POLITÉCNICA

Alternative plasma facing material for nuclear fusion reactors

R. Gonzalez-Arrabal, R. Iglesias, J. Suarez-Recio, C. Cupak, M. Fellinger, J. Brötzner, A. Lopez-Cazalilla, F. Granberg, F. Aumayr, K. Nordlund and J. M. Perlado

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Outlook

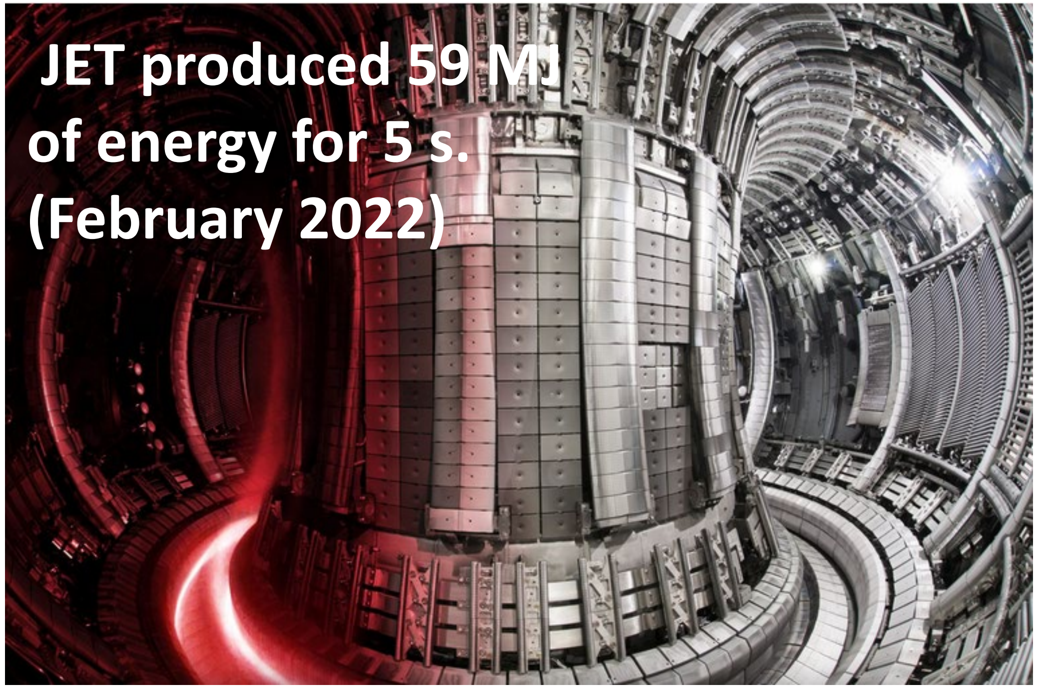
- Plasma Facing Materials in magnetic and inertial fusion
- PFM main threats
- The need to look for new materials alternative to coarse grained W: limitations of coarse grained W
- Capabilities of nanostructured W
- Conclusions

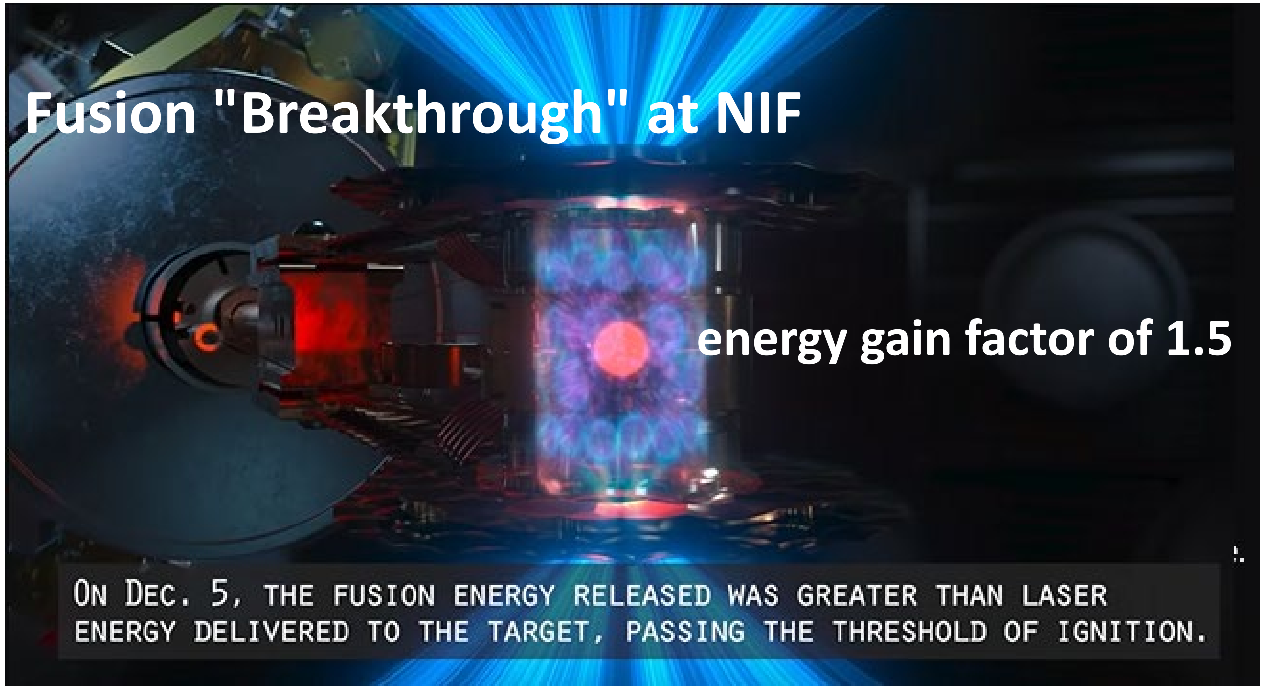
Motivation

2022: a Good year for fusion

Magnetic

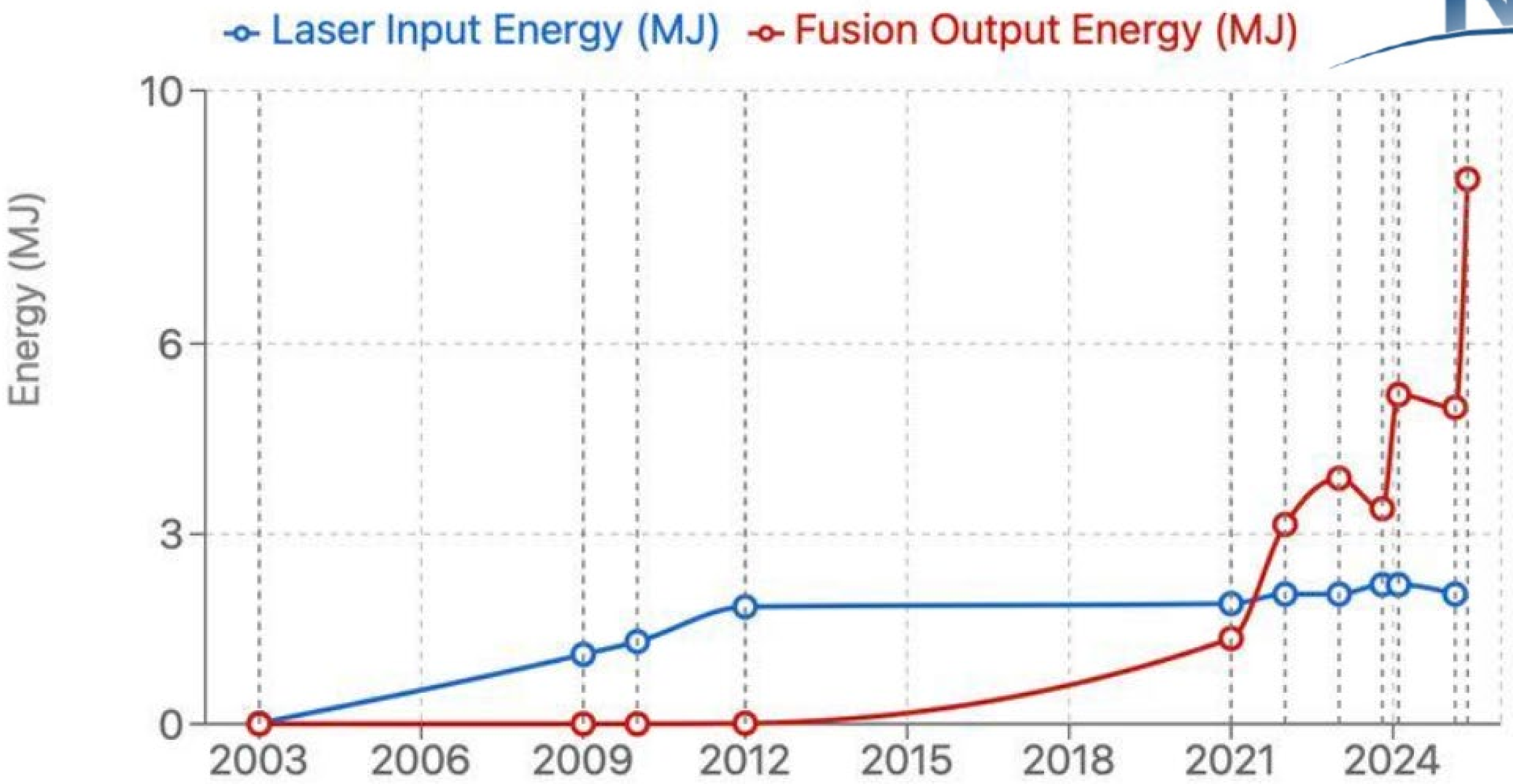
Inertial

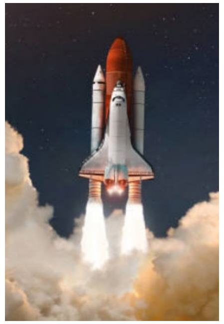




February 2023. Wendelstein 7-X reaches milestone: Power plasma with 1.3 GJ energy turnover generated for 8 minutes

Motivation





https://lasers.llnl.gov/about/keys-to-success/nif-sets-power-energy-records

Motivation

Despite the achievements, there is still a number of challenges that need to be addressed prior to up-scaling to a commercial facility:

- Define the reactor operation mode and configuration
- Select durable materials, which withstands the harsh environment expected in these reactors
- Create the needed support infrastructure

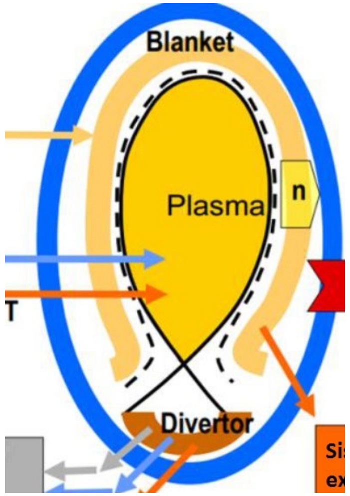
•Materials qualifications in existing facilities

Plasma facing materials (PFM/FW)

Plasma facing materials are those directly exposed to:

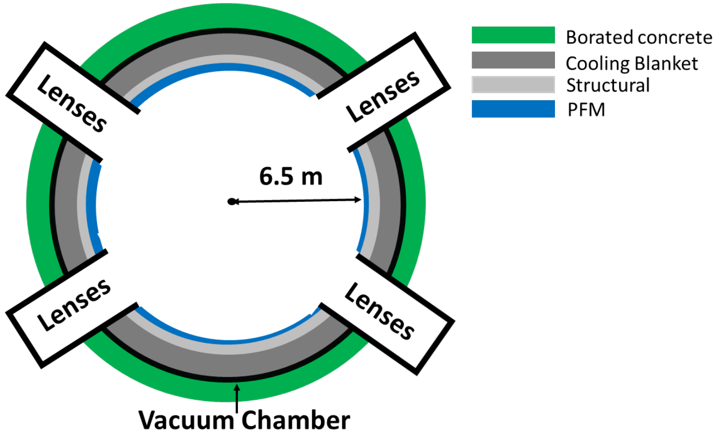
- The plasma in magnetic fusion (PFM)
- To the explosion threats in inertial fusion confinement (PFM or FW)

MCF



ICF

HiPER Prototype/Demo



Assignment: protect the structural materials located underneath

Plasma facing materials main threats

- The main threats depend on the radiation conditions → reactor configuration

- Fusion
  - Magnetic confinement
    - PFM Steady state — 1-30 e-V; $<10^{24} m^{-2}s^{-1}$; continuos
    - Divertor — 1-30 keV; $<10^{24} m^{-2}s^{-1}$; $0.2\text{-}1\times10^{-3}$s
  - Inertial (laser) confinement
    - Direct drive — keV-MeV; $10^{21}\text{-}10^{25} m^{-2}s^{-1}$; Hundres of ns
    - Indirect drive — (gas) — keV; Hundres of ns

"Neutrons are not real threats"

Plasma facing materials damage

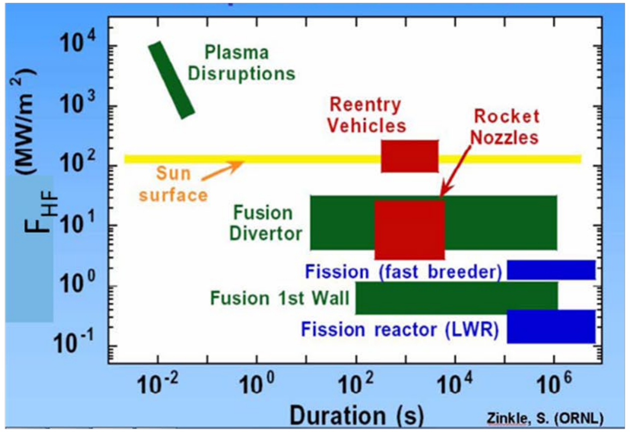
Ion arrival
Synergistic effects

Thermal loads

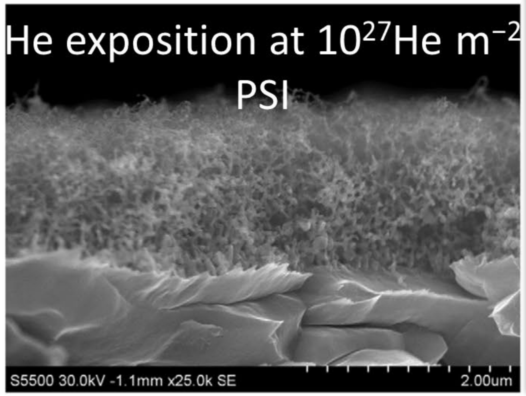
Atomistic damage

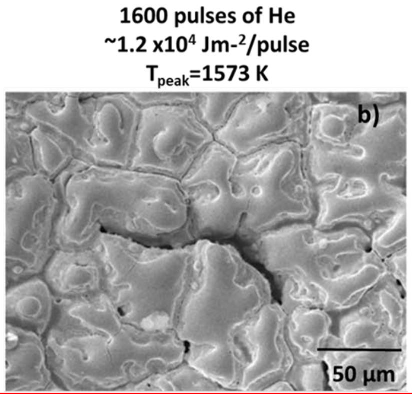
MCF
Close to the materials Surface

ICF
Deeper into the sample



Y. Gasparyan *et al* Nucl. Fusion **56** (2016) 054002





T. J. Renk et al. Fusion Science and Technology, 61:1(2012) 57-80

PFM: requirements

The main requirements are:

- Good structural stability always have to be there
- Highly resistant thermal shocks
- High thermal conductivity
- High melting point
- Low physical and chemical sputtering
- Compatibility with the refrigerant
- Low retention of Tritium

Candidate: W

Coarse grained W as PFM: drawbacks

- Oxidation at elevated temperatures→WO_3 (highly volatile and radioactive)
- Low recrystallization temperature (~1300 K)
- High ductile-brittle transition temperature (423-673 K)
- Low elastic limit
- **High capacity to retain light species (He and H)**

Objectives

Our work:

- Estimate the lifetime of W as PFM in foreseen HiPER scenarios.

- Identify the main threats

- Develop more radiation resistant materials

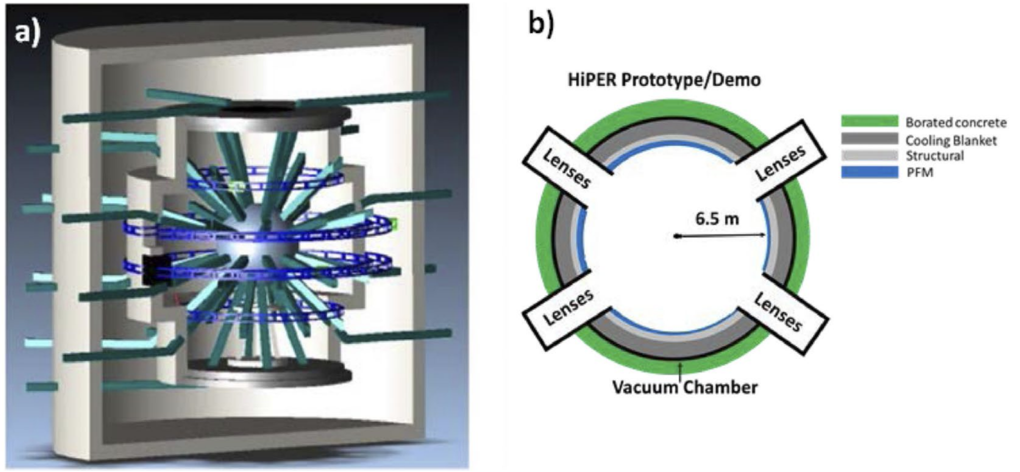
The HiPER Project

HiPER (high-power laser energy research)

Mission: the European project to demonstrate the feasibility of inertial nuclear fusion (direct-drive and drywall evacuated chamber)

Three scenarios to help identify open problems and select appropriate technologies to solve them:

Parameter	Experimental	Prototype	Demo
Frequency	Few shots per bunch	1 Hz	10 Hz
Shot energy (MJ)	20	50	154
Chamber radius (m)	5	6.5	6.5



J. M. Perlado *et al.* Proc. SPIE 8080, 80801Z (2011)

Plasma facing materials (PFM/FW)

Pulsed irradiation (hundred to miles of ns) of **high flux** (10^{22}-10^{25} $m^{-2}s^{-1}$) **high energy** (keV-MeV) **ions**

Table 2. Energy, pulse duration, depth range and energy fluence for the different irradiation types in the HiPER scenarios.

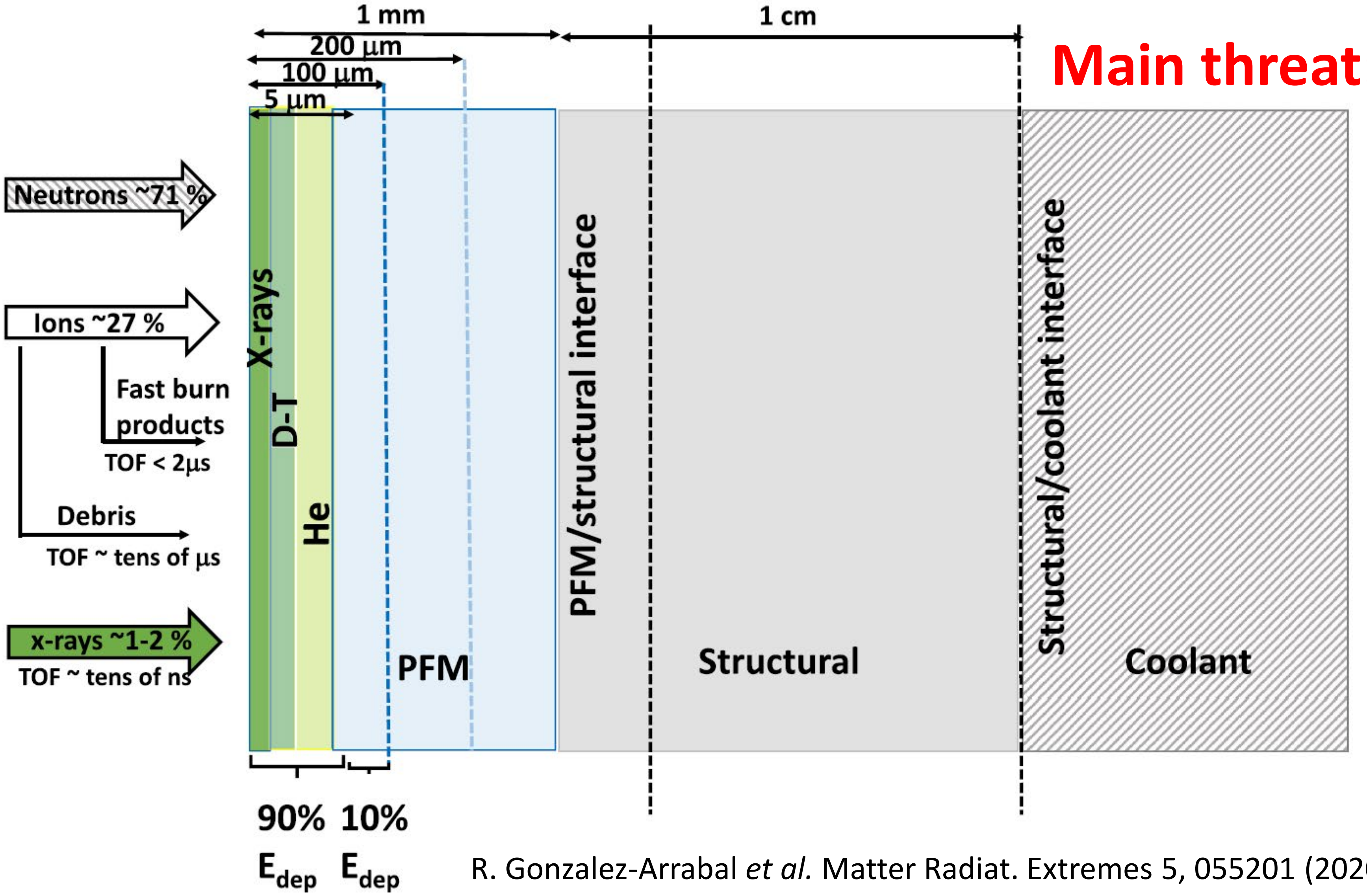
Radiation form		Energy (%)	Mean energy (MeV)	Pulse width (ns)	Mean depth range (μm)	Energy fluence (J cm^{-2}) Exp.	Proto.	Demo
Burn	H	0.4	2.55	500	10	0.02	0.03	0.1
	D	3.1	3.46	600	20	0.2	0.3	0.90
	T	2.8	2.66	600	10	0.2	0.3	0.8
	He	6.4	3.81	600	1.8	0.4	0.6	1.9
Burn total		12.7	3.40	600	8	0.8	1.2	3.7
Debris	H	0.1	0.09	1500	0.2	0.00	0.01	0.02
	D	5.8	0.14	2000	0.4	0.4	0.5	1.7
	T	7.2	0.19	2000	0.5	0.5	0.7	2.1
	He	0.9	0.23	1500	0.2	0.05	0.1	0.25
Debris total		14.4	0.17	2000	0.5	0.9	1.3	4.0
Ions total		27.1	0.29	3000	4	1.7	2.5	7.7
	X-rays	1.4	0.007	0.1	2	0.1	0.1	0.4
	Neutrons	70.8	12.4	60	10^5	4.5	6.7	20.5

Note: Radiation spectra are from the ARIES project [34].

D. Garoz *et al.* Nucl. Fusion 56 (2016) 126014

PFM: main threats

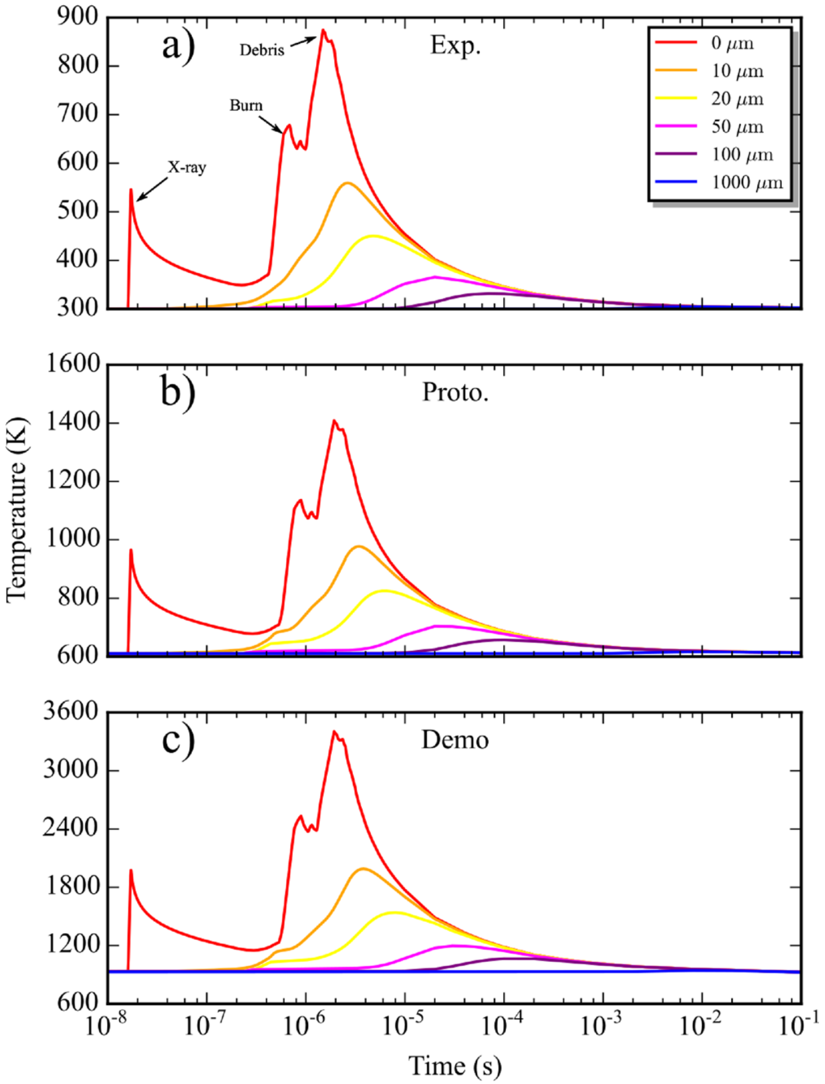
Neutrons are not real threats for PFM



Main threat: ions

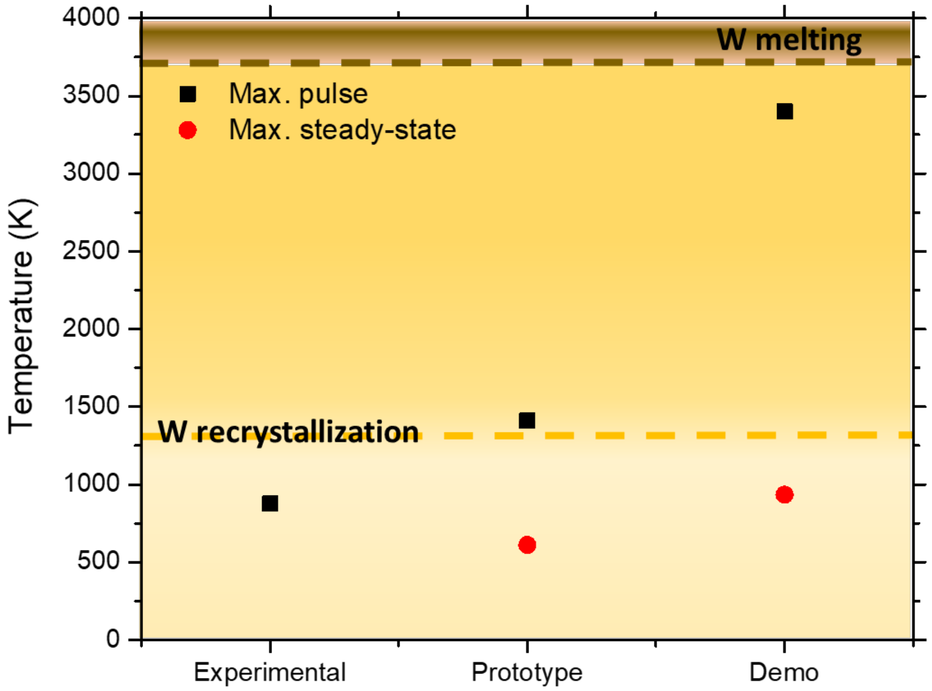
R. Gonzalez-Arrabal *et al.* Matter Radiat. Extremes 5, 055201 (2020)

Thermomechanical behavior of the tungsten in HiPER scenarios



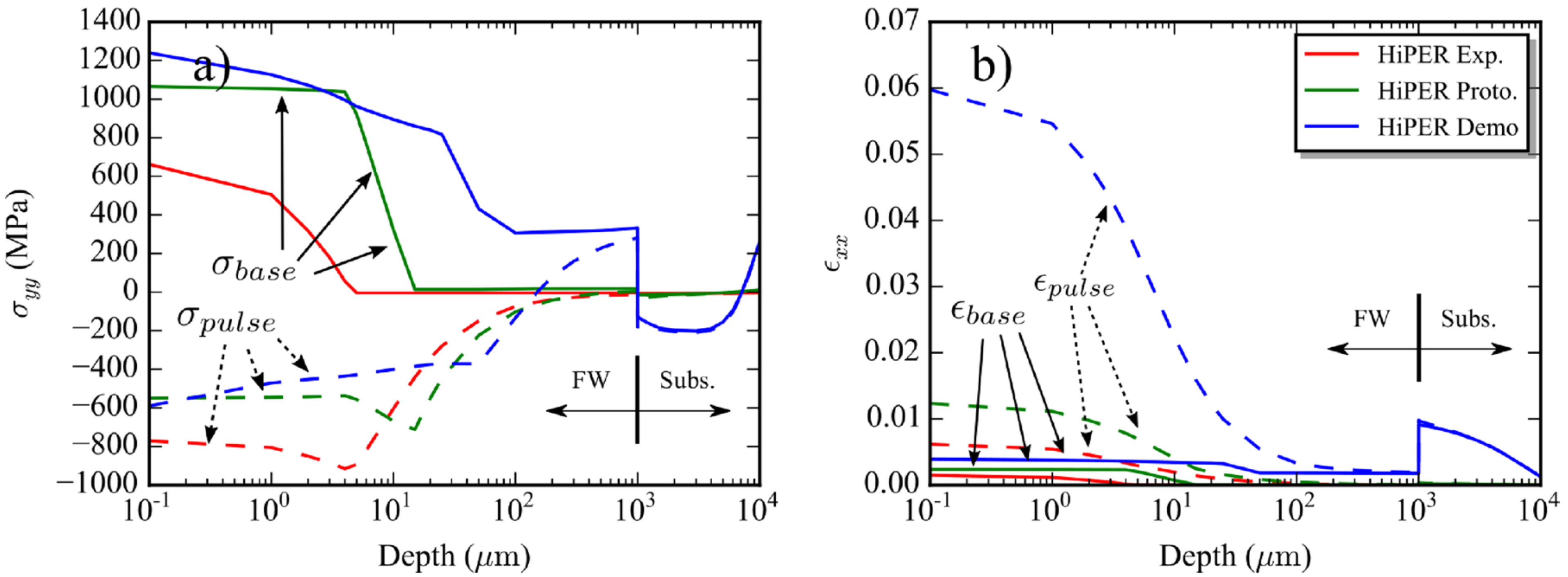
D. Garoz *et al.* Nucl. Fusion 56 (2016) 126014

- W melting temperature = 3700K
- W recrystallization temperature 1300 –1800 K



R. González-Arrabal *et al.* Matter Radiat. Extremes 5, 055201 (2020)

PFM: Strain and stress



- The FW expands until the irradiation ceases and the material cools down, leading to a tensile state due to the appearance of a plastic region which, affects the first microns of the FW.
- Fatigue appears due to the cyclic nature of the irradiation.
- **The lifetime of the FW in HiPER s is limited by fatigue loading (Prototype 580 d, Demo 28 h)**

D. Garoz *et al.* Nucl. Fusion 56 (2016) 126014

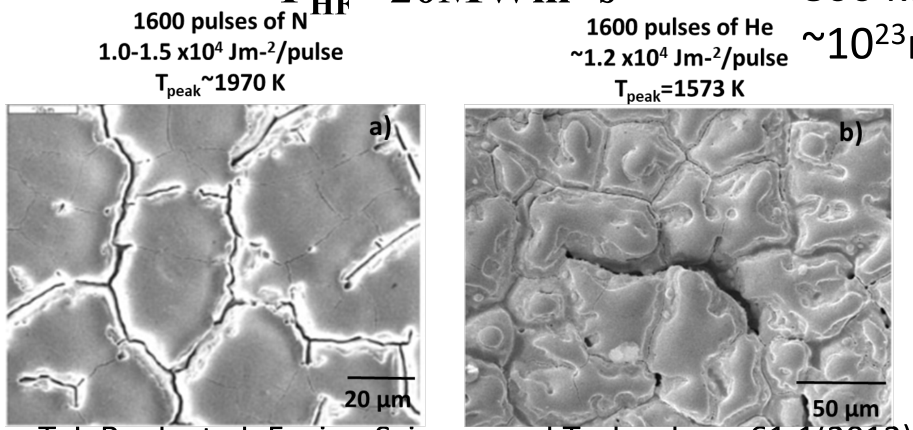
Combined effects of thermal loads and atomistic damage

High flux 10^{21}-10^{25} $m^{-2}s^{-1}$
High energy (keV-MeV) ions

Surface deterioration

F_{HF} ~$20 MWm^{-2}s^{0.5}$

800 keV
~$10^{23} m^{-2}s^{-1}$



T. J. Renk et al. Fusion Science and Technology, 61:1(2012) 57-80

Damage fluence threshold <$10^{19}m^{-2}$
(two orders of magnitude lower than the one described for PFM in MC)

HiPER			
	Experimental	Prototype	Demo
Frequency	Few shots /bunch	1Hz	10Hz
Shot Energy (MJ)	20	50	154
Inner chamber radius	5	6.5	6.5
Operation time limit based on synergistic effects (thermal loads + He irradiation)	~$1x10^3$shots	**minutes**	**seconds**

R. Gonzalez-Arrabal *et al* . Matter Radiat. Extremes **5**, 055201 (2020)

Conclusion Coarse grained W does not work

PFM

Thermal loads can be attenuated by:

- Optimizing the chamber geometry,
- Using radiation mitigation strategies
- **Materials engineering**
- Using lower target yield

- **But ions???** In particular light ions (H-isotopos and He)

PFM: new approaches

- **Challenge: Develop more radiation resistant materials.**

- Can we develop somehow a more radiation resistant material? What are we aiming to?

  – More radiation resistant materials

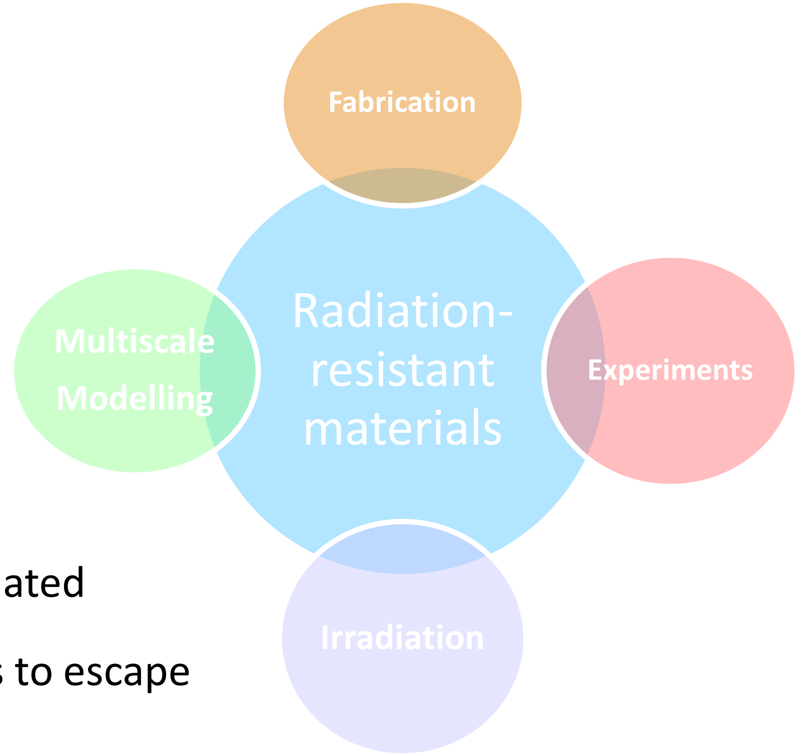
    - Self-healing

    - **Delay blistering**

      – Increasing the effective area where light ions can be accommodated

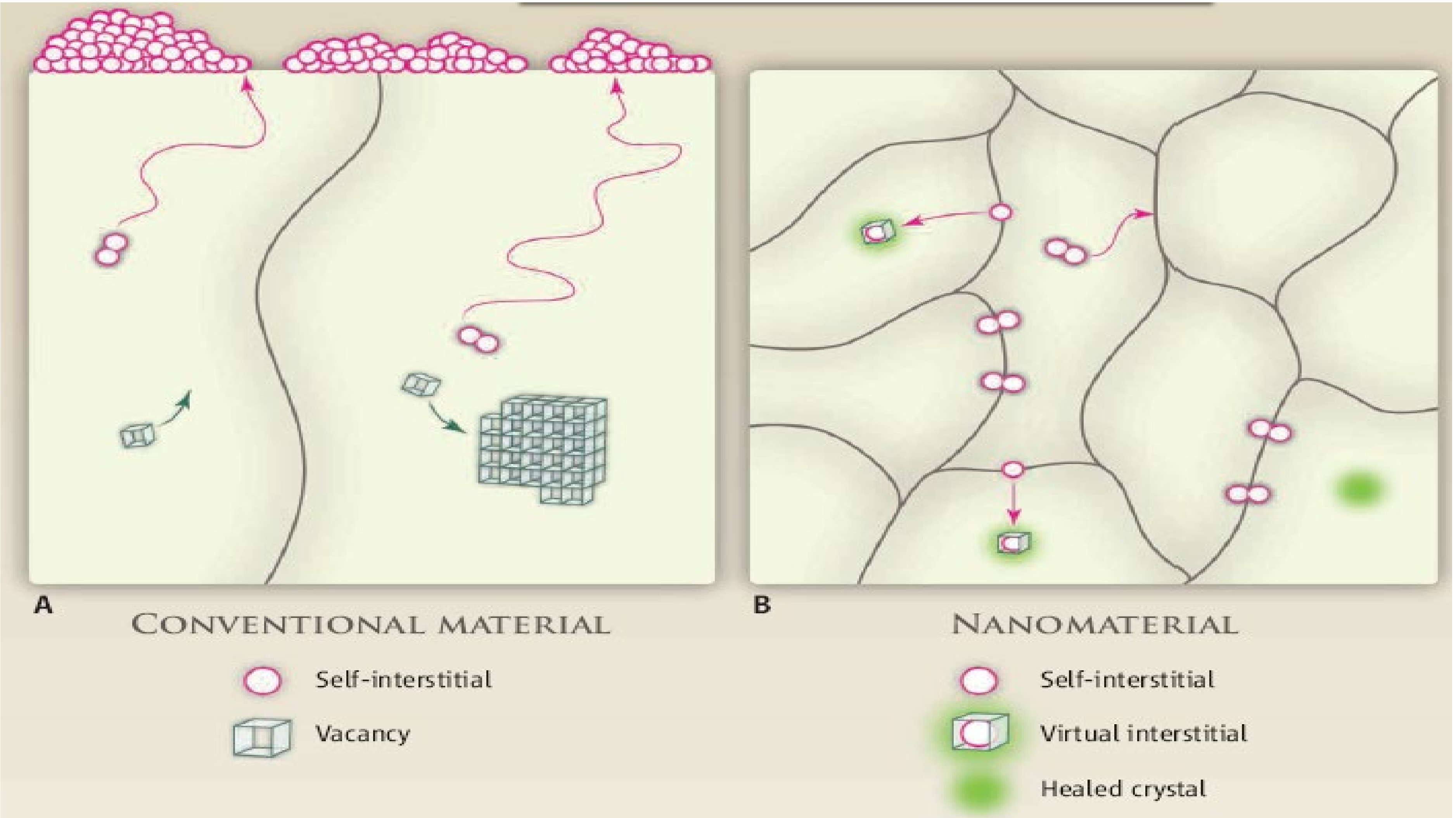
      – Creating effective diffusion channels that allow the light species to escape

  – Able to better accommodate the thermal loads $\rightarrow$ increasing the surface area



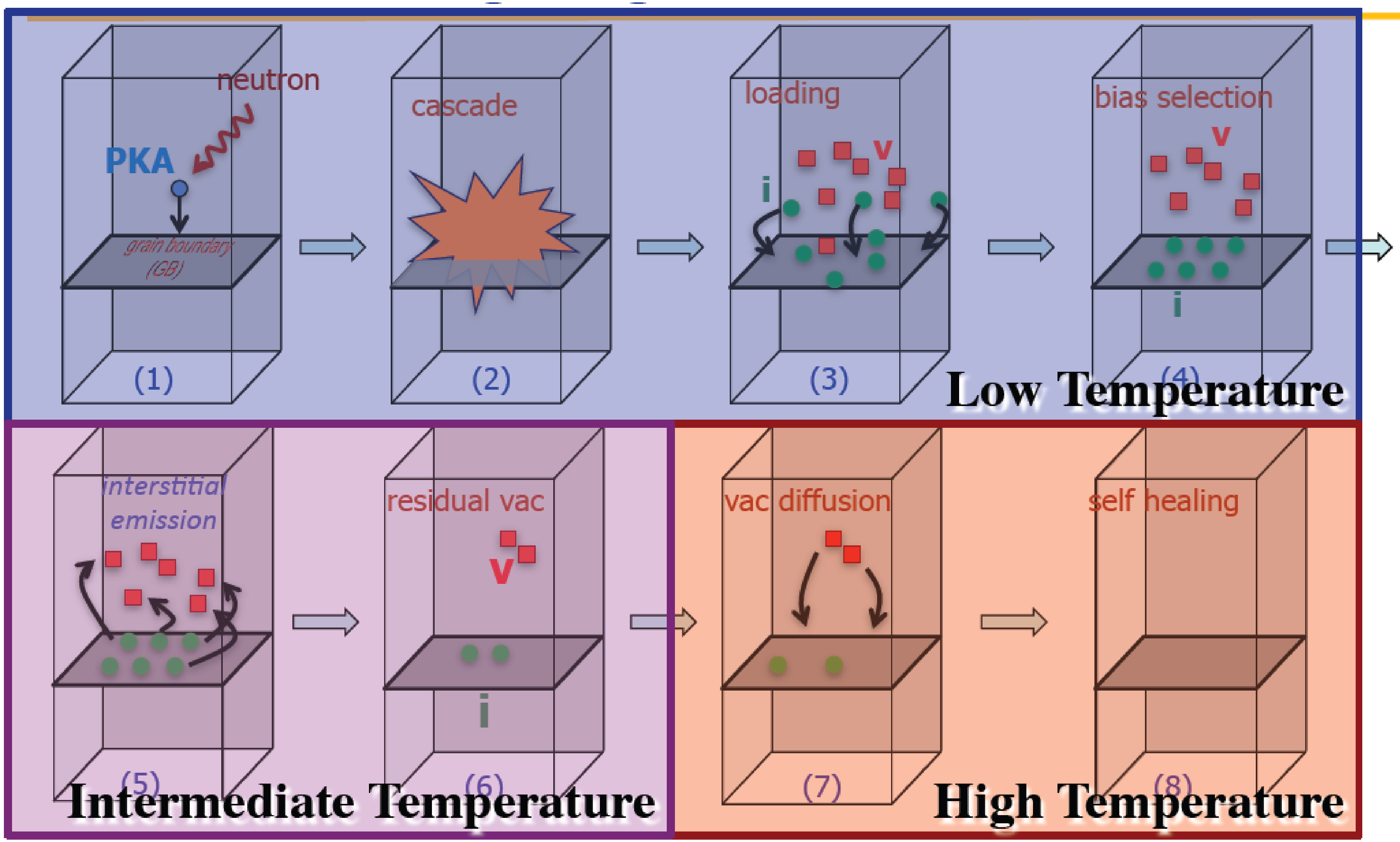
Nanomateriales under irradiation: interstitals and vacancies

Under certain circumstances



G. Ackland, Science 327, 1587 (2010)

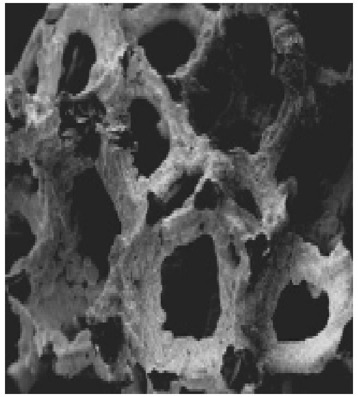
Nanomateriales under irradiation: the Beyerlein´s model



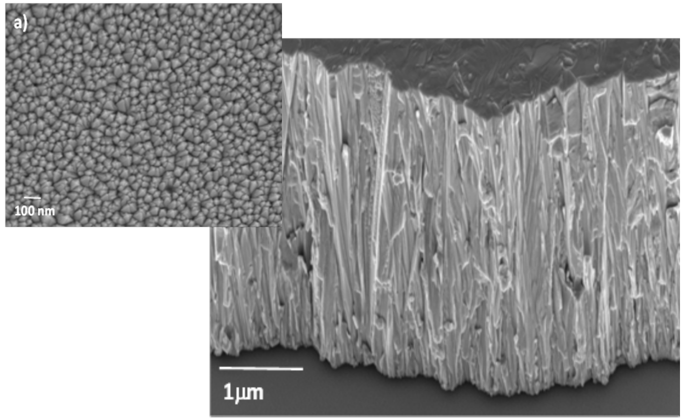
I. J. Beyerlein *et al.* Materials Today 16 (2013) 443–449.

PFM: new approaches

Foams



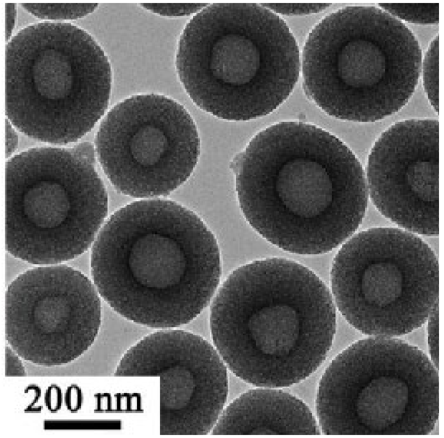
Grain size in the nm range



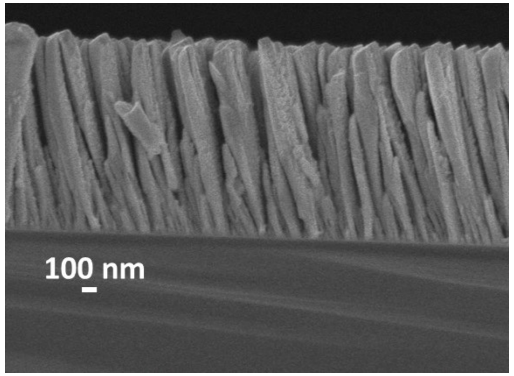
N. Gordillo *et al.* Applied Surface Science 316 (2014) 1–8

Nanoestructures

Hollow nanoparticles



P Díaz-Rodríguez *et al.* Nucl. Fusion 60 (2020) 096017



Nanoneedles

R. Gonzalez-Arrabal *et al.* Nuclear Materials and Energy 40 (2024) 101704

(IFN-GV)

Methods

- **Methods**
- Combination of experimental and computer simulations
- Study two set of samples (nano-, and mono- crystalline)

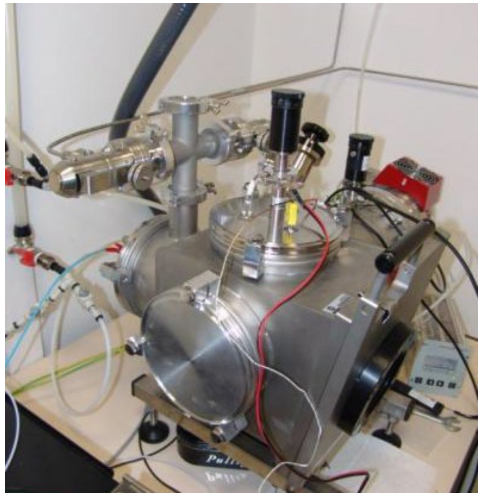
Experiments

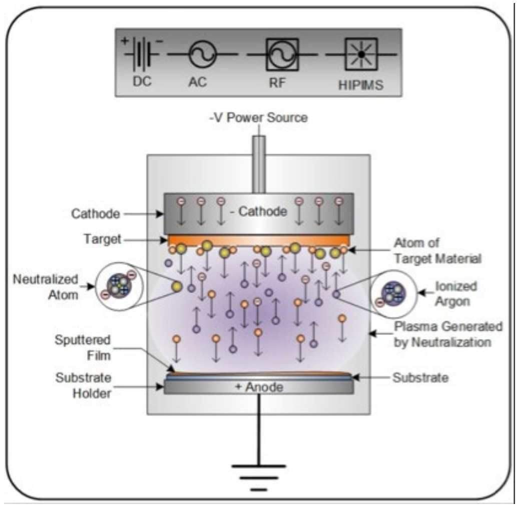
- Fabrication of nanostructured W samples by sputtering
- Implantations conditions selected to mimic as much as possible IFE conditions:
  - Sequential implantation: **C** (665KeV@RT) **and H** (170KeV@RT)
- Annealing of the samples after implantation at 473 K$\leq$ T $\leq$ 573 K
- Determination of the H depth profile by nuclear reaction analysis (NRA)
- Helium ion microscope (HiM)

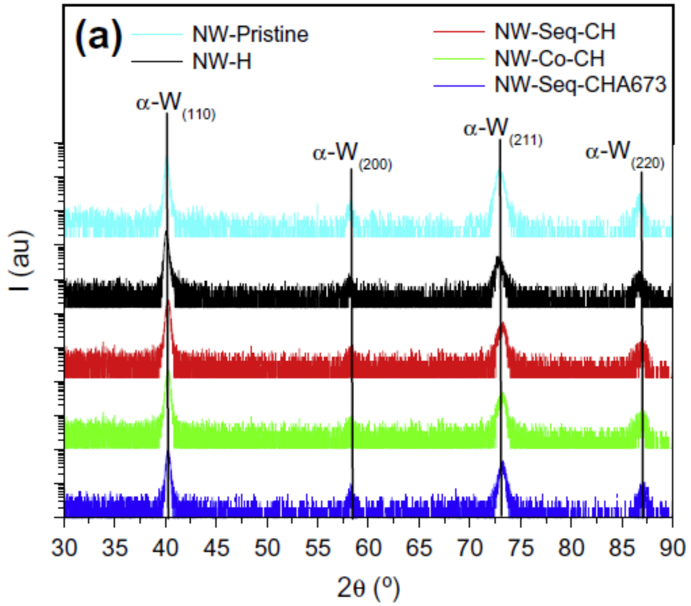
Computer simulations

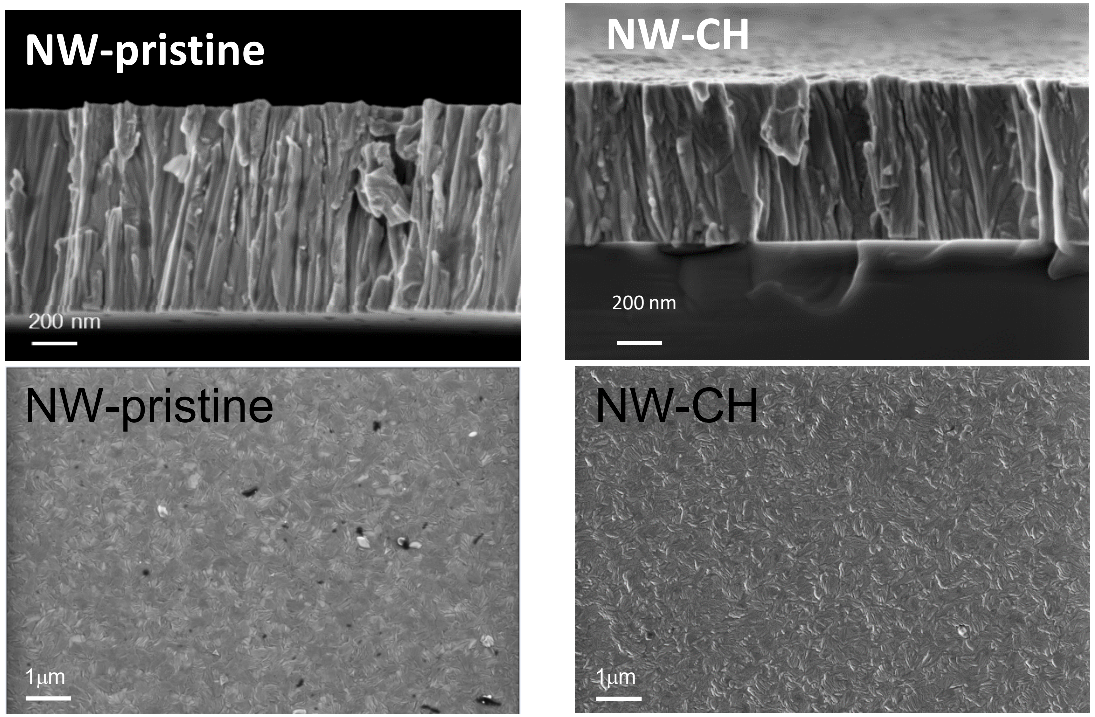
- Multiscale (DFT-MD-OKMC)
- Machine learning techniques. We have developed a MLIP to account for the role of GBs on radiation-induced damage and light species behavior. arXiv:2505.13744

Fabrication of nanostructured W coatings









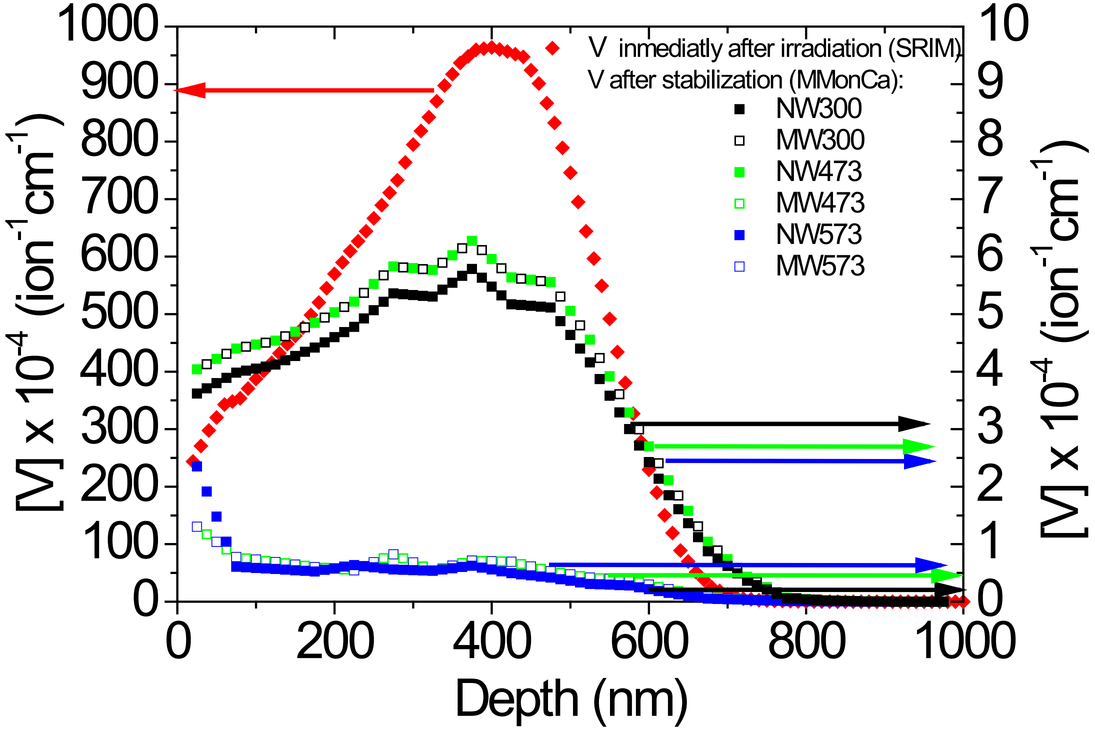
R. Gonzalez-Arrabal *et al.* JNM453 (2014) 287–295

- Nanostructured mono-phase (stable bcc α-W) samples fabricatedby sputtering at room temperature
- The morphology of the NW stable after irradiation
- No secondary phases in implanted samples

Influence of the GBs on the vacancy concentration

W irradiated with C (665 keV) and H (170 keV)

GBs and vacancies



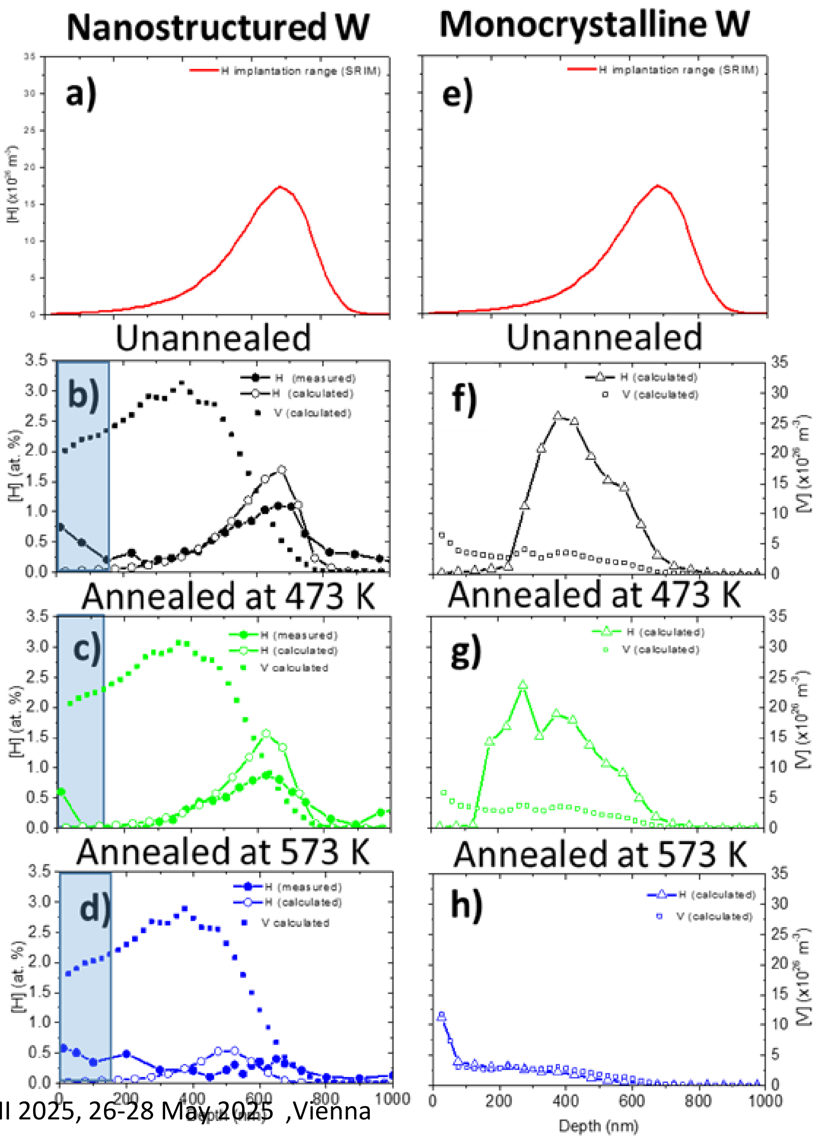
M. Panizo *et al.* Nucl. Fusion **59** (2019) 086055

- The number of Vs immediately after irradiation is two orders of magnitude higher than that after 10 d of stabilization
- NW have a larger density of Vs in the whole studied temperature range
- Small reduction in the Vs number is only observed for NW after being annealed at T=573 K

Influence of the GBs on the H behaviour

W irradiated with C (665 keV) and H (170 keV)

M. Panizo *et al*. Nucl. Fusion **59** (2019) 086055

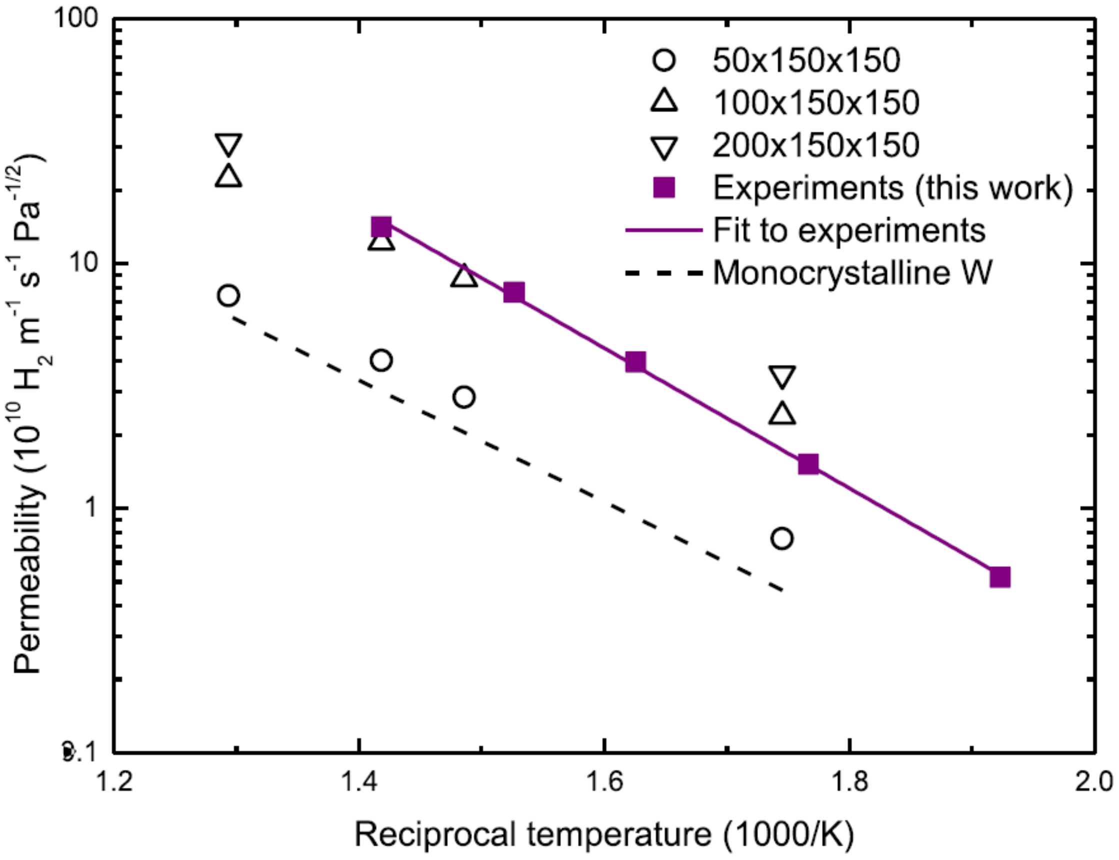


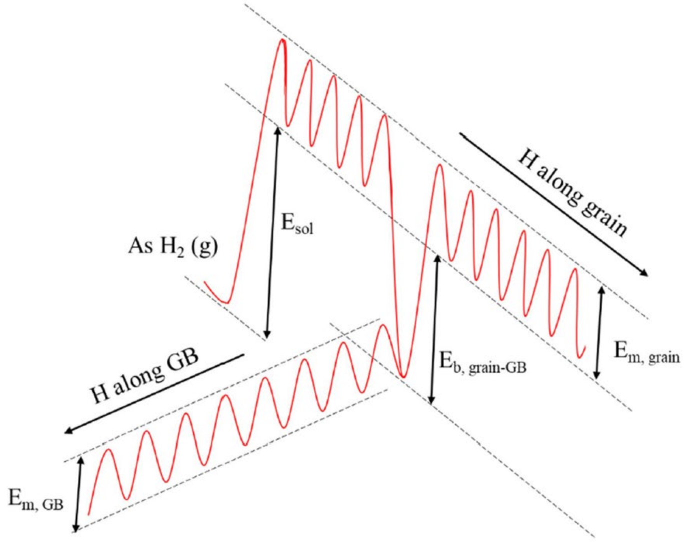
- In NW reasonable agreement between calculated and experimental data only if GBs are considered as effective diffusion channels
- At T≤ 473 K the retained H fraction is larger for MW than for NW→H release only via GBs
- At T=573K the H retained fraction negligible for all samples→ H outdifussion via sample surface as effective as via GBs
- Shape of the H depth profile → H accumulates in Vs located in the interior of the grains

Conclusion: GBs behave as effective diffusion channels for H

M. Panizo *et al.* Nucl. Fusion **59** (2019) 086055

Influence of the GBs on the H behaviour



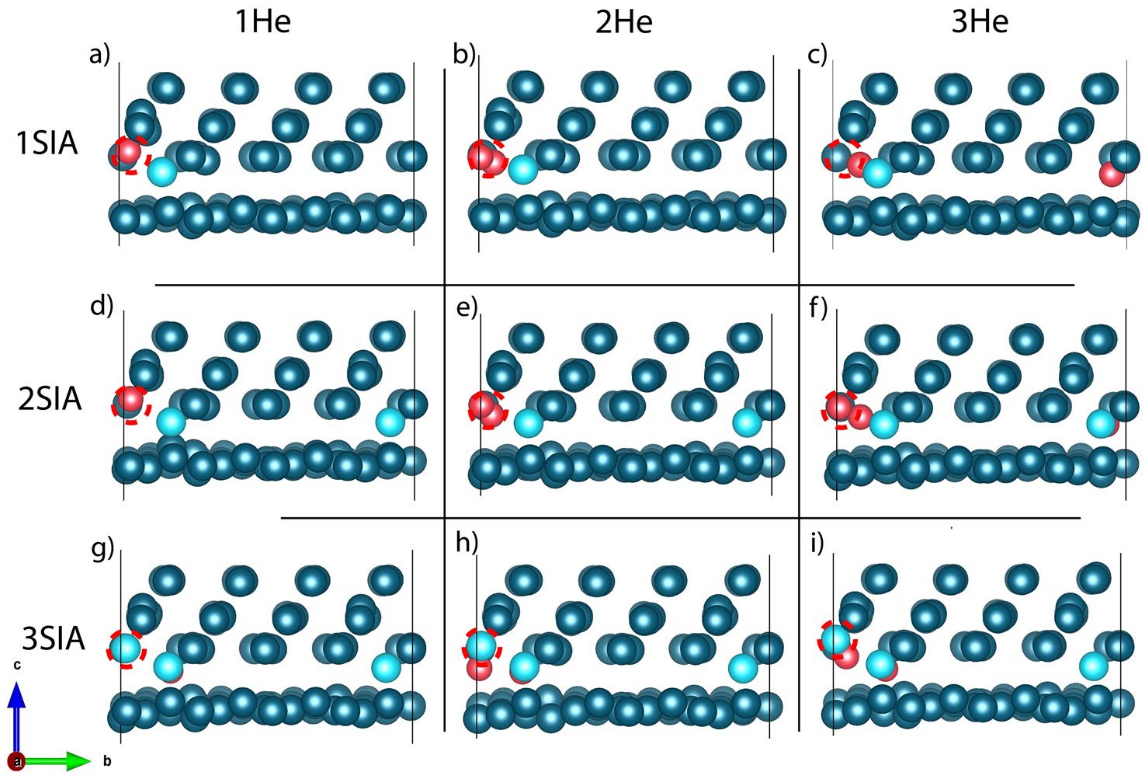


Conclusion: Grain boundaries in NW act as effective diffusion channels for H. But He?

P. Diaz-Rodriguez *et al.*, Emergent Materials, https://doi.org/10.1007/s42247-021-00344-w

V+SIA+He at GBs (DFT)

What will happen when the vacancy reaches the border and the He and the SIAs are found there?



- The presence of more than 3 SIAs prevent He to occupy the vacancy.
- He remains in the vacancy (DFT) → high temperature studies MD

J. Suárez-Recio *et al. Journal of Nuclear Materials 604 (2025) 155471*

- The behaviour of He depends on the number of He and SIAs atoms at the GB
- We have developed a Machine learning interatomic potential to study this case (work in progress)

MLIP to study defects at GBs: defect energetics benachmark

We develop a new IP, dubbed MLIPW, based on the Deep Potential methodology and trained on quantum mechanicalDFT data.

- MLIP-W **accurately** reproduces key defect energetics, matching DFT and experimental values
- Only MLIP-W predicts a negative V–V binding energy at 2nd nearest neighbor

Property	DFT	MLIP-W	EAM [48]	Tersoff [49]	Exp.
a_0 (BCC) (Å)	3.17	3.16	3.14	3.16	3.17 [51–53]
$E_f(V)$ (eV)	3.34	3.30	3.49	3.71	3.15 [54]
$E_{f,db110}$ (eV)	11.04	10.97	10.86	10.16	
$E_{f,db111}$ (eV)	10.76	10.86	10.40	9.50	
$E_{f,octa}$ (eV)	13.11	12.80	12.73	10.39	
E_b(V-V) 1nn (eV)	0.41	0.29	0.49	0.47	0.7 [55]
E_b(V-V) 2nn (eV)	−0.19	−0.21	0.38	0.41	

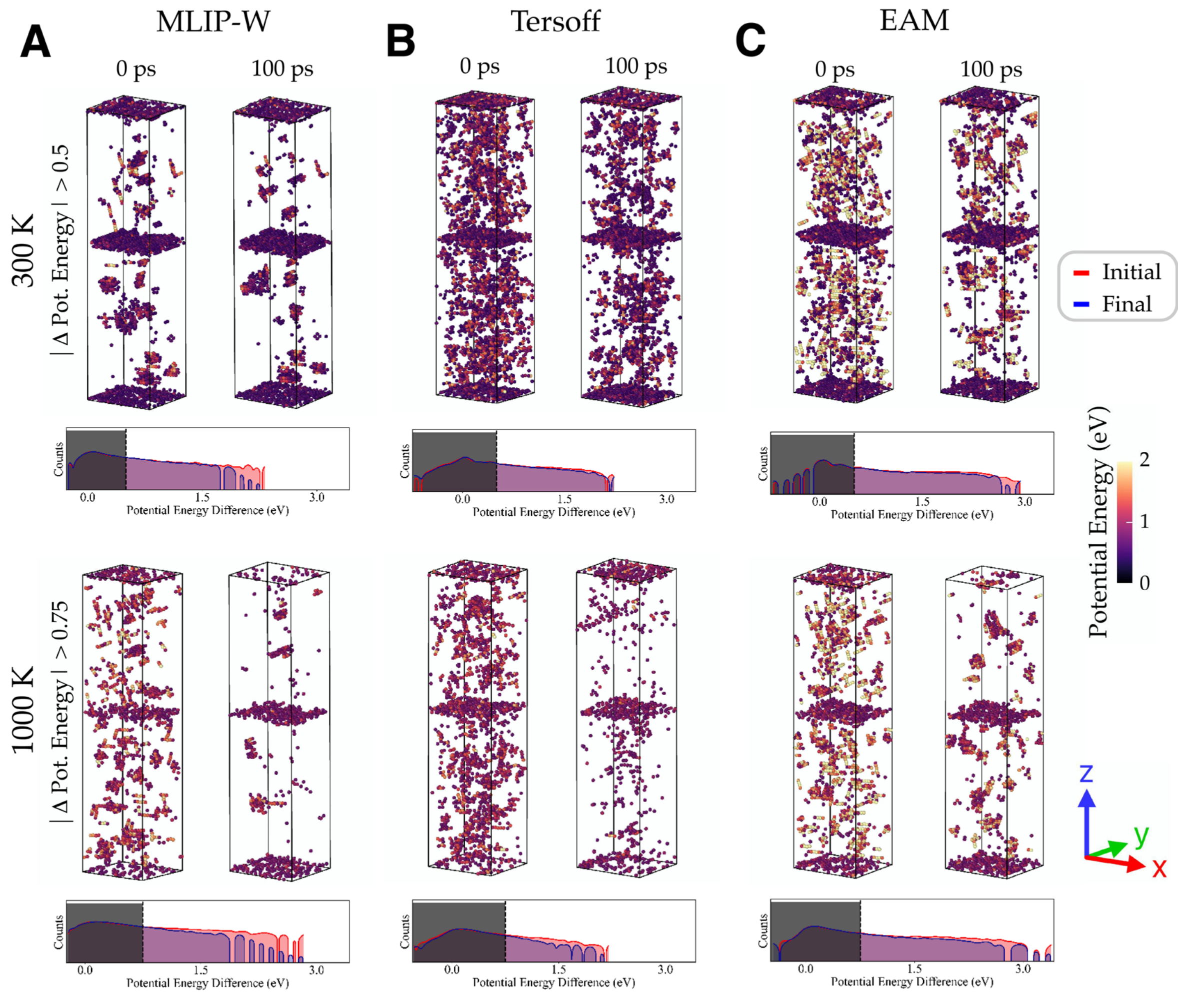
arXiv:2505.13744

Even if these static benchmarks provide an initial validation, **they alone don't necessarily guarantee accurate defect kinetics**

- Dynamic simulations are **required** to validate the **performance** of the potential

Raquel Gonzalez-Arrabal

MLIP: to study defects at GBs



- *Δ Pot* is the potential energy difference relative to the bulk for each potential.
- Only show atoms with *Δ Pot* > 0.5 eV for 300 K and 0.75 eV for 1000 K are shown in order to highlight defected or strained regions

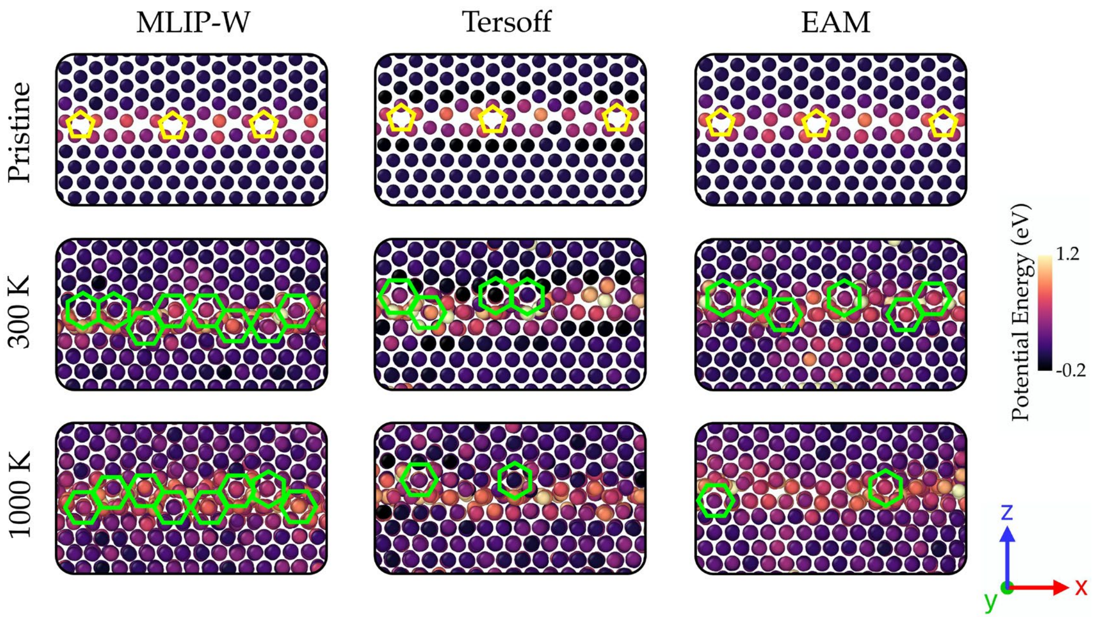
Different potentials lead to different defect evolution

arXiv:2505.13744

MLIP: to study defects at GBs

We develop a new IP, dubbed MLIPW, based on the Deep Potential methodology and trained on quantum mechanicalDFT data.

GB structure after defect migration



arXiv:2505.13744

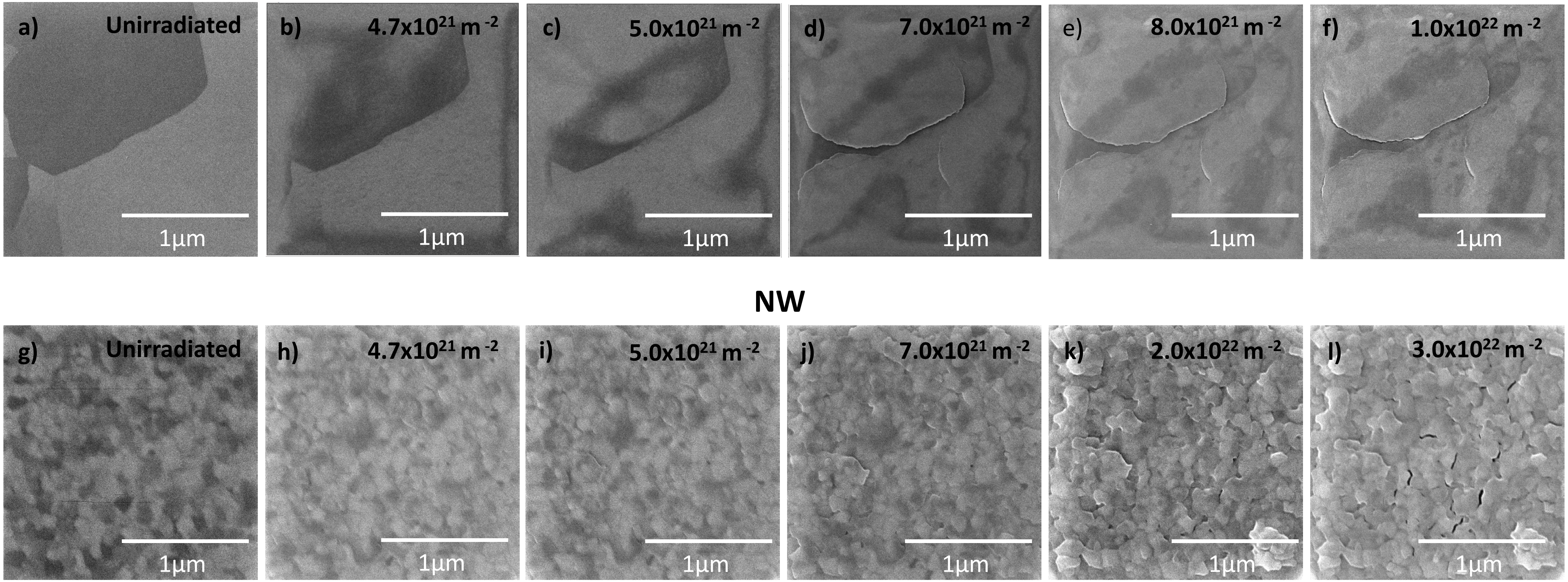
- For the MLIPW, SIAs are observed to effectively reach the GB and align along these grooves. In particular, at finite temperatures, atoms near both the W⟨112⟩ and W⟨110⟩ layers adjacent to the SIAs row shift into slightly arc-shaped crowdions to minimize the energy of the system.

- The ability of these empirical IPs to reproduce the GB structure decreases with increasing temperature to such an extent that they predict a compromised integrity of the GB, which is unexpected at the temperatures studied (up to 1000 K)

Influence of the GBs on the He behaviour

Helium ion microscope experiments: He irradiation at 30 keV and RT

CGW

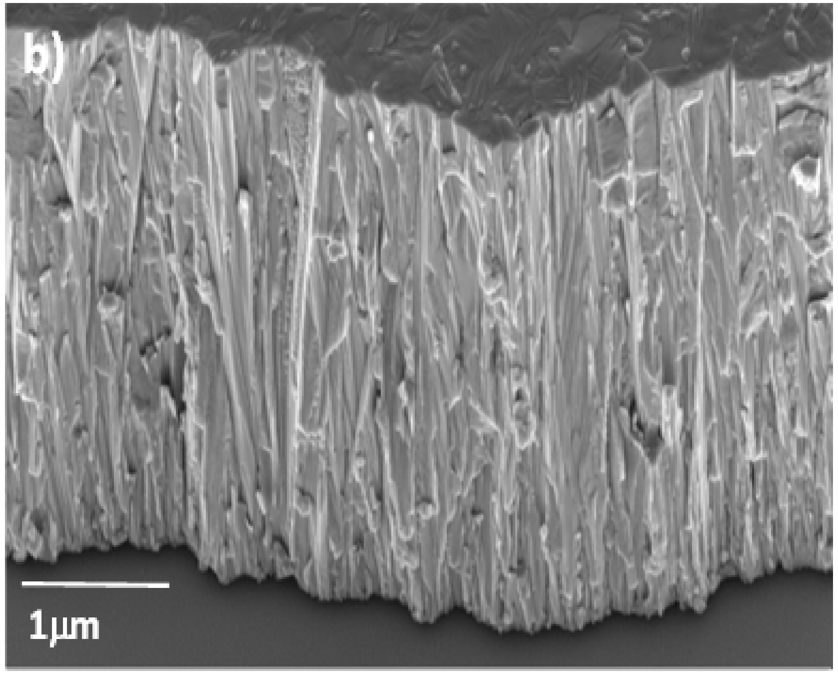


- CGW: Fluence damage threshold ~5 x10^{21} m^{-2} → blister within the grains
- NW: Fluence damage threshold ~2 x10^{22} m^{-2} → cracks long the GBs

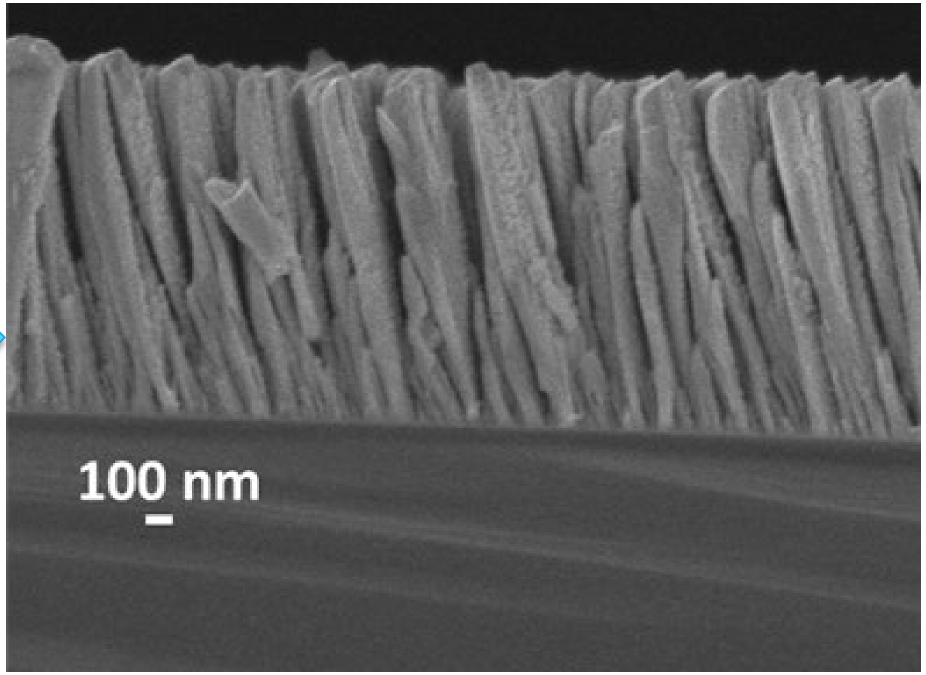
Raquel Gonzalez-Arrabal

PFM: future research lines

From GRAIN BOUNDARIES to FREE SURFACES



N. Gordillo *et al.* Applied Surface Science 316 (2014) 1–8



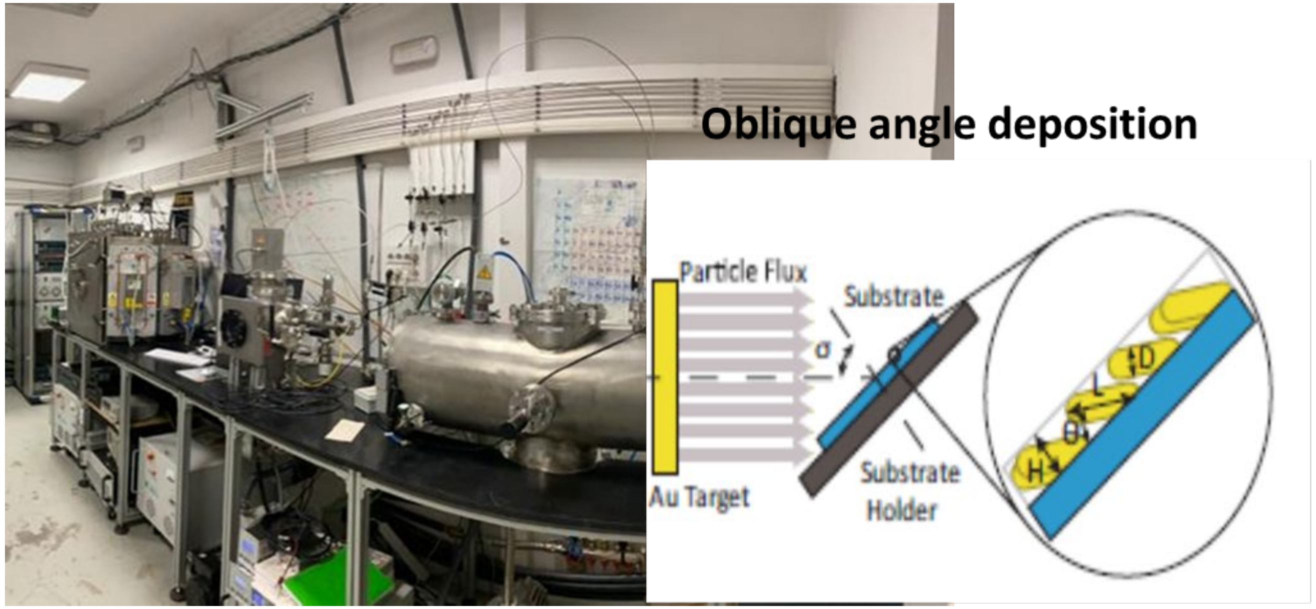
R. Gonzalez-Arrabal *et al.* Nuclear Materials and Energy 40 (2024) 101704

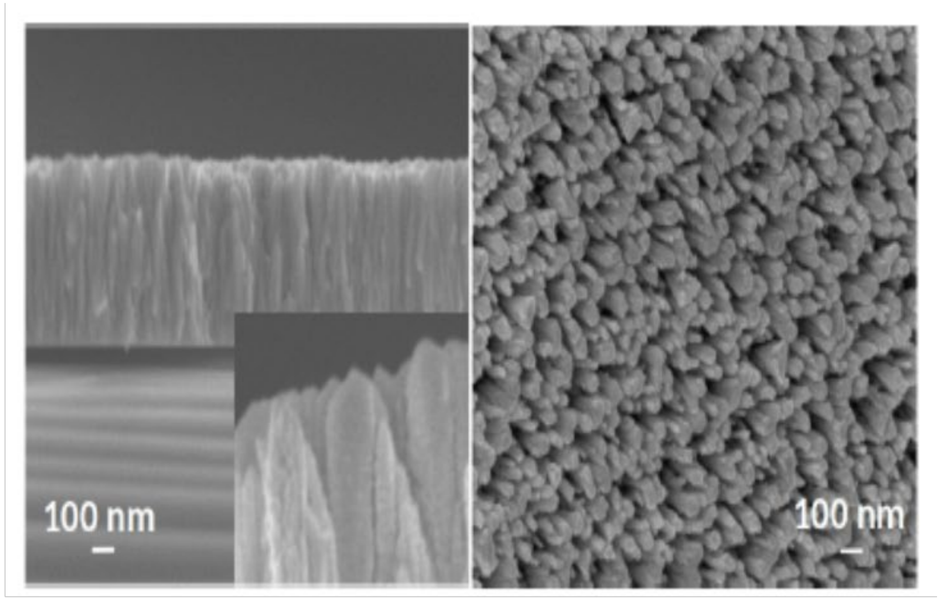
Objectives

- **Objective:** Study the capability of 3D W isolated nanostructures as PFM

- Questions

- How do free surfaces affect light species behavior (He)?
- **How does the 3D W nanocolumns affect the sputtering yield?**
    - Operational temperature range for nanostructured tungsten?





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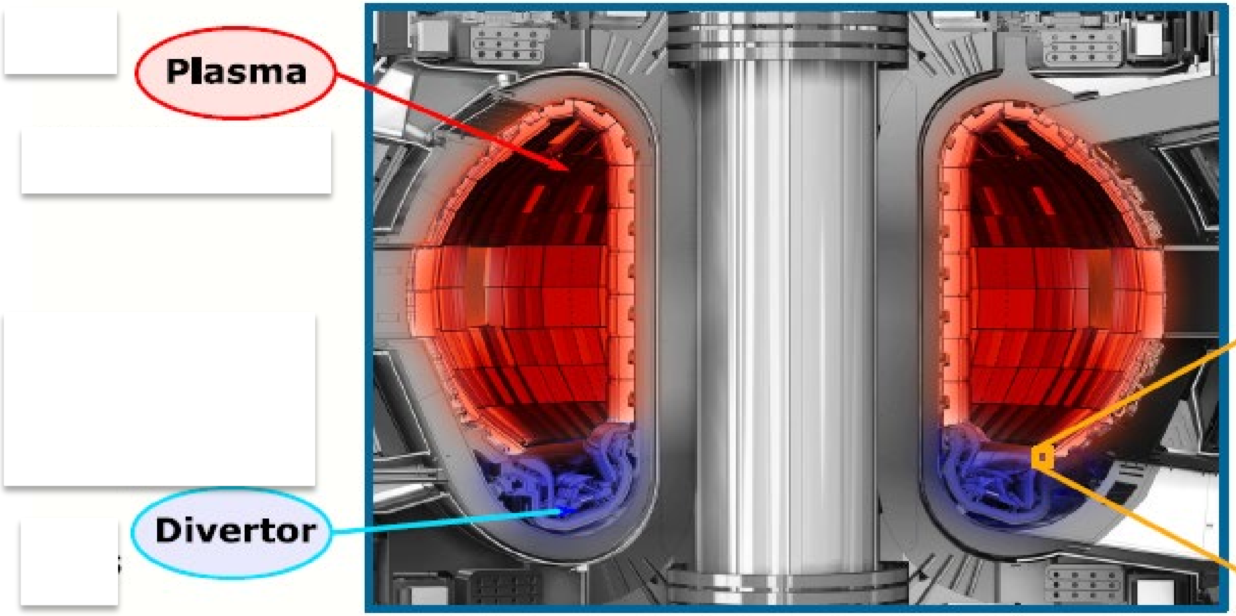
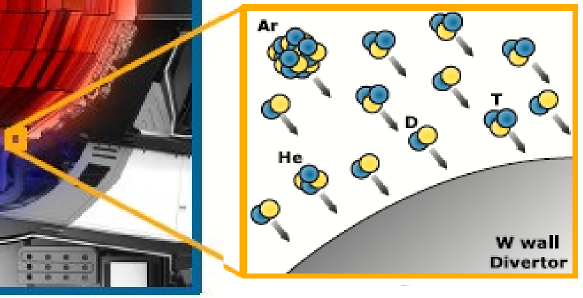
3D nanostructured W: sputtering yield

How does the 3D W nanocolumns affect the sputtering yield?



TOKAMAK reactor concept [2]

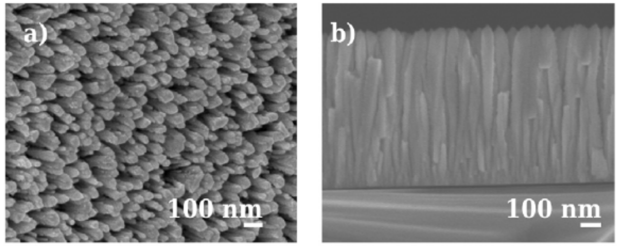


Wirh permission of C. Cupak

Heat load mitigation

- Heat loads smaller than 10MW/m^2 desired
- Seeding gases (like Ar) necessary for radiative cooling
- Sputtering by seeding gas needs to be investigated

Collaborators



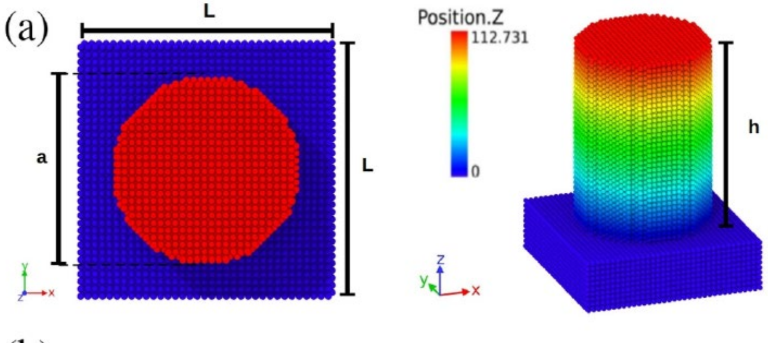
Sample fabrication and characterization

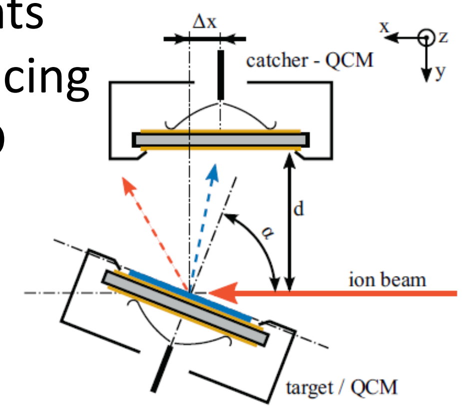
UNIVERSITY OF HELSINKI

MD Computer simulations

TECHNISCHE UNIVERSITÄT WIEN

Sputtering yield measurements
Computer simulations ray-tracing code SPRAY and SDTrimSP-3D





3D nanostructured W: sputtering yield

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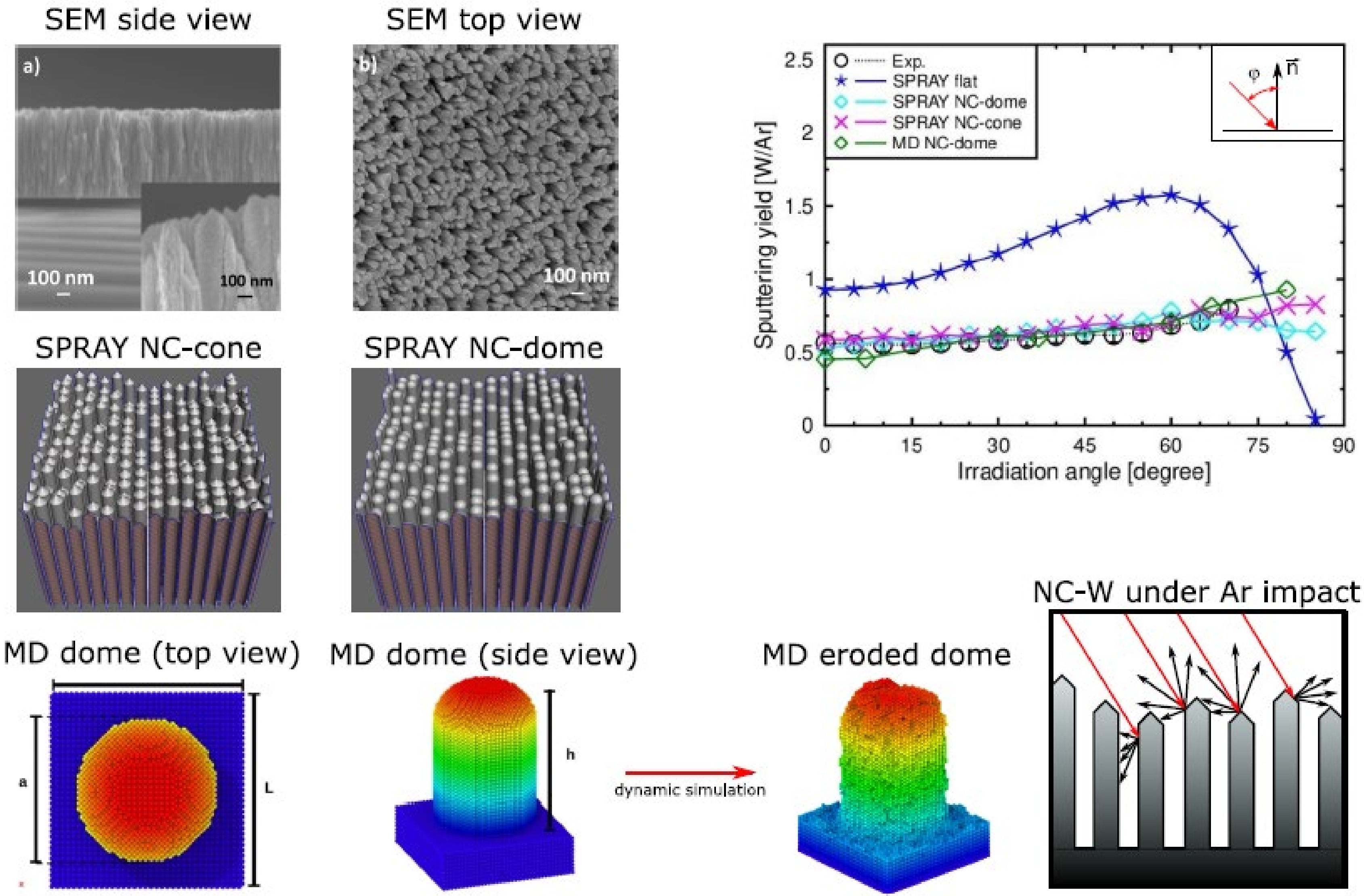
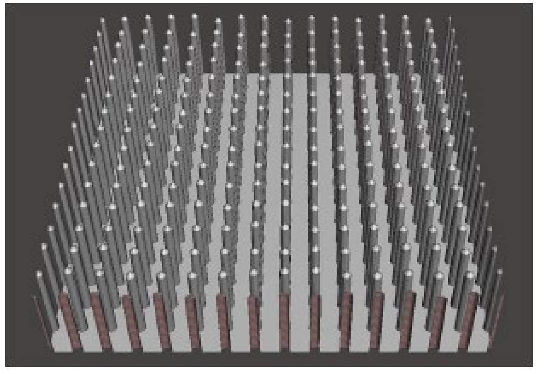


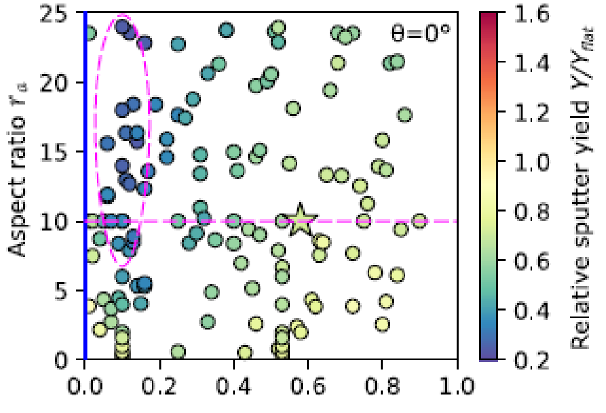
3D nanostructured W: sputtering yield



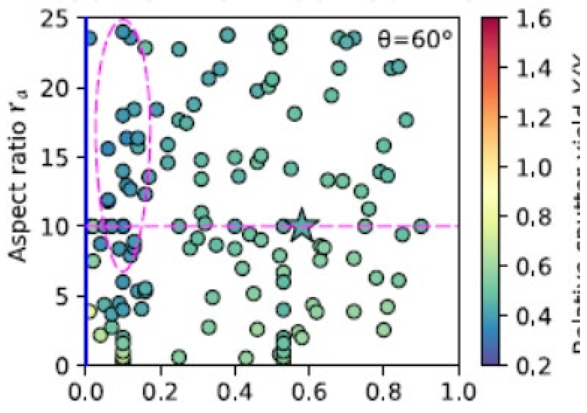
2 keV Ar^+ irradiation at 1.1×10^{20} m^{-2}

Aim: fin out the lowest sputtering by tuning:

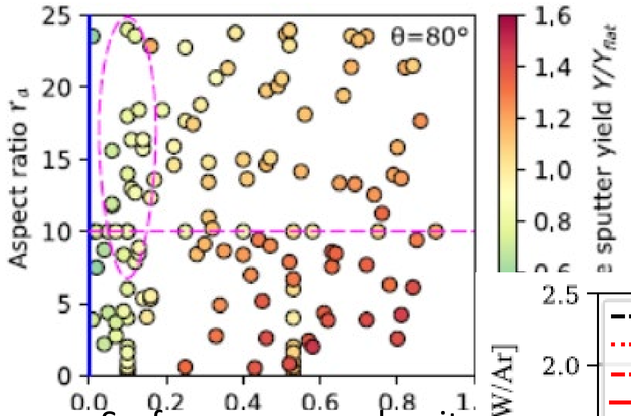
- Separation between nanocolumns
- Aspect ratio



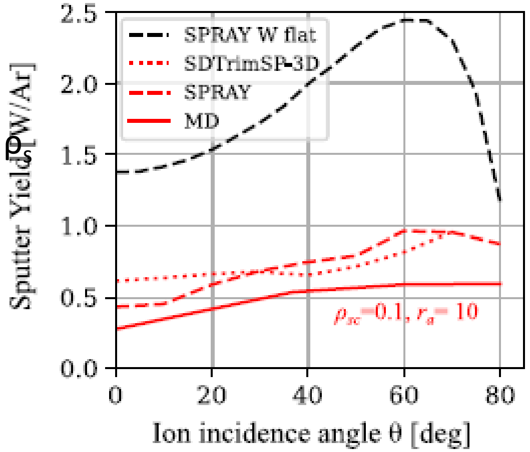
Surface coverage density ρ_s



Surface coverage density ρ_s



Surface coverage density ρ_s



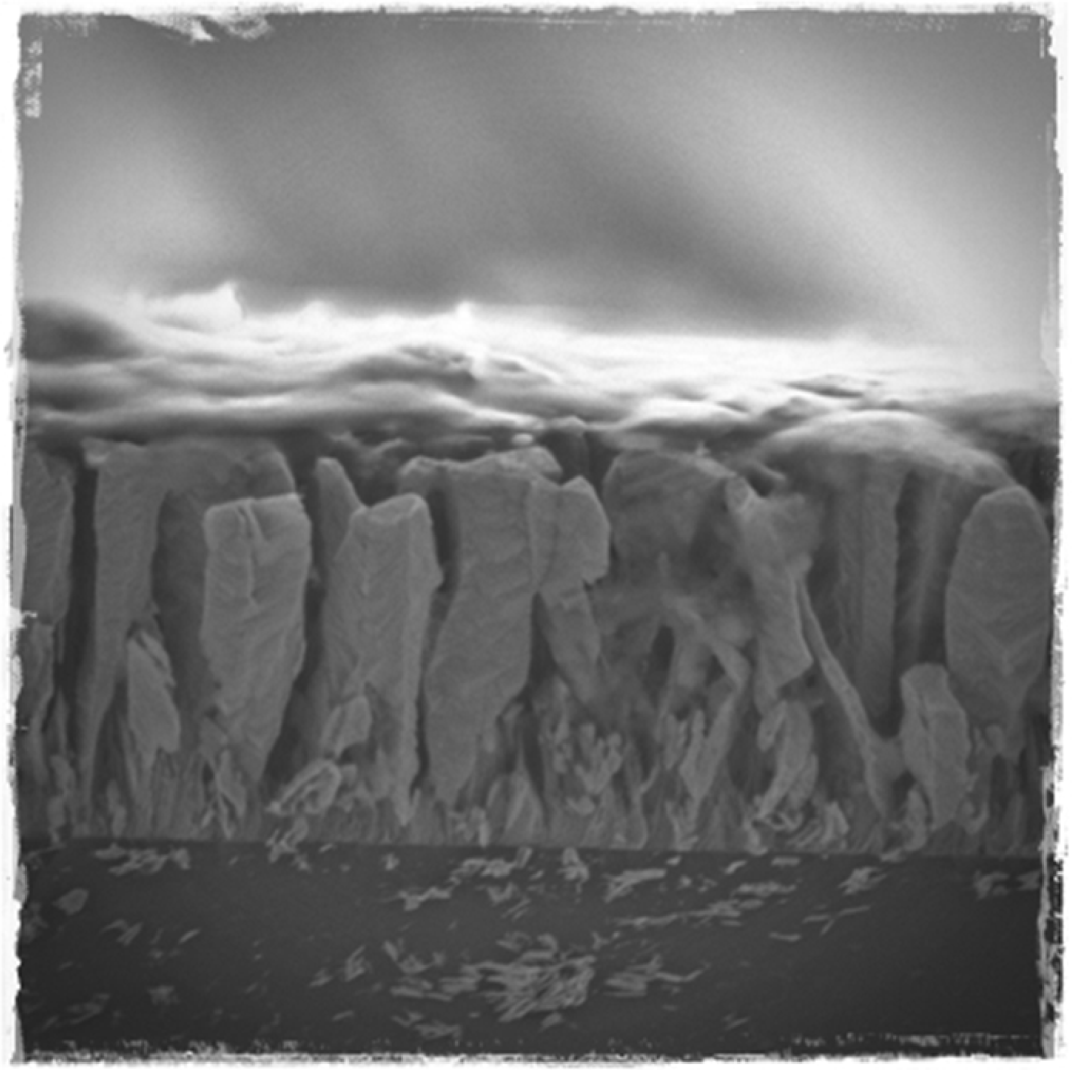
C. Cupak *et al.* Physical Review Materials, 7, 065406 (2023)

Conclusions

- Currently there is no known material able to withstand the harsh conditions of a PFM. CGW is not foreseen to properly work , at least in ICF.
- The presence of GBs may shift the fluence threshold for blistering to happen to higher values (higher radiation resistance)
  - GBs favor H outdiffusion
  - GBS seems, at low temperatures to favor the H retention in low populated vacancies
- The influence of GBs on He retention need to be further investigated.
- W nanocolumns strongly reduced the sputtering yield and flatten its angular dependence.
- **For fusion to become a reality it is necessary:**
  - **To define a realistic roadmap for advanced materials development**
  - **To establish experimental facilities to test materials under conditions as close as posible to those expected in nuclear fusion reactors**
  - **Join efforts to enhance progress, save money, and avoid duplication of results**

Thank you for your attention

Nanostructured W film



Upsala Glacier