Overview of the Fusion Materials Sciences Program

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Fusion Energy Sciences Advisory Committee meeting

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Gaithersburg, MD

OUTLINE

- Overview of Materials Sciences program: 1995-2001
  - Response to FESAC review (summer, 1998)
  - Summary of recent program restructuring (ongoing evolutionary process)
- Materials science highlights
  - Simultaneous scientific excellence: research directly relevant for fusion and of interest to the broader materials science community

Key findings from 1998 FESAC review

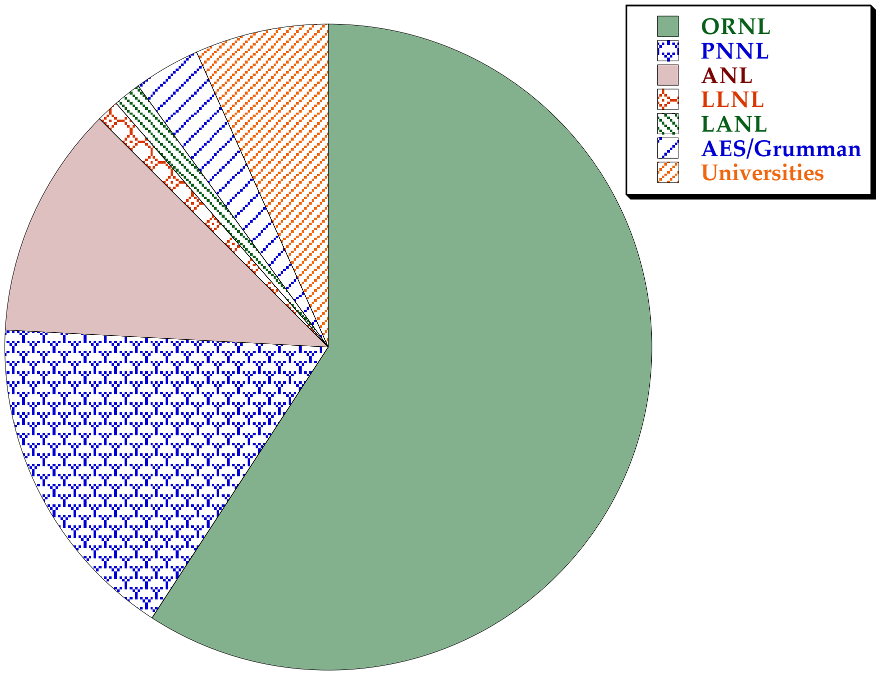
- Overall scientific quality of research is high
- R&D activities should be part of an integrated program in enabling technology
- Research focus should be expanded to include a wide variety of materials for MFE and IFE
  - Seek opportunities to interact & benefit from other government and industrial materials programs
- Budget should be increased by 1-2 M$/yr to support new initiatives in modeling and exploratory concepts

Fusion Materials Restructuring

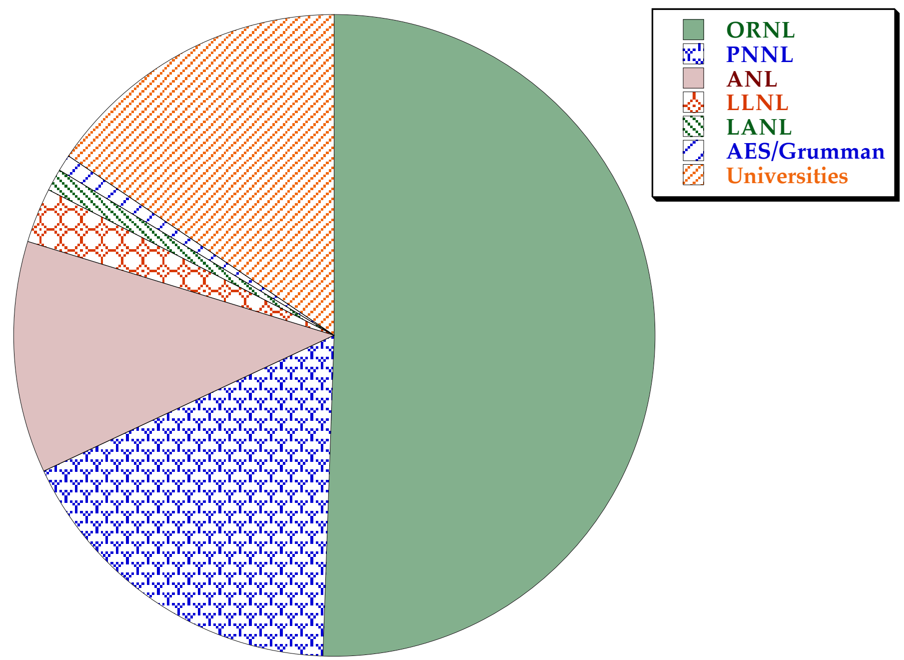
"As new discoveries are made, new truths discovered, and manners and opinions changed with the pace of circumstances, institutions must advance also to keep pace with the times"

Thomas Jefferson

Fusion Materials Sciences Institutional Budgets



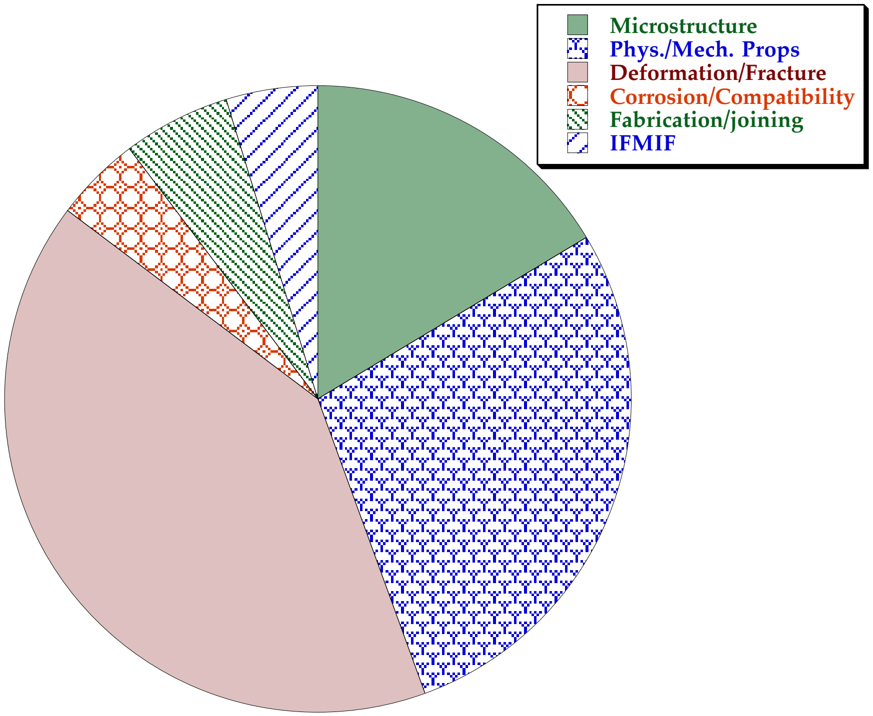
Total FY98



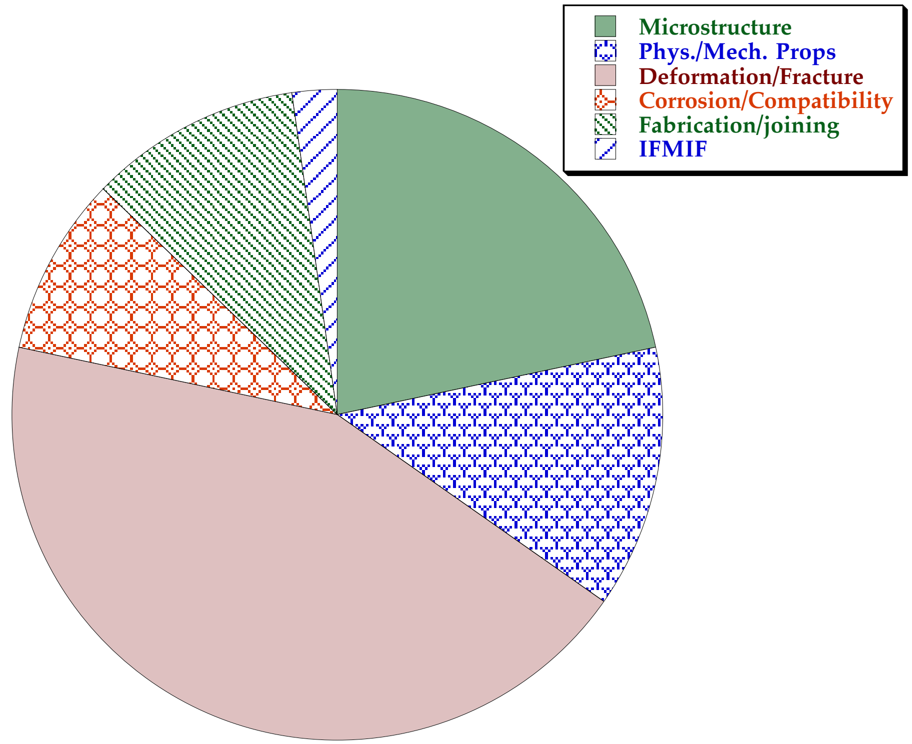
Total FY01

- University funding has tripled in the past 3 years
- Significant personnel changes have occurred at institutions
  - e.g., ORNL: 18 scientists with average support of 0.4 FTE/yr; 11 staff removed and 9 new researchers added since FY98

Fusion Materials Sciences R&D Portfolio



FY98 funding



FY01 funding

- Continued emphasis on mechanical properties

Materials Restructuring Process

1998 (external events, policy changes)	**Events**	**Comments**
	• End of U.S. participation in ITER activities	• Beginning of technology program restructuring from energy development to science-oriented.
	• FESAC panel review of Materials Program	• Recommended increased effort on theory/modeling and road-mapping
1999	• Materials Program road-mapping	• Identified key feasibility issues
	• White paper on theory/modeling initiative	• Modeling call for proposals released December 1999

Materials Restructuring Process

2000 (restructuring implementation begins)	**Events**	Comments
	• Theory/modeling competitive solicitation ($1M) • Guidance from OFES to accelerate restructuring process • Develop concept for reorganizing along cross-cutting technical issues	• outreach to broad materials community
2001	• Theory/modeling awards made • Peer review to be conducted • Initiate outreach to plasma research and IFE	• 3 new participating institutions

Materials Science Restructuring Themes

	Pre-Restructuring	**Restructured**
Orientation	Fusion Materials ***Development***	Fusion Materials ***Science***
Mission	Schedule-driven development of materials for fusion power (ITER blanket test modules, DEMO, …)	Fundamental understanding of scientific underpinnings of materials for fusion
Organization	Lead lab for each candidate structural materials class (V alloy, F/M, SiC/SiC)	Integrated national teams focused on key cross-cutting issues
Approach	Experiments for semi-empirical correlations	Experiments to guide/ validate theory and modeling

Fusion Materials Science Mission Statement

- Advance the materials science base for the development of innovative materials and fabrication methods that will establish the technological viability of fusion energy and enable improved performance, enhanced safety, and reduced overall fusion system costs so as to permit fusion to reach its full potential
- Assess facility needs for this development, including opportunities for international collaboration
- Support materials research needs for existing and near-term devices

Example of Change in
Approach to Materials Research
V alloy (a BCC metal)

Old Approach (*Development*)	**New Approach (*Science*)**
• Select reference alloy (V-4Cr-4Ti)	
• Focus most research on this alloy (narrow scope)	• Focus research on fundamental understanding of BCC materials
• R&D planning based on need to develop materials to meet device construction schedule	• Research planning based on theory and modeling requirements of BCC materials
• Experiment-based R&D to build engineering data base	• Experiments used to guide and validate scientific theory and models
	• Study model BCC alloys/ surrogate materials encompassing V alloys

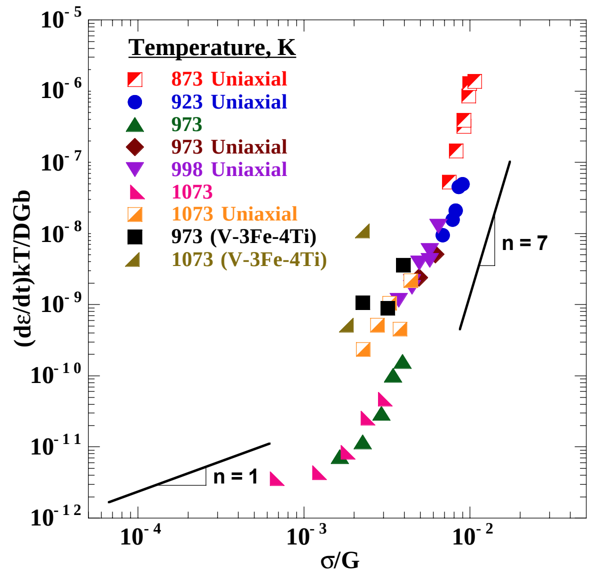
Investigation of Thermal Creep Mechanisms in V-4Cr-4Ti

Diffusion-Controlled Creep Mechanisms

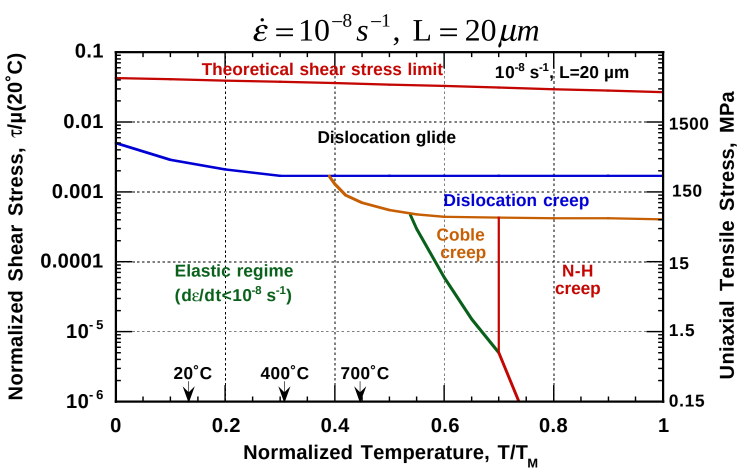
$$\frac{\dot{\varepsilon}kT}{DGb} = A\left(\frac{b}{d}\right)^m\left(\frac{\sigma}{G}\right)^n$$

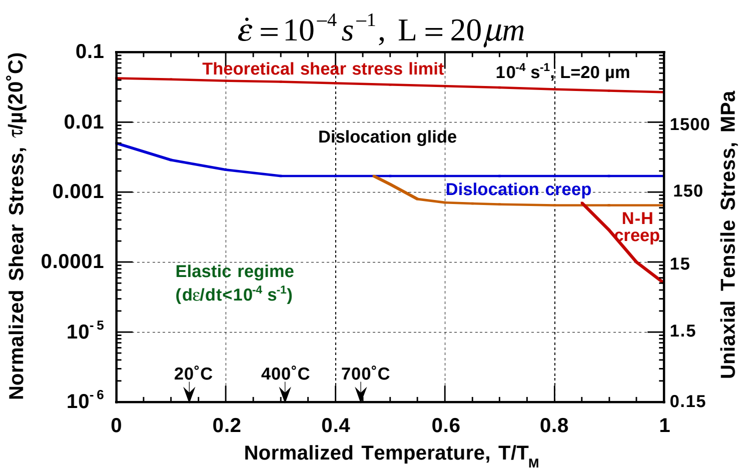
Mechanism	D	n	A	m
Climb of Edge Dislocations	D_L	5	$6x10^7$	0
Viscous Glide (Microcreep)	D_S	3	6	0
Low-Temperature Climb	D_d	7	$2x10^8$	0
Harper-Dorn	D_L	1	$3x10^{-10}$	0
Nabarro-Herring	D_L	1	12	2
Coble	D_b	1	100	3
GBS (Superplasticity)	D_b	2	200	2
Nabarro-Subgrain	D_L	1	12	2
Nabarro-Bardeen-Herring	D_L	3	10	0

Experimental Creep Data



Deformation Mechanism Maps for V-4Cr-4Ti





PNNL / ORNL / ANL / UCSB collaboration

Features of Restructured Fusion Materials Science Program

- Science-based materials research
- Principal product is *basic knowledge, theory, and models* needed to resolve feasibility issues of fusion materials
- Primary role of experiments is to guide and validate theory and models
- Utilize, leverage, and expand on revolutionary advances in computational and experimental methods (e.g.,nanoscience) for fusion materials design
- While focusing on long-term viability and attractiveness issues of fusion materials, apply expertise in near-term to current issues of plasma research and IFE studies

Fusion Materials Science has Similarities with the Fusion Plasma Science Philosophy

	Fusion Plasma Science	Fusion Materials Science
Basic Goal	**Understand fourth state of matter as it relates to fusion**	**Understand first state of matter as it relates to fusion**
Key Issues		
• Basic properties and microscopic phenomena	– particle/energy confinement and transport	– dislocation propagation, phonon transport, … – microstructural stability
• System properties and macroscopic phenomena	– MHD stability	– fracture and deformation
• Creation and sustainment	– plasma-wave interactions	– physical metallurgy and thermodynamics
• Interactions with environment	– plasma-wall interactions	– corrosion & compatibility; radiation effects on materials

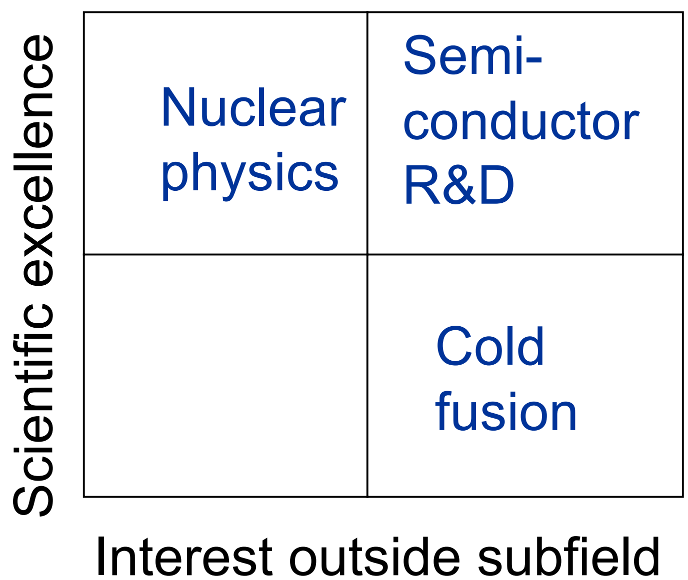
Fusion Materials Science Program

	Theory-Experiment Coordinating Group*				
	Microstructural Stability	**Physical & Mechanical Properties**	**Fracture & Deformation Mechanisms**	**Corrosion and Compatibility Phenomena**	**Fabrication and Joining Science**
Materials for Attractive Fusion Energy					
• **Structural Alloys*** - Vanadium Alloys - F/M and ODS Steels - High T Refractory Alloys - Exploratory Alloys	■	■	■	■	■
• **Ceramic Composites*** - SiC/SiC, other CFCs	■	■	■	■	■
• **Coatings**		■		■	■
• **Breeder/multiplier Materials**					
• **Neutron Source Facilities**					
Materials for Near-Term Fusion Experiments					
• **PFMs (Refractory Alloys, etc.)**		■	■	■	■
• **Copper Alloys**	■	■	■	■	■
• **Ceramic Insulators**		■			■
• **Optical Materials**		■			■

*asterisk denotes Fusion Materials Task Group

Simultaneous excellence is central to the R&D portfolio of the fusion materials science program

- Provide valuable product for fusion energy sciences (build knowledge base)
- Provide excellence in materials science
  - This also helps to build support for fusion energy within the broad materials science community



Fusion Materials Science is the Vital Link Between the Fusion Energy Sciences and Materials Science Communities

- Researchers in the Fusion Materials Science program are housed in materials science departments at their institutions (provides access to the broader materials science community)

- Researchers in the Fusion Materials Science program are also actively involved in numerous non-fusion cutting-edge materials science endeavors (provides targeted leveraging)

- Fusion Materials research is contributing to several materials science “grand challenges”

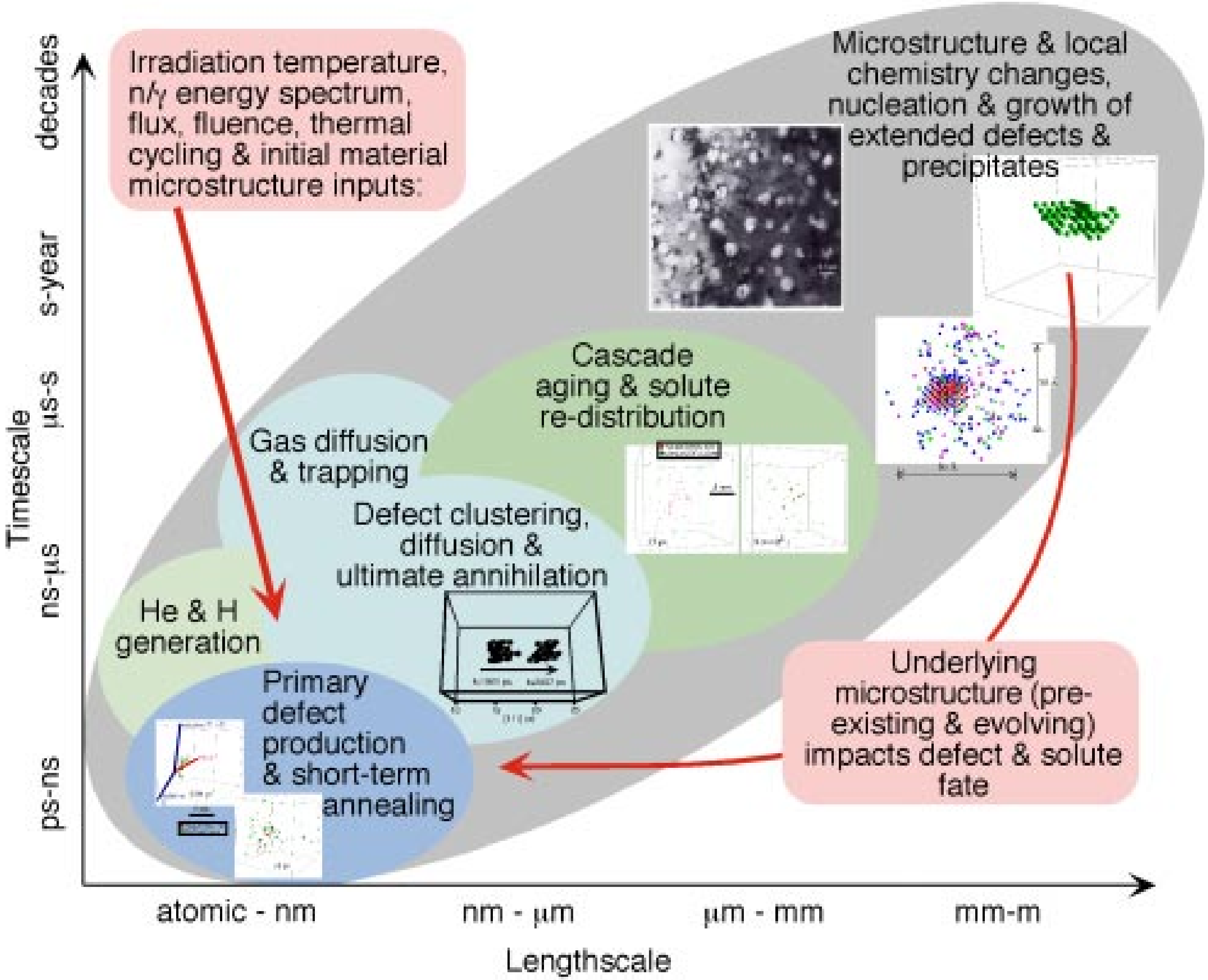
Fusion Materials Science is Strongly Integrated with other Materials Science programs (research synergy)

- No one engaged in fusion materials research is supported 100% by OFES funding; all fusion materials scientists actively interact with other research communities
- BES (ceramic composites, radiation effects in materials, electron microscopy, deformation physics, nanoscale materials)
- NERI (deformation mechanisms in irradiated materials, damage-resistant alloys)
- EMSP program (radiation effects in nuclear waste materials, including modeling relevant for SiC and other ceramics)
- Naval programs (radiation effects in SiC/SiC, refractory alloys, cladding materials)
- NRC (fracture mechanics and radiation effects in pressure vessel alloys)
- EPRI (stress corrosion cracking in alloys)
- APT, SNS (effects of He and radiation damage on structural integrity of materials)
- Defense programs (stockpile stewardship materials issues)

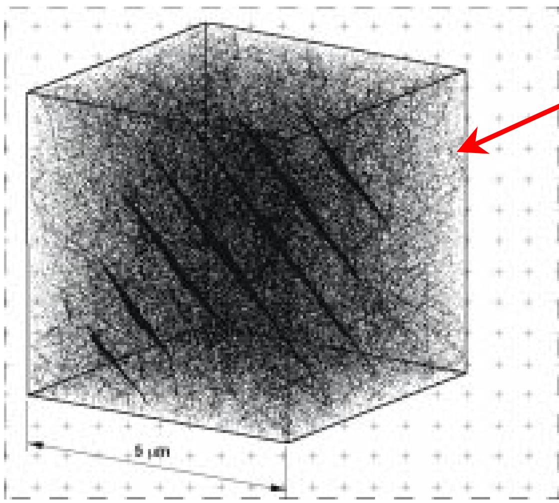
Fusion Materials Scientists are Contributing to the Resolution of Several Grand Challenges in the General Field of Materials Science

- **What are the maximum limits in strength and toughness for materials?**
  - Dislocation propagation, interaction with matrix obstacles
- **How are the "laws" of materials science altered under nanoscale and/or nonequilibrium conditions**
  - Critical dimensions for dislocation multiplication
  - Nonequilibrium thermodynamics
- **What is the correct physical description of electron and phonon transport and scattering in materials?**
  - Thermal and electrical conductivity degradation due to point, line and planar defects
- **What is the effect of crystal structure (or noncrystallinity) on the properties of matter?**

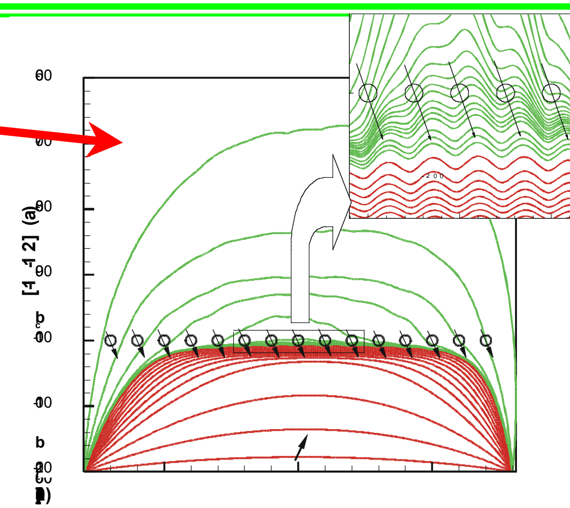
Radiation damage is inherently multiscale with interacting phenomena ranging from ps-decades and nm-m

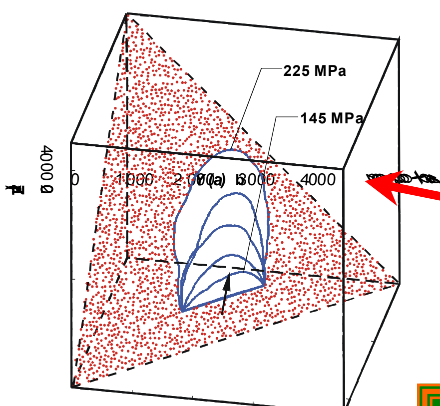


Dislocation Dynamics (DD) is a new computer simulation method developed at UCLA for modeling fundamental microscopic mechanical properties. Successful fusion applications: (1) Mechanisms of dislocation interaction with radiation defects; (2) Radiation hardening; (3) Localization of plastic flow.

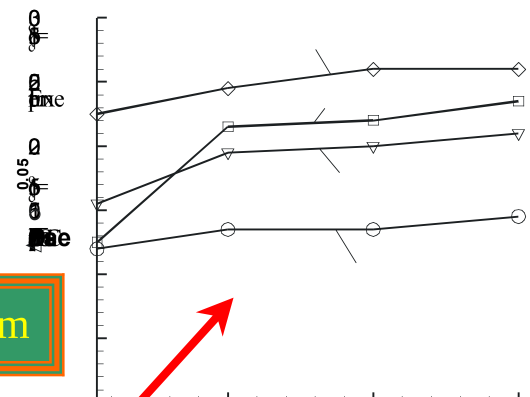


Simulations & experiments on flow localization



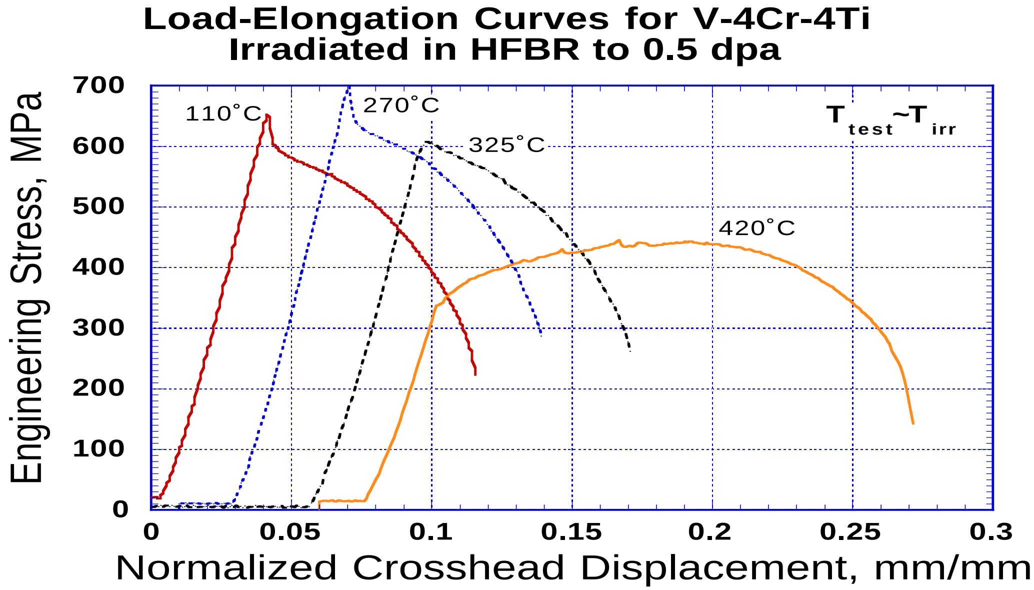


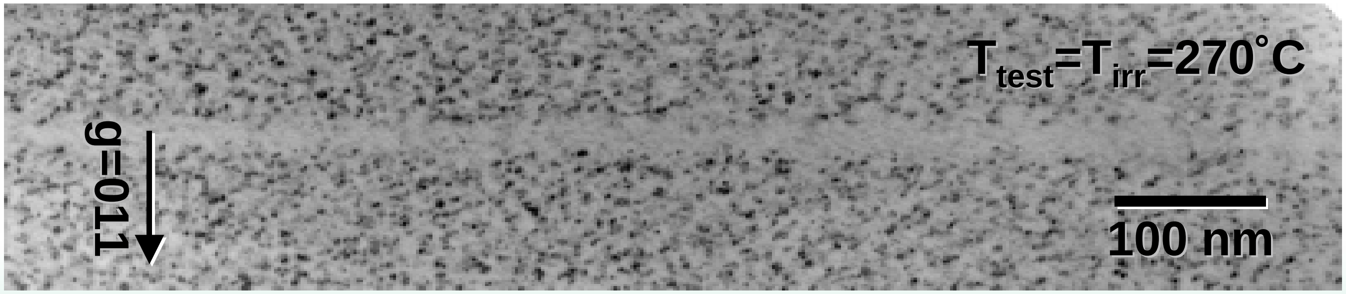
Flow Localization Mechanism



Comparison between simulations & radiation hardening experiments

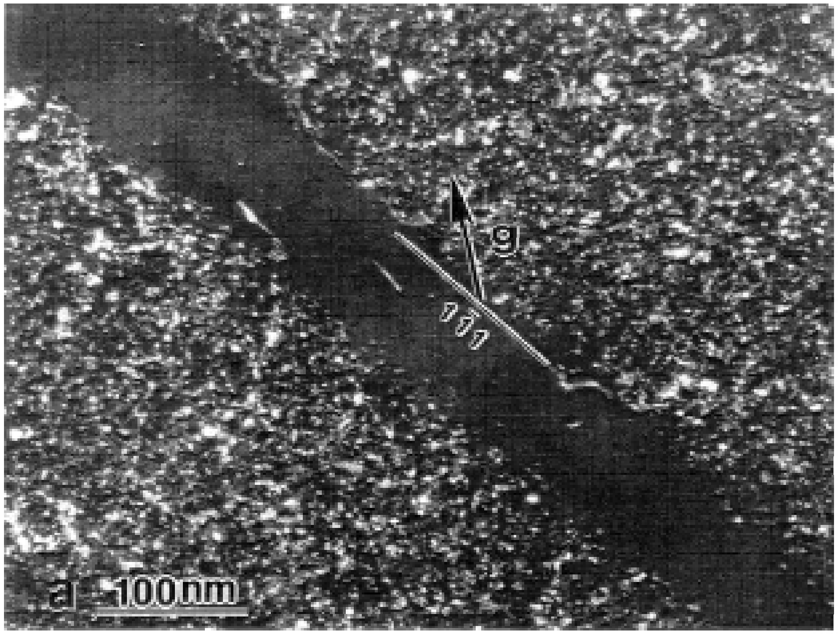
Irradiated Materials Suffer Plastic Instability due to Dislocation Channeling

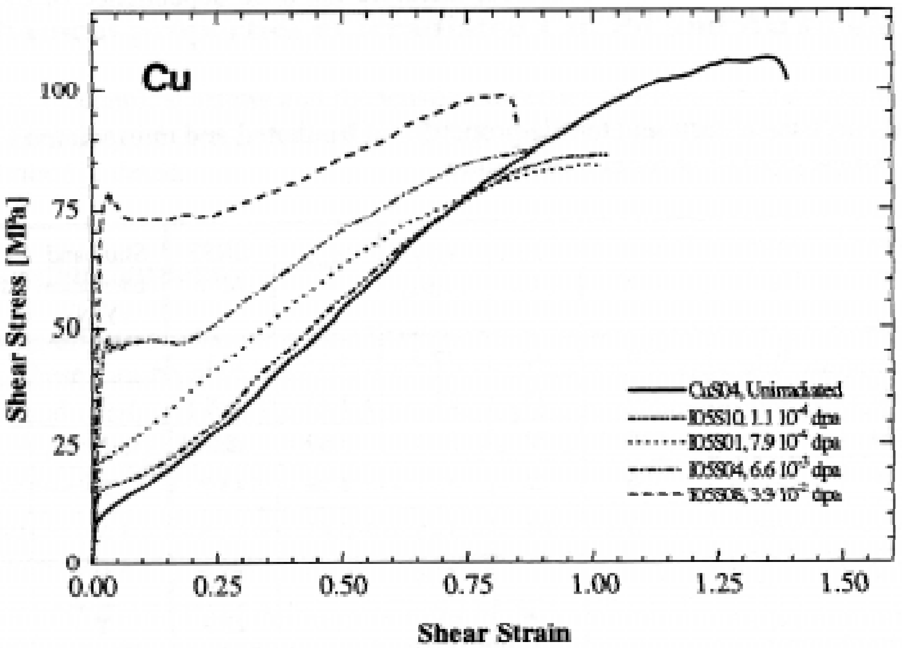




Irradiated materials undergo plastic instability and failure due to dislocation channel formation

Plastic flow localization in irradiated metals - An unresolved issue for >30 yrs



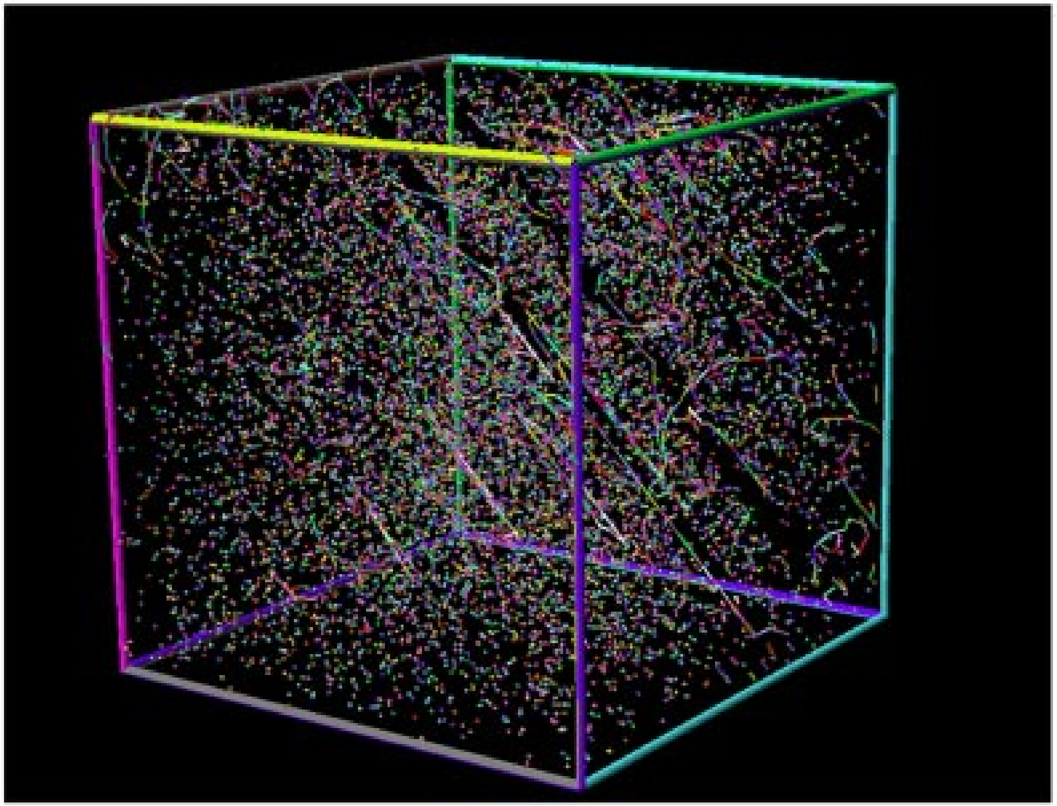


Outstanding questions:

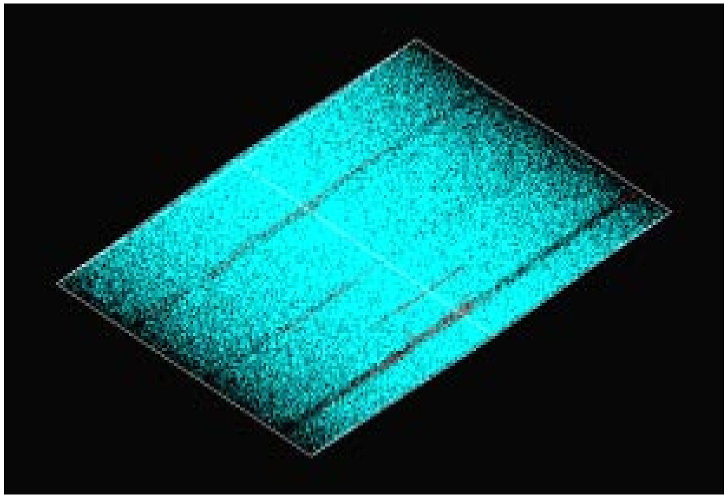
- **What governs the appearance of a yield point?**
- **What governs the dose dependence of yield point onset?**
- **What governs dislocation channel initiation?**
- **What governs dislocation channel growth? (cross-slip in fcc metals is not well understood)**
- **What controls channel width?**

Plastic flow localization in defect free bands appears in the Dislocation Dynamics (DD) simulations

The implementation of cross-slip into DD gives rise to the formation of defect free bands (channels) with a width of 200-300 nm

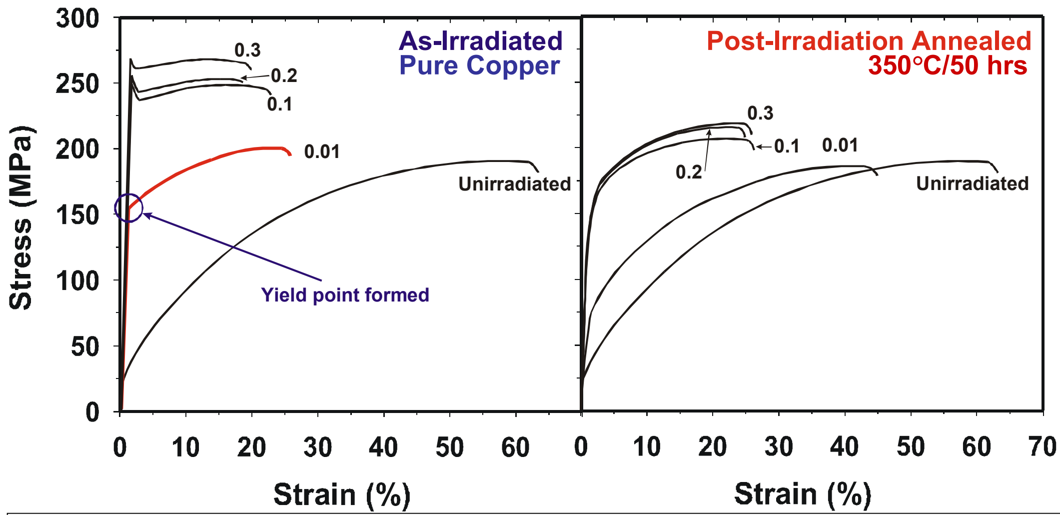


Spreading of the channels is restrained by the formation of dipole segments and the remaining radiation induced defect distribution



Nature, August 24, 2000

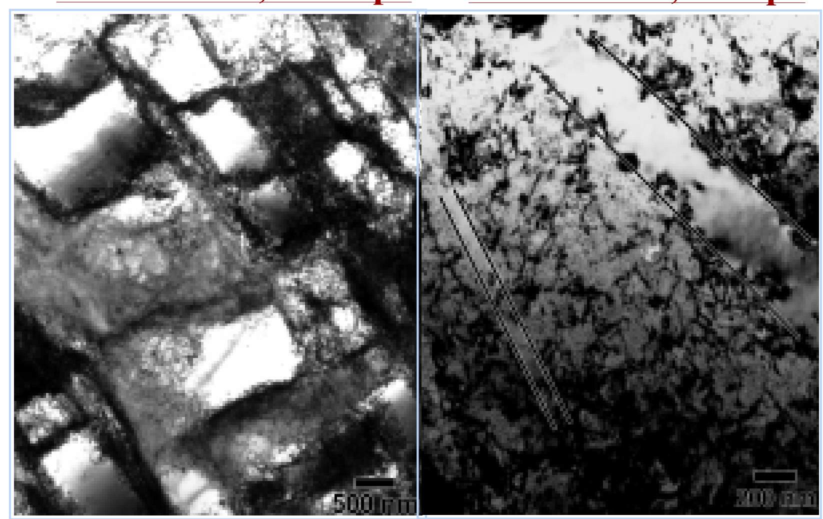
Deformation Behavior in As-Irradiated and Post-Irradiation Annealed Pure Copper (PNNL & Risø National Laboratory)



Post-Irradiation Annealed Condition

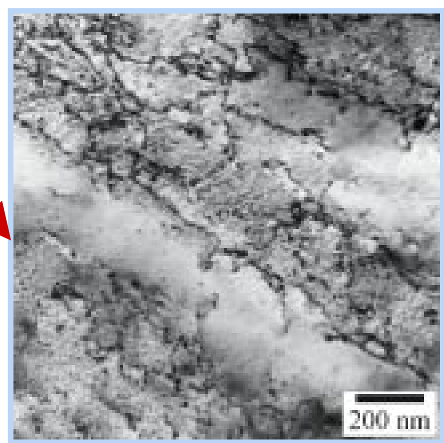
- Dislocation cell structure: material deforms homogeneously at 0.01 dpa
- Mixture of channeling and homogeneous deformation at 0.3 dpa

PI Annealed, 0.01 dpa   PI Annealed, 0.3 dpa

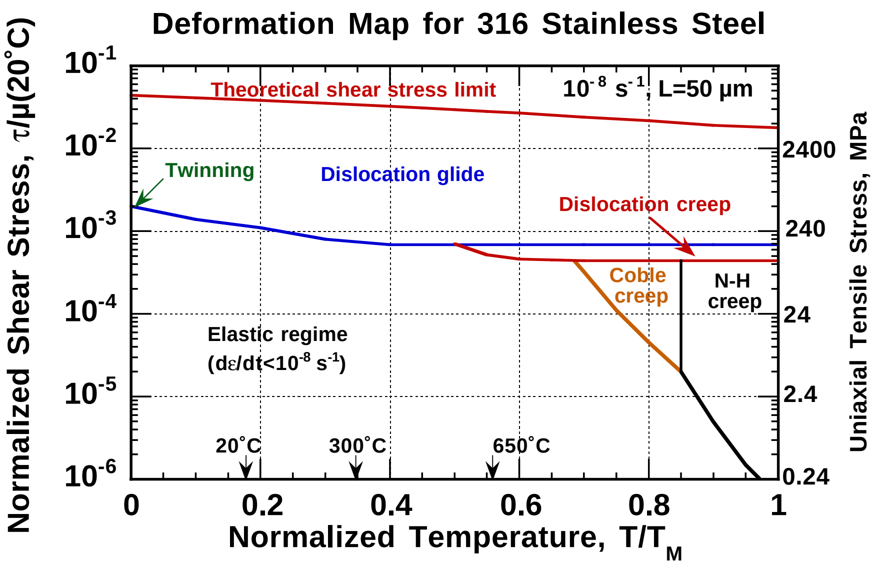


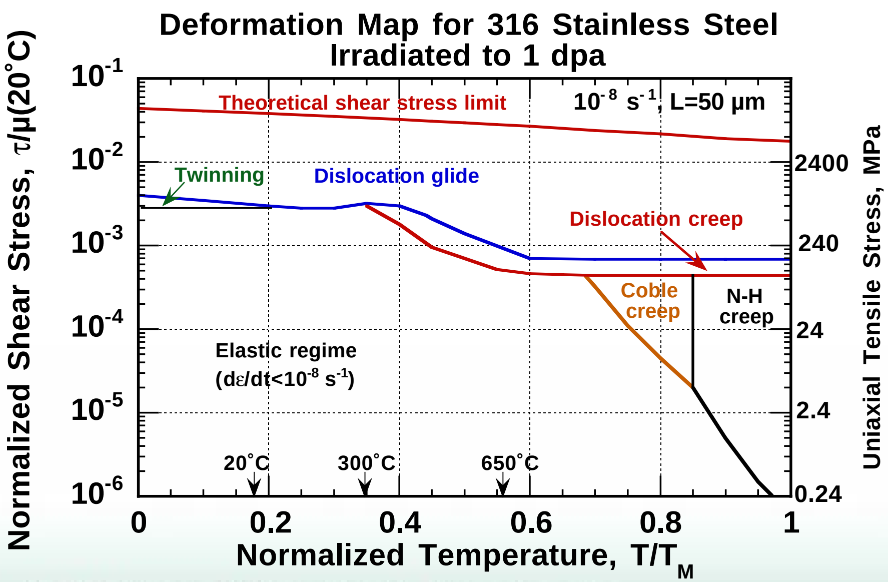
As-Irradiated, 0.3 dpa

- Cleared channels with little to no dislocation movement between the channels; localized deformation
- Large increases in strength (6 to 8x)
- Loss of uniform elongation and work hardening capacity
- Formation of a clearly defined yield point

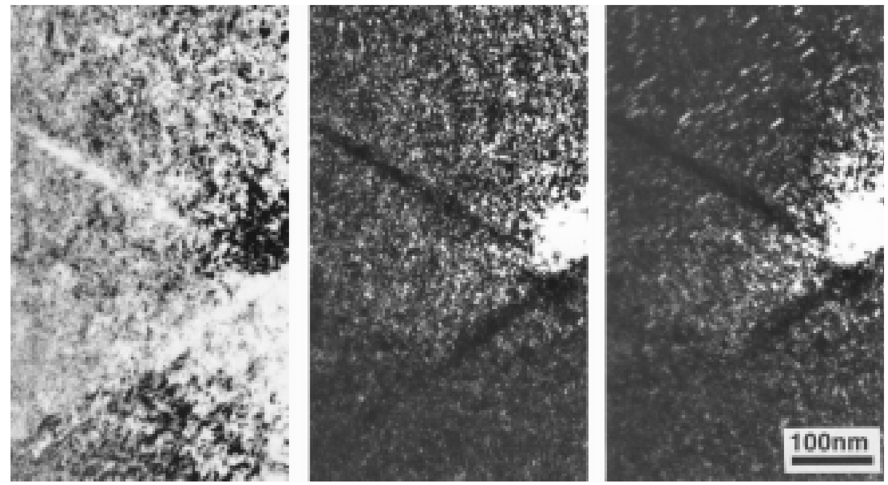


Deformation mechanisms in FCC metals

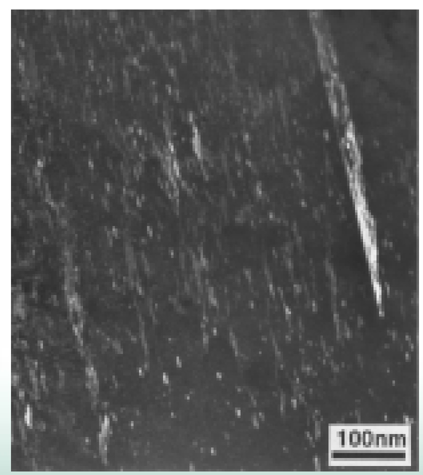




Irradiation is a useful tool to produce controlled microstructures for deformation mechanics studies



Channeling (Disln glide) occurs at higher temperatures (~300˚C)

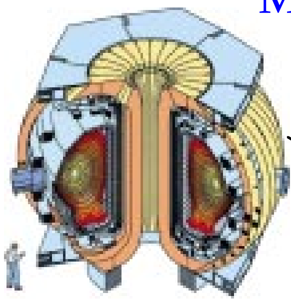


Twinning occurs at lower temperatures (<200˚C) and high strain rates

Multiphysics - Multiscale Fracture Modeling - I

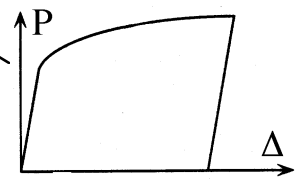
10 m

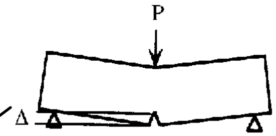
Macroscopic Scale



10^{-2} m

structure





specimen

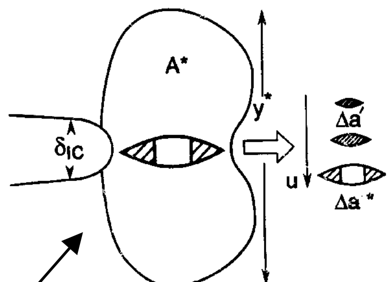
Elastic-plastic deformation and fracture of a cracked body as a function of temperature and loading rate as characterized by material macro constitutive and fracture toughness properties.

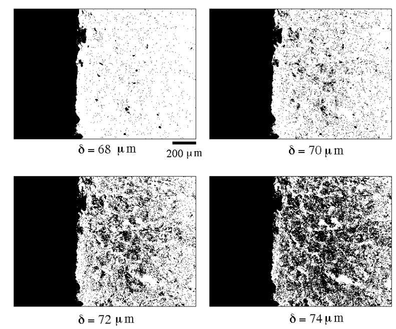
FEM: load-displacement

Large scale bridging

10^{-3} m

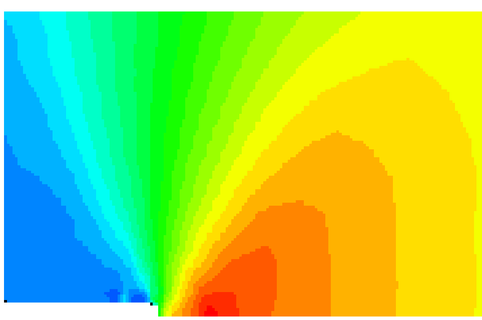
Mesoscopic Scale

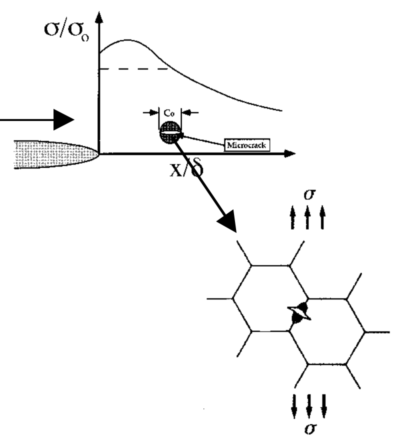


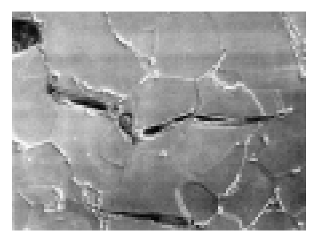


Local multiaxial plasticity at blunting macro-crack tip resulting in stress-strain field concentrations that crack mm-scale brittle trigger particles. Many micro-cracks arrest at particle-ferrite interfaces, lath packets, and grain boundaries. Ultimate process zone damage development and collective instability cause macro-cleavage.

FEM: blunting fields







Trigger particle mechanics

$$\sigma^* = K_{micro}/C\sqrt{\pi a}$$

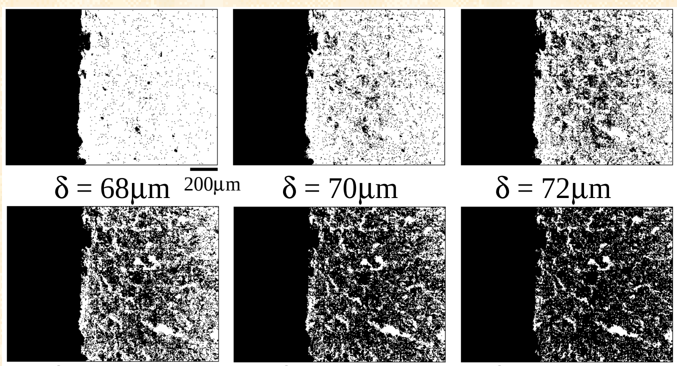
10^{-10} m

UCSB

Multiscale Research on Fracture Mechanisms, Mechanics, Models and Structural Integrity Assessment Methods

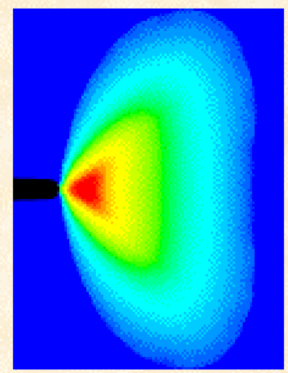
Fracture involves multiple processes interacting from atomic to structural scales. UCSB is developing multiscale physical fracture models and new engineering methods of fracture control using small-scale tests. Research combines theory, models, measurements and characterization of key processes at all pertinent length scales.

Tomographic Imaging of Cleavage

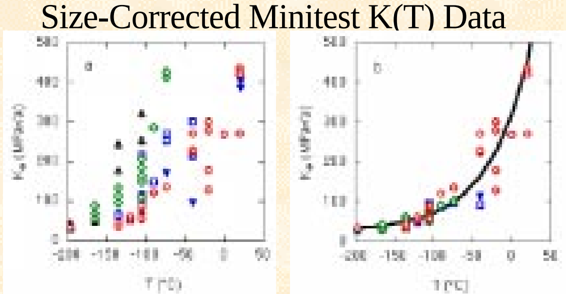


δ = 74μm δ = 76μm δ = 78μm

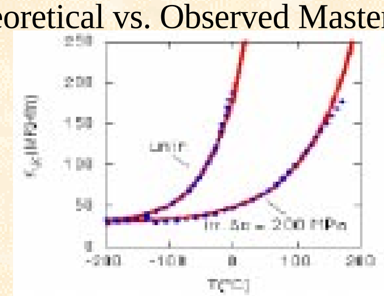
FEM Simulations of Crack Fields



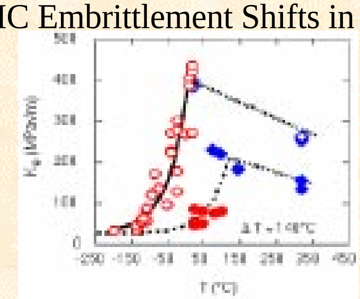
Size-Corrected Minitest K(T) Data



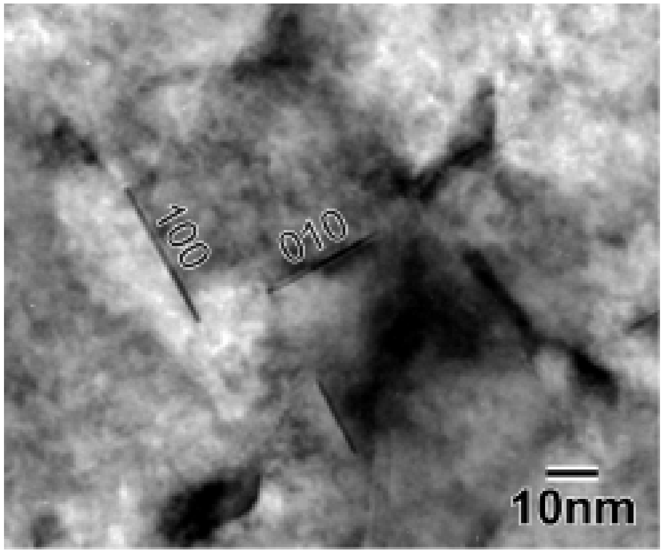
Theoretical vs. Observed Master Curve

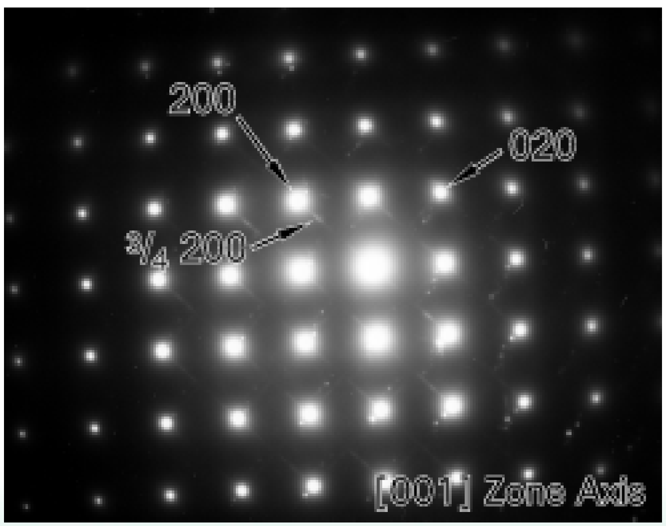


MC Embrittlement Shifts in F82H

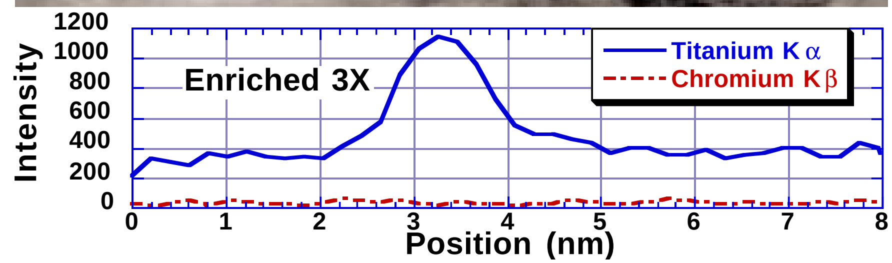


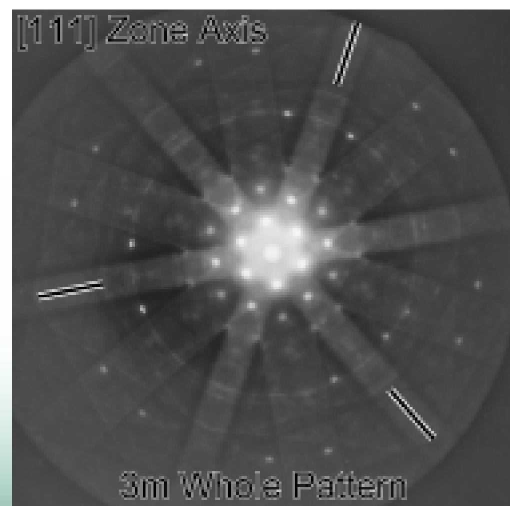
Advanced Analytical Electron Microscopy Techniques are being used to Examine Precipitates in V alloys





Solute Segregation Was Detected in V-4Cr-4Ti Following Neutron Irradiation to 0.5 dpa at Elevated Temperatures

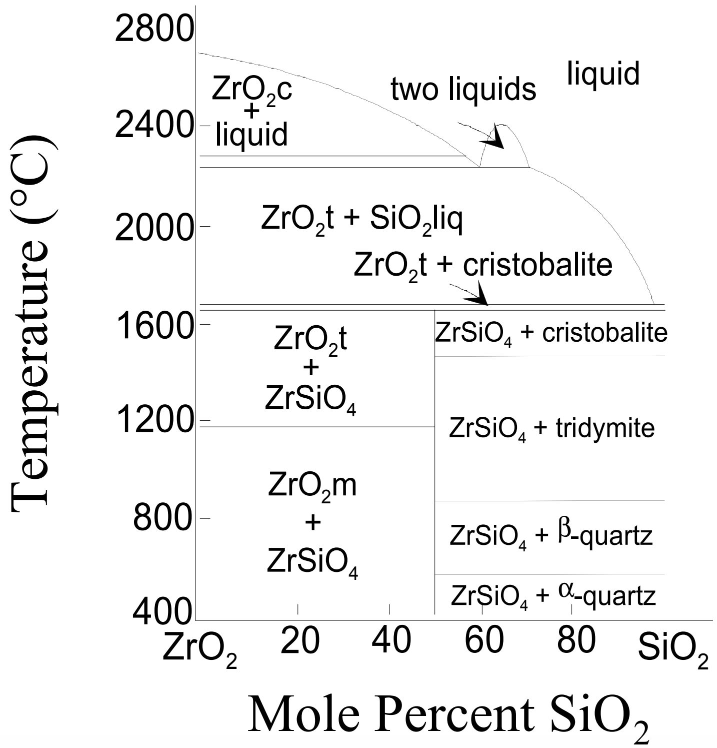




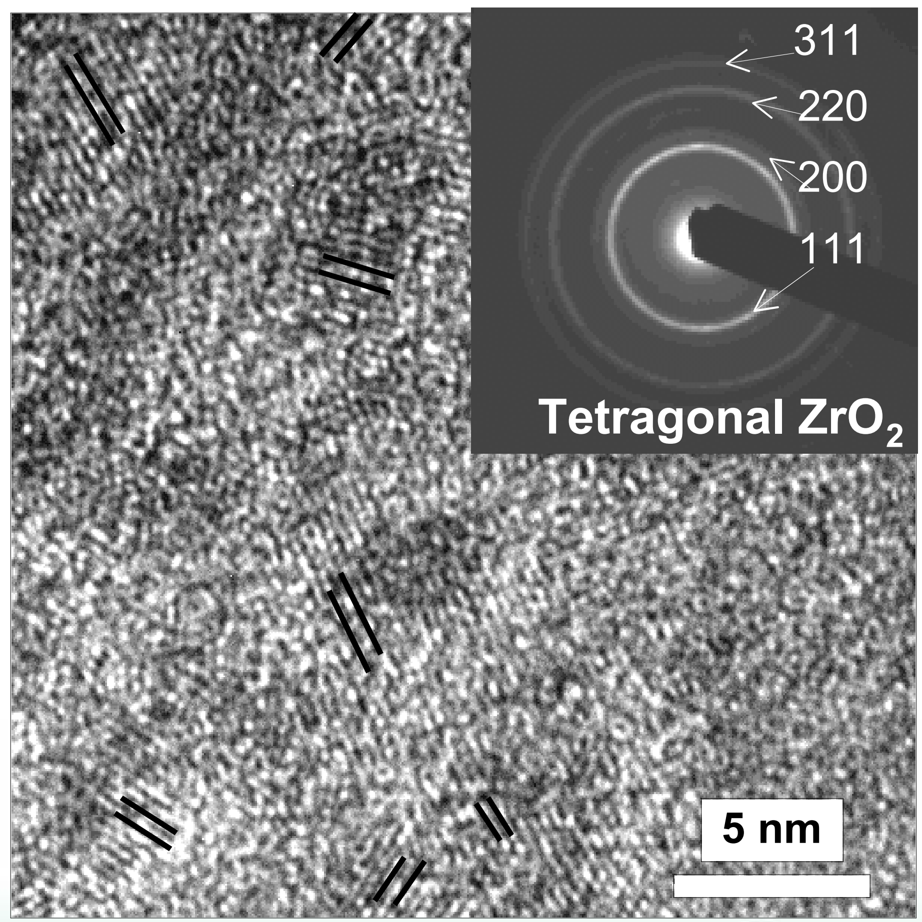
Analytical microscopy reveals Ti-rich precipitates with Fm3m space group

Experimental evidence for nanoscale melting during atomic collisions has been obtained

ZrO_2-SiO_2 Phase Diagram



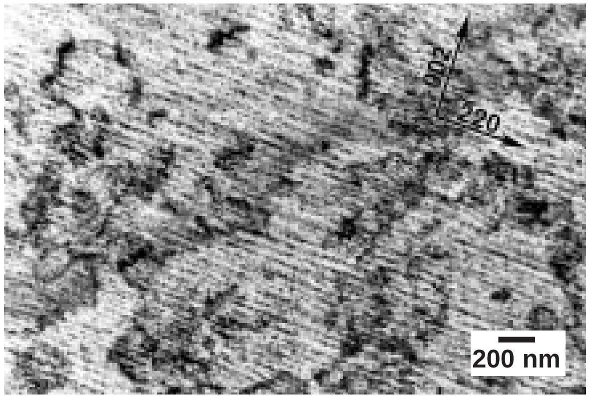
Microstructure of Zircon Irradiated at 800 °C



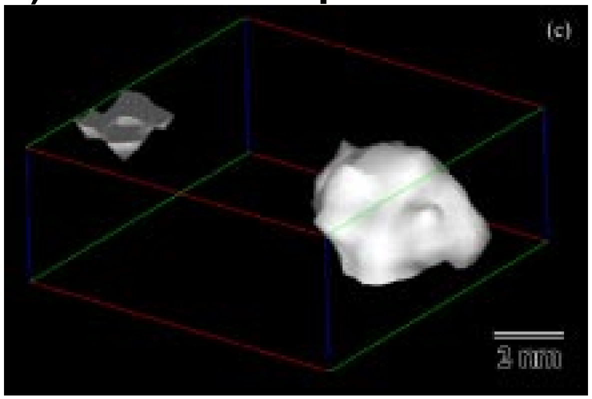
Nature, vol. 395, Sept 5. 1998, p. 56

Nanoscience appears in numerous places in the fusion materials science program

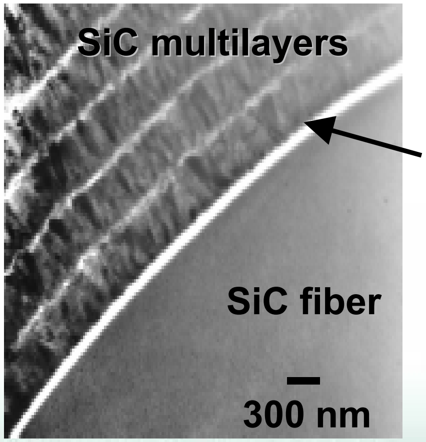
Nanoscale self-organization of defect clusters in neutron-irradiated Ni



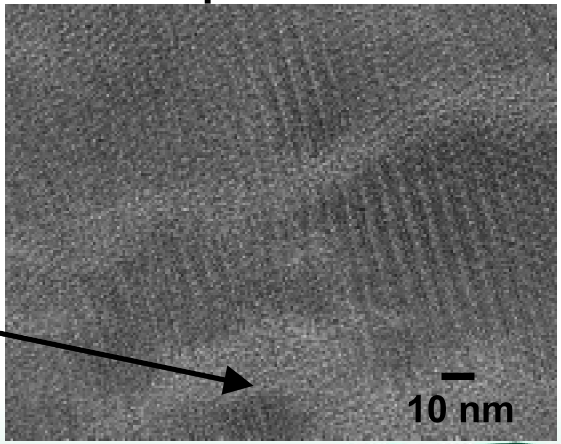
3-D atom probe iso-composition contour (Y, Ti, O) for nanocomposited ferritic steel



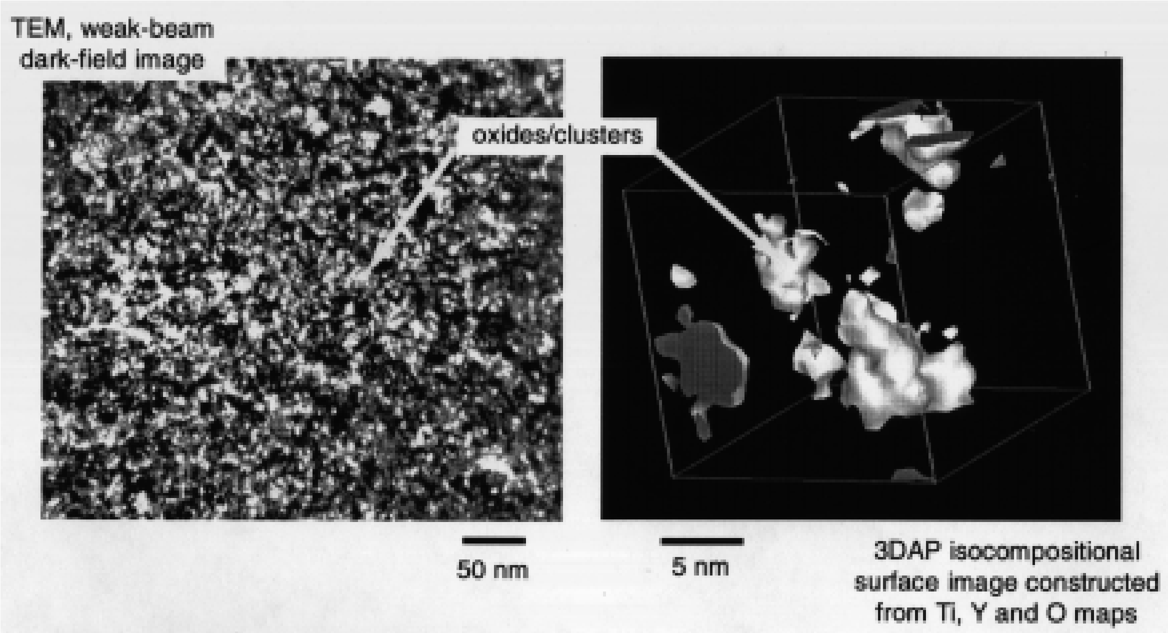
Crack-deflecting interfaces in ceramic composites give improved toughness



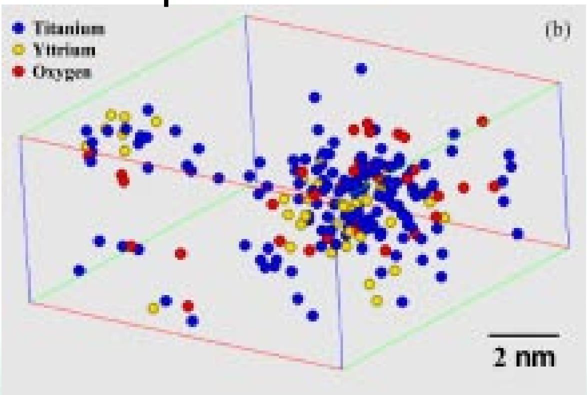
Atomic resolution analysis of crystal-amorphous transition in SiC



Recent work at ORNL suggests that thermodynamics may be significantly altered at the nanoscale

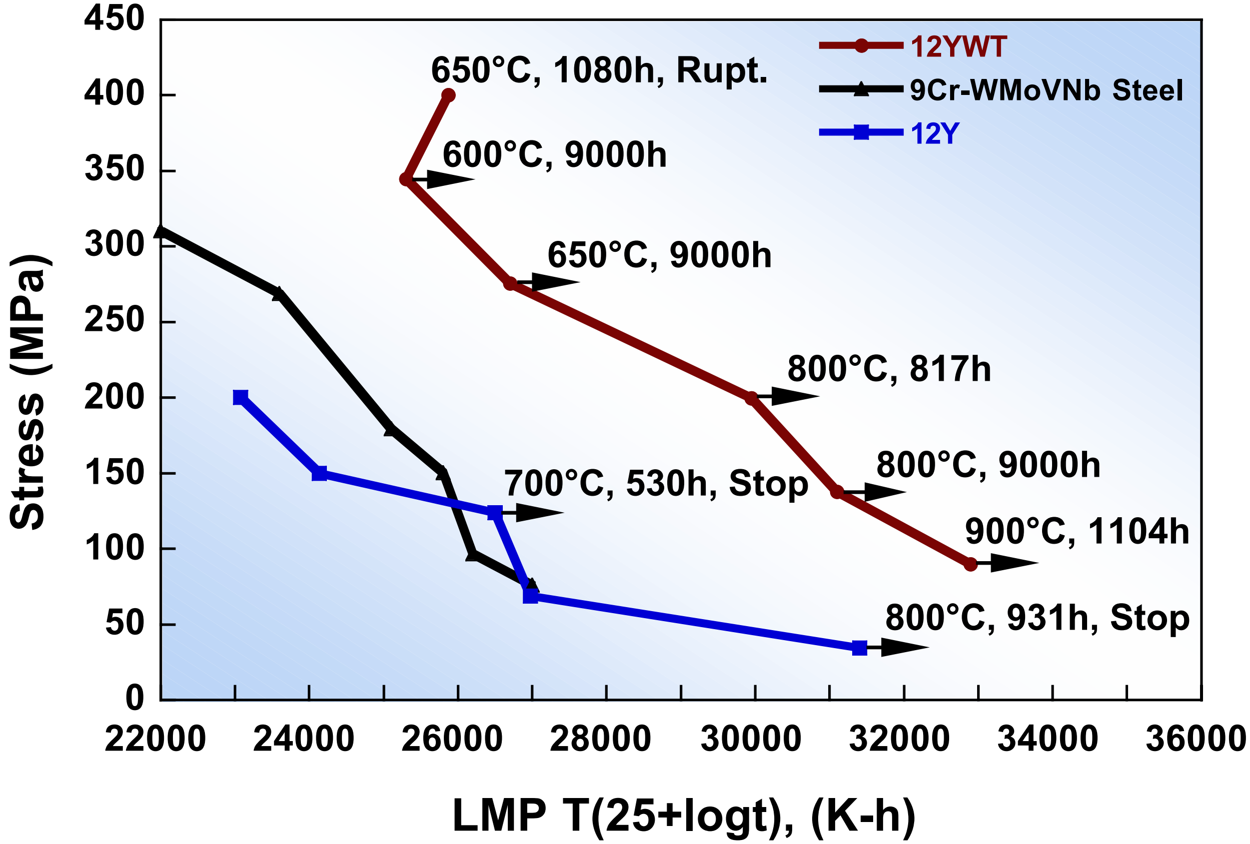


Atomic composition of nanoclusters



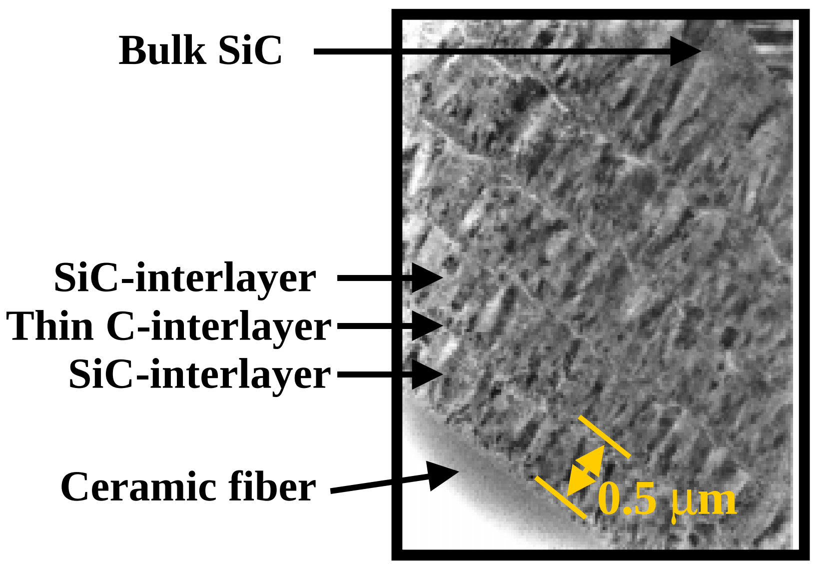
Atomic analysis of new nanocomposited ferritic steel provides clues to its outstanding creep strength (6 orders of magnitude lower creep rate than conventional steels at 600-900˚C)

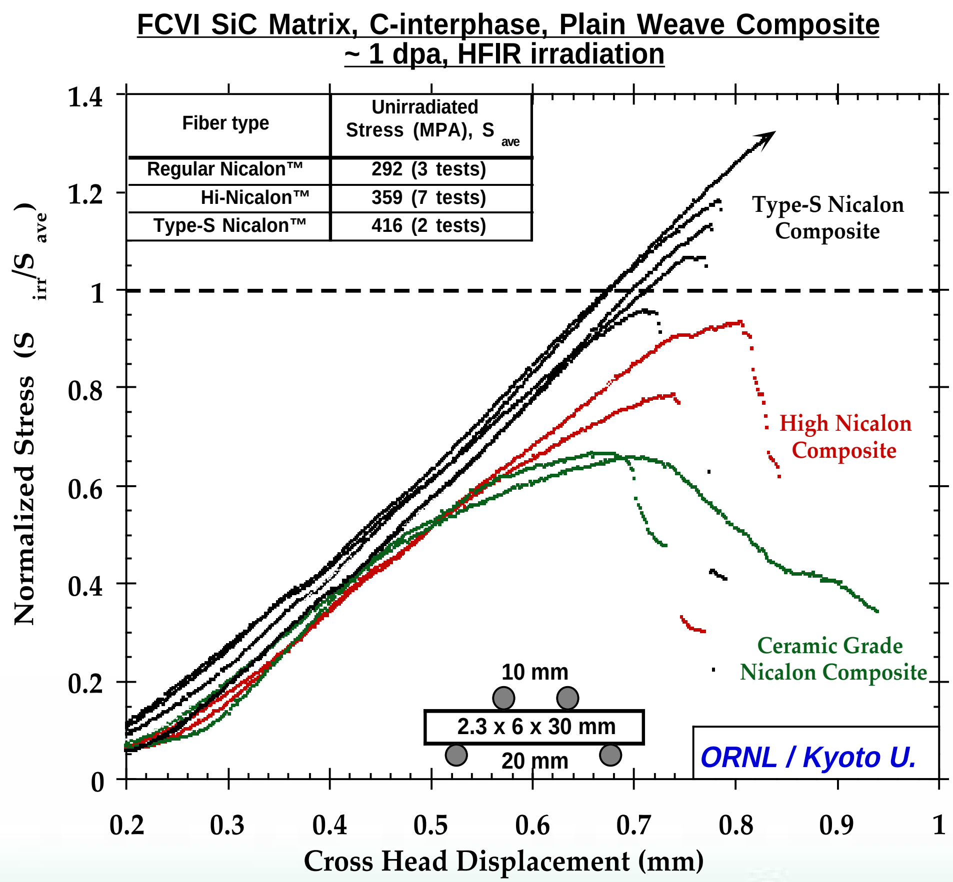
Discovery of Unprecedented Strength Properties in Iron Base Alloy



- Time to failure is increased by several orders of magnitude
- Potential for increasing the upper operating temperature of iron based alloys by ~200°C

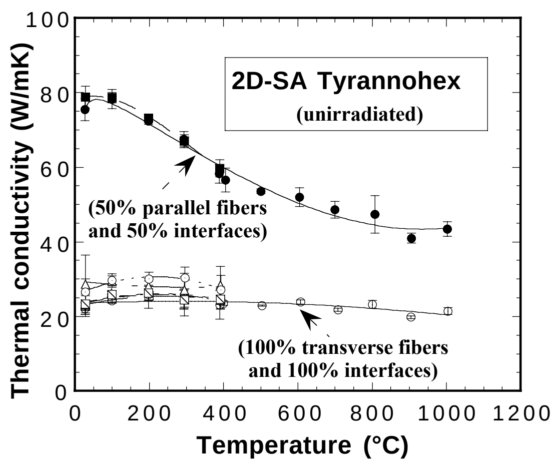
A science-based program involving tailored nanoscale microstructures is producing remarkable advances in radiation-stable ductile ceramic composites (SiC/SiC)





Thermal Conductivity of 2D SiC/SiC Composites

Fusion Materials Program



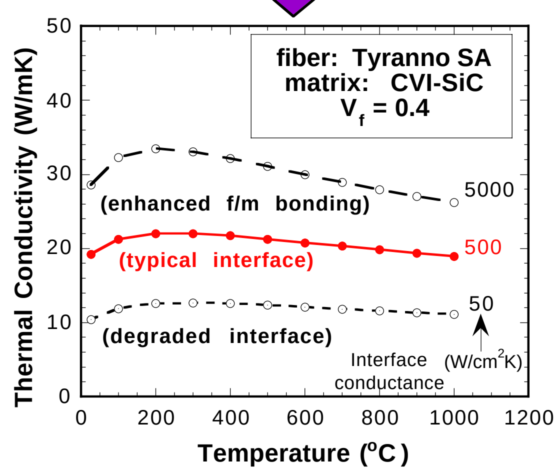
Experimental:

- Number and quality of interfaces important
- Fibers parallel to conduction path useful (3D architecture)
- Samples currently being irradiated

NERI Program

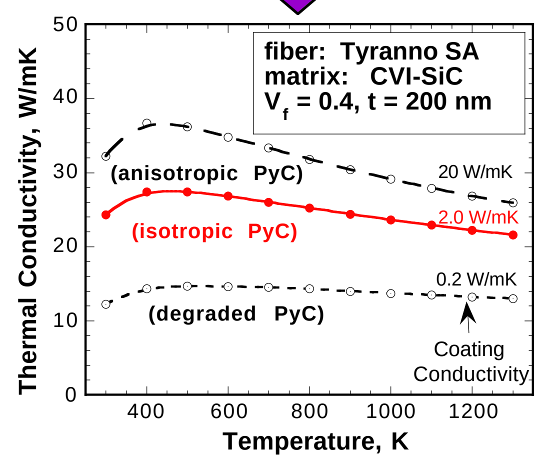
Model 1: Thin Interface Conductance

- Strong bonding due to fiber surface treatment useful
- Degraded interface due to irradiation or fiber/matrix mismatch



Model 2: Interphase Conductivity

- Preferred orientation of graphitic crystallites
- Strong interface cohesion
- Degraded interphase due to irradiation or oxidation



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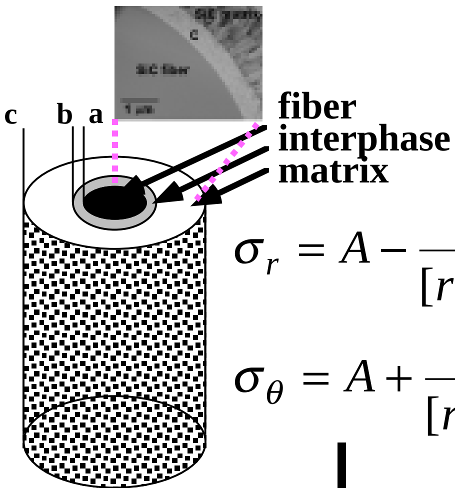
U.S. Department of Energy
Pacific Northwest National Laboratory

Crack Growth in Ceramic Composites is a Potential Lifetime-Limiting Mechanism Controlled by Microscale Phenomena

microscale

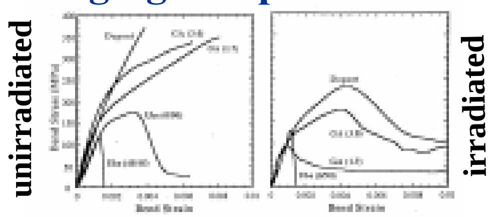
Analytical modeling of internal stresses

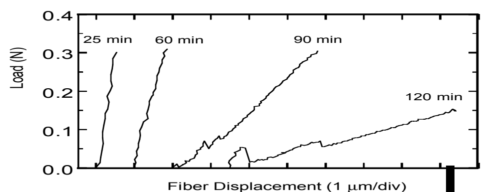


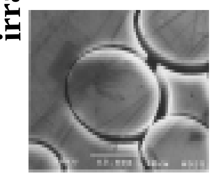
$$\sigma_r = A - \frac{B}{[r(dpa)]^2}$$

$$\sigma_\theta = A + \frac{B}{[r(dpa)]^2}$$

Experimentally determined, semi-empirical, bridging-compliance relations





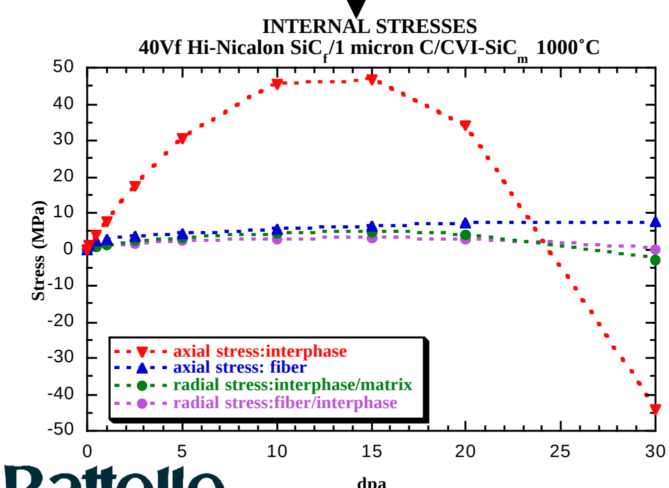


Micromechanical model for predicting subcritical crack growth due to microscale mechanisms.

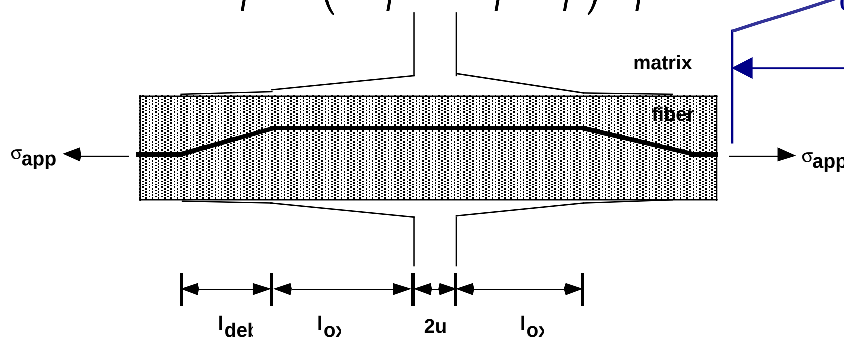
+

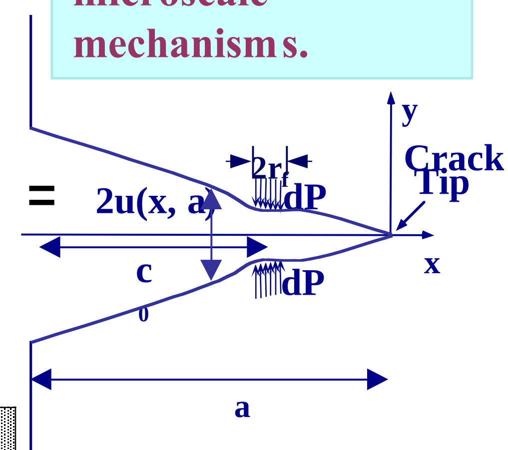
=

macroscale



$$u_f = \left(\Phi^l_f + P_f \Phi^n_f\right) P_f$$

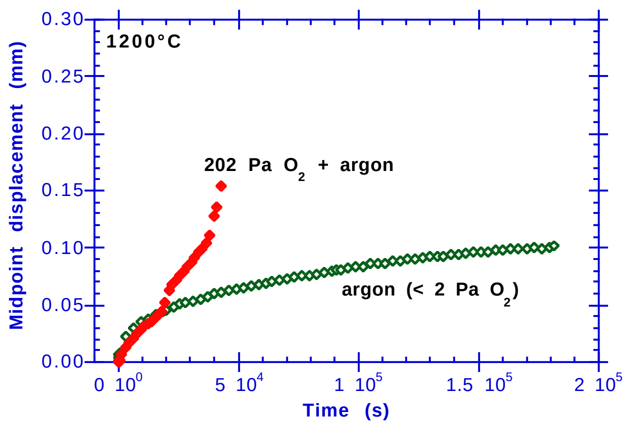




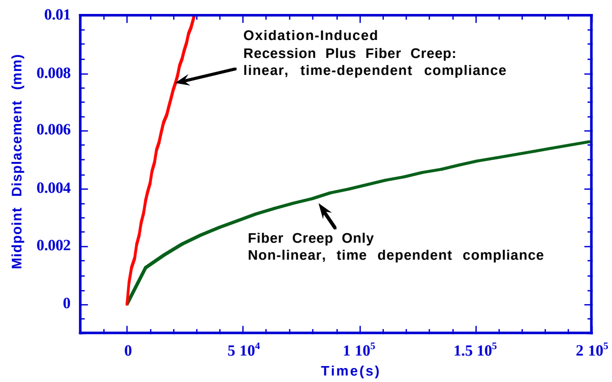
Micromechanical Modeling Allows Prediction of Component Lifetime of Ceramic Composites

Model verification

experiment



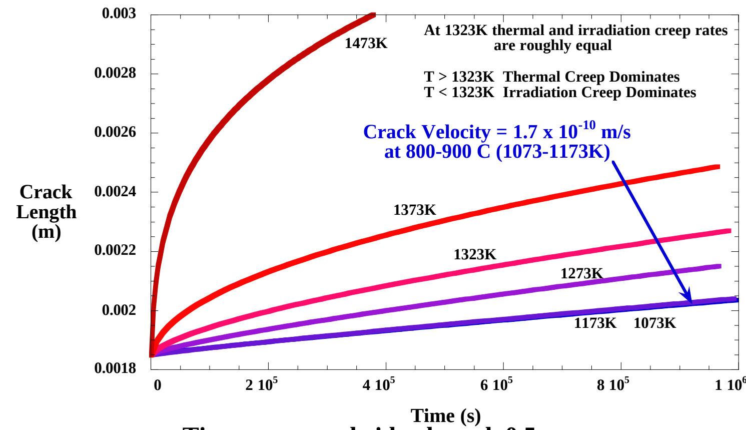
model



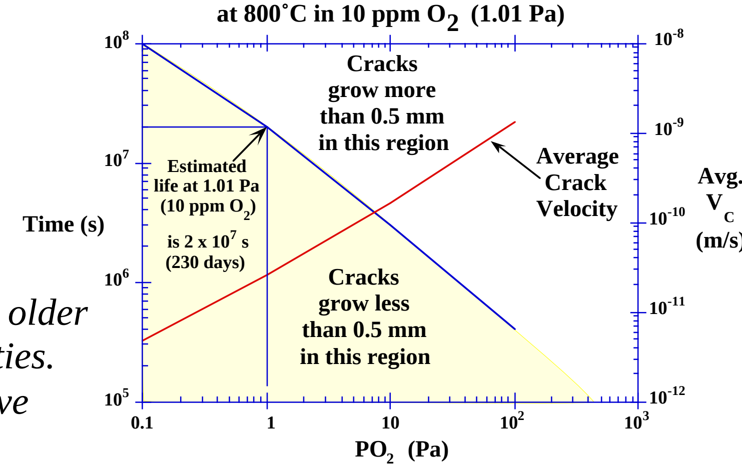
Oxygen atmosphere investigated in conjunction with DOE office of Basic Energy Science Program

Predictive capabilities

Irradiation-enhanced creep of fibers controls crack growth below ≈ 1073 K



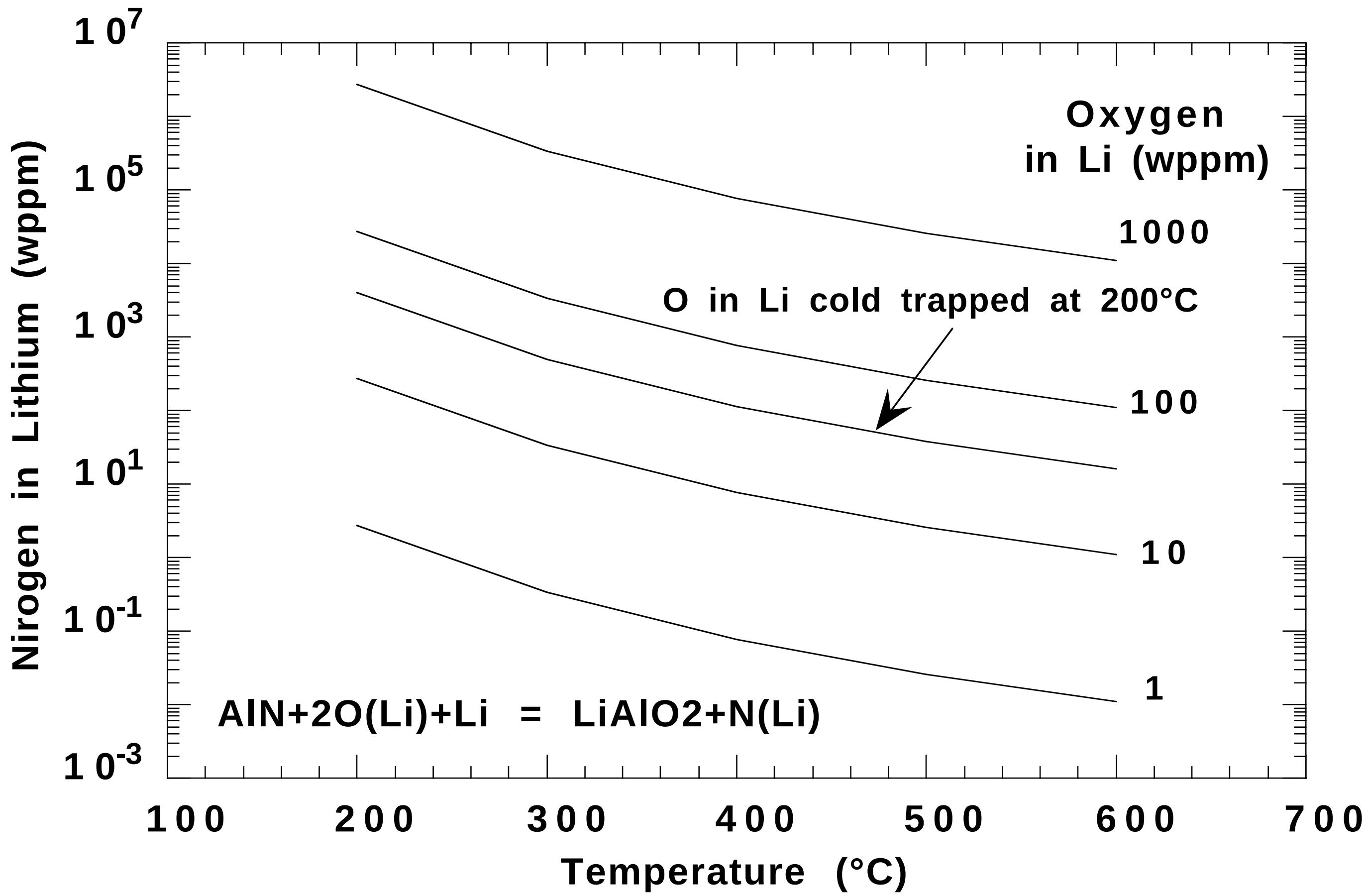
Time to grow a bridged crack 0.5 mm at 800˚C in 10 ppm O_2 (1.01 Pa)



Model predicts crack velocity and crack length

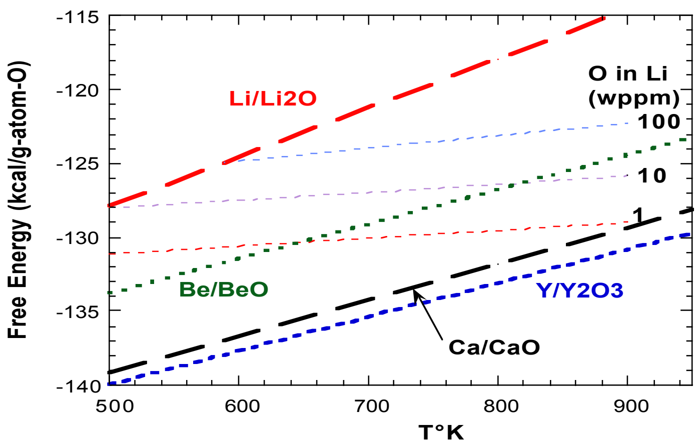
NOTE: Lifetime predicted for older generation material properties. More recent materials have enhanced lifetimes.

Calculated Regions of Thermodynamic Stability for AlN in oxygen-enriched Li

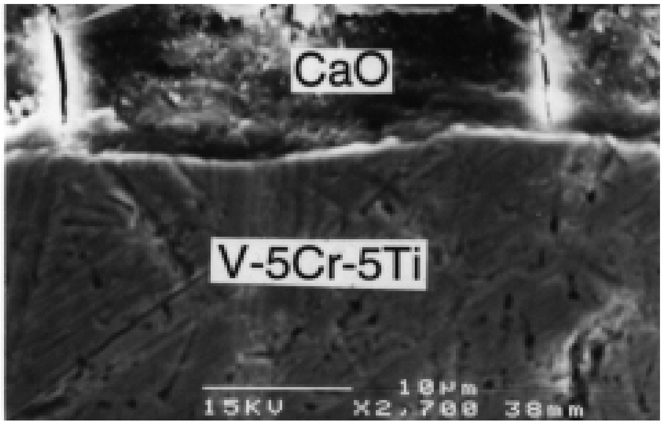


Argonne National Laboratory

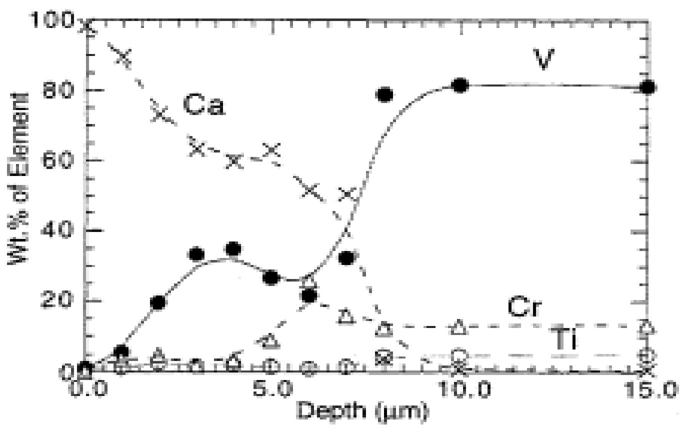
Thermodynamic Stability, Microstructure Characterization, and Property Evaluation of In-situ Formed "CaO" Insulating Coating on Vanadium Alloys



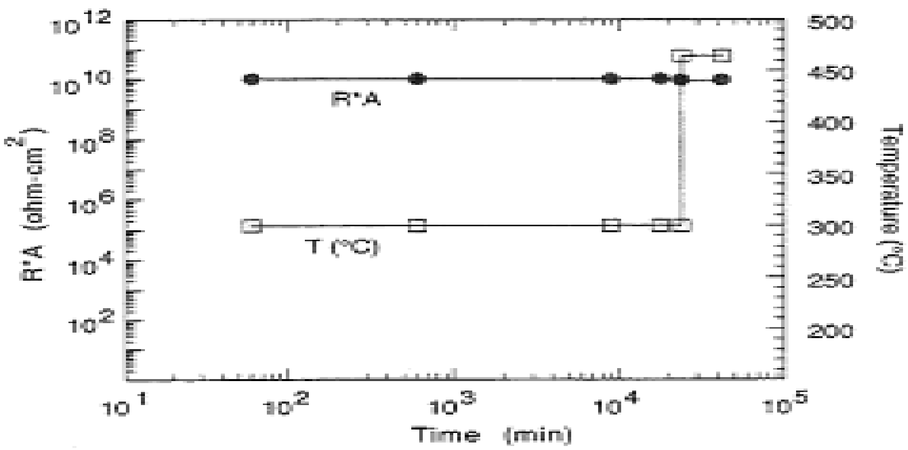
- Calculated thermodynamic stability of candidate oxides in lithium as function of oxygen content



- Microstructure of "CaO" coating on V-alloy



- **Composition from EDS analysis vs depth for in-situ formed "CaO" coating on V-alloy**



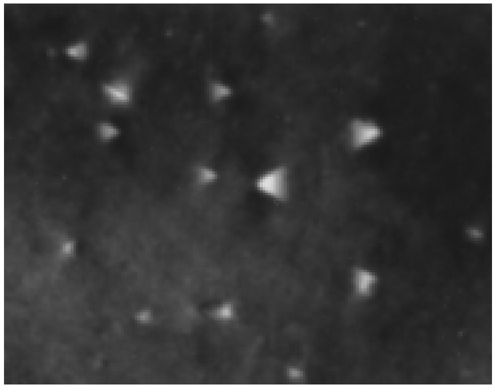
- In-situ resistance of "CaO' coating in lithium

Argonne National Laboratory

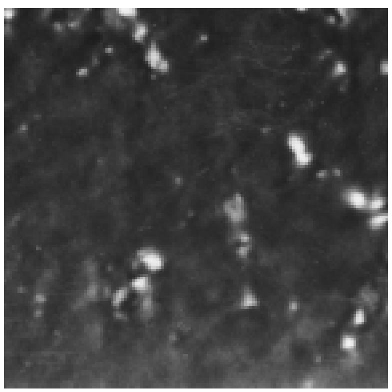
One of the Most Important Scientific Results From the US/Japan Collaborations on Fusion Materials has been the Demonstration of Equivalency of Displacement Damage Produced by Fission and Fusion Neutrons

Similar defect clusters produced by fission and fusion neutrons as observed by TEM

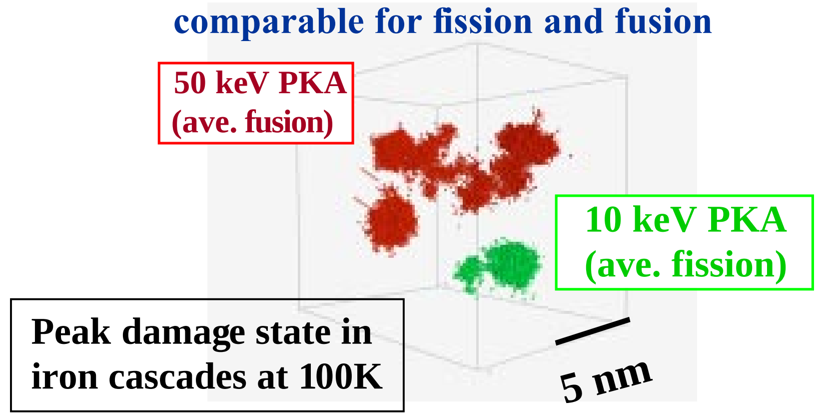
Fission (0.1 - 3 MeV)



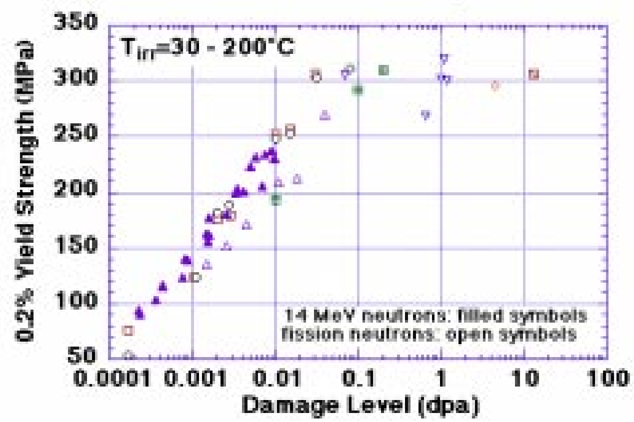
Fusion (14 MeV)



MD computer simulations of the displacement events show that subcascades and defect production are comparable for fission and fusion



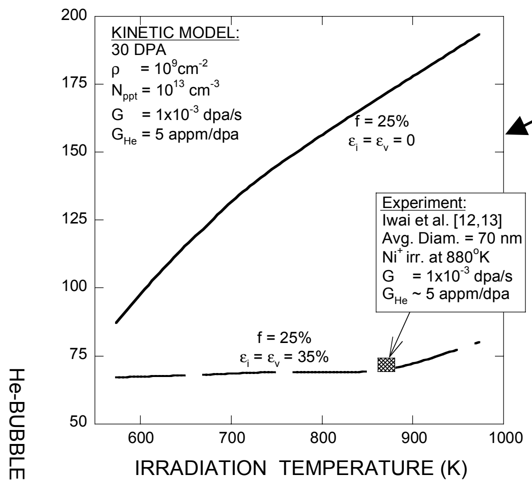
Similar hardening behavior confirms the equivalency

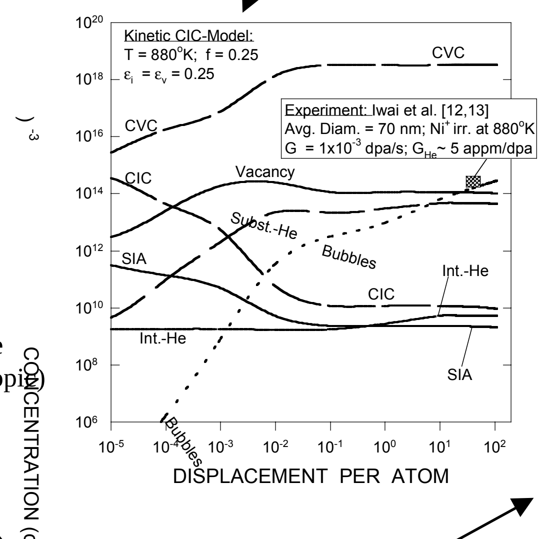


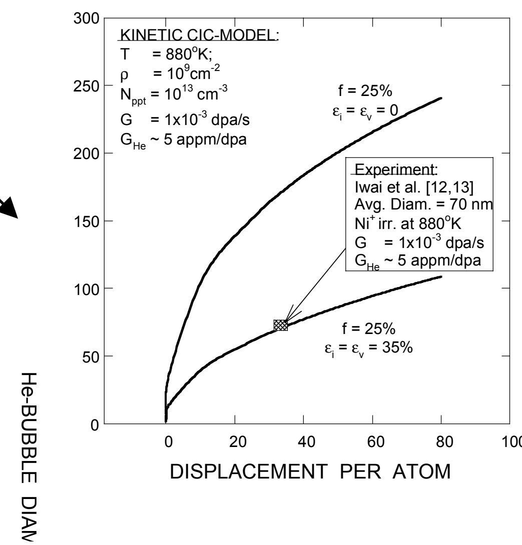
A critical unanswered question is the effect of higher transmutant H and He production in the fusion spectrum

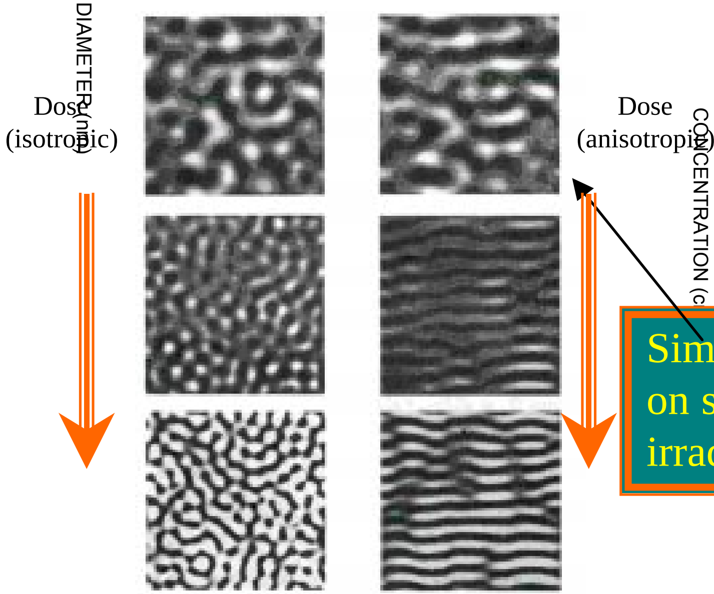
UCLA Advanced Rate Theory Modeling of Microstructure Evolution: Main features (1) Mobile cascade-induced clusters (CIC); (2) Continuous helium generation; (3) Coupled Nucleation & Growth; (4) Spatial self-organization.

Simulations & experiments for microstructure evolution in vanadium with helium effects

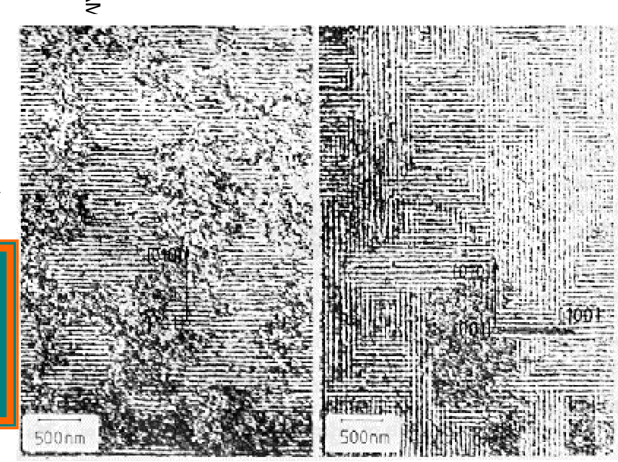








Simulations & experiments on self-organization of irradiated Cu microstructure.

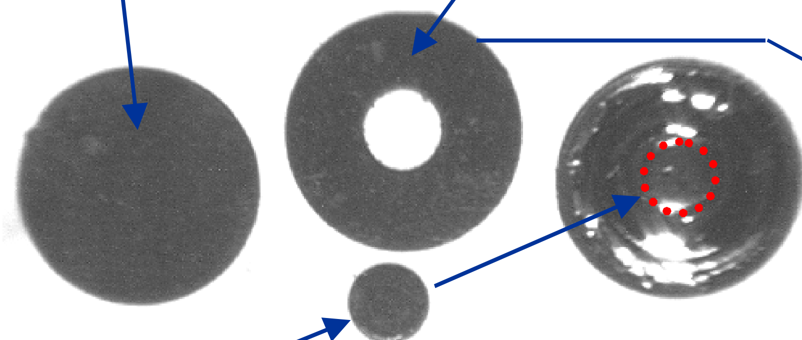


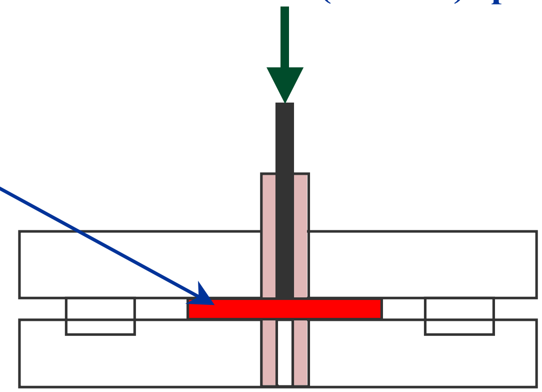
Newly Developed Techniques Allow Greater Materials Science Output From Smaller Irradiation Volumes

3 mm TEM disk is irradiated in fission reactor

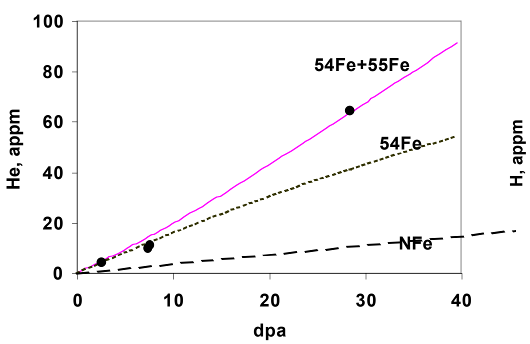
He and H analyses on outer rim

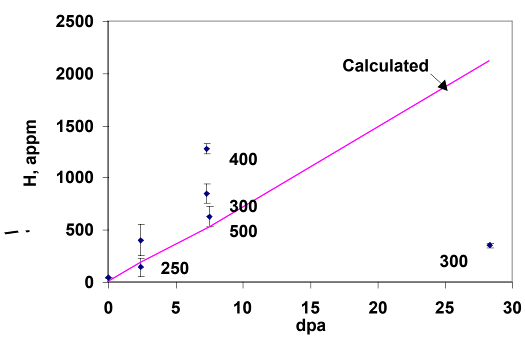
Shear punch test yields mechanical properties data that correlate with tensile data and can be correlated with data on conventional (full size) specimens

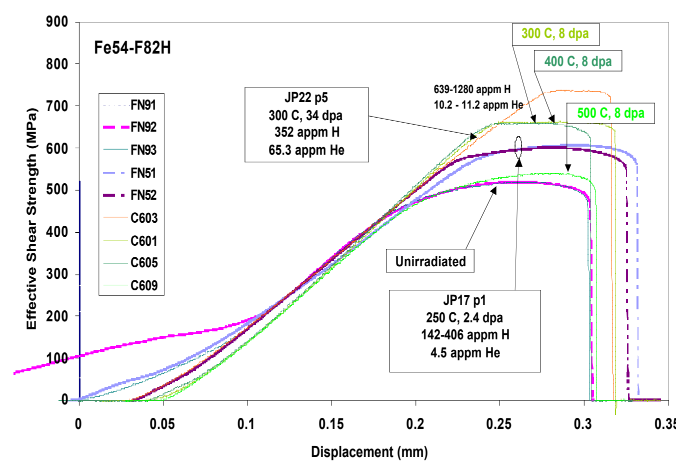




Bonded into unirradiated disk to reduce radioactivity levels and waste generation in evaluation of microchemistry and microstructures







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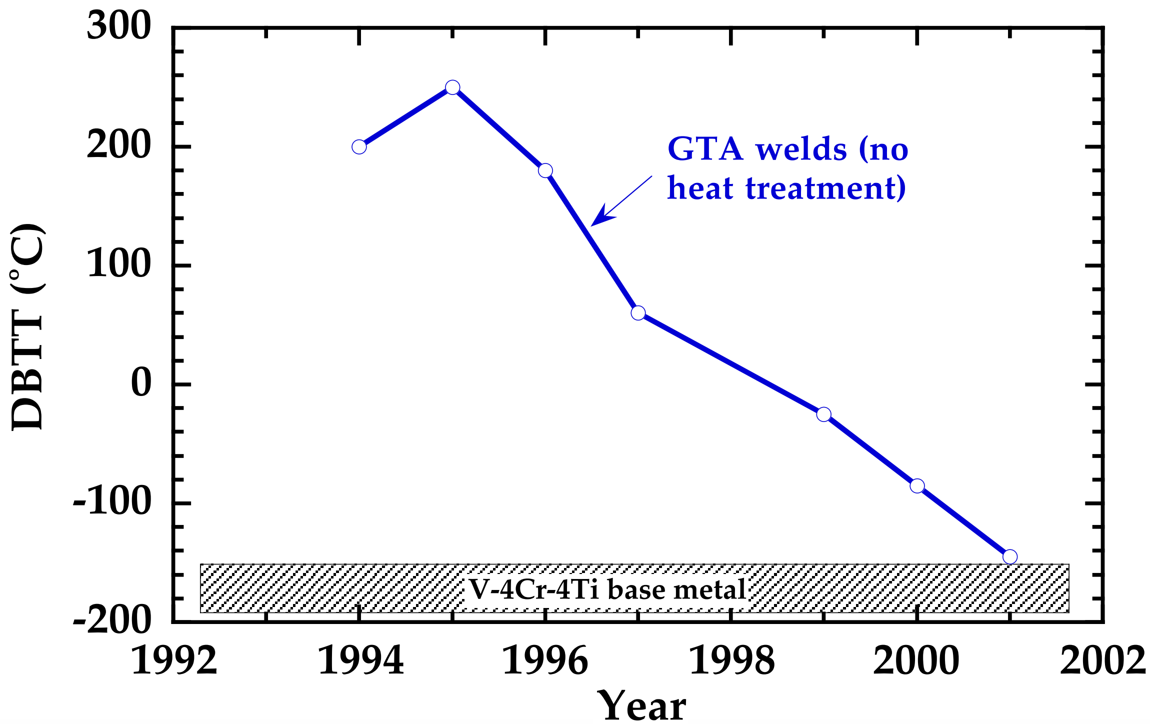
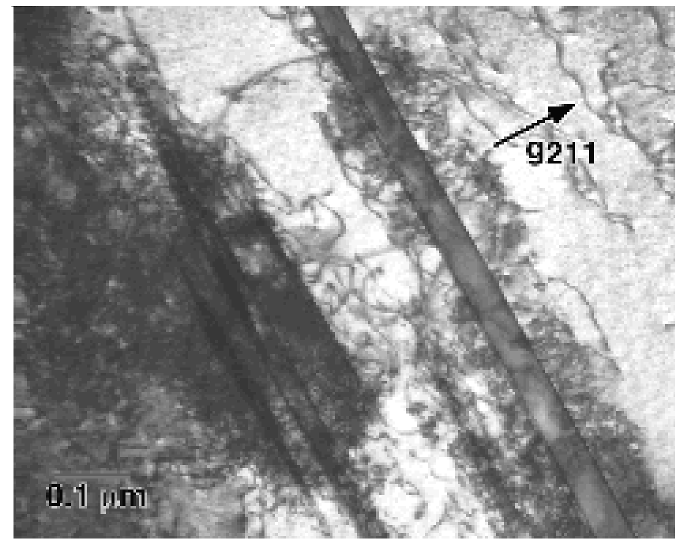
Hydrogen and Helium analysis results

U.S. Department of Energy
Pacific Northwest National Laboratory

A focussed, science-based welding program has successfully resolved one of the key feasibility issues for V alloys



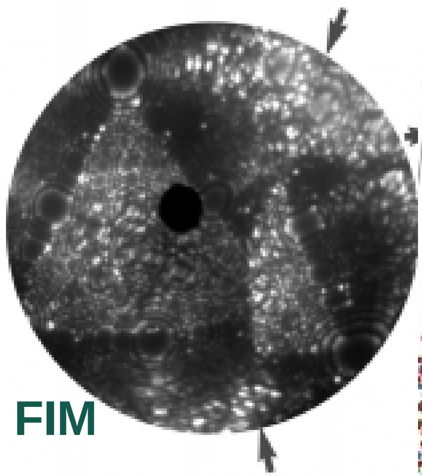


– Results are applicable to other Group V refractory alloys (Nb, Ta)

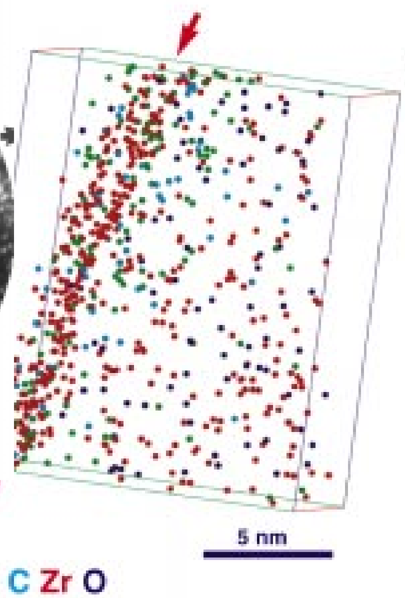
Atom Probe Tomography Reveals Zr, B and C Segregation to Grain Boundaries Produces Improved Mo Weldments

- B, Zr (and C) segregation inhibits O embrittlement of grain boundaries
  - E_{tot}~20%, transgranular fracture mode instead of typical e_{tot}~3%, intergranular fracture for Mo welds
- Bulk alloy composition: 1600 appm Zr, 96 appm C, 53 appm B, 250 appm O

BASE METAL



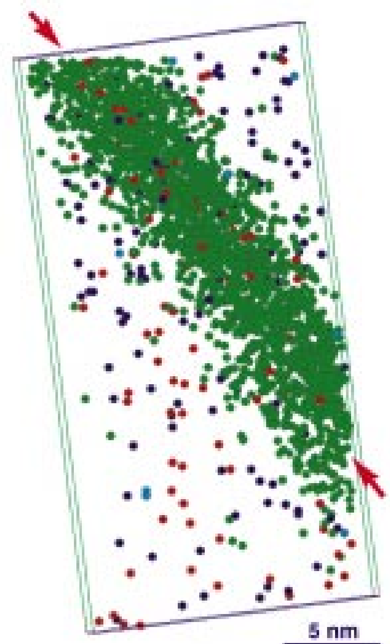
FIM



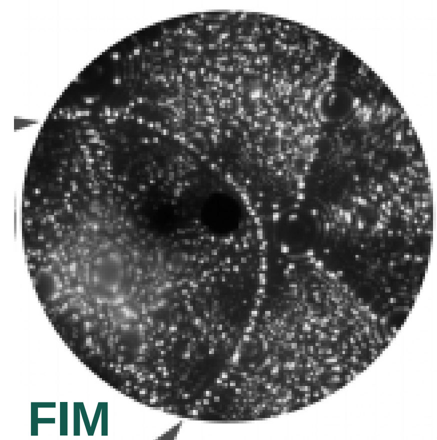
GIE (atoms m^{-2})

Zr	7.6 x 10^{13}
B	7.3 x 10^{12}
C	1.1 x 10^{13}
O	-3.9 x 10^{12}

HEAT AFFECTED ZONE



APT atom maps



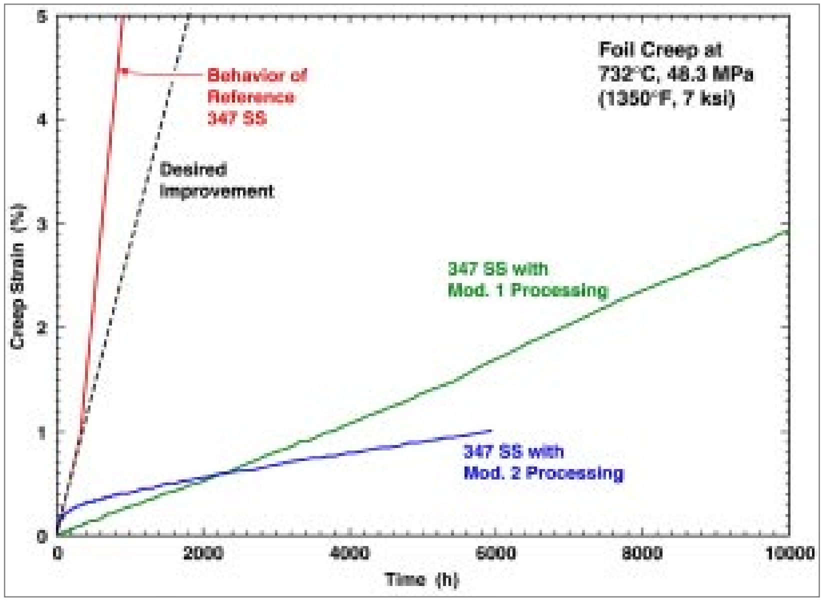
FIM

GIE (atoms m^{-2})

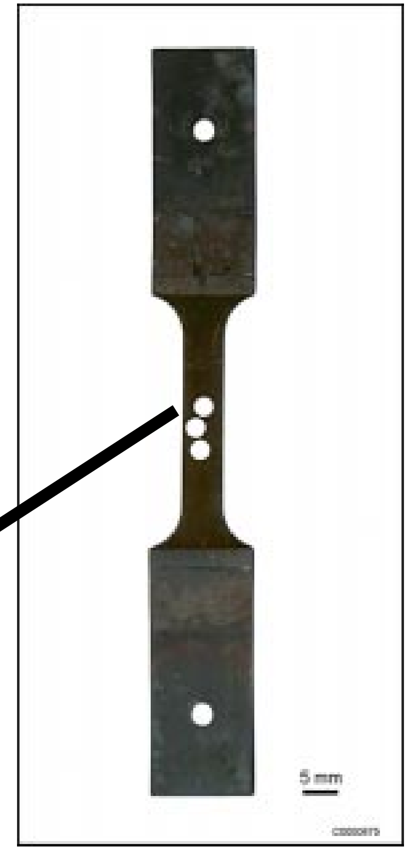
Zr	1.3 x 10^{13}
B	9.9 x 10^{14}
C	9.9 x 10^{11}
O	1.1 x 10^{13}

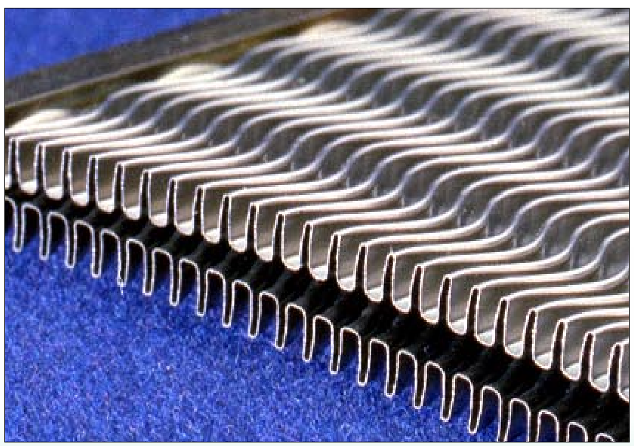
Research performed by
M. K. Miller, Oak Ridge National Laboratory
and A. J. Bryhan, Applied Materials

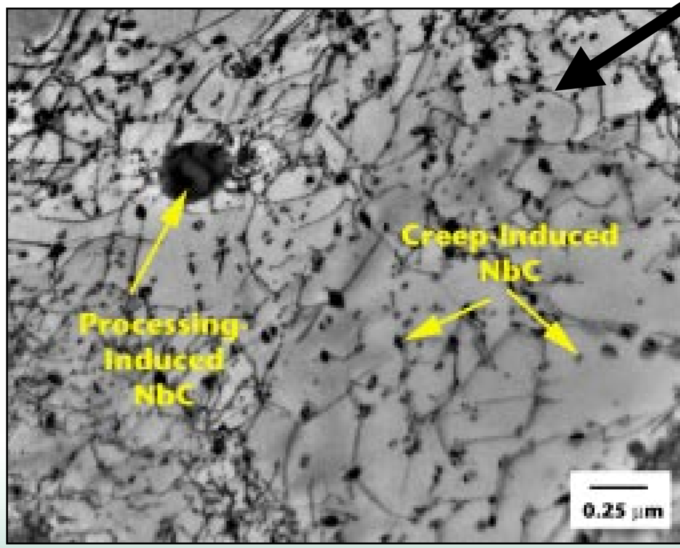
Microstructure-Mechanical property knowledge derived from Fusion Materials Science investigations is being transferred to US Industry



Precipitate stability knowledge derived from radiation effects studies can be used to develop highly creep resistant alloys (microturbine recuperator)







The Materials Science Program Provides the Underlying Materials Science Knowledge Base within the VLT

Technology Program Element	Types of Materials Addressed	Key Materials Issues
• Materials Science	**• Structures • Coatings • Insulating ceramics • Optical materials**	**•deformation,fracture mechanisms • thermodynamic, kinetic stability • electric, dielectric degradation • F center formation, stability**
• Plasma Technology	• Plasma facing/high heat flux components • Magnet components • ICH/ECH launcher/ antennas	• plasma interactions, heat transport • critical current, insulator perform. • low-loss coatings and feedthroughs
• Fusion Technology	• Fuels (tritium) • Breeder systems	• tritium permeation • thermal, neutronics, hydrodynamics
• IFE	• Chamber wall • Final optics	• durability, tritium retention • surface crazing, bulk defects
• Safety	• Structure, coolant, breeder	• volatization, decay heat
• Advanced Design	• Overall integration	• compatibility, performance limits

Interactions with International Fusion Materials Community

Science issue	**Activity**	**US**	**Japan**	**EU**	**Russia**	**China**
Deformation & fracture	V alloys	IEA working gp.			IEA working gp.	
		DOE/Monbusho				
Deformation & fracture, Nanoscience (ODS)	Ferritic steel	IEA working group				
		DOE/JAERI				
Deformation mechanisms, enhanced thermal cond.	SiC/SiC	IEA working group				
		DOE/Monbusho				
		DOE/JAERI				
Cross-cutting theory & modeling phenomena	Theory & modeling	IEA working group				
Electric, dielectric props.	Ceramic insulators	IEA working group				
		DOE/Monbusho				
Accelerator physics, liquid jet thermohydraulics, He gas cooling technology	Neutron source (IFMIF)	IEA working group				

The Fusion Materials Science Program will use its expertise to help address materials issues of plasma and IFE studies

- **Early 2001:** send out requests for expressions of interest in using expertise of materials program
- **Mid-2001:** review EOI's and prioritize
- **Fall 2001:** initiate work on highest priority tasks

Conclusions

- **The program has been responsive to the 1998 FESAC panel recommendations**
  - **Enhanced theory & modeling effort is underway**
  - **FY02 strawman budget will not allow both international commitments and theory & modeling to be maintained at current levels**
- **The Fusion Materials Sciences program is pursuing simultaneous scientific excellence (fusion energy and materials science)**
- **Very strong ties have been established with the broader materials science community**
- **Fusion materials science research will serve as an increasingly valuable Enabling Technologies complement to the plasma science research program**