

# Modelling of fusion reactor material performance

Matti Paljakka, Tommi Lyytinen, Anssi Laukkanen et al.

16/04/2026 VTT – beyond the obvious

# We create solutions in three business areas

We help our clients and partners build new businesses and find sustainable solutions to global challenges through science and technology.

Our mission is to promote the application and commercialisation of research and technology in business and society.

## Carbon neutral solutions



## Digital technologies



## Sustainable products and materials



# VTT in numbers

Creating impact over 80 years!

**306 M€**

operating income

**2,390**

employees

**488**

patent families



Carbon neutral  
solutions

**51%**

of the net turnover  
from abroad

**1,100**

customers

**60+**

start-ups



Digital  
technologies

**81**

Net promoter  
score (NPS)

**646**

scientific articles /  
year



Sustainable  
products and  
materials

# Overview of fusion at VTT

Fusion is strong and growing:

- ✓ Volume >3 times larger than in 2020
- ✓ ~100 people
- ✓ Research Professor and Lead positions

Versatile project portfolio

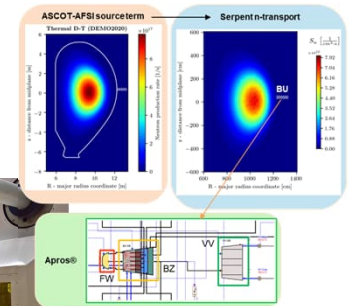
- ✓ EUROfusion, domestic research instruments
- ✓ Long history with ITER & F4E
- ✓ Commercial work for private companies

VTT coordinates fusion research in Finland

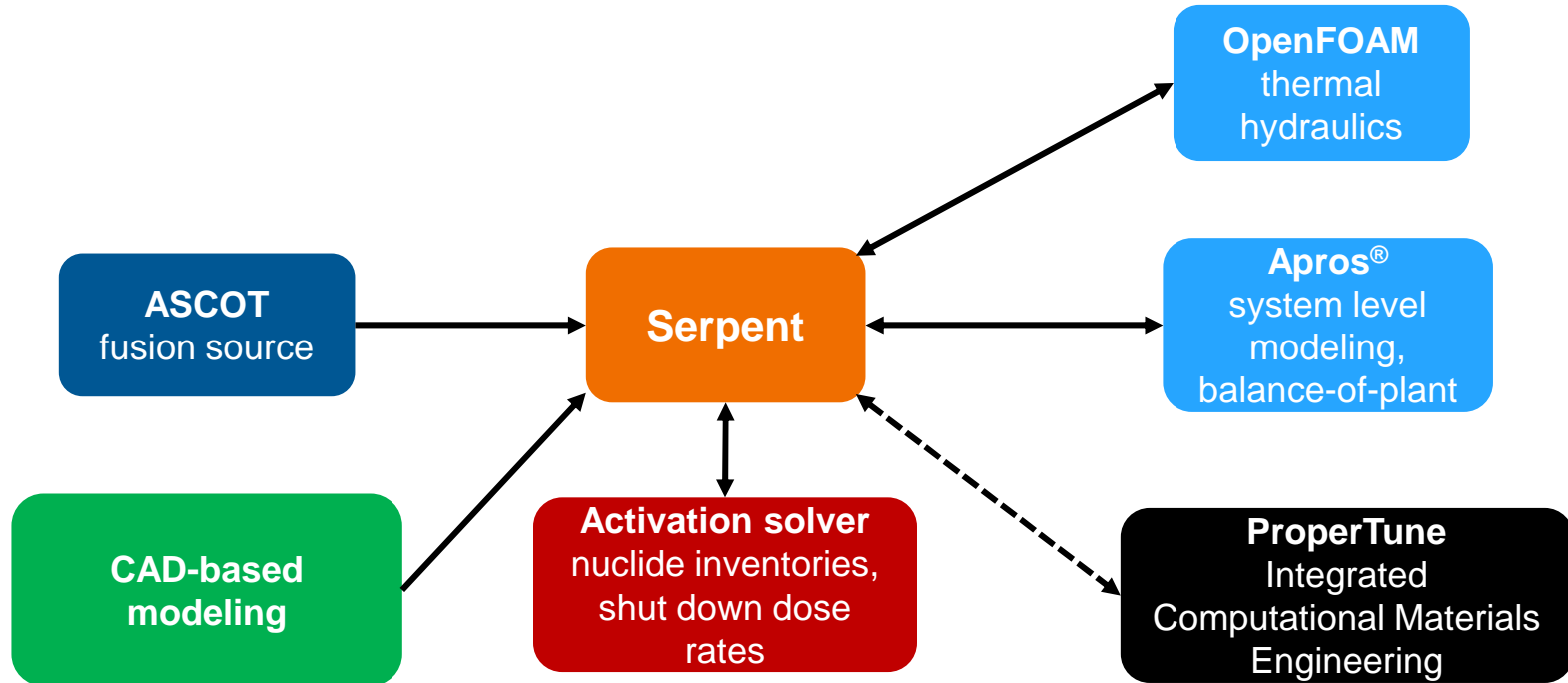
- ✓ FinnFusion Consortium <https://finnfusion.fi/>

Topical areas:

- ✓ Remote Handling
- ✓ Fusion physics
- ✓ Safety and licensing
- ✓ Engineering analysis
- ✓ Material research

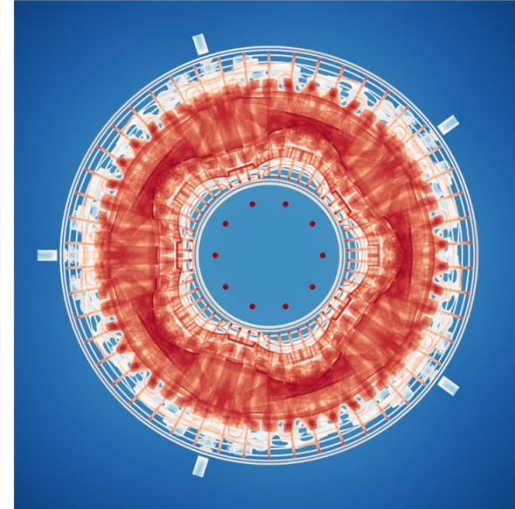


# VT's Fusion Simulation Framework



# Serpent Monte Carlo code

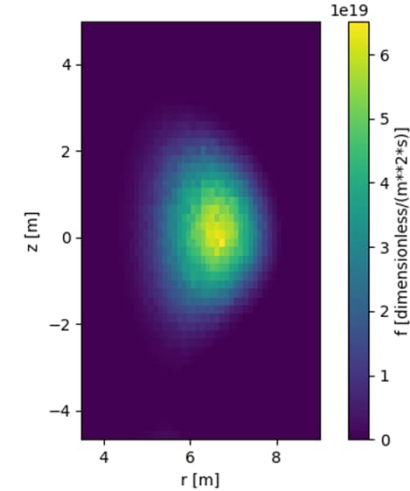
- Monte Carlo code developed at VTT since 2004
- Origin in fission reactor modeling -> nowadays applied in fusion and other radiation transport problems
- Features related to fusion
  - Coupled neutron-photon transport
  - Weight-windows-based variance reduction techniques (heavy shielding problems)
  - Built-in neutron activation solver
  - Transport mode using CAD-based STL (stereolithography) geometry format and unstructured mesh geometry (polyhedra)
  - Coupled via Python interface to thermal-hydraulics (e.g. OpenFoam) and system codes (e.g. Apros®) in the Kraken framework



**Fig:** Total collision rate of W7-X stellarator visualized with Serpent plotter S. Äkäslompolo et al. *Fus. Eng. and Des.*, **167**, 2021.

# From plasma to neutronics: ASCOT-Serpent

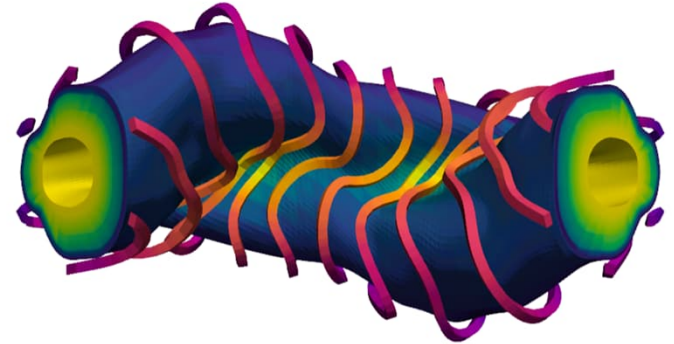
- ASCOT Fusion Source Integrator (AFSI) calculates the 5D phase-space distribution of the fusion products
  - Directly used as source input in Serpent
    - Reactions:(DT, He4n); (DHe3,He4p); (DD,Tp); (DD,He3n)
- Source modeling capabilities:
  - 1) Thermal fusion source (burning plasma operation)
  - 2) Beam-thermal source (external heating e.g., NBI, ICRH)
    - Ionization of the beam in the plasma (BBNBI)
    - Slowing-down simulation of ionized beam particles (ASCOT)
    - Calculating fusion product distribution (AFSI)



**Fig:** Example neutron r-z-distribution in ITER obtained with AFSI

# CAD-based modeling

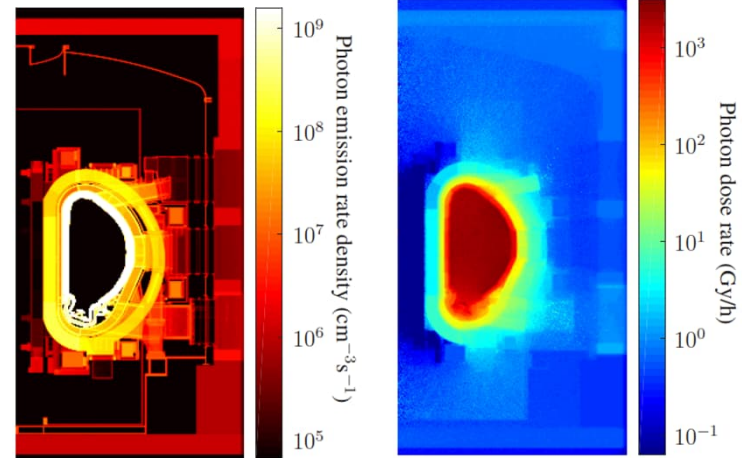
- Serpent can perform transport simulation in CAD-based mesh geometries (STL mesh, polyhedral mesh)
  - Eliminates the need for conversion to simplified Monte Carlo formats (e.g. CSG)
  - Enables high-fidelity modeling without geometry simplification
  - Supports rapid and consistent design iteration cycles
- Support for advanced mesh formats (e.g. AMF, 3MF)
  - Transfer component material information from the CAD to Serpent simulations



**Fig:** Shielding calculation example in SQUID stellarator using STL mesh format.

# Activation analyses and shutdown dose rates

- Serpent has a built-in activation solver
  - Activation and radioactive waste inventories as a function of time
- Radioactive decay source automatically generated from activated material compositions and decay data
  - Serpent photon transport simulation -> Shut down dose rates



Left: Photon emission rate density from radioactive decay at the moment of reactor shut-down.

Right: Photon dose rate from radioactive decay at the moment of reactor shut-down

J. Leppänen, T. Kaltiaisenaho, PHYSOR 2016

# Multiphysics couplings with Serpent

- OpenFOAM – Thermal Hydraulics Coupling
  - High-fidelity CFD for flow, temperature and density fields
  - Direct mapping of Serpent energy deposition onto the OpenFOAM mesh
  - Feedback loop: updated material properties (temperature, density) returned to Serpent
  - Enables consistent neutronics–thermal hydraulics coupling on a shared mesh
  
- Apros – System-Level Modeling
  - Dynamic balance-of-plant and system behavior simulation
  - Serpent provides volumetric energy deposition as source terms
  - Apros evaluates system response (e.g. cooling performance, transients)

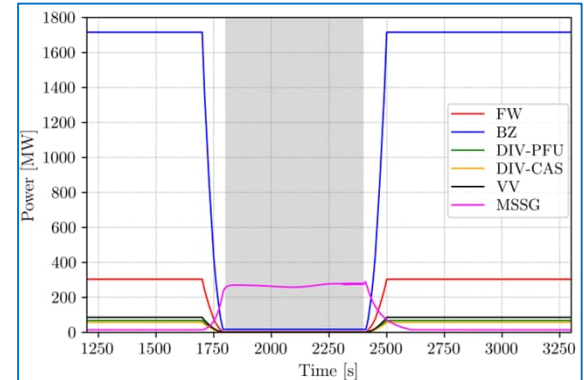
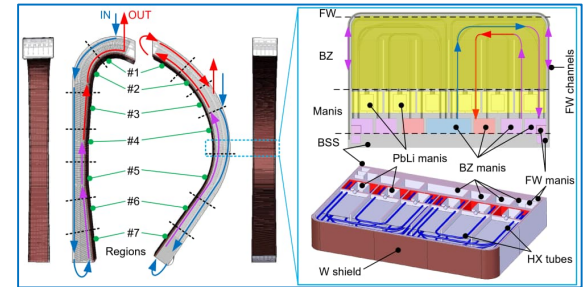
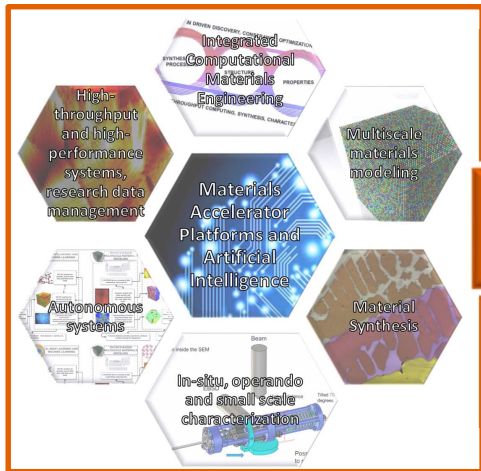


Fig: Apros DEMO BoP calculations.

# VTT ProperTune

- Integrated Computational Materials Engineering (ICME) concept that uses multiscale modelling for optimal computational material design
- Energy deposition conditions from Serpent (fusion environment)
- Irradiation effects (dpa, flux), helium formation, etc. as inputs for ProperTune
- Finding optimal materials for neutronics design with ProperTune (lifetime endurance, wear and corrosion resistance and fracture and fatigue durability)

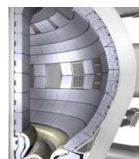
# VTT Technical Research Centre of Finland Ltd – biased view to materials engineering @ VTT



## VTT is developing 3 Materials Accelerator Platforms:



Powder metallurgical and structural materials



Potential use cases:  
Materials for extreme operating conditions



Synthetic biology and bioengineered materials



Materials from sustainable feedstock and renewable sources

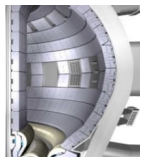


Functional materials, energy storage

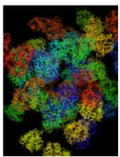


Novel semiconductors, microelectronics and energy storage materials

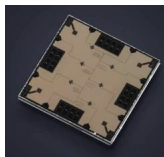
## Selected example activities, projects and programmes:



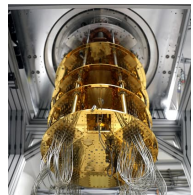
Eco-fusion R4B: EU-MACE, and HEU, Arpa-E activity



SynbioMAP and biotech: HEU and investment program activity



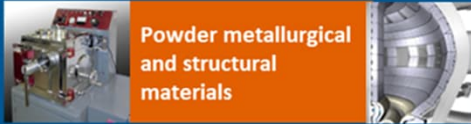
Quantum Nova, future pilot facility, FULL MAP (HEU)



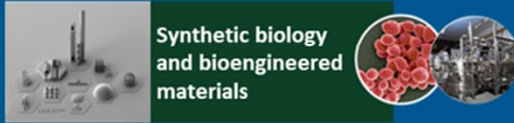
Quantum computing infrastructure

# VTT Technical Research Centre of Finland Ltd – biased view to materials engineering @ VTT

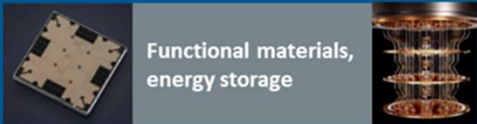
Building 3 Material Accelerator Platforms and unique infrastructure such as quantum computing



**Powder metallurgical and structural materials**

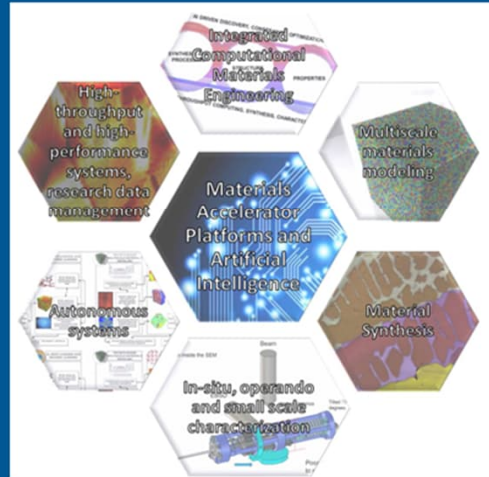


**Synthetic biology and bioengineered materials**

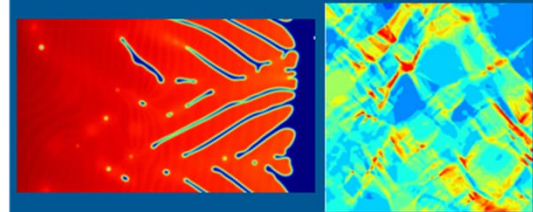
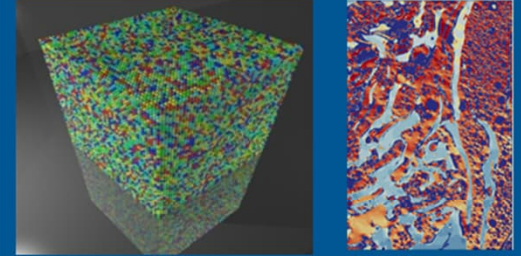


**Functional materials, energy storage**

AI-driven materials science and engineering with VTT properTune in collaboration with industry

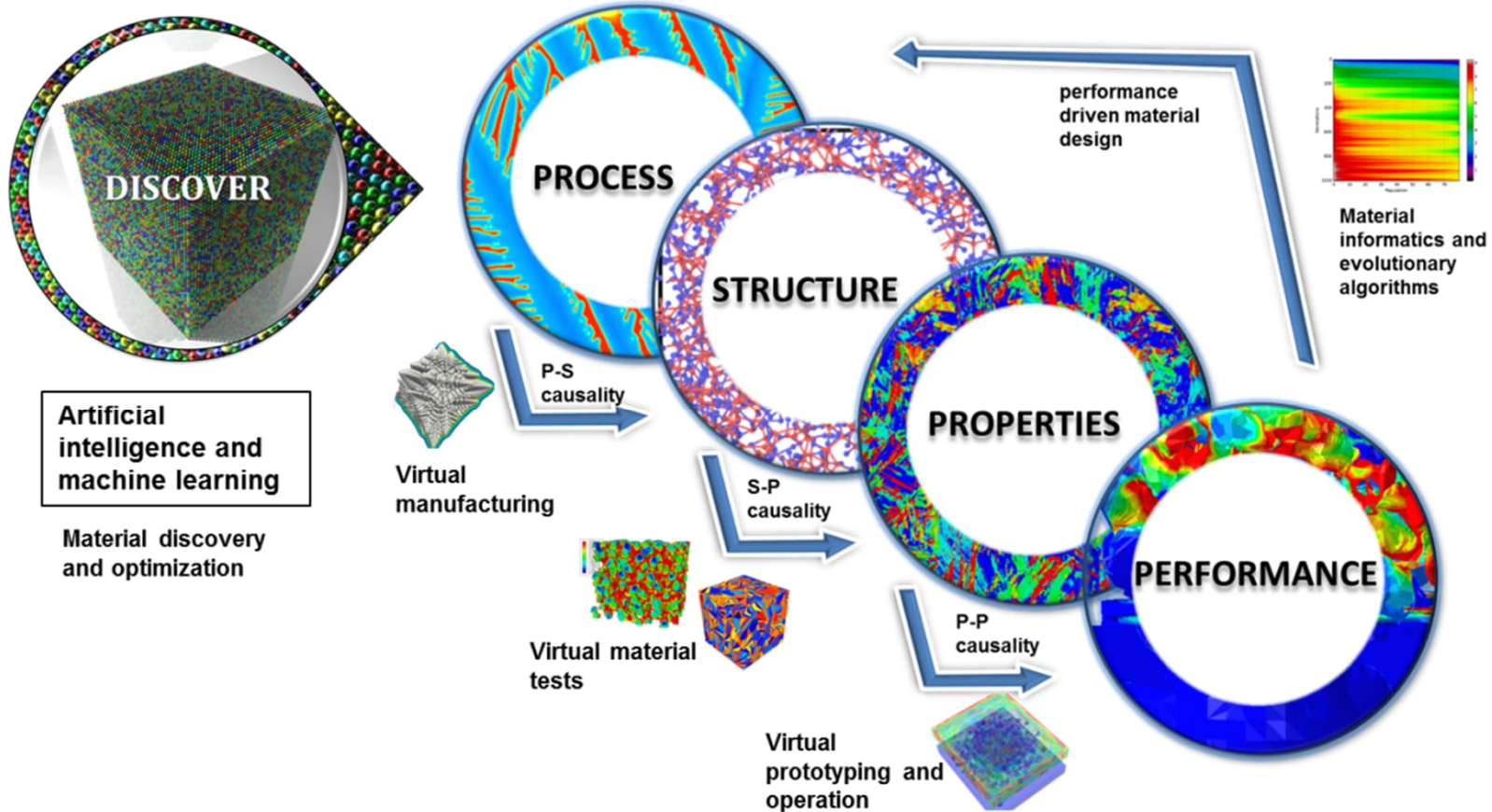


Multiscale capabilities for modeling, testing and characterization, piloting for material manufacturing



Materials Acceleration Platforms (MAPs): Accelerating Materials Research and Development to Meet Urgent Societal Challenges, Stier et al., [doi.org/10.1002/adma.202407791](https://doi.org/10.1002/adma.202407791)  
Interface morphology and dislocation-mediated processes during rapid solidification of thin films, Nittala et al., [doi.org/10.1016/j.actamat.2025.121581](https://doi.org/10.1016/j.actamat.2025.121581)  
Dislocation density in cellular rapid solidification using phase field modeling and crystal plasticity, Lindroos et al., [doi.org/10.1016/j.jplplas.2021.103139](https://doi.org/10.1016/j.jplplas.2021.103139)

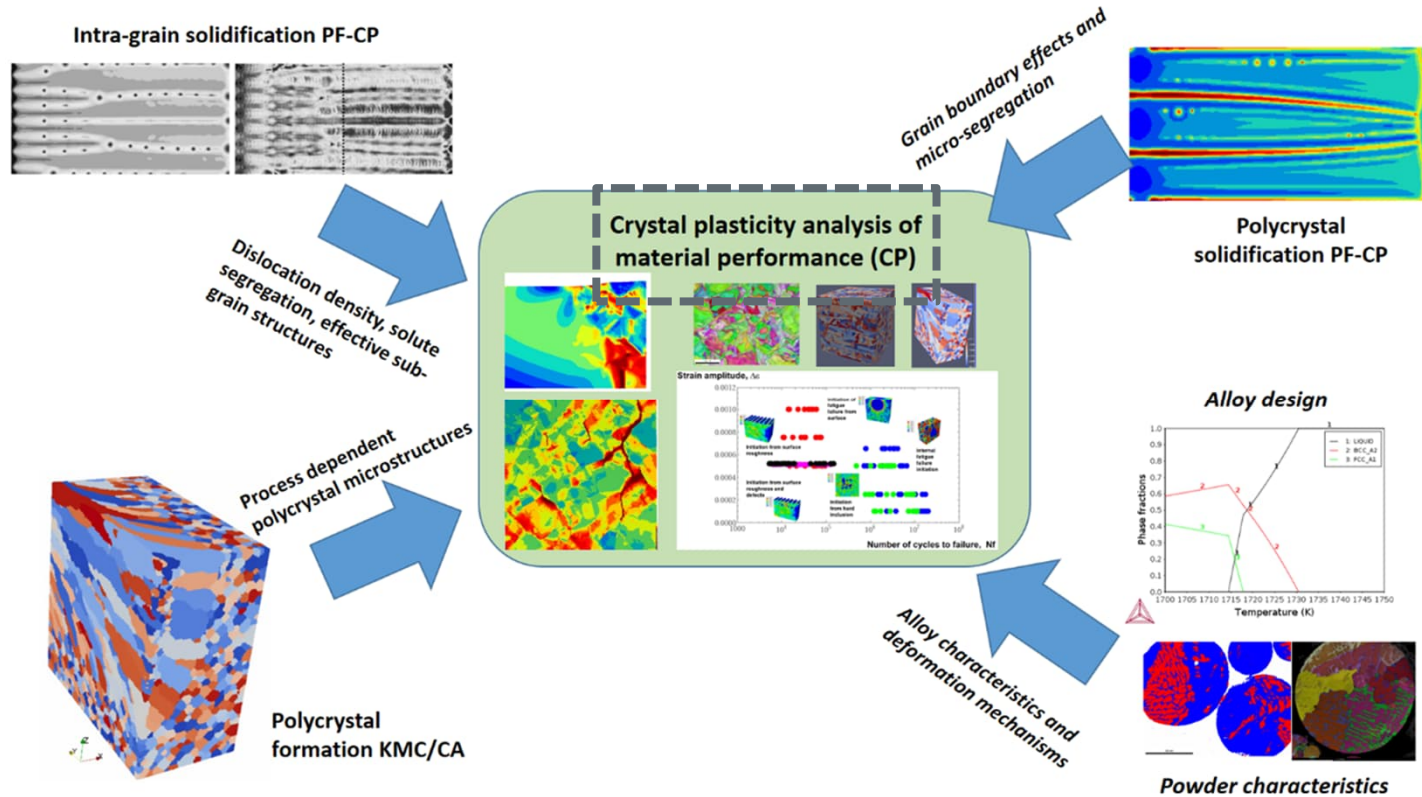
# VTT properTune modeling and simulation solution for digitalization of materials



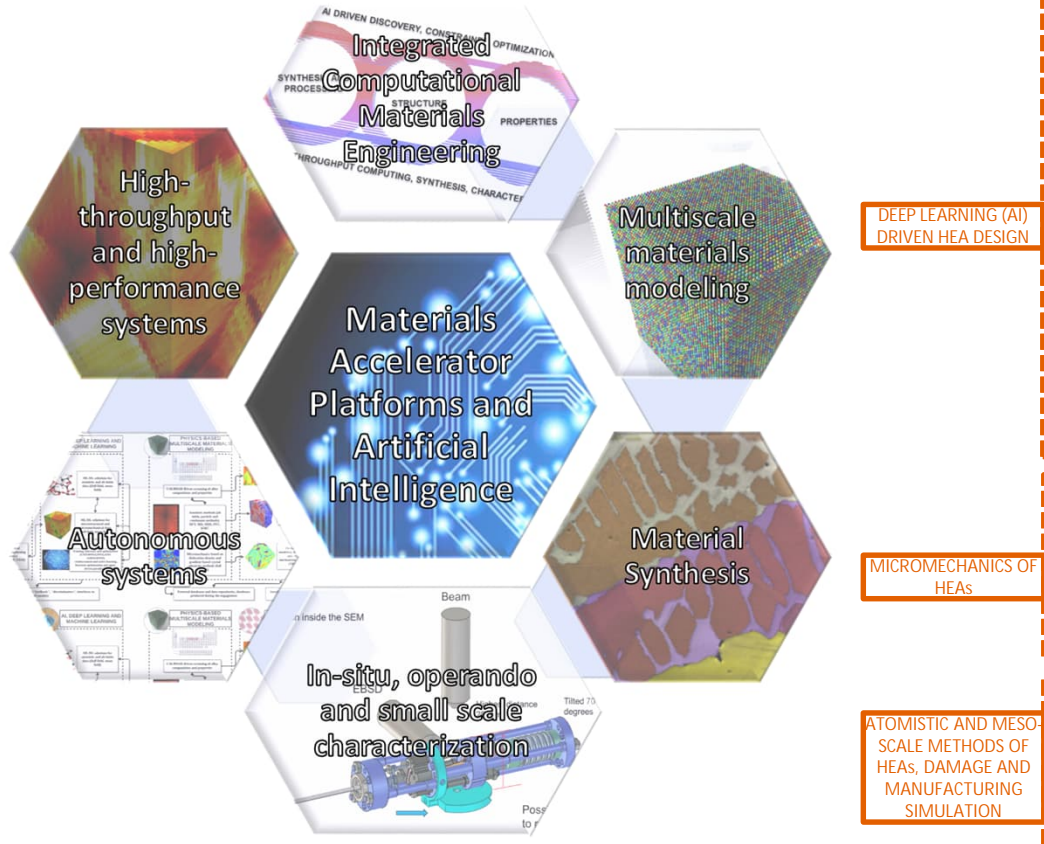
# Materials for fusion, examples and use cases

# Process-property modeling workflow

Modeling material properties and performance based on integration to alloy design, processing and manufacturing models



# Activities overall tie in and develop Materials Accelerator Platform related concepts for fusion materials to digitalize and accelerate innovation – for example, materials modeling and design of CCAs/HEAs



Examples of application:

WPMAT: 1) development of high heat-flux materials (HHFMs) and solutions, 2) developing manufacturing processes (casting, forging, heat treatments, ...) while improving material properties (mechanical, electrical etc.)

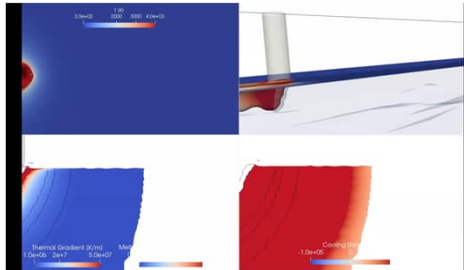
WPPRD: 1) novel HHFMs – W, W-alloys, refractory high entropy alloys, 2) development of printable tungsten (alloys) and additive manufacturing processes for tungsten

IREMEV: deformation and fracture mechanisms of irradiated tungsten and fusion materials in general

WPMAG: insulation materials and modeling of performance criticalities by way of multiscale methods

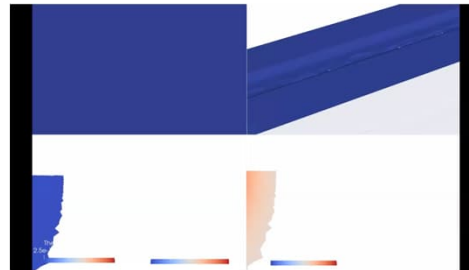
# Example: WPPRD – Prospective R&D / Tungsten and RHEAs, beam shaping for manufacturability

Gaussian Profile



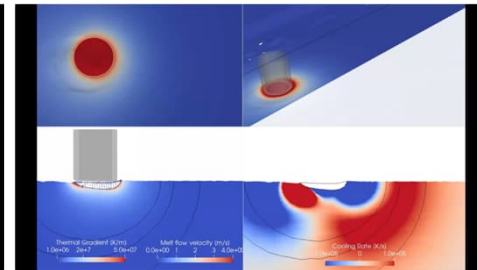
Gaussian beam drills a narrow and deeper hole

Double-ring Profile



Double-ring beam leads to a wider and stable "indentation"

Double-ring Wobbling Profile

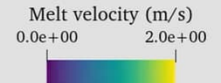
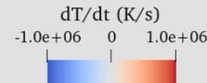
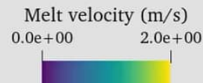
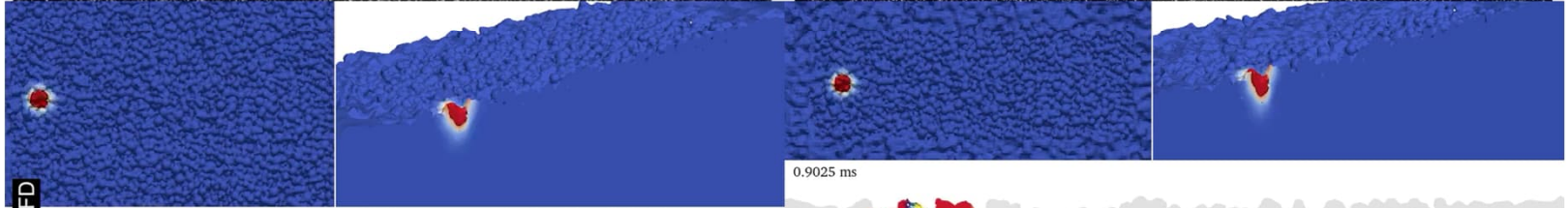
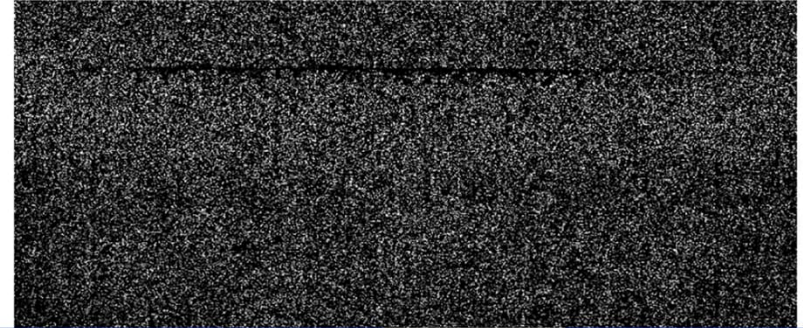
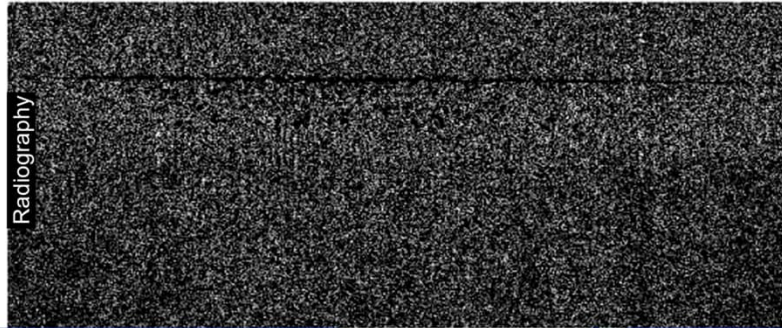


Double-ring Wobbling Profile leads to a much wider and more stable "indentation"

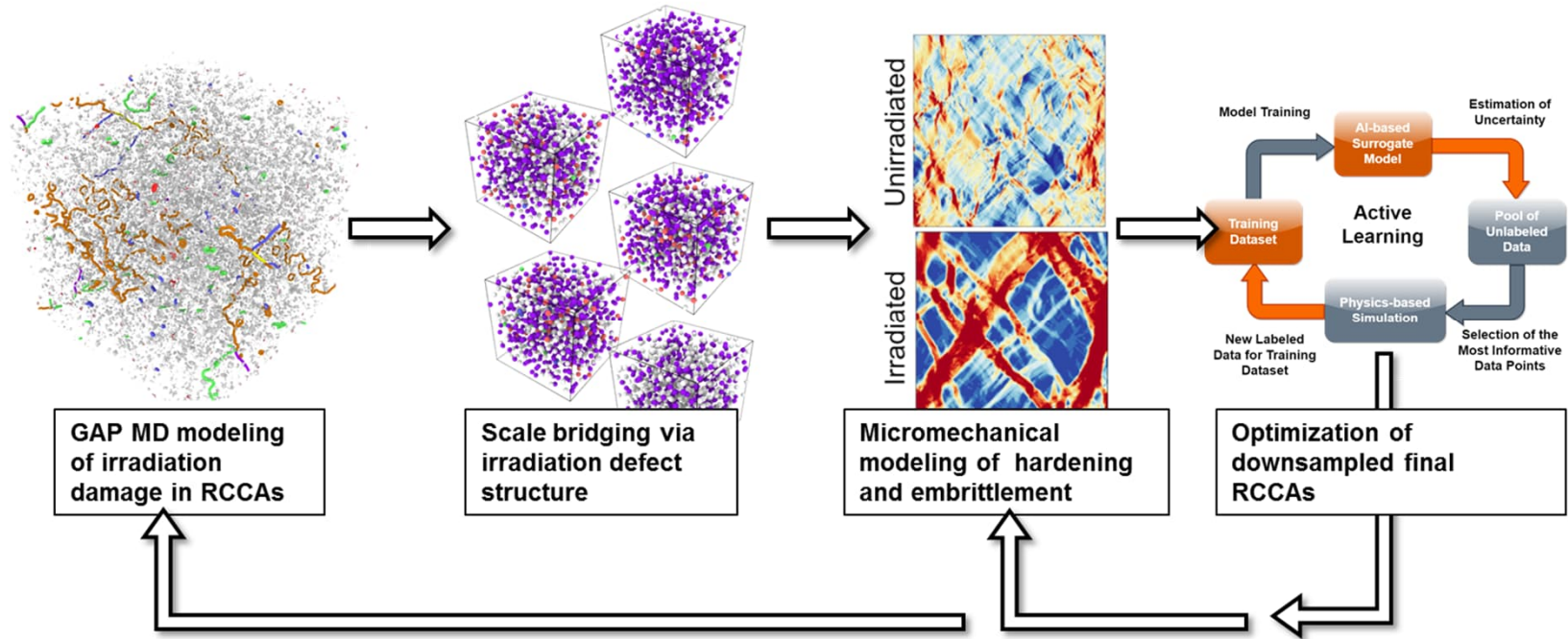
# Example: WPPRD – Prospective R&D / Tungsten and RHEAs, beam shaping for manufacturability

Laser speed 0.3 m/s  
 $t = 0.82$  ms

Laser speed 1.0 m/s  
 $t = 0.82$  ms



# Example: ENR – enabling research, novel irradiation resistant and ductile refractory complex concentrated alloys (RCCAs)



# Example: IREMEV – Modeling programme / crystal plasticity fundamentals, non-irradiated vs. heavily irradiated

Principal behavior of unirradiated reference vs. heavily irradiated microstructure: von Mises stress, 1<sup>st</sup> principal stress, cumulative plastic slip, SSD density, GND density

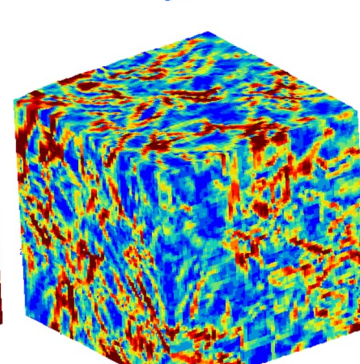
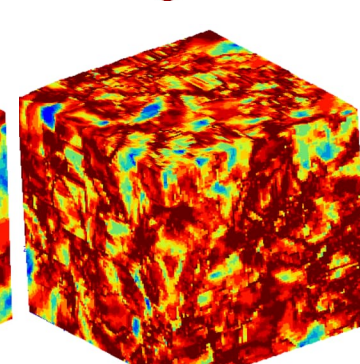
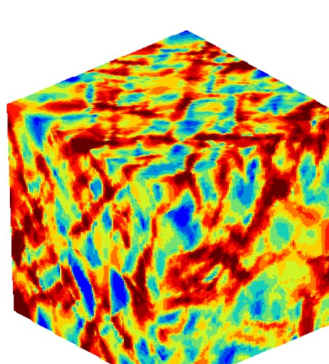
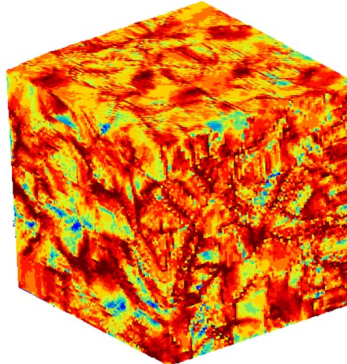
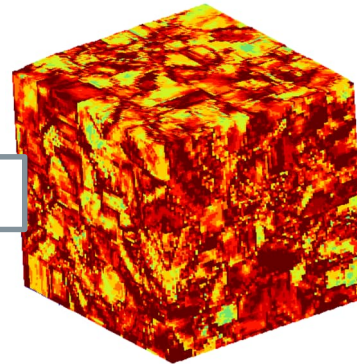
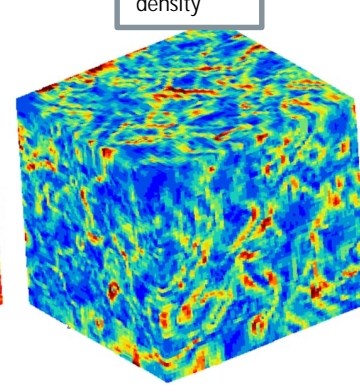
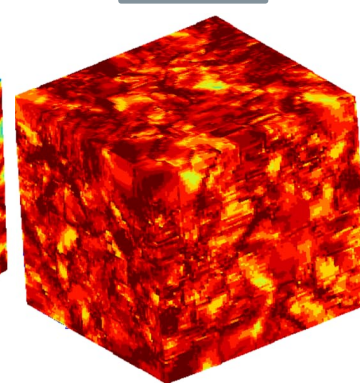
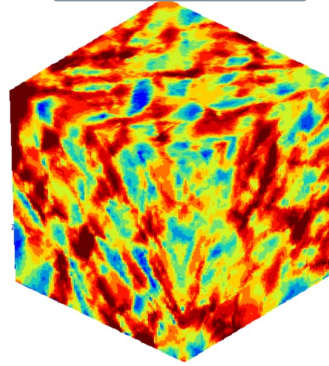
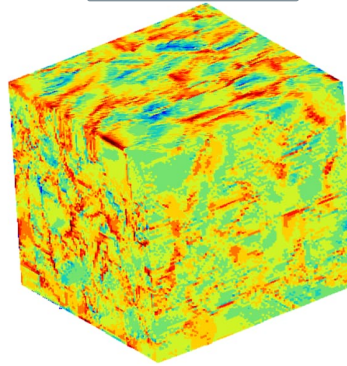
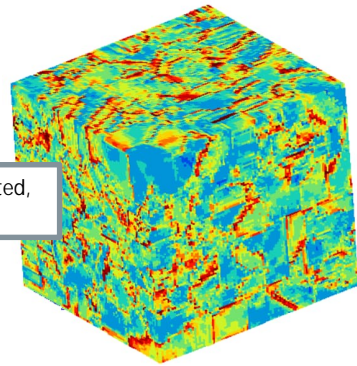
von Mises stress

1st principal stress

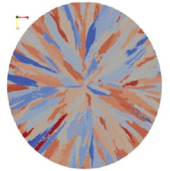
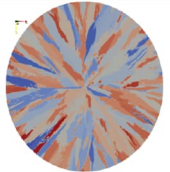
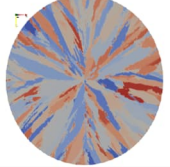
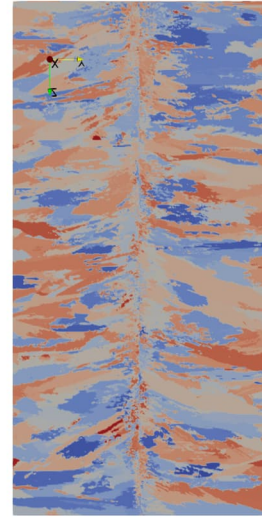
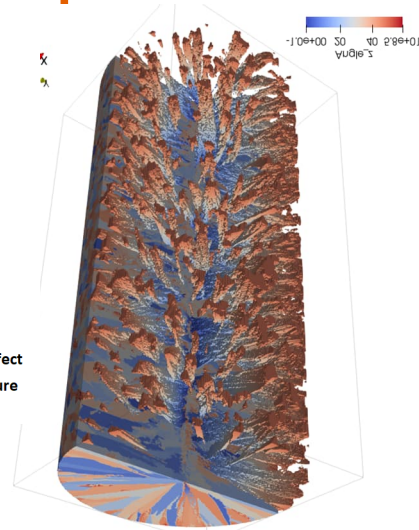
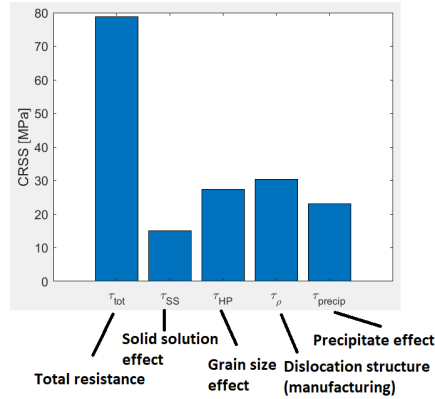
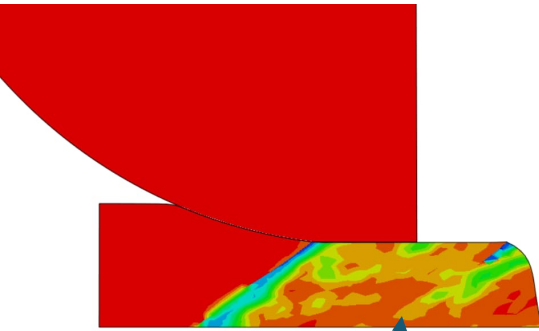
Cumulative plastic slip

SSD density

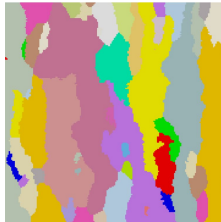
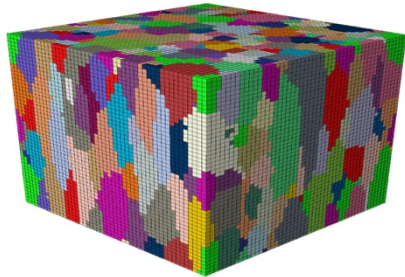
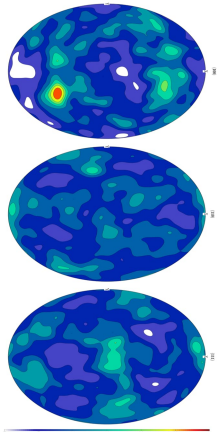
GND density



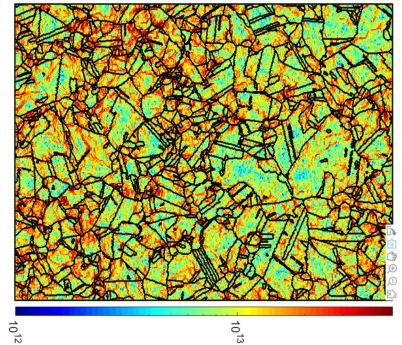
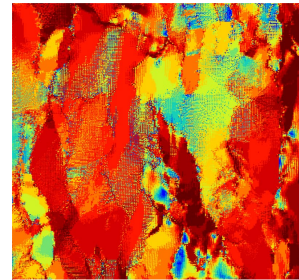
# Example: WPMAT – Materials/ Novel copper alloys, manufacturing technologies and properties



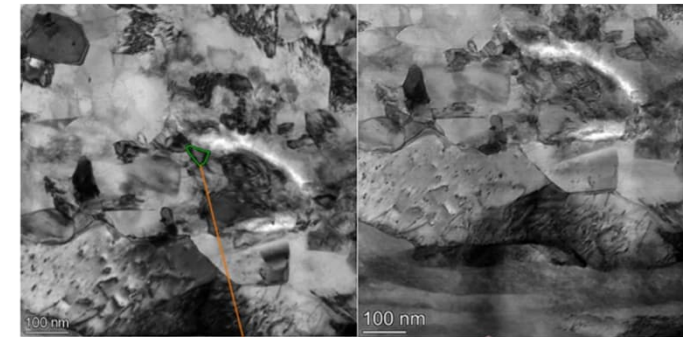
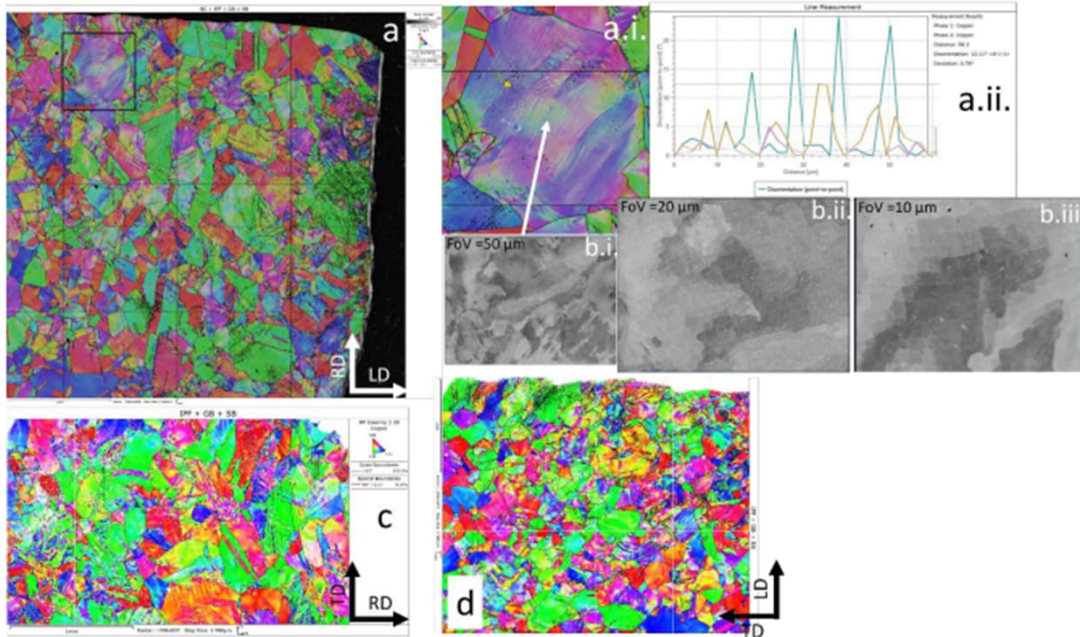
Grain structure heterogeneities



Reconstruction of grain structure

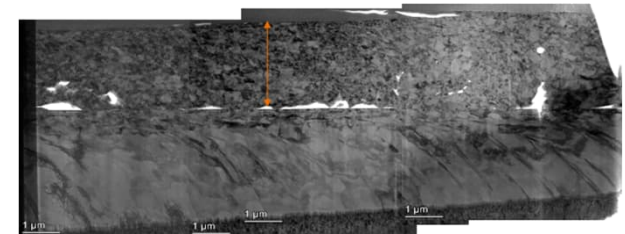


# Example: WPMAT – Materials/ Novel copper alloys, manufacturing technologies and properties



Dislocation density  
=  $3.02 \times 10^{15} \text{ m}^{-2}$

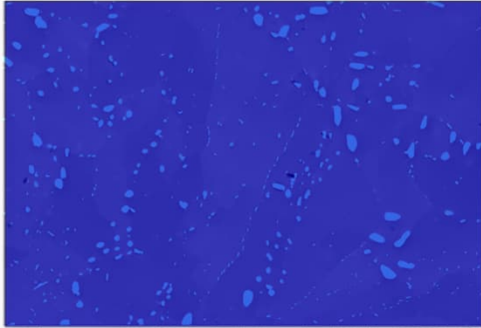
Dislocation density  
=  $1.18 \times 10^{15} \text{ m}^{-2}$



Microstructure evolution during loading have been studied with TEM and SEM-EBSD techniques. Focus has been put for understanding the material reorientation and grain size evolution

# Example: WPMAT – Materials/ Novel copper alloys, manufacturing technologies and properties

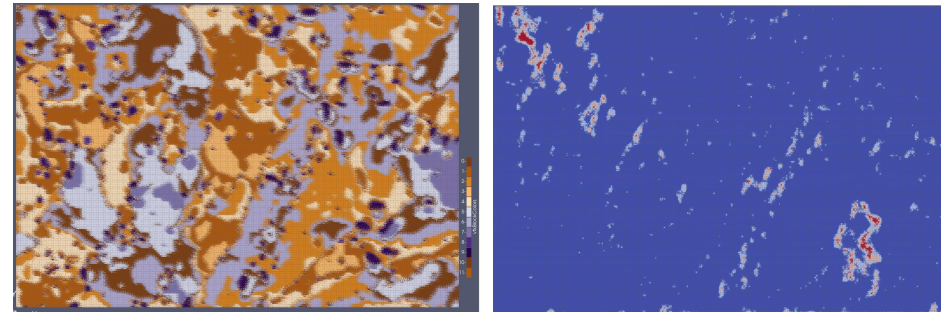
Step: Zpost Frame: 0  
Total Time: 1.181882



Crystalline damage (e.g. RPVsteels / EUROFER) with carbides

## Ductile fracture (CuCrZr)

Step: Zpost Frame: 0  
Total Time: 2.079890



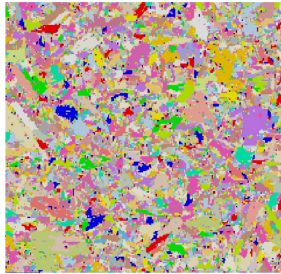
Phase field fracture (for all materials)  
brittle / (semi-)ductile

Peridynamics fracture including  
precipitates or defects etc

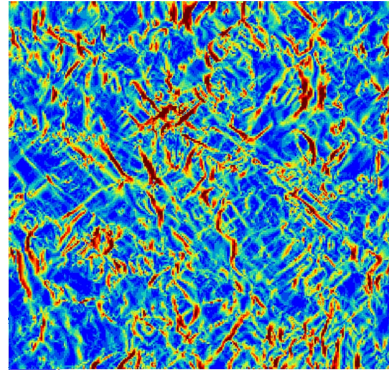
# Example: EEG – Engineering programme, micromechanics based integrity assessment of irradiated structural components

Differences in plastic deformation behavior and localization as expressed by the GND dislocation density

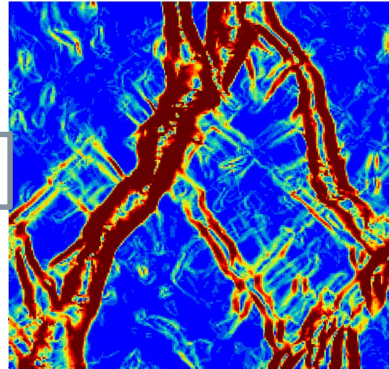
2D EBSD based model (EUROFER)



Unirradiated, reference

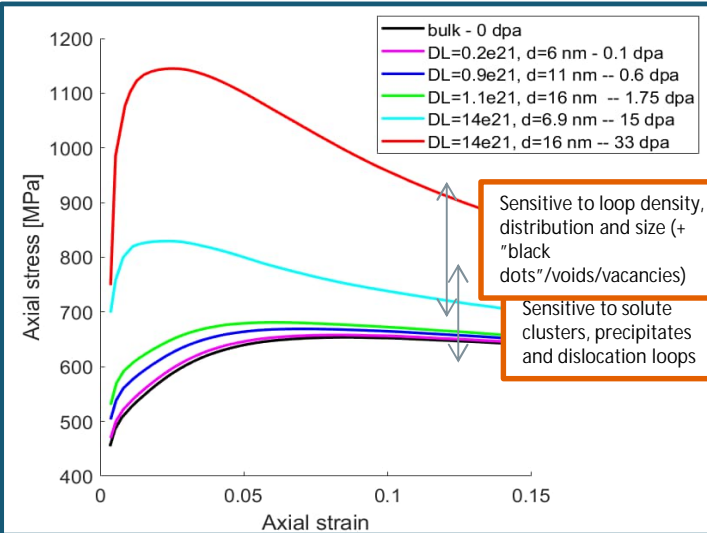


Irradiated 13 dpa



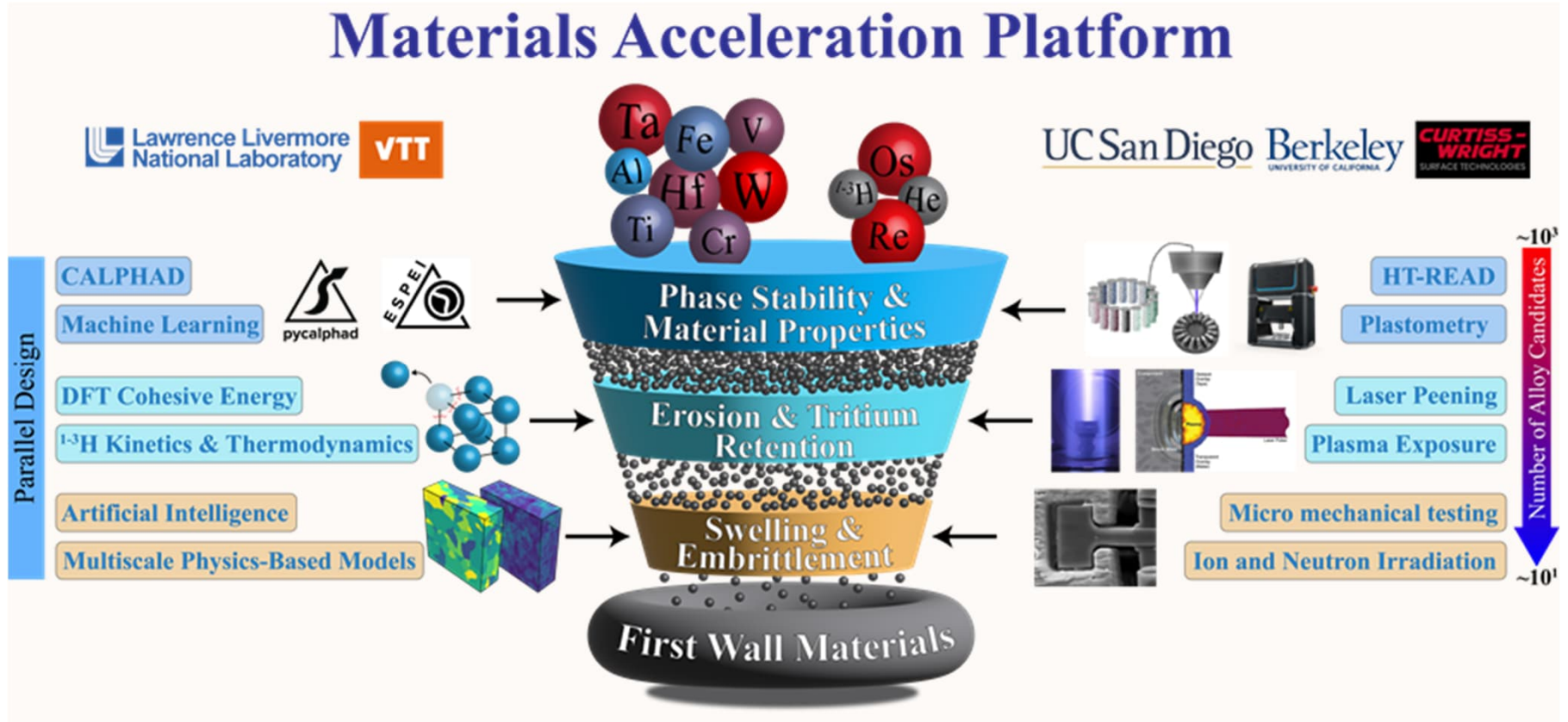
GND density

Engineering stress-strain calculations with the EBSD model as a function of dose and sensitivity analyses for different input property datasets



# Example: Arpa-E – First wall materials Material Acceleration Platform (MAP)

## Materials Acceleration Platform



# bey<sup>0</sup>nd

## the obvious

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