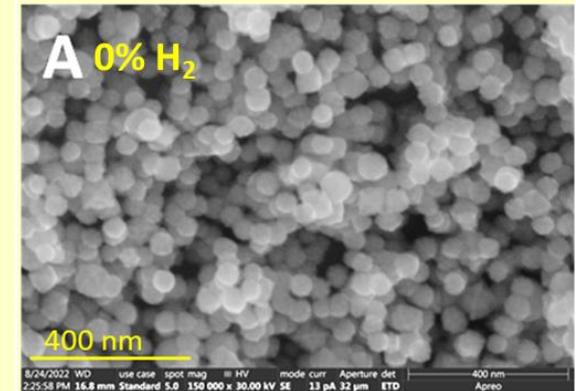
Synthesis rate of the W dust in H₂/Ar mixtures. Experimental Set-up.

Schematic view of the MSGA nanoparticle source

Usual working gas : Ar



spot on collector



SEM, particles

Source of material:

Surface process:

Gas phase processes:

Transport:

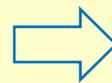
Tungsten (W magnetron target);

sputtering of target atoms by the ions

nucleation, accretion, coagulation;

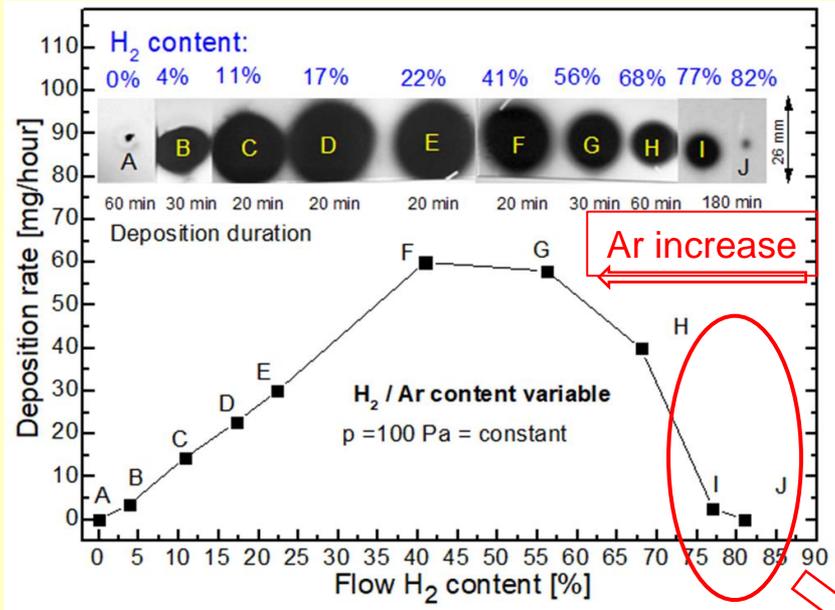
diffusion, convection

Relevant for the project, go to H₂ with Ar admixtures!



- Influence of Ar on particle formation rate in H₂ ?
- Influence of Ar on particle size and morphology ?

Producing W nanoparticles from sputtered W : rate



The dependence of the W dust synthesis rate over the H₂ content in the MSGA discharge. The dust mass was obtained by sample weighting

- Using only H₂ the deposition rate is low;
- Adding Argon the deposition rate (mg/hour) of particles increases compared with H₂ only, then decreases;
- W dust is obtained even for high H₂ content (measured up to 88%) in the MSGA setup;

How the rate behaves in Ar/H₂ mixtures?

Experimental Parameters:

Pressure in aggregation chamber: 100 Pa;

Exit aperture diameter: 2 mm;

RF power applied to magnetron: 80 W

Variable :

- H₂ / Ar ratio : 0 – 100 % (H₂ (0 -10 sccm) mixed with Ar (2 - 5 sccm)) ;

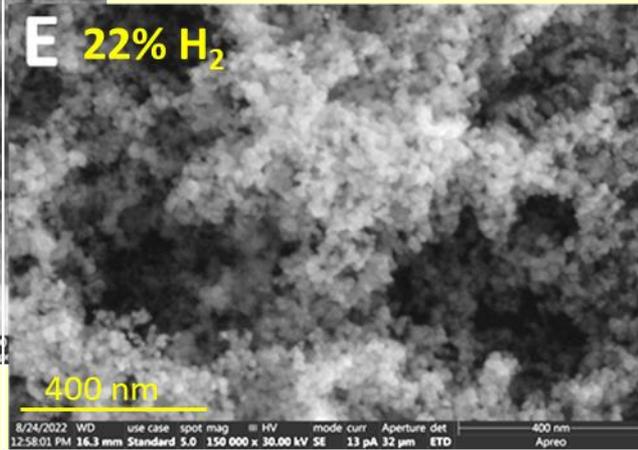
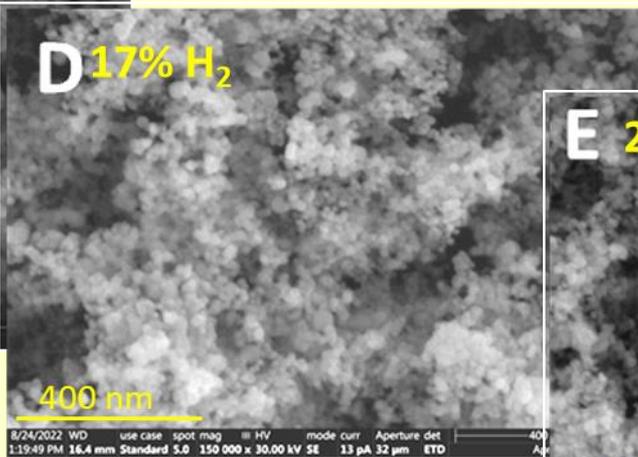
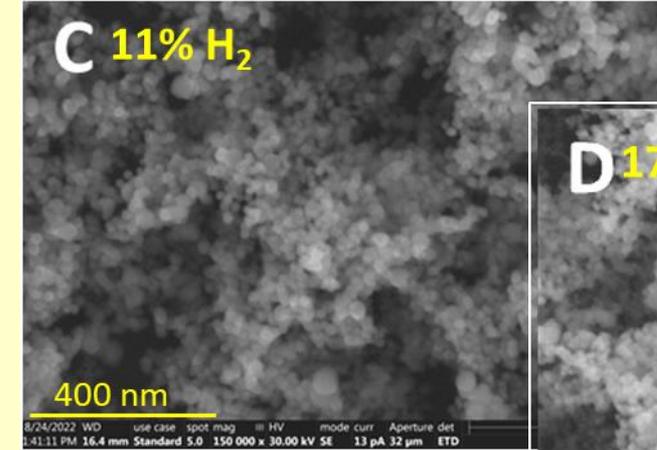
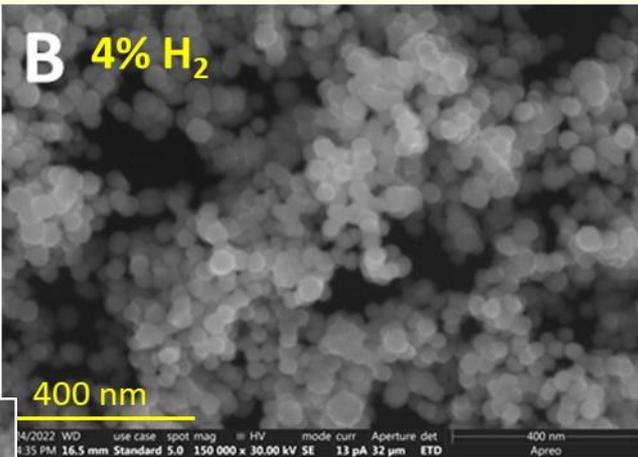
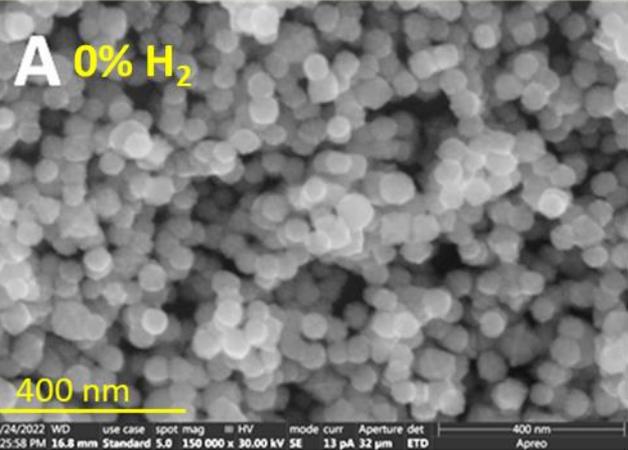
- Time (for collecting the dust): 20 -180 min.

Interest for the region dominated by H₂ where Ar is injected in small amounts, as in plasma detachment experiments;

Conclusion: Comparing with H₂ only, the admixing of Ar in H₂ favors the nanoparticle production process.

Producing W nanoparticles from sputtered W : particle morphology

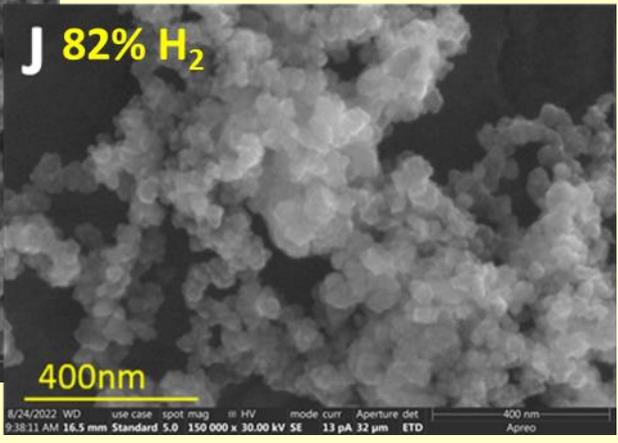
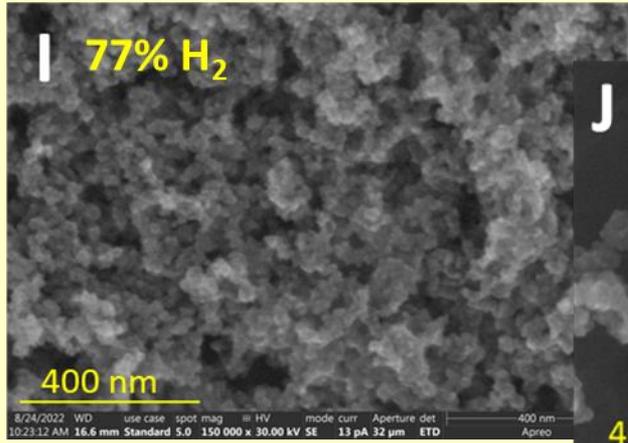
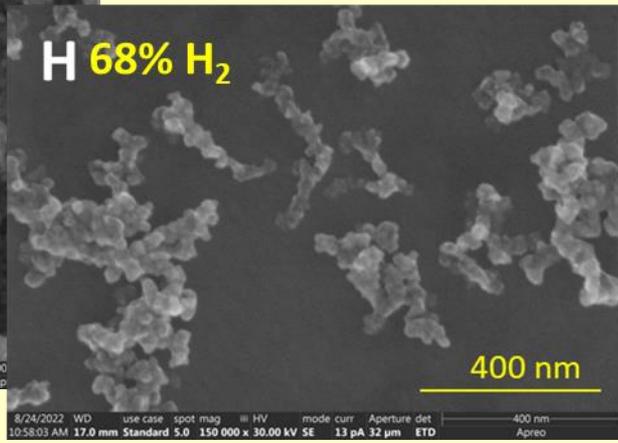
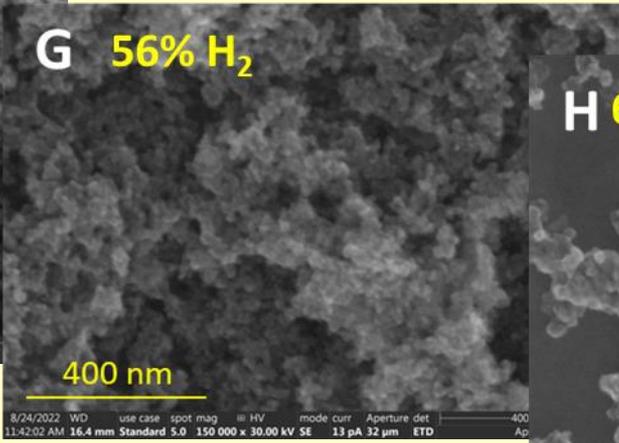
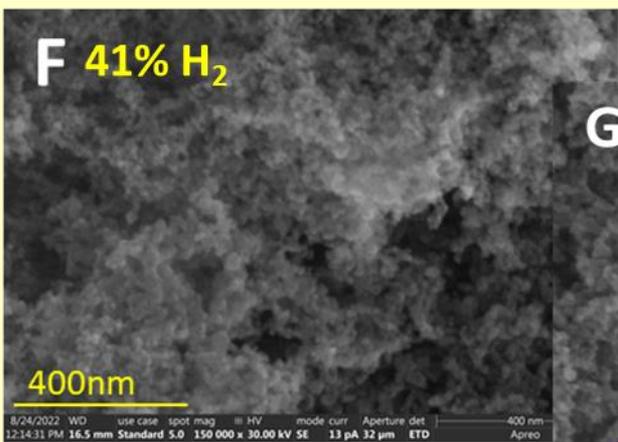
How the rate influences the nanoparticles morphology?



- Individual dust particles are obtained in discharges containing up to 22% H₂ ;
- The particles size decreases when H₂ content increases.

Argon dominated atmosphere

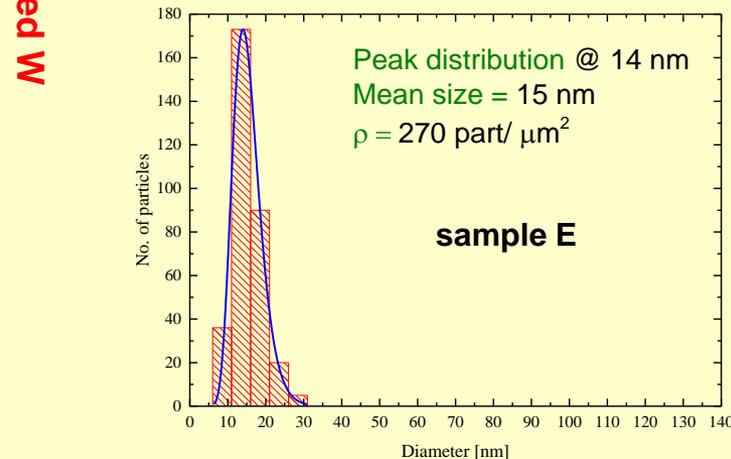
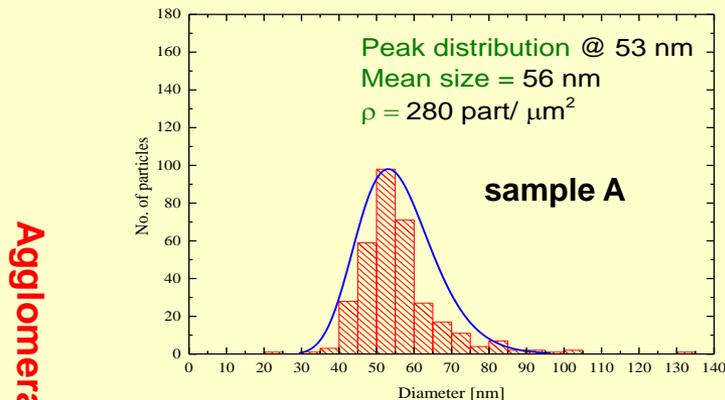
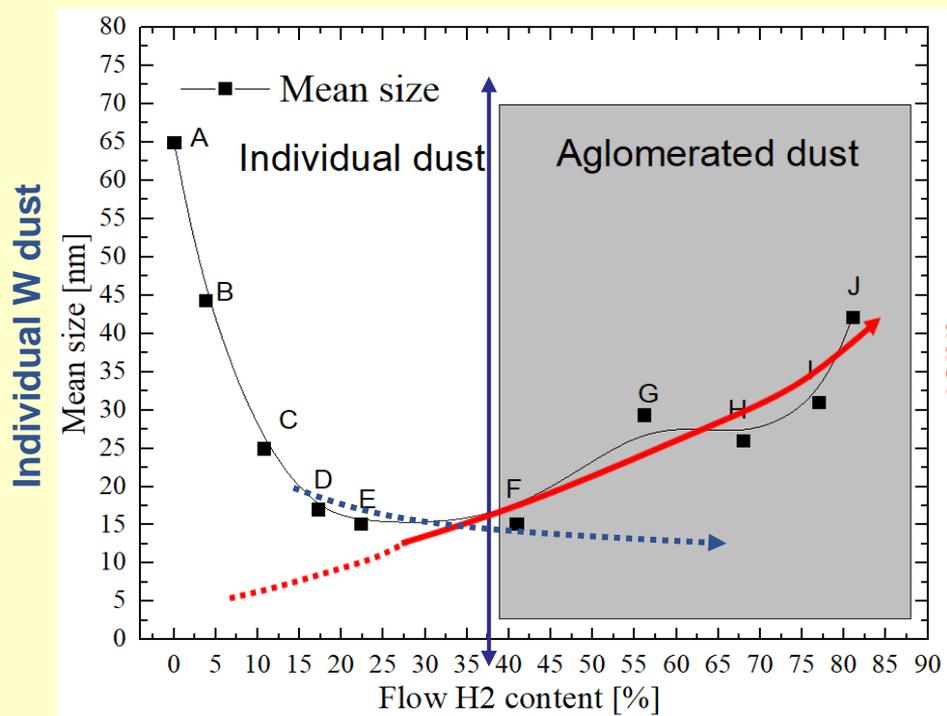
Producing W nanoparticles from sputtered W : particle morphology



The dust becomes agglomerated for higher amount of H₂ in discharge (40-80%)

Hydrogen dominated atmosphere

Producing W nanoparticles from sputtered W : particle size distribution upon $H_2/(Ar+H_2)$ ratio



For higher amount of H_2 in discharge (40-80%) is observed apparition of agglomerated dust.

Conclusions:

- Admixing Ar in H_2 favors the production process, in comparison with H_2 only,
- In hydrogen dominated H_2/Ar mixtures the particles size is much smaller compared to Argon rich atmosphere;
- In hydrogen dominated H_2/Ar mixtures the agglomeration process is favored;

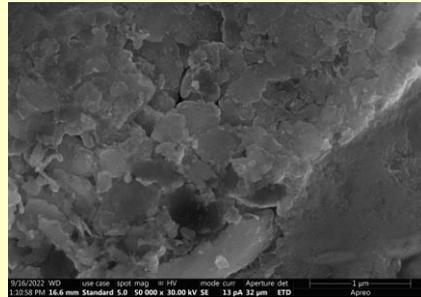
Retro-deposition of dust ?

Question: Ar effect on retrodeposition ?

Experiments performed in H₂ dominant atmosphere (80-90%)



Optical image of the sputtered target

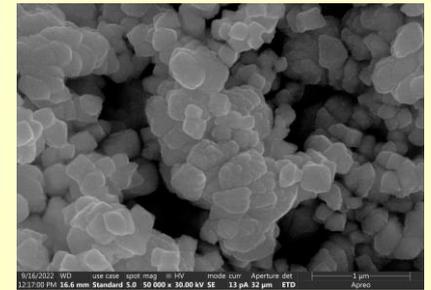


SEM image of the retro-deposited dust collected from the target

Experiments performed in Ar (with only traces of H₂)



Optical image of the sputtered target



SEM image of the retro-deposited dust collected from the target

Conclusion: Admixing Ar gas in H₂ promotes nanoparticles retro-deposition !

Estimation of the erosion rate during sputtering in H₂ dominated atmosphere made by measuring the profile of the eroded track: 2-3 mg / cm²min:

Formation of W and Be nanoparticles by deposition of energy onto W, Be surfaces by a laser beam (PLA-W, PLA-Be)

Working with Be needs special conditions, use of BeH (Beryllium Handling Facility);

W ablation by laser used for preliminary trials before setting-up the system at facility

Producing W nanoparticles under high energy laser deposition on W surfaces

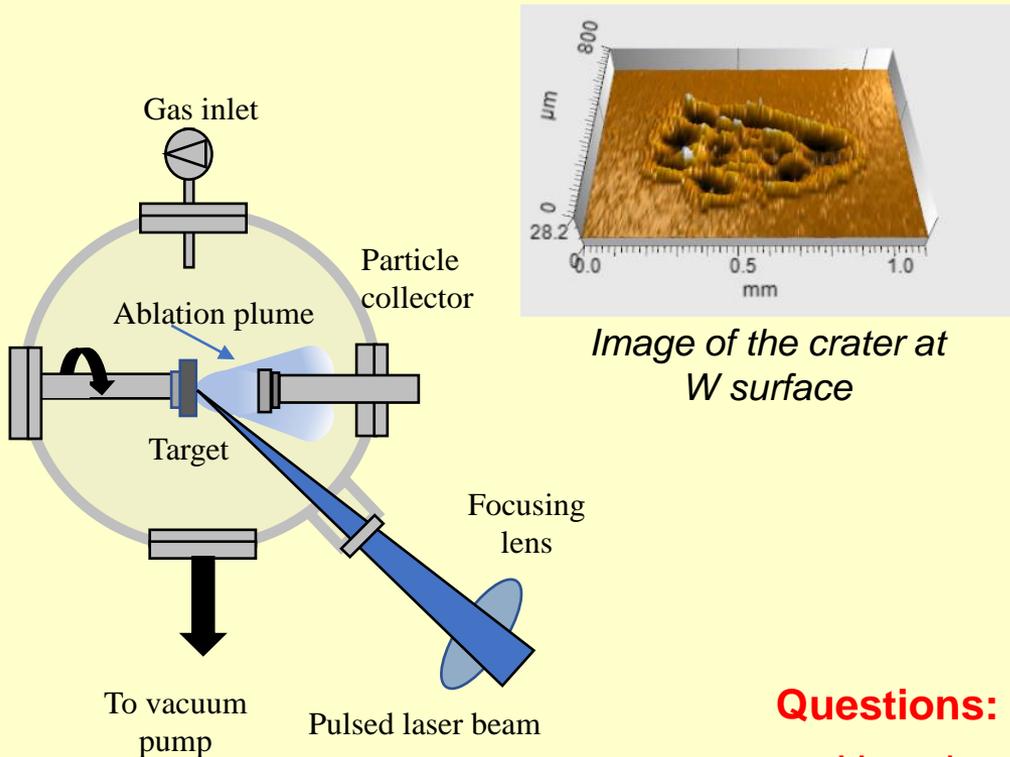


Image of the crater at W surface

Source of material: W target
Surface processes: melting, vaporization;
Particle evolution: gas phase;

Fixed parameters

- Nd - YAG pulsed laser
- $\lambda=266$ nm, 4-6 ns pulse duration,
- 10 Hz repetition rate
- Fluence= 2.5 J/cm² (~ 400 MW/cm²)
- Distance target - substrate = 4.5 cm

Variable parameters

- Different Z-gases: vacuum, H₂, He, Ne, Ar ...
- Different gas pressure: 10⁻², 1,3, 5, 7 mbar...

Questions:

- How the nature of background gas influences the nanoparticles production ?
- How the pressure influences the nanoparticles production ?
- Chemical composition?

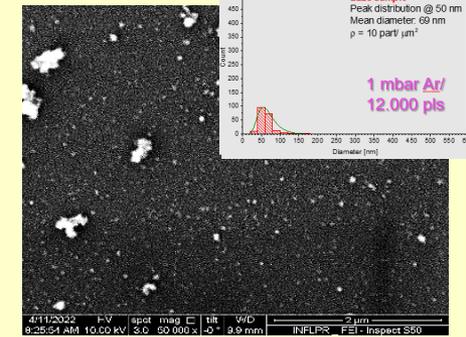
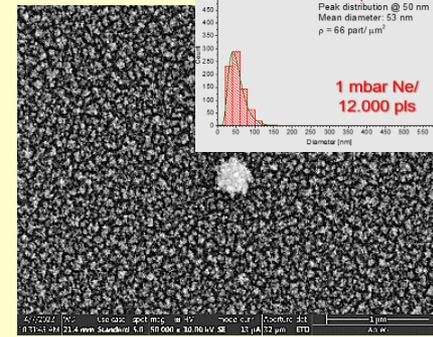
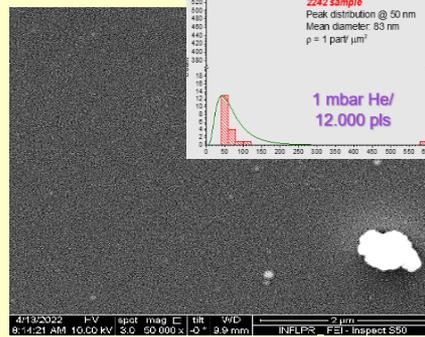
Producing W nanoparticles under high energy laser deposition on W surfaces – morphology dependence upon gas type and pressure

H₂

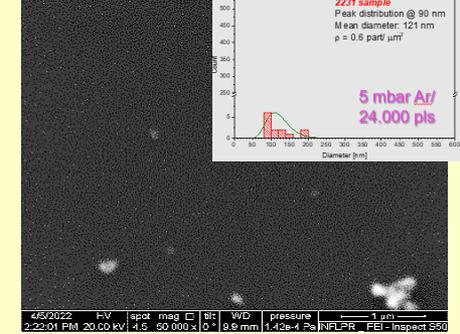
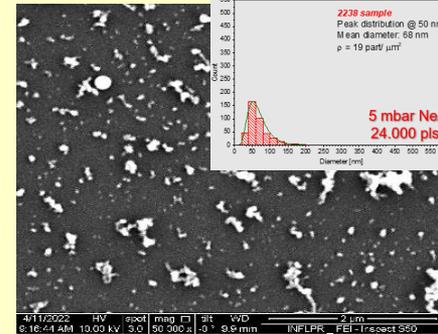
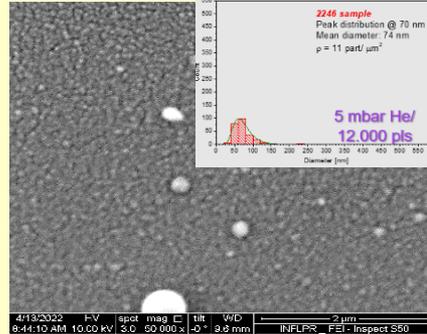
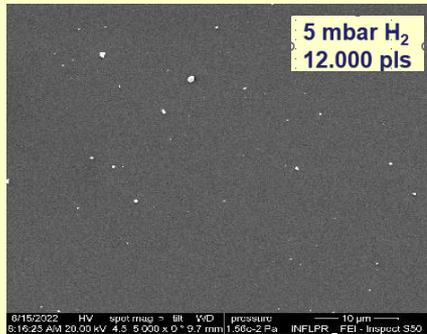
He

Ne

Ar



pressure 1 mbar



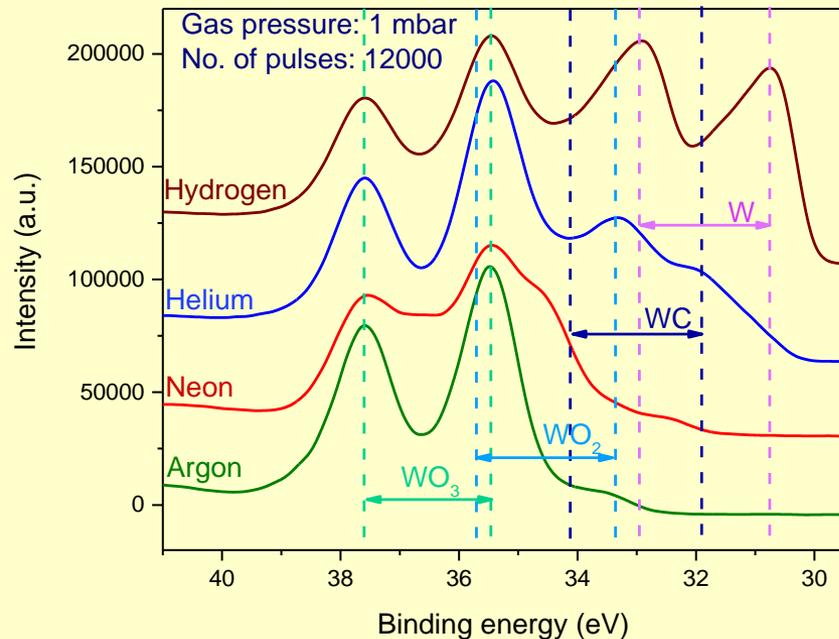
pressure 5 mbar

- Hydrogen (H₂) promote thin film deposition, not particles;
- Tungsten particles (sizes 20-100 nm, cluster-film like) are found mainly in high-Z gases and at larger pressure;
- The particles are arranged in agglomerated cluster geometries; some droplets may appear, mainly in He.

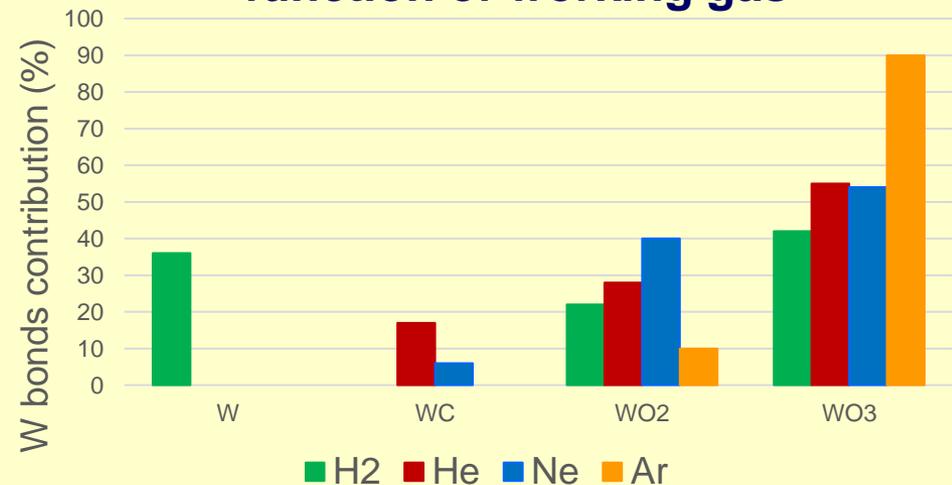
Chemical investigation of the collected material

Comparative high-resolution W4f XPS spectra for all investigated gases, Ar, Ne, He, and H₂ respectively

W-related components as resulted upon deconvolution of the XPS spectra for the W4f region for all investigated gases



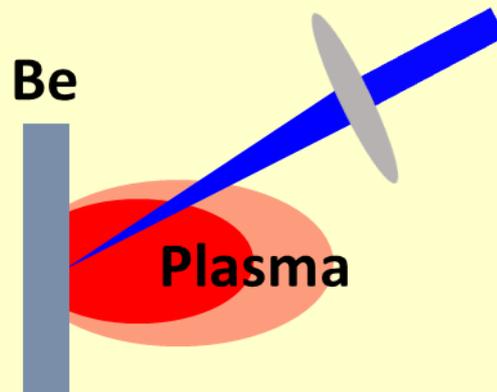
Tungsten oxidation states as a function of working gas



- Ablation in H₂ atmosphere promotes the metallic state of tungsten;
- Ablation in He, Ne, Ar leads to WC, WO₂ and WO₃ production;

First attempts at Be particle production via high energy laser deposition on surface

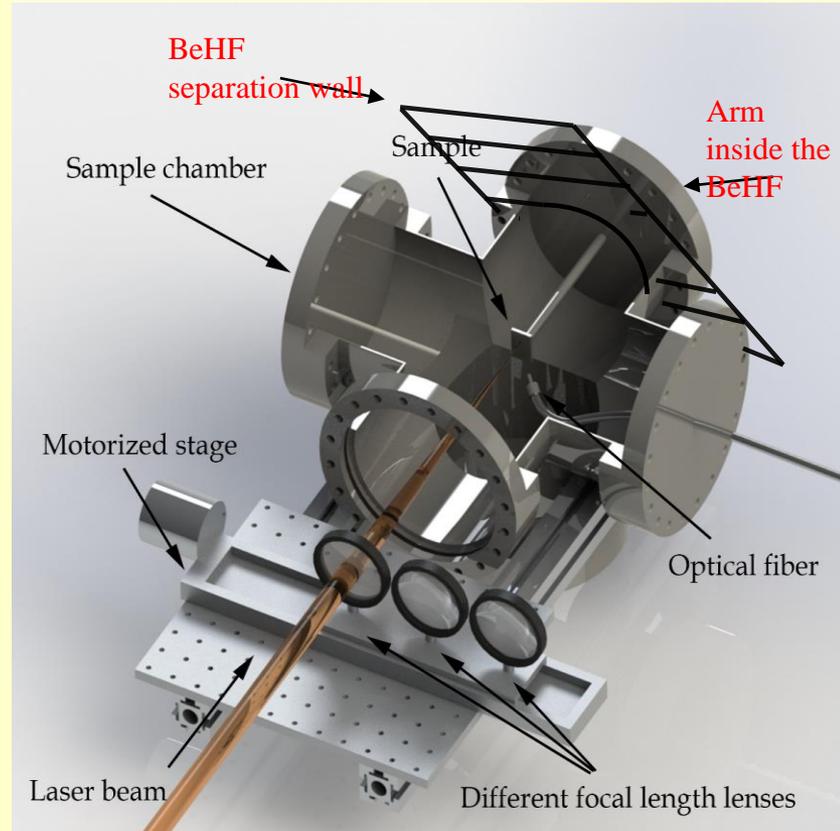
Setting up the laser ablation system at Be facility
Particles obtained: influence of background gas and pressure



Upgrade for Nanoparticle Production by Laser Experiments



How to avoid working with the whole laser setup in Beryllium Handling Facility (BeHF) ?



The setup distributed over two spaces:

- only one arm of the chamber enters the Be working area, it is used for targets mounting and samples extraction;
- outside the Be working area are placed the laser, the optics, the diagnostics;

Upgrade of the BeHF facility for nanoparticle production by high energy laser deposition at Be targets

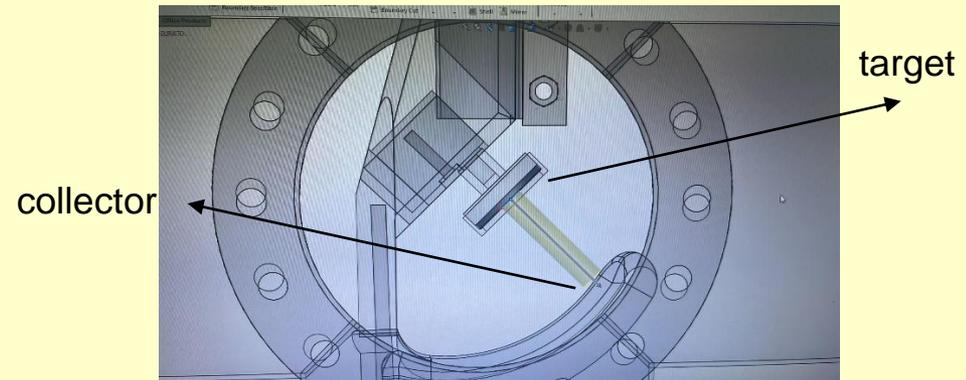


PLA system configured at BeHF (INFLPR)

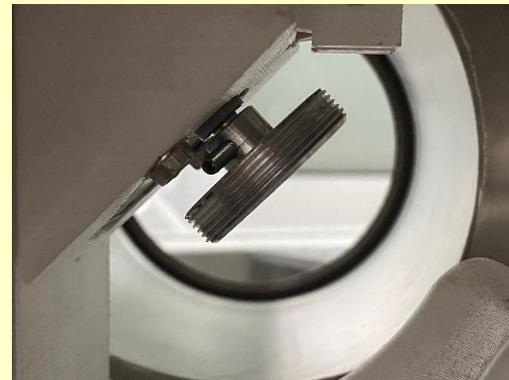
The setup includes:

i) The laser itself ; ii) Optical line for handling the laser beam and its focusing on the target; iii) 45° sample holder with tunable rotating speed;

- independent gas inlets for 3 gases;
- vacuum system (mechanical and turbo pumps);



CAD sketch of the target and collector arrangement

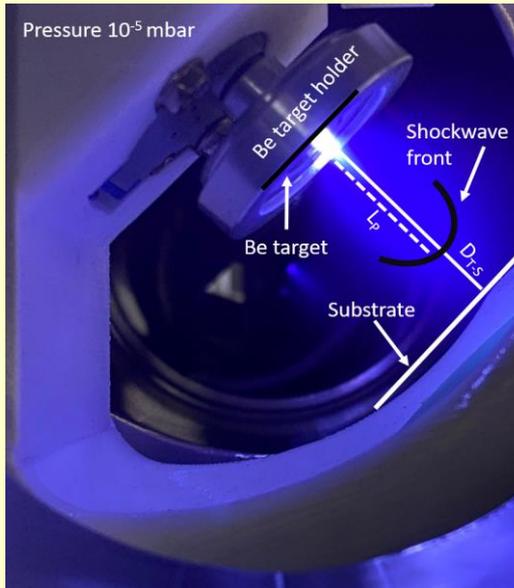


Side-view image of the Be target holder mounted in the chamber

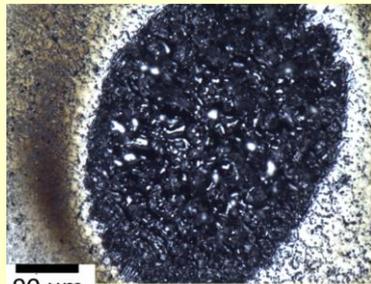


Front side view image of a Be target ablated

Producing Be nanoparticles by high energy laser deposition at Be targets



Side-view image of plasma during Be irradiation with a Nd:YAG laser working at 1064 nm, in vacuum at a base pressure of 1×10^{-5} mbar



on target



Target surface morphology after laser impact on Be (120 pulses, optical microscope 50x)

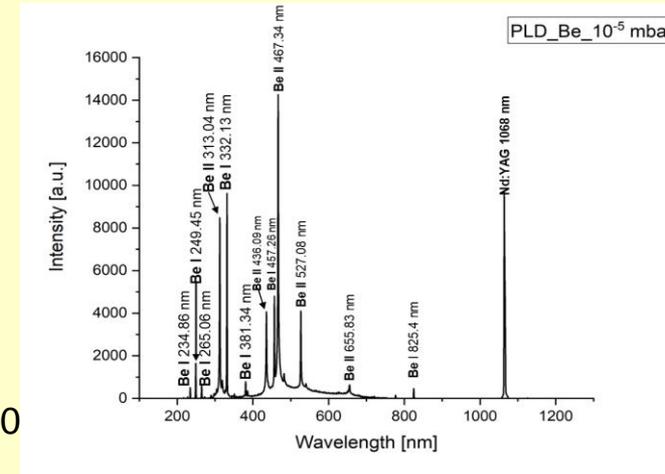
Processes:

- Source of material: Be target
- Processes: melting/vaporization
- Particle collected on substrate

Experimental parameters:

- Laser: 1064 nm Nd:YAG, 5-7 ns, 10 Hz
- Target collector distance $D_{T-S} = 3.5$ cm
- Laser fluence 3 J/cm^2 ($\sim 528 \text{ MW/m}^2$)
($A_{\text{spot}} = 0.63 \text{ mm}^2$)
- Laser pulse no.: 3000, 6000, 9000, 12000
- Background gas: H_2 , He, Ne, Ar
- Pressures: 10^{-2} mbar, 0.5 mbar, 7 mbar

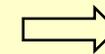
inside plasma



Clear evidence of Be I and Be II lines by emission spectroscopy

on collector

Be dust collected on a Si(100) substrate after testing the PLA system built at the Be facility from INFLPR



Gas nature and pressure influence on the deposited Be material

H₂

He

Ne

Ar

10⁻² mbar

10⁻² mbar

10⁻² mbar

10⁻² mbar

droplets & compact

droplets & compact

droplets & compact

droplets & microstructured

7 mbar

7 mbar

7 mbar

7 mbar

droplets & np

agglomerated np

sponge-like
agglomerated np

agglomerated np

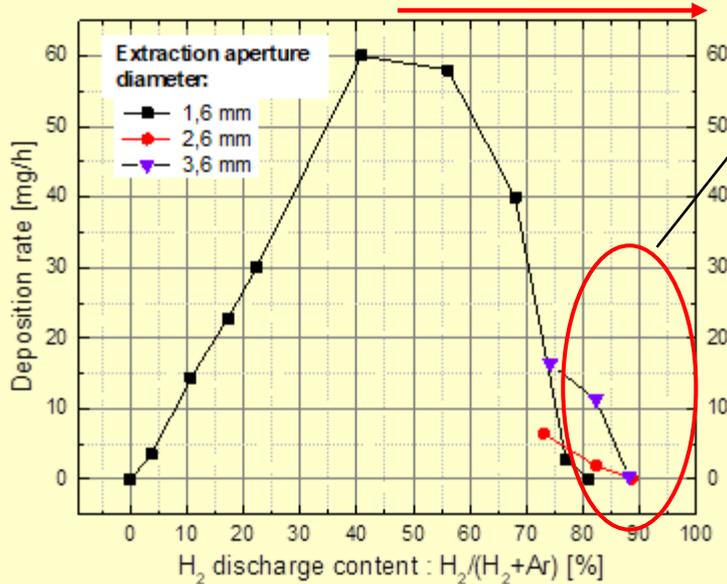
Results:

- Be is prone to producing droplets and thin films at low pressure, whatever the gas;
- At higher pressure the nanoparticles and nanostructured are agglomerated;

Further work

W sputtering: Significant increase of sputtering in H₂ dominated plasma injected with small Ar amounts:

Increase of H₂ percentage



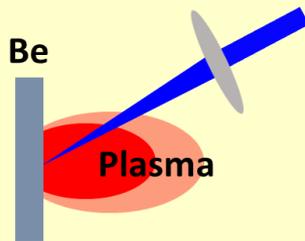
1) To explore in detail the hydrogen dominated region with H₂/Ar at ratios similar to those used for plasma detachment;

2) Answer to questions:

Is the sputtering rate increase related to the higher mass Ar ions or to chemistry?

(Mass Spectrometry Measurements not presented here indicate that plasma becomes dominated by ArH⁺ ions)

How the sputtering rates and particles characteristics compare in case of other gases used in detachment, in the series: He, Ne, Ar, Kr...



Be, laser: Complete the setup with a dedicated laser and with diagnostic;

-Explore the setup capabilities in terms of laser parameters;

-Explore the Be particle production in conditions used in detachment experiments in hydrogen dominated plasmas injected with He, Ne, Ar, Kr...

Research questions:

How the nanoparticles are produced?

Which is the fate of nanoparticles ?

WP2. Physical models for nucleation and growth (responsible for WP: Khaled Hassouni, LSPM)

Understand the production mechanism of Tungsten and Beryllium nanoparticles in different plasma regimes

- Models for nucleation of particles from W vapors;
- Results of calculations for binding energy of W dimers, and higher mass clusters ;

DFT – Density Functional Theory and DTF-TD - Time dependent DFT
MD - Molecular Dynamic calculations for cluster growth

A view behind the particle formation

Metal atoms formation

- atomic vapors from the target
- mixing with the buffer (H₂, D₂, Ar, Ne, Kr...) gas, cooling



Nucleation

- produce the initial embryos for particle growth;
- take place near the target.

A) Homogenous nucleation

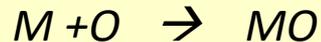


(enhanced by three body collisions)

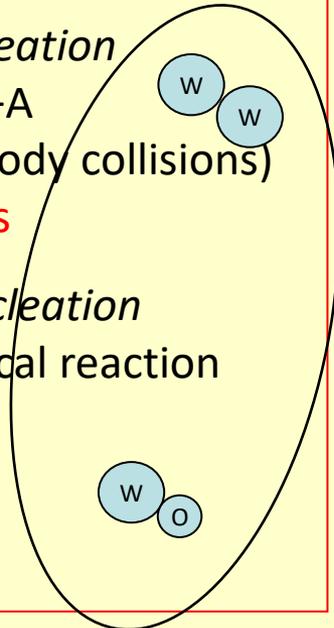
RESULT : W-W dimers

B) Heterogeneous nucleation

(triggered by a chemical reaction with a foreign gas)

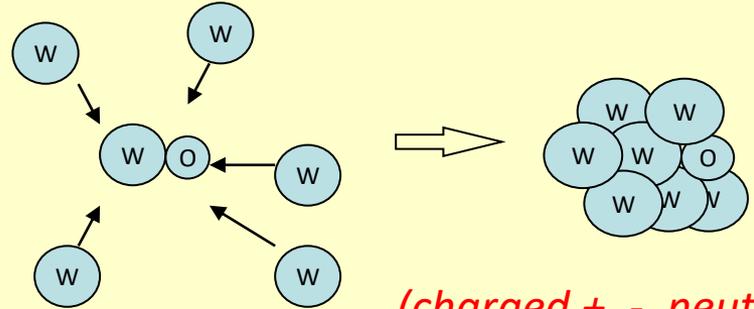


RESULT : W-O dimers



Accretion

- attachment of W atoms or ions to dimers

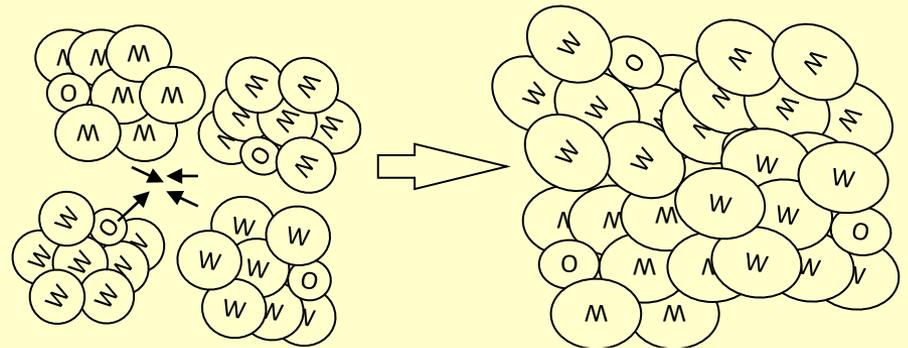


(charged +, -, neutral)

RESULT: Small W nanocrystals (~2-10 nm)

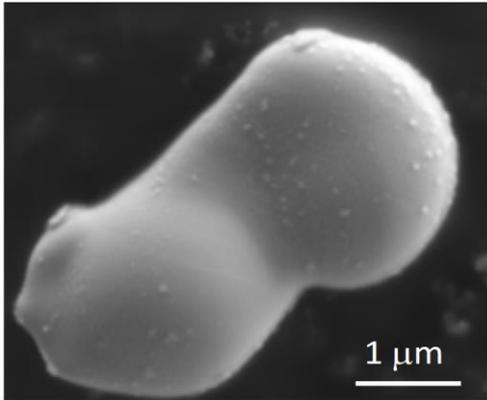


Coagulation



RESULT: particles

Research topic 1: Formation of nanoparticles in the presence of droplets



Particle collected from WEST - solidified droplet displaying nanoparticles on the surface (from Cecile Arnas - PIIM)

Process: Condensation in the vapor cloud around the droplets emitted in the plasma phase during anomalous events : disruptions (Coll. IRFM)

Possible steps:

1- Liquid droplet and vapor emission → 2- Evaporation around the droplet → 3- Vapor expansion → supersaturation → 4- NPs Nucleation → 5- growth/coagulation

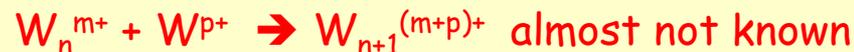
Investigation tools :

- **Nucleation theories ; Transport models; Aerosol dynamics**

Research topic 2 : Nanoparticles production in the presence of enhanced sputtering (semi-detached or detached regime)

Steps: Presence of High-z charged ions → sputtering enhancement → emission of atoms, may be clusters from PFCs → fate of the emitted species - molecular growth ? → nucleation ?

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



Some data exist for neutral clusters for which MD may be use

Work performed since 01/01/2022: clustering kinetics in the case of W

- Determine the stable neutral and charged structure by MD with prescribed interaction potential and/or DFT
 - calculate the bonding energy for such structures to evaluate their stability;
- Determine the interaction potential for W^+/W_n & W_n^+/W systems?
 - a prerequisite for the estimation of the coagulation cross sections

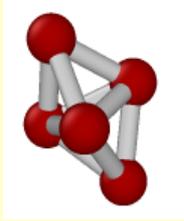
Type of structures: $W_2, W_3, W_4, W_5, W_{10}, \dots$

Methodology: Use of Molecular Dynamics (MD) calculations
 Use of Density Functional Theory (DFT) calculations;

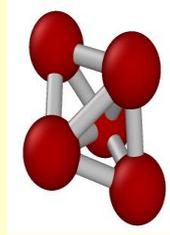
A comparison between MD and DFT approaches, W5 and W10

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

EAM potential Thersoff potential

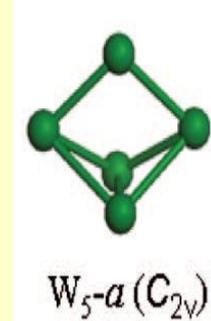


$E = -5.77$
eV/atom

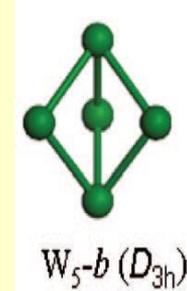


$E = -4.99$
eV/atom

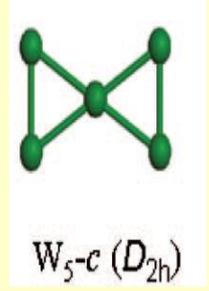
DFT (article Jiguang Du et al, 2009),
method: Gradient corrected DFT



$E = -4.61$
eV/atom

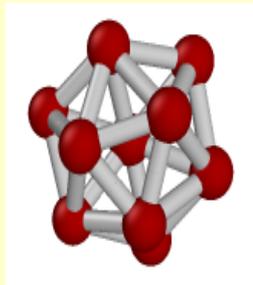


$E = -4.39$
eV/atom



$E = -4.05$
eV/atom

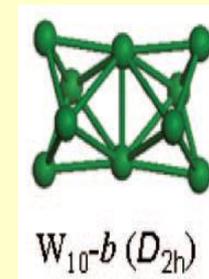
EAM potential



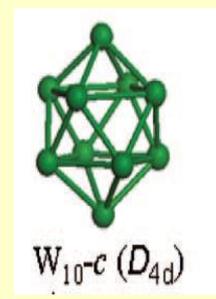
$E = -6,57$ eV/atom



$E = -5.44$
eV/atom

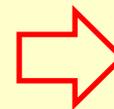


$E = -5.42$
eV/atom



$E = -5.42$
eV/atom

- MD and DFT produce different results !.
- It is likely that DFT results describe better the reality because it is more based on fundamental principle.



Conclusions
Use DFT first for
further activities!

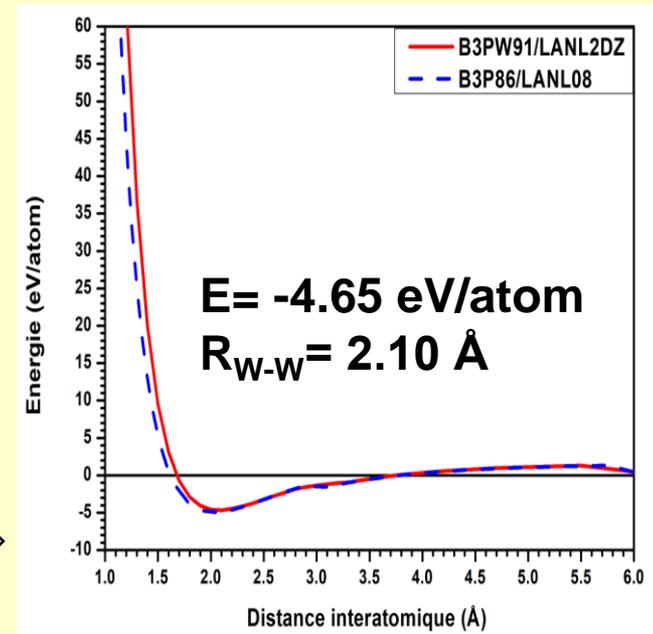
Research methodology

Uses a selected XC (exchange correlation) functionals basis set and calculates: Bond energy, bond length, PES - potential energy surface

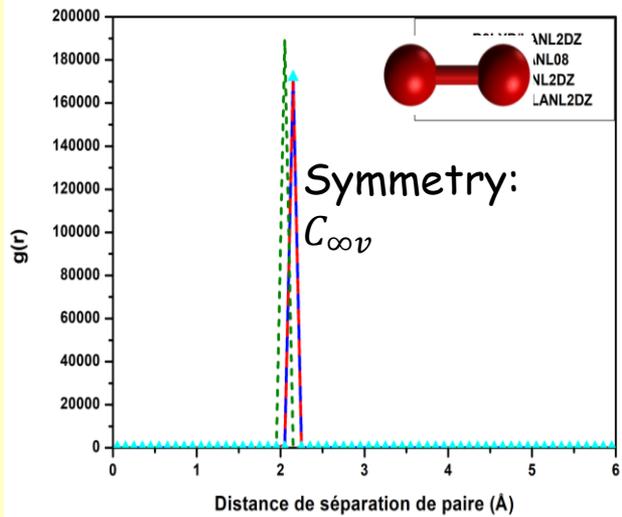
- First step DFT :determine the 'best' exchange correlation-XC functional and basis set. Perform calculations for stable state determination
- Second step DFT determine the whole PES (Potential Energy Surface) for the interaction $W_n^-W^+/W_n^+ - W$
- Third step : perform Molecular dynamic simulation for growth

Results - DFT. The case of W-W and W-W+

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

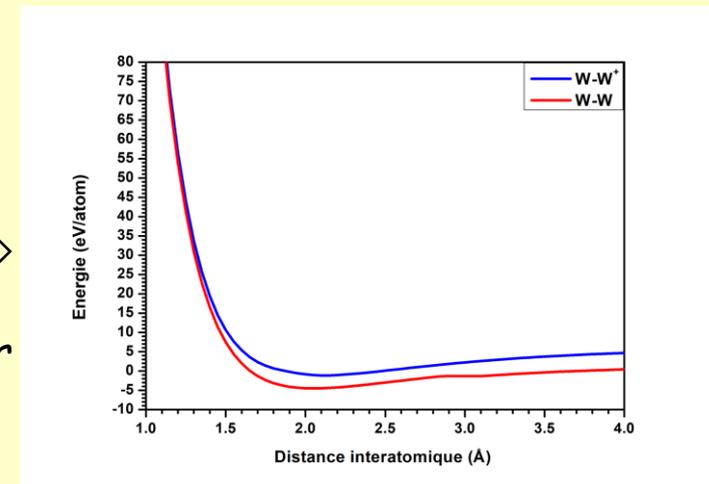


W-W potential energy as a function of W-W distance \rightarrow



Bond length \leftarrow

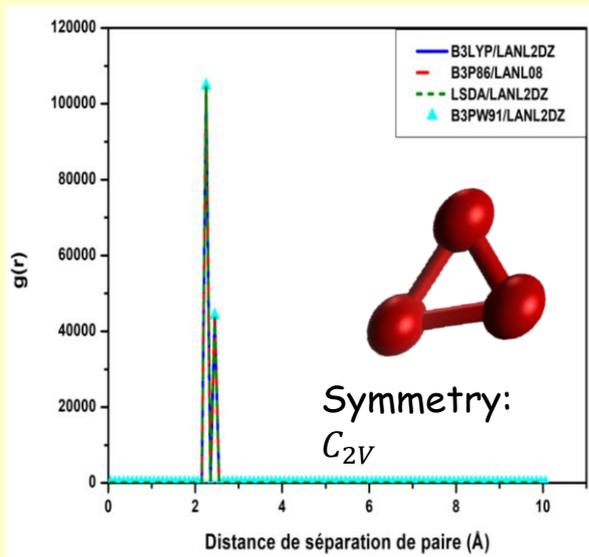
Comparison PES for W-W and W-W+ \rightarrow



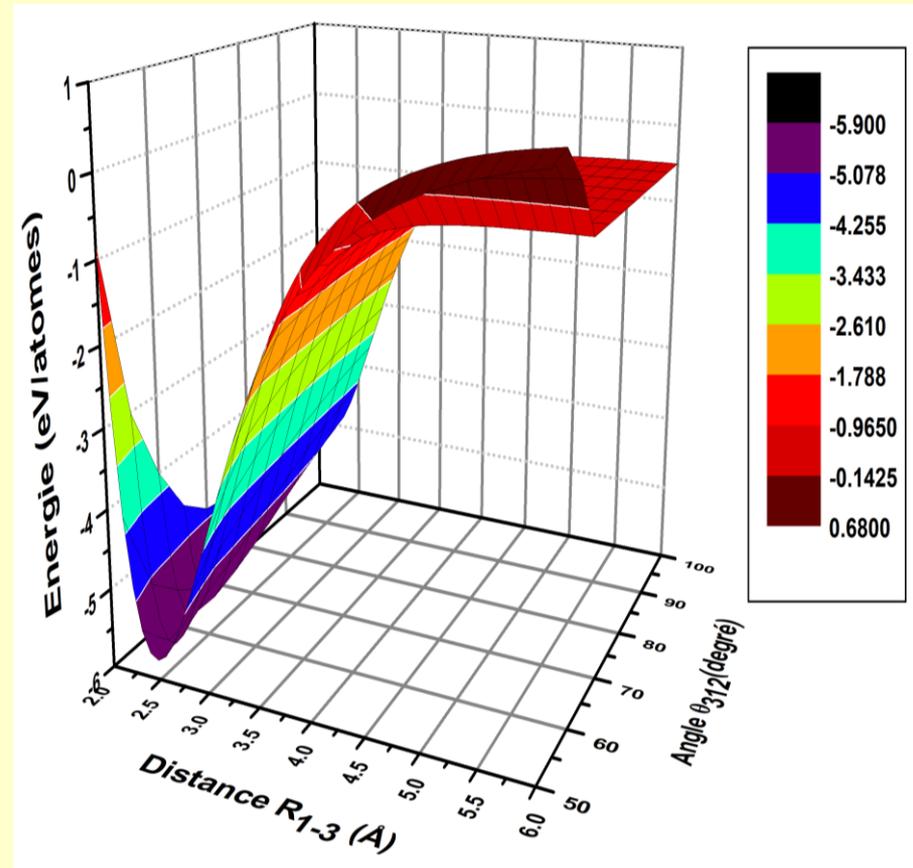
Results - DFT (Case W3)

The case of W3

XC functionals	Basis set	Bond energy (eV/atom)	Bond length (Å)
B3LYP	LANL2DZ	-5.36	$R_{12}=2.253$ $R_{13}=2.254$ $R_{23}=2.454$
B3PW91	LANL2DZ	-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	LANL2DZ	-7.52	$R_{12}=R_{13}=2.244$ $R_{23}=2.428$



PES -The case of W_2-W^+

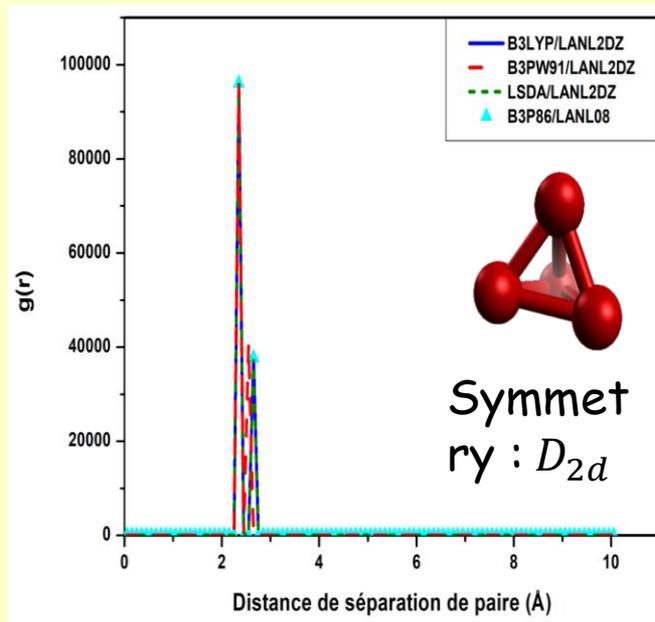


PES using **B3P86/LANL2DZ** XC functional/Basis set as a function of W_1-W_3 distance and (1-2,1-3) angle

Results - DFT (case W5)

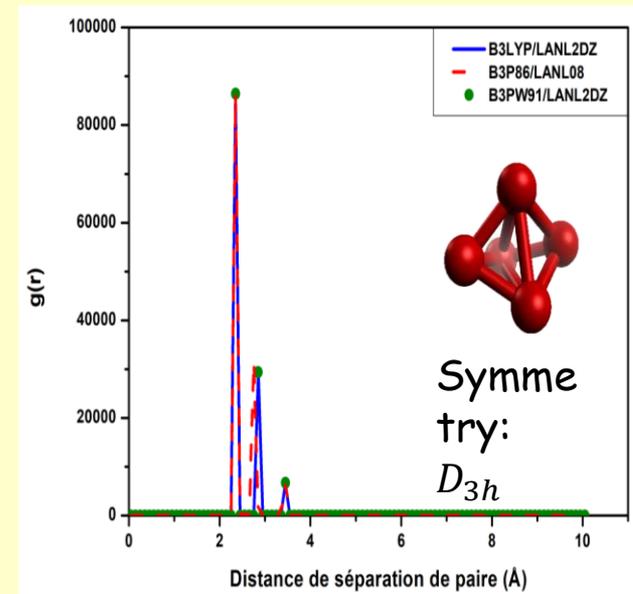
The case of W4

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

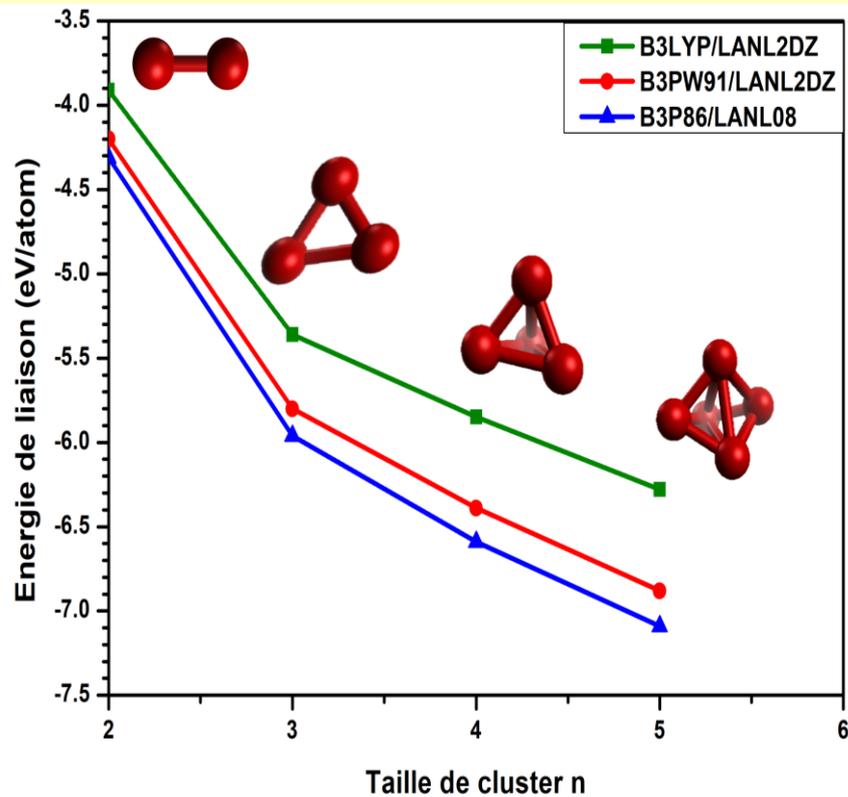


The case of W5

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

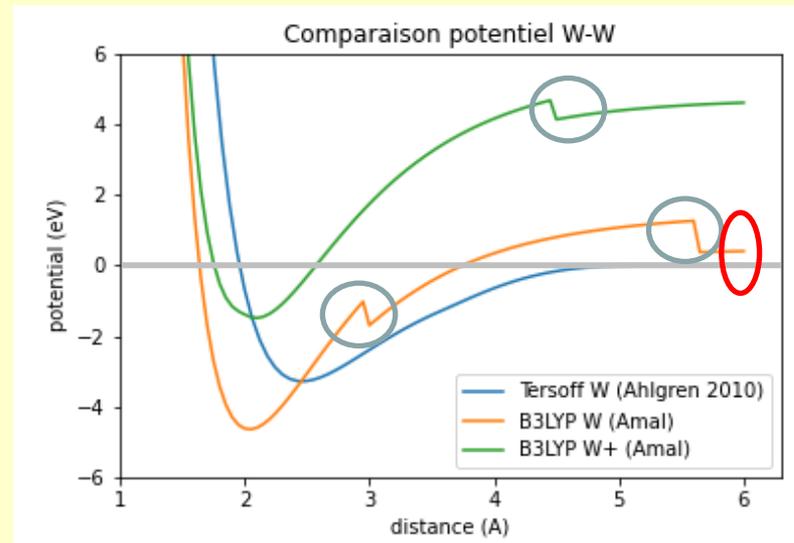


Conclusions and work in the near future



- The basis sets and XC functionals selected through stable state optimization;
- Some PES calculated;

1. Solve issue on PES:



I1- Jumps in the PES

I2- The energy does not go to zero when increasing W-W distance

2. Calculate PES for small clusters up to W5;
3. PerformMD simulations on these PES

II. Start the investigation of Evaporation/Condensation/Solidification of tungsten around a tungsten droplet emitted after an anomalous event

Research questions:

How such nanoparticles influence the edge plasma?

WP1. Edge plasma integrated simulation with impurity and dust transport (IRFM - responsible of the WP - *Nicolas Fedorzack*, PIIM, LSPM)

Edge plasma simulation:

codes SOLEDGE3X- EIRENE, Te, ne, n_W ... (in WEST and ITER)

Monte Carlo simulation for sputtering

ERO2 code, DUMBO code - creation, transport, survival time of particles in detached/semidetached plasma;



DE LA RECHERCHE À L'INDUSTRIE

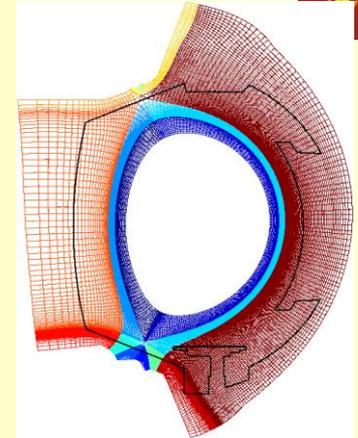


SOLEEDGE simulations of WEST plasma background

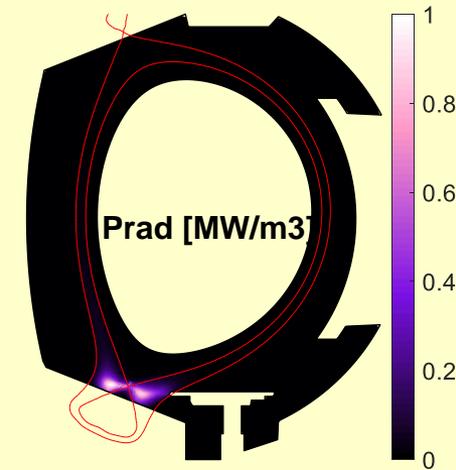
N. Fedorczak, G. Ciraolo, Hao YANG

SOLEEDGE modeling tool for plasma background

H. YANG

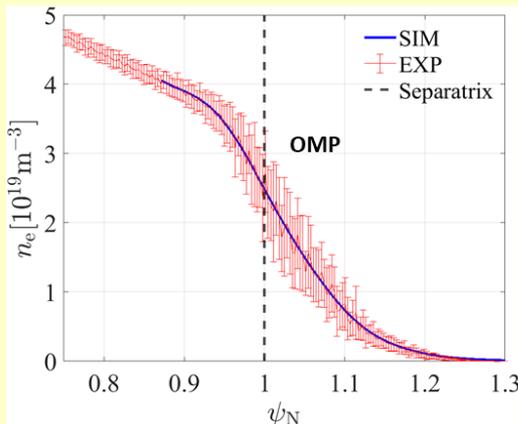


Grid used in simulations

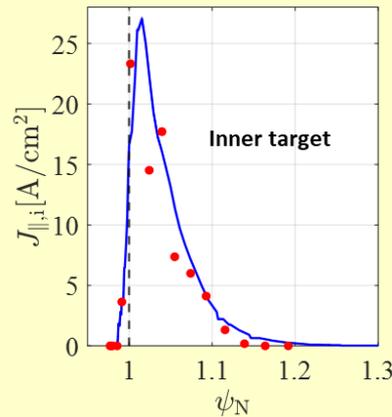


Map of the radiated power

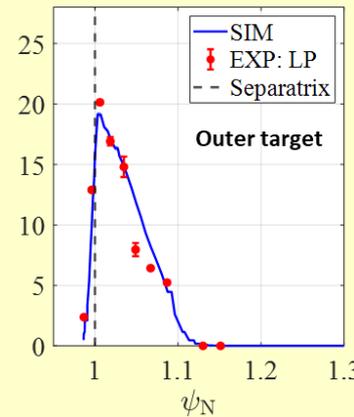
- SOLEEDGE-EIRENE : 2D plasma solver across the entire chamber
- Applied to WEST, constrained against a few experimental cases, with good success



Upstream density plasma profile: simulation versus experiment



Particle flux to divertor targets: simulation versus experiment



Experiment: data measured by spectroscopy, Langmuir probe, interferometry...

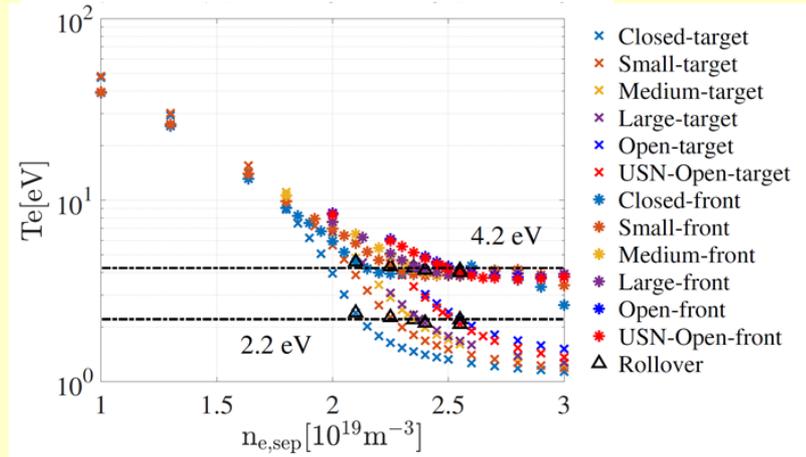
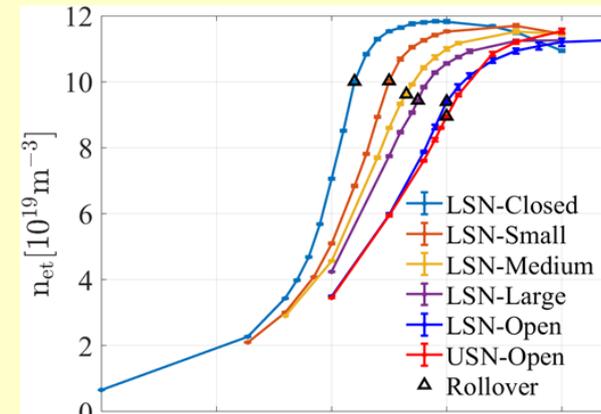
Extensive scans of divertor conditions initiated by Hao Yang



H. YANG

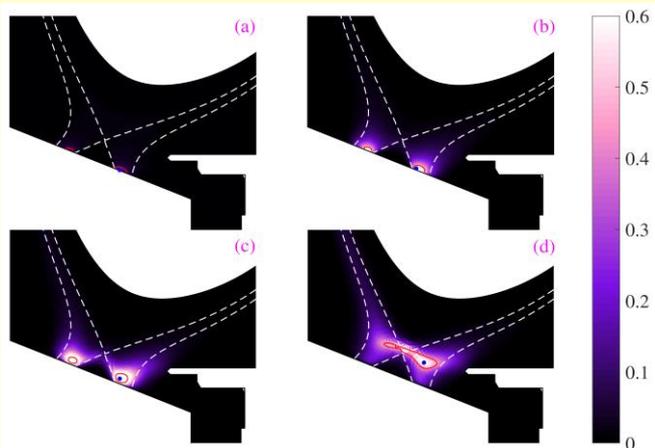
- At given power, scan gaz fuelling in pure Deuterium case
- Continuous variation of steady-state divertor conditions
- divertor detachment well identified
- Power scan also performed,
- with light impurity (Oxygen)

Calculated electron density at the outer target at different levels of fuelling for various baffling geometries



Electron temperature at the radiation front location (circles) and outer target (crosses). Detachment occurs at about 2.2 eV at target and 4.2 eV at the radiation front

Radiation power [MW/m³]



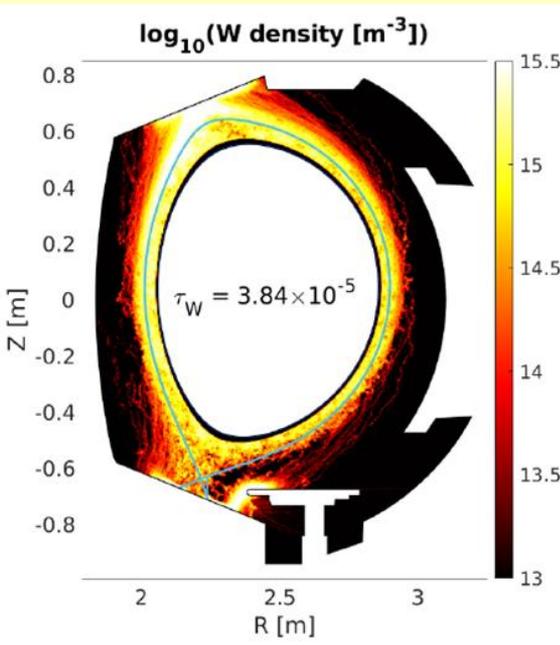
Radiation maps at different levels of fuelling

Tungsten sputtering and migration solved with ERO2.0

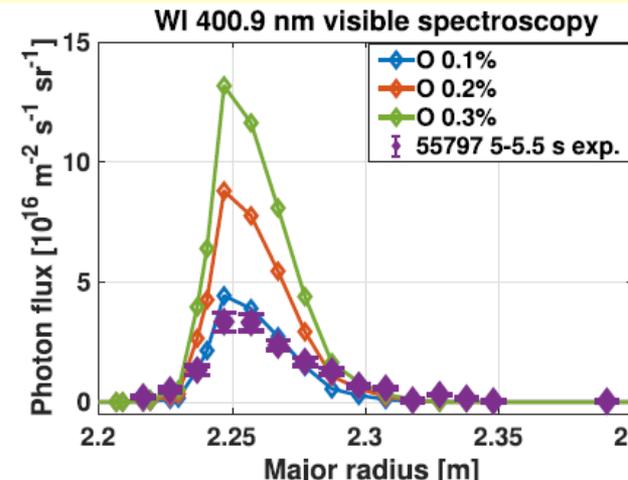
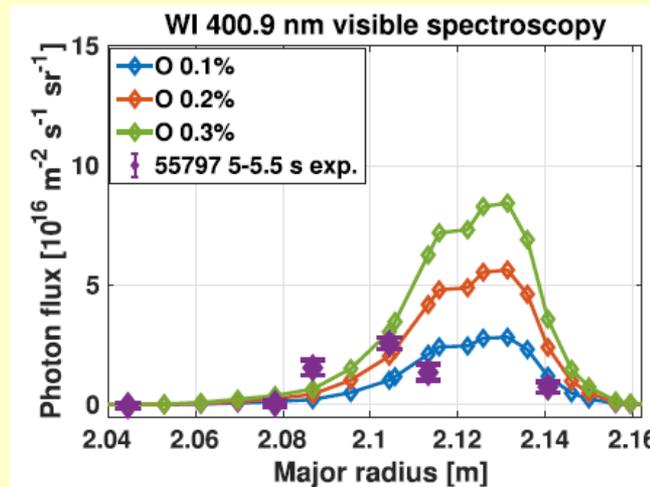


S. DI GENOVA

- Monte Carlo kinetic solver for tungsten sputtering and migration
- Uses SOLEDGE plasma background (no self consistent coupling yet, especially on radiated power)



lower divertor sources ERO2 / experiment

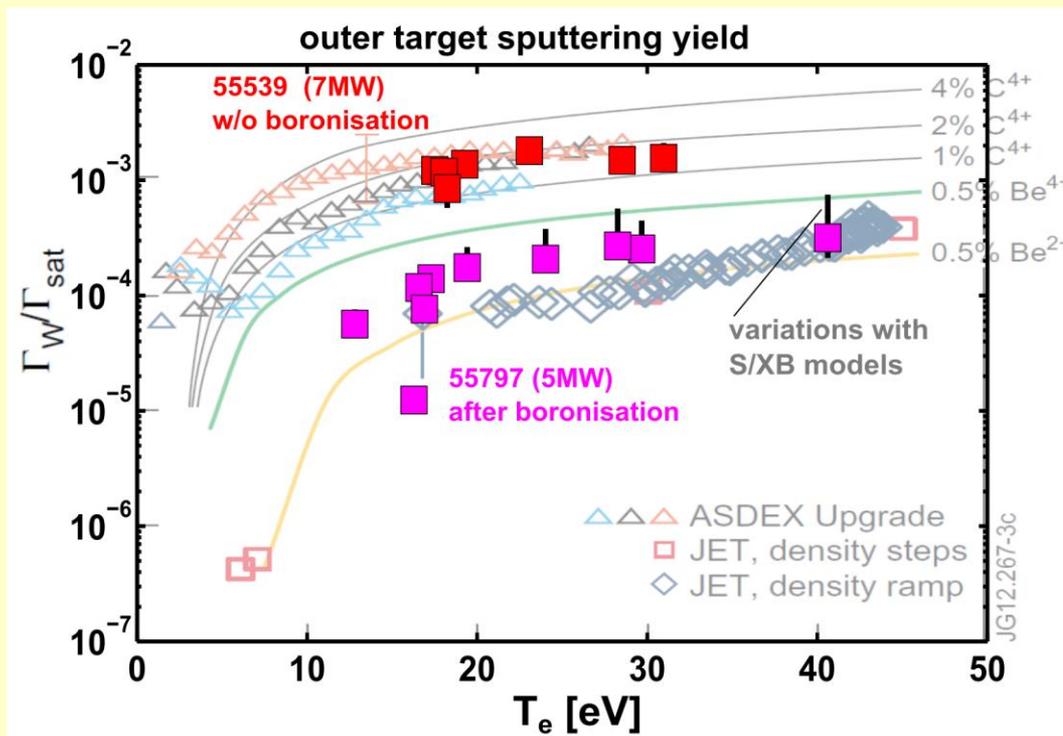


W atoms 2D density distribution calculated with ERO2

Gross surface tungsten sources (simulated with ERO2) consistent with experiment (data given by visible spectroscopy)

Standard experimental conditions in WEST gives tungsten sputtering yields of $\sim 1E-4$ - $1.E-3$ in the divertor

- Measured with visible spectroscopy and Langmuir probes
- Coherent with JET-ILW & ASDEX-Upgrade



Ratio of the tungsten flux at divertor (measured by visible spectroscopy) over the deuterium flux striking the target (measured by Langmuir probes)

Summary and Further work

- Large simulation database performed by Hao YANG for WEST
- Covers different detachment conditions with or without light impurity
- ERO2.0 is currently used to infer tungsten ion concentrations in the divertor, including state of the art sputtering, redeposition & migration processes
- Large experimental database from WEST to check models. So far, no dedicated experimental sessions focusing on plasma detachment, but significant plasma time (of past experiments) showed detachment
- Number of transient events on divertor though (disruptions) → specific dust formation



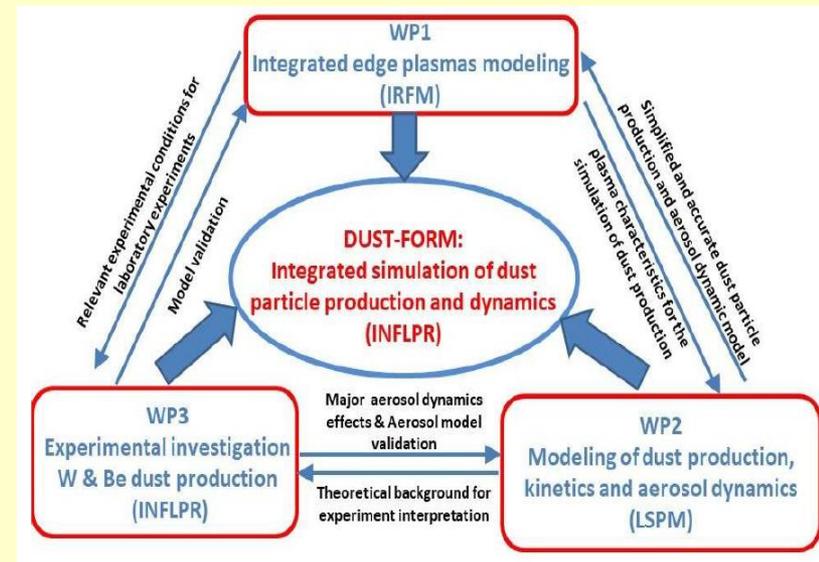
Further work

- Continue with simulation of shots in WEST in different conditions, appropriate for plasma detachment;
- Elaborate procedures of inclusion of impurities and dust formed by sputtering and transient levels in the simulation codes.

Handling challenge 2: Advances in integration across the research directions

Corroboration of the works developed in the three Research directions (WPs)

1. Are the experiments performed in laboratory (WP3) significance for the simulation codes (WP1) ?
2. Are the experiments performed in laboratory relevance for, and compatibility with the input parameter entering in modelling (WP 2)?



1. Are the physical models for nucleation and growth (WP2) compatible with the integration in the plasma edge simulation codes (WP1) ?
2. Are the growth models (WP2) compatible with the verification – calibration in laboratory experiments (WP3) ?
 1. Are the quantities used in the simulation codes (WP1) compatible with the usage in particle growth modelling (WP2) ?
 2. Are the parameters used in the simulation codes (WP1) compatible with the range of parameters used in experiments (WP3) ?

Challenge: selection of parameters relevant for the integration of works!

Integration

Two project meetings (July 26,2022 and September 5, 2022) devoted to work integration, work ongoing on:

Setting of common parameters to work with:

-definition of **ranges of relevant quantities** used in fusion plasma simulation, models for dust growth and laboratory experiments: **number densities, pressures, plasma parameters, power densities deposited on surfaces, time scales.**

Critical comparison between the physics of dust creation in laboratory, in models, and in Tokamak:

- **what is common, what is different in the physics of processes ?**
- compare laboratory dust formation conditions with those of Tokamak as shown by the collected dust.

Selection and elaboration of simplified models and experiments to be cross-validated:

- definition of **laboratory experiments producing results useful for calibration of the nanoparticle growth models;**
- elaboration of **nanoparticles growth models and hypothesis compatible with insertion in the simulation codes;**

Some questions answered...

Discharge sputtering

- adding Ar in H₂ increases significantly the particles production;
- adding Ar in H₂ increases the nanoparticles size;
- adding Ar in H₂ decreases the agglomeration of dust;
- adding Ar in H₂ increases the retro-deposition;

Recent results (not presented here, mass spectrometry) indicate:

- in presence of even small amounts of Ar, hydrogen plasma is dominated by the ArH⁺ ion;
- hydrogenated W species appear, can be centers for heterogenous nucleation?

Plasmas created by deposition of high energy at substrate with lasers:

- increasing the Z of the gas atomic, collected material begins to show an open and porous structure, i.e., evolving progressively towards clusters and particles;
- increased pressures leads to limitation of (W, Be) plasma extension during laser deposition of power, more pronounced in higher-Z gases;
- Be plasmas are prone to droplets formation; sponge like material in Ne.

Modeling of clusters growth

- DFT calculations for stability of W₂, W₃, W₄, W₅ clusters

Milestones and deliverables 2022

Milestones -2022

WP-1: Numerical simulation that accurately describes the details of edge plasma-surface interaction processes that drive the production of dust particles (**M1-1-1 - 31.12.2022 & 30.06.2023**);

2022: 60%; continuing 2023..

WP-2: Numerical code that describes the details of clustering and aerosol dynamics of nanoparticles that may be produced along with micrometer spherical particles generated after anomalous events (**M2-1-1-31.12.2022 & 30.06.2023**);

2022: 60%; continuing 2023...

WP-2: Numerical code that describes the details of clustering and aerosol dynamics of nanoparticles that may be produced through enhanced sputtering by high-z seed in semi-detached or detached regime conditions (**M2-2-1 - 31.12.2022**);

2022: 100%;

WP-3: Decision on the final design and operating parameters for the magnetron sputtering installation (**M3-1-1 - 31.12.2022**)

2022: 100%;

Deliverables – 2022 – will be reported on time:

WP-1 - Interim report on the edge plasma-surface interaction processes that drive the production of dust particles. Also an interim report on dust particle production and dynamics in the plasma will be provided;

WP- 2 – Report on the detailed physical models of clustering and aerosol dynamics of nanoparticles that may be produced along with micrometer spherical particles generated after anomalous events;

WP-3 – Interim report on W dust formation in magnetron plasmas and the description of process parameters as well as the initial assessment of Be dust formation in plasma by melting/evaporation. The first report on dust sampling on WEST will also be included;

Thank you for your attention !

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and all team members