



Project code: ENR-MAT.01.IAP

Progress in the project DUST-FORM "NanoDust in Metallic Tokamak" in 2023, and plans for 2024

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(presenter from behalf of the team)

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Research directions and project structure

Research questions:

Is dust production enhanced when using gases for divertor detachment (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;

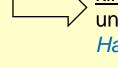
How nanoparticles nucleate, growth, evolve in plasmas?

- consider physical phenomena: melting, evaporation, nucleation, growth, and transport;

How such nanoparticles influences the edge plasma? -consider the behavior of particles in the edge plasma;

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.



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

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

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





Experimental investigation of W and Be dust particles production through plasma-surface and laser-surface interaction. Particles collection in tokamak (WP3)

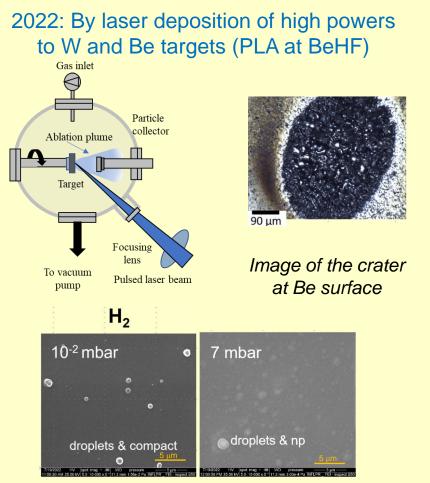




Content

- Progress in the experimental methods
- Highlights on tungsten species in hydrogen plasmas in contact with tungsten surfaces
- Assessment of tungsten dust formation rates in hydrogen plasmas in contact with tungsten surfaces in presence of small percentages of Kr
- Insights in dust formation mechanisms: surface versus volume processes
- Relevance for fusion research
- Ideas for further research

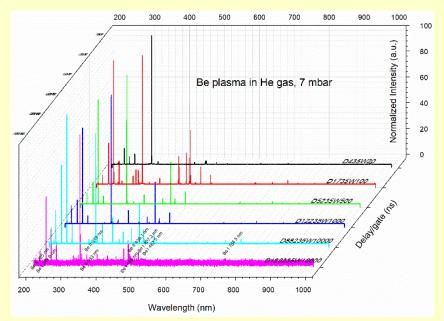
Be particles production and process diagnostics



Be particles produced by PLA

Source of material: Be target; Surface processes: ablation, melting, vaporization; Particle evolution: gas phase.

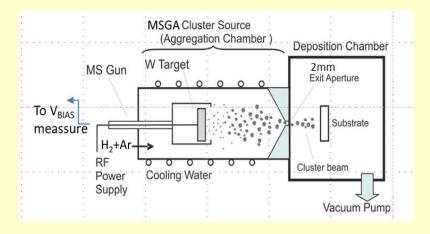
2023: added OES diagnostics with space and time resolution



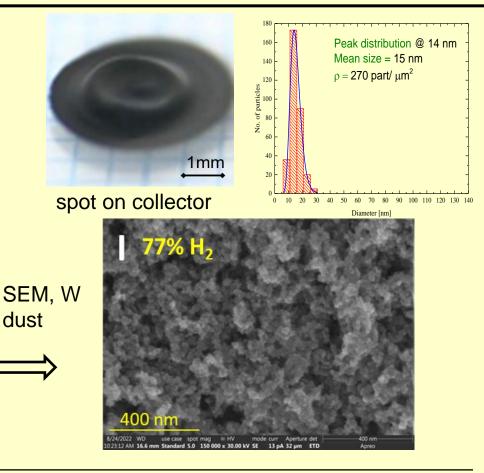
Overall spectra of the beryllium plasma plume generated in He at high pressure (7 mbar), at various moments from the laser interaction with the target (at 235 ns).

<u>Milestone:</u> Decision on the final design and operating parameters for the laser ablation– achieved for 2023, continuation in 2024. Progress in the setups for W dust production and process diagnostics – 1 - previous results

2022 – dust synthesis – via Magnetron Sputtering Gas Aggregation with W target



Schematic view of the MSGA nanoparticle source W particles produced by MSGA

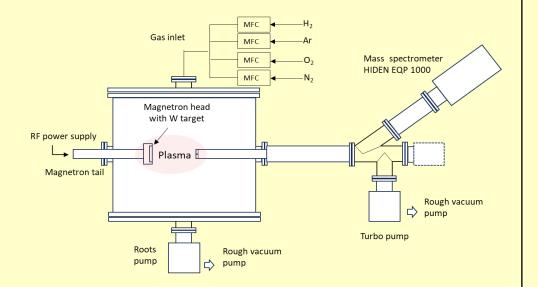


Species investigation tools 2022 – limited to OES

Evaluation of dust production rates 2022: by weighing dust collectors

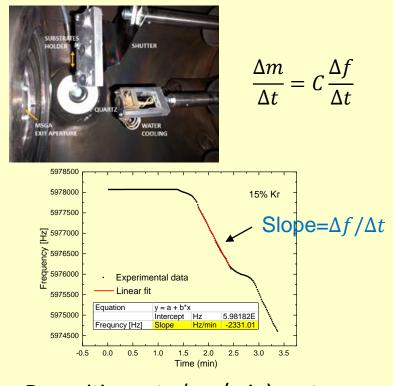
Progress in the setups for W dust production and process diagnostics - 2 – new accomplishments

2023 – Species investigation: Mass Spectrometry added to a magnetron sputtering setup



Mass spectrometer Hiden EQP 1000, 0-300 amu

2023 – Dust production rates - by using a Quartz Crystal Microbalance system QCM)



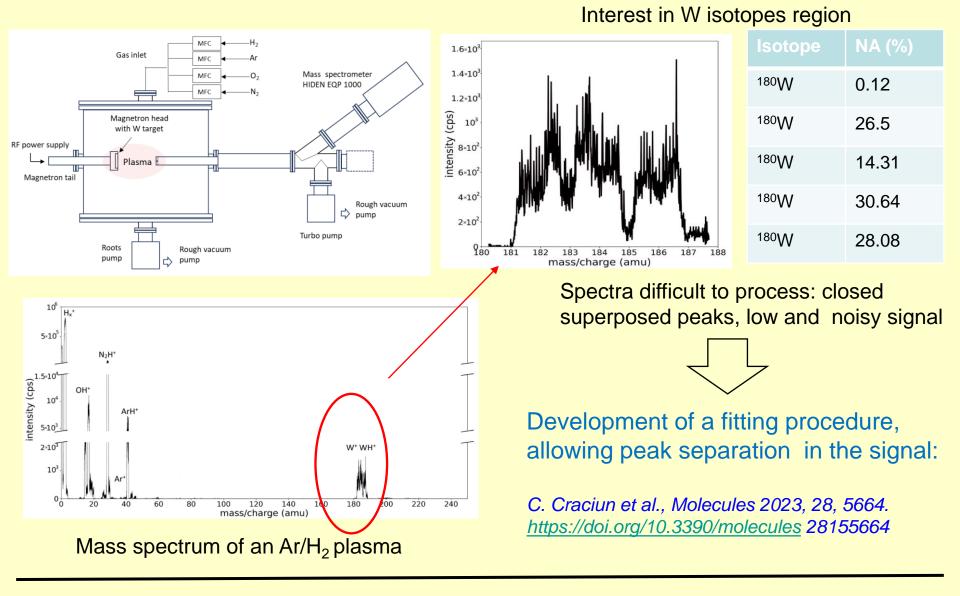
Deposition rate (mg/min)~ rate of frequency variation (Hz/min)



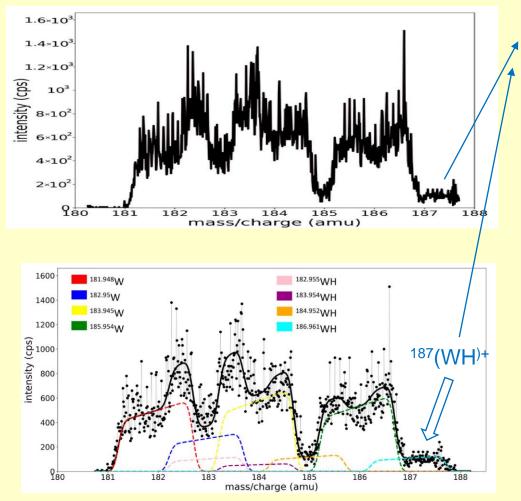


Highlights on tungsten species in hydrogen plasmas in contact with tungsten surfaces

Illustration of Mass spectra recorded in sputtering H₂ - dominated plasma with W target



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By applying the fitting procedure it results that there are two contributions in the signal: 1) one is assignable to W⁺ peaks, 2) a separate one assignable to WH⁺ species.

Estimation from MS: not-negligible WH⁺ percentages: WH⁺/W⁺ ~15- 25 % for gas ratios $Ar/(Ar+H_2) \sim 10-20\%$

WD detected in Tokamak (OES):

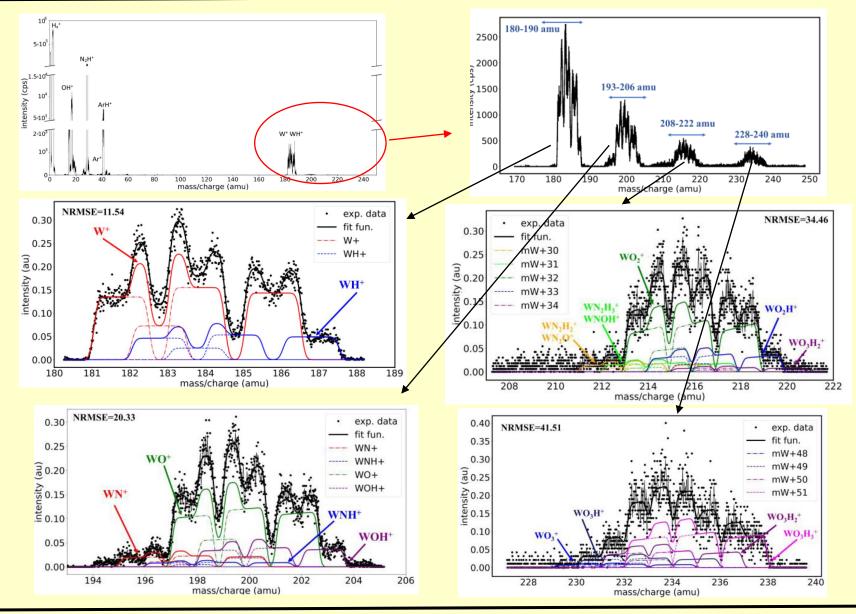
ASDEX, TEXTOR: S. Brezinsek et al. Nuclear Materials and Energy, vol. 18, pp. 50-55, 2019.

EAST: Q. Zhang et al. Nuclear Materials and Energy, vol. 33, p. 101265, 2022.

<u>Conclusion</u>: Part of the released W is found in plasma as tungsten hydride WH molecules.

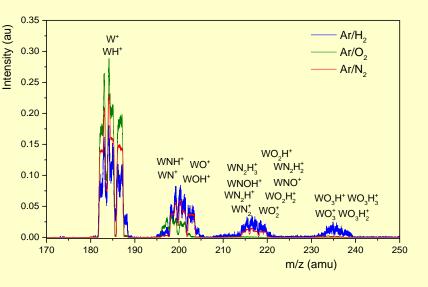
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Fitting of mass spectra in the range 180-250 amu: evidence for $WH_xN_yO_z^+$ molecular species

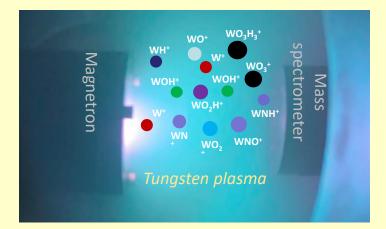


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Evidence for high mass ionic molecular species in W sputtered plasmas in presence of impurities



Molecular W species identified in plasma



-		30-189 amu 206 amu	Region 210-222 amu		Region 225-240 amu	
Dete io		Isotopic Mass	Detected ion	Isotopic Mass	Detected ion	Isotopic Mass
W	/+	182, 183, 184, 186	WN ₂ ⁺	210, 211, 212, 214	WO ₃ ⁺	230, 231, 232, 234
w	H⁺	183, 184, 185, 187	WN₂H⁺	211, 212, 213, 215	WO₃H⁺	231, 232, 233, 235
w	N ⁺	196, 197, 188, 200	WN ₂ H ₂ ⁺ WNO ⁺	212, 213, 214, 216	WO ₃ H ₂ ⁺	232, 233, 234, 236
WN	IH⁺	197, 198, 189, 201	WN₂H₃ ⁺ WNOH ⁺	213, 214, 215, 217	WO ₃ H ₃ ⁺	233, 234, 235, 237
W	0+	198, 199, 200, 202	WO ₂ ⁺	214, 215, 216, 218		
wo)H⁺	199, 200, 201, 203	WO₂H⁺	215, 216, 217, 219		
			$WO_2H_2^+$	216, 217, 218, 220		

Conclusion, new finding:

- The material removed from the W wall can be found in plasma, not only as metallic atoms, but also as tungsten molecular compounds formed in reactions with hydrogen, oxygen, and nitrogen gas;
- The molecular species were identified for the mass range 180-250 amu and can be described by the general formula $WH_xN_yO_z$ (x=0-5; y=0-3; z=0-3).

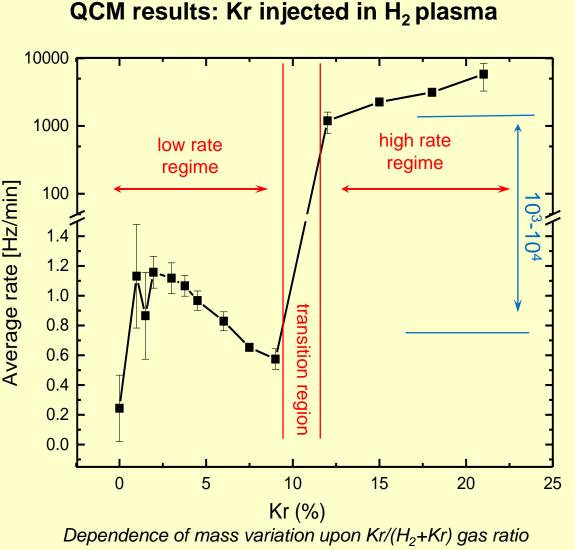
Details in: S.D. Stoica et al., Plasma Processes and Polymers, 2024, in press





Assessment of tungsten dust formation rates in hydrogen plasmas in contact with tungsten surfaces in presence of small percentages of Kr

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(average upon 3 independent measurements)

Experimental details: MSGA system, Sputtering power=100 W, p=0.07 mbar, gas ratios Kr/(H₂+Kr) = 0 - 22 %

Remarks:

-at Kr percentages less than ~10% the dust collection rates are very low (QCM frequency variations ~1Hz/min) - low rate regime;

-at Kr percentages higher than ~15% the dust collection rates are extremely high $(10^{3}-10^{4} \text{ Hz/min}) - \text{high rate regime};$

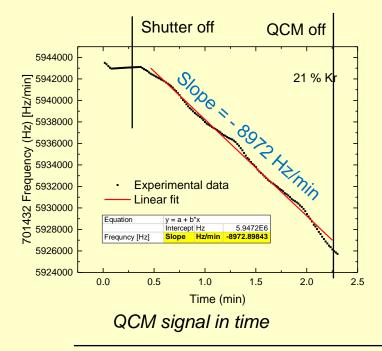
- there is a transition region in the process, associated with a critical Kr percentage in the range 10-13%; once exceeded the critical value explosive increase (-10³-10⁴ times) of dust production rate is observed.

<u>Conclusion:</u> There is a critical value of Kr percentage leading to explosive increase of dust formation rate

Kr injected in H₂ dominated plasma – dust collection versus dust morphology

High rate regime (21% Kr)

Experimental details: MSGA system, Sputtering power=100 W, p=0.07 mbar, gas ratios Kr/(H₂+Kr) = 21 %



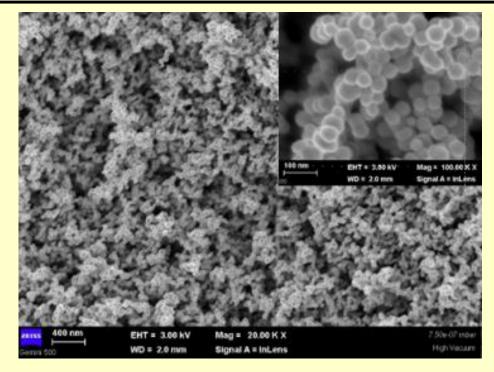


Image of the dust deposited on the QCM crystal during a high rate deposition (21% Kr)- Well individualized, round particles with sizes in the range 50-100 nm are well distinguished.

Continuous mass increase

Dust aspect: uniform, continuous coverage of the substrate with nanoparticles

Kr injected in H₂ dominated plasma – dust collection versus dust morphology

gas ratios $Kr/(H_2+Kr) = 3\%$ Shutter off 5982584 Slopes 7.2 Halmin 5982582 3 % Kr 5982580 5982578 Frequency [Hz] 5982576 5982574 5982572 Experimental data Linear fit 5982570 Equation $v = a + b^*x$ 5982568 Intercep Hz 5.98258E6 Frequency (Hz 5982566 -2 6 10 12 14 Time [min] QCM signal in time

Low rate regime (3%Kr)

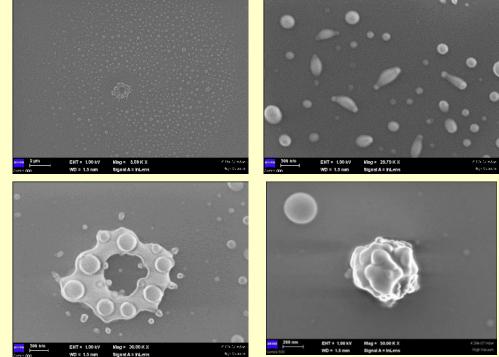
Experimental details:

Sputtering power=100 W,

MSGA system,

p=0.07 mbar,

Dust collecting time 3 h



- Various size particles, many nanometric and also a few of micron size. The small nanoparticles surround the big particles; they seem melted;
- The high-size particles are made from many fused small-size nanoparticles

QCM: Continuous mass increase Dust aspect: Discontinuous and non-uniform coverage

<u>Contradiction:</u> QCM indicates a continuous increase of mass on substrate; SEM indicate discontinuous surface coverage, big particles, even micron size!





Insights in dust formation mechanisms: surface versus volume

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Dust growth mechanisms

Low rate regime -

- the W atoms migrate on the surface and concentrate around centers of nucleation;

- small-size clusters and nanoparticles quasi-uniformly distributed on the surface are formed;

-clusters and small-size nanoparticles move on the substrate and stick to each other, coalesce forming larger particles by coalescence;

- larger particles keep increasing in size ending eventually in a reduced number of large particles, even of micron size. - Growth by a surface mechanism -

High rate regime -

-high concentration of W species in the gas phase, favours nanoparticle formation by volume nucleation and growth by atom addition;

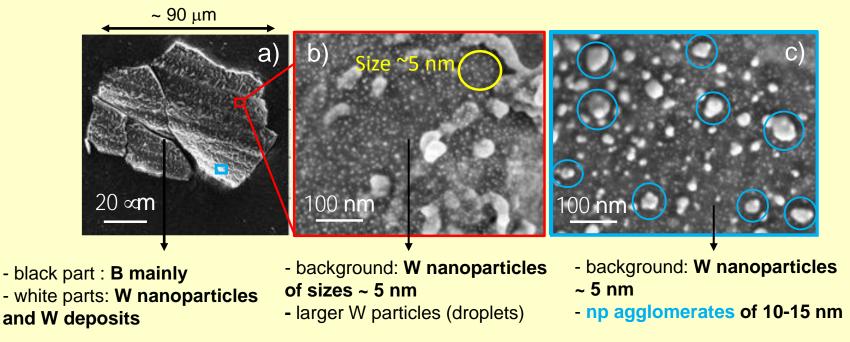
-volume processes prevail on surface processes and particles formed in volume are collected; - Growth by volume processes



<u>Conclusion</u>: with increasing sputtering rate a **critical value of the W species concentration** in plasma is reached, when the mechanism of particle formation switches from surface-dominated processes, to volumedominated processes!

Nanoparticles collected in WEST (Cecile Arnas)

SEM images from ITER-like W monobloks (2020): W micron-sized particle covered with B layer and W nanoparticles



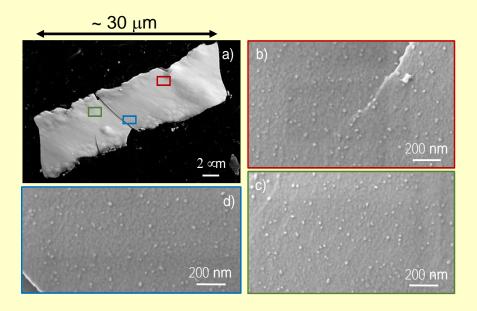
Two classes of dust collected with the vacuum technique after each plasma campaign:

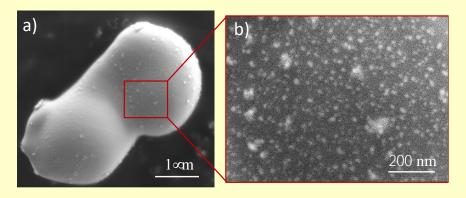
- i) micron-sized dust dominant in mass
- ii) nanoparticles of smallest size ~ 5 nm, dominant in number

Assumption: nanoparticle growth from W sputtering and agglomeration in low temperature plasma regions

West

Nanoparticles collected in WEST





a) Small piece of W delaminated layer (2019)

b), c), d): nanoparticles on size range: 10-25 nm

Assumption: nanoparticle growth from W sputtering in plasma region of low temperature

- a) Merging of two W droplets of 2 μ m each (2019)
- b) nanoparticles everywhere on the surface
 - size in the background ~ 20 nm

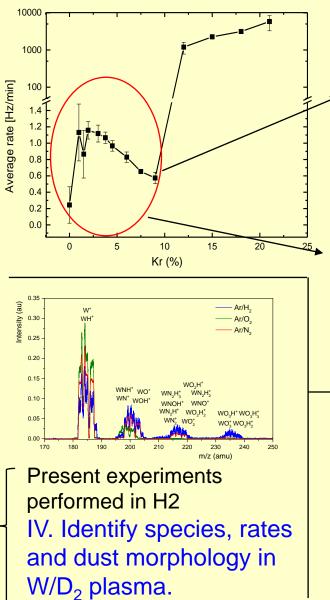
Assumption: nucleation in oversaturated W vapor, followed by condensation during the cooling of W vapor on droplets:

Conclusion: the two mechanisms hypothesis explain characteristics of the dust collected in tokamak, for example micron – size particles covered with nanometric particles;

Relevance for fusion, opportunities

- 1. How do the higher mass molecular W species impact the Tokamak studies and experiments?
- Q: Should be mass spectrometry experiments adapted for the detection of higher-mass tungsten species? (Presently, W species in fusion plasma are assessed mostly by emission spectroscopy, atomic W lines)
- Q:Are the W molecular species enough important to be included (and how) in modeling?
- Q: How dust formation rates are influenced by the molecular species? (Laboratory experiments on dust formation in conjunction with mass spectrometry are feasible!)
- 2. We are on the way to clarifying the debate regarding the existence of both micron and nanometer-size particles collected in Tokamak!
- Consolidate the two mechanism hypothesis by dedicated experiments, based on comparing QCM and SEM investigations of particles collected on tungsten surfaces!
- 3. Even in the absence of anomalous events (arcing, ELMs) micron size dust can be present, because of sputtering followed by the surface growth mechanism;
- 4. The high dust formation rate sustained by volume processes must be prevented!
- Q: How to evaluate the critical value of the amount of tungsten released in plasma when the mechanism of dust formation changes from surface (low rates of dust formation) to volume (high rates of dust formation)?.

Open questions and further laboratory work

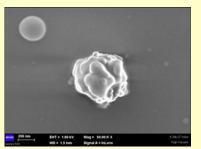


The minimum observed in the collected dust can be useful for selecting conditions of the detachment experiments. Is the observed behavior common to other injection gases, like Ne, Ar, Kr ?

I. How do the dust formation rates compare to other gases used in detachment, in the series: Ne, Ar, Kr...

The non-monotonic behavior of the rate al low Kr injected value is due to hydrogen modification of the W surface? Is this due to ions energy change because plasma composition is changed?

II. Focus on sputtering phenomena at the W/H_2 plasma interface...



Nucleation and dust formation at low rate were assessed on Si surfaces. How nucleation and dust formation behaves on W surfaces? III. More insight in the dust formation mechanisms





Modeling of dust particle production kinetics (WP2) Khaled Hassouni - LSPM

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Tasks and milestones

Three Milestones

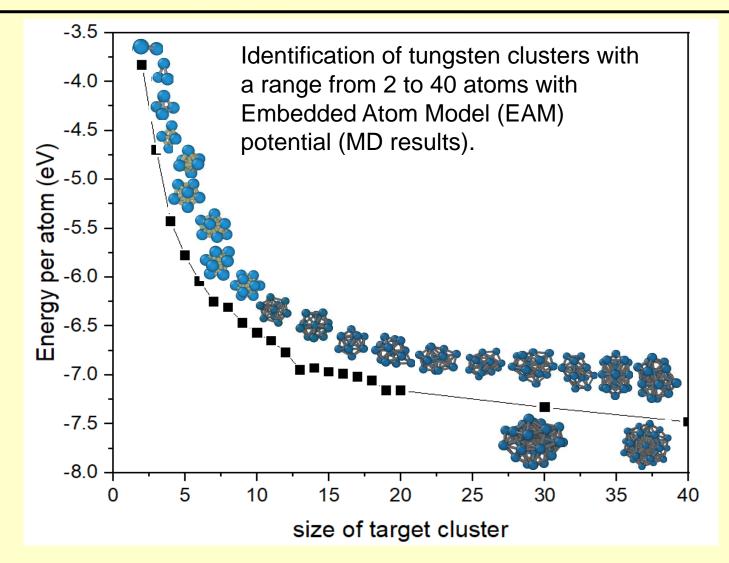
- *M2-1-1 :* A numerical code that describes the details of clustering and aerosol dynamics of nanoparticles that may be produced along with micrometer spherical particles generated after anomalous events.
- → almost achieved : simulations are being performed → report expected 15 February
- *M2-1-2 :* A simplified and yet accurate clustering/aerosol model that may be used in integrated model of edge plasma estimates of nanoparticle density and characteristic size
- → A simplified bimodal model has been developed: G. Tetard et al. J. Phys. D accepted

→ Need to be applied to edge plasma conditions : in progress

- M2-2-2 : A simplified and yet accurate clustering/aerosol dynamics model that may be used in integrated edge plasma modeling to investigate nano-particle formation and evolution under semi-detached or detached regime insured by high-z element seeding
- → sticking cross-sections for molecular growth processes involving neutral clusters were determined possibility of tungsten cluster growth by W_n-W collision up to a collision-energy of 30 eV
- ➔ Infer the sticking cross section for charge species, W_n-W⁺, from neutral species in good progress

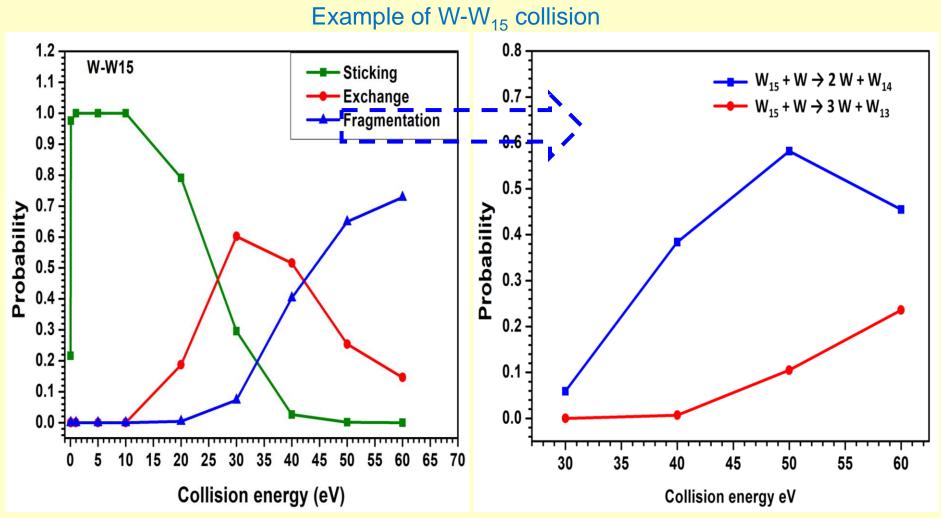
Determine cross sections for charged and neutral species through quantum MD: started

Structure of the tungsten clusters and potential energy per atom



- The most stable compact tungsten clusters likely to be involved in the growth process were identified by MD and DFT.
- The energy per atom decreases with the size of the cluster indicating a stabilization.

Probabilities of the different processes taking place during W_n-W collision as function of the collision energy



- Probabilities of various processes subsequent to the collision of a W atom with a W₁₅ cluster.
- The fragmentation may proceed on several routes with different probabilities.

Cross sections for the sticking between charged/charged or charged/neutral clusters

Cross sections are inferred from neutral/neutral sticking, by applying a correction procedure:

A correction factor η^{pq} : $\sigma^{p,q} = \eta^{p,q} \sigma^{0,0}$ is used, where:

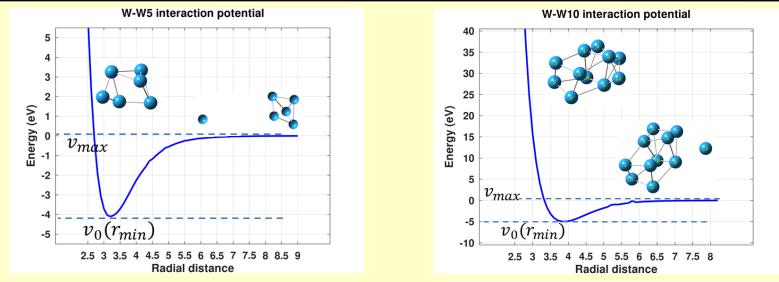
- $\sigma^{0,0}$ is the cross section for the sticking between neutral determined by MD simulation (previous slide)
- $\sigma^{p,q}$ is the cross section for the sticking between clusters with the same sizes but with charges p and q
- $\eta^{p,q}$ is determined from the interaction potential between the two charged clusters

$$\eta^{p,q} = exp\left(-\frac{v_{max}}{kT}\right)\left[1 + \frac{v_{max} - v_0(r_{min})}{kT}\right]$$

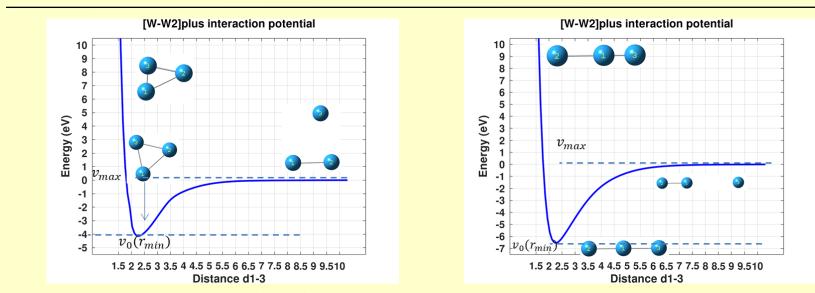
 v_{max} and $v_0(r_{min})$ are inferred from the potential surface of the cluster pair interaction

➔ One needs to determine the <u>surface potential</u> of the cluster-pair interaction. This is in progress for W⁺-W_{n=1-40} collisions, a few examples follow.

Examples of calculated potential surfaces



Estimation of v_{max} and $v_0(r_{min})$ from the variation of the potential energy versus the distance



Estimation of v_{max} and $v_0(r_{min})$ from the variation of the potential energy versus the distance for two interacting trajectories of charged species (W-W₂)⁺ leading to linear and triangular cluster





Edge plasma integrated simulation with impurity and dust transport (WP1) Nicolas Fedorczak, IRFM

WP1 Edge plasma integrated modelling with impurity and dust transport

Scientific deliverable:

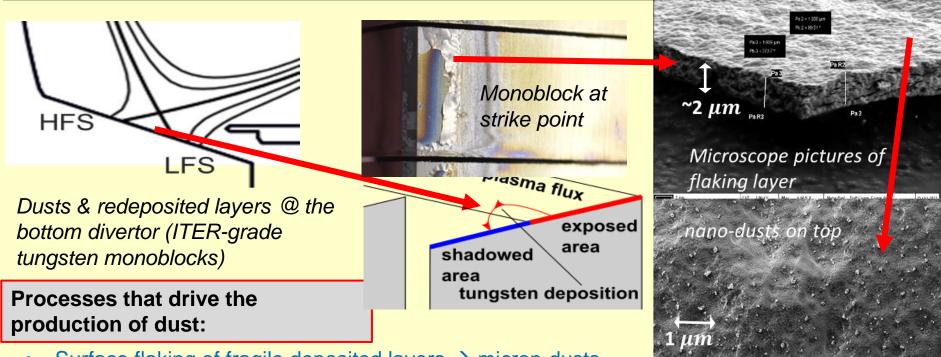
Simulation that describes the details of edge plasma-surface interaction processes that drive the production of dust particles. Partially achieved

Milestones:

T1-1: A numerical simulation that accurately describes the details of edge plasma-surface interaction processes that drive the production of dust particles. **Achieved**

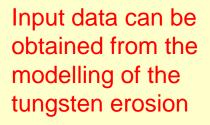
T1-2: A numerical code that comprehensively describes dust particle production and dynamics in the plasma. Not achieved (no competences available in 2023 \rightarrow 2024)

Task 1-1: model the driving of dust production in edge plasma Focus on dust formation conditions in WEST.



- Surface flaking of fragile deposited layers → micron-dusts
- Volume aggregation of tungsten ions/atoms → nano-dusts ?
- \rightarrow Needs for modelling the aggregation and dust transport:
- Local volume density of W ions in plasma (aggregation)
- Redeposition in divertor (flaking) modeling

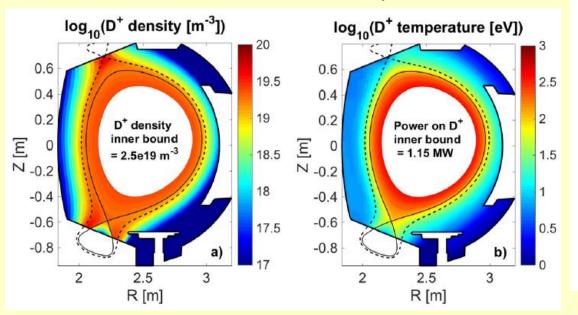
The dominant process producing tungsten ions in the divertor volume, and leading to local redeposition of these ions on the target, is the local erosion of the divertor.



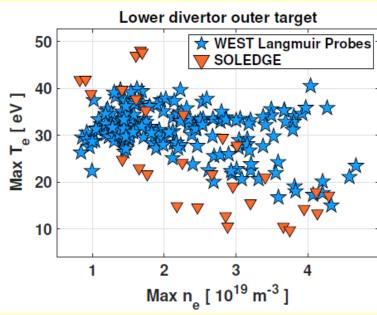
Modeling tungsten erosion : ERO2 applied on SOLEDGE plasma backgrounds

Data about erosion are provided by ERO2.0 code. In order to apply ERO2.0 plasma backgrounds have to be produced in advance by SOLEDGE code.

SOLEDGE plasma backgrounds (~30 cases), scanning input power & plasma density (pure D) have been produced



SOLEDGE: extended domain plasma solutions

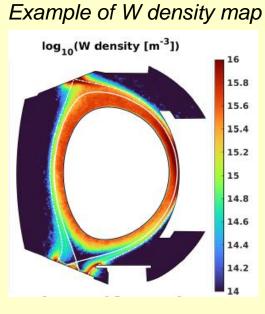


2D maps of plasma density and temperature (observed good agreement with Langmuir probe measurements) Maximum electron temperature as a function of maximum density at the outerstrike point

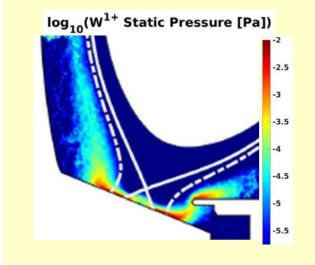
Results are coherent with WEST divertor conditions covering representative scenarios

ER02.0 simulations ran on every SOLEDGE cases: W maps

To enhance sputtering 3% of oxygen ions added into incident fluxes used in ERO2.0



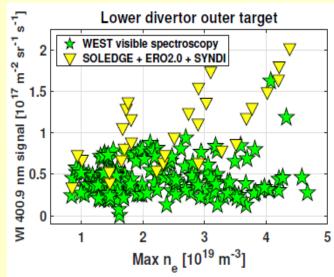
Example of W⁺ ion pressure



2D map of tungsten density provided by ERO2

Results:

Thermodynamic pressure of the W⁺ ions (~ 10mPa) above the target plates, which could serve as input to aggregation models. Check: W sources (photons) ERO2.0 vs WEST



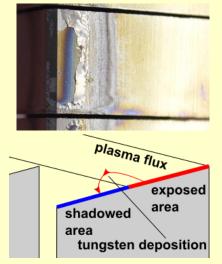
- Green stars are experimental data,
- Yellow triangles are produced by applying a synthetic optical diagnostic to ER02.0 / SOLEDGe simulations
- Adding oxygen (3%) for sputtering lead o divertor W sources coherent with data $(\approx 10^{19}m^{-2}s^{-1})$
- Provides BOTH volume distributions (for the aggregation model) & deposition profiles (for redeposition in flakes).

T1-2: modelling dust production and dynamics : Further possible work

- From ER02.0 maps of W ion densities, aggregation model developed in WP2 may provide:
 - Possibility of aggregation under relevant WEST plasma conditions;
 - Dynamics & localization of aggregation.
- Then, dust dynamics can be simulated by DUMBO code *:
 - Check dynamics consistency (trajectories, time of existence, etc) function of nano-dust localisation, size & plasma background
 - Statistics on domain of existence → predict dust production (/m2) over campaign the * A. Autricque et al. Nuclear Materials and Energy 12 (2017)]

Data for comparison with experiment available

- Evaluation of the redeposition: Gross erosion flux ≈ 10¹⁹m⁻²s⁻¹. Campaign ~3h of plasma (high fluence, creating deposits) shows range of 10 microns of effective gross erosion. So, 2 microns in the shadowed parts of monoblocks would correspond to 20% of ions deposited in this area
- Consistency needs 3D modelling (2024)



SUMMARY OF THE RESULTS

WP1

WP2

- Significant progress in the experimental methods for W and Be dust production investigation (space and time resolution OES, MS, QCM)
- Mass spectrometry, identification for the first time of tungsten molecular species in H₂ plasmas in contact with W surfaces;
 - QCM two regimes of dust formation and deposition low and high rate;
 - Two mechanisms of dust formation explain micron size and nanometer size dust formation from W atoms.
- Identification of stable tungsten clusters with a range from 2 to 40 atoms with Embedded Atom Model (EAM) potential (MD results);
- Probabilities of the different processes taking place during W_n-W collision as function of the collision energy; ;
 - Cross sections for the sticking between charged/charged or charged/neutral clusters in progress.
- A complete set of ER02.0 / SOLEDGE simulations have been performed, scanning a representative range of operational conditions on WEST;
- WP3 Data to run aggregation models in WEST for nanometric dust formation (from WP2) are available;
 - Dust dynamics can be further simulated with the DUMBO code (using seeded dust, or a surrogate equation for the aggregation).

Published papers

- C. Arnas et al. *Micron-sized dust and nanoparticles produced in the WEST tokamak* Nuclear materials and Energy, 10.1016/j.nme.2023.101471, pinboard: 34689
- C. Craciun et al. Mass Spectra Fitting as Diagnostic Tool for Magnetron Plasmas generated in Ar and Ar/H2 Gases with Tungsten Targets, 10.3390/molecules28155664, pinboard 35342
- S.D. Stoica et al. *Evidence for molecular tungsten species presence in impurity*seeded hydrogen plasma in contact with W surfaces Plasma Processes and Polymers, in press;
- G. Tetard et al. An effective approach for aerosol dynamics modelling in dusty plasma J.Phys. D. Appl. Phys, in press.

Conferences

• C. Arnas, et al. Dust of nano-micron sizes produced during the C4 and C5 plasma campaigns, WEST Task Force Meeting, January 26th 2023, slides in WEST portal

Thank you for your attention !

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Milestones and deliverables 2023

Deliverables (2023) - all reports were PROVIDED. **Milestones (2023)**

W1, M1-1-1 A numerical simulation that accurately describes the details of edge plasma-surface interaction processes that drive the production of dust particles – Achieved

W1, M1-2-1 A numerical code that comprehensively describes dust particle production and dynamics in the plasma - Not achieved (no competences available in 2023 \rightarrow 2024)

W2, M2-1-1 A 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- almost achieved: simulations are being performed → report expected 15 February

W2, M 2-1-2 A simplified and yet accurate clustering/aerosol model that may be used in integrated model of edge plasma - estimates of nanoparticle density and characteristic size – Achieved, a simplified bimodal model has been developed; in progress to be applied to edge plasma.

W2, M2-2-2 A simplified and yet accurate clustering/aerosol dynamics model that may be used in integrated edge plasma modeling in order to investigate nano-particle formation and evolution under semi-detached or detached regime insured by high-z element seeding - sticking cross-sections for molecular growth processes involving neutral clusters were determined possibility of tungsten cluster growth by W_n-W collision up to a collision-energy of 30 eV

W3- M3-2-1 Decision on the final design and operating parameters for the laser ablation installation 31.12.2023 & 30.06.2024 – achieved for 2023, to be finalized in 2024.