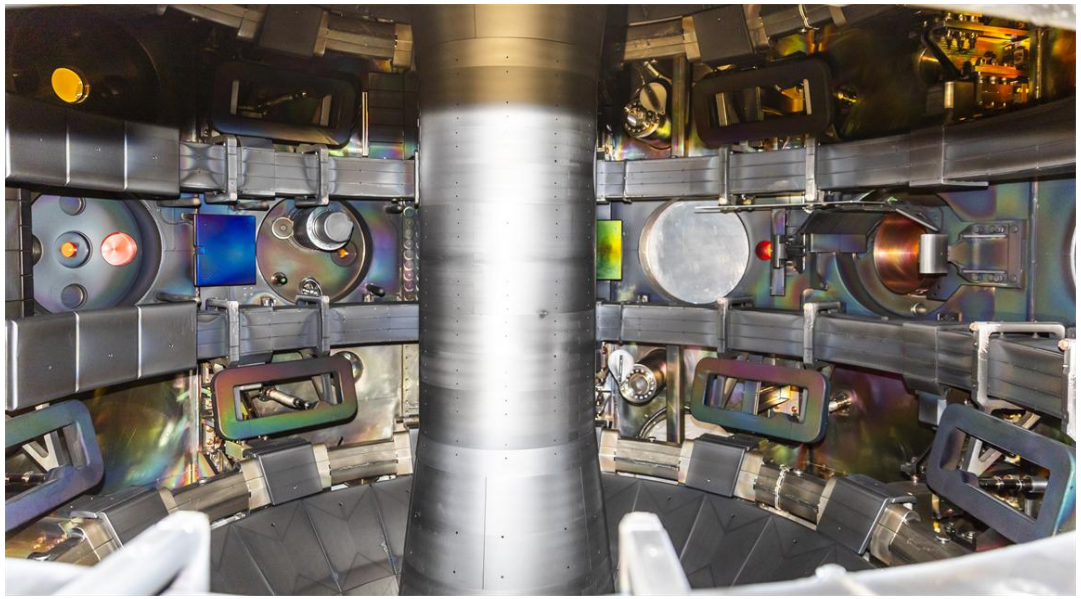
Multiscale models for materials *and* DONES: microstructural observables, environmental conditions, and interpretation of observations

S. L. Dudarev

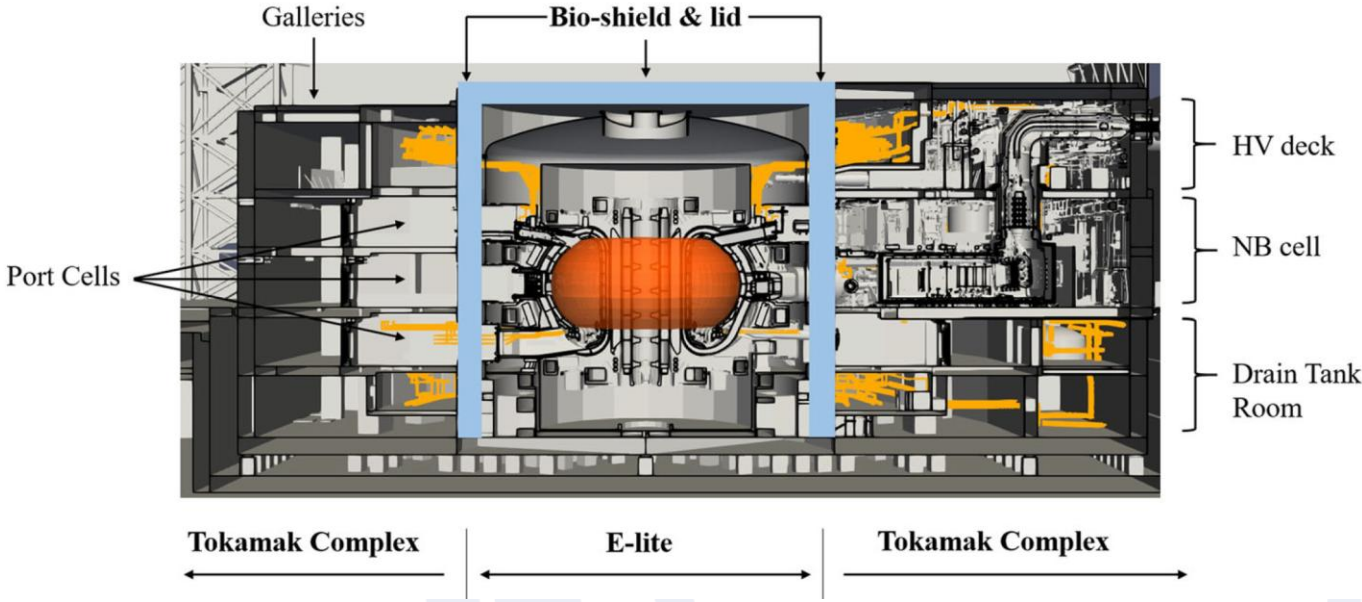
UK Atomic Energy Authority, Culham Campus,
Oxfordshire OX14 3DB, UK

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Objectives: modelling and observation



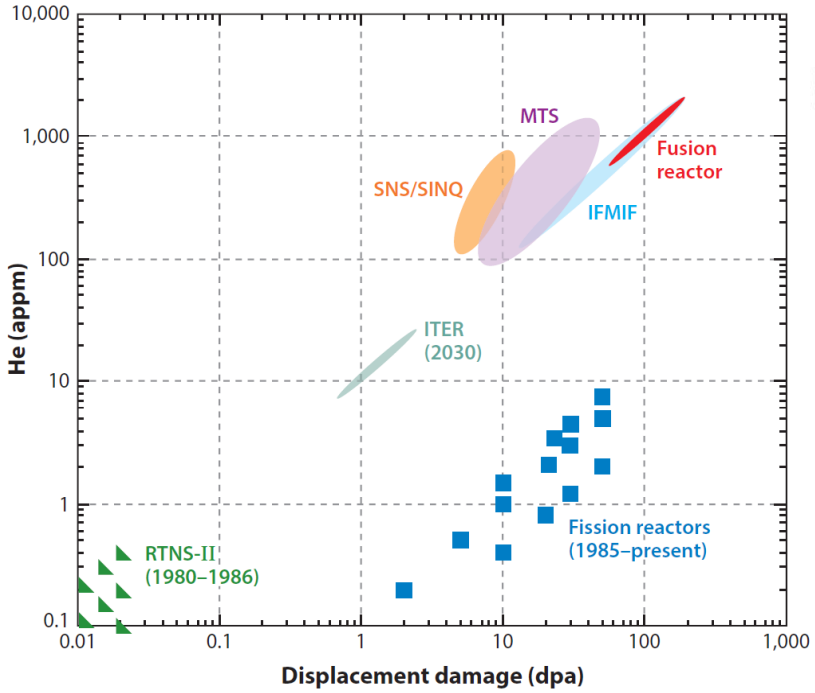
Interior view of MAST-U tokamak at UKAEA, August 2026



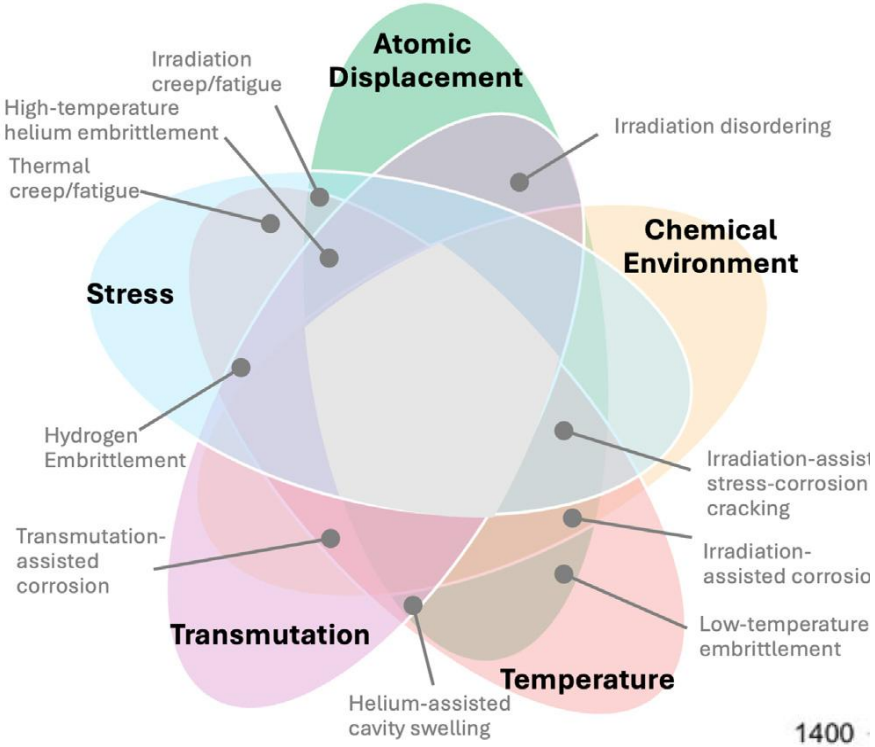
R. Juarez *et al.*, Nature Communications **15** (2024) 8563

- Present generation of fusion devices explore plasma performance. D-T experiments are still rare, with neutron fluence in the ~10^{-5} dpa range (cf. ~10^{-2} dpa for fission pressure vessel and ~10 dpa for fuel cladding).
- Complexity of a fusion device is greater than that of a fission reactor.
- Engineering data on materials performance under high neutron exposure are still scarce – and the central question about ***what to test*** has not yet been answered definitively.

Operating conditions for structural materials

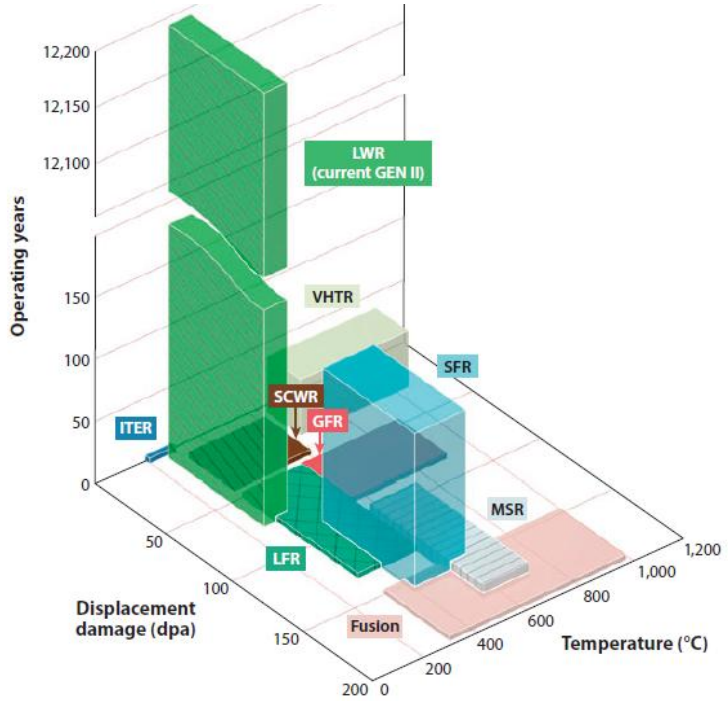


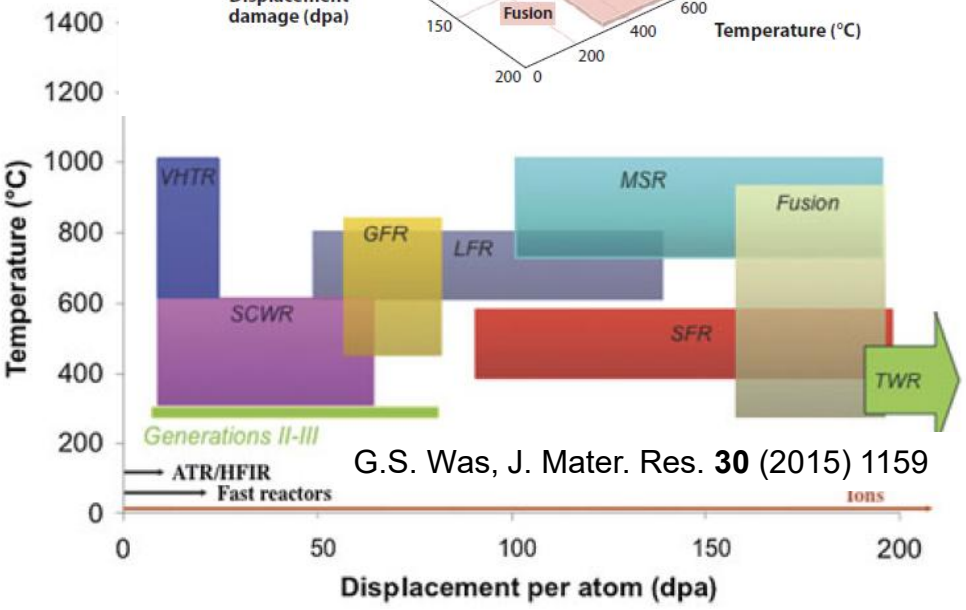
S.J. Zinkle and L.L. Snead, Annu. Rev. Mater. Res. **44** (2014) 241–67



S.E. Ferry *et al.*, Current Opinion in Solid State and Materials Science **43** (2026) 101291

S.J. Zinkle and L.L. Snead, Annu. Rev. Mater. Res. **44** (2014) 241–67

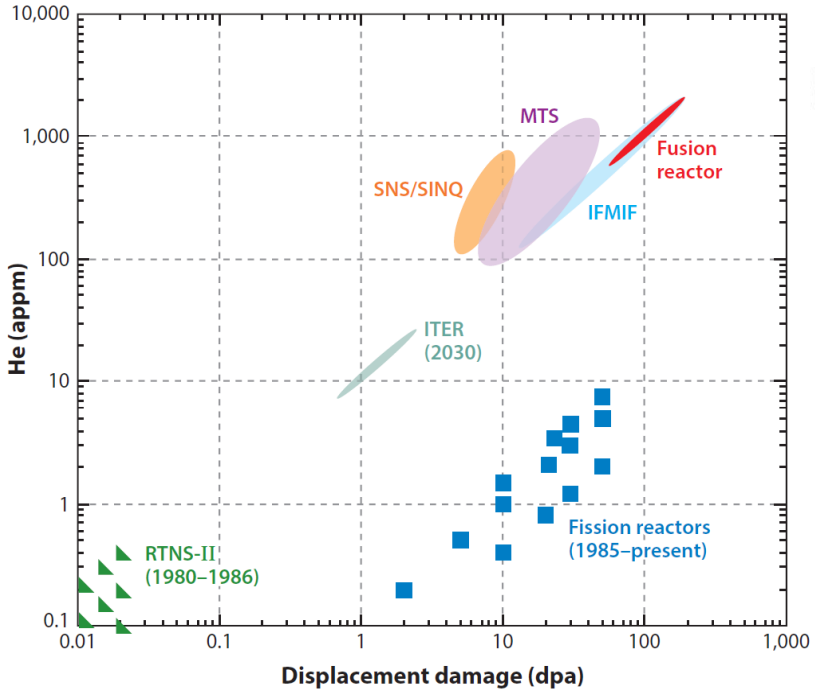


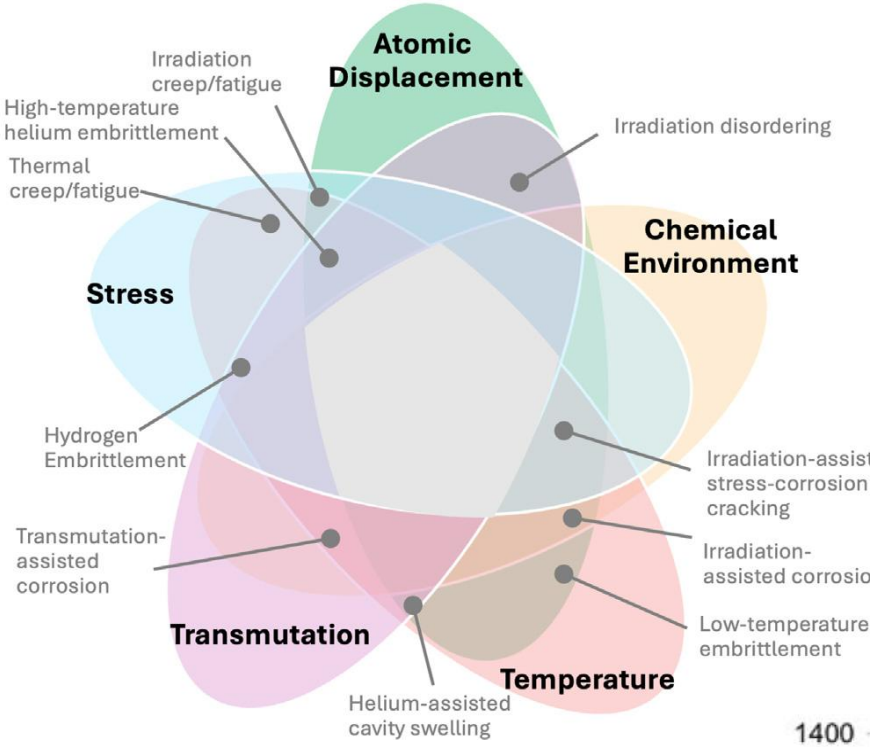


G.S. Was, J. Mater. Res. **30** (2015) 1159

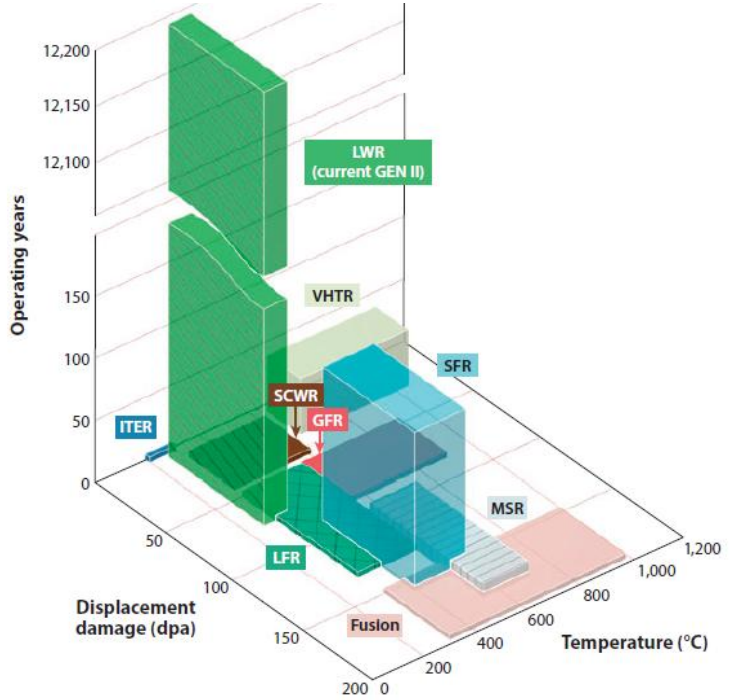
How to define the operating conditions for materials in a fusion device?

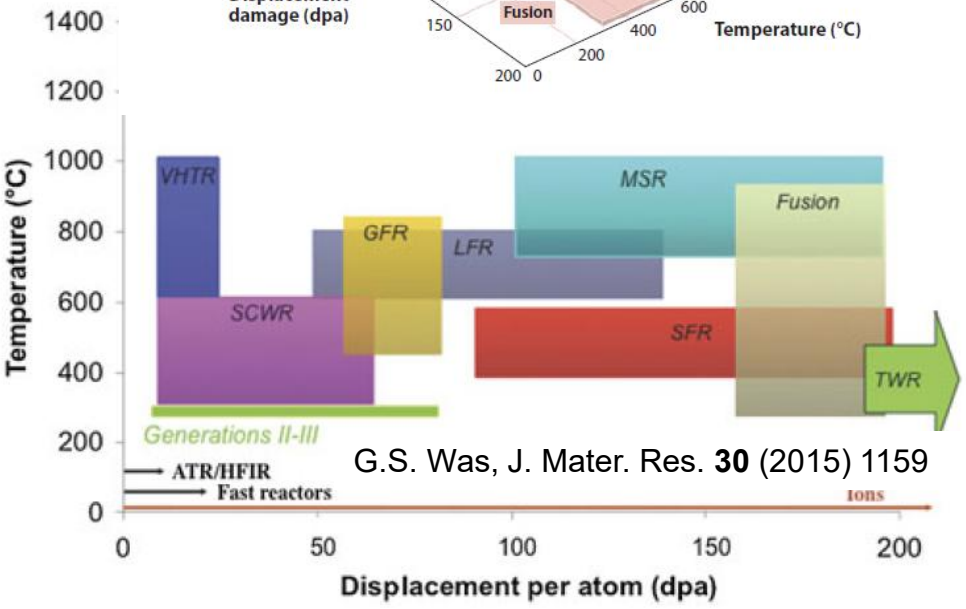
Operating conditions for structural materials





S.J. Zinkle and L.L. Snead, Annu. Rev. Mater. Res. **44** (2014) 241–67





G.S. Was, J. Mater. Res. **30** (2015) 1159

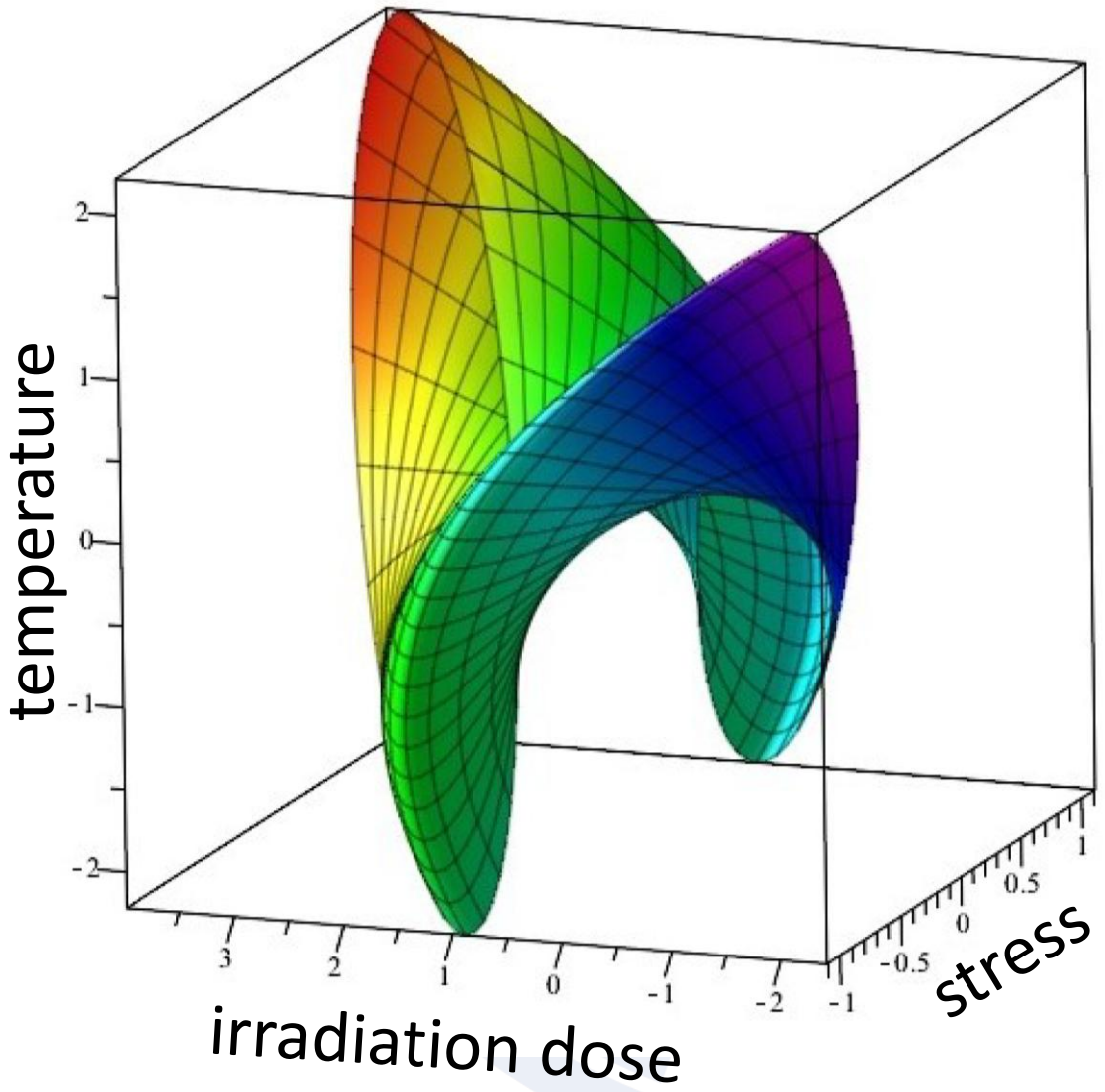
Analysis assumes steady state operation; neglects fast time-dependent transients.

Assessments are sketchy; order of priorities is hard to define.

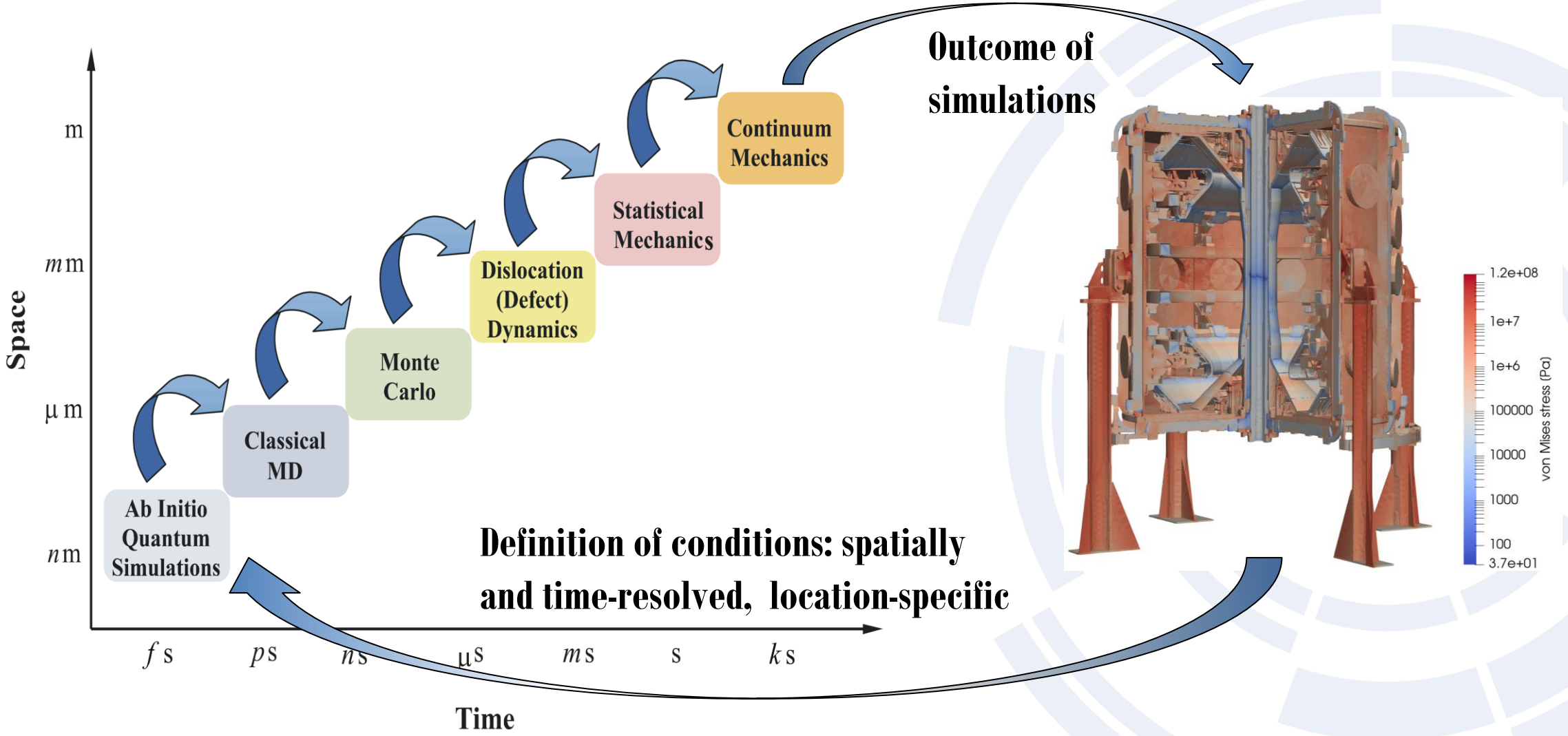
1960s design vs modern data analysis

1. Construct and test
2. Think
3. Improve and refine

- Various factors hard to evaluate before a full device is constructed and tested.
- Parameter space with many variables, hard to explore uniformly
- Functional materials, HTS, electrical insulation etc.
- Multi-dimensional optimization as a part of planning the programme of tests.

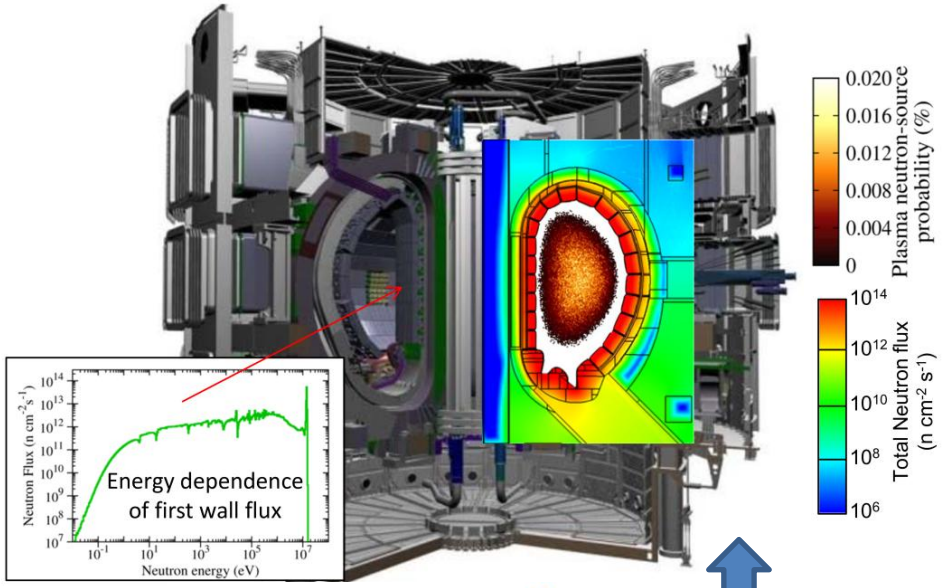


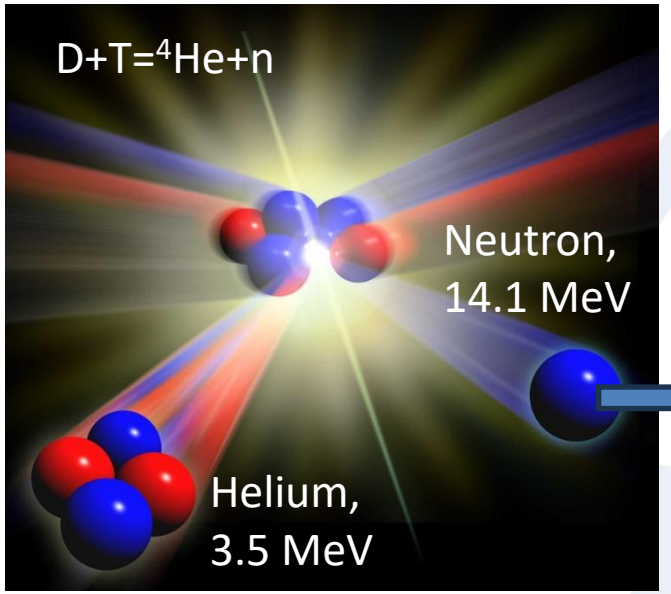
How to optimize? A self-consistent simulation:

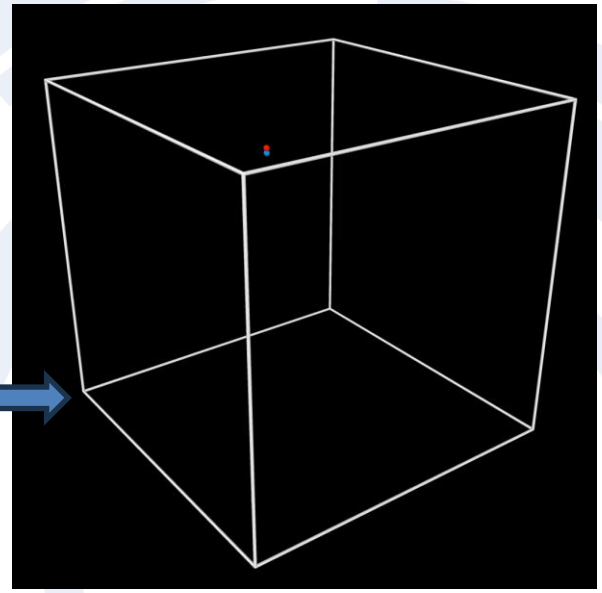


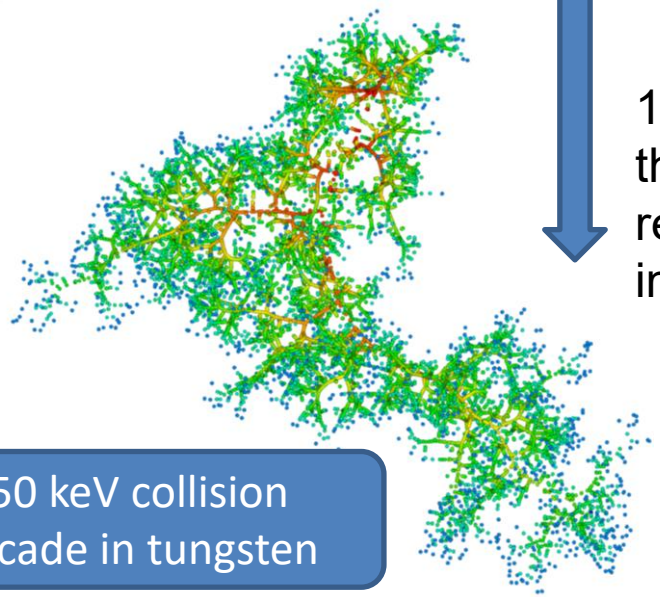
To define the spectrum of operating conditions, one needs to perform a self-consistent full device simulation. The simulation also defines the content of microscopic models required to perform it.

Can a full device simulation be realised?









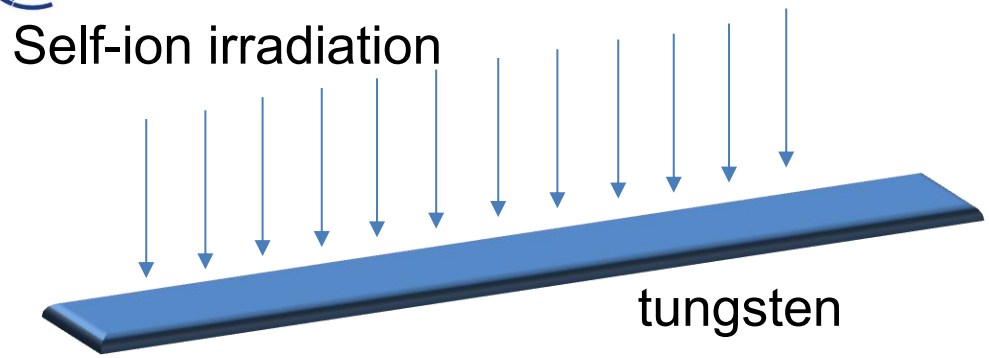
150 keV collision cascade in tungsten

10^9 difference between the length scales of a reactor and a neutron impact cascade event

1. The gap between the length and time scales is so large that the problem appears intractable. Data transfer, through a hierarchy of multiscale models, is not a practical solution.
2. Experimental information is too limited to provide the required input to Finite Element Models.

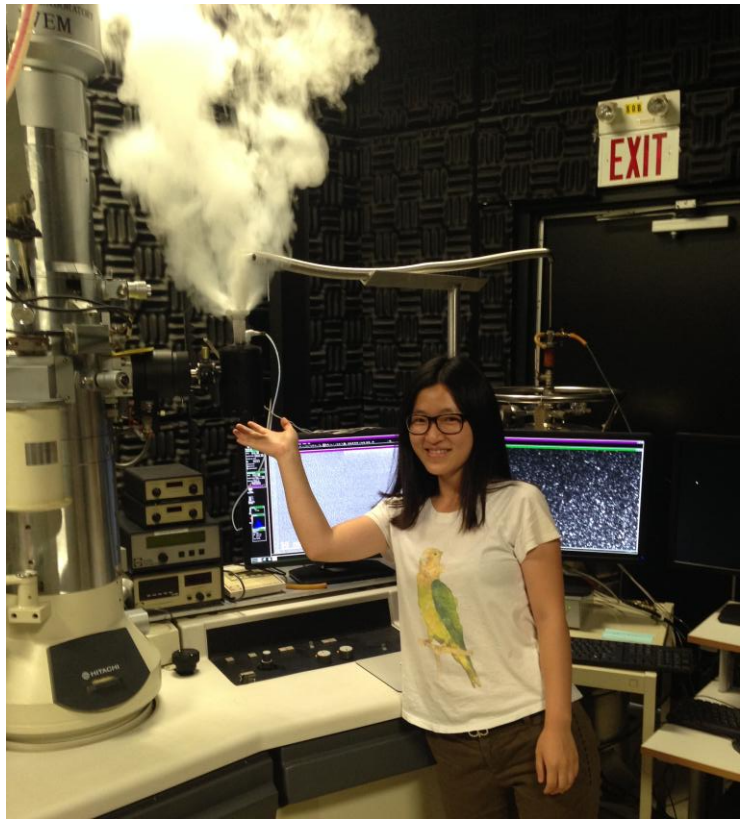
A. E. Sand *et al.*, EPL, **103** (2013) 46003

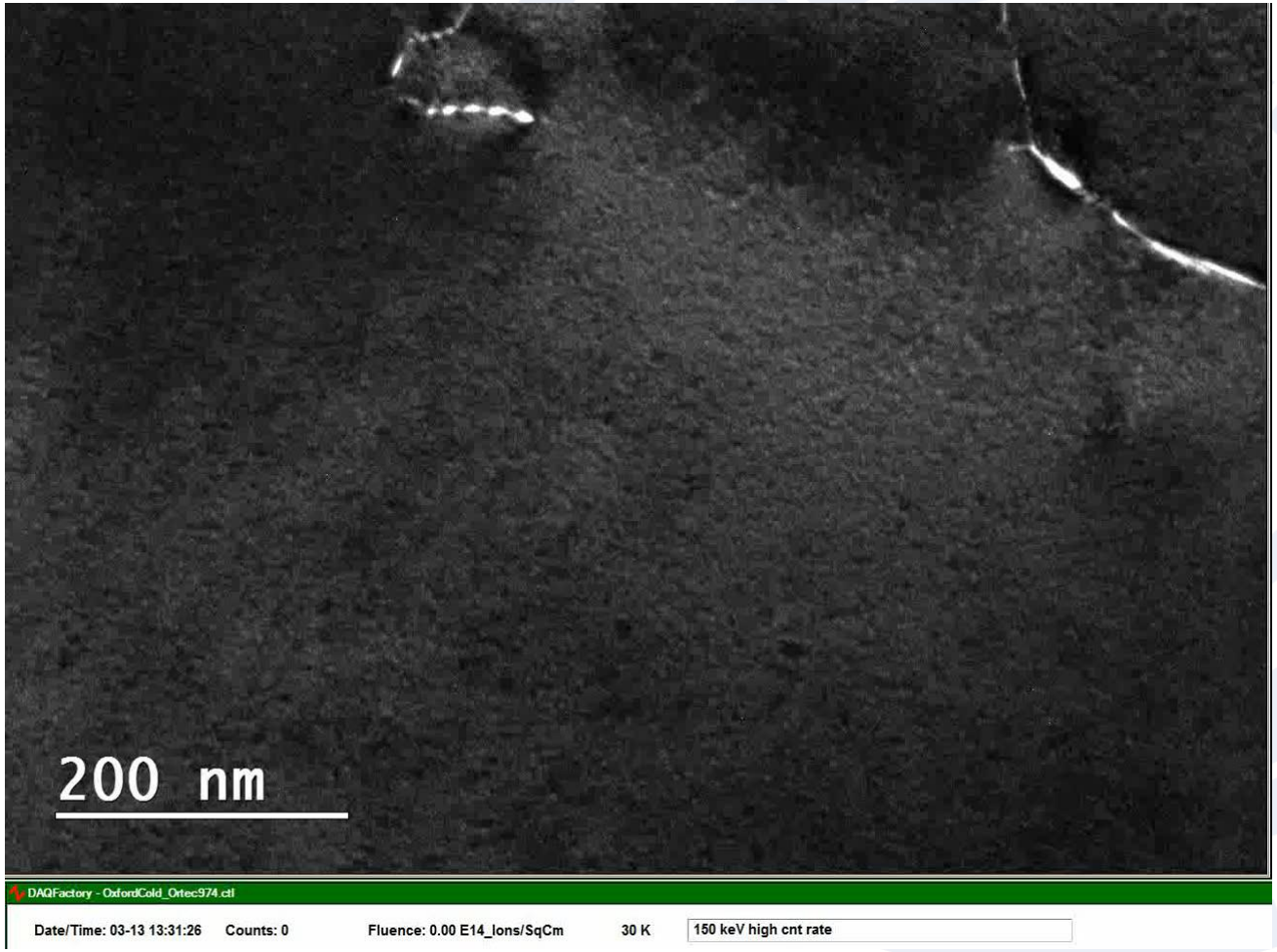
Exposure of materials to impacts of microscopic particles



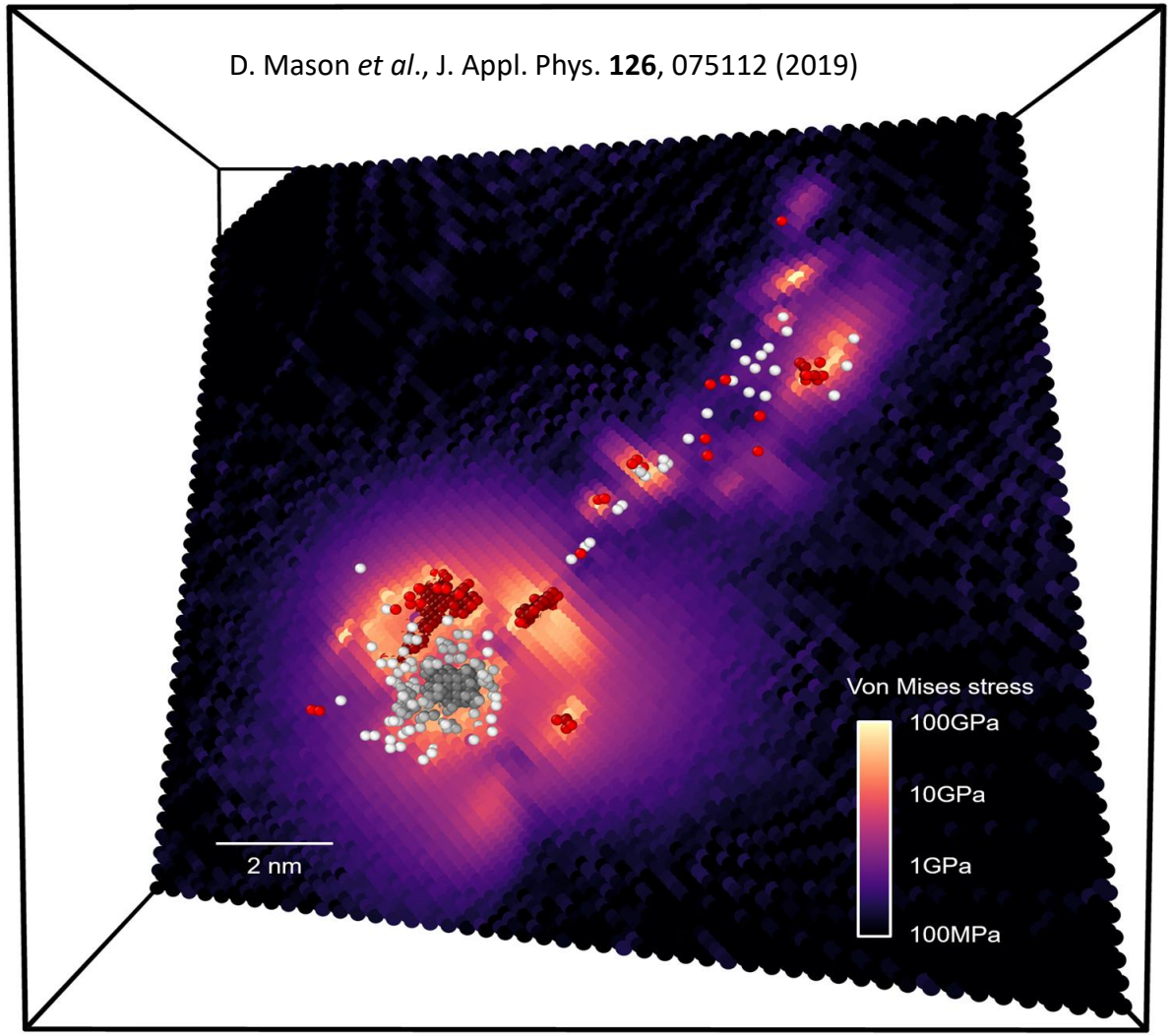
X. Yi *et al.*, EPL **110**, 36001 (2015)

In situ transmission electron microscope observation of pure tungsten bombarded by 150 keV W+ ions at 30K.





Stress produced by a neutron collision cascade event



Stress field generated by the defects formed in a collision cascade in tungsten.

Defects as sources of stress and strain

The *relaxation volume tensor* is the change of the volume enclosed by the external surface of a crystal, caused by a source of strain inside it.

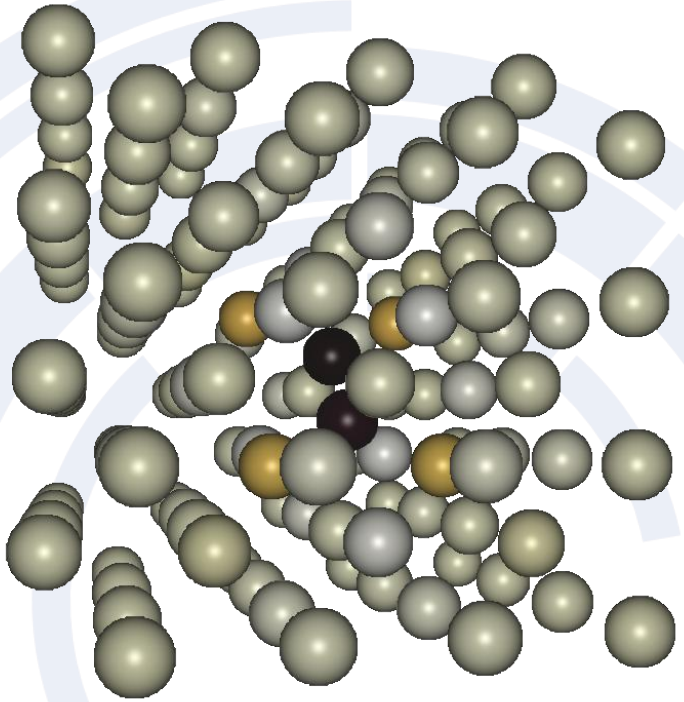
$$\Omega_{ij} = \frac{1}{2}\int_S [u_i(\mathbf{x})n_j(\mathbf{x}) + u_j(\mathbf{x})n_i(\mathbf{x})]dS.$$

From the divergence theorem, this equals the integral of the total strain over the volume of the crystal (the shape is arbitrary)

$$\Omega_{ij} = \int_V \varepsilon_{ij}(\mathbf{x})\, d^3x$$

Relaxation volume tensor of a defect = (volume of the body) × (average strain). The relaxation volume of a defect (a scalar) is the sum of diagonal elements of the relaxation volume tensor.

$$\Omega = \mathrm{Tr}(\mathbf{\Omega}) = \Omega_{ii}$$



M. Boleininger *et al.*, Phys. Rev. Materials **6** (2022) 063601
T. Mura, *Micromechanics of defects in solids* (Kluwer, 1991)

Lattice distortions due to defects: *ab initio* analysis

TABLE XXIV. Elements of the dipole tensor P_{ij} (in eV units), the relaxation volume tensor Ω_{ij} (in Å^3 units), eigenvalues of the relaxation volume tensor $\Omega^{(i)}$ (in Å^3 units), and the relaxation volume of the defect Ω_{rel} (in atomic volume units Ω_0) computed for Fe.

Fe	P_{11}	P_{22}	P_{33}	P_{12}	P_{23}	P_{31}	Ω_{11}	Ω_{22}	Ω_{33}	Ω_{12}	Ω_{23}	Ω_{31}	$\Omega^{(1)}$	$\Omega^{(2)}$	$\Omega^{(3)}$	Ω_{rel}
⟨111⟩d	23.465	23.465	23.472	5.850	5.851	5.851	6.327	6.327	6.335	4.362	4.363	4.363	1.964	1.964	15.051	1.673
⟨111⟩c	23.186	23.186	23.193	5.903	5.904	5.904	6.252	6.252	6.259	4.402	4.402	4.402	1.850	1.850	15.056	1.653
⟨110⟩d	25.832	21.143	21.150	0.000	5.122	0.000	9.777	4.294	4.302	0.000	3.819	0.000	9.777	0.475	8.122	1.620
Tetra	21.396	23.331	23.339	0.000	0.001	0.000	4.607	6.871	6.880	0.000	0.000	0.000	4.607	6.871	6.880	1.619
⟨100⟩d	32.284	22.931	22.937	0.000	0.000	0.000	14.316	3.378	3.385	0.000	0.000	0.000	14.316	3.378	3.385	1.858
Octa	23.273	23.273	31.302	0.000	0.000	0.000	3.869	3.869	13.258	0.000	0.000	0.000	3.869	3.869	13.258	1.851
Vac	−3.081	−3.081	−3.081	0.000	0.000	0.000	−0.831	−0.831	−0.831	0.000	0.000	0.000	−0.831	−0.831	−0.831	−0.220

A self-interstitial defect in iron expands the material by 1.62 atomic volumes.

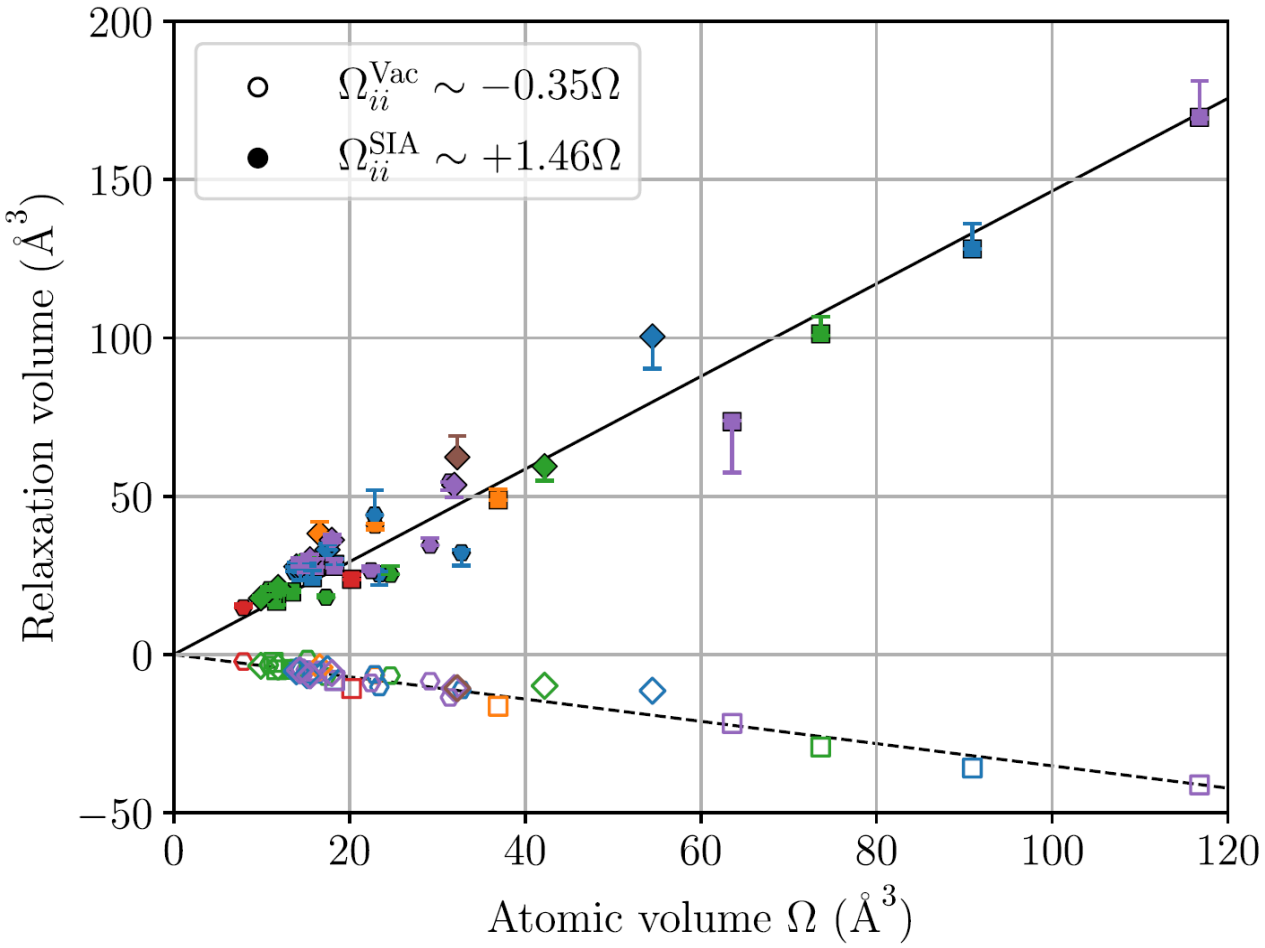
TABLE XX. Elements of the dipole tensor P_{ij} (in eV units), the relaxation volume tensor Ω_{ij} (in Å^3 units), eigenvalues of the relaxation volume tensor $\Omega^{(i)}$ (in Å^3 units), and the relaxation volume of the defect Ω_{rel} (in atomic volume units Ω_0) computed for W.

W	P_{11}	P_{22}	P_{33}	P_{12}	P_{23}	P_{31}	Ω_{11}	Ω_{22}	Ω_{33}	Ω_{12}	Ω_{23}	Ω_{31}	$\Omega^{(1)}$	$\Omega^{(2)}$	$\Omega^{(3)}$	Ω_{rel}
⟨111⟩d	52.754	52.754	52.754	13.128	13.128	13.128	9.209	9.209	9.209	7.402	7.402	7.402	1.808	1.808	24.012	1.712
⟨111⟩c	52.745	52.745	52.745	13.151	13.151	13.151	9.207	9.207	9.207	7.414	7.414	7.414	1.793	1.793	24.036	1.711
⟨110⟩d	56.960	52.557	52.557	0.000	11.277	0.000	10.908	8.693	8.693	0.000	6.358	0.000	10.908	2.335	15.050	1.753
Tetra	47.359	59.114	59.114	0.000	0.000	0.000	5.693	11.606	11.606	0.000	0.000	0.000	5.693	11.606	11.606	1.791
⟨100⟩d	65.920	53.379	53.379	0.000	0.000	0.000	14.254	7.945	7.945	0.000	0.000	0.000	14.254	7.945	7.945	1.868
Octa	52.741	52.741	67.209	0.000	0.000	0.000	7.623	7.623	14.901	0.000	0.000	0.000	7.623	7.623	14.901	1.868
Vac	−9.984	−9.984	−9.984	0.000	0.000	0.000	−1.743	−1.743	−1.743	0.000	0.000	0.000	−1.743	−1.743	−1.743	−0.324

A vacancy in tungsten contracts the crystal by -0.324 atomic volumes.

P.-W. Ma *et al.*, Phys. Rev. Mater. **3** (2019) 013605;
P.-W. Ma *et al.*, Phys. Rev. Mater. **5** (2021) 013601

Defect relaxation volumes across the Periodic Table



Relaxation volumes of defects in metals are well correlated with atomic volumes; the total relaxation volume of a Frenkel pair is close to 1 atomic volume.

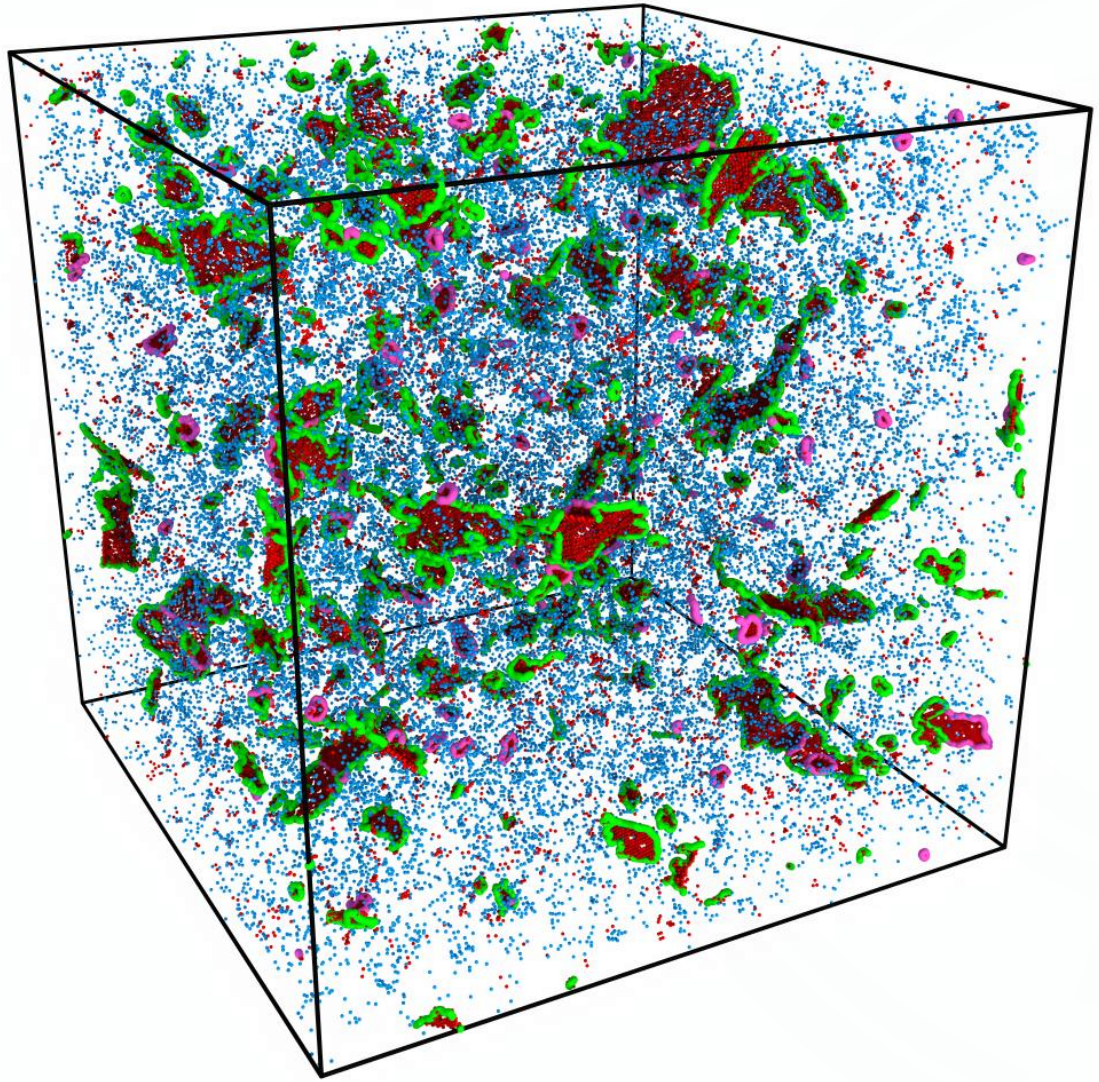
A.R. Warwick *et al.*, Phys. Rev. Mater. **9** (2025) 093605; Phys. Rev. Mater. **10** (2026) 045402

Evolution of microstructure at high irradiation dose

Blue particles are vacancies; red particles are self-interstitial defects.

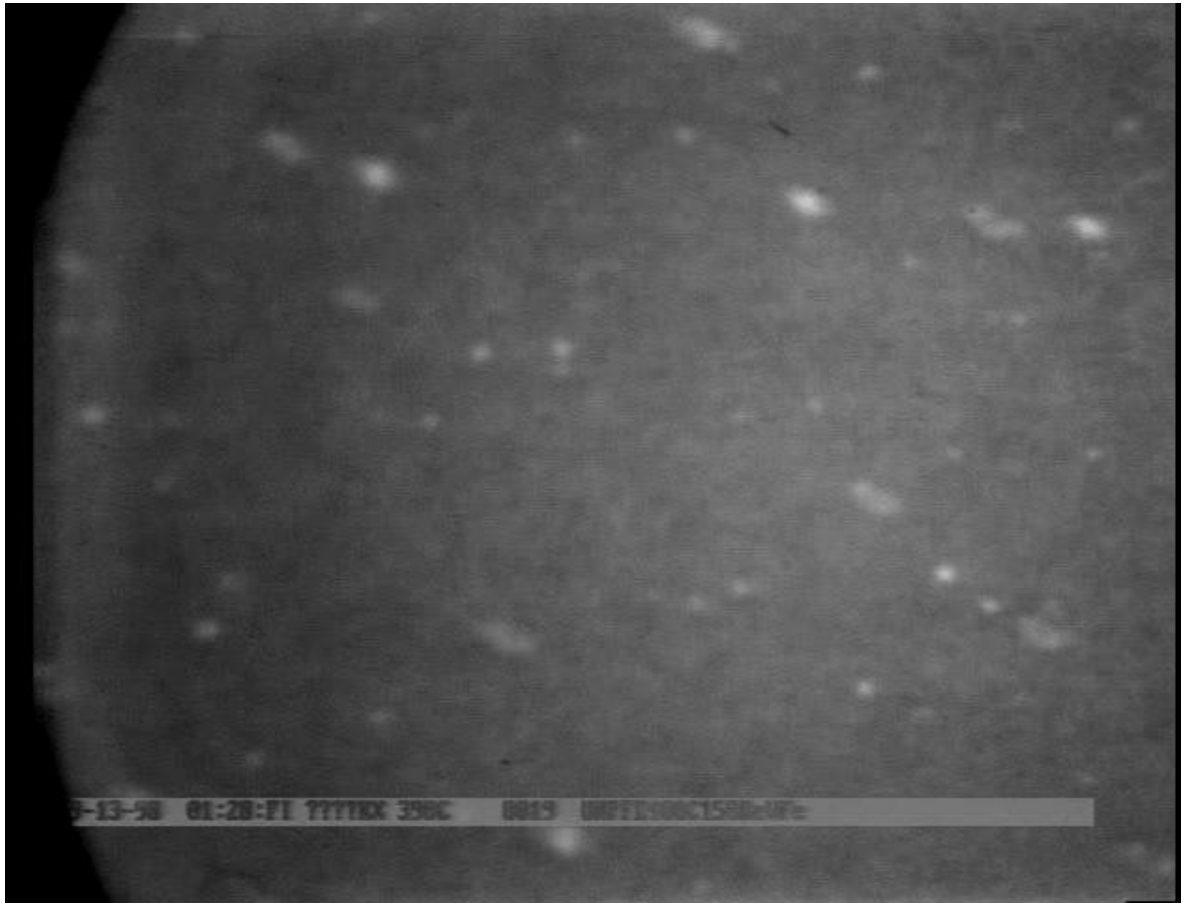
Self-interstitial defects interact and coalesce into dislocation loops.

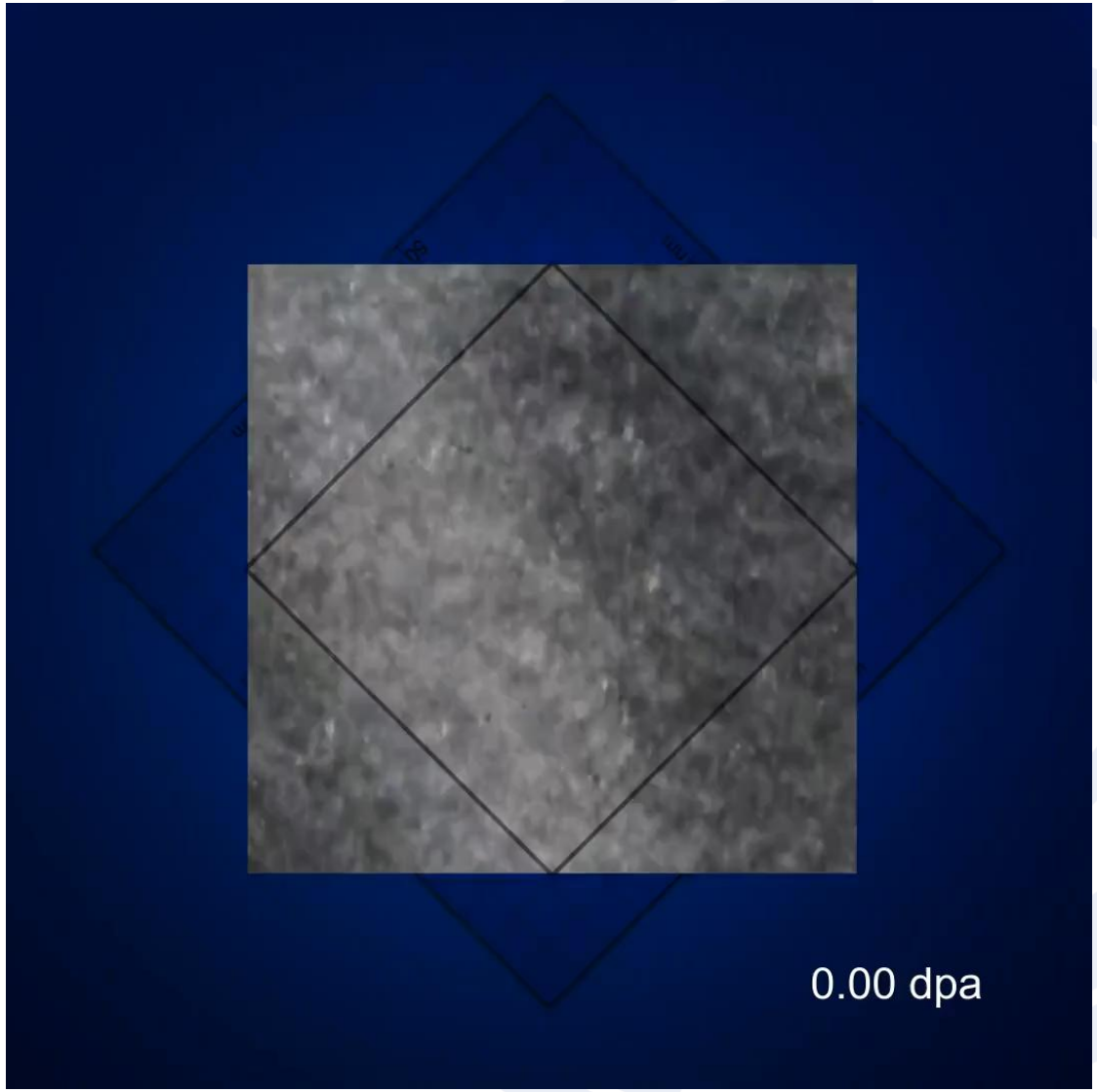
Vacancies remain dispersed in the lattice.



M. Boleininger *et al.*, Scientific Reports **13** (2023) 1684

Evolution of microstructure at high irradiation dose



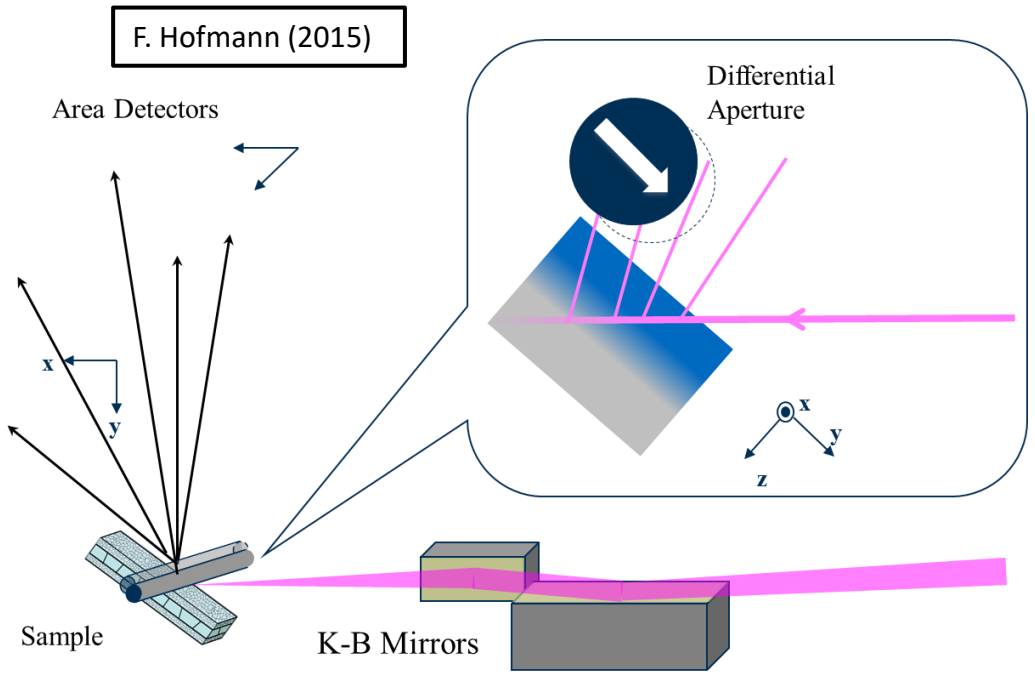


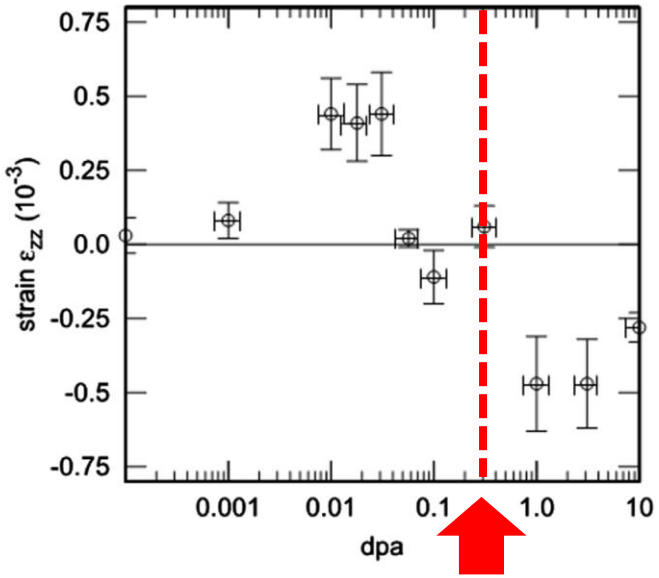
Comparison of observed and simulated transmission electron microscope visualisations of evolution of microstructure in the high dose limit.

M. Hernández-Mayoral *et al*., Philos. Mag. **88** (2008) 2881

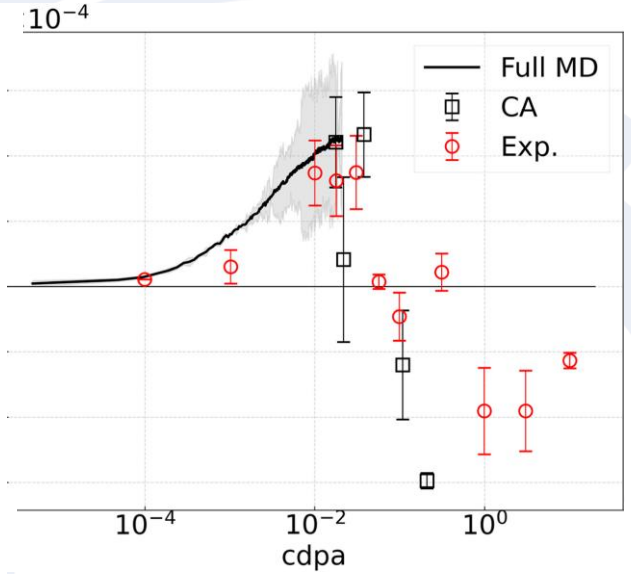
D.R. Mason *et al*., Acta Materialia **277** (2024) 120162

Negative (vacancy) lattice strain dominates at high dose

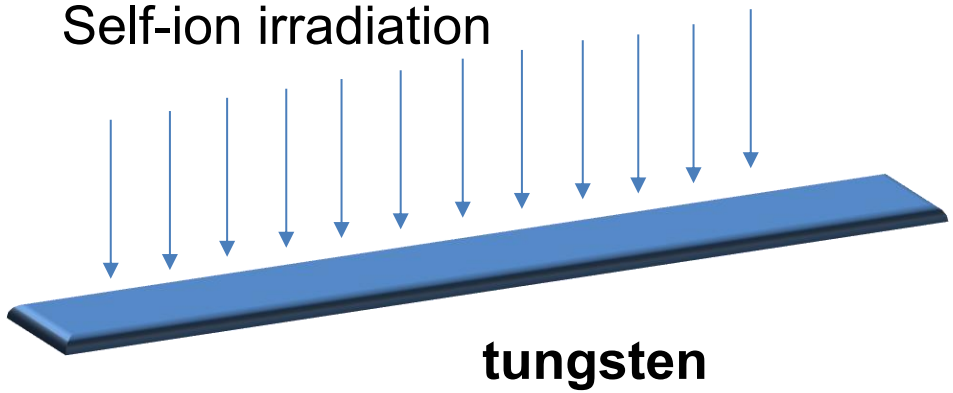




0.3 dpa



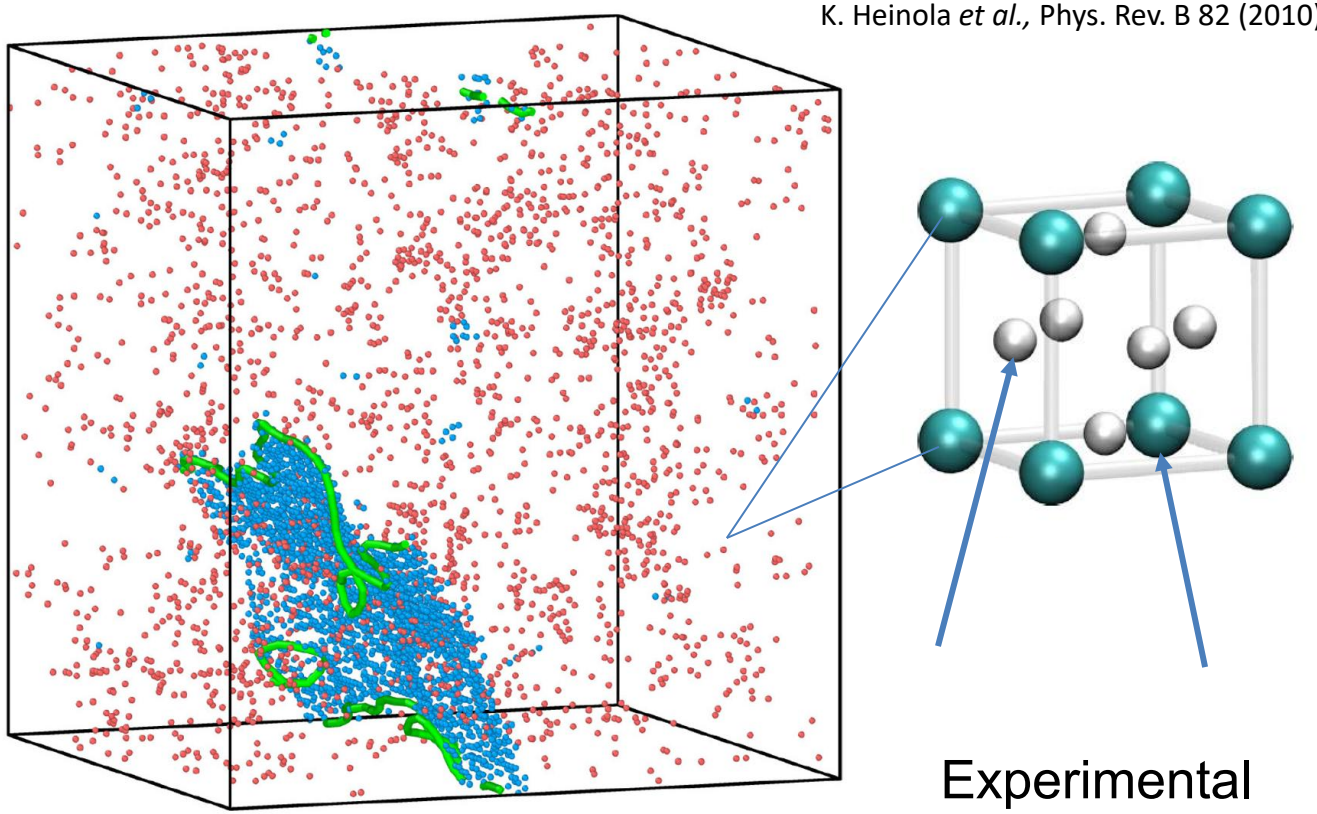
D.R. Mason *et al.,* PRL **125** (2020) 225503;
J. Wu *et al.,* Comp. Mat. Sci. 251 (2025) 113738



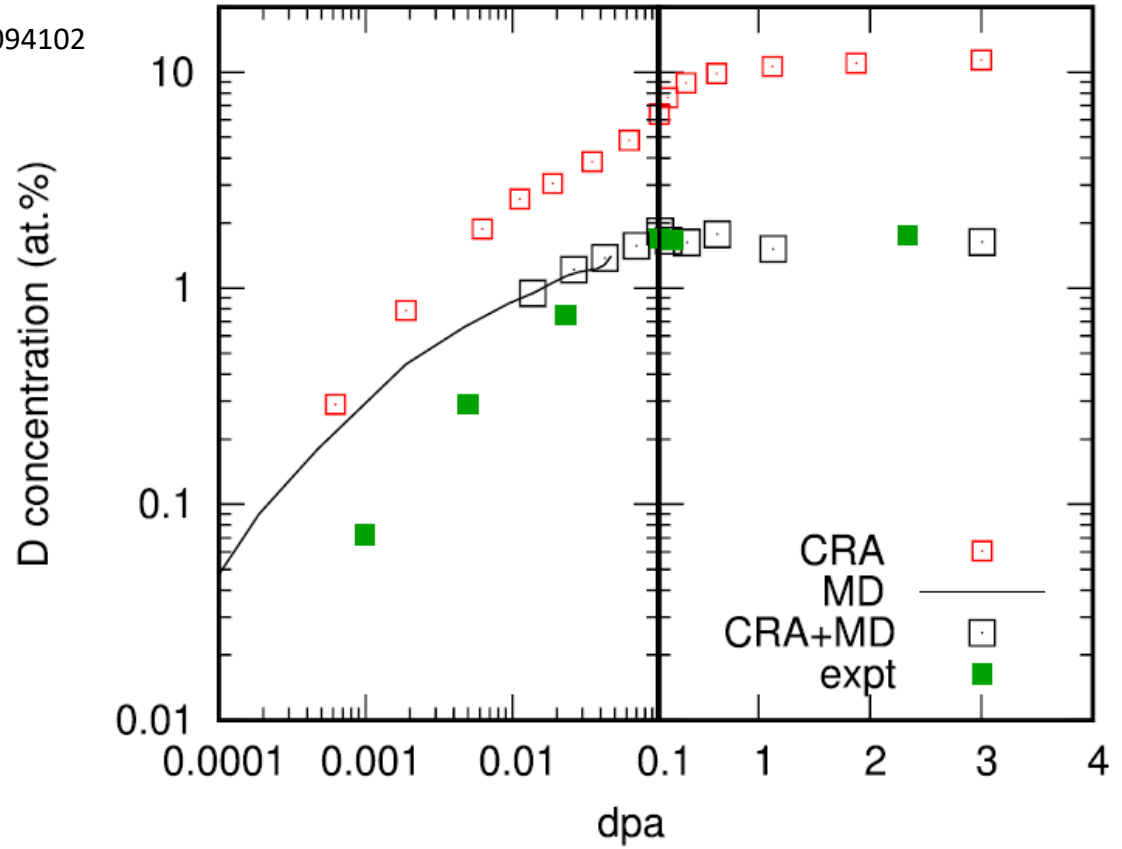
- Experimental definition of “high dose”
- Evolution of materials under irradiation is non-linear
- Above ~0.3 dpa, lattice strain is dominated by vacancies, producing an apparent contraction

Hydrogen retention in vacancies at high dose

K. Heinola *et al.,* Phys. Rev. B 82 (2010) 094102



Experimental

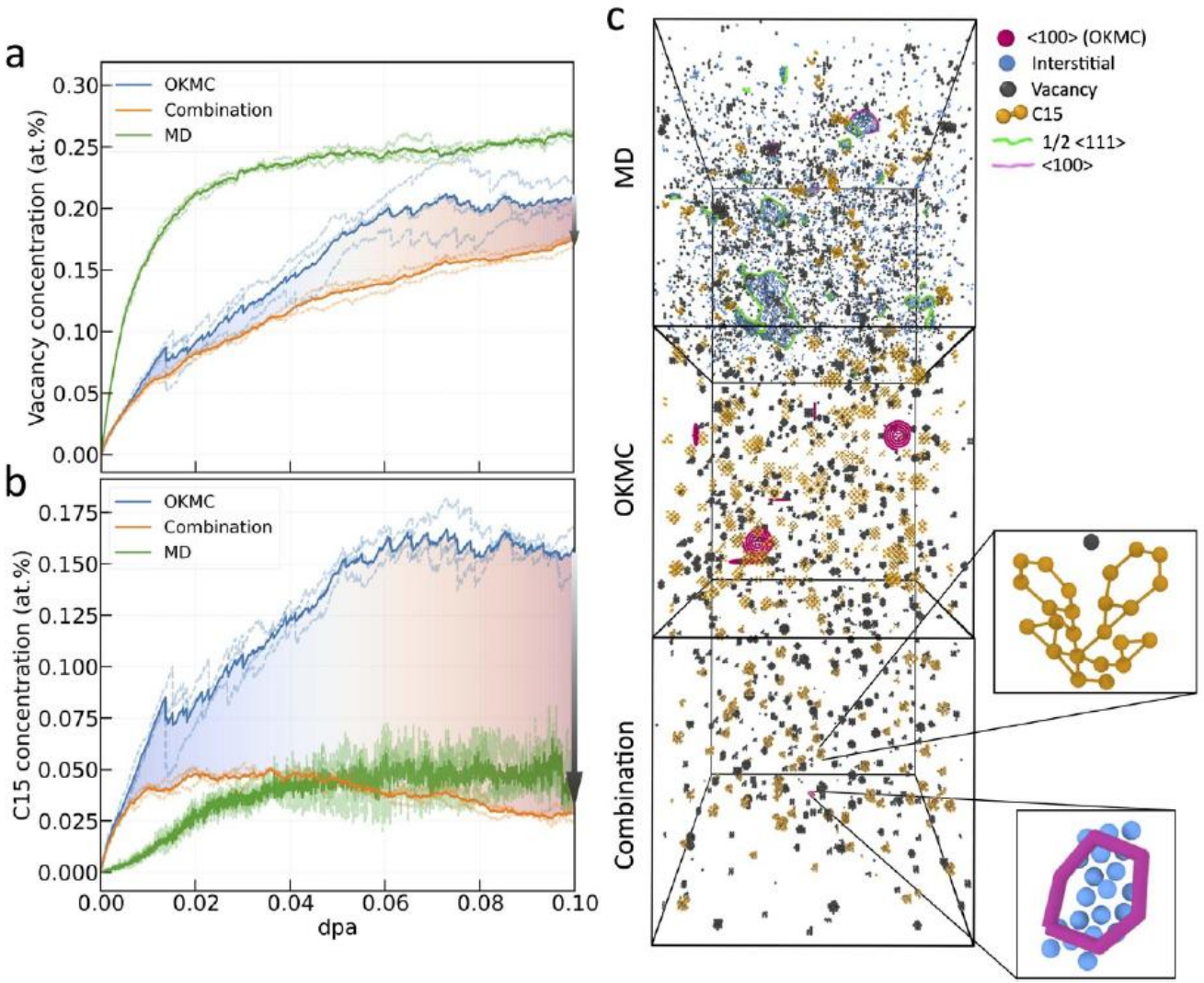


V. Lindblad and F. Granberg, J. Nucl. Mater. **630** (2026) 156710

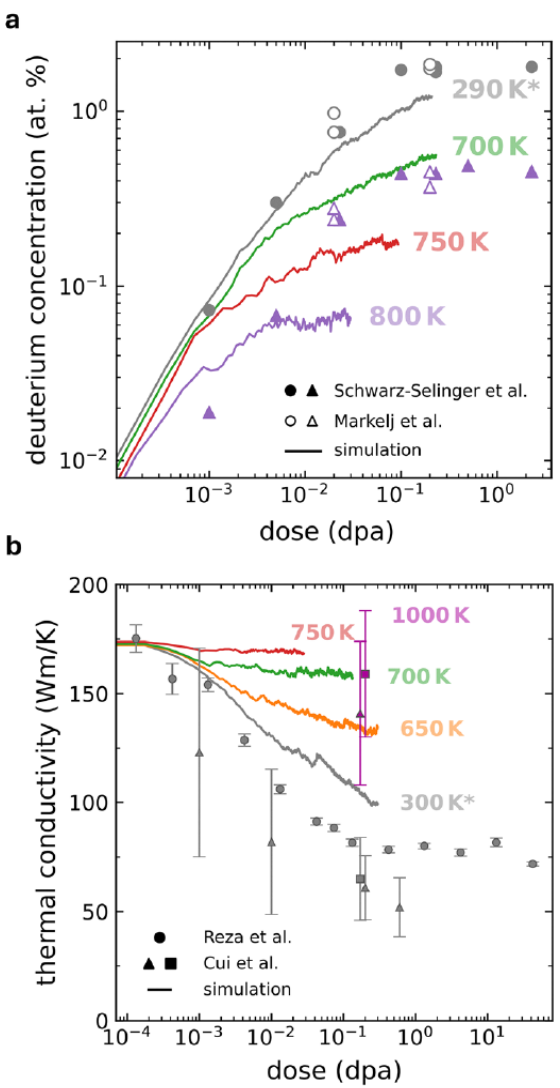
D.R. Mason *et al.,* Phys. Rev. Mater. **5**, 095403 (2021)

High concentration of vacancies in irradiated materials makes them susceptible to hydrogen retention. Heinola *et al.* (2010) showed that a vacancy in tungsten retains up to 6 hydrogen atoms; Mason *et al*. (2020) predicted how much hydrogen can be retained in irradiated tungsten

Evolution of microstructure: vacancy migration effects

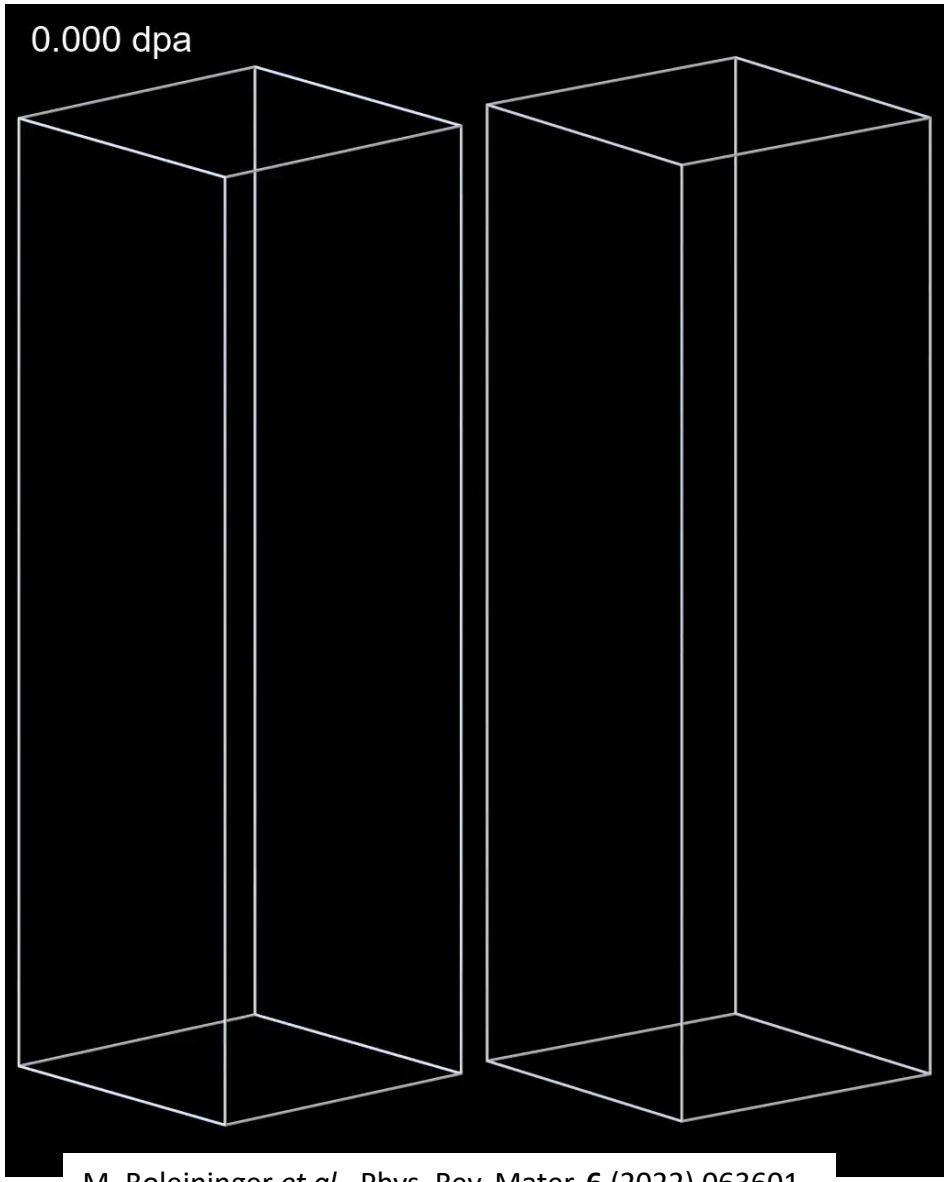


J. Wu, ..., M.J. Caturla... *et al.,* Nucl. Fusion **66** (2026) 086045

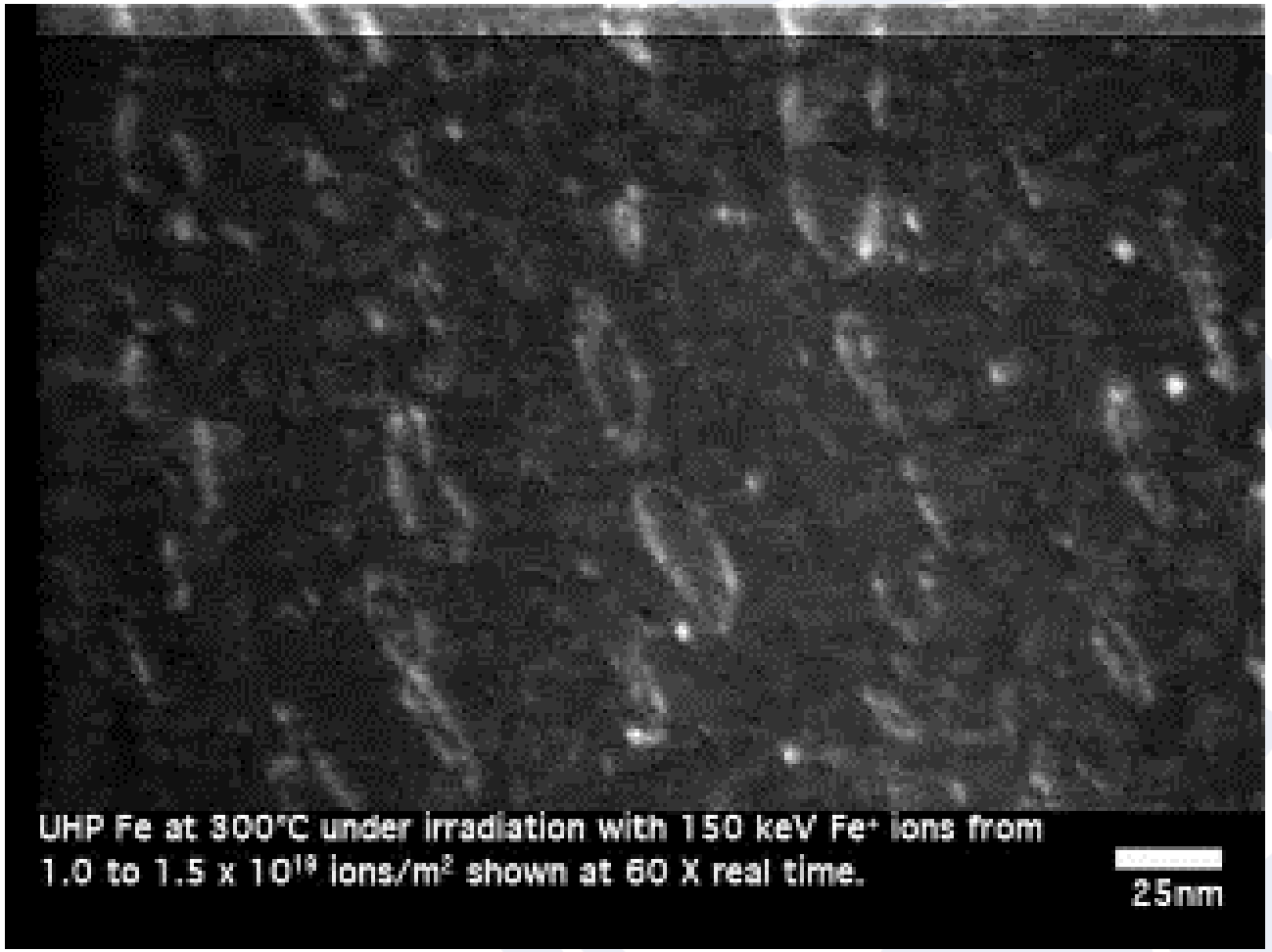


M. Boleininger *et al.,* Mater. Advances (2026) 10.1039/d5ma00677e

Microstructure under irradiation *and* stress



M. Boleininger *et al*., Phys. Rev. Mater. **6** (2022) 063601

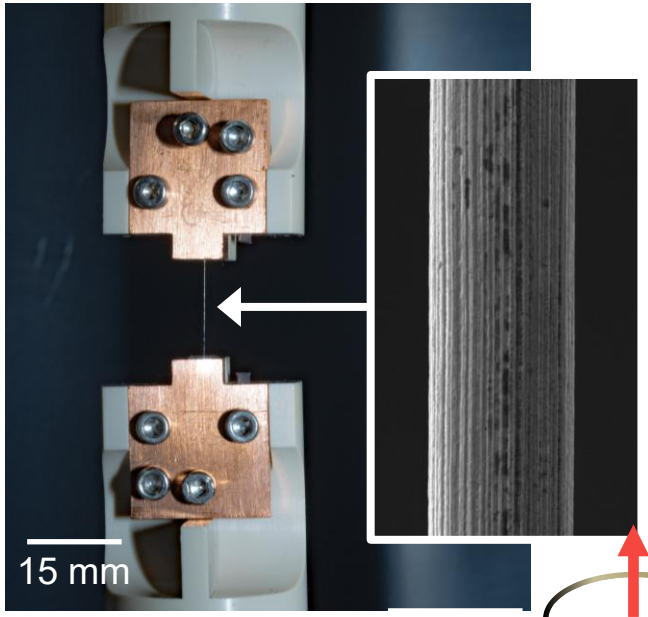


Simulated and observed microstructures developing in a bcc metal under irradiation in the limit of high dose. Dislocation network forms through the coalescence of dislocation loops.

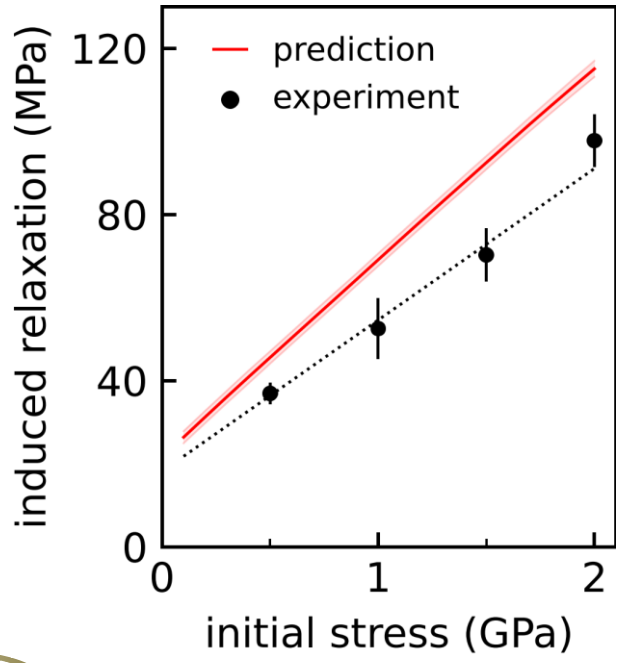
M. Hernández-Mayoral *et al*., Philos. Mag. **88** (2008) 2881

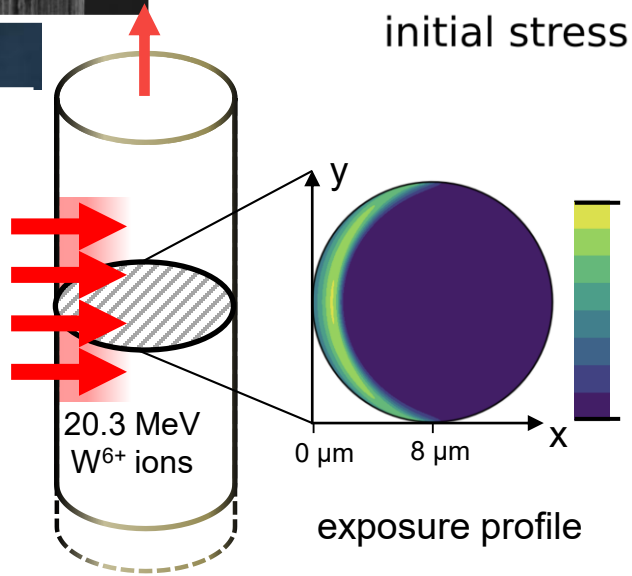
Microstructure under irradiation *and* stress

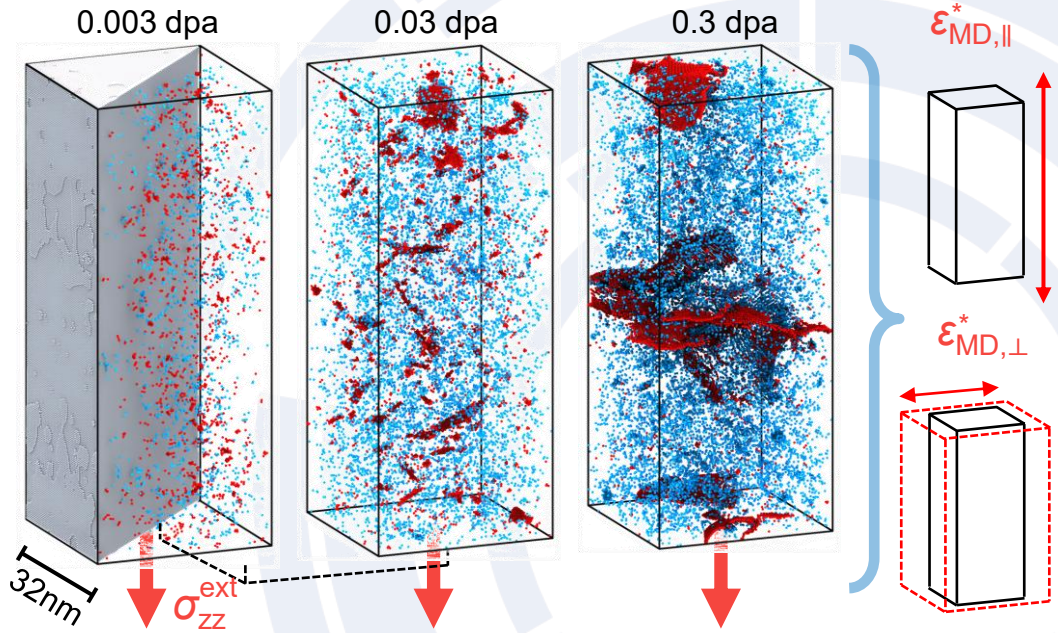
A. Feichtmayer, M. Boleininger *et al.*, Communications Materials **5** (2024) 218;
https://www.nature.com/articles/s43246-024-00655-5

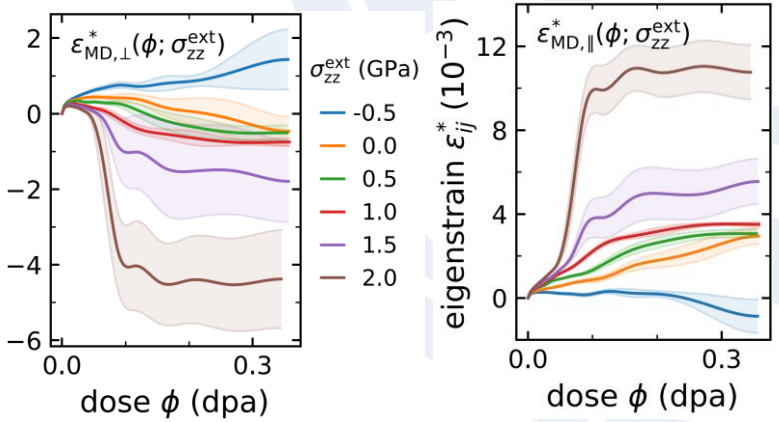


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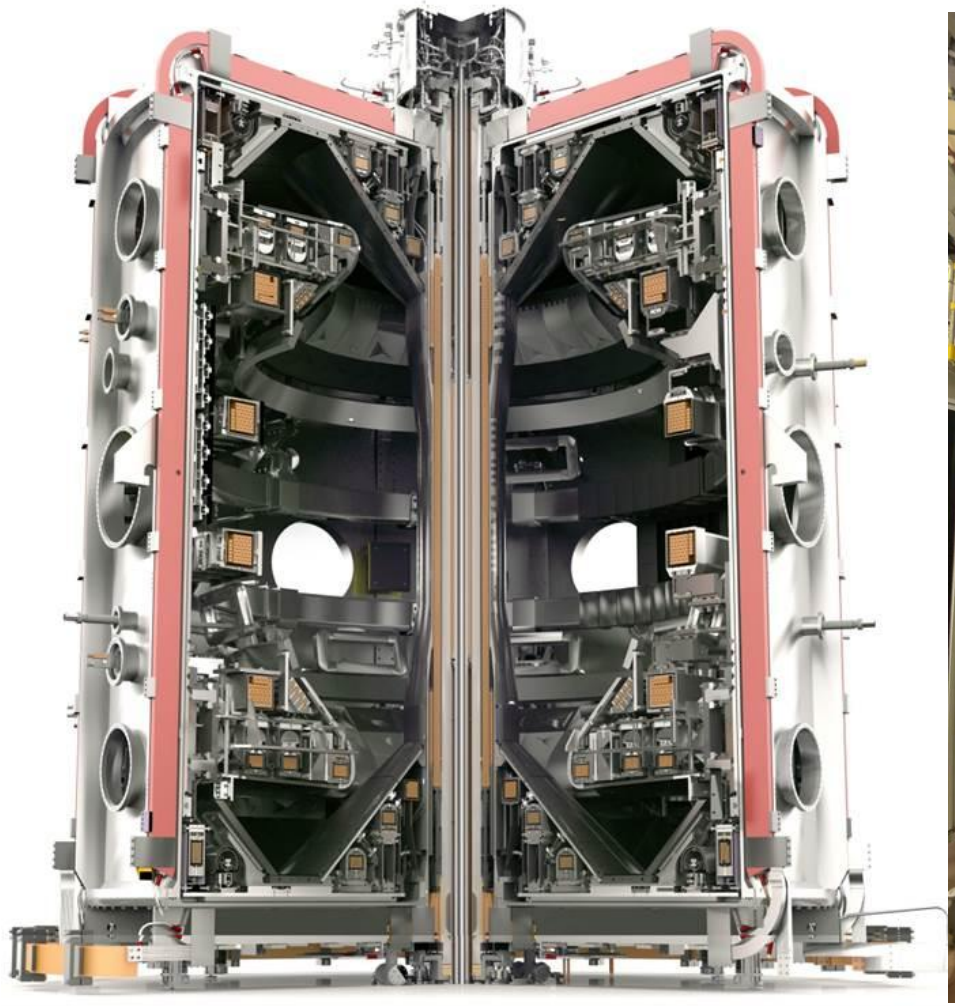


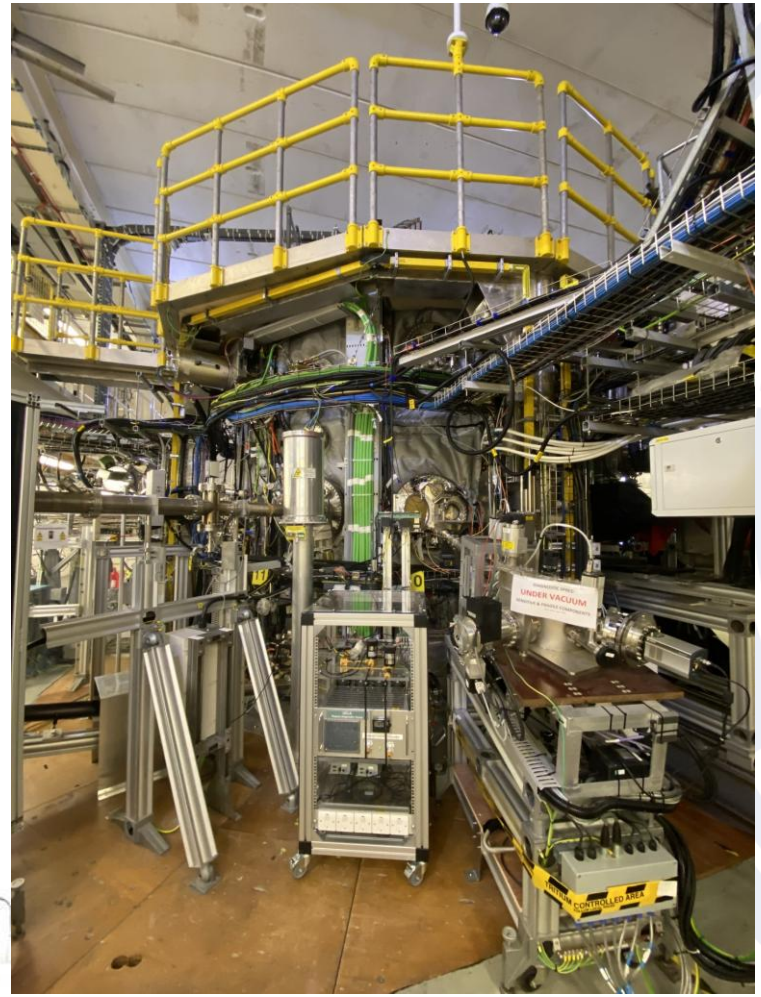
Experiment

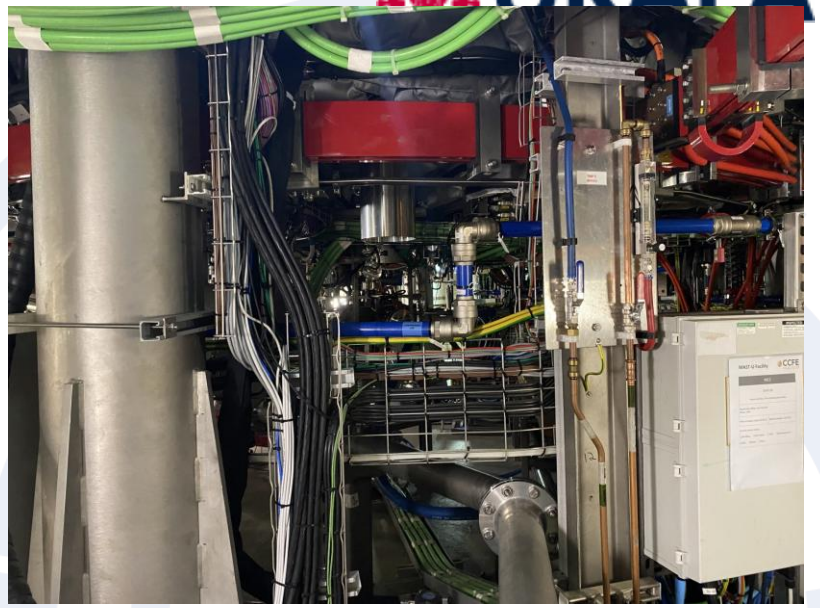
Simulation

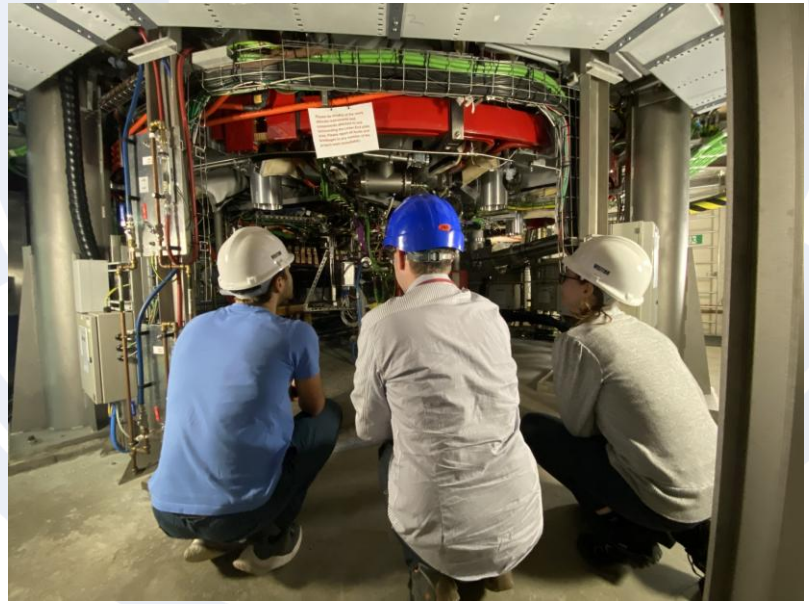
A full fusion device simulation: MAST-U case study

A deformable model for a tokamak



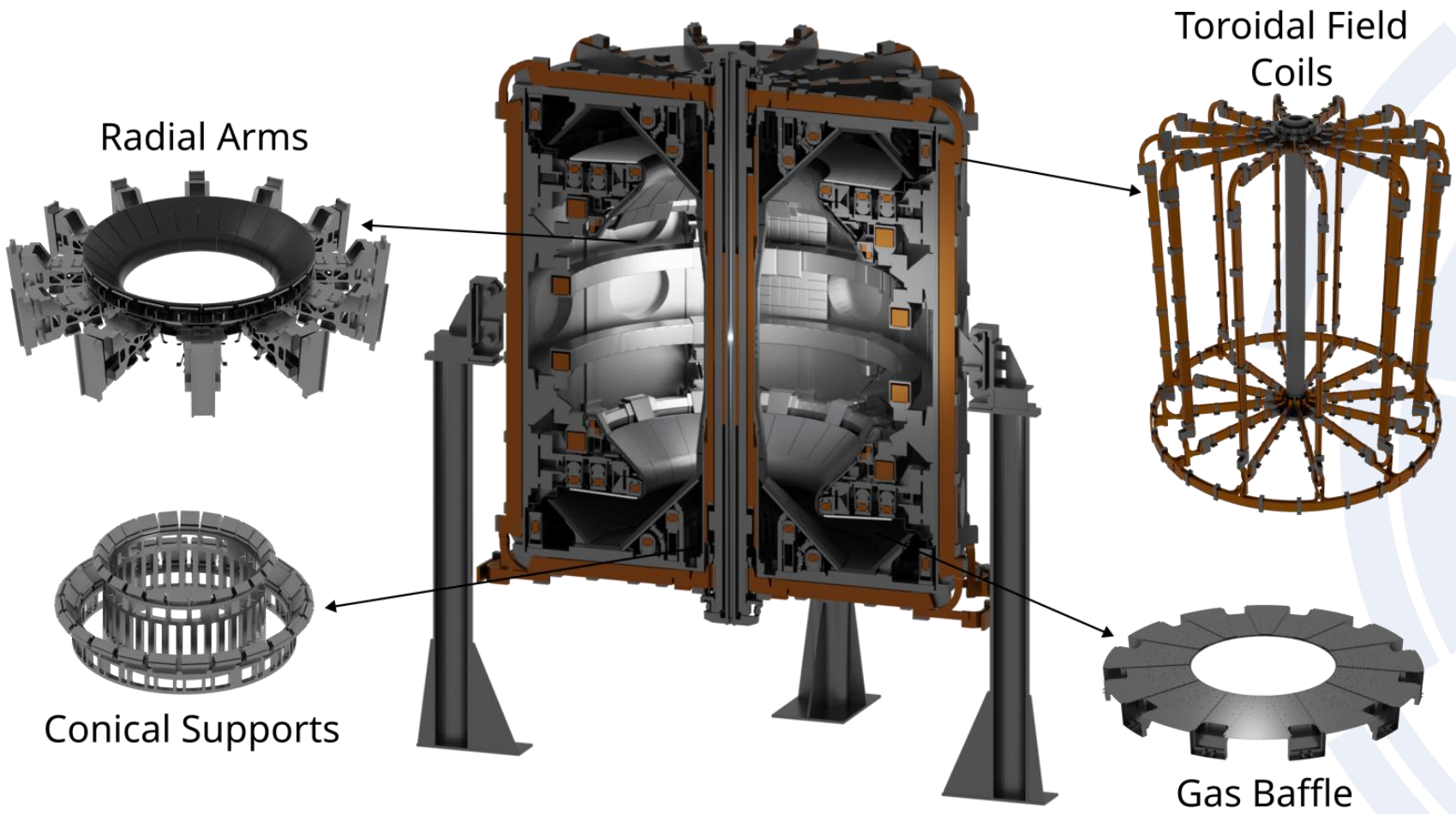






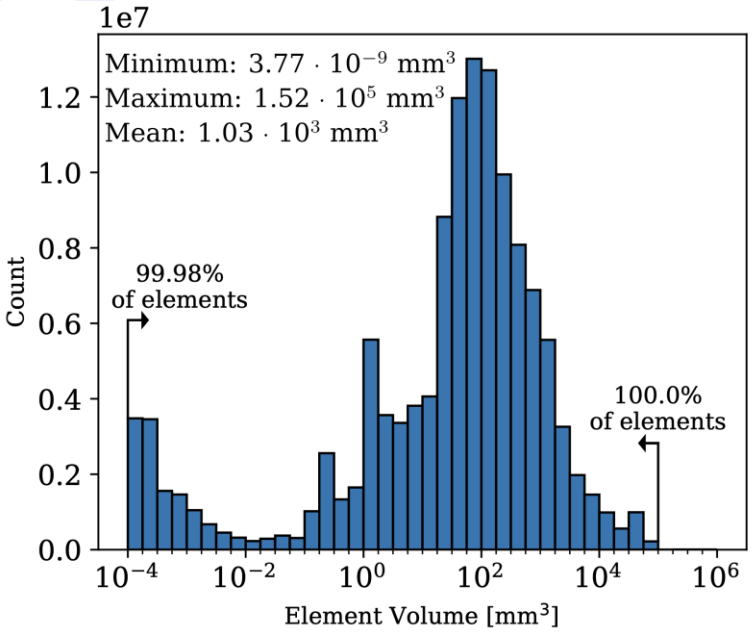
From an un-deformable CAD to a model able to treat deformations

A full device FEM model



Average linear element size is ~10 mm

127 million finite elements



W.M.E. Ellis *et al.*, Nucl. Fusion **65** (2025) 036033, https://doi.org/10.1088/1741-4326/adb443
L. Reali *et al.*, https://doi.org/10.1051/epjconf/202430206002

Mathematical formulation

Algorithmic steps linking microscopic defects to macroscopic continuum elasticity:

- Compute the elastic dipole tensor of a defect P_{kl} $\quad u_i(\mathbf{r}) = -P_{kl}\dfrac{\partial}{\partial x_l}G_{ik}(\mathbf{r}-\mathbf{R})$

- Compute the relaxation volume tensor, related to dipole tensor as $\quad P_{kl} = C_{klmn}\Omega_{mn}$

volume tensor

- Define the density of elastic relaxation volume tensors, analogous to charge density

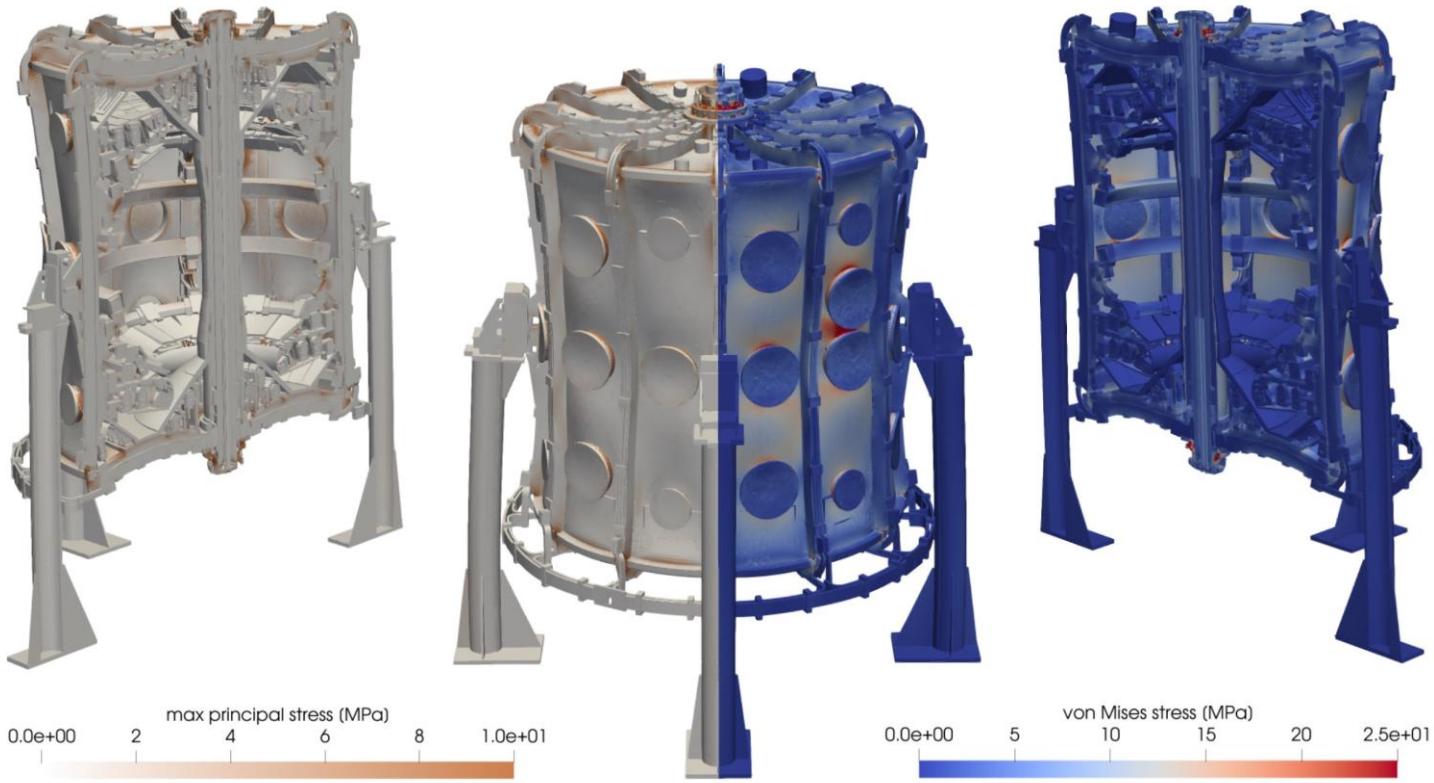
$$\omega_{mn}(\mathbf{x}) = \sum_a \Omega_{mn}^{(a)}\delta(\mathbf{x}-\mathbf{R}_a) \quad \Longleftrightarrow \quad \rho(\mathbf{r}) = \sum_a q_a\delta(\mathbf{r}-\mathbf{r}_a)$$

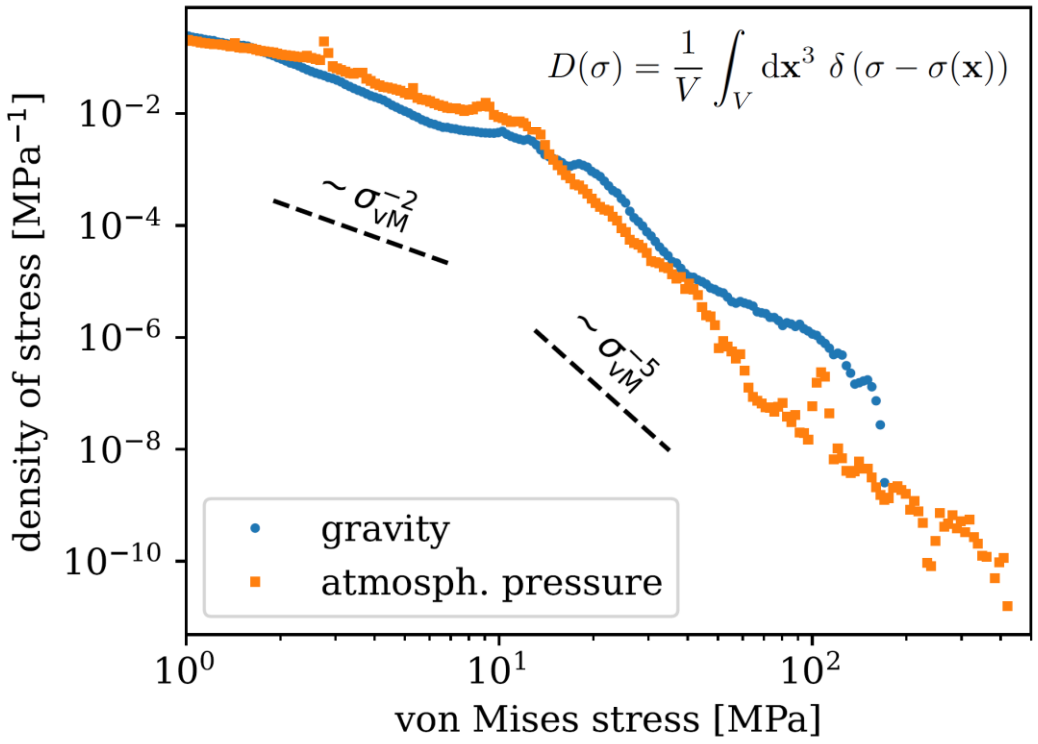
- Using the condition of mechanical equilibrium, compute the effective body forces

$$\partial\sigma_{ij}(\mathbf{x})/\partial x_j = 0 \qquad f_i(\mathbf{x}) = -C_{ipmn}\frac{\partial\omega_{mn}(\mathbf{x})}{\partial x_p}$$

S.L. Dudarev *et al.*, Nucl. Fusion **58** (2018) 126002; https://doi.org/10.1088/1741-4326/aadb48
L. Reali *et al.*, Nucl. Fusion **62** (2022) 016002; https://doi.org/10.1088/1741-4326/ac35d4

Statistics of stress in a tokamak structure: gravity



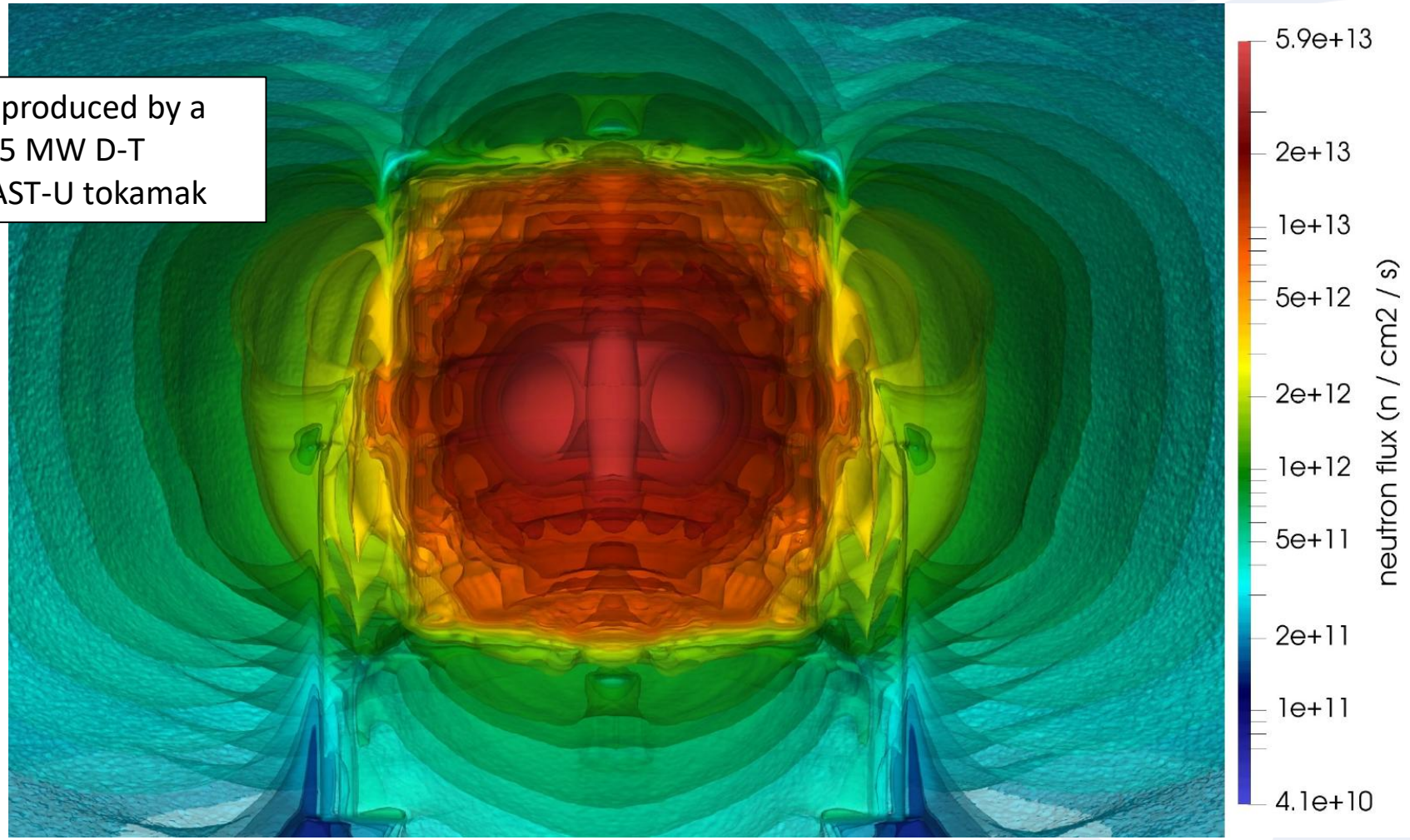


Stress as an operating condition for materials. The *density of stress* computed for a full tokamak structure. The statistics is not Gaussian; there is no “characteristic value” of stress.

W.M.E. Ellis *et al*., Nucl. Fusion 65 (2025) 036033, https://doi.org/10.1088/1741-4326/adb443
L. Reali *et al*., https://doi.org/10.1051/epjconf/202430206002

Gradients of neutron exposure

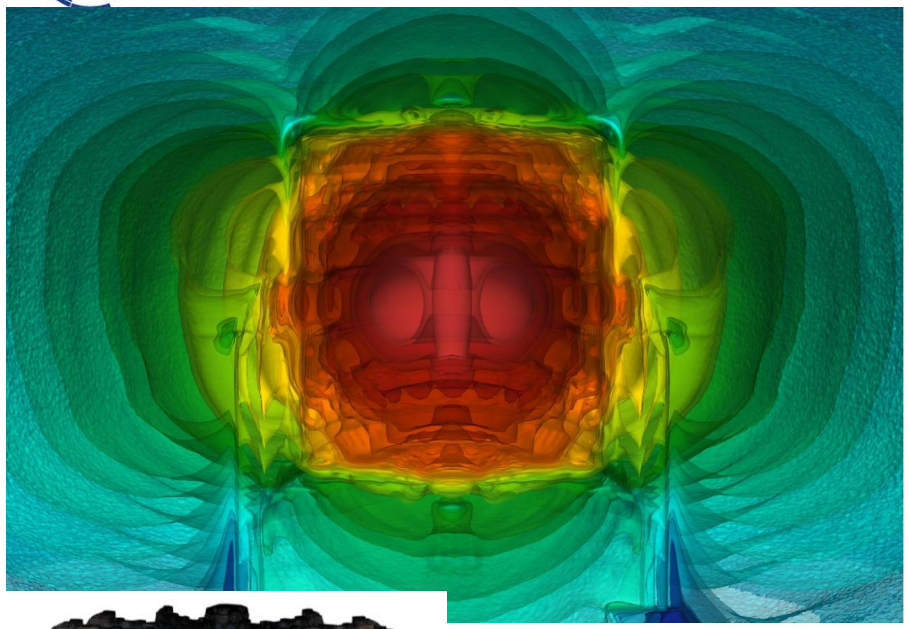
Neutron flux produced by a hypothetical 5 MW D-T plasma in MAST-U tokamak

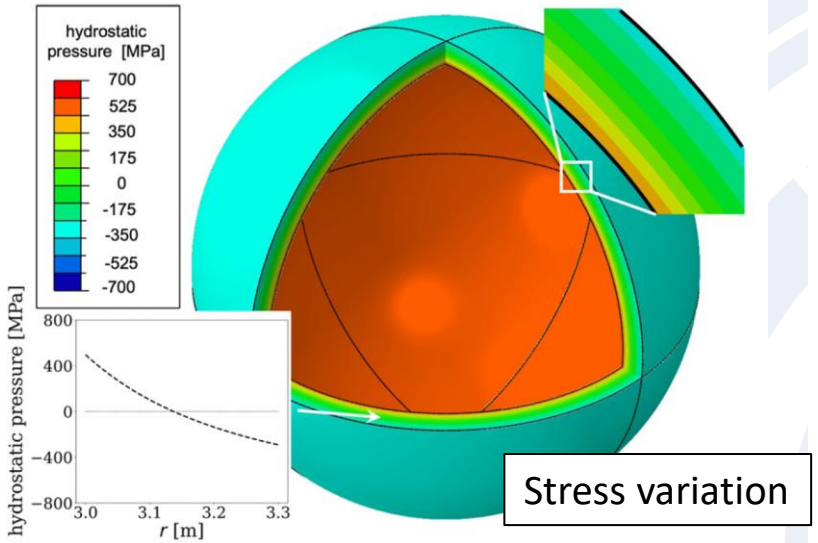


L. Reali *et al*. (2026) PRX Energy, accepted for publication

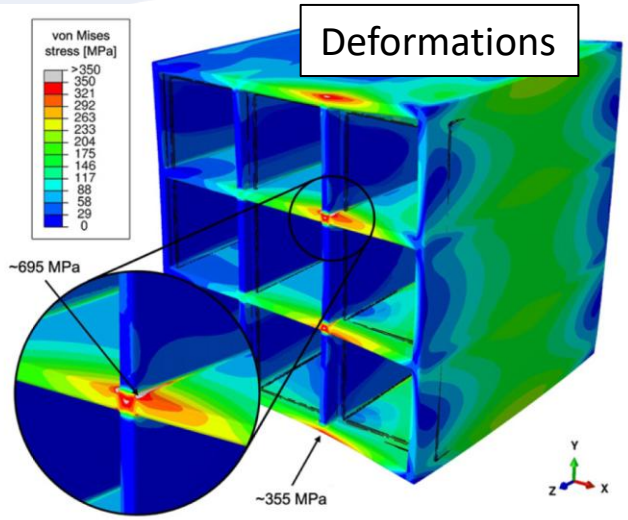
A bespoke two-stage method, transferring the data generated by an OpenMC neutron transport simulations to the FEM mesh at 0.1mm, or even finer, spatial resolution.

Gradients of neutron exposure





Stress variation



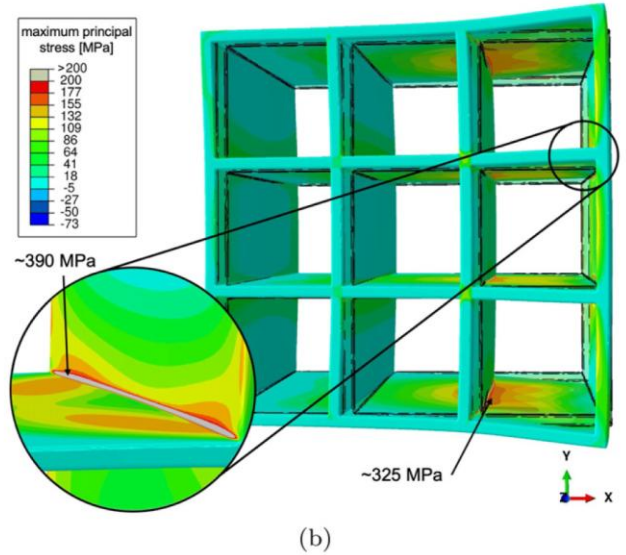


$$p(r) = -\frac{1}{3}\sigma_{ii}(r) = -\frac{1}{3}\left[\sigma_{rr}(r) + \sigma_{\phi\phi}(r) + \sigma_{\theta\theta}(r)\right]$$

$$p(r) = \frac{4\mu}{9}\left(\frac{1+\nu}{1-\nu}\right)\left[\omega(r) - \overline{\omega}\right]$$

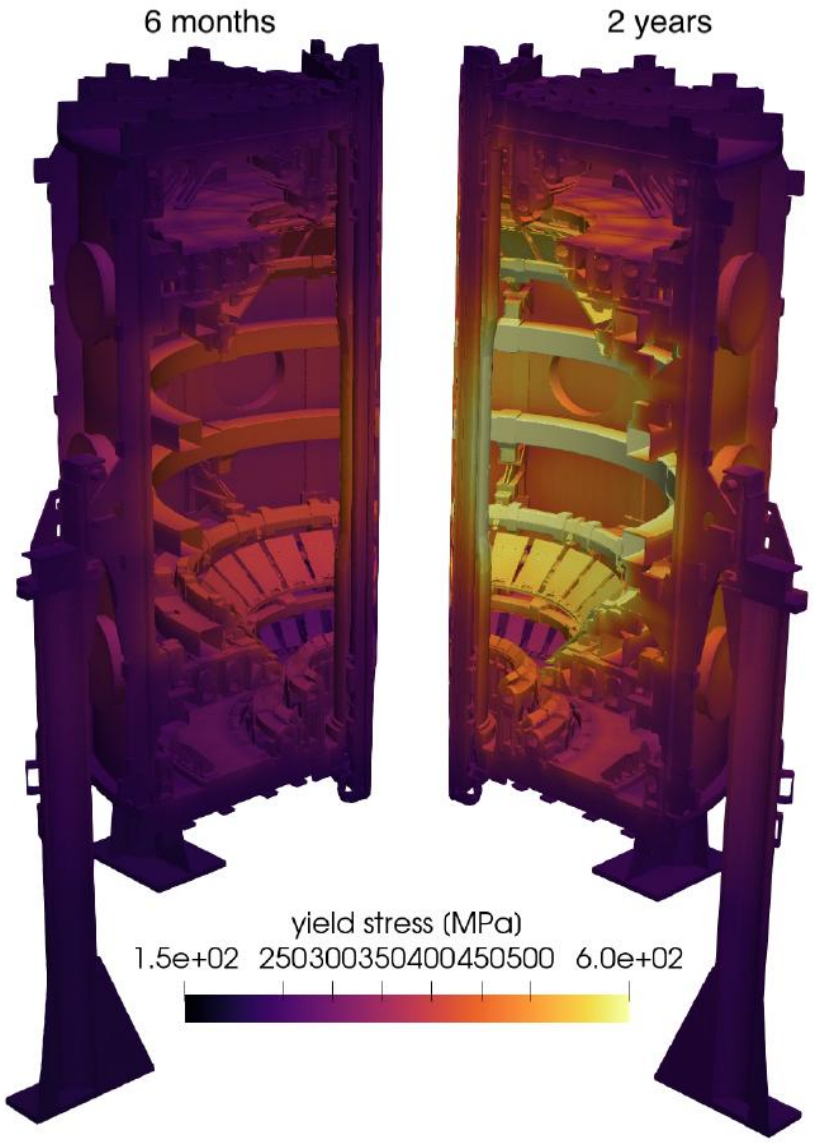
FEM simulations highlight the effect of *gradients of radiation exposure*, hard to realise in small specimen tests.

Gradients produce potentially high stress σ≈μ[ω-ϖ]; μ is the shear modulus.

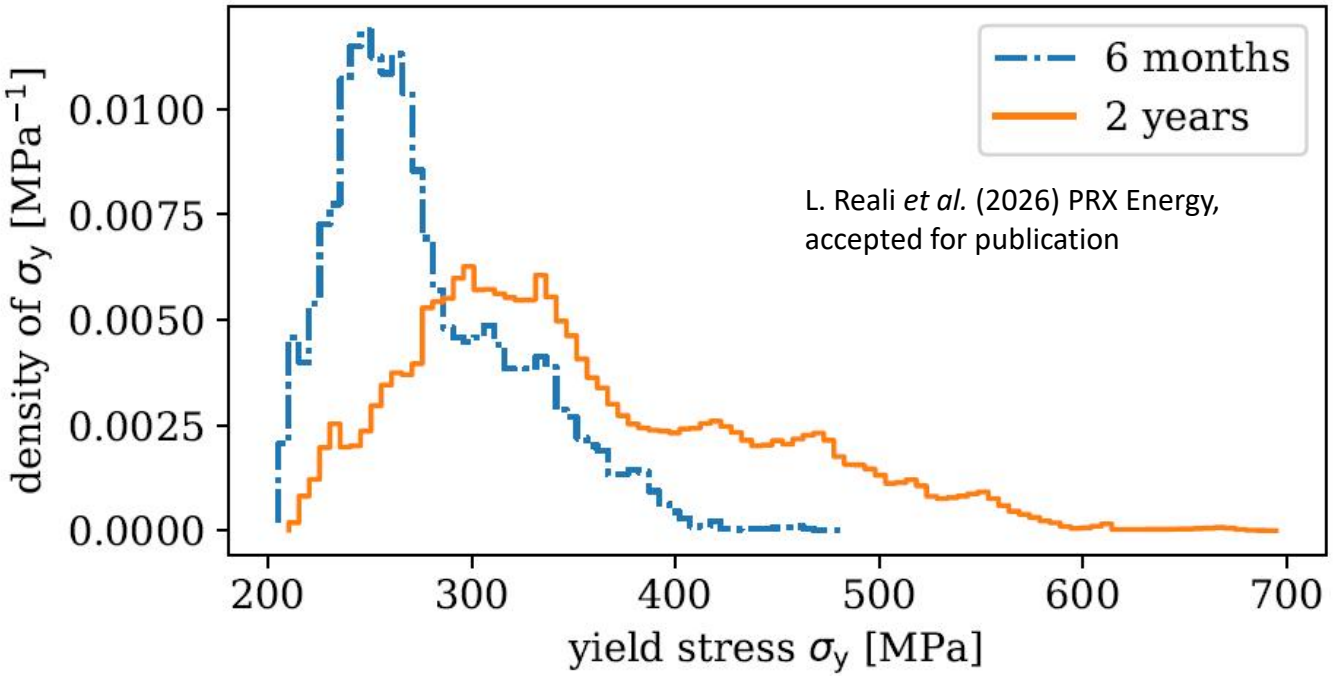


L. Reali *et al.*, Nucl. Fusion **62** (2022) 016002; https://doi.org/10.1088/1741-4326/ac35d4

Radiation hardening of the tokamak steel vessel



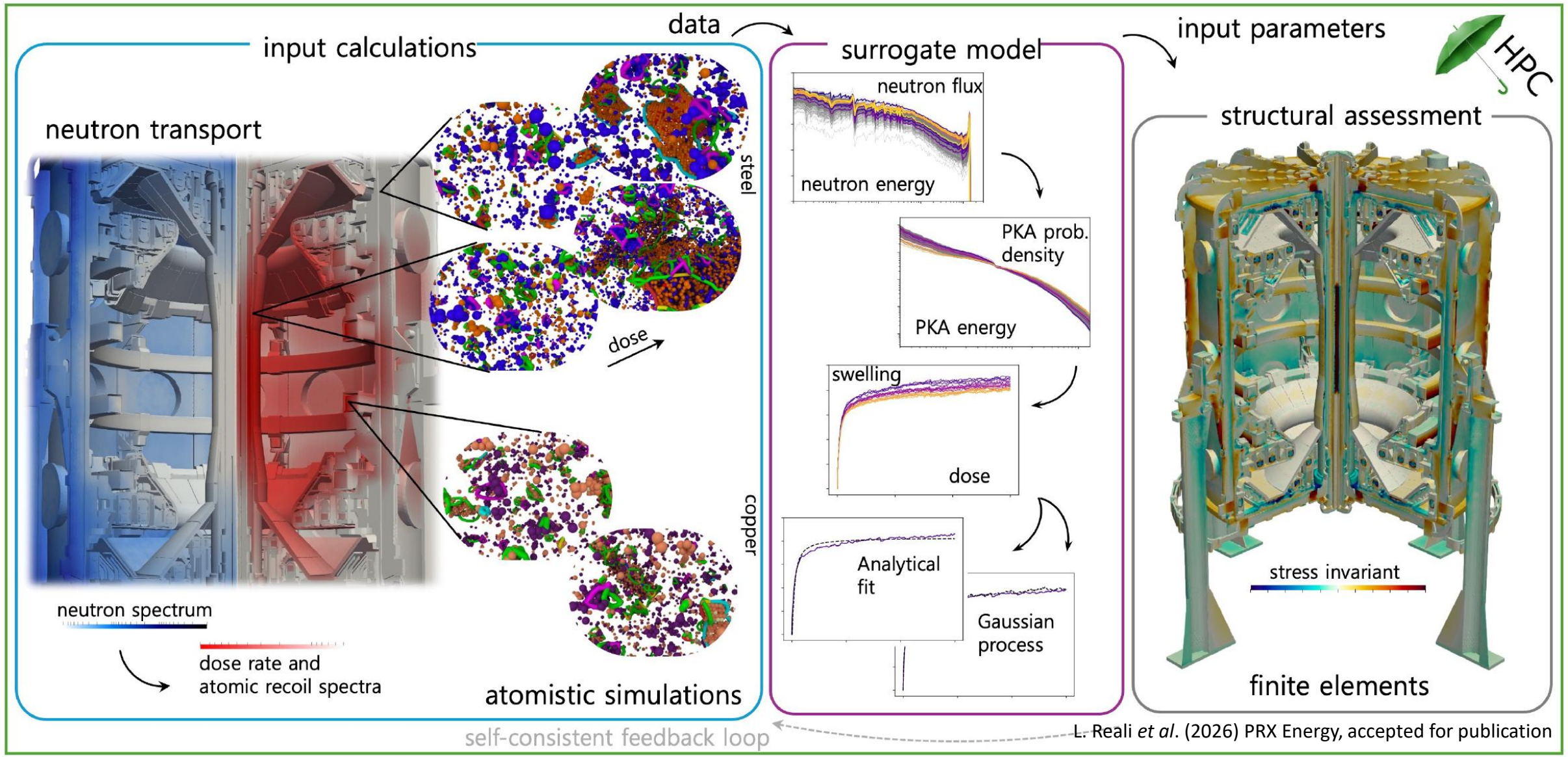
$$D(\sigma_y) = \frac{1}{V}\int_V \delta\left[\sigma_y - \sigma_y(\mathbf{x})\right]\,\mathrm{d}^3x$$



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Since neutron exposure varies across a fusion device, hardening does not follow a *curve* but presents a *spectrum* of values. Converting a 3D image into a spectrum – hardness vs dose in a full tokamak.

Compatibility with FEM and the role of self-consistency



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