Overview of the Fusion Materials Sciences Program

Presented by S.J. Zinkle,

Oak Ridge National Lab

Fusion Energy Sciences Advisory Committee meeting

February 27, 2001

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

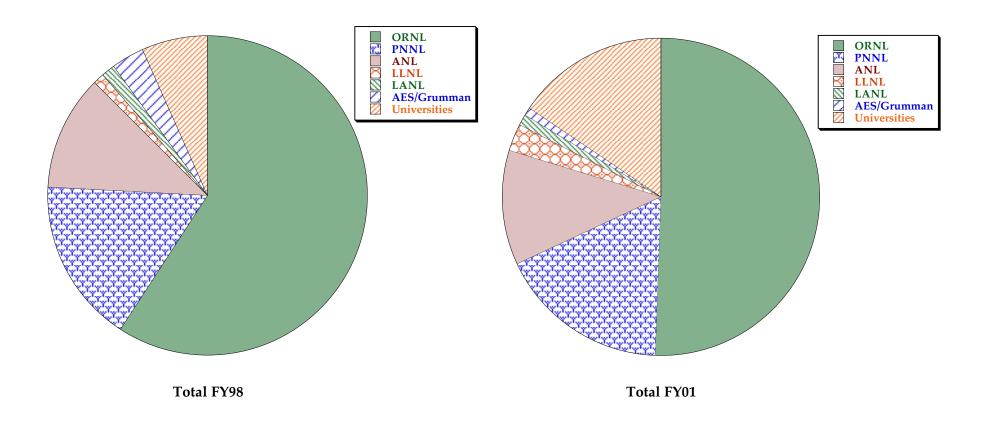
- Overall scientific quality of research is high
- R&D activities should be part of an integrated program in enabling technology
- •Research focus should be expanded to include a wide variety of materials for MFE and IFE
 - —Seek opportunities to interact & benefit from other government and industrial 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"

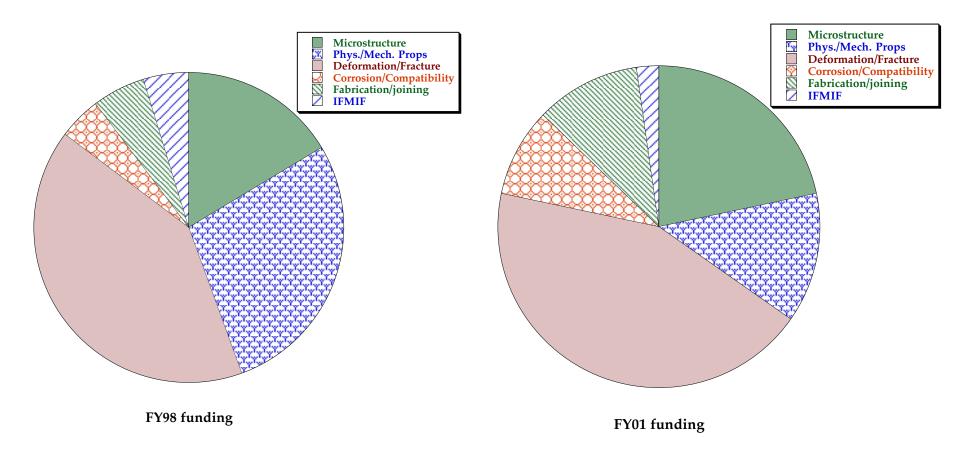
Thomas Jefferson

Fusion Materials Sciences Institutional Budgets



- 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



Continued emphasis on mechanical properties

Materials Restructuring Process

1998	<u>Events</u>	<u>Comments</u>
(external events, policy changes)	 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	<u>Events</u>	<u>Comments</u>
implementation begins)	 Theory/modeling competitive solicitation (\$1M) Guidance from OFES to accelerate restructuring process Develop concept for reorganizing along crosscutting 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
<u>Orientation</u>	Fusion Materials	Fusion Materials
	Development	Science
Mission	Schedule-driven	Fundamental
	development of	understanding of
	materials for fusion	scientific
	power (ITER blanket	underpinnings of
	test modules, DEMO,	materials for fusion
)	
<u>Organization</u>	Lead lab for each	Integrated national
	candidate structural	teams focused on
	materials class (V	key cross-cutting
	alloy, F/M, SiC/SiC)	issues
<u>Approach</u>	Experiments for	Experiments to
	semi-empirical	guide/ validate theory
	correlations	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)

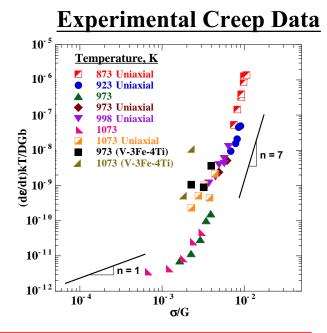
Old Approach (Development)	New Approach (Science)
 Select reference alloy (V-4Cr-4Ti) 	
 Focus most research on this alloy (narrow scope) 	 Focus research on fundamental understanding of BCC materials
 R&D planning based on need to develop materials to meet device construction schedule 	 Research planning 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

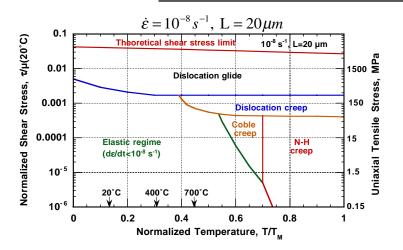
Diffusion-Controlled Creep Mechanisms

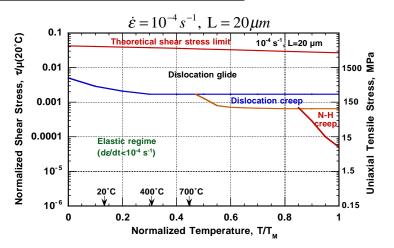
$$\frac{\dot{\varepsilon}kT}{DGb} = A\left(\frac{b}{d}\right)^m \left(\frac{\sigma}{G}\right)^n$$

Mechanism	D	n	A	m
Climb of Edge Dislocations	D _L	5	6x10 ⁷	0
Viscous Glide (Microcreep)	Ds	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



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	Understand first state of nmatter as it relates to fusion
<u>Key Issues</u>	matter as it relates to rusion	initaties as it relates to lusion
 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.) Coppor Alloys					
Copper Alloys Ceramic Insulators Ontical Materials					
• 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

xcellence	Nuclear physics	Semi- conductor R&D
Scientific excellence		Cold fusion

Interest outside subfield

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)

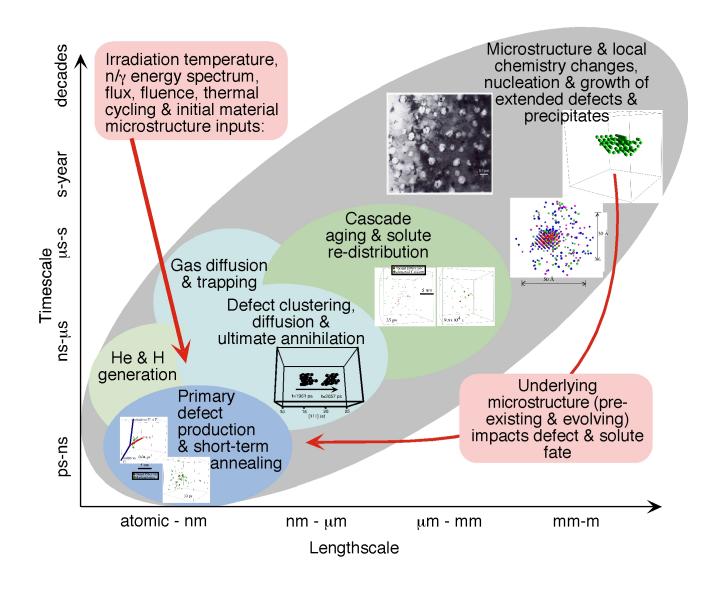
- No one engaged in fusion materials research is supported 100% by OFES funding; all fusion materials scientists actively interact with other research communities
- BES (ceramic composites, radiation effects in materials, electron microscopy, deformation physics, nanoscale materials)
- NERI (deformation 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

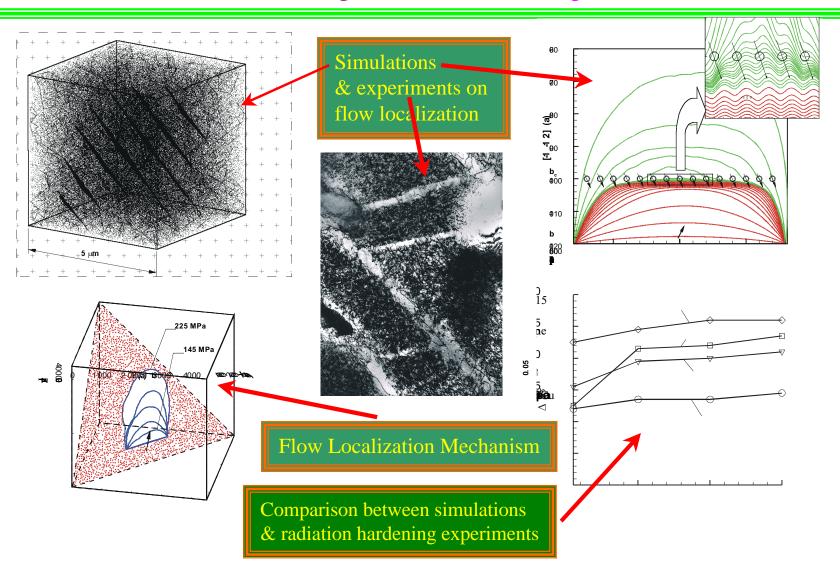
- What are the maximum limits in strength and toughness for materials?
 - Dislocation propagation, interaction with matrix obstacles
- How are the "laws" of materials science altered under nanoscale and/or nonequilibrium conditions
 - -Critical dimensions for dislocation multiplication
 - Nonequilibrium 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

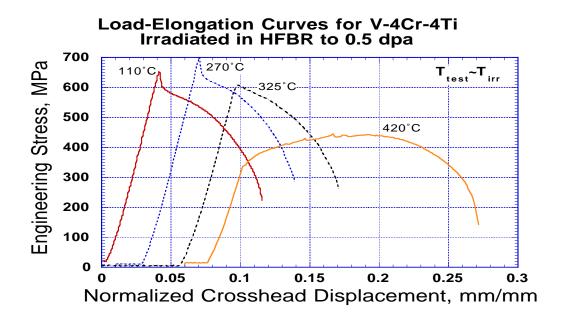


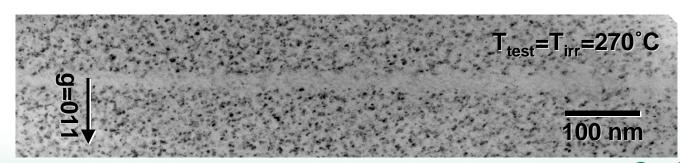


Dislocation Dynamics (DD) is a new computer simulation method developed at UCLA for modeling fundamental microscopic mechanical properties. Successful fusion applications: (1) Mechanisms of dislocation interaction with radiation defects; (2) Radiation hardening; (3) Localization of plastic flow.



Irradiated Materials Suffer Plastic Instability due to Dislocation Channeling



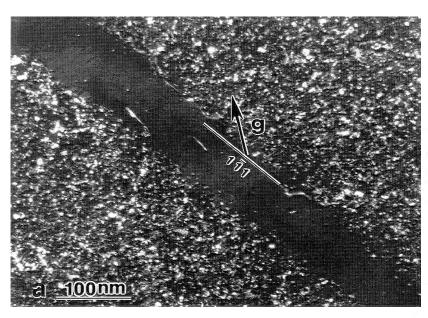


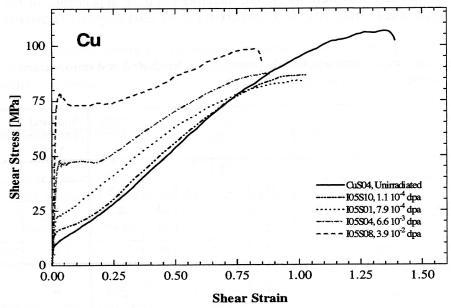


Irradiated materials undergo plastic instability and failure due to dislocation channel formation



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





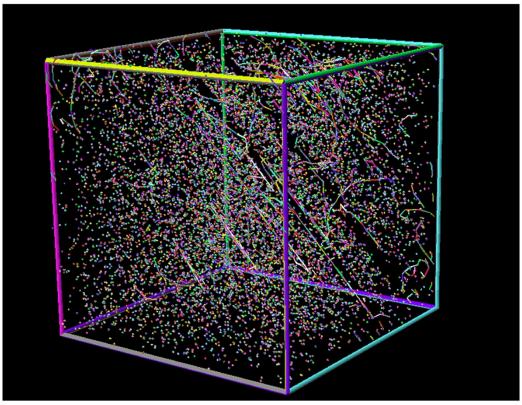
Outstanding questions:

- 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?

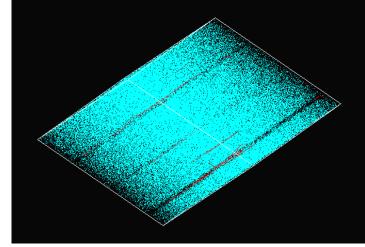
Plastic flow localization in defect free bands appears in the Dislocation Dynamics (DD) simulations



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

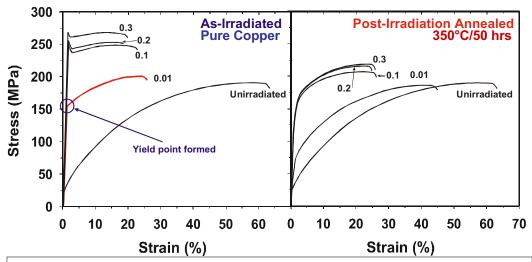


Spreading of the channels is restrained by the formation of dipole segments and the remaining radiation induced defect distribution



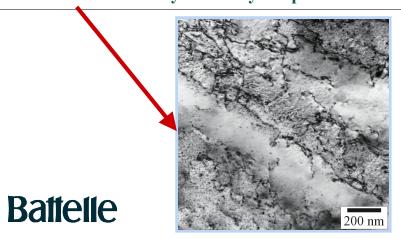
Nature, August 24, 2000

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



As-Irradiated, 0.3 dpa

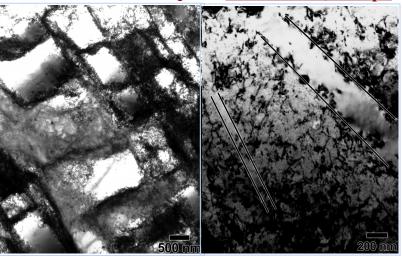
- Cleared channels with little to no dislocation movement between the channels; localized deformation
- Large increases in strength (6 to 8x)
- Loss of uniform elongation and work hardening capacity
- Formation of a clearly defined yield point



Post-Irradiation Annealed Condition

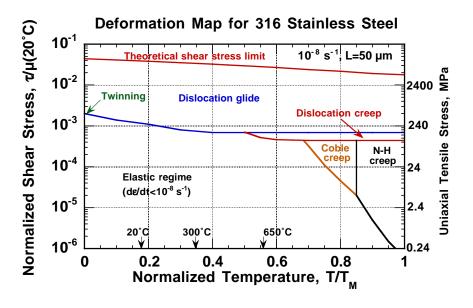
- Dislocation cell structure: material deforms homogeneously at 0.01 dpa
- Mixture of channeling and homogeneous deformation at 0.3 dpa

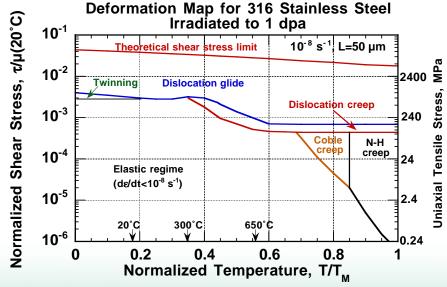
PI Annealed, 0.01 dpa PI Annealed, 0.3 dpa



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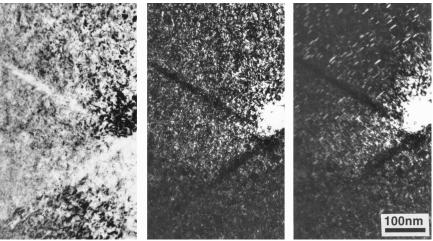
Deformation mechanisms in FCC metals



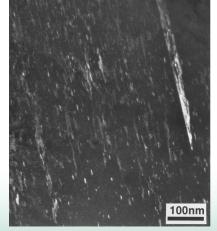


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Irradiation is a useful tool to produce controlled microstructures for deformation mechanics studies



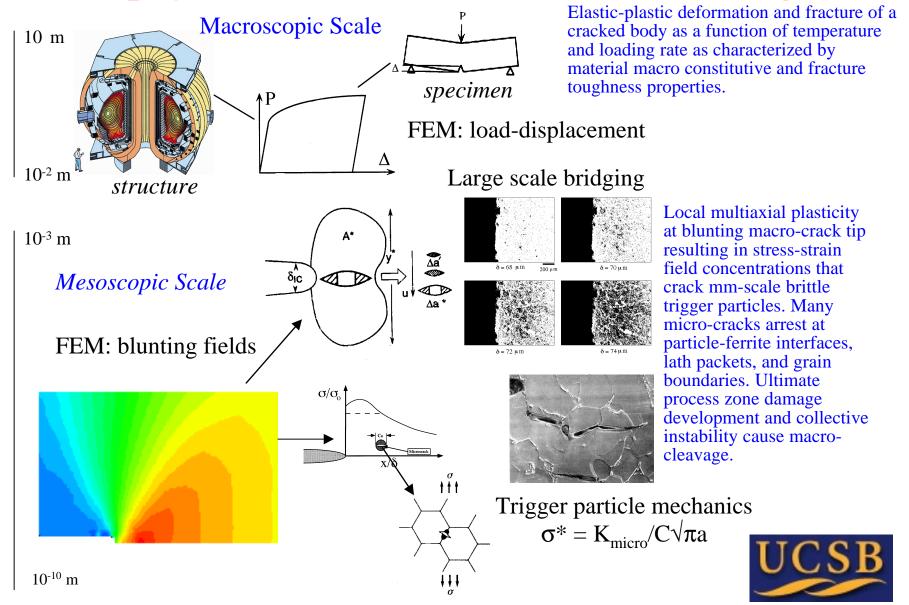
Channeling (Disln glide) occurs at higher temperatures (~300°C)



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

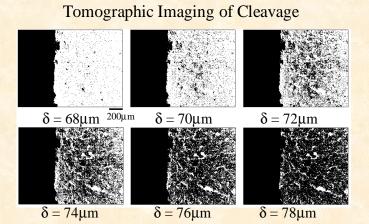


Multiphysics - Multiscale Fracture Modeling - I

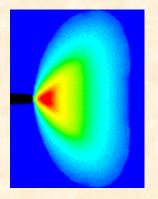


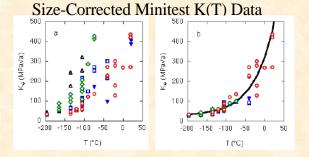
Multiscale Research on Fracture Mechanisms, Mechanics, Models and Structural Integrity Assessment Methods

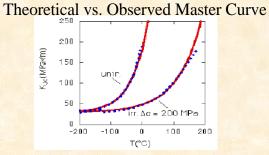
Fracture involves multiple processes interacting from atomic to structural scales. UCSB is developing multiscale physical fracture models and new engineering methods of fracture control using small-scale tests. Research combines theory, models, measurements and characterization of key processes at all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



FEM Simulations of Crack Fields



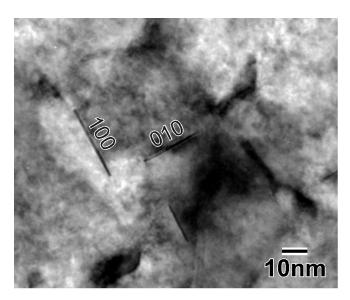


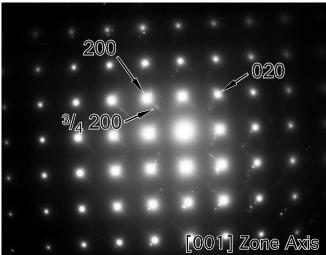


MC Embrittlement Shifts in F82H



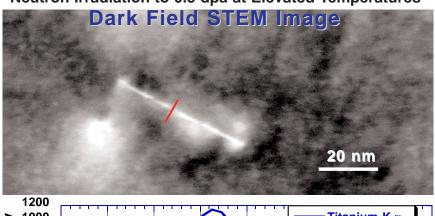
Advanced Analytical Electron Microscopy Techniques are being used to Examine Precipitates in V alloys

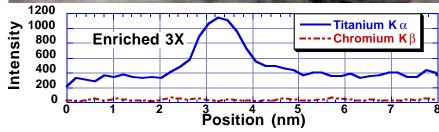




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Solute Segregation Was Detected in V-4Cr-4Ti Following Neutron Irradiation to 0.5 dpa at Elevated Temperatures





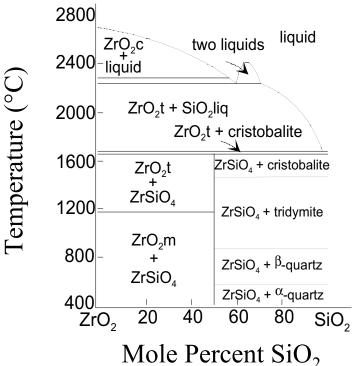


Analytical microscopy reveals Ti-rich precipitates with Fm3m space group

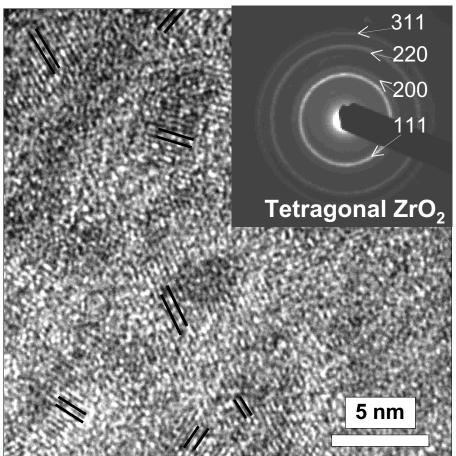


Experimental evidence for nanoscale melting during atomic collisions has been obtained





Microstructure of Zircon Irradiated at 800 °C



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

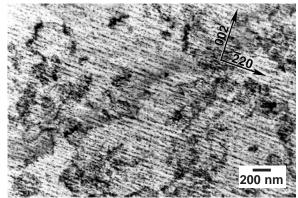
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Nanoscience appears in numerous places in the fusion materials science program

region

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



Crack-deflecting interfaces in ceramic composites give improved toughness

SiC multilayers

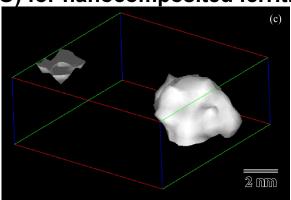


SiC fiber

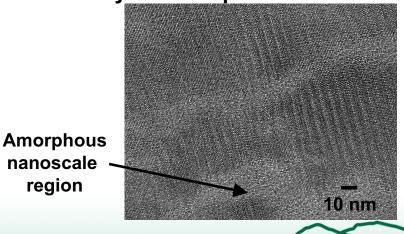
300 nm

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

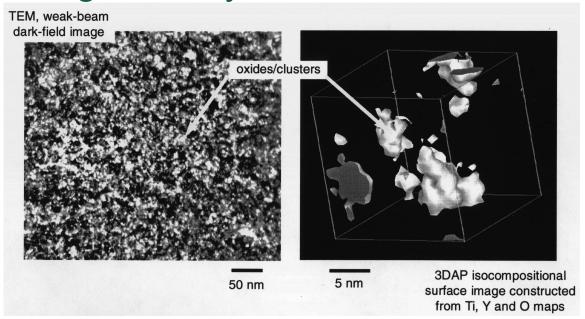


Atomic resolution analysis of crystal-amorphous transition in SiC

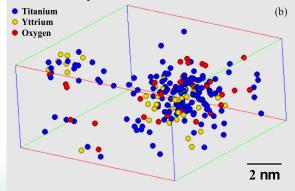




Recent work at ORNL suggests that thermodynamics may be significantly altered at the nanoscale



Atomic composition of nanoclusters

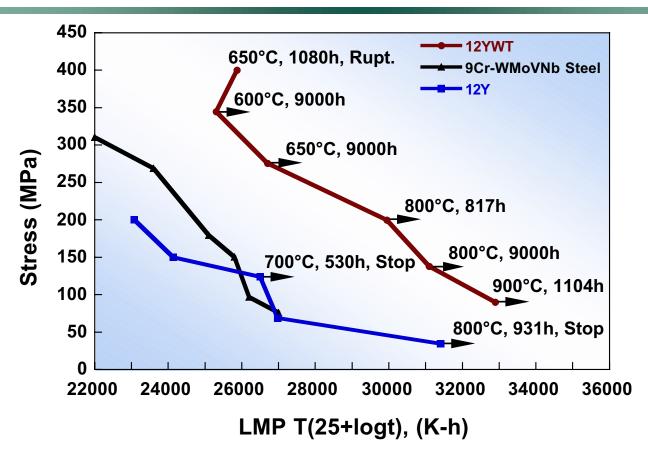


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Atomic analysis of new nanocomposited ferritic steel provides clues to its outstanding creep strength (6 orders of magnitude lower creep rate than conventional steels at 600-900°C)

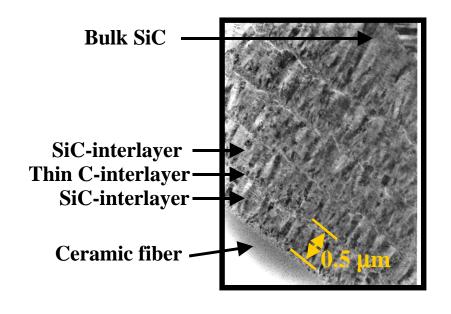


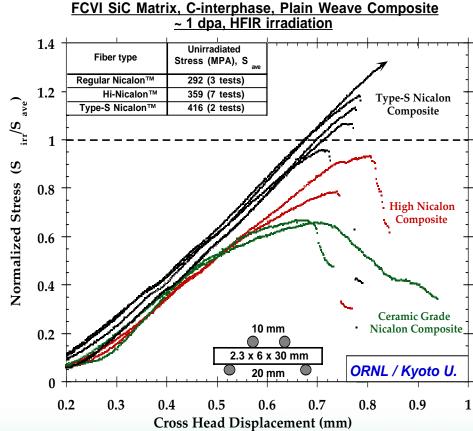
Discovery of Unprecedented Strength Properties in Iron Base Alloy



- 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)

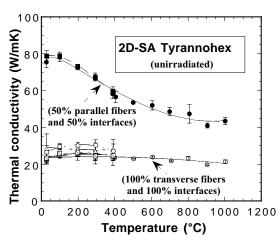




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Thermal Conductivity of 2D SiC/SiC Composites

Fusion Materials Program



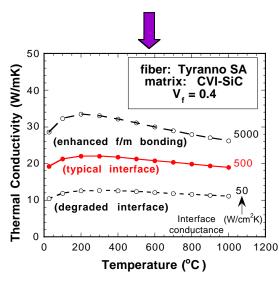
Experimental:

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

NERI Program

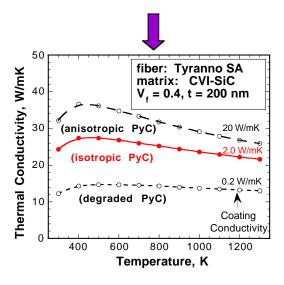
Model 1: Thin Interface Conductance

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



Model 2: Interphase Conductivity

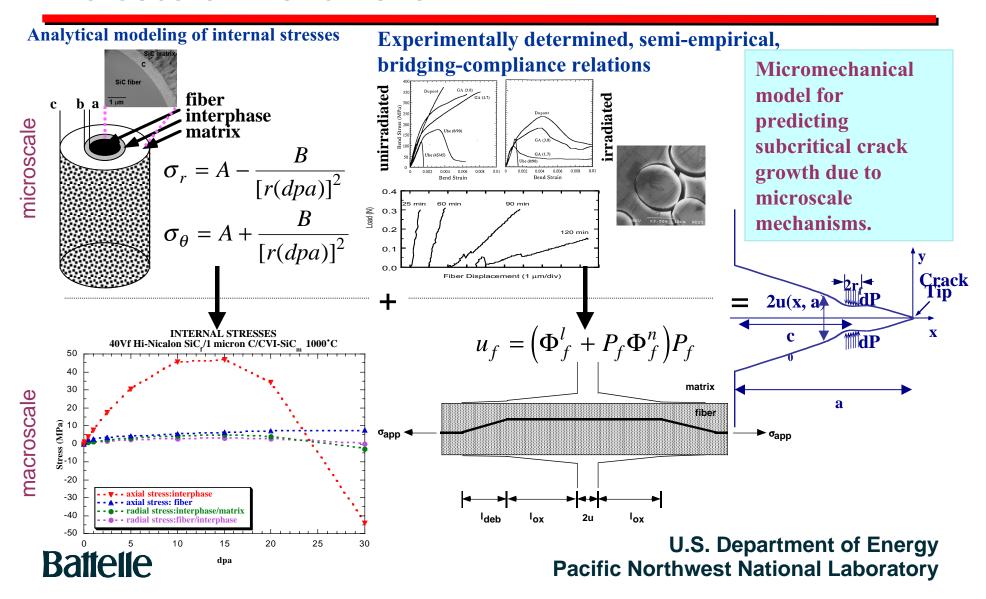
- Preferred orientation of graphitic crystallites
- Strong interface cohesion
- Degraded interphase due to irradiation or oxidation



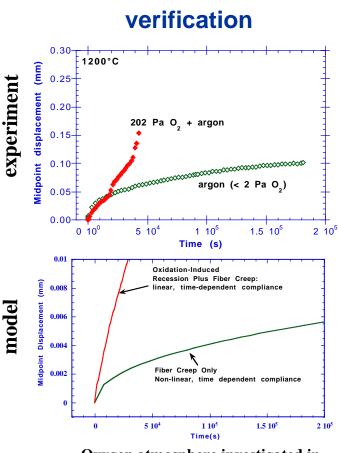


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Crack Growth in Ceramic Composites is a Potential Lifetime-Limiting Mechanism Controlled by Microscale Phenomena



Micromechanical Modeling Allows Prediction of Component Lifetime of Ceramic Composites

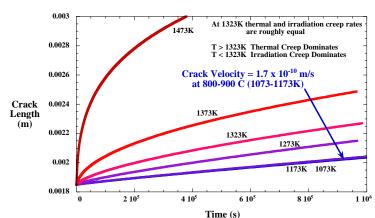


Model

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

Predictive capabilities

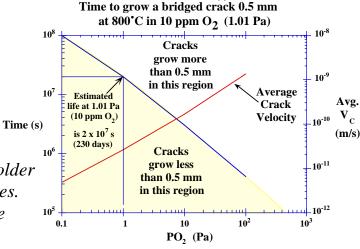
Irradiationenhanced creep of fibers controls crack growth below ≈ 1073 K



Model predicts crack velocity and crack length

NOTE: Lifetime predicted for older generation material properties.

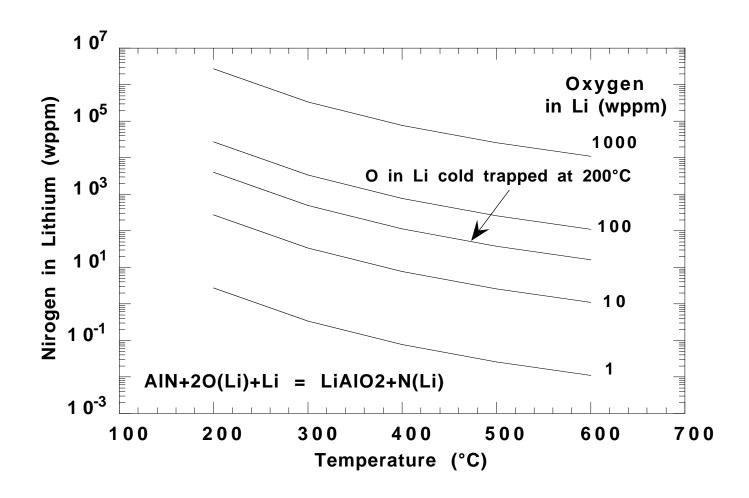
More recent materials have enhanced lifetimes.



Battelle

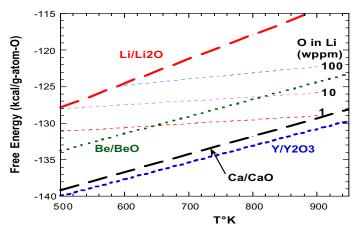
U.S. Department of Energy Pacific Northwest National Laboratory

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

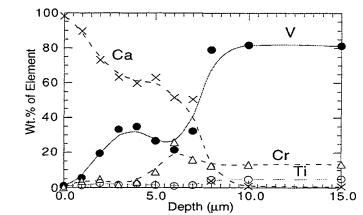


Argonne National Laboratory

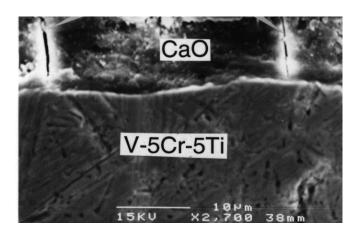
Thermodynamic Stability, Microstructure Characterization, and Property Evaluation of In-situ Formed "CaO" Insulating Coating on Vanadium Alloys



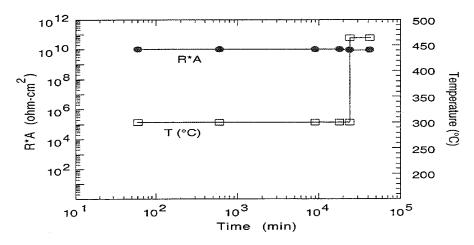
• Calculated thermodynamic stability of candidate oxides in lithium as function of oxygen content



• Composition from EDS analysis vs depth for insitu formed "CaO" coating on V-alloy



Microstructure of "CaO" coating on V-alloy

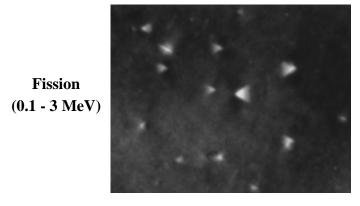


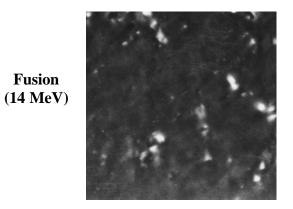
In-situ resistance of "CaO' coating in lithium

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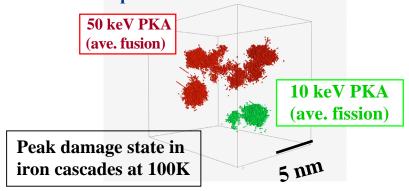
One of the Most Important Scientific Results From the US/Japan Collaborations on Fusion Materials has been the Demonstration of Equivalency of Displacement Damage Produced by Fission and Fusion Neutrons

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

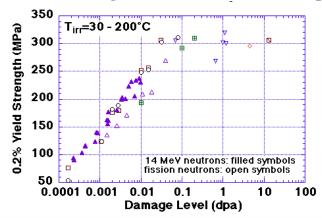




MD computer simulations of the displacement events show that subcascades and defect production are comparable for fission and fusion



Similar hardening behavior confirms the equivalency

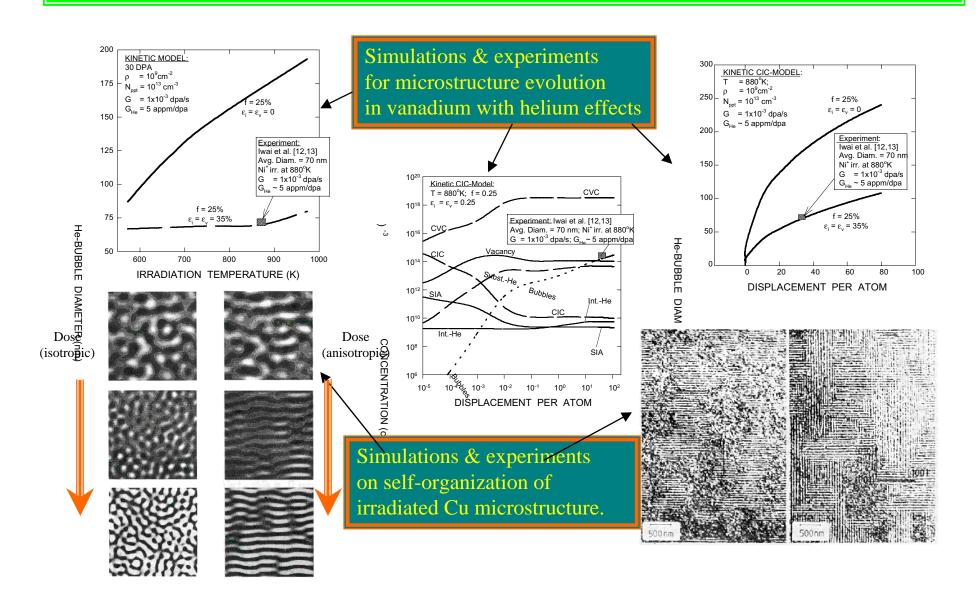


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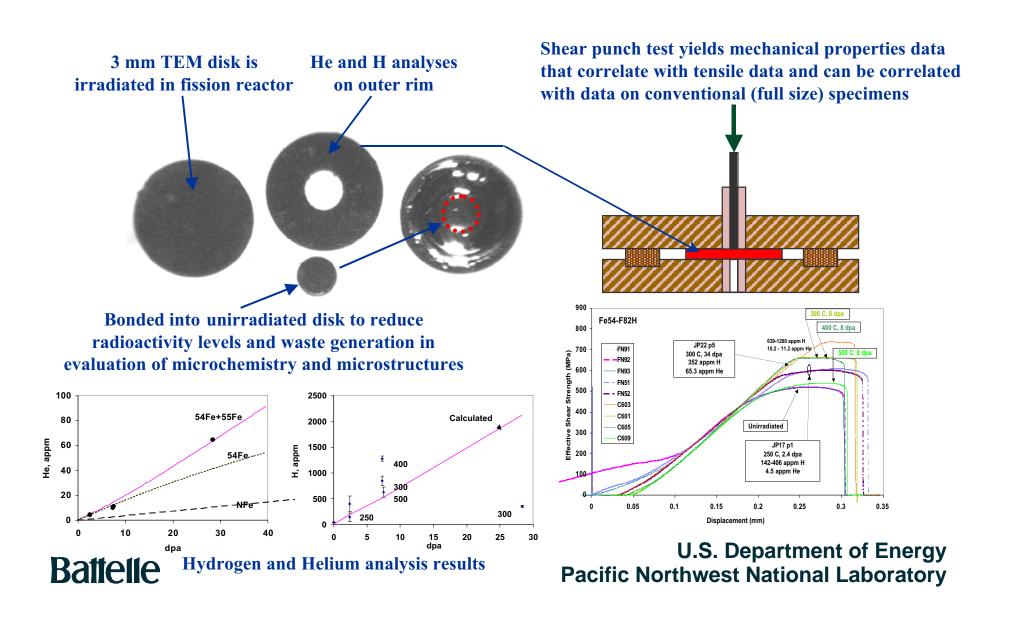
A critical unanswered question is the effect of higher transmutant H and He production in the fusion spectrum



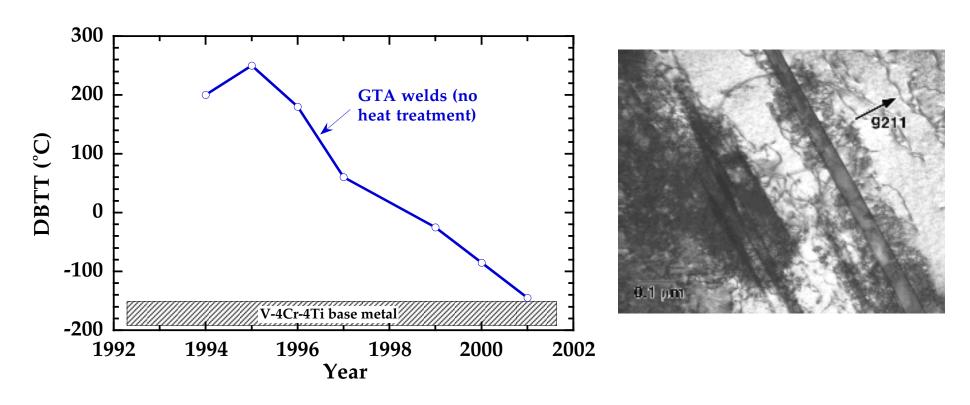
UCLA Advanced Rate Theory Modeling of Microstructure Evolution: Main features (1) Mobile cascade-induced clusters (CIC); (2) Continuous helium generation; (3) Coupled Nucleation & Growth; (4) Spatial self-organization.



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



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)

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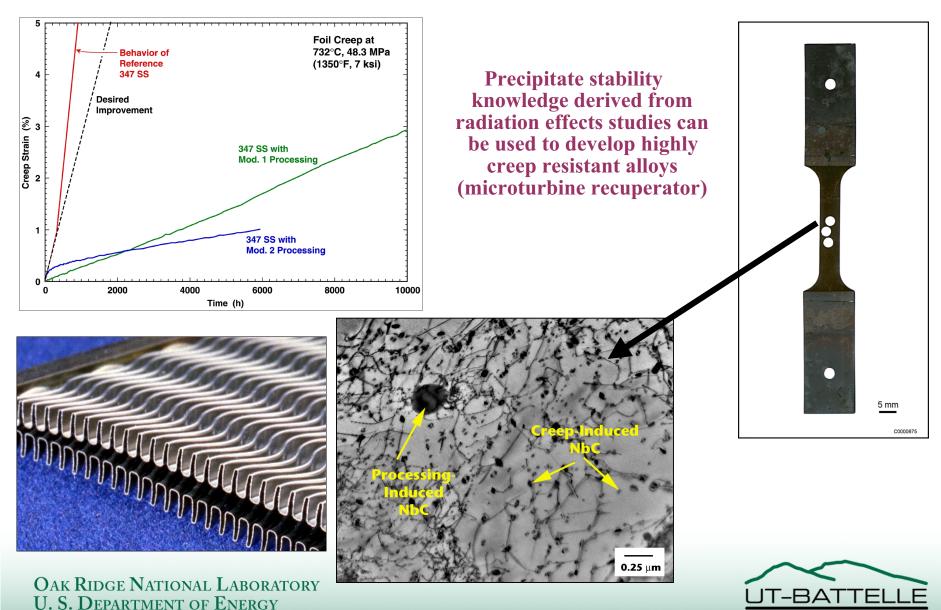


Atom Probe Tomography Reveals Zr, B and C Segregation to Grain Boundaries Produces Improved Mo Weldments

- •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 HEAT AFFECTED ZONE FIM GIE (atoms m⁻²) GIE (atoms m⁻²) 1.3×10^{13} 7.6×10^{13} 9.9×10^{14} B C Zr O B 7.3×10^{12} 9.9×10^{11} 5 nm 1.1×10^{13} **APT atom maps** 1.1×10^{13} -3.9×10^{12} Research performed by OAK RIDGE NATIONAL LABORATORY M. K. Miller, Oak Ridge National Laboratory JT-BATTELL U. S. DEPARTMENT OF ENERGY and A. J. Bryhan, Applied Materials

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



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	StructuresCoatingsInsulating ceramicsOptical 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 permeationthermal, neutronics, hydrodynamics
• IFE	Chamber wallFinal optics	durability, tritium retentionsurface 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	
					gr).
		DOE/N	lonbusho			
Deformation & fracture,	Ferritic	IEA working g			group	
Nanoscience (ODS)	steel	DOE	/JAERI			
Deformation	SiC/SiC	IEA w	orking gro	oup		
mechanisms, enhanced		DOE/N	lonbusho			
thermal cond.		DOE	/JAERI			
Cross-cutting theory & modeling phenomena	Theory & modeling	IEA working group				
		IEA working group				
Electric, dielectric props.	Ceramic insulator s			g gro	up	
		DOE/M	Ionbusho			
Accelerator physics, liquid Neutron		IEA working group				
jet thermohydraulics, He gas cooling technology	source (IFMIF)					

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

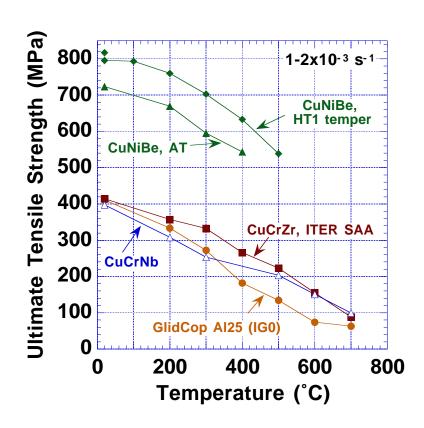
Mid-2001: review EOI's and prioritize

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

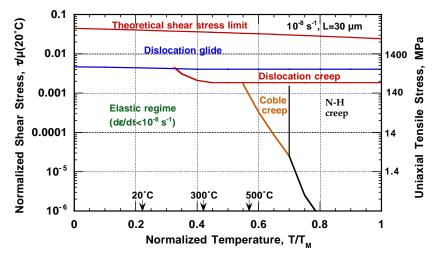
Mechanical behavior of copper alloys can be understood on the basis of current materials science models of deformation



Applications to US industry (e.g., USCAR) as well as fusion energy sciences program

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Deformation Map for CuNiBe (Brush-Wellman Hycon 3HP)



Deformation Map for Oxide Dispersion-strengthened Copper (GlidCop Al25)

