Structural Materials Development for Fusion Energy: A Historical Perspective and Opportunities to Accelerate Materials Development through Computational Multiscale Materials Modeling

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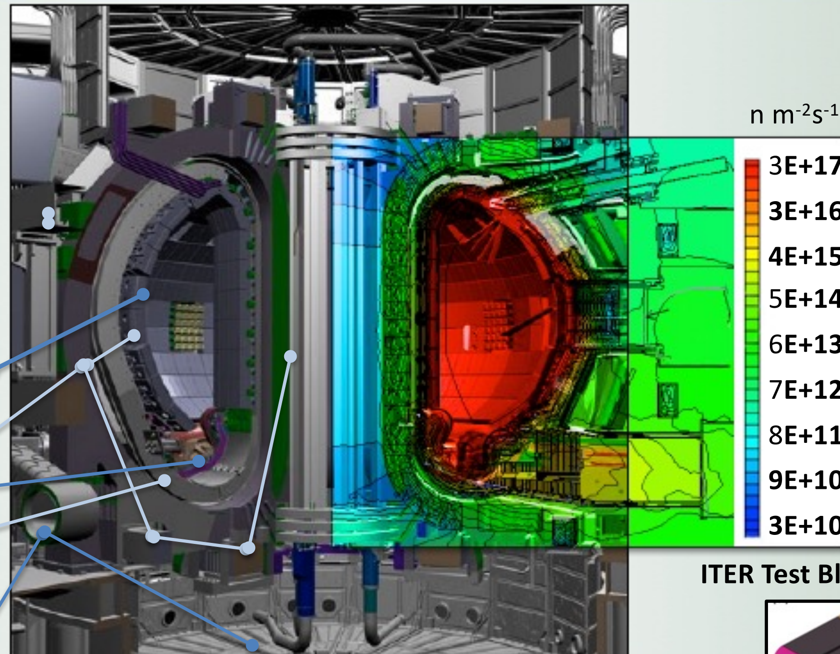
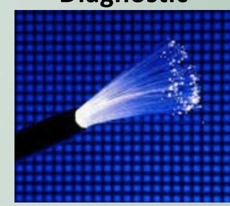
The significant gap bridging materials from ITER to Fusion Power Plant
- virtually no materials systems currently used are reactor viable

ITER Lifetime Neutron Fluence (nm^{-2})	Fusion Power Reactor Annual Neutron Fluence (nm^{-2})	
3.7E+21	5E+22	Blanket
5.1E+14	7E+15	Magnet
1.9E+21	2.6E+22	Divertor
1.1E+19	1.5E+20	Vacuum Vessel
3.4E+11	4.5E+12	Cryostat

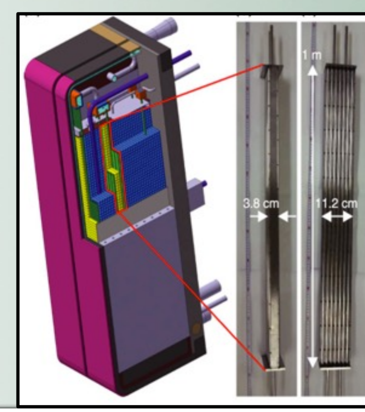


Magnet

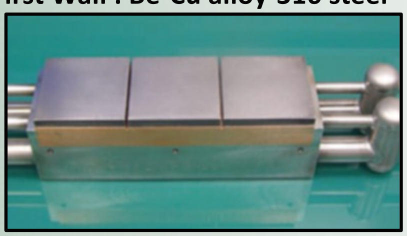
Diagnostic



ITER Test Blanket Module: RAF Steel



First Wall : Be-Cu alloy-316 steel



Divertor: W-Cu alloy-316 steel

Fusion Materials Development Challenges

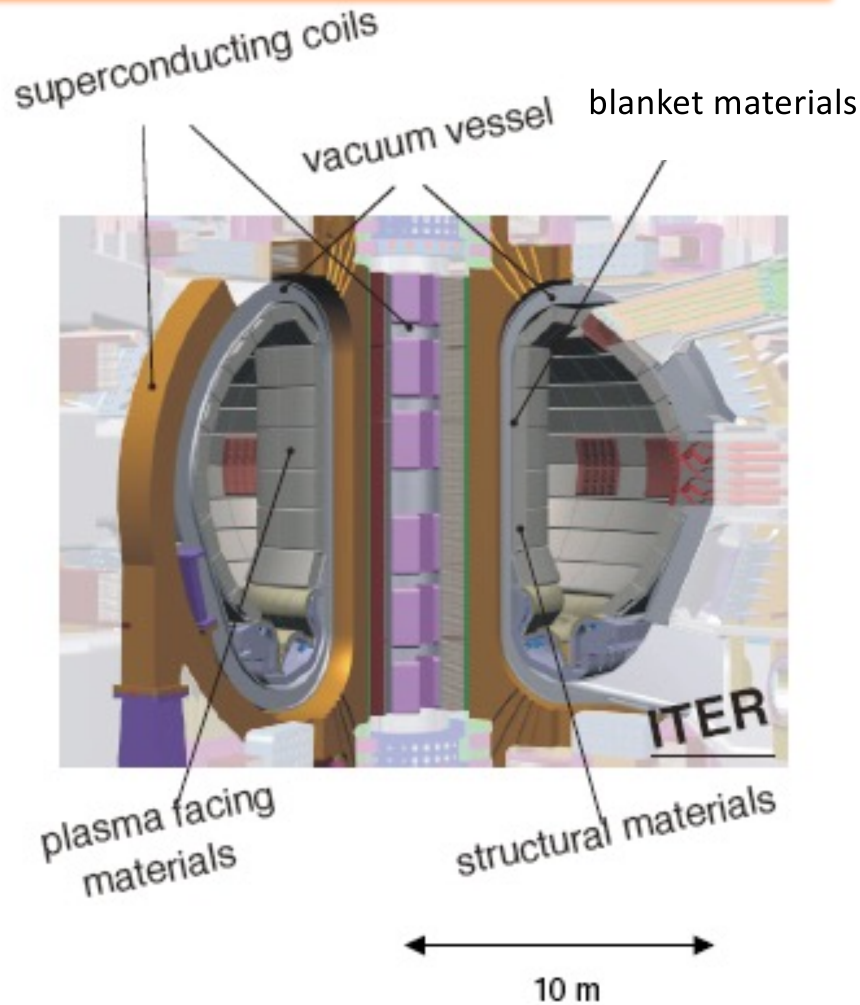
• Plasma – materials interactions
- Sputtering, re-deposition & tritium implantation/retention
- High heat flux
- Varying thermomechanical stress

• Nuclear & non-nuclear degradation to materials and structures
- Structural stability to intense fusion neutron exposure (including transmutant H/He)
- Reduced activation mandate
- Corrosive environments, with possible radiation enhanced corrosion
- Large, time varying thermomechanical stresses and high Temperatures

• Harness fusion energy
- Minimize tritium inventory in blanket structures, PFCs, etc.
- Efficiently extract tritium from hot coolant
- Thermohydraulic and magnetohydrodynamic instabilities

Fusion Materials Development Challenges

- **Magnetic fusion energy presents many materials challenges, including:**
  - High thermal heat fluxes
  - Low induced radioactivity
  - Sputtering/blistering of plasma facing components
  - Radiation damage
  - Chemical compatibility
  - Joining/Welding



*Ref: H. Bolt, Max-Planck Institute for Plasma Physics, Garching, Germany

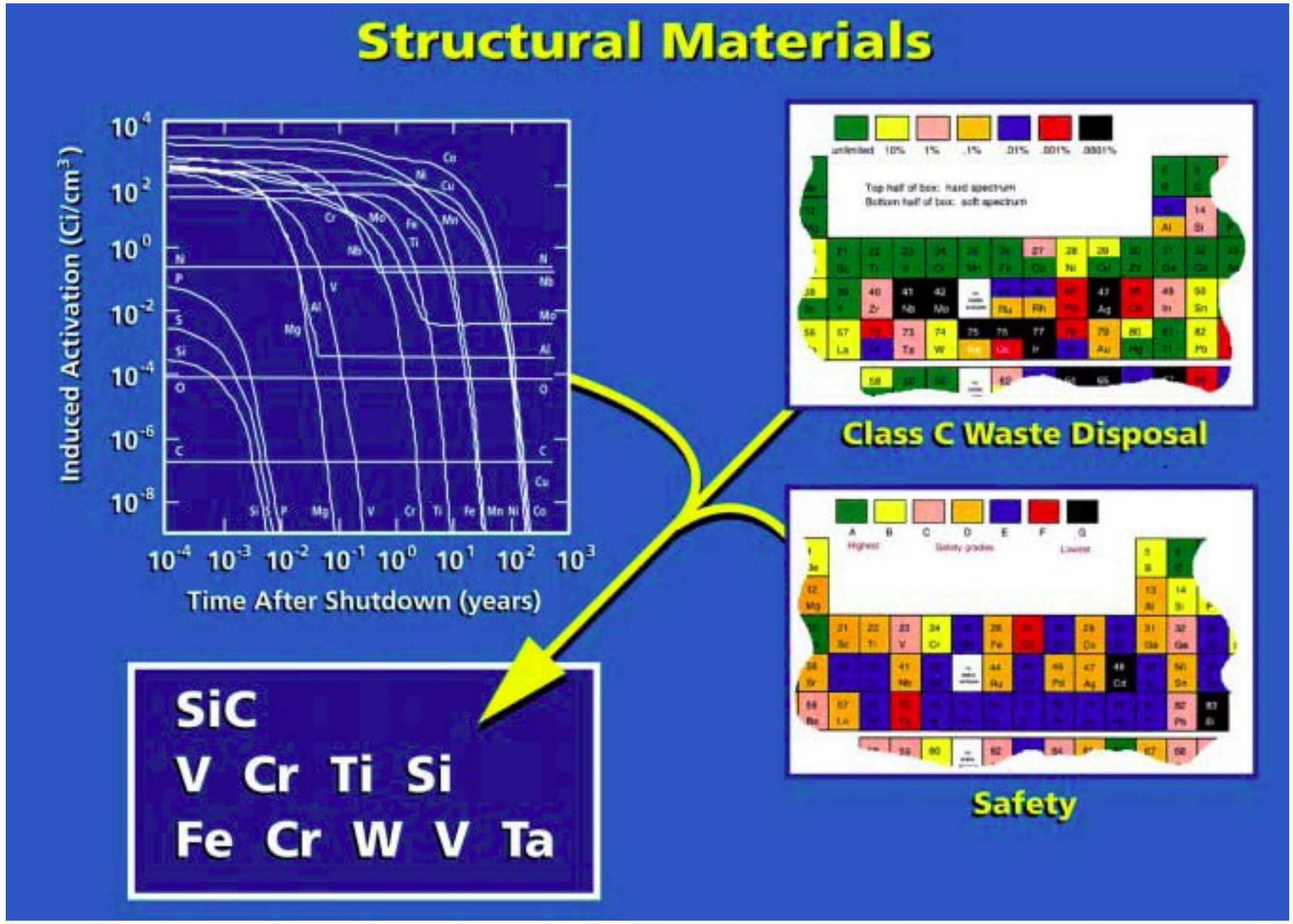
Fusion Materials Engineering Challenges: low-induced radioactivity

• Structural materials selection strongly impacts the economic & environmental attractiveness of fusion power

• Many materials are not suitable for various technical reasons

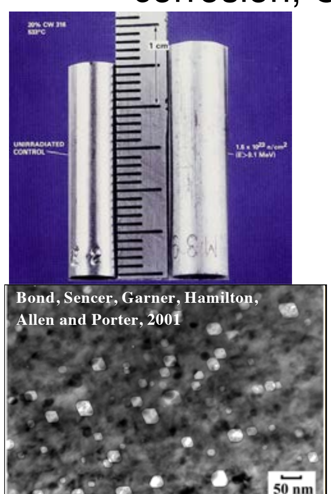
• Based on safety, waste disposal and performance considerations, the leading candidates are:

- RAF/M and NFA steels
- Tungsten alloys
- Vanadium alloys
- SiC/SiC composites

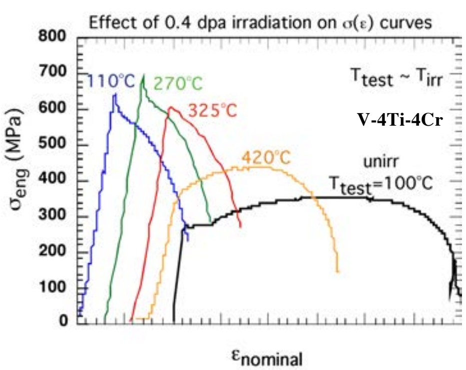


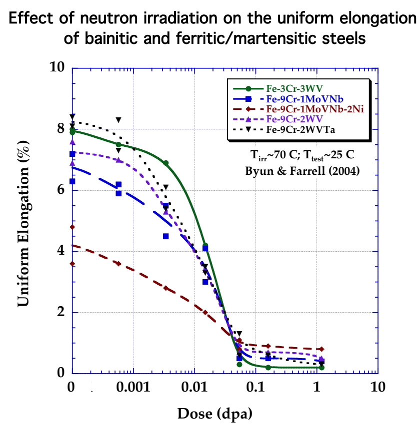
Irradiation effects on structural materials

- Exposure to neutrons degrades the mechanical performance of structural materials and impacts the economics and safety of current & future fission power plants:
  - Irradiation hardening and embrittlement/decreased uniform elongation (< 0.4 T_m)
  - Irradiation (<0.45 T_m) and thermal (>~0.45 T_m) creep
  - Volumetric swelling, dimensional instability & growth (0.3 - 0.6 T_m)
  - High temperature He embrittlement (> 0.5 T_m); Specific to fusion & spallation accelerators
- Additional environmental degradation due to corrosive environments (SCC, uniform/shadow corrosion, CRUD)



304 Stainless steel irradiated in EBR-II, 380°C, ~22 dpa, 1% swelling





Variables

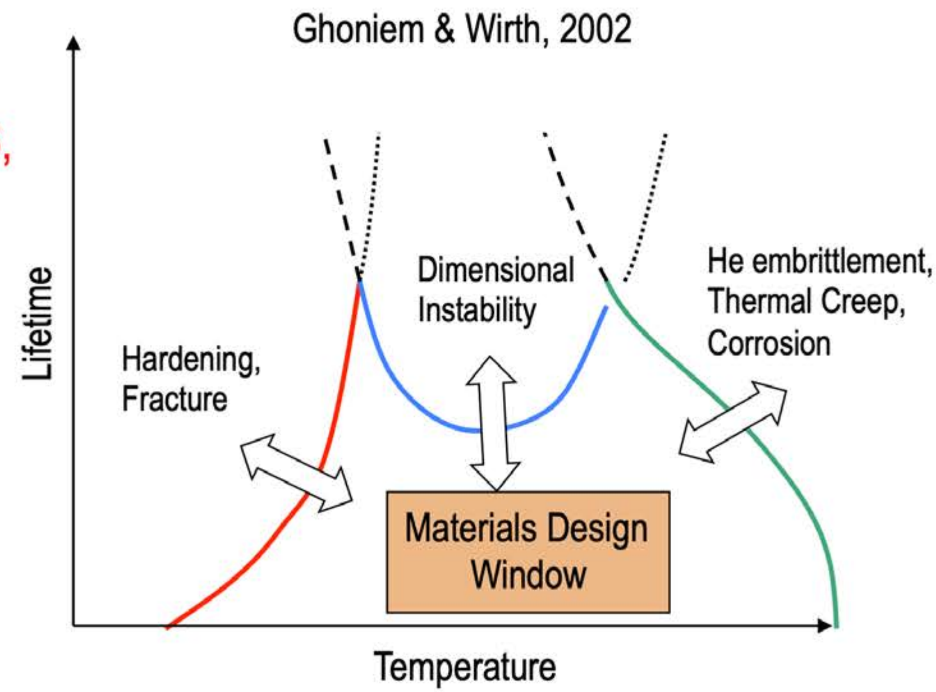
- Structural Materials (Fe-based steels, Vanadium and Ni-based alloys, Refractory metals & alloys, SiC) and composition
- Zr alloy cladding
- Initial microstructure (cold-worked, annealed)
- Irradiation temperature
- Chemical environment & thermal-mechanical loading
- Neutron flux, fluence and energy spectrum
  - materials test reactor irradiations typically at accelerations of 10^2 - 10^4

Synergistic Interactions

Irradiation effects on structural materials

Unique to fusion: displacement damage (displacements per atom or dpa) and He coupled with stress results in considerable microstructure and property changes.

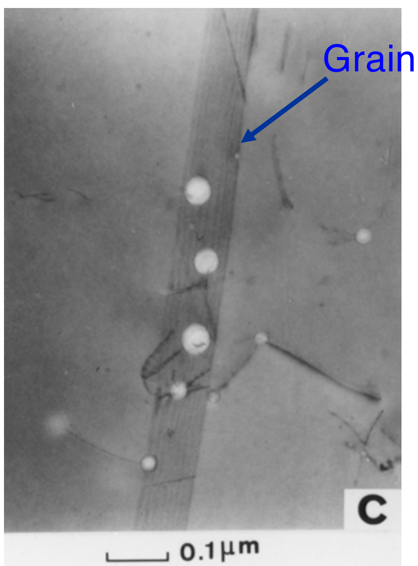
- Low temperatures ($< 0.4\ T_m$, < 0.1 dpa):
  - Hardening + He embrittlement
  - Loss of ductility
  - Loss of fracture resistance
- Intermediate temperatures ($0.3 < T_m < 0.6$, > 10 dpa):
  - Swelling + He
  - Irradiation creep + He
- At high temperatures ($> 0.4\ T_m$):
  - Thermal creep
  - He embrittlement (> 10 dpa)
  - Fatigue and creep-fatigue, crack growth
  - Corrosion, oxidation and impurity embrittlement



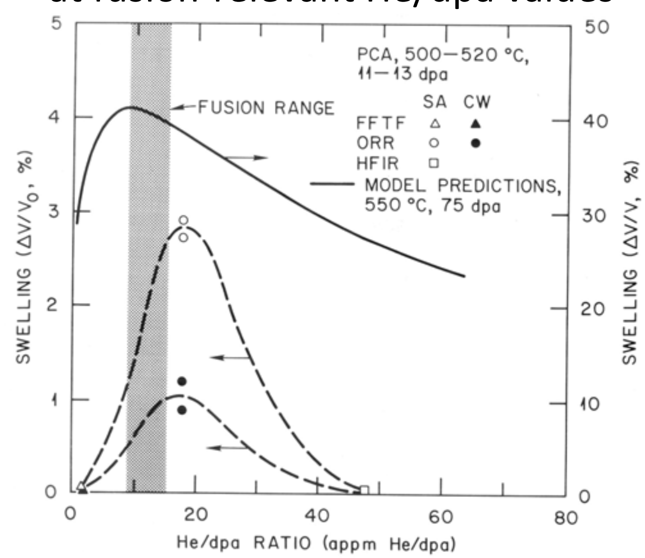
Why is He/dpa ratio such an important parameter for materials R&D?

- He generation can alter the microstructural evolution path of irradiated materials (pronounced effects typically occur for >100 appm)
  - Cavity formation (matrix and grain boundaries)
  - Precipitate and dislocation loop formation
- He can also increase hardening and embrittlement at low Temperature

He bubbles on grain boundaries can cause severe embrittlement at high temperatures



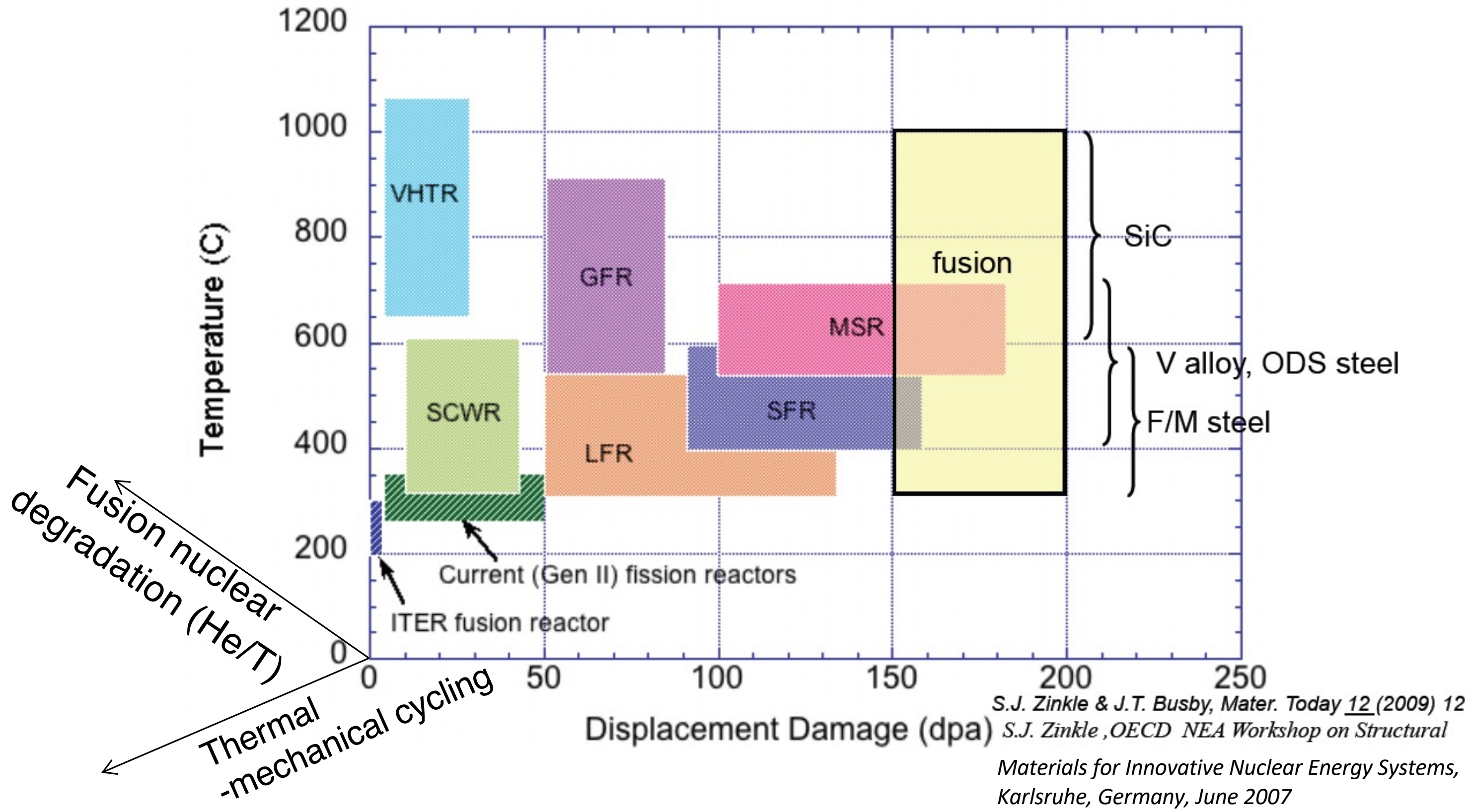
Swelling in stainless steel is maximized at fusion-relevant He/dpa values



R.E. Stoller, J. Nucl. Mater. 174 (1990) 289

Nuclear structural materials degradation shares commonality

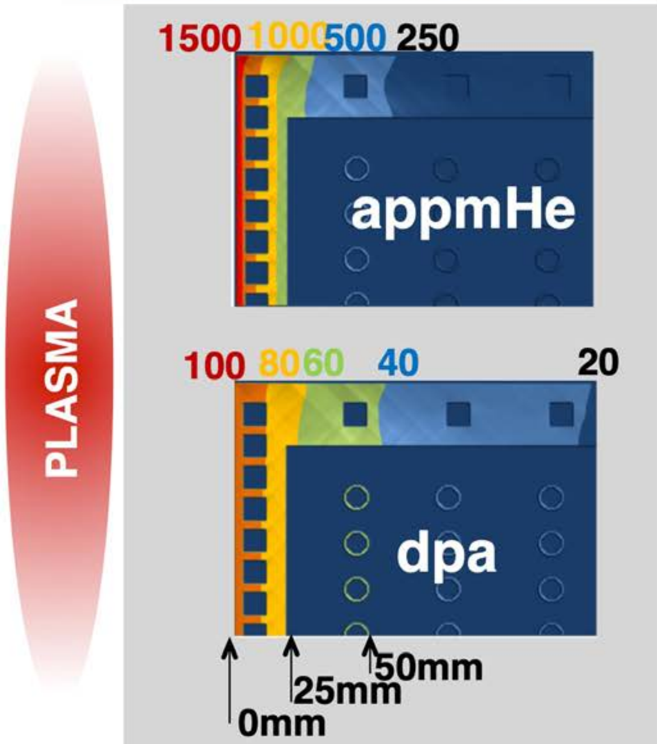
But, the fusion nuclear environment incorporates additional degradation concerns (He/transmutants, thermo-mechanical cycling and tritium) that are more (to much more) extreme in the fusion environment than fission, even without the initially large extrapolation to DEMO neutron irradiation conditions



S.J. Zinkle & J.T. Busby, Mater. Today 12 (2009) 12
S.J. Zinkle ,OECD NEA Workshop on Structural Materials for Innovative Nuclear Energy Systems, Karlsruhe, Germany, June 2007

Irradiation effects on structural materials: commonality between fusion & fission

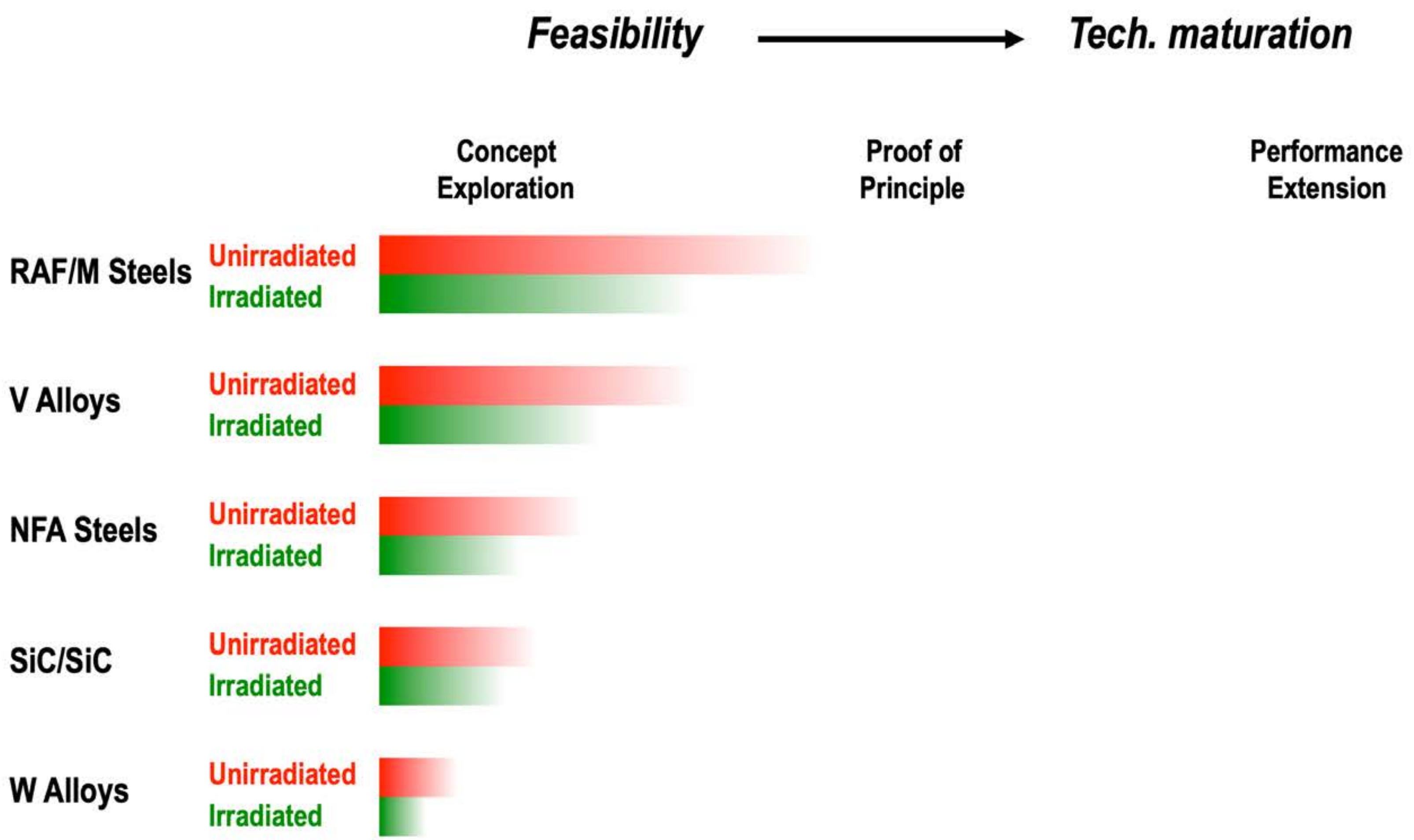
Helium production (appm) for
100 dpa at plasma facing side



H. Tanigawa, E.Wakai 2012

- "Only" the first few centimeters have a high He/dpa ratio
- In addition this part of the blanket carries the highest thermo-mechanical loads
- Therefore,
  - fission reactor irradiations are still meaningful for a significant fraction of in-vessel components
  - Nevertheless, a dedicated fusion neutron source is indispensable, but has to focus on plasma-near materials and loading conditions

Fusion Materials Current Readiness



Fusion Materials Current Readiness: Radiation Effects

Data Base Need	0 – 5 years: 10 dpa/100 appm He						5 – 15 years: 50 dpa/500 appm He						>15 years: 150 dpa/1500 appm He					
	RAF/M	NFA	V	W	SiC	Adv Mat	RAF/M	NFA	V	W	SiC	Adv Mat	RAF/M	NFA	V	W	SiC	Adv Mat
Radiation Effects																		
Hardening & Embrittlement	Green	Yellow	Yellow	Red	Yellow	Red	Yellow	Red	Yellow	Red	Yellow	Red	Red	Red	Red	Red	Red	Red
Phase Instabilities	Green	Red	Yellow	Red	Yellow	Red	Yellow	Red	Red	Red	Yellow	Red	Red	Red	Red	Red	Red	Red
Irradiation Creep	Green	Yellow	Yellow	Red	Yellow	Red	Yellow	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
Volumetric Swelling	Green	Red	Yellow	Red	Yellow	Red	Yellow	Red	Yellow	Red	Yellow	Red	Yellow	Red	Red	Red	Red	Red
High T Helium Effects	Green	Red	Red	Red	Red	Red	Yellow	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red

• Table focuses on structural materials for first wall/vacuum vessel, but radiation stability & degradation of magnet (conducting coils & insulators) and on diagnostics (optical/electronic properties) are needed in the near term (< 10 dpa, up to 10^9 Gy)

Note: He levels are for RAF/M, lower and higher values for other materials

Green = Adequate Knowledge Base Exists
Yellow = Partial Knowledge Base Exists
Red = Knowledge Base Does Not Exist of Completely Inadequate

Fusion Prototypic Neutron Source (FPNS)

- The need for an irradiation source to test and qualify materials has been recognized since the 1970's.

- Many facilities have been proposed, but in the U.S., only RTNS (I & II) was built and operated at < 0.1 dpa between 1979 and 1987

- IFMIF is being designed and technology prototyped by the Japan/EU (IFMIF EVEDA)
  - IFMIF cost estimated at >$1.25B
  - DONES (essentially half-IFMIF) currently being pursued, estimated at ~$700M

- Multiple FESAC & community reports (e.g., RENEW, Gaps and Priorities, etc.) have promoted material testing in a prototypic fusion neutron spectrum
  - More recently, the US APS-DPP Community Planning Process reiterated that FPNS is needed and assigned a high(est) priority ranking among needed new start facilities
  - In summer/fall 2022, EPRI hosted a 2-part workshop series to further discuss requirements for an FPNS and build consensus on timeline, with the emergence of private fusion companies

Fusion Prototypic Neutron Source (FPNS)

EPRI

Program on Technology Innovation: 2022 Fusion Prototypic Neutron Source (FPNS) Performance Requirements Workshop Summary

Washington, D.C., September 20–21, 2022

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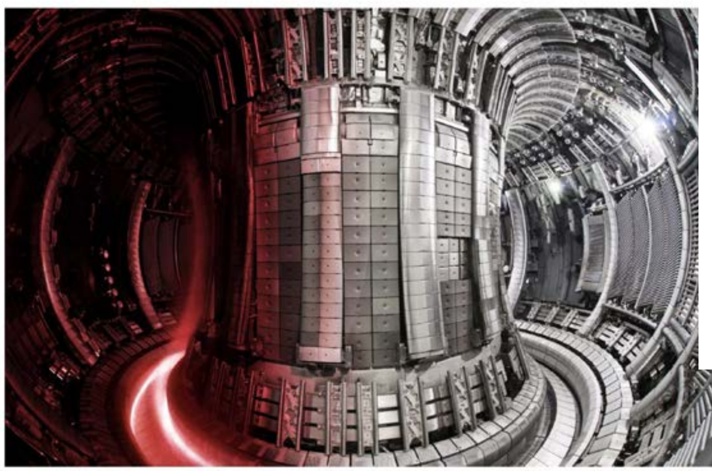

Refined FPNS requirements resulting from the 2018 FES workshop [4], 2020 APS DPP CPP [5] and 2021 *MASCO* [6] reports

Parameter	2018 Workshop Guidelines [4]	2021 Augmented Recommendations [6]
Damage rate	~ 8–11 dpa/calendar year (Fe)	Time averaged rate during beam-on period. Integrated over irradiation time. Required for >70% of sample volume.
Spectrum	~10 appm He/dpa (Fe)	~40 appm H/dpa(Fe)
Sample volume in high flux region	≥50 cm3	Ability to accommodate in situ control and measurement capabilities
Temperature range	~300–1000°C	–
Temperature control	Three independently monitored and controlled regions	Ability to maintain within 5% of target temperature (Kelvin) at a reference point in each temperature zone.
Flux gradient	≤20%/cm in the plane of the sample	Spatial variation <10% along 6 mm length in beam-normal plane within at least 70% of all temperature zones.

Fusion Materials Current Readiness

• Thermo-mechanical properties of candidate structural materials (RA/FM: Reduced activation ferritic-martensitic steels, NFA: Nanoscale oxide dispersion strengthened ferritic alloys, V: Vanadium alloys, W: Tungsten, SiC: Silicon Carbide, Adv Mat: ***to be developed*** advanced material)

	0 – 5 years						5 – 15 years						>15 years					
Data Base Need	10 dpa/100 appm He						50 dpa/500 appm He						150 dpa/1500 appm He					
	RAF/M	NFA	V	W	SiC	Adv Mat	RAF/M	NFA	V	W	SiC	Adv Mat	RAF/M	NFA	V	W	SiC	Adv Mat
Thermo-Mechanical Effects																		
Fatigue	Yellow	Red	Red	Red	Yellow	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
Thermal Creep	Yellow	Yellow	Yellow	Yellow	Yellow	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red
Creep-Fatigue Interaction	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red	Red

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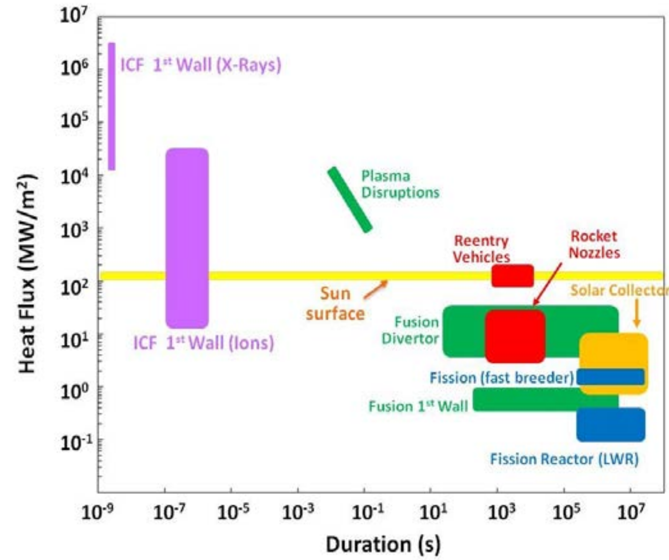
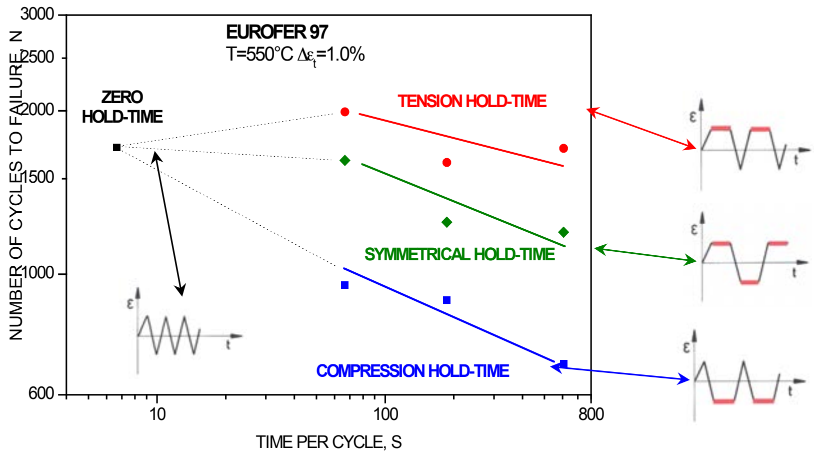
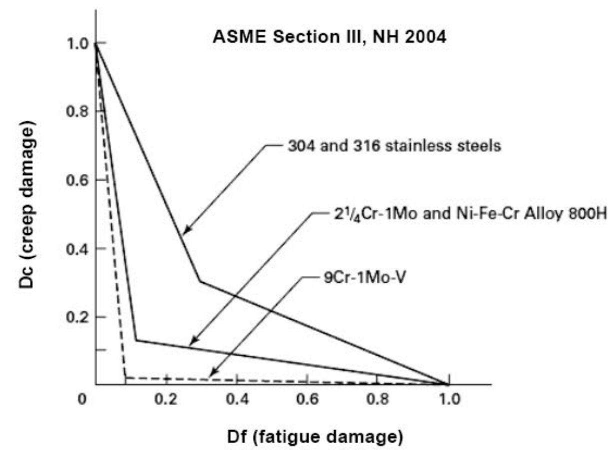
Fusion Materials Action Item: High Temperature design rules

- Current high-temperature design methods are largely empirical.
- New models of high-temperature deformation and fracture are needed for:
  - Creep-fatigue interaction.
  - Elastic-plastic, time-dependent fracture mechanics.
  - Materials with low ductility, pronounced anisotropy, composites and multilayers.
- Integrated materials-component-structure development, design and testing approach needed.



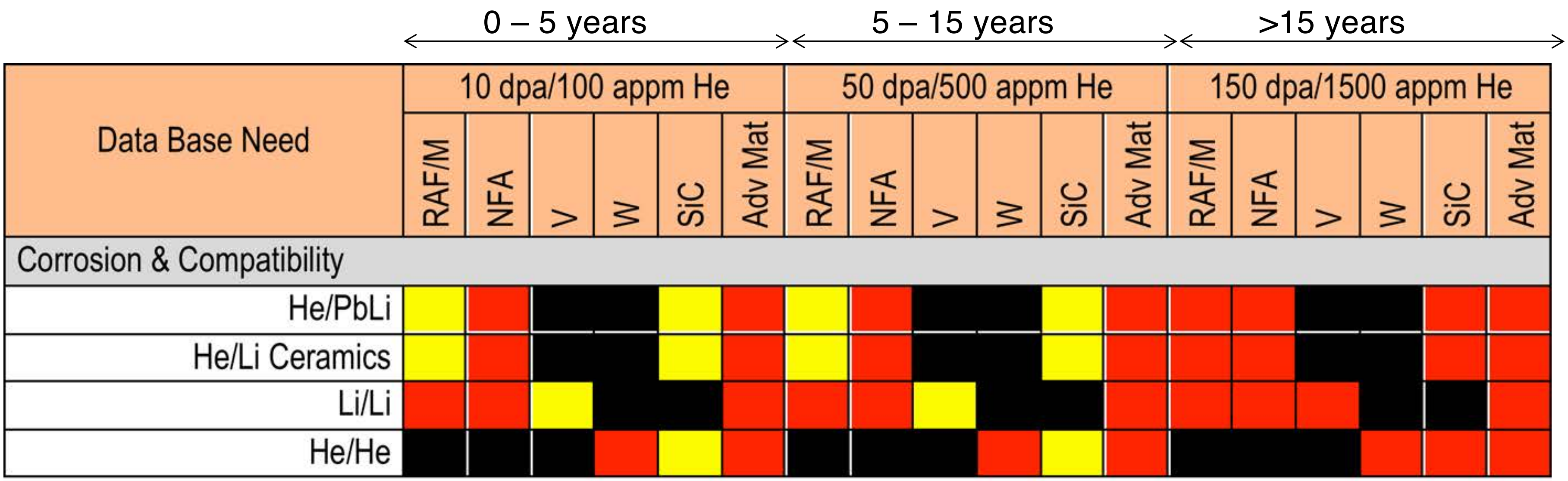
J. Aktaa & R. Schmitt, 2004





Fusion Materials Current Readiness

- Corrosion/compatibility knowledge to data largely based on isothermal exposures
- Significant need for flowing loop testing + coupled MHD/E-M effects (See Bruce Pint presentation)



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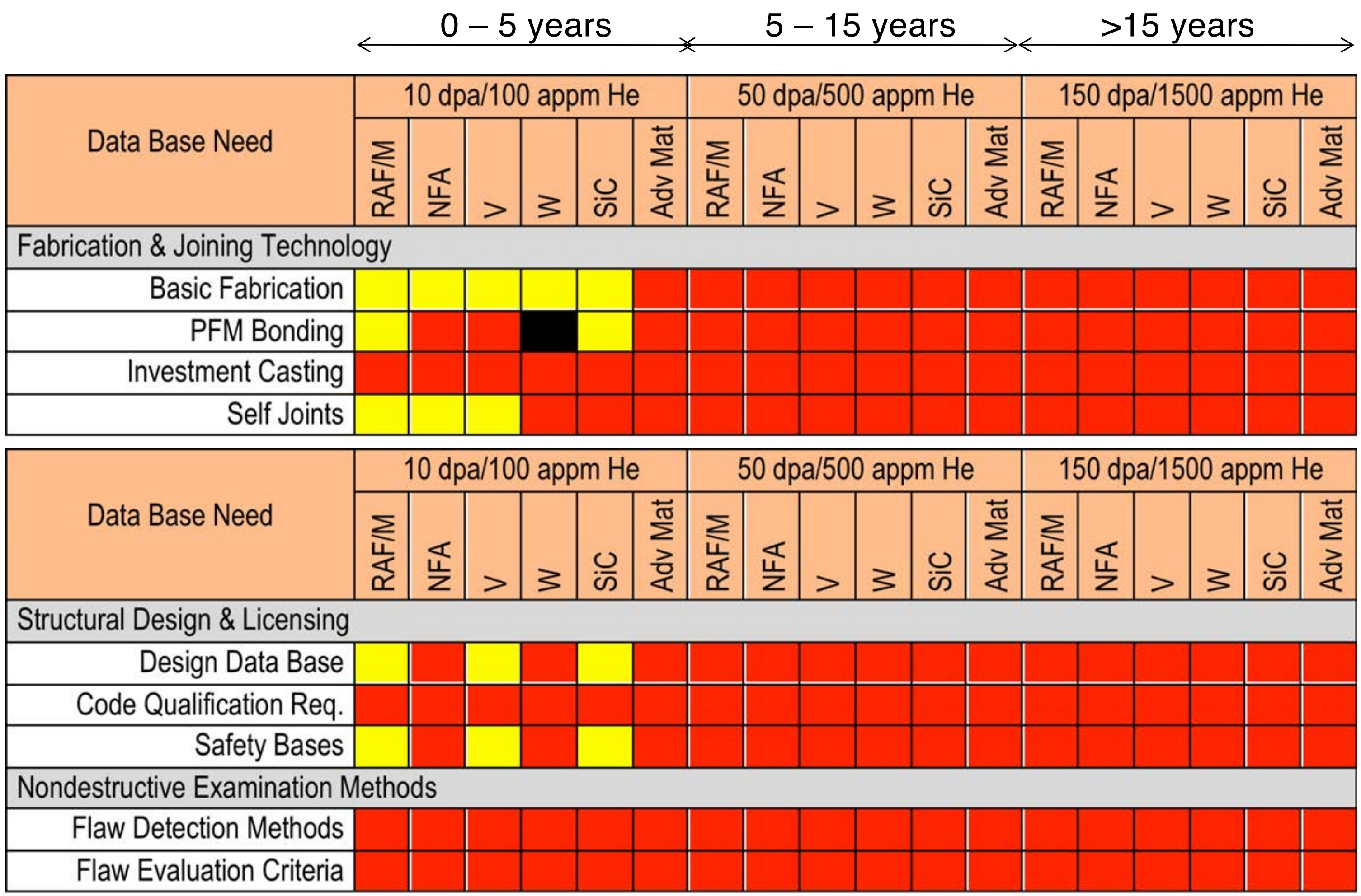
Fusion Materials Database: Current Readiness



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*Status of Vanadium alloys in fusion blankets**

Coolant	Compatibility	Effects of magnetic field	Tritium leakage	Tritium recovery	Tritium inventory in V-alloy	Technological challenge
Liquid Li	Minor	Critical (MHD pressure drop)	No	Critical	Minor	MHD coating T recovery
Li–Pb	Critical (oxidation, Pb attack)	Critical (MHD pressure drop)	Moderate to critical	Moderate	Moderate to critical	MHD coating Corrosion protection T permeation barrier
FLiBe	Critical (fluoridation, oxidation)	Moderate (thermofluid)	Critical	Moderate	Critical	Corrosion protection T permeation barrier
He	Critical (oxidation, nitriding)	No	No	Critical	Minor	Corrosion protection T recovery

- Corrosion, MHD and tritium barrier coatings require substantial R&D effort, and lack of stable coating technology led U.S. Fusion Materials Program to de-prioritize V-4Cr-4Ti alloys *(shifted to dual-cooled lead-lithium blanket with SiC flow channel inserts and RAF/M structure)*

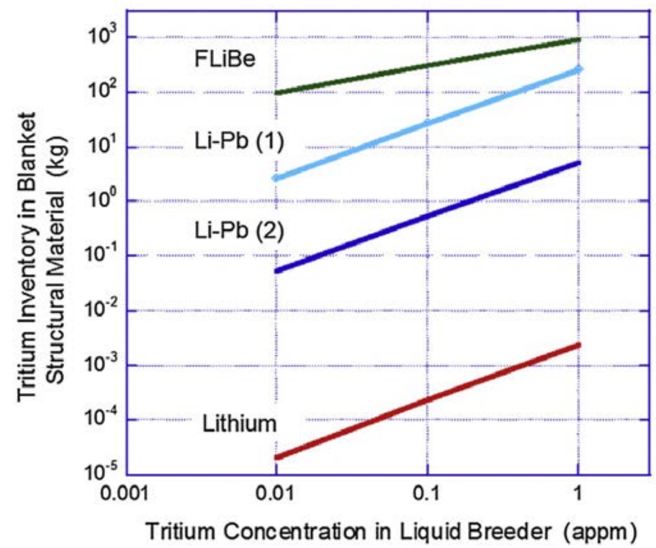


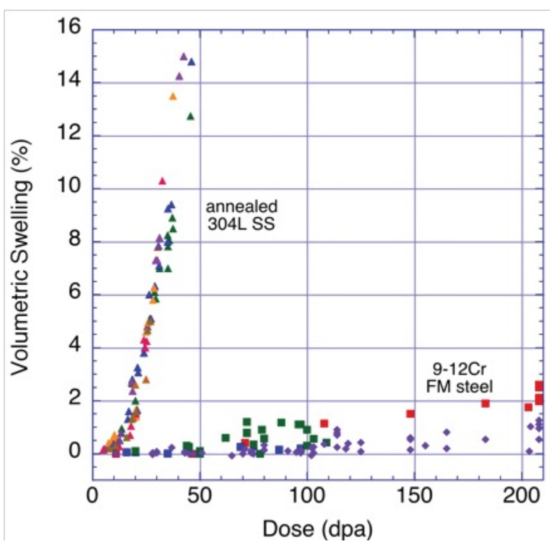
Fig. 1. Equilibrium tritium inventory in V–4Cr–4Ti structural materials at 1000 K for three tritium breeders as a function of tritium level in the breeders assuming self-cooled FFHR reactor [16]. The physical values assumed were shown in the text.

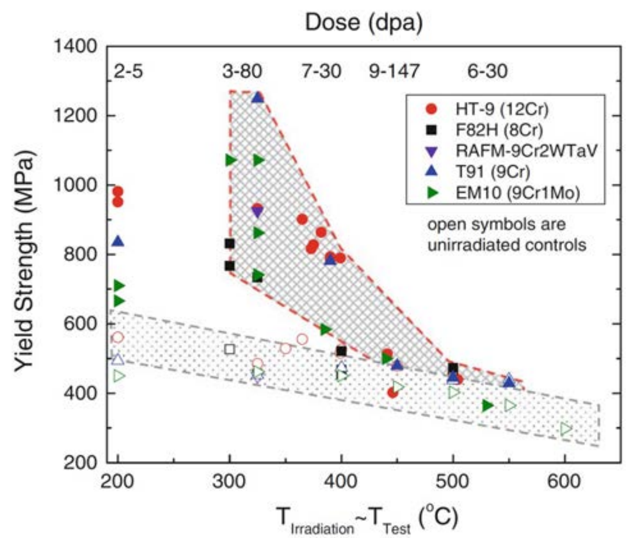
*Ref: T. Muroga, J.M. Chen, V.M. Chernov, R.J. Kurtz, M. Le Flem, *J. Nucl. Mater.* **455** (2014) 263-286.

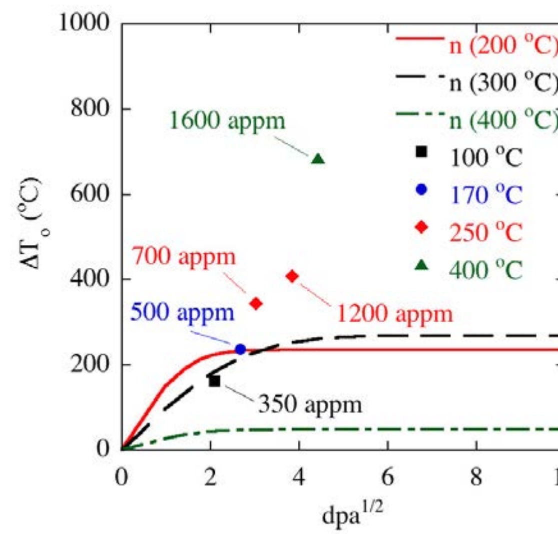
Reduced Activation Ferritic Martensitic Alloys for FPP

• NASEM pilot plant report notes “The scientific understanding of the neutron-induced degradation provides confidence up to a dose of 50 dpa/500 appm He (~5 MW-year m^{-2}) within the temperature range from 400 to 550°C”

- The data shown below **“provides confidence in RAFM structural materials for use in a fusion pilot plant, although the degradation service limit is not yet established.”**
- “However, RAFM materials have not been fully demonstrated in the complex environmental loading conditions of a fusion pilot plant, which include multiple combined degradation modes including neutron degradation, He and H gas generation from nuclear transmutation, injected ions and permeating tritium, significant and potentially time varying heat flux, complex mechanical loading, magnetic fields and corrosive coolants, including the effects of radiolysis. Materials development efforts must focus on meeting all the requirements of a recognized code standard.”







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Finding: Confidence exists in the ability of low-activation ferritic martensitic alloys to survive D-T neutron-induced degradation up to a dose of 50 dpa/500 appm He (~5 MW-year m^{-2}) at temperatures between 400 and 550°C; however, partially integrated testing is required to provide confidence in the performance of reduced activation ferritic martensitic components to the cyclic loading and environmental degradation required for Phase 1 and 2 operation of the pilot plant.

Finding: Due to the anticipated higher operating temperature of a fusion pilot plant, the design criteria and licensing will be significantly different than for light water fission reactors or ITER, and will require development to address unique components, higher operating temperature and time varying stress state, corrosive coolants and stress/temperature gradients.

Recommendation: The materials engineering community, supported by the fusion community and the Department of Energy, should develop high temperature structural design criteria that incorporate creep, fatigue, and corrosion behavior of in-vessel and ex-vessel structural and functional components to enable the engineering design and licensing of a fusion pilot plant as part of the conceptual design activities.

Materials – tritium issues require additional research

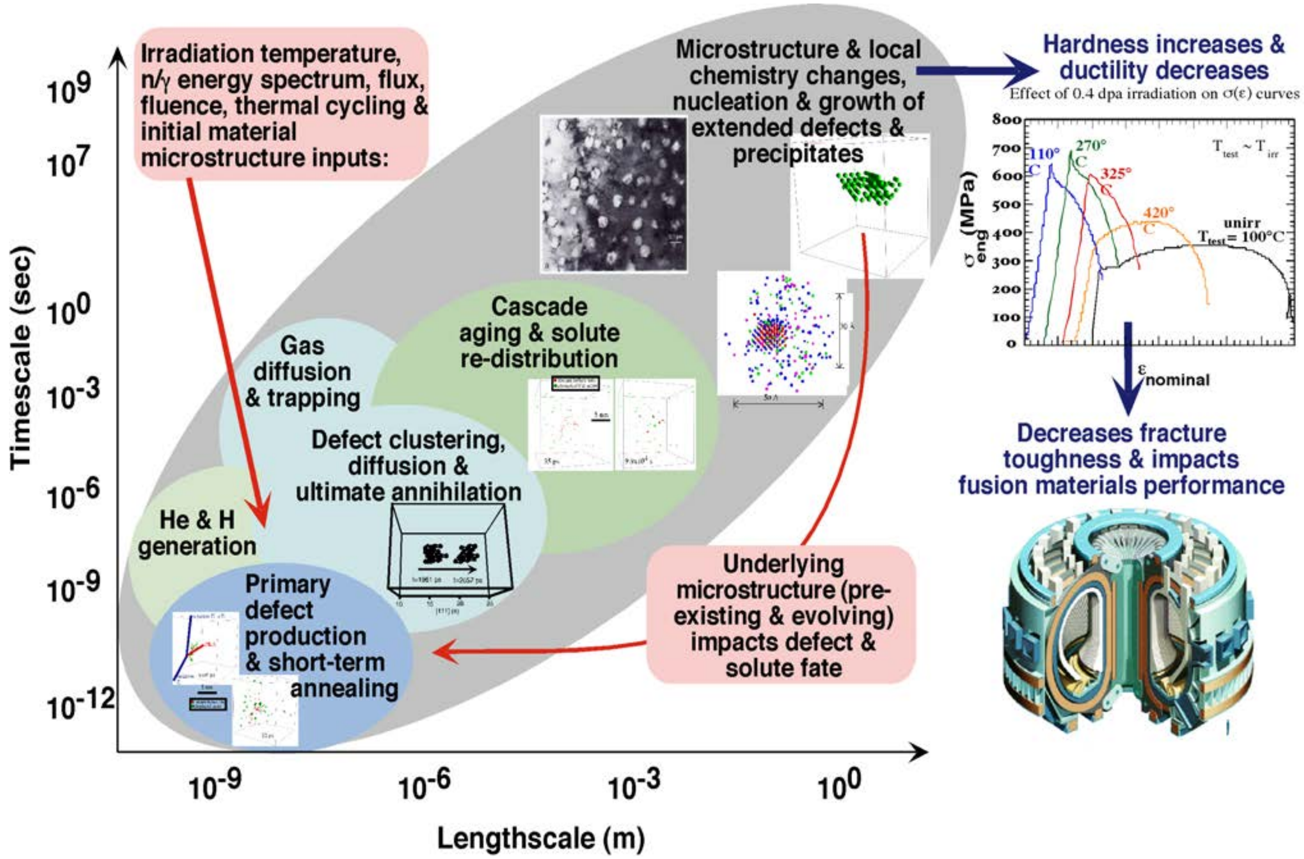
- Identification of a robust, efficient and economic method for extraction of tritium from high temperature coolants
  - Large number of potential tritium blanket systems is both advantageous and a hindrance
- Current materials science strategies to develop radiation-resistant materials may (or may not) lead to dramatically enhanced tritium retention in the fusion blanket
  - Fission power reactors (typical annual T_2 discharges of 100-800 Ci/GW_e; ~10% of production) are drawing increasing scrutiny
  - A 1 GW_e fusion plant will produce ~10^9 Ci/yr; typical assumed releases are ~0.3 to $1x10^5$Ci/yr (<0.01% of production)
  - Nanoscale cavity formation may lead to significant trapping of hydrogen isotopes in the blanket structure
  - Tritium trapping efficacy of precipitates and nanoscale solute clusters (blanket & piping) is poorly understood from a fundamental perspective

Integrated simulation for Fusion technology

Recommendation: To meet the challenge of having a viable design by 2028 and initial pilot plant operation in the 2035-2040, innovations in fusion confinement concepts and technology to extract fusion power and close the fusion fuel cycle should be developed in parallel. This will enable the engineering design of a pilot plant and the construction decisions to be accelerated by a combination of government and private funding.

- Modeling and simulation incorporating multiple physics and multiscale phenomena with increasing fidelity into simulations to evaluate and refine design options
  - High fidelity simulations will benefit from exascale computing and enable reduced models including via artificial intelligence.
- Physics, system and process models can be combined into comprehensive full device models which will likely contribute to evaluating the operations and maintenance of the pilot plant
- Engineering computer aided design, structural analysis and process and control modeling will provide an important opportunity to optimize the design and integration of the fusion pilot plant

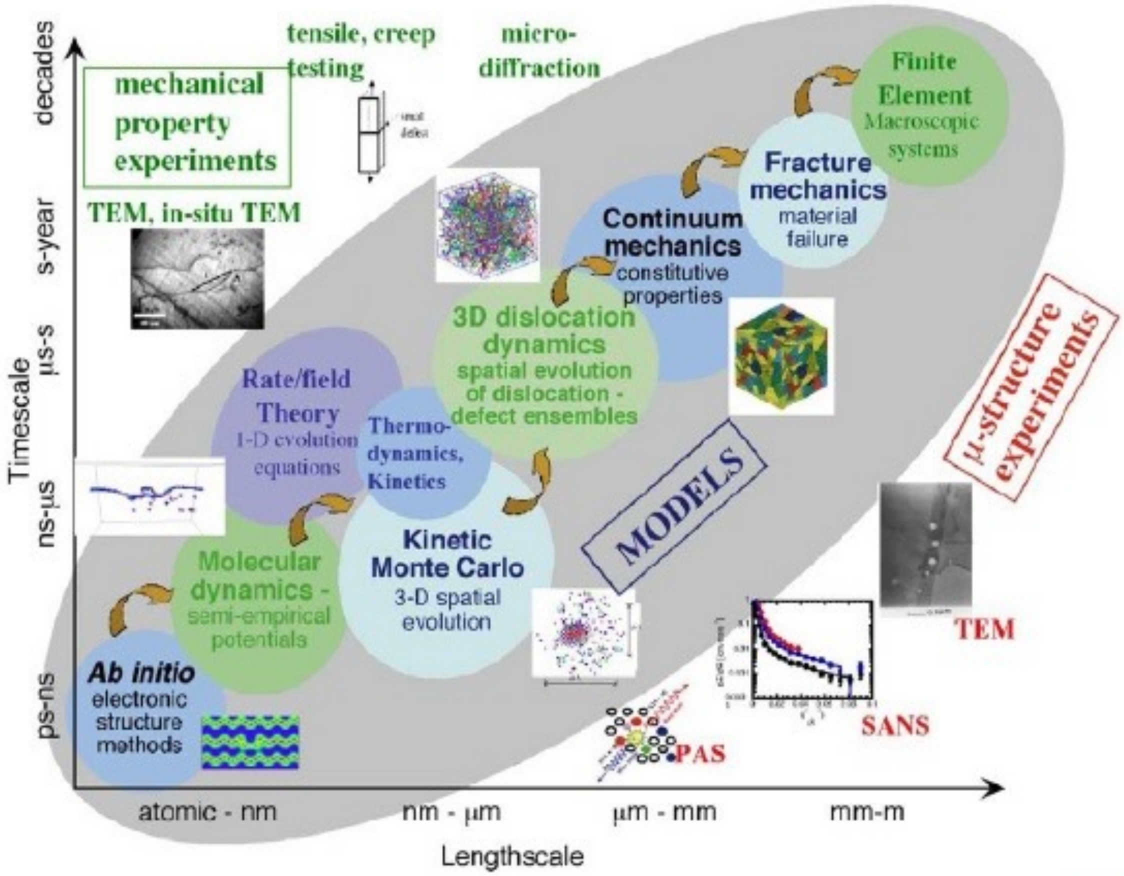
Fusion materials degradation is multiscale



Radiation damage produces atomic defects and transmutants at the shortest time and length scales, which evolve over longer scales to produce changes in microstructure and properties through hierarchical and inherently multiscale processes

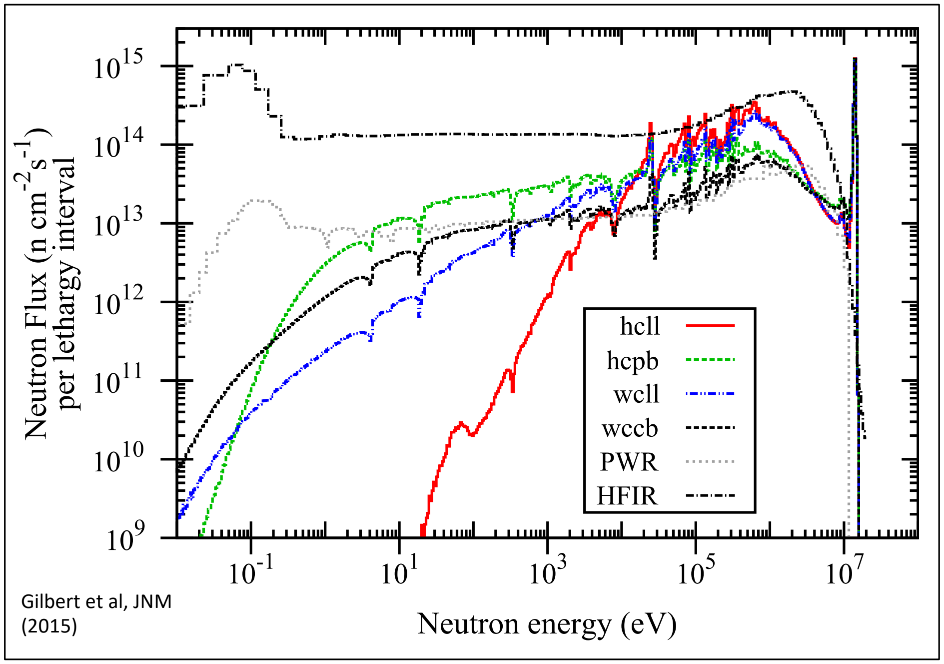
Fusion materials degradation is multiscale

Uncertainties and errors are found –and ideally must be quantified– at every possible level



Significant opportunity for & examples of computational thermodynamics to tailor improved materials properties (advanced ferritic/martensitic alloys, Cu-based alloys, etc.)

Primary damage & opportunities to utilize multi-ion beams

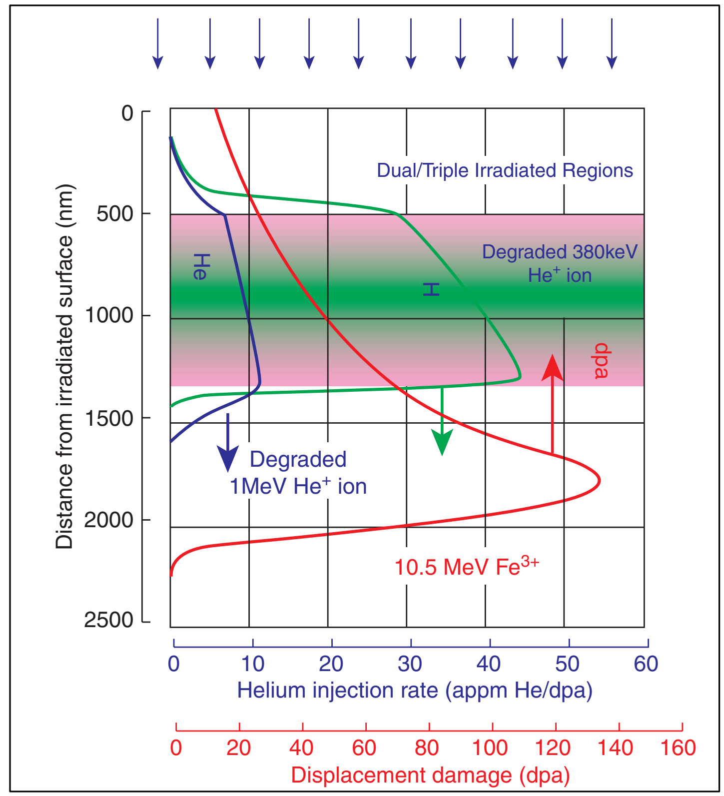


$$k = \rho_a \int \sigma_d(E)\phi(E)dE$$

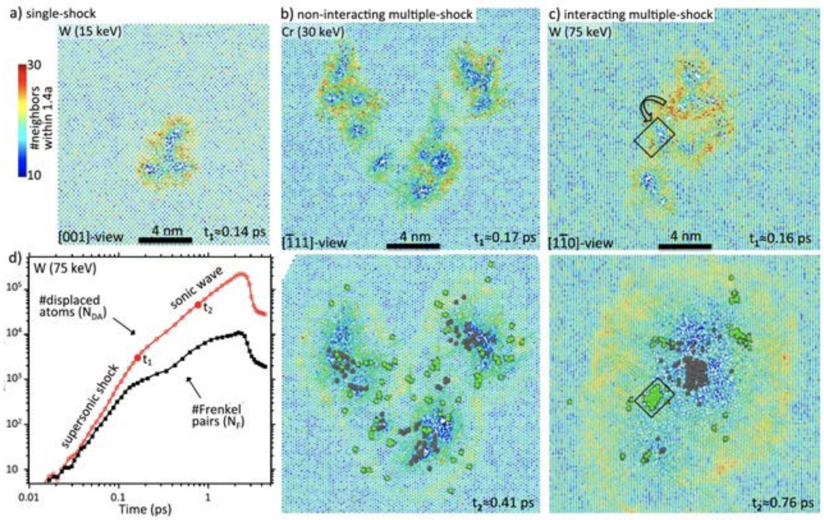
$$\sigma_d(E) = \int_{E_{th}}^{E_{\max}} \sigma_n(E,T)\nu(T)dT$$

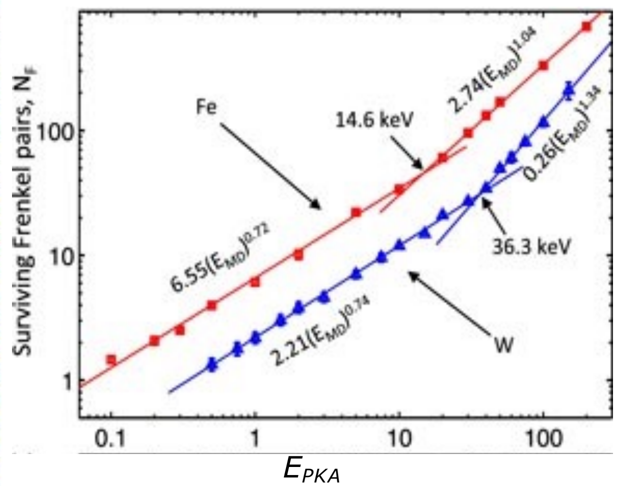
Neutron data libraries

Multiple ion beam irradiations can provide additional scientific data about coupled defect – He – H radiation effects

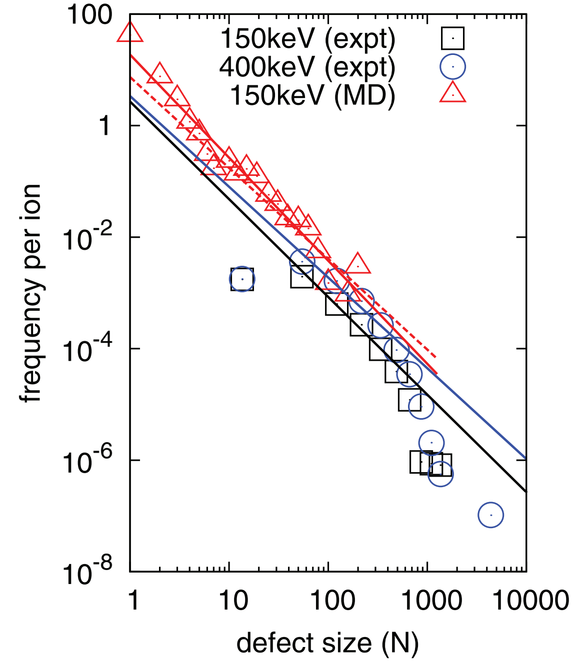


MD simulations of initial damage state





Setyawan et al, JPCM **27** (2015) 225402

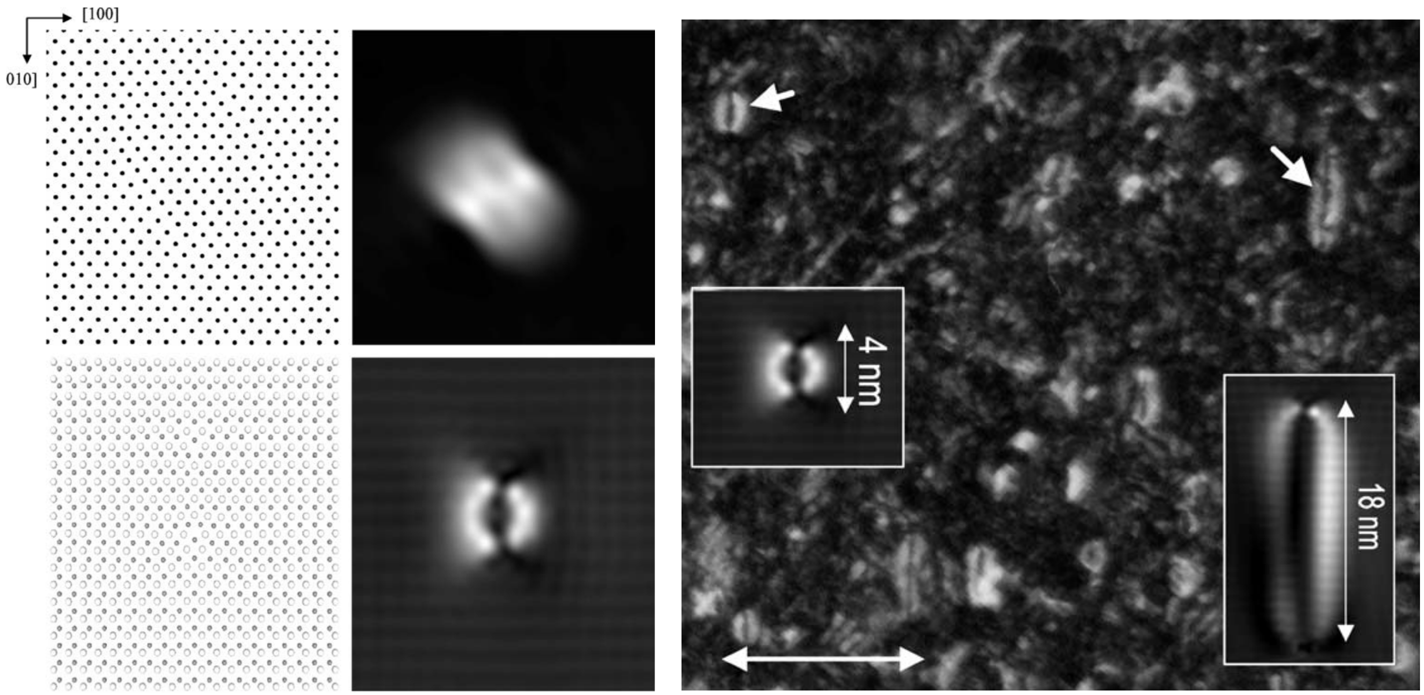


Yi et al, EPL (2015)

- Extensive simulation data exists for initial defect distributions and defect production

MD can also accurately simulate the structure of large defects

Marian, Schaublin, Wirth, Perlado (2002-2005)



Molecular dynamics can be used to validate structure of complex defects such as large dislocation loops (results for Fe-Cr alloy neutron irradiated to 8.8 dpa)

DFT calculations for fundamental defect properties

- Advantages

  Can give the most reliable estimate currently available for quantities not accessible through experiments:

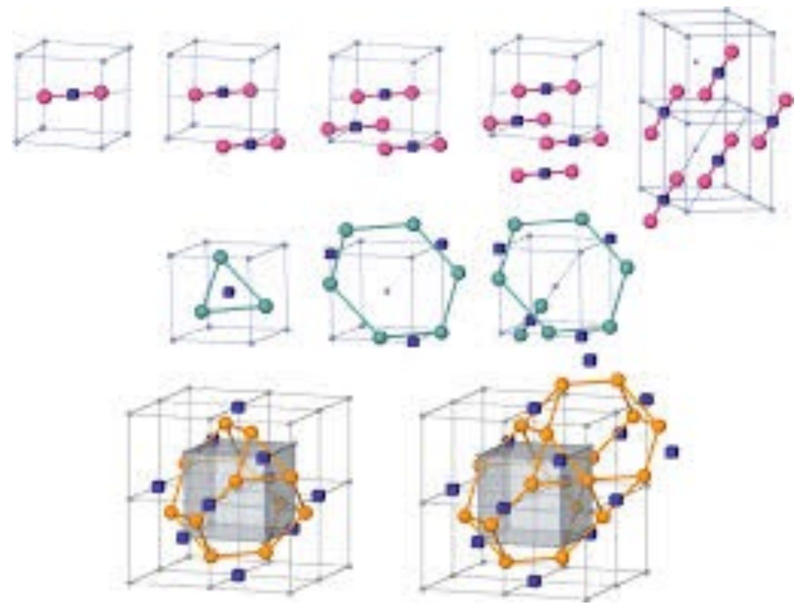
  – Defect formation energies, binding energies, saddle point energies, …

- Drawbacks

  Numerically very expensive:

  – Size of the system limited to max. ~10^3 atoms (less for metals)

  – Essentially used only for static calculations



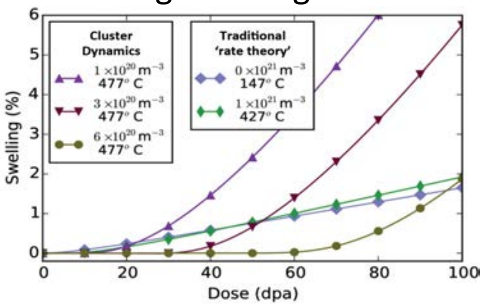
DFT methods have been crucial in predicting the structure of primary defects in metals.

Ventelon et al, 2010, 2012, 2013,2015

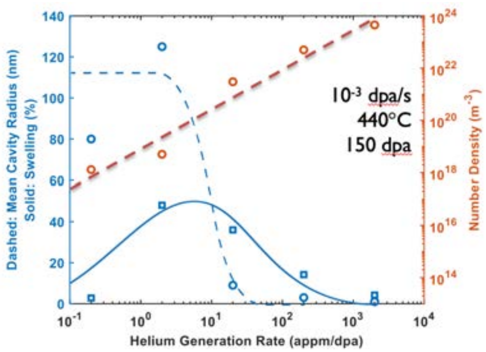
Mesoscale cluster dynamics can simulate defect cluster evolution

Array of rate equations: $\frac{dC_n}{dt} = \underbrace{D_n \nabla^2 C_n}_{\text{Spatial Diffusion}} + \underbrace{R_n(C)}_{\text{Aggregation and recombination}} - \underbrace{D_n k_n^2 C_n}_{\text{Loss at sinks}} + \underbrace{g_n}_{\text{Production in cascades}}$

Modeling Swelling in F-M steel

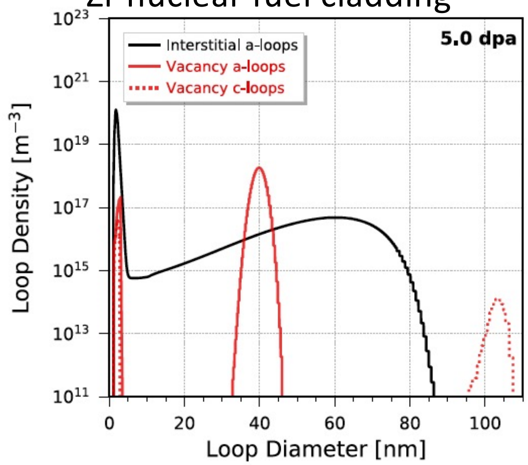


Modeling Swelling in dual-beam irradiated F-M steel



S. Taller et al., *Scientific Reports* **11** (2021) 1-14.

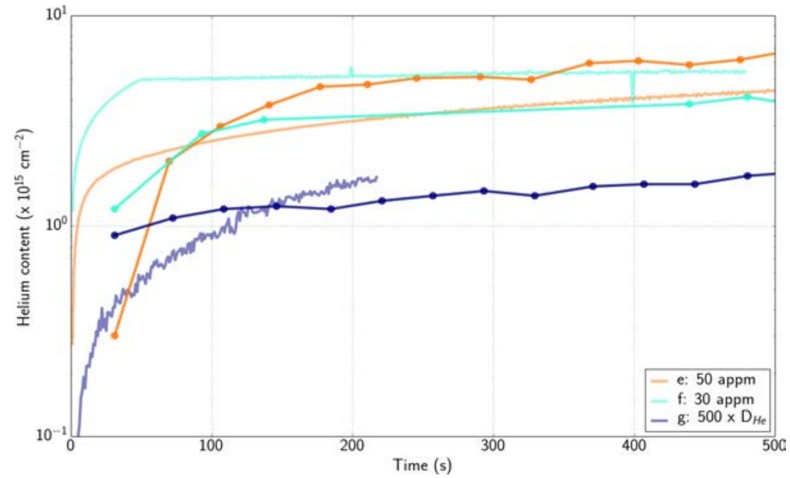
Modeling interstitial and vacancy loop evolution in α-Zr nuclear fuel cladding



Xolotl is open-source cluster dynamics code developed by Plasma Surface Interaction SciDAC and applied to divertor surface evolution and gas content, nuclear fuel swelling and radiation damaged microstructures

https://github.com/ORNL-Fusion/xolotl

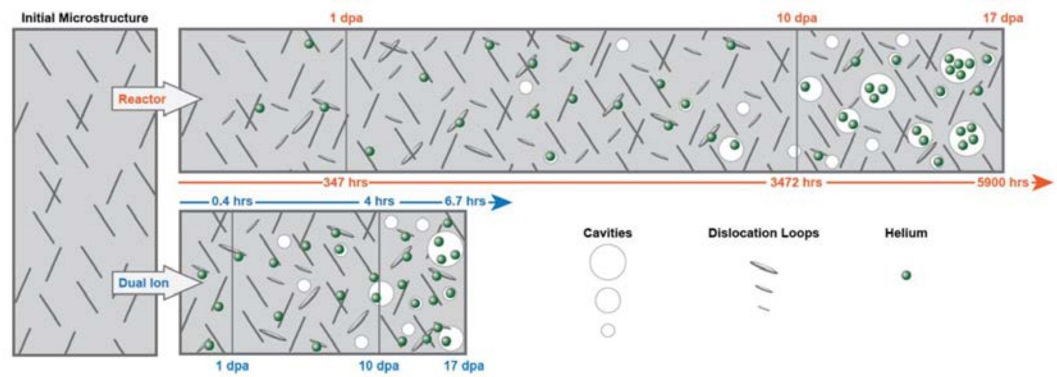
He content in plasma-exposed Tungsten

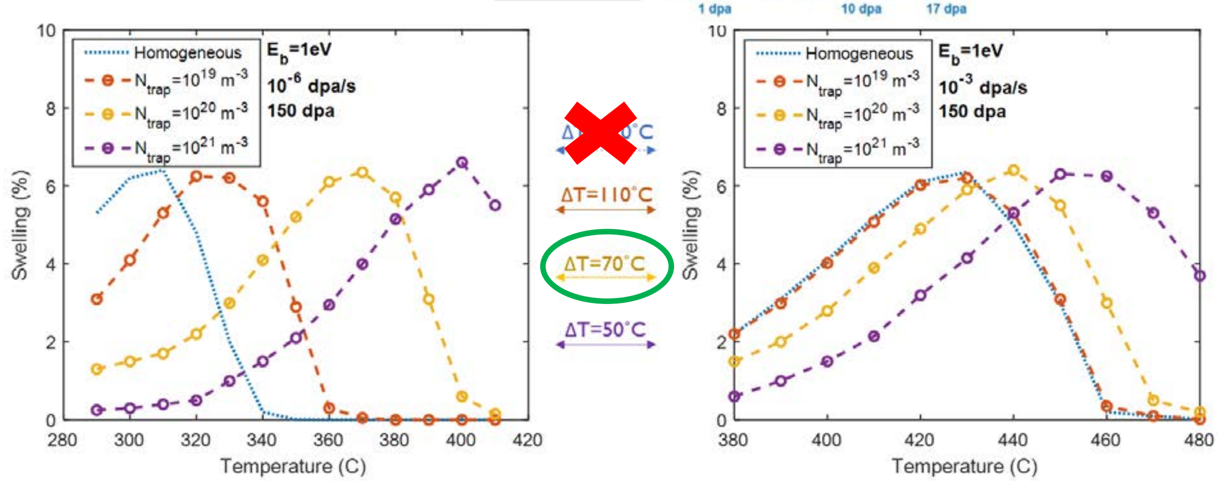


S. Blondel et al., *Nuclear Fusion* **58** (2018) 126034.

*Modeling predictions of Ion irradiation temperature shift – relative to fast neutron irradiation**

- Incorporation of helium trapping sites to account for He partitioning in microstructure & provides effective cavity nucleation sites at high dose rates (ion irradiation)





Enhanced nucleation from helium trapping predicts experimentally observed temperature shift that leads to ion irradiation replicating Bor-60 irradiated microstructures

*S. Taller, G. Van Couvering, B.D. Wirth and G.S. Was, *Scientific Reports* **11** (2021) 1-14.

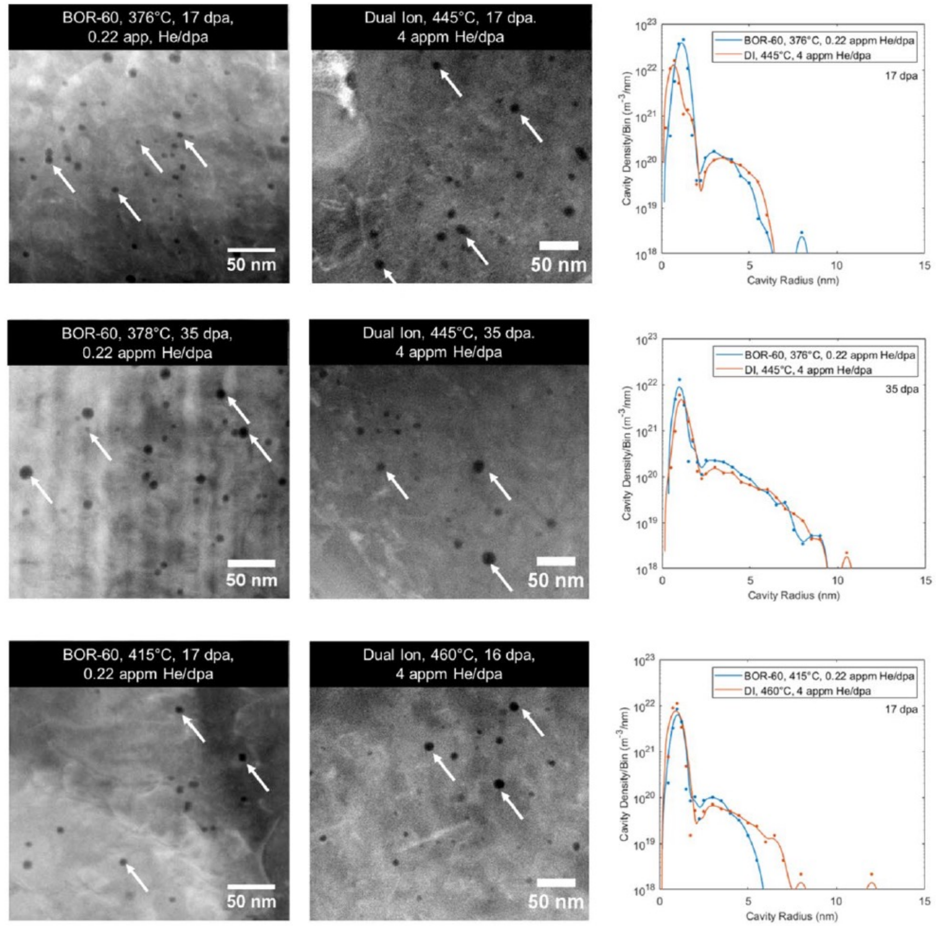
Good agreement results between dual ion & fast reactor irradiated microstructures*

BOR-60 DI

BOR-60: 376°C:17 dpa
DI: 445°C:17 dpa

BOR-60: 378°C:35 dpa
DI: 445°C:35 dpa

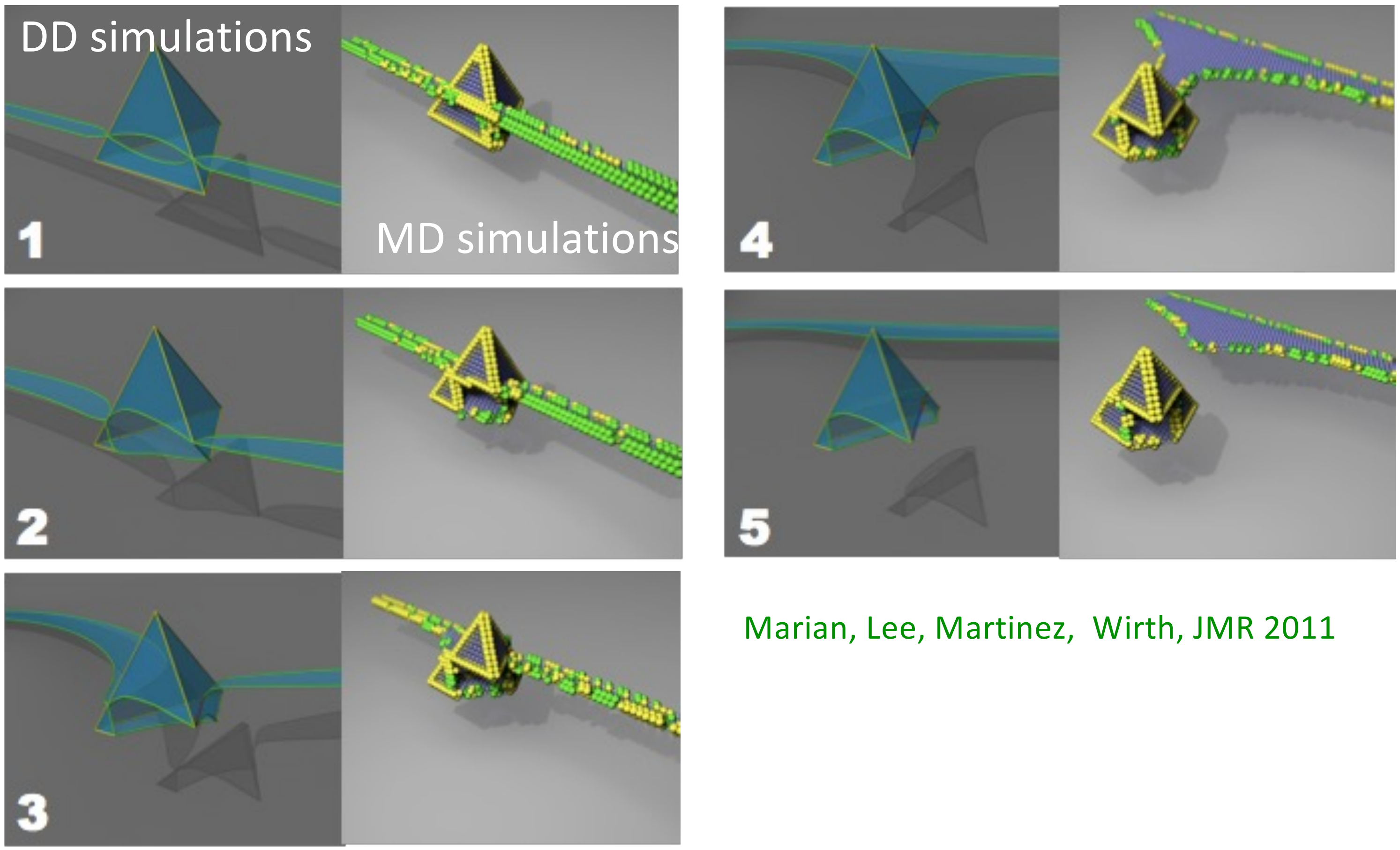
BOR-60: 415°C:17 dpa
DI: 460°C:16 dpa



*S. Taller, G. Van Couvering, B.D. Wirth and G.S. Was, *Scientific Reports* **11** (2021) 1-14.

Connecting atomic and continuum scale dislocation plasticity

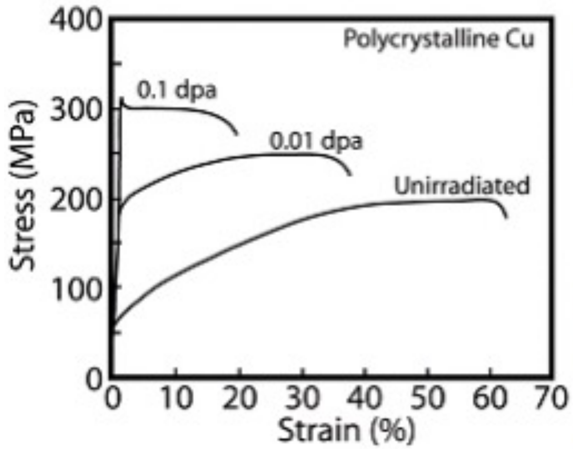
Simulations of dislocation-SFT interactions in irradiated Cu



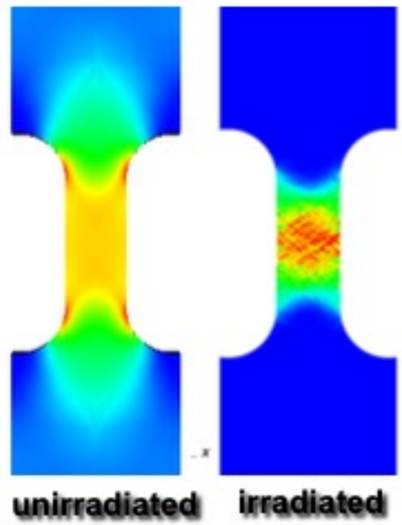
Marian, Lee, Martinez, Wirth, JMR 2011

Polycrystal plasticity to predict stress-strain response

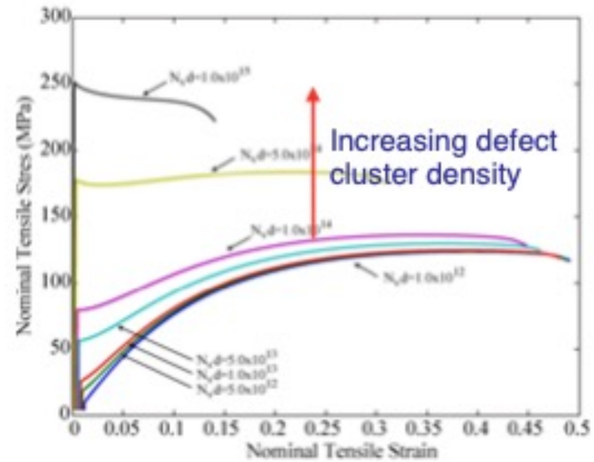
Tension Experiments*



B. N. Singh et al,
J. Nucl. Mat. **224,** 131 (1995).



Full FEM Tension Simulations



Plastic instability in tension geometry leads to flow localization and failure

•Isotropic polycrystal plasticity incorporates coarse grained scaling laws governing dislocation density evolution and interactions determined for single crystals
•Dislocation - (radiation damage) defect interactions included based on MD simulations
•Resulting models can be further modified to include the effects of dispersed particles, solute atoms, and other known resistance mechanisms

Arsenlis, Wirth and Rhee, *Phil. Mag*. **84**, 3617 (2004).

Summary: Structural Materials development status & needs

- Recent community prioritization has emphasized the need, and the urgency, for expanding efforts in fusion technology related to materials development for applications in PMI, blankets, structural components, including the use of multiscale-multiphysics modeling & simulation

- Reviewed status of reduced activation structural materials development & outstanding issues
  - Confidence in reduced activation ferritic/martensitic alloys for use in a fusion pilot plant (for few environmental cycles), although the degradation service limit is not yet established. And, many unresolved questions with dose rate & He/dpa (thermal/radiation cycling)
  - Vanadium alloys have promise, but require substantial R&D for MHD & tritium barrier coatings (also controlling impurity/embrittlement effects)
  - Significant effort needed to develop high temperature materials design rules in creep/fatigue deformation regimes & to further evaluate He embrittlement limits

- Most significant development needs include: Blanket technology, structural materials development for blankets, including environmental degradation and tritium permeation/retention, and 14 MeV prototypic neutron source

Summary: Computational Multiscale Materials Modeling

• Computational multiscale materials modeling has demonstrated ability to model complex, radiation effects in Fe-Cr based alloys and Cu across a range of length and timescales, and is nearing the point of confidence that models could be used in alloy design and prediction of 14-MeV radiation damage response in fusion environment, but require further quantification of uncertainties at each scale & propagated

- Defect production physics well established and transmutation cross-sections known
- Computational thermodynamics is a powerful tool within alloy design (not shown here)
- Successful demonstration of atomistically-informed meso-scale cluster dynamics modeling of defect cluster evolution and He-dpa synergies in cavity nucleation
- Demonstration of crystal plasticity and dislocation dynamics coupling to atomistic and meso-scale models is able to predict mechanical property (stress-strain) changes
- Biggest modeling challenges relate to multiscale time integration across rare dynamics and modeling multi-component alloys with transmutant impurities

• Integrated scientific approach utilizing computational modeling & experimental irradiations and characterization is required to further develop and qualify structural materials for commercial fusion reactors (High Performance Computing in and of itself will not be sufficient to bridge the gap)

- Substantial opportunities to extend systematic modeling & experiments towards other fusion power plant components, most notably in the blanket & tritium handling systems, which also face extreme neutron fluxes and chemical environments