Recent Advances in Radiation Materials Science from the US Fusion Reactor Materials Program

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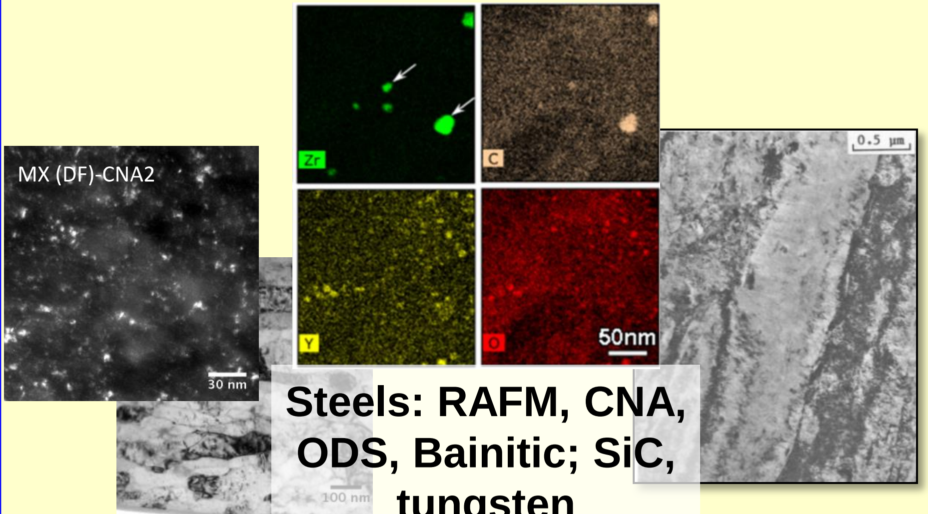
Introduction

- US fusion reactor materials (FRM) program coordinates efforts across several institutions, employs an integrated approach of computational materials science and extensive irradiation programs (primarily HFIR)
- augmented by research on plasma-materials interaction and reactor design studies, extensive international collaborations
- focused on radiation effects in candidate materials with emphasis on:
  - advanced ferritic-martensitic (FM) steels, including oxide-dispersion-strengthened (ODS) and castable nanostructured alloy (CNA) variants,
  - SiC and SiC/SiC composites
  - tungsten and possible W alloys
  - properties of interest include: microstructural stability, dimensional stability (e.g. swelling and creep), mechanical properties (e.g. strength and ductility), physical properties (e.g. thermal conductivity), response to high heat flux testing
- primary international collaborations:
  - Nat. Inst. for Quantum and Radiological Science and Technology (Japan)
  - PHENIX (Japanese universities)
  - EUROfusion/KIT (EU, in preparation)

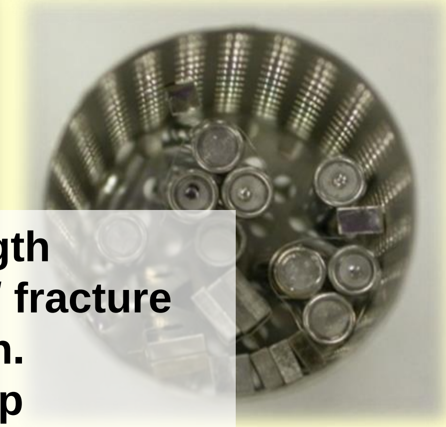
Current US Program Activities – FM Steels

Alloy (Material) Development



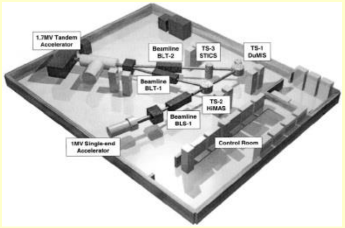
Steels: RAFM, CNA, ODS, Bainitic; SiC, tungsten

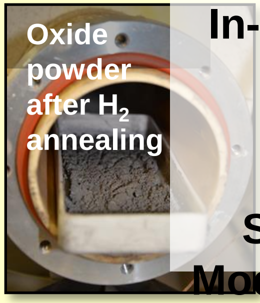
Fission Neutron Irradiation

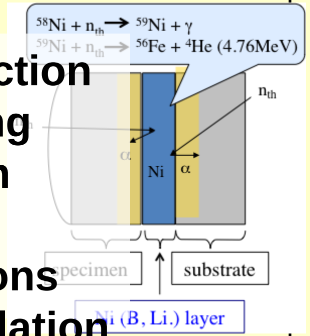


Strength
Toughness / fracture mech.
Creep
Microstructures

He Effects

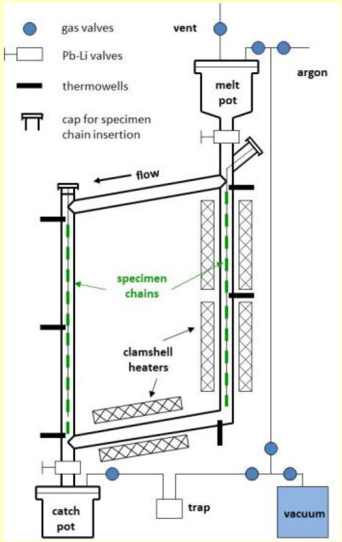


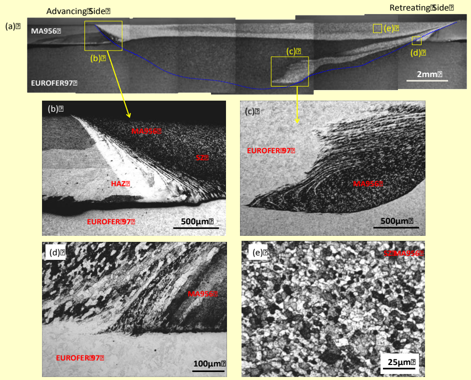




In-situ helium injection
Isotopic tailoring
Multi-beam ion irradiation
Spallation neutrons
Modeling and simulation

Others

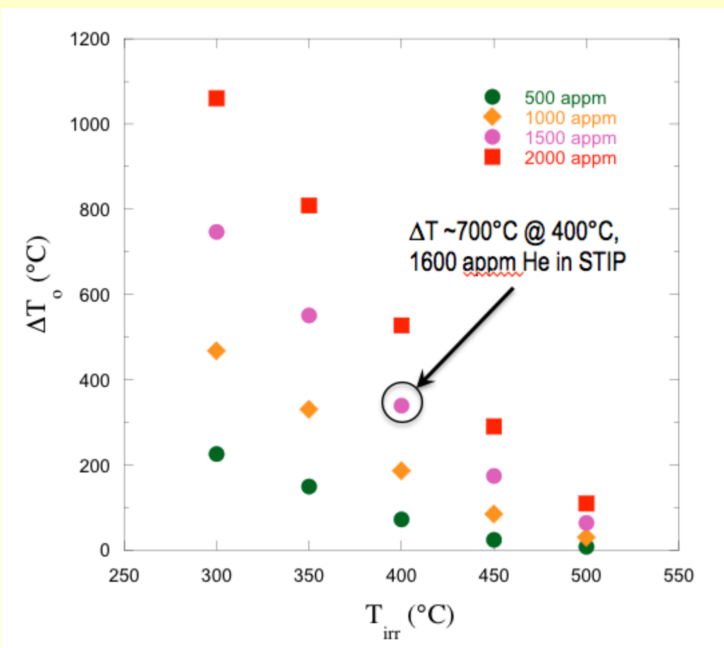


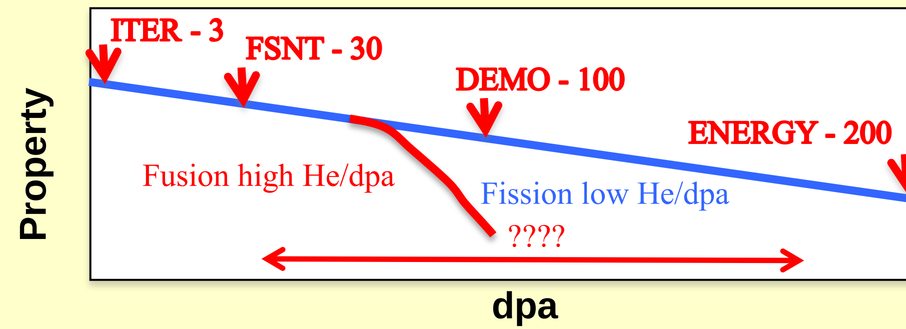


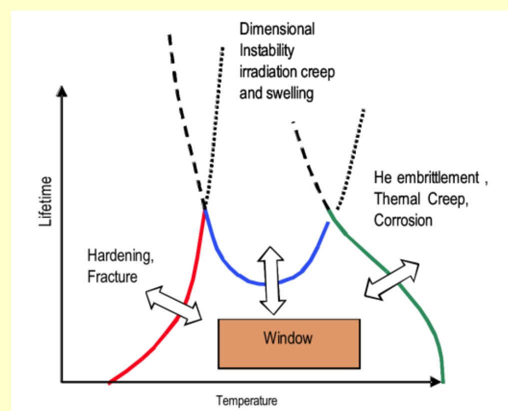
Chemical compatibility
Joining and welding

Helium: Fusion Materials Grand Challenge

- He effects remain a major unquantified challenge for fusion structural materials – **<u>lack of fusion-relevant irradiation facility</u>**
- Scientific challenge - understanding and modeling
- Engineering challenge - predicting and mitigating
- Developing quantitative physically based predictive models for how properties change as f(dpa, He, T_i, alloy, test conditions).

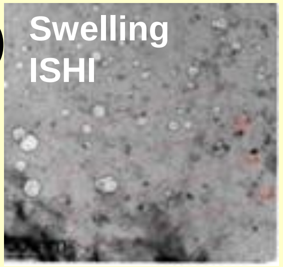


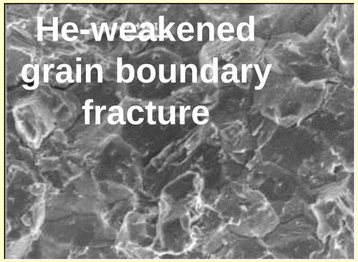




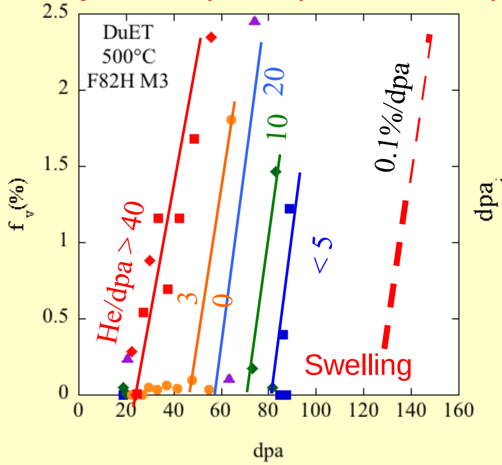
FM He Effects: Swelling, Hardening and Fracture

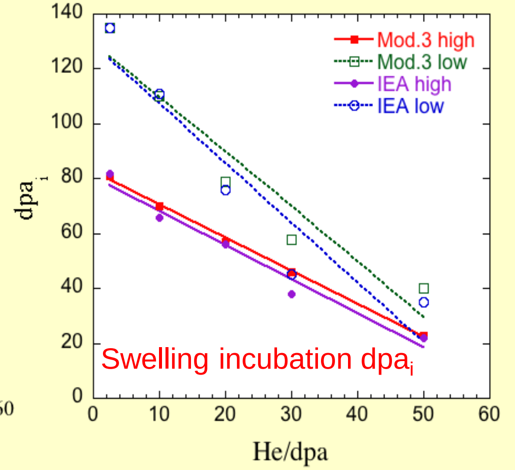
- ISHI[1], DI[2], STIP[3] ΔV/V incubation dose=f(He/dpa)
- High He expands $\Delta\sigma_i$ dpa and T-range (STIP)
- Possible He threshold ≈ 500 appm
- He transport-fate-consequences master model

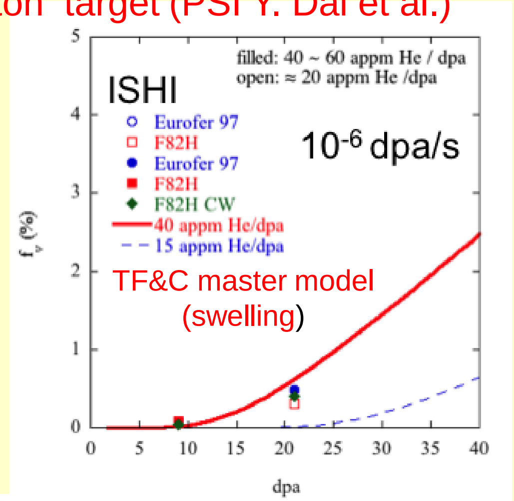


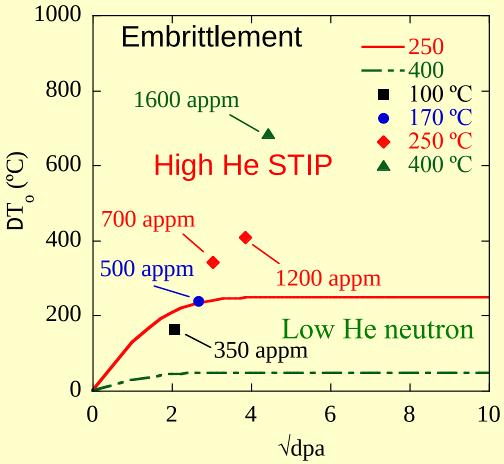


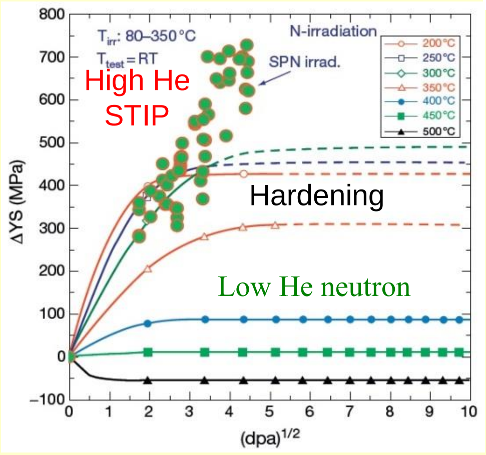
[1]In situ He injection (HFIR) [2]Dual ion (DuET Kyoto) [3]Spallation proton target (PSI Y. Dai et al.)

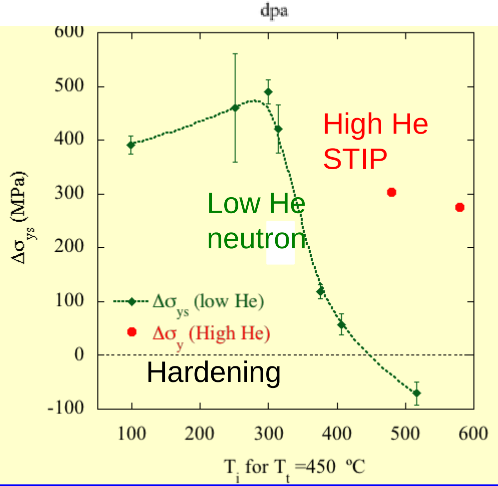






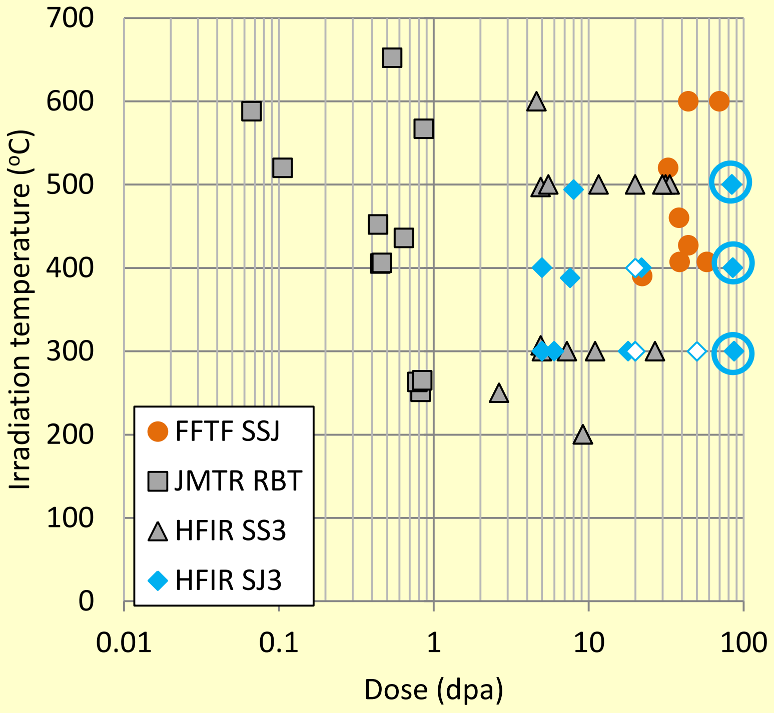




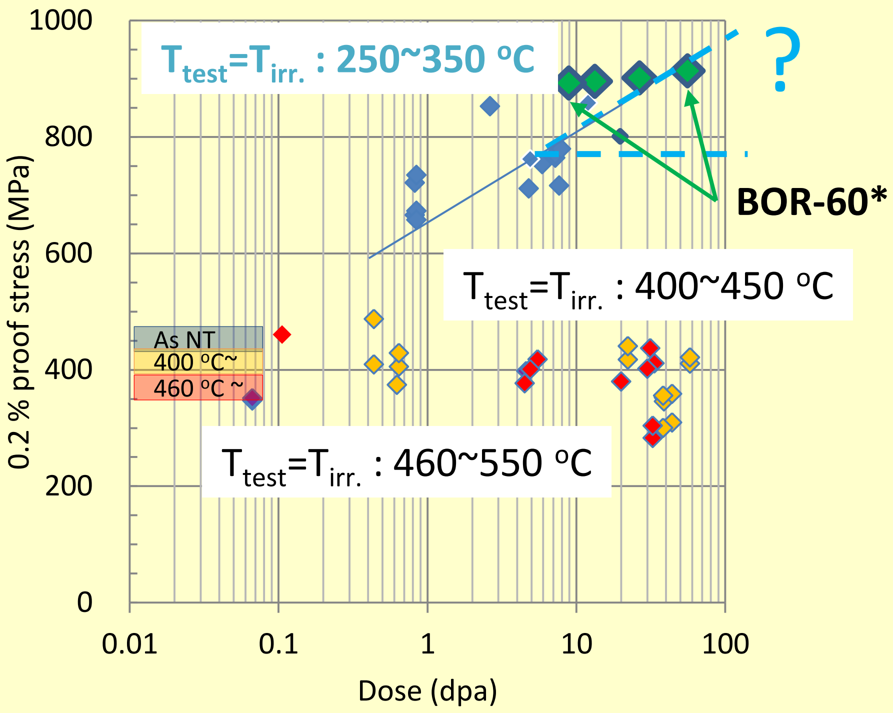


Radiation Effect Studies in FM Steels

Irradiation test matrix for F82H



Post irradiation tensile tests on F82H



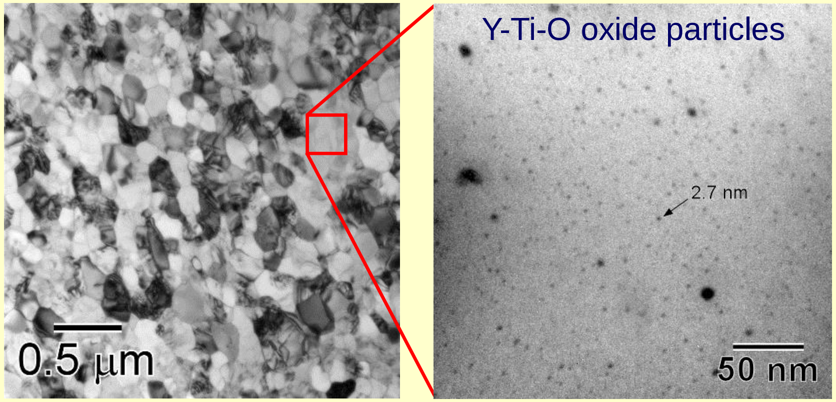
- Neutron irradiation studies on fusion steels are conducted HFIR primarily in DOE-QST collaboration.

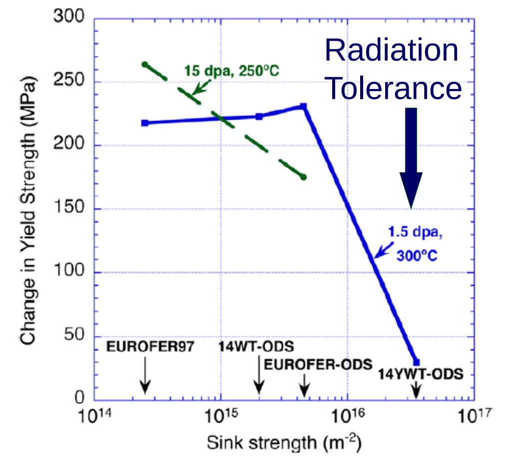
Development of ODS alloys for fusion systems

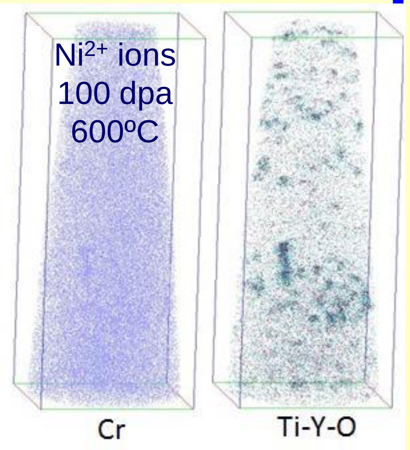
Two paths are being pursued

1) ODS Fe-Cr for very high performance: 14YWT developed starting in 2001

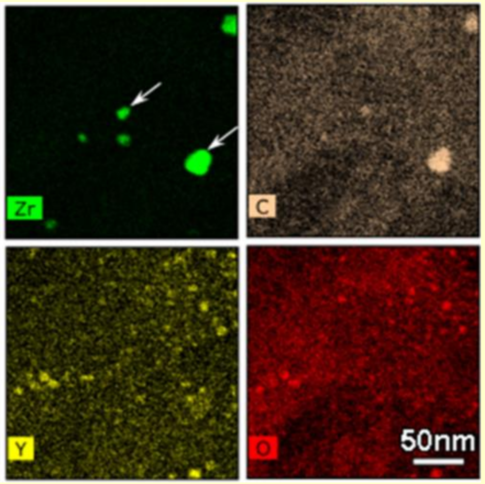
Ultra-small grains & high ND of nano-size oxides → High sink strength → Radiation Stability



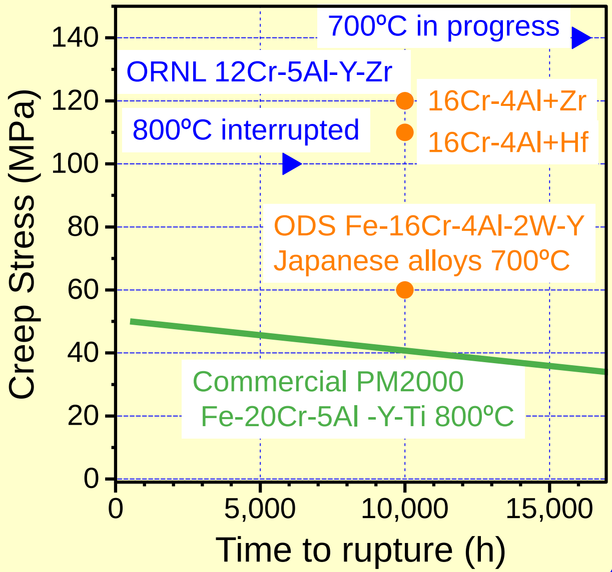




2) ODS Fe-Cr-Al for Pb-Li compatibility

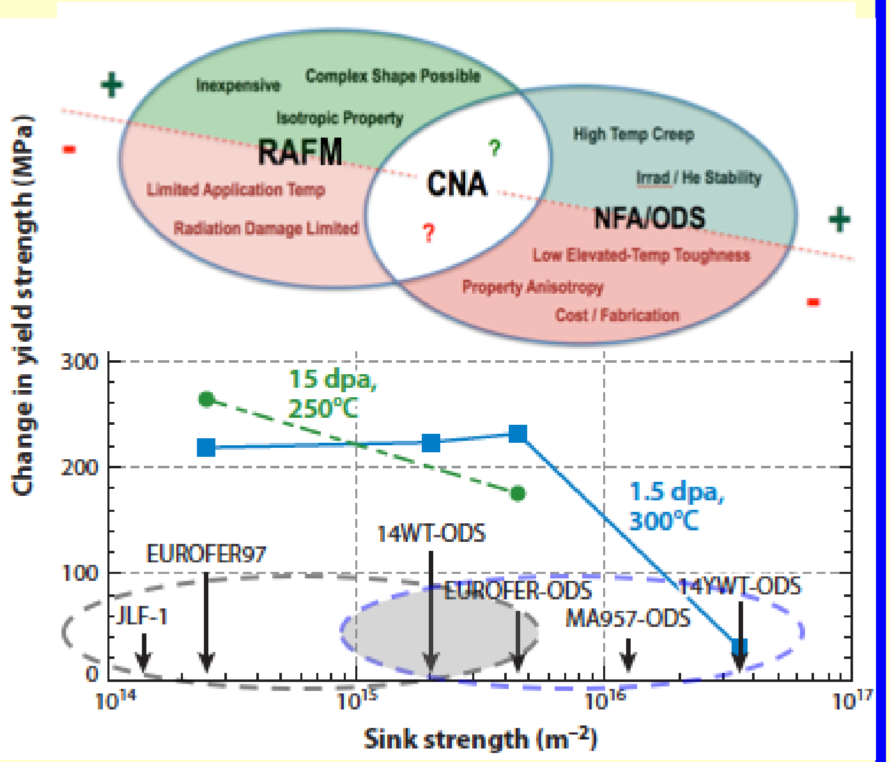


- ODS Fe-12Cr-5Al-Zr alloy exhibited unprecedented creep resistance at 700-800°C due to fine $Y_3Al_5O_{12}$ precipitates
- Co-precipitation with Zr(C,N) increased oxide particle number density
- Need irradiation testing



Castable Nanostructured Alloys (CNAs)

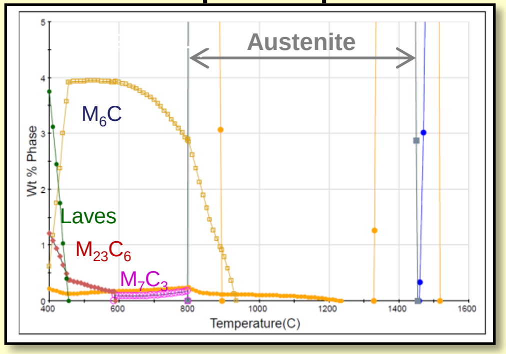
- With the aid of computational thermodynamics, CNAs are being developed to significantly increase the density of MX-type ultrafine precipitates.
  – It's expected to fill the gap between current FM steels and developmental NFA/ODS alloys in terms of radiation resistance and high-temperature strength.
- Strength and toughness are screened to down-select alloys for detailed studies.
- Preliminary ion irradiation experiment and weldability study showed promising results.
- Detailed property tests will be pursued on new heats from the down-selected alloys.

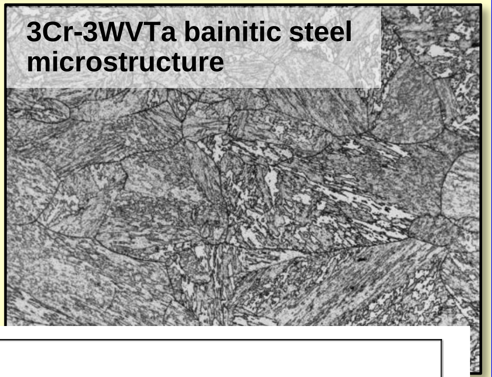


[L. Tan, L.L. Snead, Y. Katoh, *J. Nucl. Mater.* 478 (2016) 42.]

Bainitic Steel Development

Calculated phase equilibrium





Objective: to develop a new PWHT-free bainitic steel with improved properties

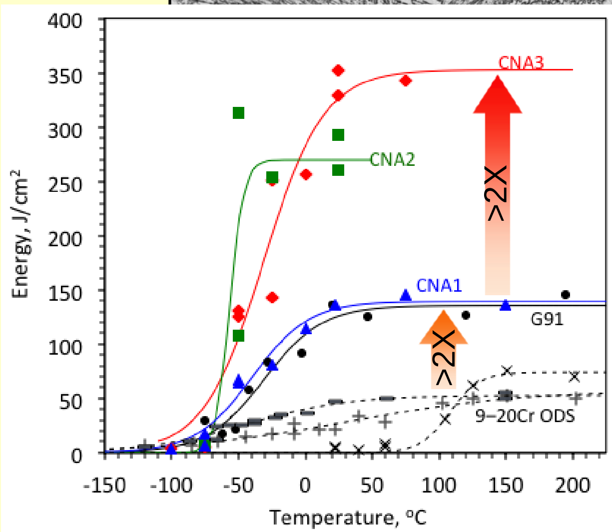
- possible application to vacuum vessel and support structure
- based on 3Cr-3WVTa bainitic steel
- control microstructure evolution via compositional optimization

Task 1: Alloy Design

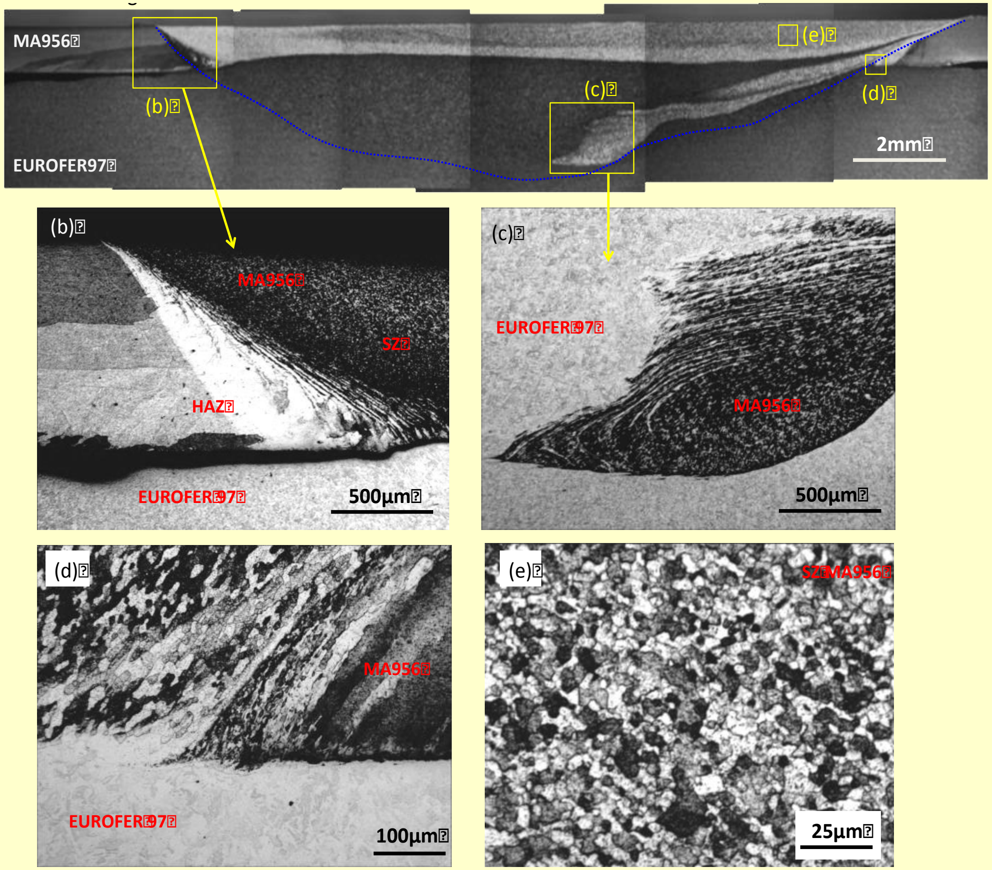
- utilize computational thermodynamics to predict phase equilibrium and transformation kinetics
- support from broad steel development expertise at ORNL (Mod. 9Cr-1Mo, 9Cr–2WVTa, 14YWT, HT-UPS, AFA, CNA, etc.)

Task 2: Property evaluation

- comprehensive property evaluation including tensile, creep, toughness, improved toughness observed.
- HFIR irradiation testing



Friction Stir Welding of Oxide Dispersion Strengthened and Ferritic Martensitic Steels

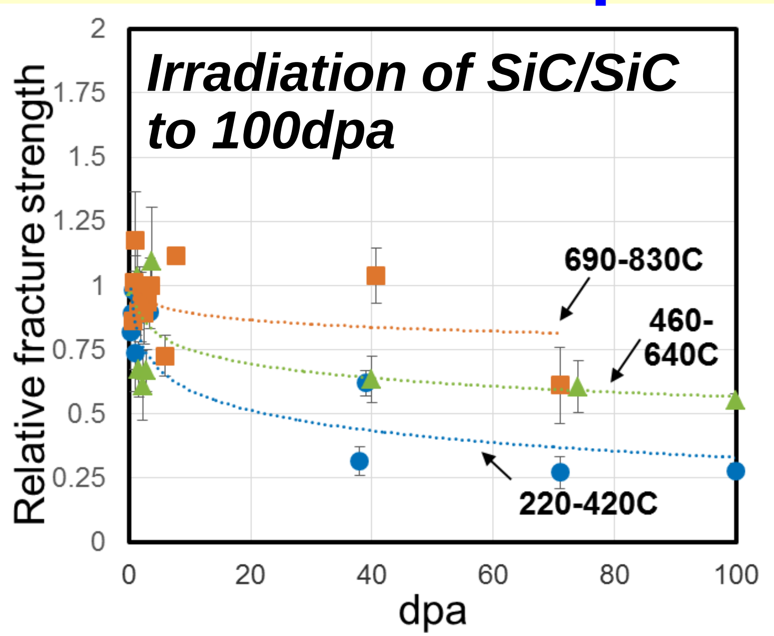


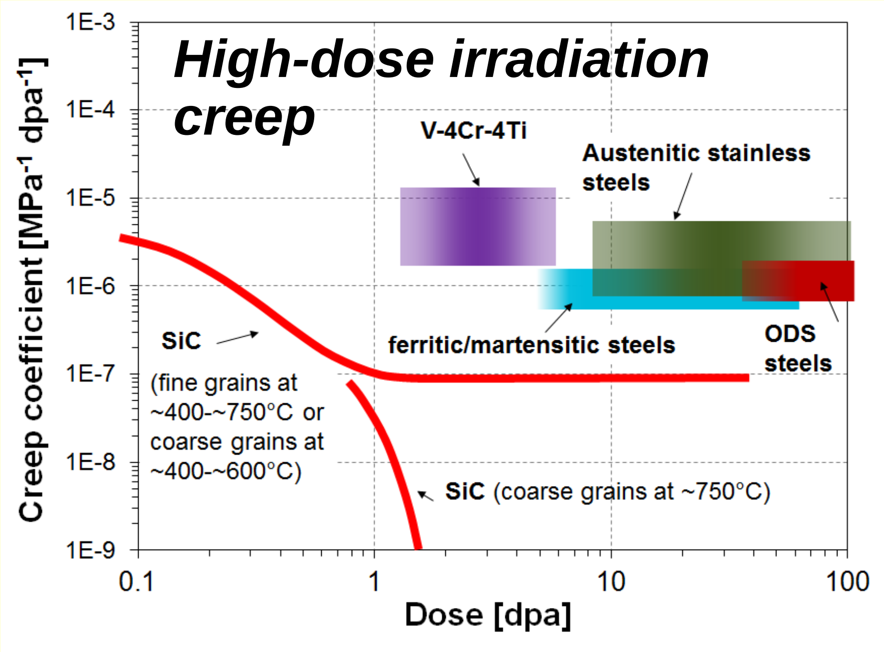
Cross sectional view of dissimilar alloy friction stir weld cross-section between two steels - ODS MA956 and RAFM EUROFER97

Z. Yu, Z. Feng, D. Hoelzer, L. Tan, M. Sokolov , "Friction Stir Welding of ODS and RAFM Steels," *Metallurgical and Materials Transactions 2E (2015)164-172 DOI: 10.1007/s40553-015-0054-9.*

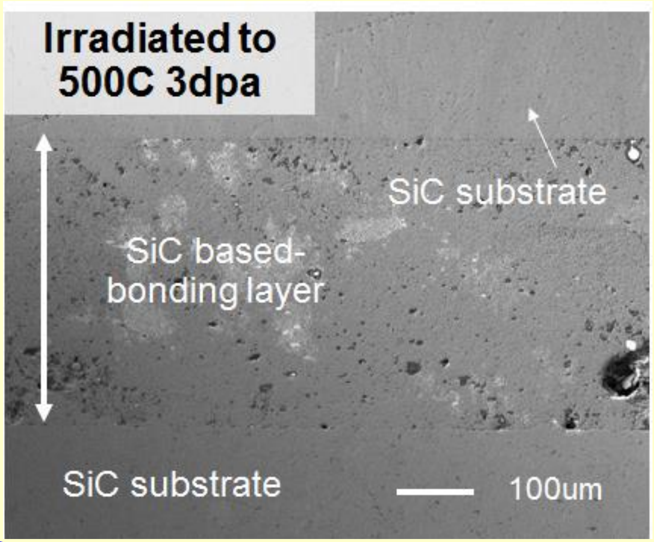
- **Scientific Achievement**
  - Demonstrated successful solid-state joining of ODS to FM steels by the friction stir welding process.
- **Significance and Impact**
  - Successful joining of ODS and FM steels removes a major engineering barrier to the use of these alloys for fusion reactors
- **Research Details**
  - Defect free welds were achieved
  - Microstructural changes induced by FSW can be minimized by post weld heat treatment
  - As-welded FSW exhibits excellent creep resistance
  - Dynamic recrystallization formed fine grains in the stir zone of ODS alloy

Development of SiC composites

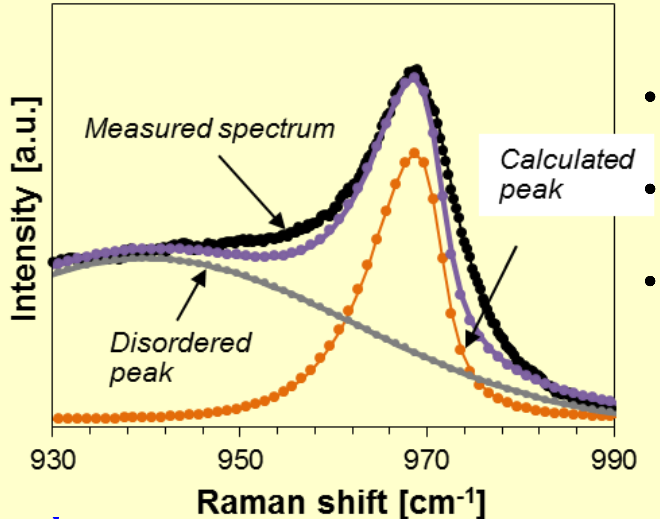




Joining technology



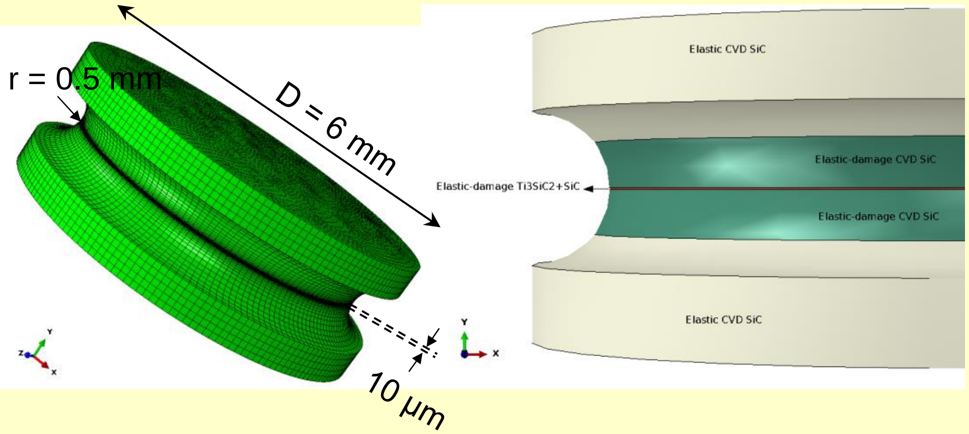
Advanced defect characterization

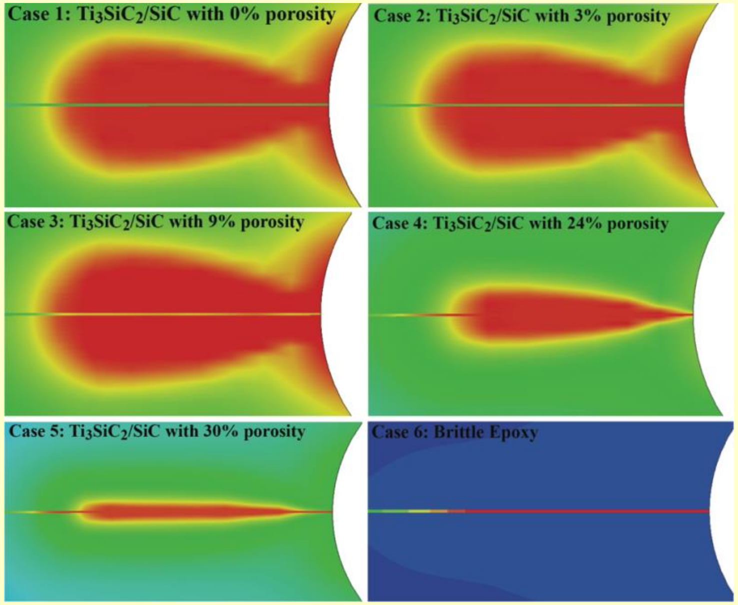


- Raman spectroscopy
- Positron annihilation
- High energy X-ray

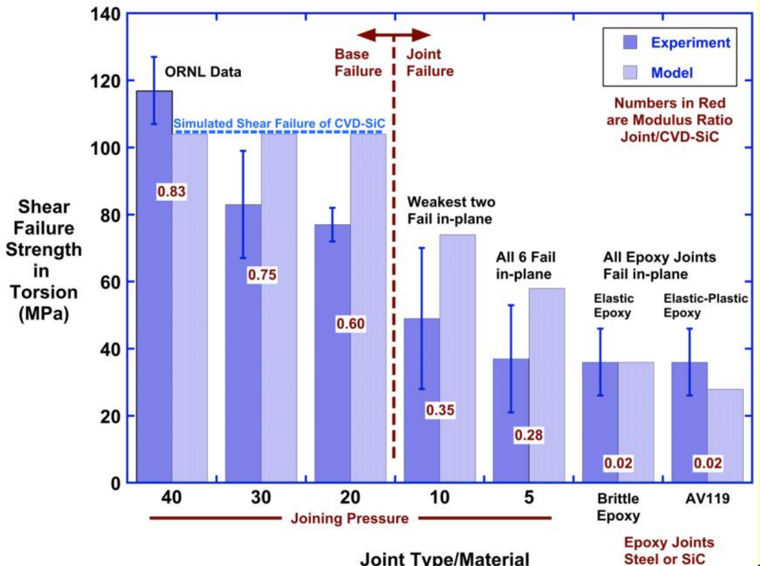
Continuum and Discrete Finite Element Damage Models of SiC Joints

- 3D finite element model subject to torsion with homogenized joint and elastic-damage models



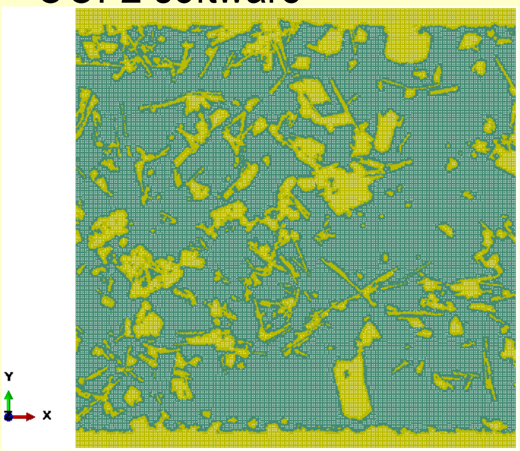


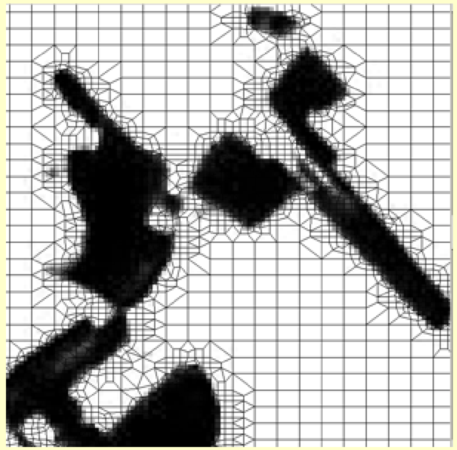
- Model correctly predicts generic response of joint failures with strong modulus effects and explains torsion specimen failure modes
  - In-plane and out-of-plane failures captured by finite element elastic-plastic damage models
- However, internal joint microstructure plays a role in joint failures and this model does not address joint microstructure



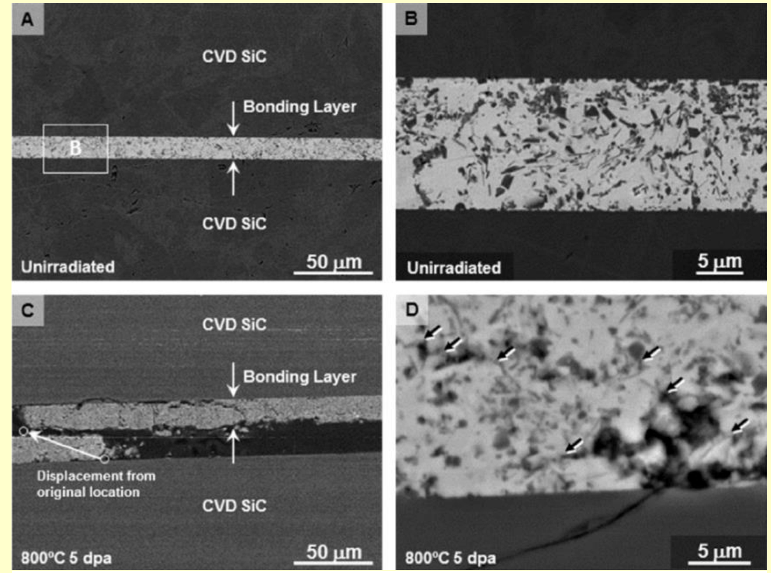
HFIR Irradiated SiC Joints Show Complex Damage at Several Length Scales

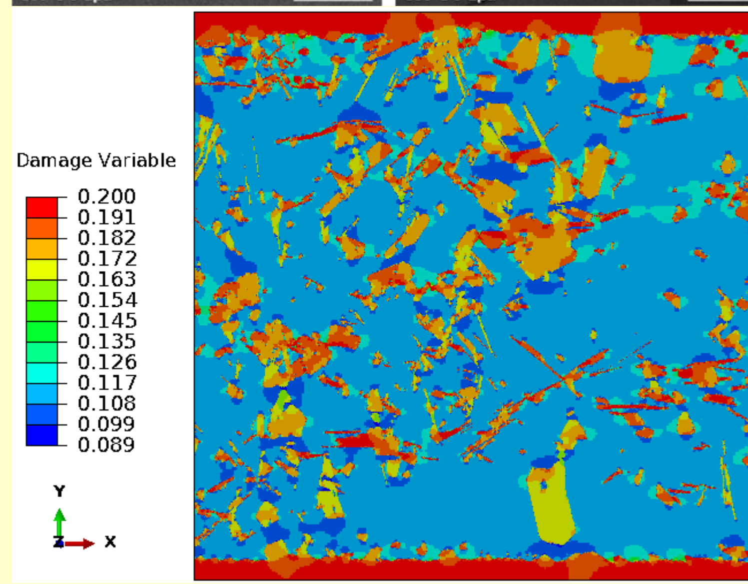
- 3D FE model is extended to include a FE mesh at the microstructural scale using digital images and NIST OOF2 software





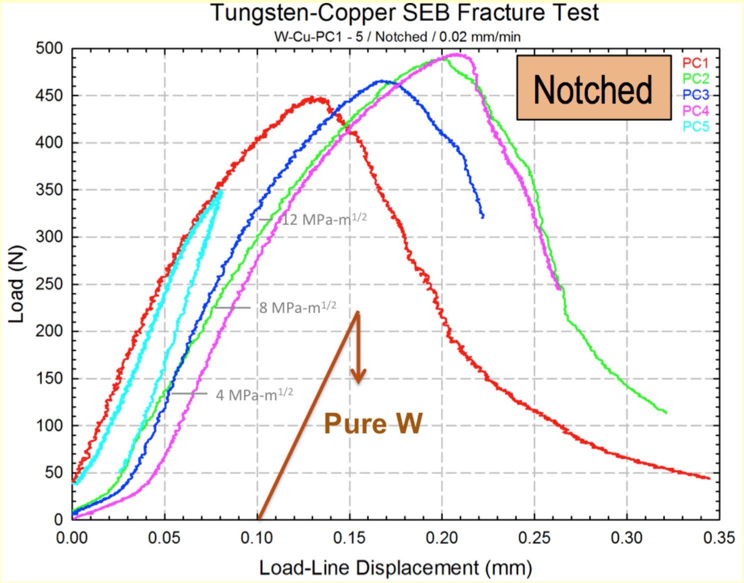
- Damage model applied to each phase separately and more failure details emerge
- Cracks (red areas) initiate in the SiC phase along the interfaces and also inside the joint at dissimilar interfaces
  - These details appear to correlate with observed damage modes after HFIR irradiation
- Future work will include thermal stresses and dissimilar irradiation-induced swelling

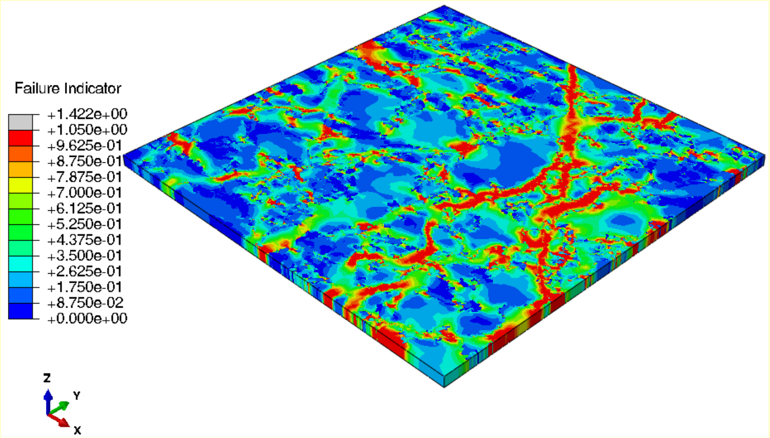




Ductile-phase Toughening of Tungsten for Fusion

- Development of tungsten-based composites with greatly improved fracture resistance relative to monolithic tungsten is underway that capitalizes on the extensive work on toughening of brittle ceramics and intermetallic phase composites
- Notched three-point bend fracture experiments have been performed on a W-Cu composite and a W-Ni-Fe alloy
- Initial results show that ductile phases contribute significantly to increasing fracture resistance
- Sophisticated crack-bridging models are being developed to treat crack growth in brittle matrix composites and design high-strength, high-ductility plasma facing components for fusion

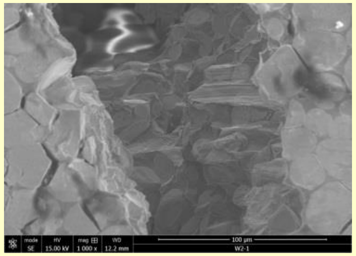




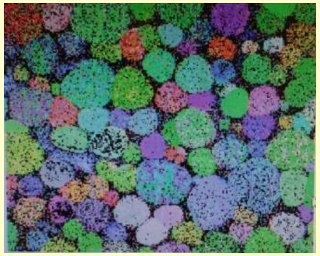
Other Ductile-phase Toughened Alloys

- 90-97 wt%W:NiFe alloys have very high initiation RT toughness, ultra-stable crack growth & good tensile strength and ductility
- Weak to modest dependence on W content
- Toughening from crack wake bridging & process zone plasticity

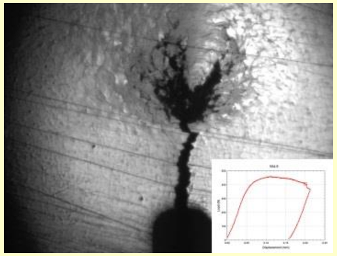
Crack wake bridging

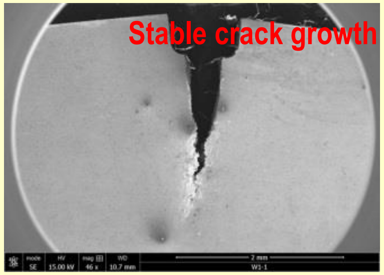


W:NiWFe

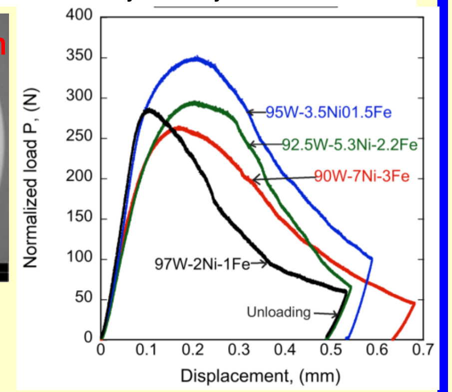


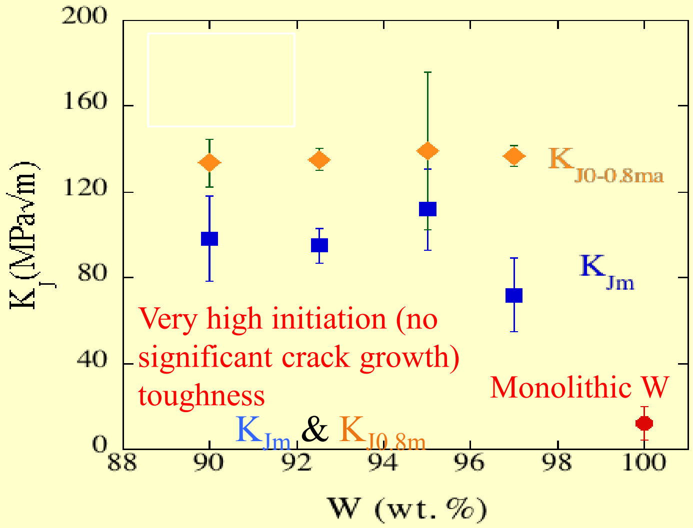
Process zone plasticity

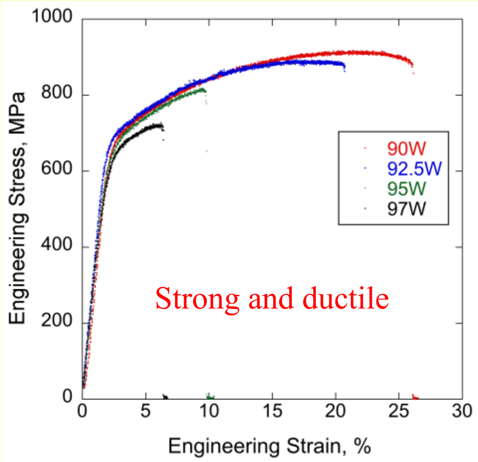


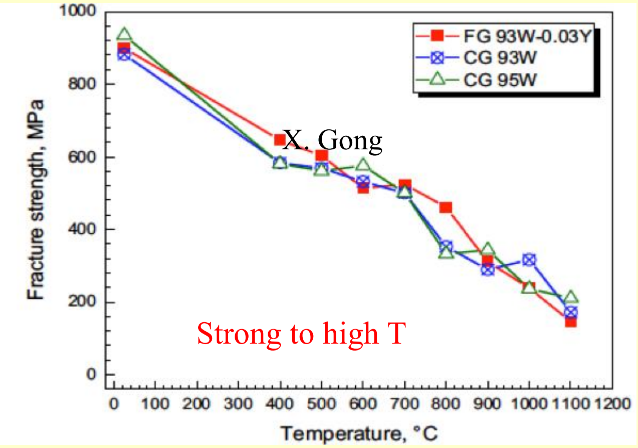


P-d curves normalized to yield P_y and d_y at a/W = 0.5



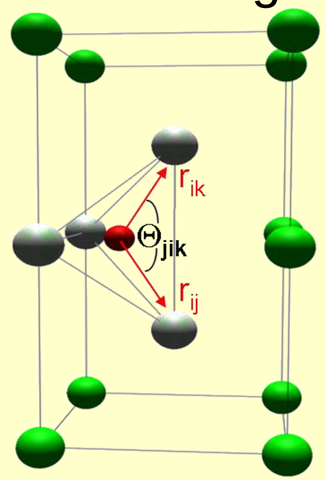






Development of new Fe-He potential and equation of state

- fitted to both energies and forces of relaxed and unrelaxed defect configurations obtained from VASP *ab initio* calculations for a range of He and He/vacancy defects, up to He_3V
- results indicate tetrahedral site is most stable for He, required addition of a 3-body term to the typical embedded atom potential

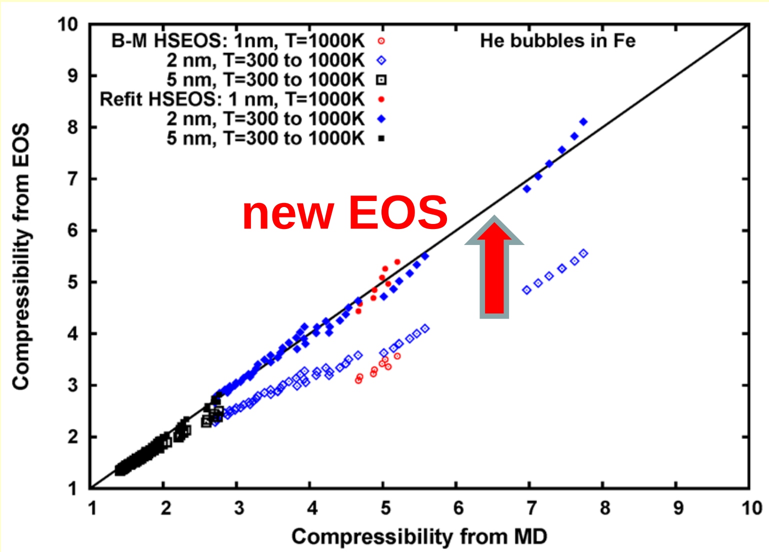


$$Y(r_{ij}, r_{ik}, \Theta_{ijk}) = \sum_{j,k \in Fe} \cos^2\left(\Theta_{ijk} - 0.44\right) f_{cut}\left(r_{ij}\right) f_{cut}\left(r_{ik}\right)$$

- potential used in MD to determine P-V behavior of He in bubbles, results used to revise previous "hard sphere" equation of state for He

$$compressibility: Z = \frac{pV}{mkT} = (1 + y + y^2 - y^3)(1 - y)^{-3}$$

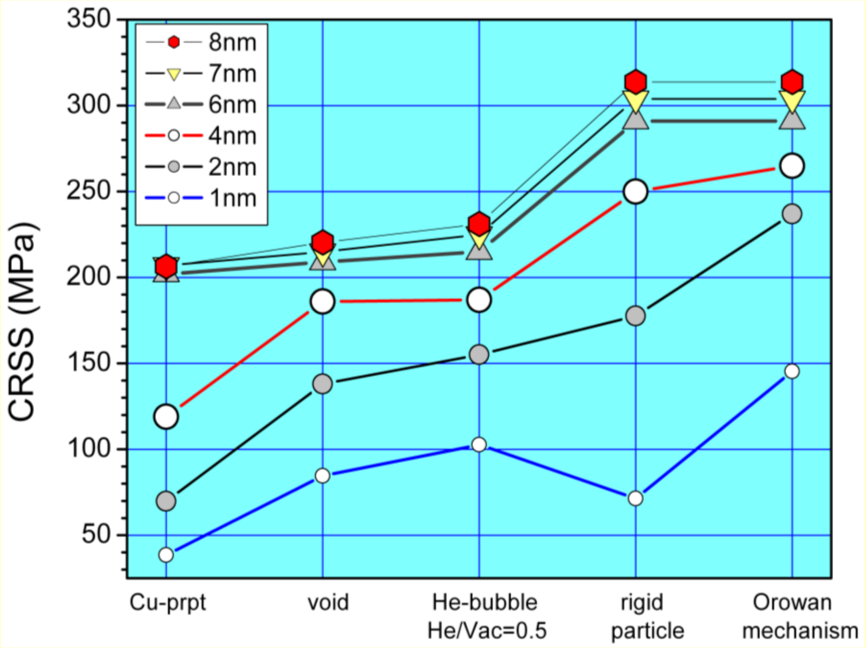
$$y = \frac{\pi d_g^{\ 3}}{6} \frac{m}{V}, \; d_g = a_1(a_2 - a_3 \cdot \ln(T(K)/a_4))$$



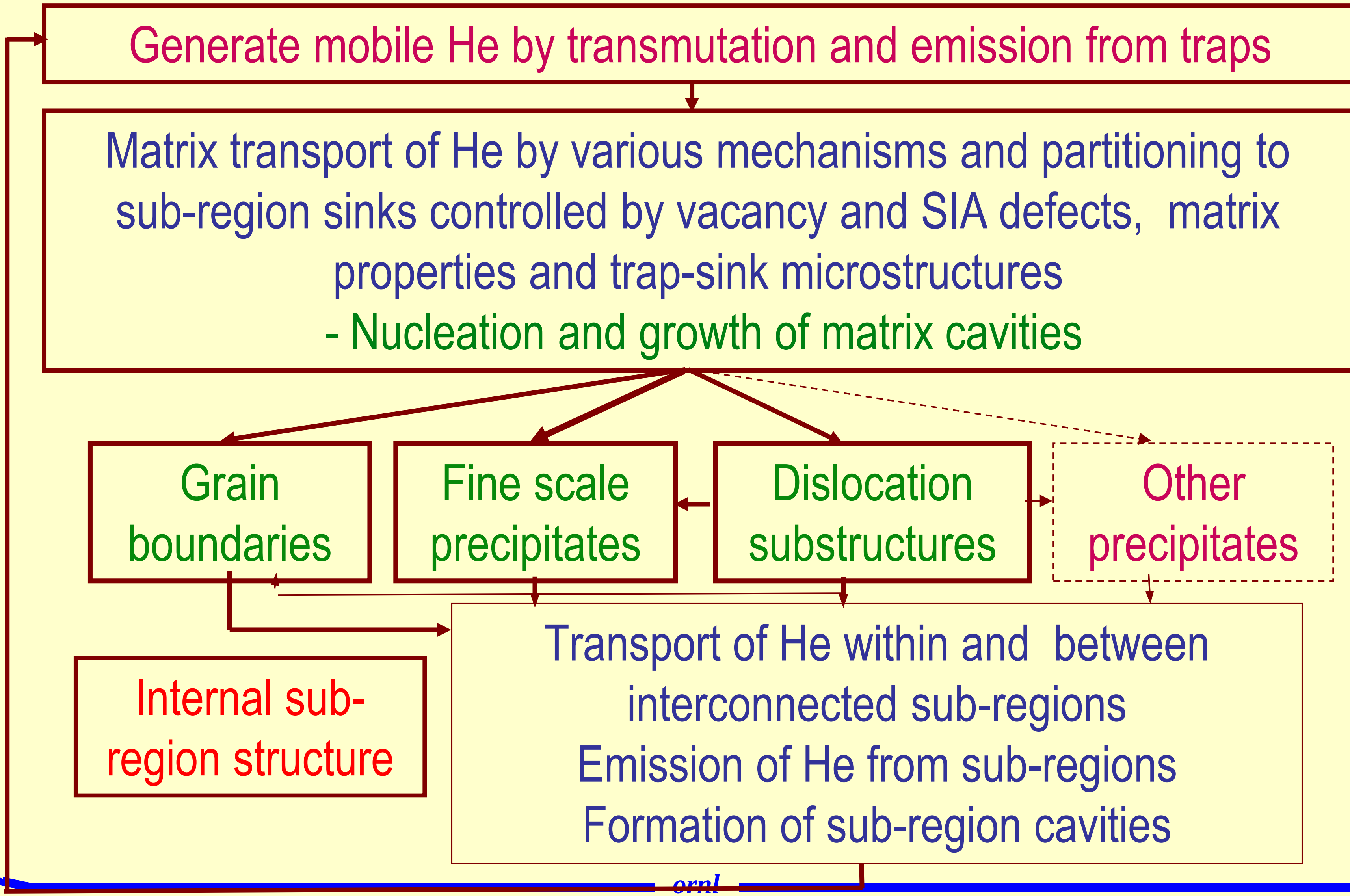
MD simulations used to investigate dislocation-defect interactions

- fundamental plastic behavior of Fe and W, dislocation structure and mobility
- strengthening and hardening of structural materials due to radiation-induced defects
- primary objectives are:
  - elucidate atomistic reactions responsible for hardening
  - provide data for coarser scale elasticity and rate theory based predictions
  - provide direct verification with specially designed experiments.

Fe strengthening due to localized obstacles

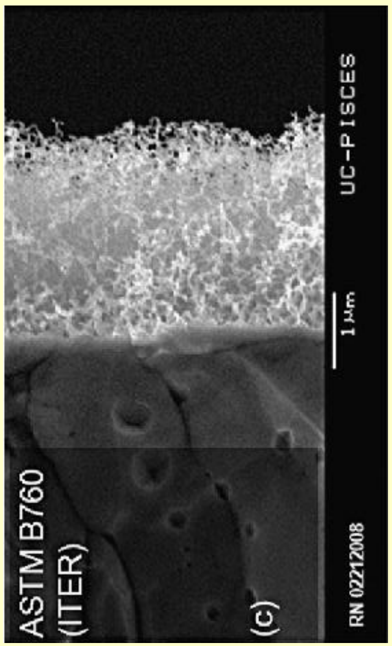


Master model framework to track generation, transport, fate, and consequences of He

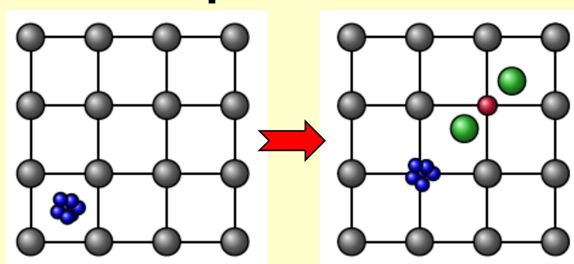


"Fuzz" formation in W plasma-facing material

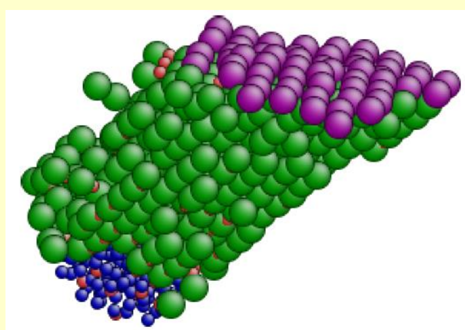
Atomistic investigations of unit mechanisms that contribute to surface roughening in tungsten exposed to low-energy He, a possible precursor to fuzz formation.



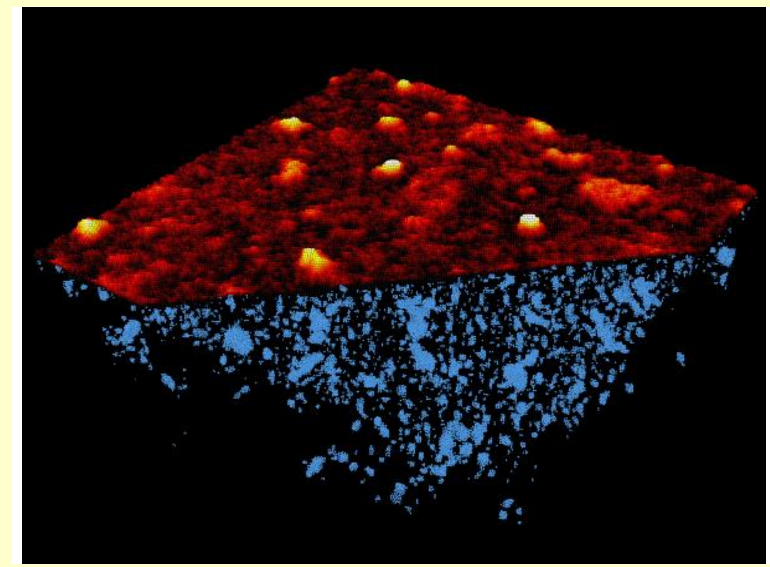
"Trap mutation"



"Loop punching"



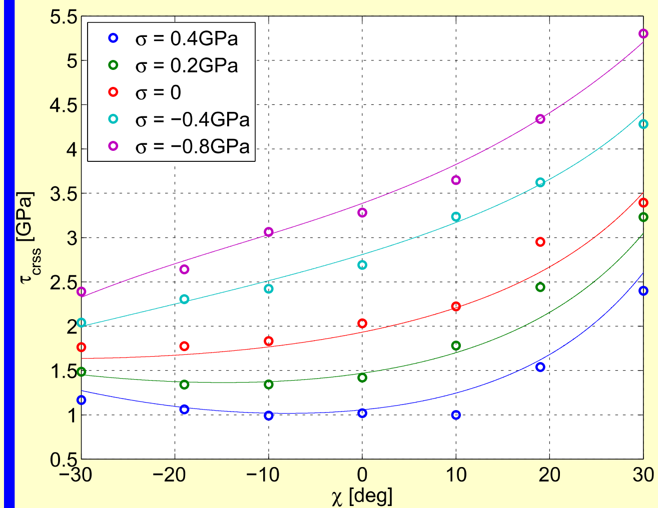
Large-scale MD simulation, 1.5 ms, W (111) surface, $f_{He}=4x10^{25}$ He/m^2/s

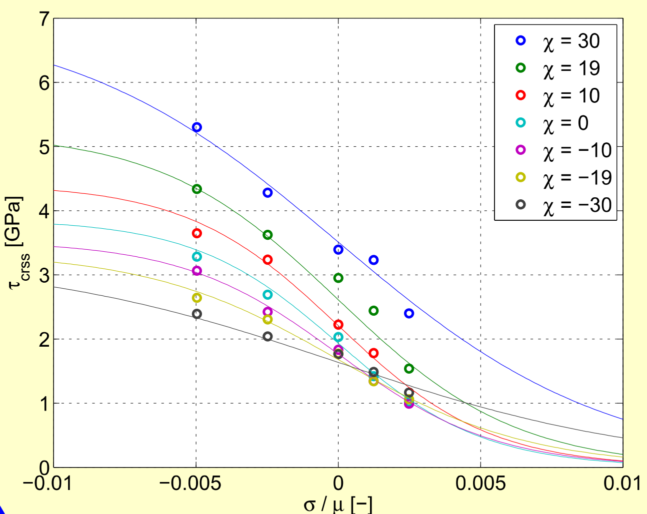


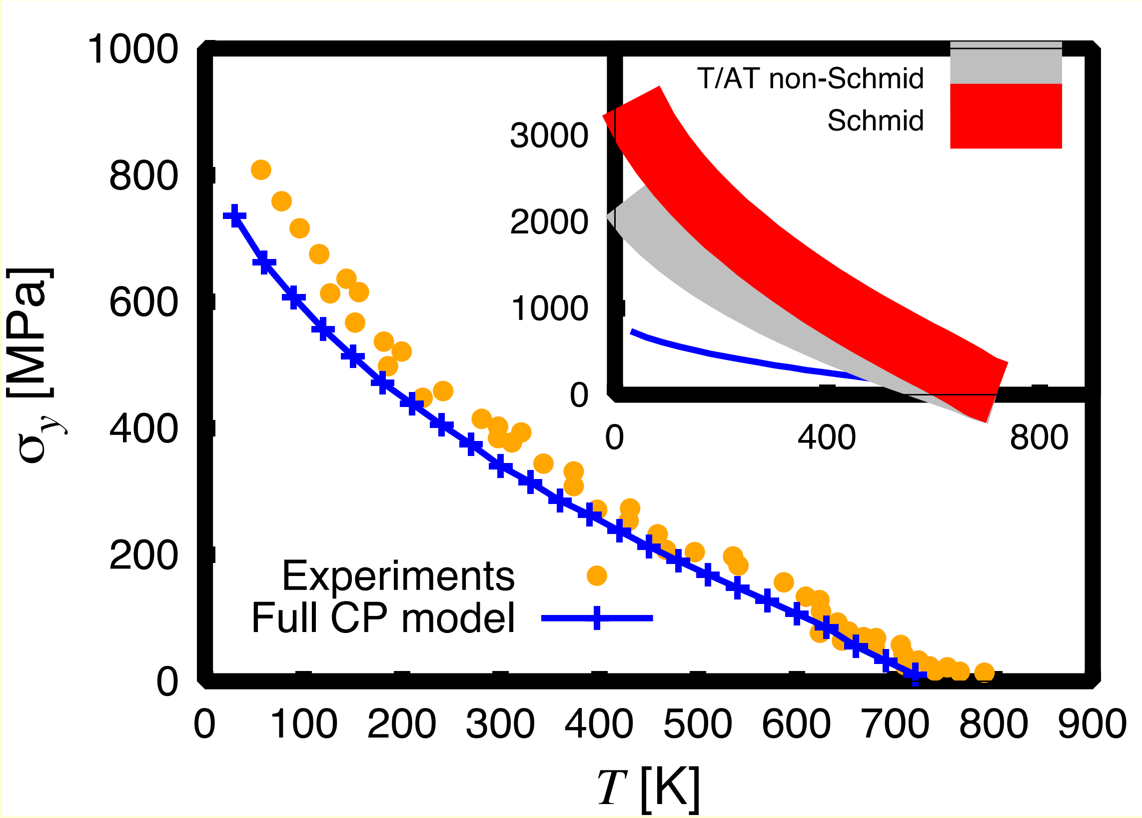
Surface morphology: red, yellow, and white are surface regions elevated to different distances by underlying He bubbles

Crystal plasticity model for single crystal W informed by atomistic calculations

Atomistic calculations of non-Schmid effects

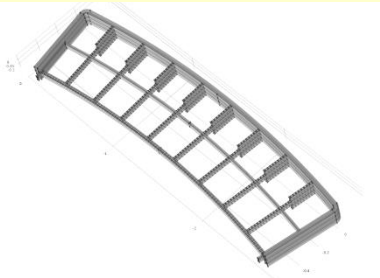




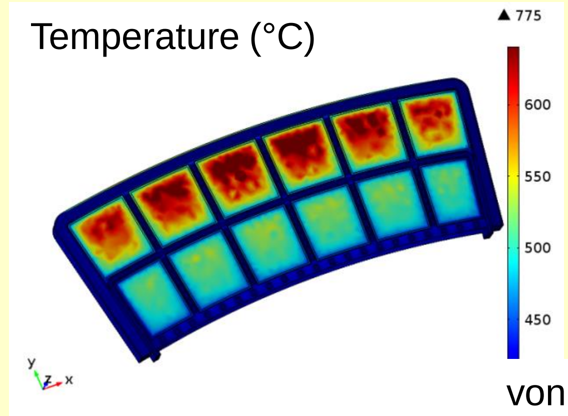


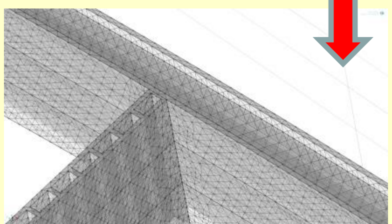
- Very successful prediction of yield strength.
- Working towards an extension of this modeling to W-Re, polycrystalline systems.

Multiscale, multiphysics mechanical design of fusion reactor components

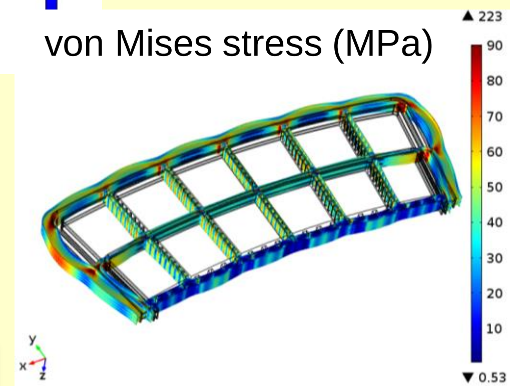


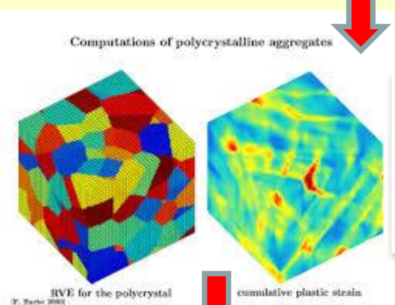
Thermo-elastic analysis & shape optimization: ~2-5 MDOF





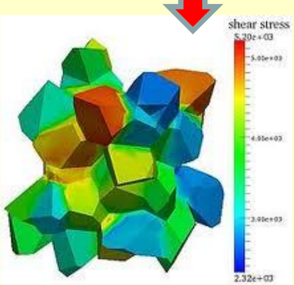
Visco-plastic model of critical region (CR) ~0.5 MDOF



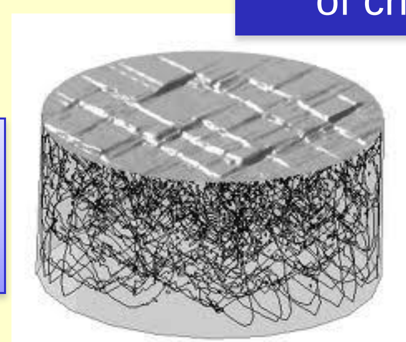


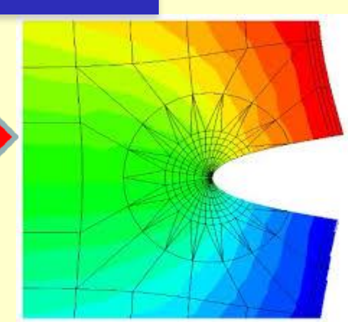
Crystal Plasticity of Macro-RVE ~0.1 MDOF

3D Elasto-plastic fracture mechanics of critical flaw



DD simulation of micro-RVE ~10K DOF





Summary

- Primary materials challenges for successful fusion energy include: (1) developing structural materials with suitably long lifetimes, (2) obtaining a plasma-facing material with sufficient ductility and low tritium retention, and (3) verifying the performance of functional materials
- Key computational results include development of:
  - a new He-Fe interatomic potential and equation of state for atomistic simulations of helium effects in irradiated steels
  - a detailed kinetic model describing the behavior of helium and its use to predict swelling and embrittlement in FM steels and their ODS variants
  - successful development of continuum and discrete finite element damage models of SiC joints
  - integrated computational approach for investigating near-surface mechanisms responsible for “fuzz” formation on W surfaces
  - atomistically informed model for crystal plasticity of W
  - integrated models for design of fusion reactor components

Summary, cont.

- Key experimental results and insights include:
  - use of dual ion, spallation, and neutron irradiation with *in situ* implantation of He demonstrates a strong correlation between He/dpa ratio and both swelling and mechanical properties, swelling is reduced in ODS relative to conventional FM steels
  - ODS and CNA variants exhibit high strength and longer creep lifetimes than conventional FM steels
  - successful use of friction stir welding on ODS and FM steel components
  - high-dose neutron irradiation of advanced nuclear grade SiC demonstrate limited effects on high-temperature strength with only modest swelling and reduction in thermal conductivity;
  - impact of He on SiC microstructure observed, impact on mechanical properties is being assessed;
  - good progress in development of radiation-resistant joints for SiC composites
  - ductility of W and alloys such as W-Re remains problematic, possible ductile-phase toughening being explored
  - progress in mechanistic understanding of "fuzz" formation on W PFC, approach to mitigation not clear
- Need for a fusion-relevant neutron source remains a high priority to enable materials qualification for machines beyond ITER