Frontiers of Fusion Materials Science

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Office of Fusion Energy Sciences
Budget Planning meeting

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INTRODUCTION

- **The mission of the Fusion Materials Sciences program is to "*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*"**
  - **Research performed on structural materials (alloys and ceramic composites), insulators, etc.**

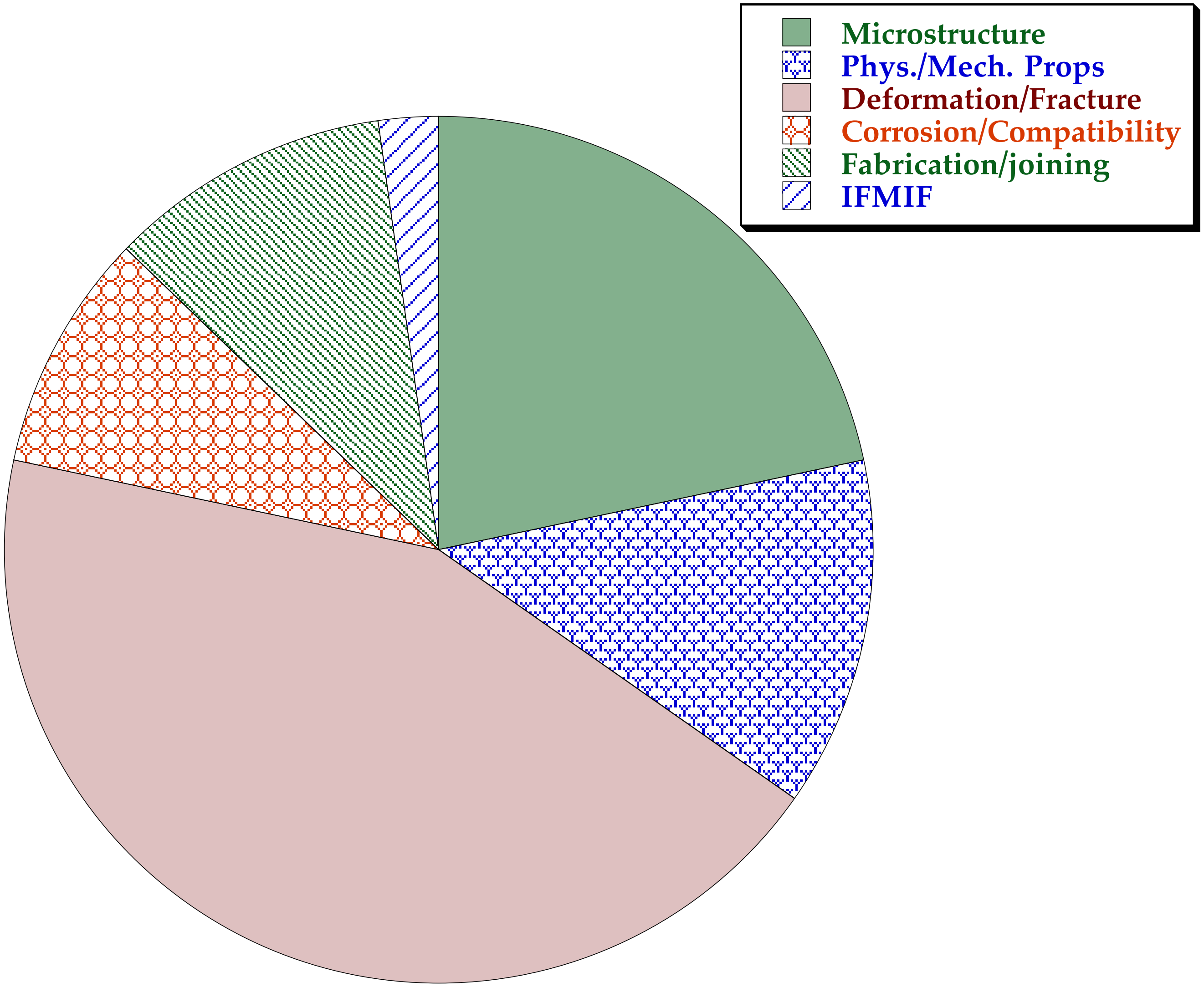
- **Today's presentation: Materials science highlights**
  - **Simultaneous scientific excellence: research directly relevant for fusion and of interest to the broader (materials) science community**

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

Fusion Materials Sciences R&D Portfolio



- Large emphasis on mechanical properties

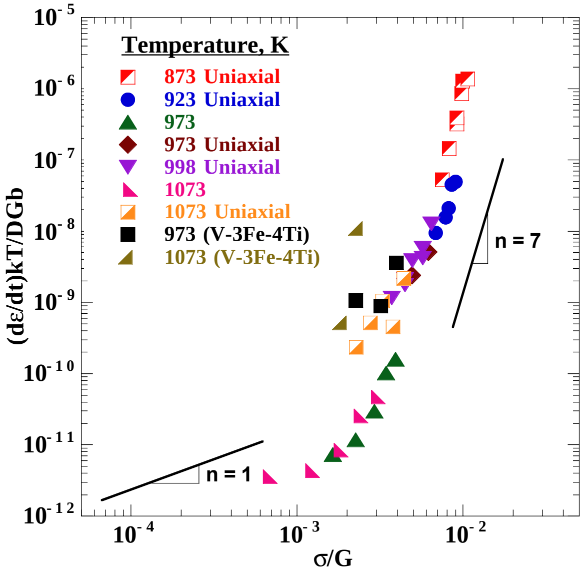
Investigation of Thermal Creep Mechanisms in V-4Cr-4Ti

Diffusion-Controlled Creep Mechanisms

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

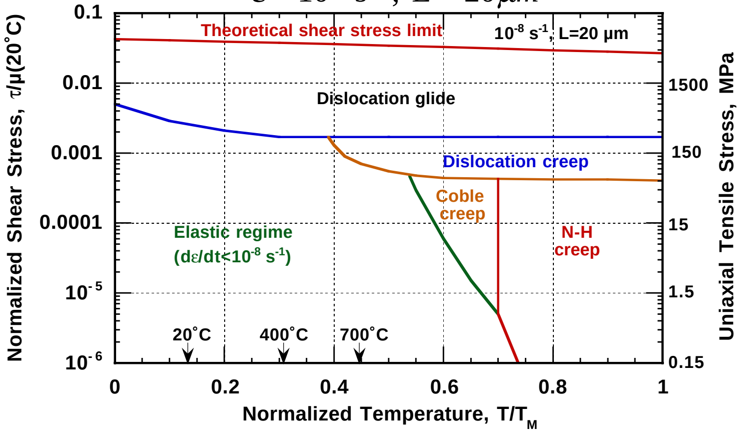
Mechanism	D	n	A	m
Climb of Edge Dislocations	D_L	5	6×10^{7}	0
Viscous Glide (Microcreep)	D_S	3	6	0
Low-Temperature Climb	D_d	7	2×10^{8}	0
Harper-Dorn	D_L	1	3×10^{-10}	0
Nabarro-Herring	D_L	1	12	2
Coble	D_b	1	100	3
GBS (Superplasticity)	D_b	2	200	2
Nabarro-Subgrain	D_L	1	12	2
Nabarro-Bardeen-Herring	D_L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

Experimental Creep Data

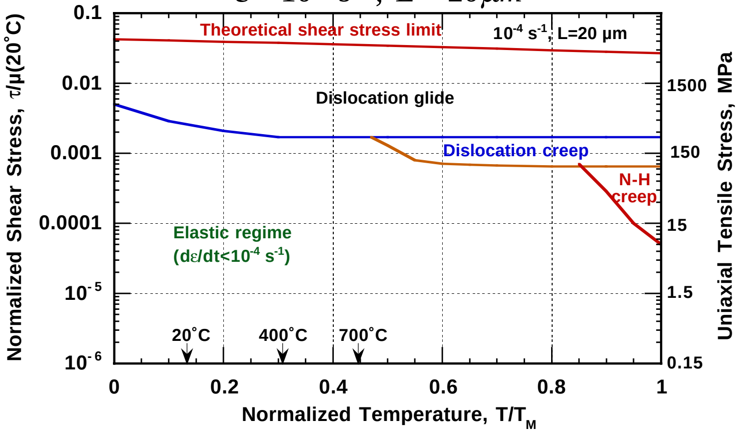


Deformation Mechanism Maps for V-4Cr-4Ti

$$\dot{\varepsilon} = 10^{-8}\,s^{-1},\ \mathrm{L} = 20\,\mu m$$



$$\dot{\varepsilon} = 10^{-4}\,s^{-1},\ \mathrm{L} = 20\,\mu m$$



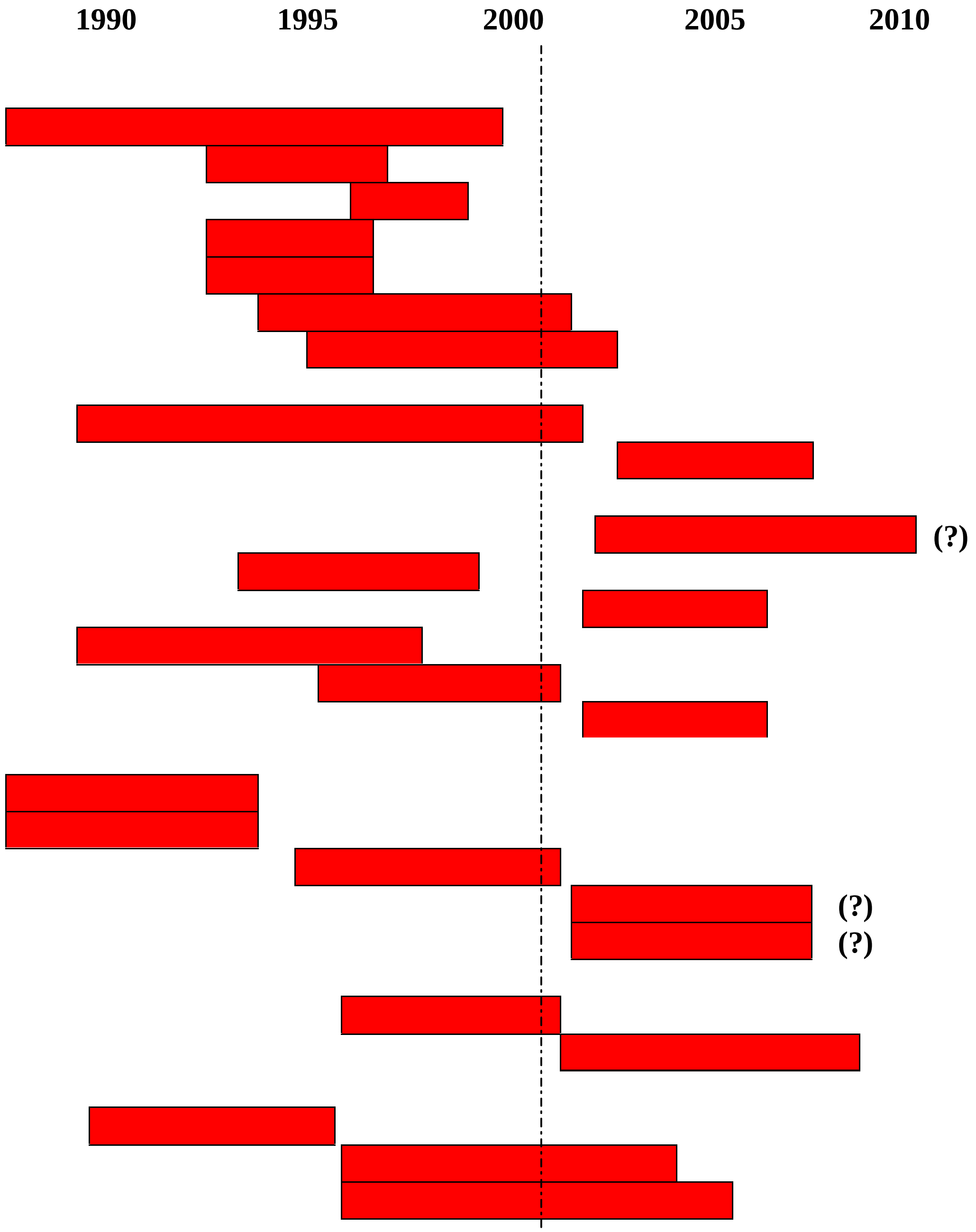
PNNL / ORNL / ANL / UCSB collaboration

The R&D portfolio of the fusion materials science program has two general guiding features

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

Topic	**Fusion benefit**	**Science aspect**
Displacement cascades	Quantification of displacement damage source term	• Is the concept of a liquid valid for time scales of only a few lattice vibrations • Transient (ps) electron-phonon coupling physics
Defect migration	Radiation damage accumulation kinetics	• 1D vs. 3D diffusion processes • ionization-induced diffusion (nonmetals)
Structural material operating limits	Identify/expand operating temperature window and mechanical stress capabilities	• Thermal creep mechanisms • Dislocation-defect interactions

V-4Cr-4Ti R&D Roadmap Snapshot



PHYSICAL/MECHANICAL PROPERTIES:

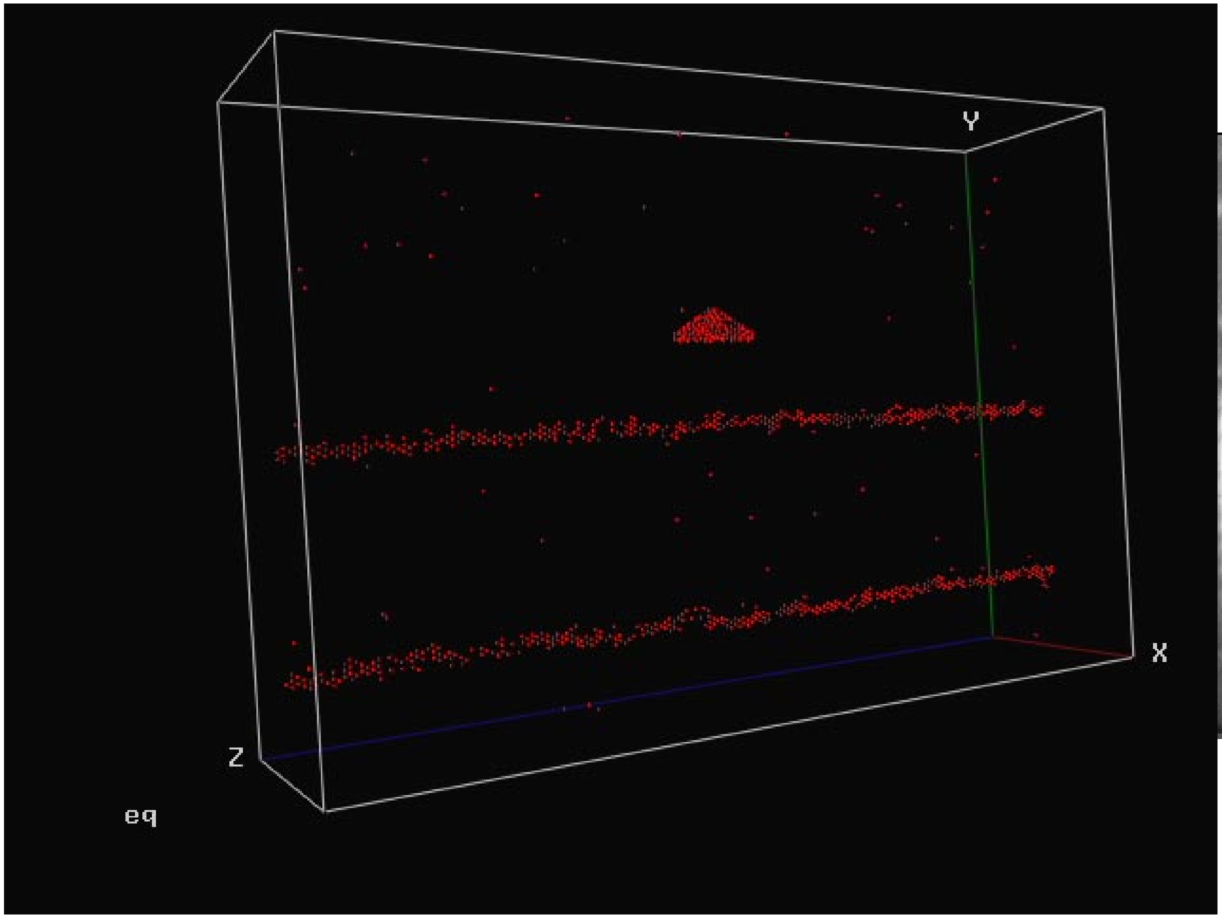
- **Unirradiated:**
  - **Tensile properties**
  - **Thermal conductivity**
  - **Electrical conductivity**
  - **Specific heat**
  - **Coeff. thermal expansion**
  - **Fracture toughness**
  - **Thermal creep**
- **Irradiated (1-30 dpa)**
  - **Tensile properties (100-600°C)**
    - **(600-750C)**
  - **Thermal creep with fusion-relevant He**
    - **(He embrittlement)**
  - **Fracture toughness T_{irr} ≤400°C**
    - **400-700°C**
  - **Microstructural stability 100-600°C**
  - **Irradiation creep - 200-500°C**
    - **500-700°C**
- **Chemical compatibility with coolants**
  - **Lithium**
  - **Pb-Li**
  - **Helium**
  - **Sn-Li**
  - **Flibe**
- **Joining**
  - **Thick plate lab welds (DBTT ≤0°C)**
  - **Field welds (friction stir welding?)**
- **MHD insulators**
  - **Initial screening**
  - **Chemical compatibility 400-700°C**
  - **In-situ formation/self-healing**

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

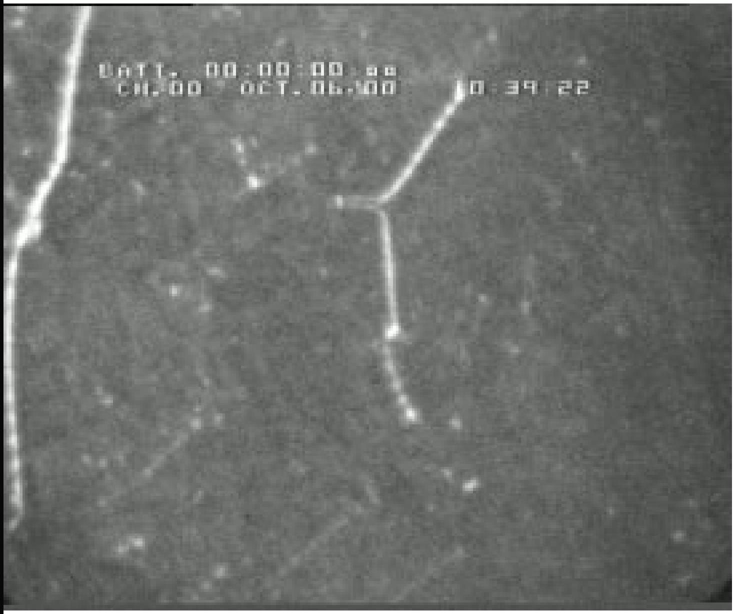
- No one engaged in fusion materials research is supported 100% by OFES funding; all fusion materials scientists actively interact with other research communities
- BES (ceramic composites, radiation effects in materials, electron microscopy, deformation physics, nanoscale materials)
- NERI (deformation mechanisms in irradiated materials, damage-resistant alloys)
- NEPO (mechanical behavior of reactor core internal structure)
- 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)

Atomistic simulations model the unit interaction of an edge dislocation with a radiation-induced defect cluster

MD simulation by Brian Wirth at LLNL



Experimental TEM image by Ian Robertson at UIUC



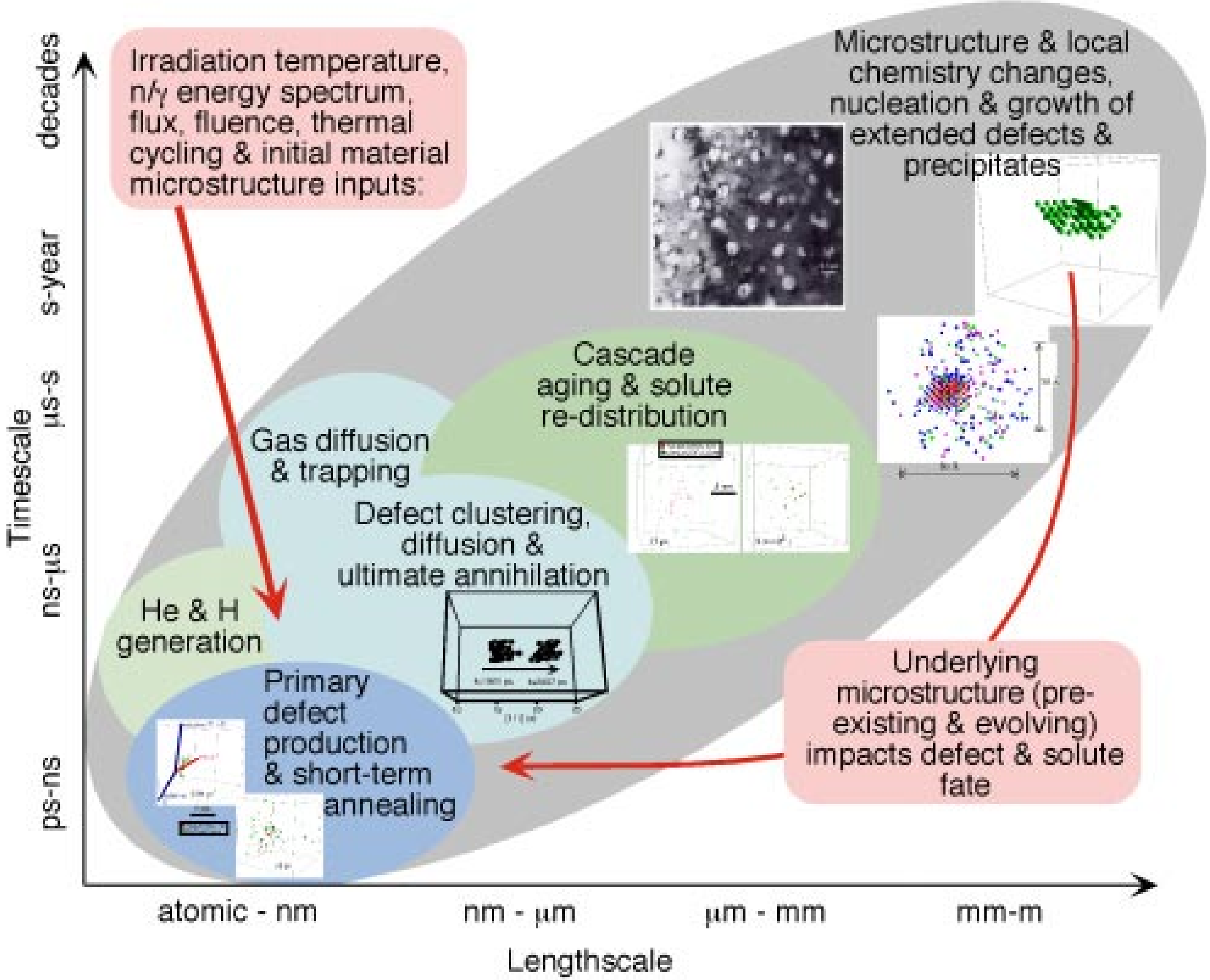
The simulations are in excellent qualitative agreement with experiments

Atomistic simulations supported by OFES and ASCI,
In-situ TEM supported by OBES

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



Irradiation temperature, n/γ energy spectrum, flux, fluence, thermal cycling & initial material microstructure inputs:

Microstructure & local chemistry changes, nucleation & growth of extended defects & precipitates

Cascade aging & solute re-distribution

Gas diffusion & trapping

Defect clustering, diffusion & ultimate annihilation

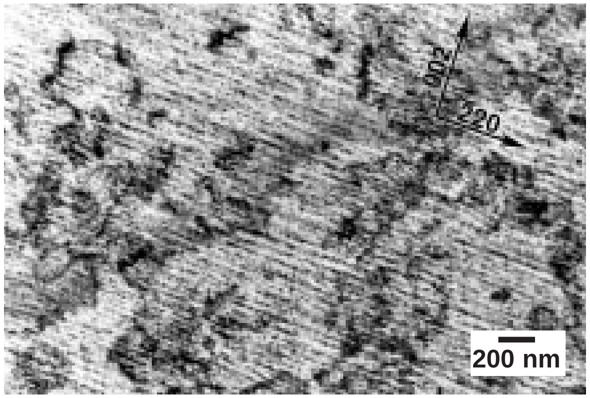
He & H generation

Primary defect production & short-term annealing

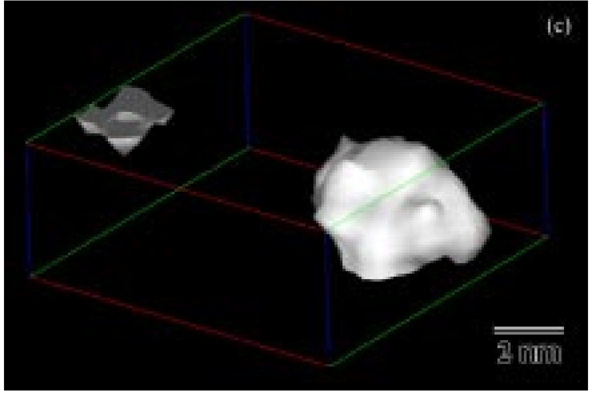
Underlying microstructure (pre-existing & evolving) impacts defect & solute fate

Nanoscience appears in numerous places in the fusion materials science program

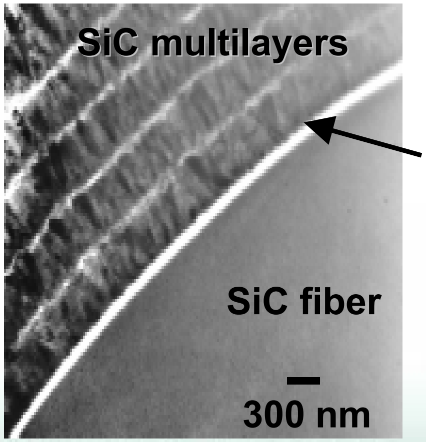
Nanoscale self-organization of defect clusters in neutron-irradiated Ni



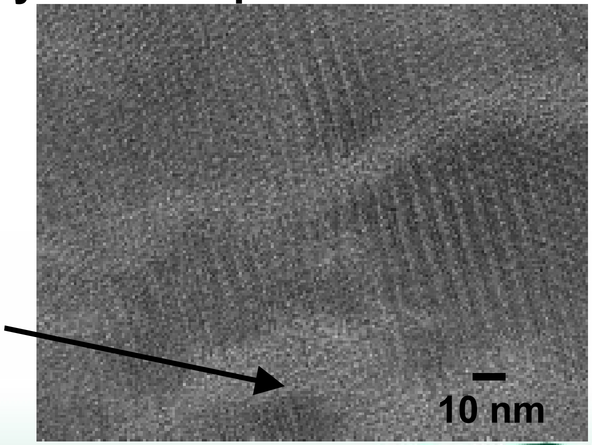
3-D atom probe iso-composition contour (Y, Ti, O) for nanocomposited ferritic steel



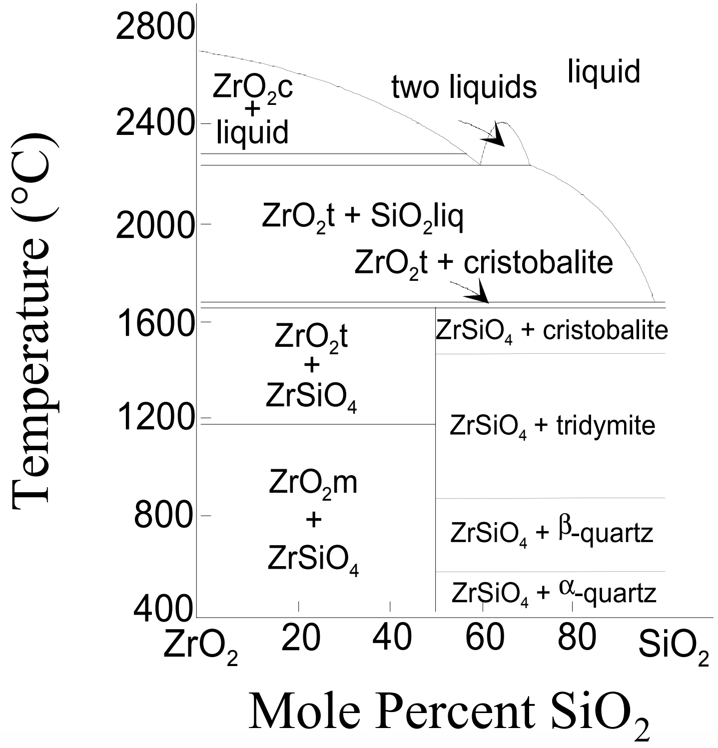
Crack-deflecting interfaces in ceramic composites give improved toughness

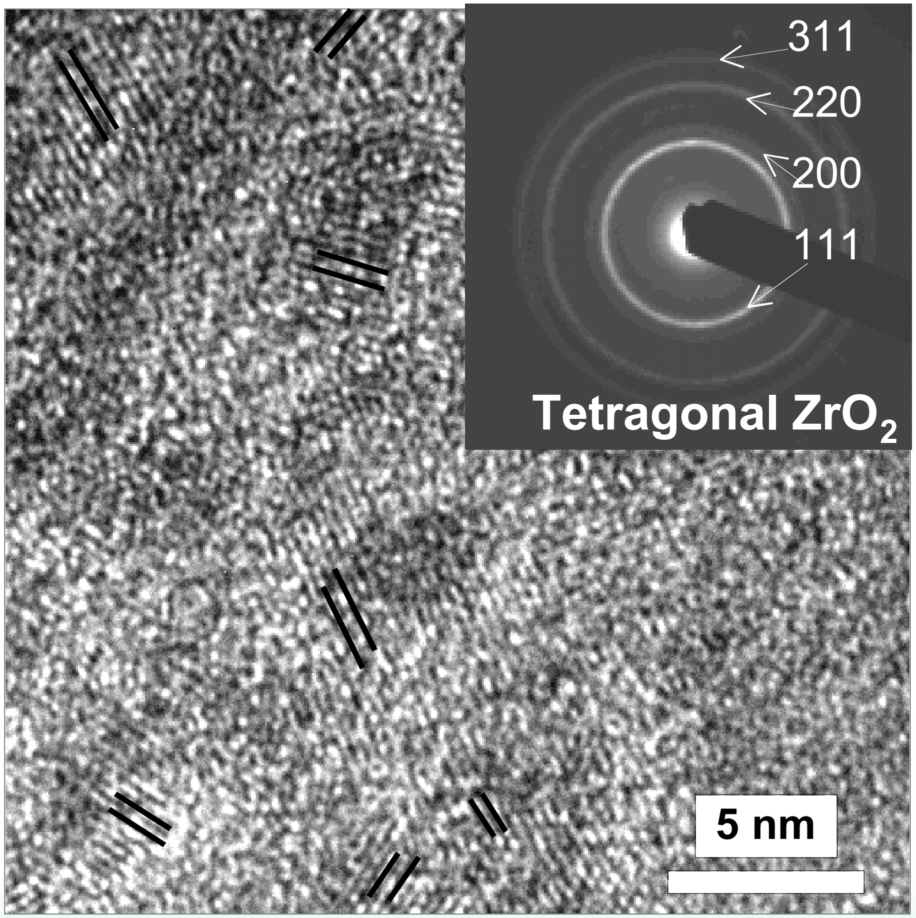


Atomic resolution analysis of crystal-amorphous transition in SiC



Experimental evidence for nanoscale melting during atomic collisions has been obtained


ZrO_2-SiO_2 Phase Diagram

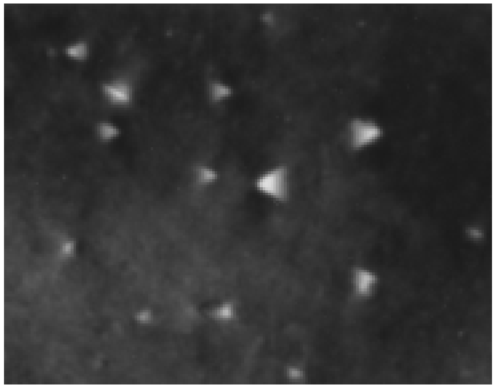

Microstructure of Zircon Irradiated at 800 °C

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

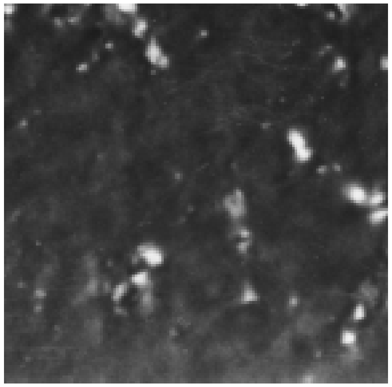
One of the Most Important Scientific Results From the US/Japan Collaborations on Fusion Materials has been the Demonstration of Equivalency of Displacement Damage Produced by Fission and Fusion Neutrons

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

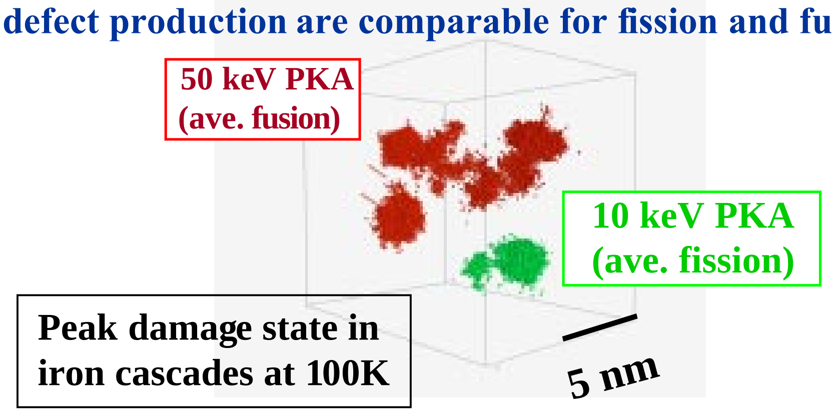
Fission (0.1 - 3 MeV)



Fusion (14 MeV)



MD computer simulations show that subcascades and defect production are comparable for fission and fusion

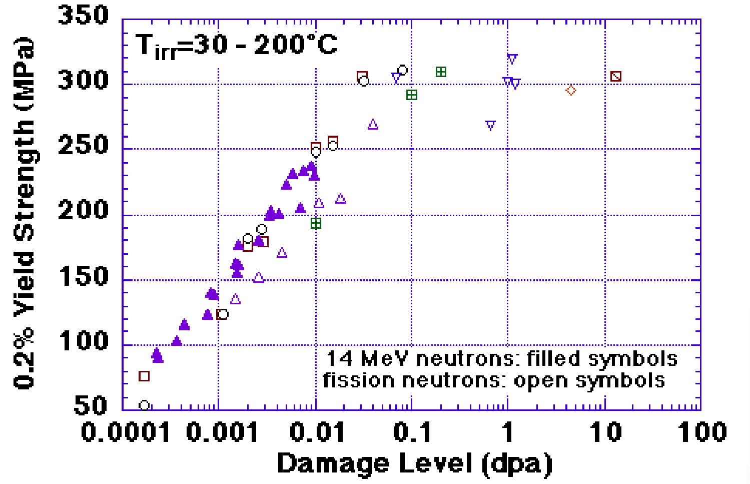


50 keV PKA (ave. fusion)

10 keV PKA (ave. fission)

Peak damage state in iron cascades at 100K

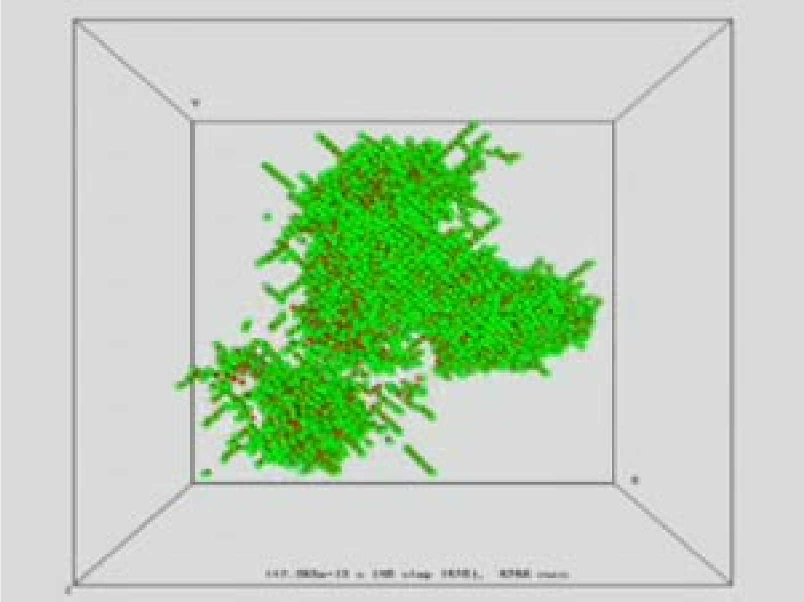
Similar hardening behavior confirms the equivalency



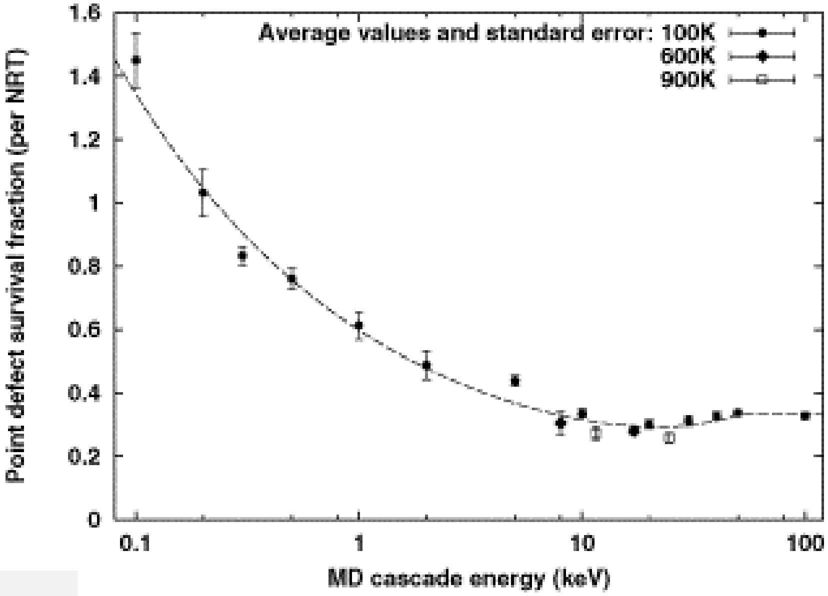
14 MeV neutrons: filled symbols
fission neutrons: open symbols

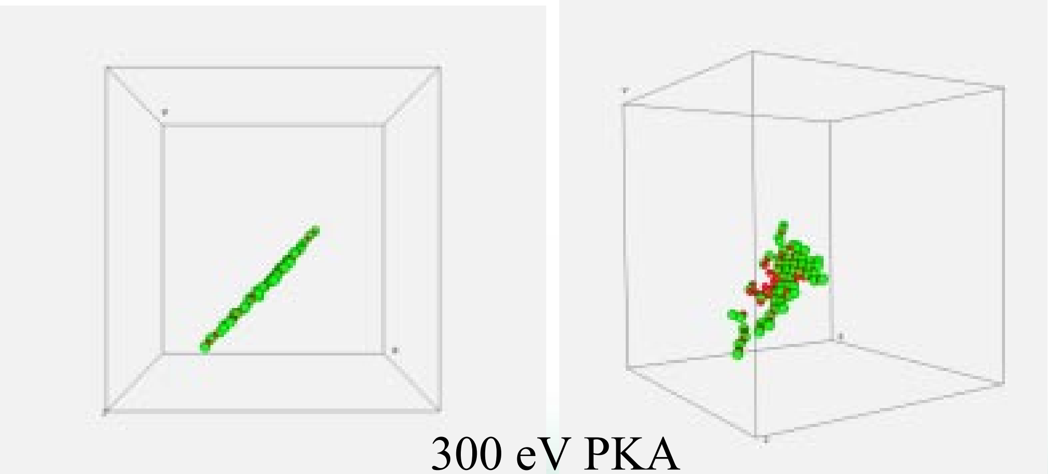
A critical unanswered question is the effect of higher transmutant H and He production in the fusion spectrum

Displacement Damage Mechanisms are being investigated with Molecular Dynamics Simulations



Damage efficiency saturates when subcascade formation occurs



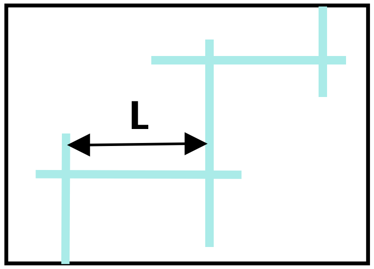


300 eV PKA

PKAs oriented in the close packed planes produce enhanced damage efficiency at low energies compared to other orientations, due to a planar defect creation process

New Defect Reaction Kinetics for Mobile Clusters

- MD simulations show that INTERSTITIAL CLUSTERS formed in cascades MIGRATE ONE-DIMENSIONALLY, but occasionally they CHANGE DIRECTION!
- **These clusters follow a new kind of reaction kinetics.**



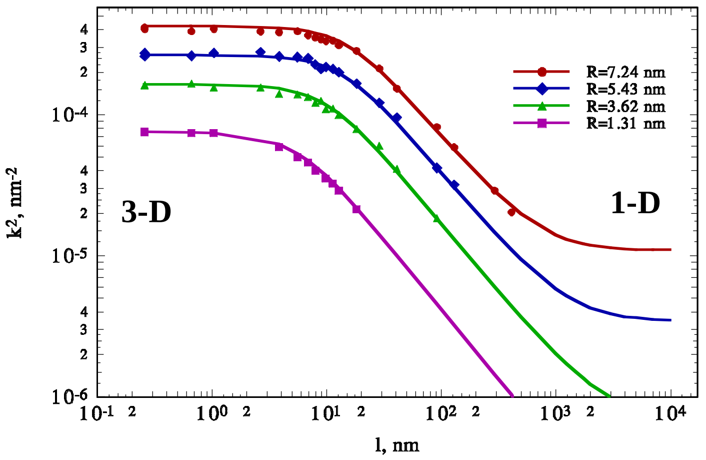
Mixed 1-D/3-D migration, average length L between direction changes

- Kinetic Monte Carlo computer simulations lead to a new analytical theory for reaction kinetics from 1-D to 3-D

Sink strength as a function of 1-D path length.

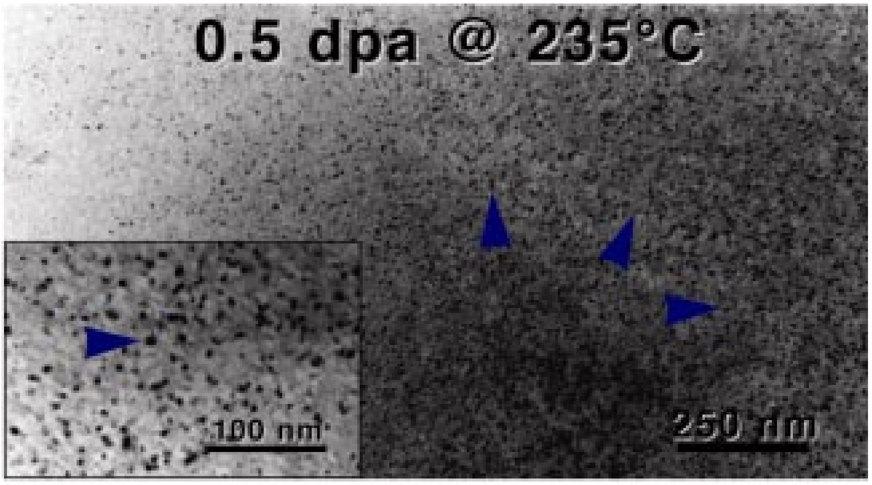
Analytical expression compared to KMC results

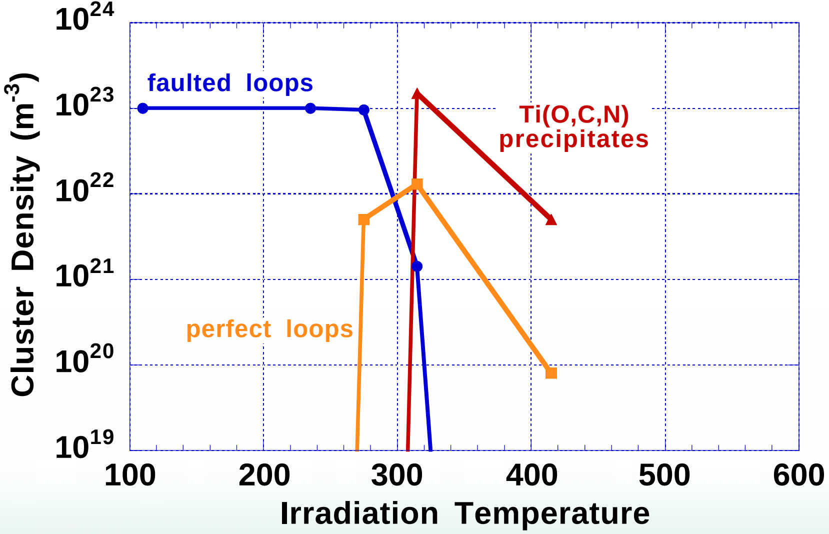
$$k_m^2 = 0.5\, k_1^2 \{ 1 + \sqrt{1 + 4/(l^2 k_1^2/4 + k_1^4/k_3^4)} \}$$



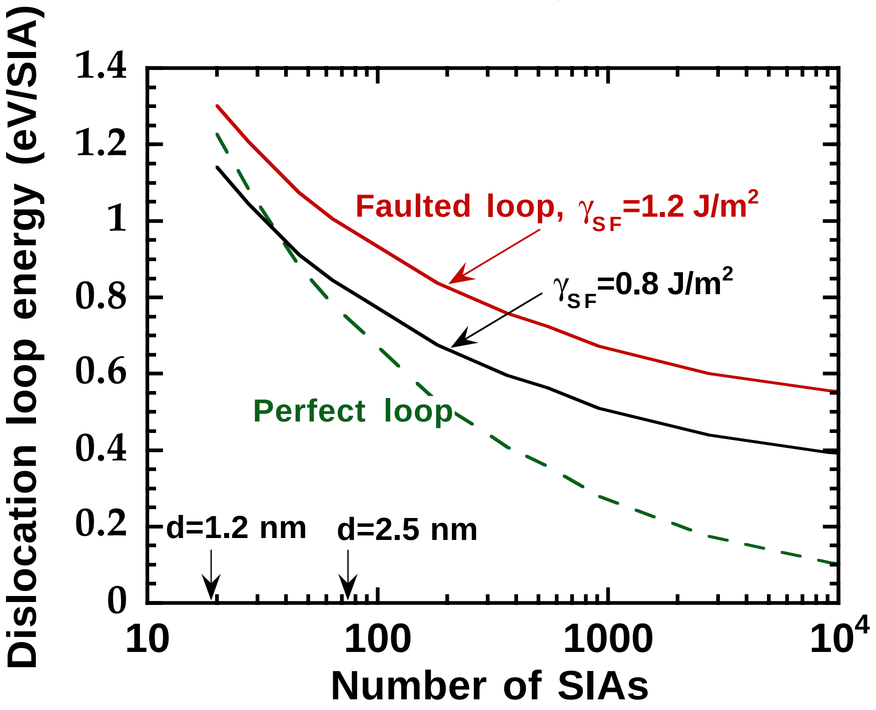
- **The new defect reaction kinetics applied in PBM rate theory rationalizes**
- Decoration of dislocations by loops
- Enhanced swelling at grain boundaries
- Dependence of void swelling on temperature, recoil energy, dose
- Void lattice formation in pure metals and complex alloys

Experimental investigation of stacking fault energies of BCC metals



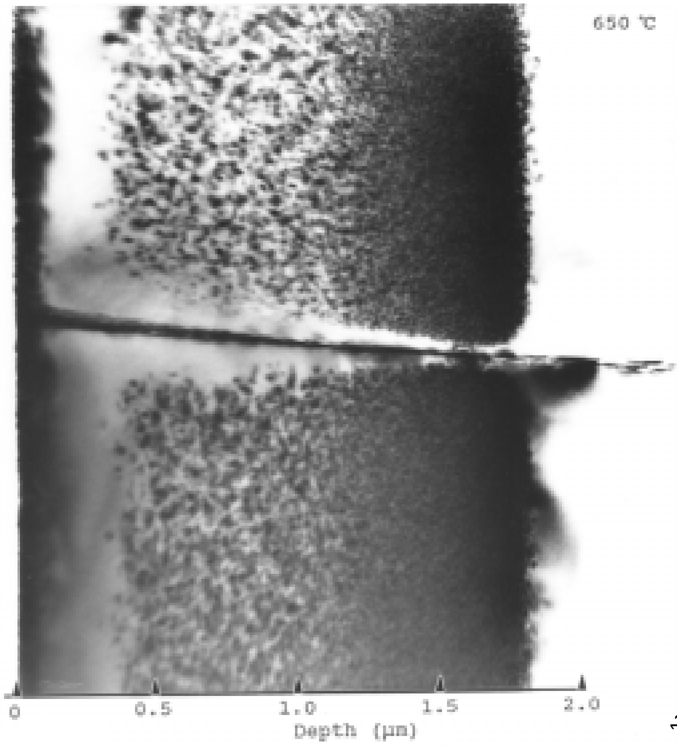

Measured Defect Cluster Densities in V-4Cr-4Ti Neutron-irradiated to 0.5 dpa

Continuum mechanics calculation of dislocation loop energies in vanadium



Determination of interstitial migration energies in ceramics

Defect-free zones in ion-irradiated $MgAl_2O_4$



- Solve steady state rate eqns:

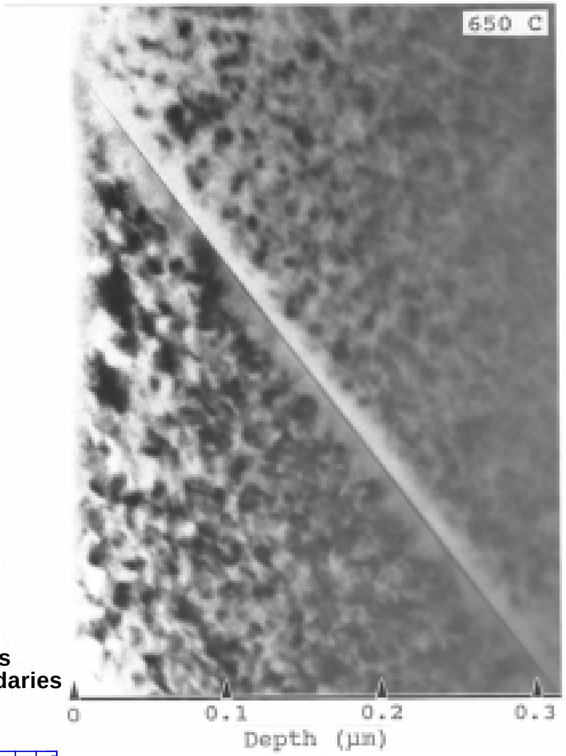
$$D_i \frac{d^2C_i}{dx^2} - \alpha C_i C_v - D_i C_i C_s + P = 0$$

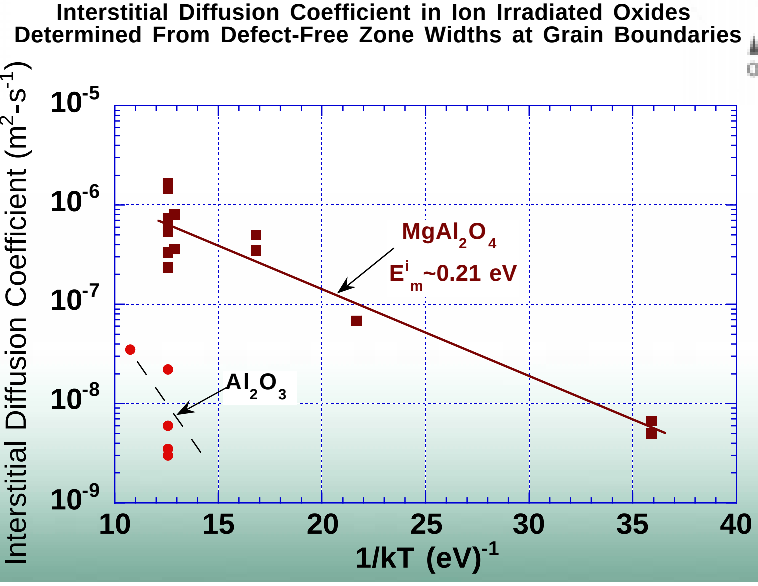
$$D_v \frac{d^2C_v}{dx^2} - \alpha C_i C_v - D_v C_v C_s + P = 0$$

- For sink-dominant conditions ($C_S > 10^{14}/m^2$), the defect-free zone width is related to the diffusivity (D_i) and damage rate (P) by:

$$D_i = \frac{L\ P}{C_i^{crit}\sqrt{C_s}}$$

Defect-free grain boundary zones in ion-irradiated Al_2O_3





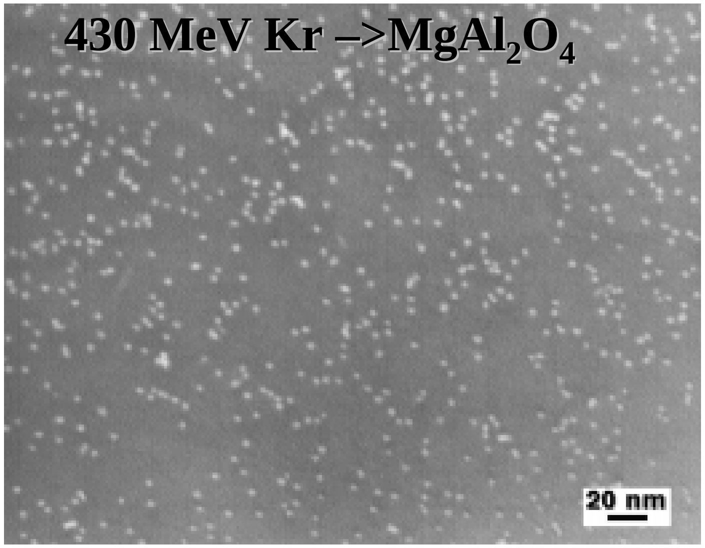
Interstitial Diffusion Coefficient in Ion Irradiated Oxides Determined From Defect-Free Zone Widths at Grain Boundaries

Ionizing Radiation can induce a myriad of effects in ceramics

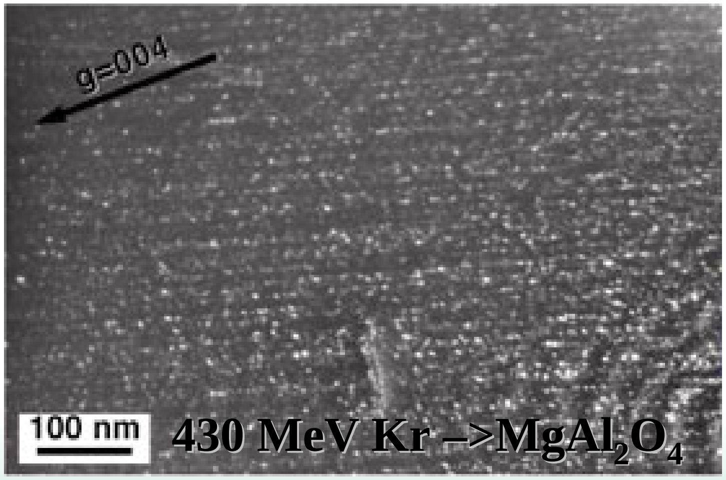
- Defect production
  - –Radiolysis (SiO_2, alkali halides)
  - –Ion track damage (swift heavy ions)

- Defect annealing and coalescence (ionization-induced diffusion)
  - –Athermal defect migration is possible in some materials

Highly ionizing radiation ($dE_{ioniz.}/dx > 7$ keV/nm) introduces new damage production mechanisms

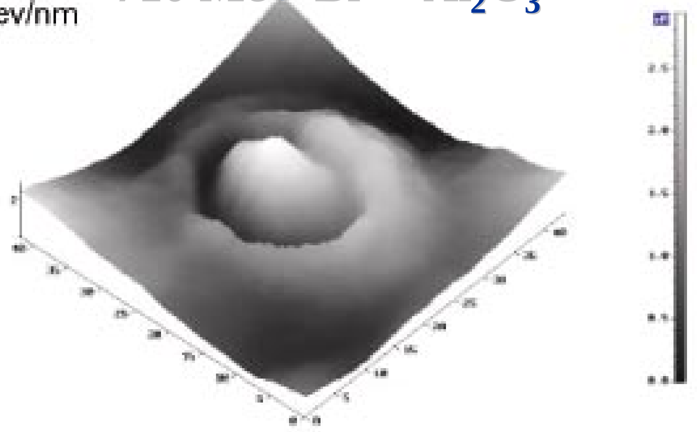


Ion tracks produce displacement damage via inelastic atomic events

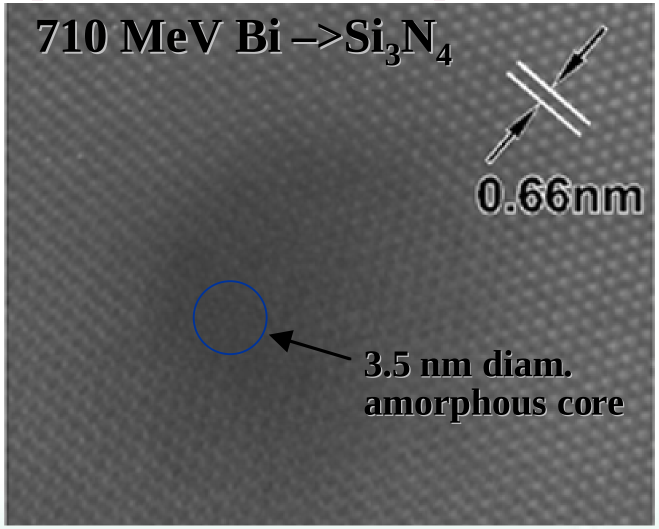


$(dE/dx)_{ion.}$ 41 kev/nm

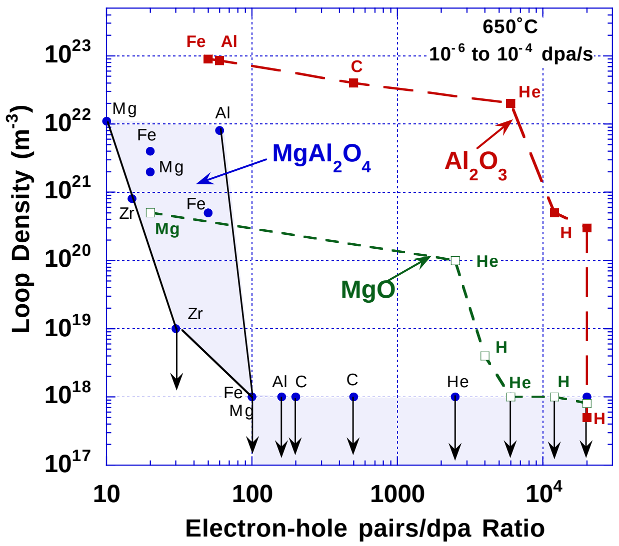
710 MeV Bi –>Al_2O_3

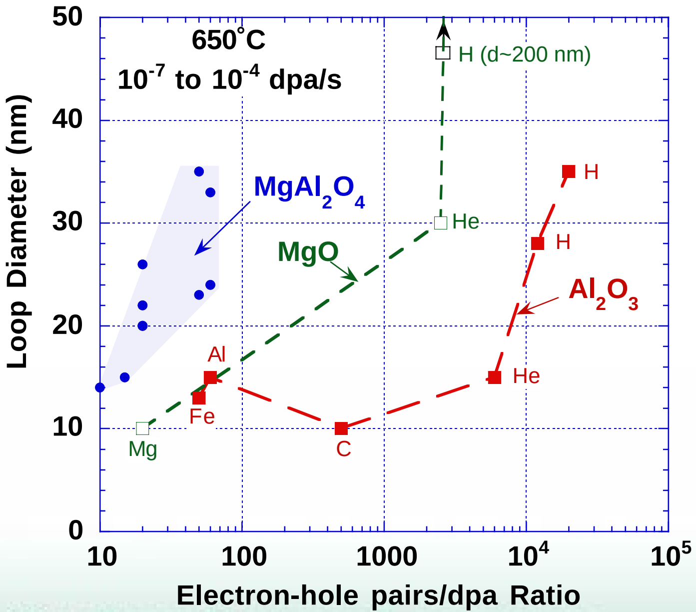


Swift heavy ions induce surface protrusions and amorphization

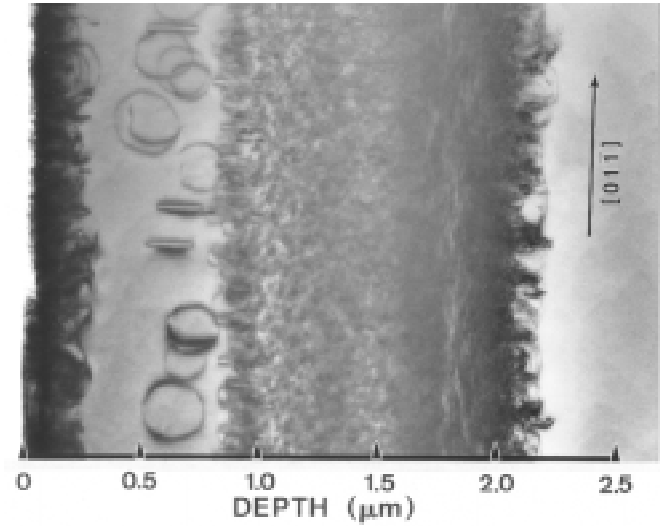


Investigation of ionization-induced diffusion in ceramics

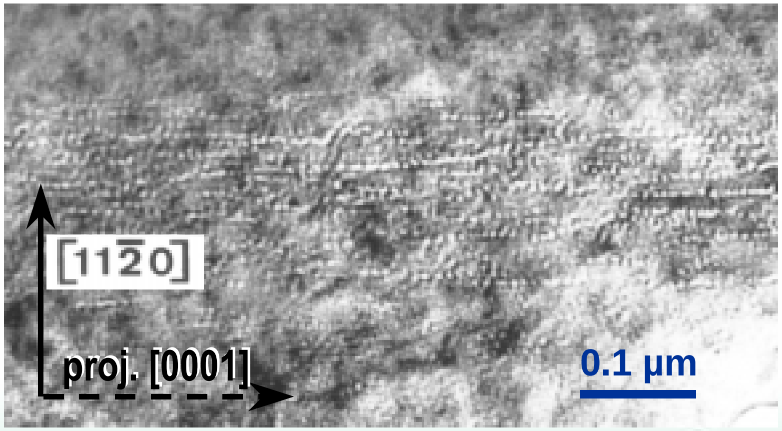




Large interstitial loops in $MgAl_2O_4$ ion-irradiated at 25˚C for regions with >100 eln.-hole pairs per dpa

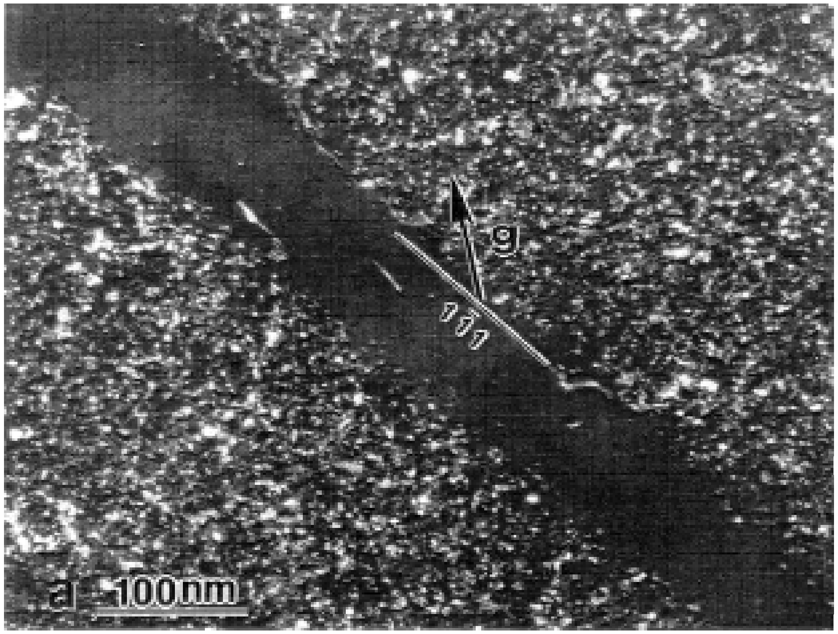


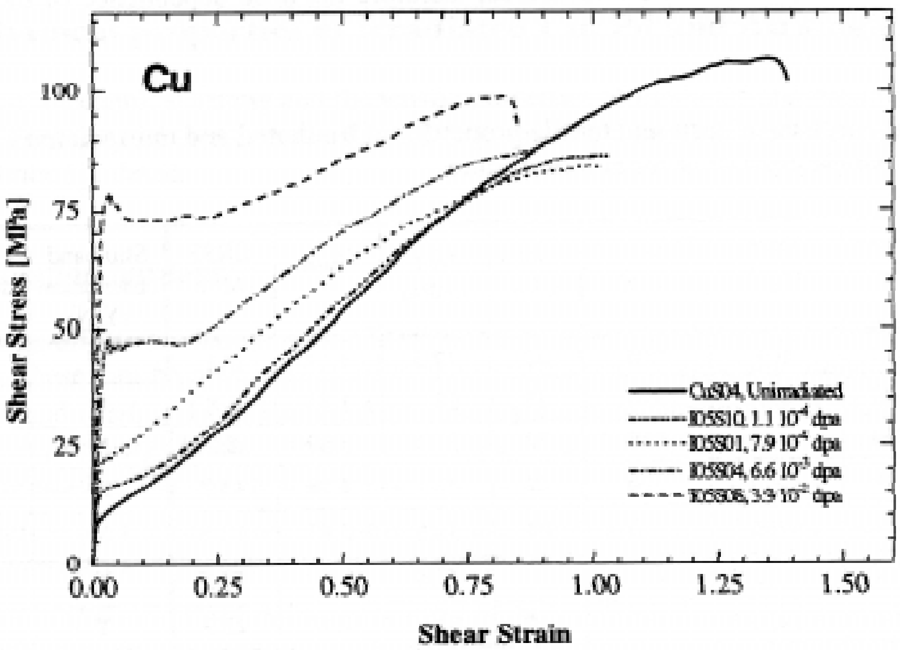
Aligned cavities in Al_2O_3 ion-irradiated at 25˚C (Al/O/He ion irradiation, >500 eln.-hole pairs per dpa)



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?

Dislocation Dynamics (DD) is a new computer simulation method developed at UCLA for modeling fundamental microscopic mechanical properties

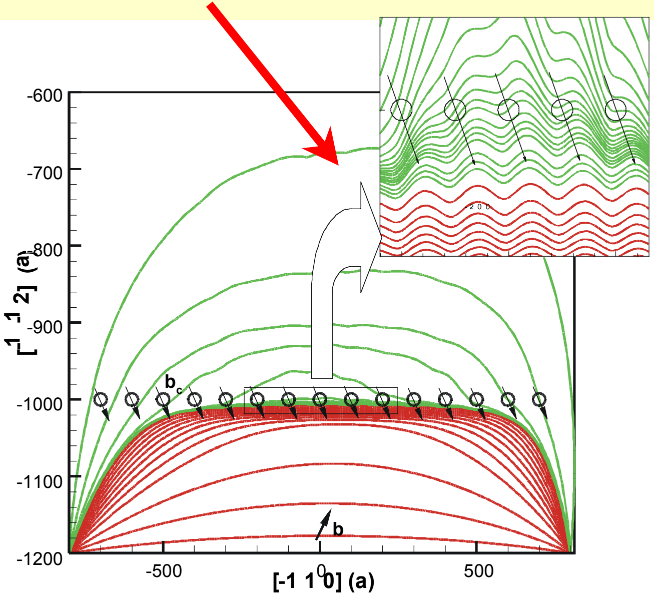
Broad Objectives of DD:

1. Understand fundamental deformation mechanisms
2. Provide a physical basis for plasticity
3. Determine stress-strain behavior without assumptions.
4. Design new ultra-strong and super-ductile materials.

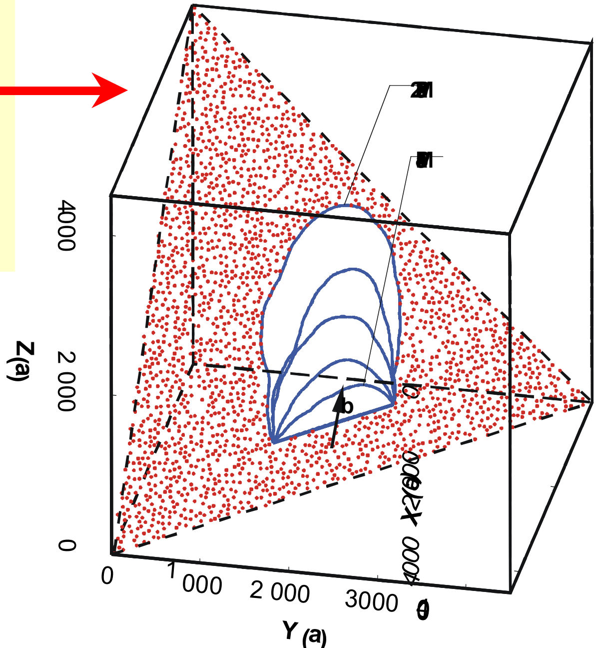
New Understanding (dislocation-defect interactions):

(a) Local heating destroys vacancy clusters;

(b) Shape instabilities allow dislocations to overcome the resistance of SIA clusters.



Leads to yield drop



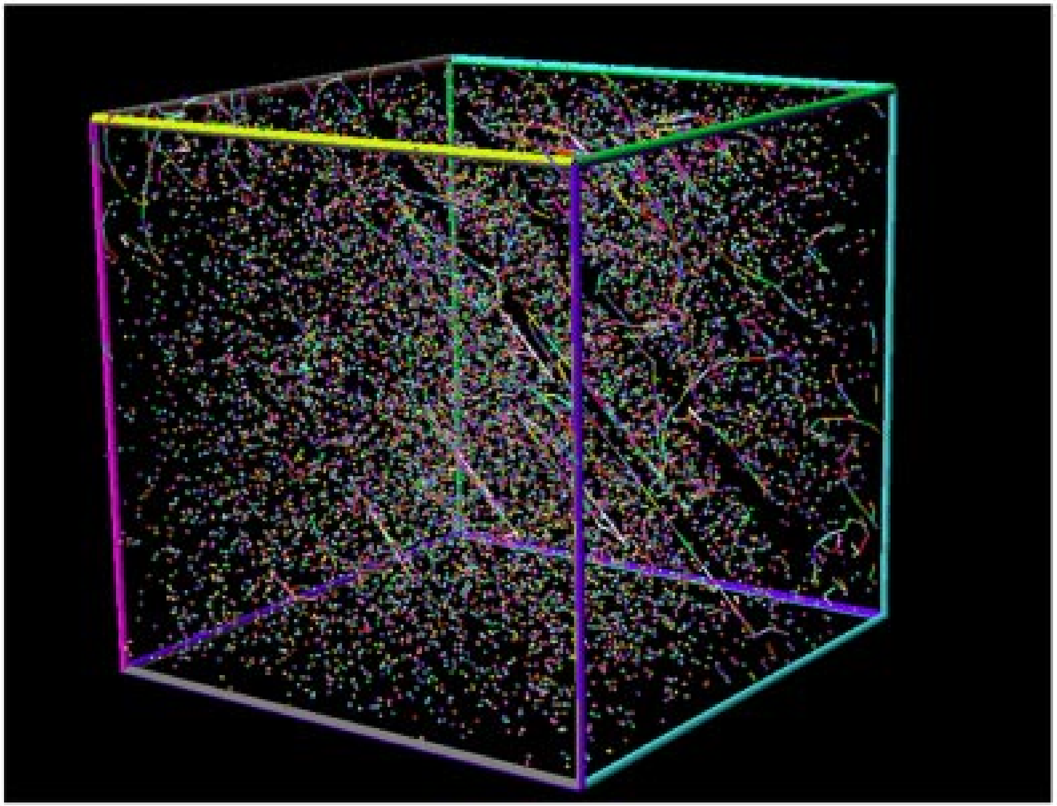
Leads to localized flow

(1) N.M. Ghoniem, B. N. Singh, L. Z. Sun, and T. Diaz de la Rubia, *J. Nucl. Mater*, **276:** 166-177 (2000).

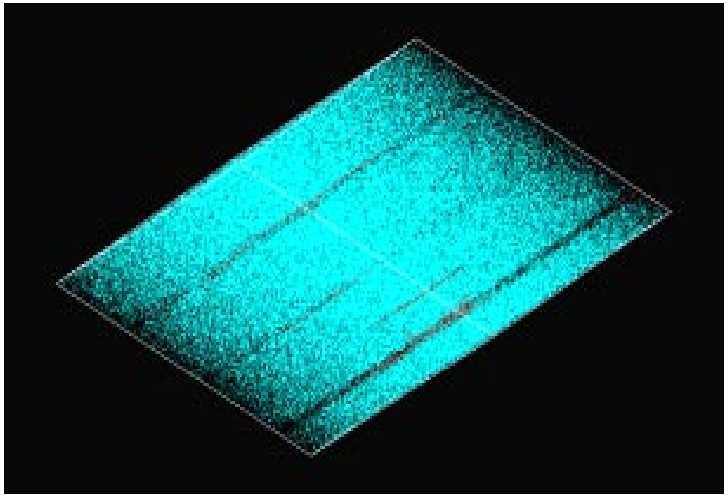
(2) N.M. Ghoniem, S.- H. Tong, B.N. Singh, and L. Z. Sun, *Phil. Mag.*, 2001, submitted

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



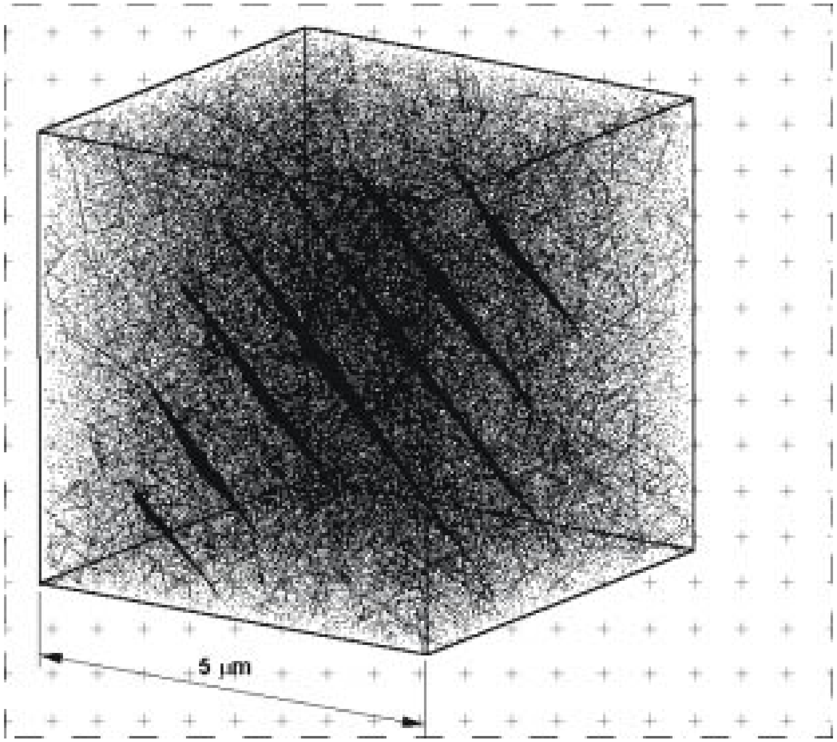
Spreading of the channels is restrained by the formation of dipole segments and the remaining radiation induced defect distribution



Nature, August 24, 2000

Successful Applications in Fusion Material Science (2)

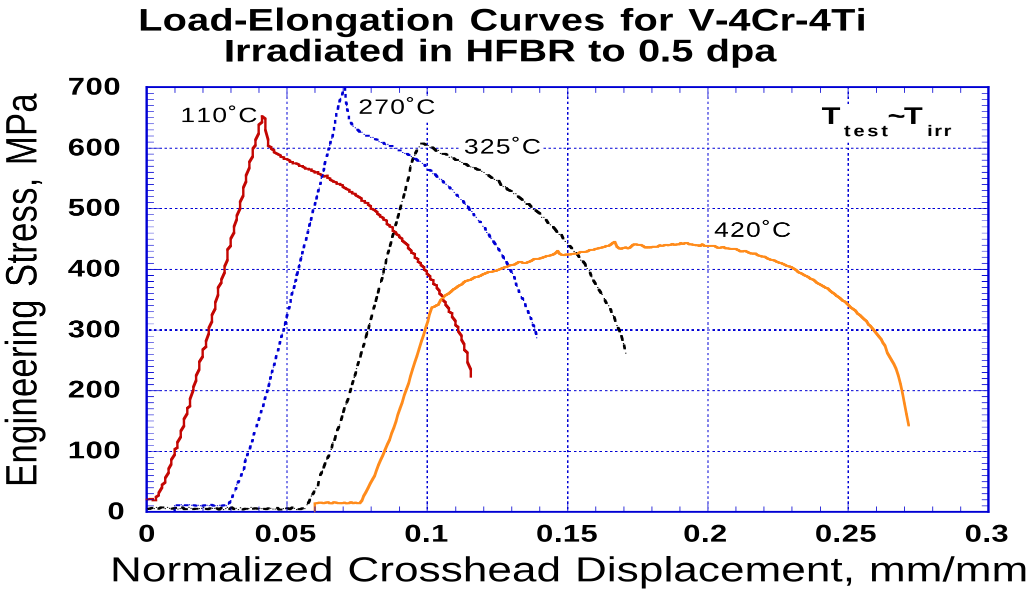
UCLA-RISO (Denmark) collaboration on localization of plastic flow

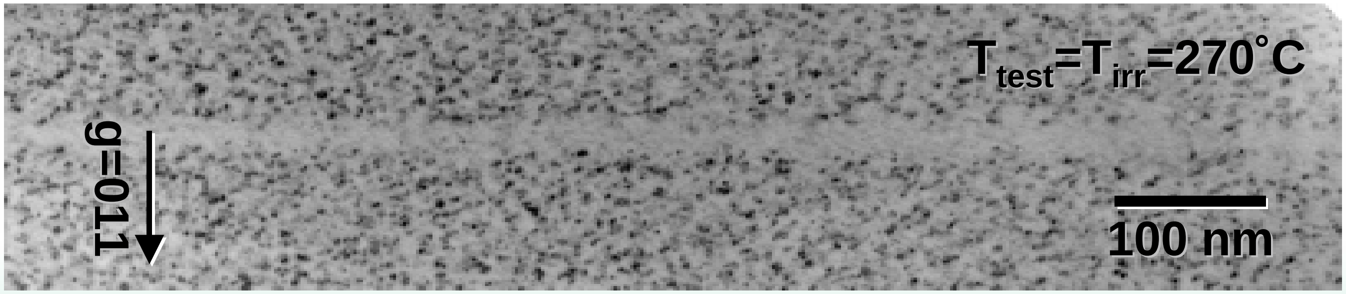


Computer Simulations

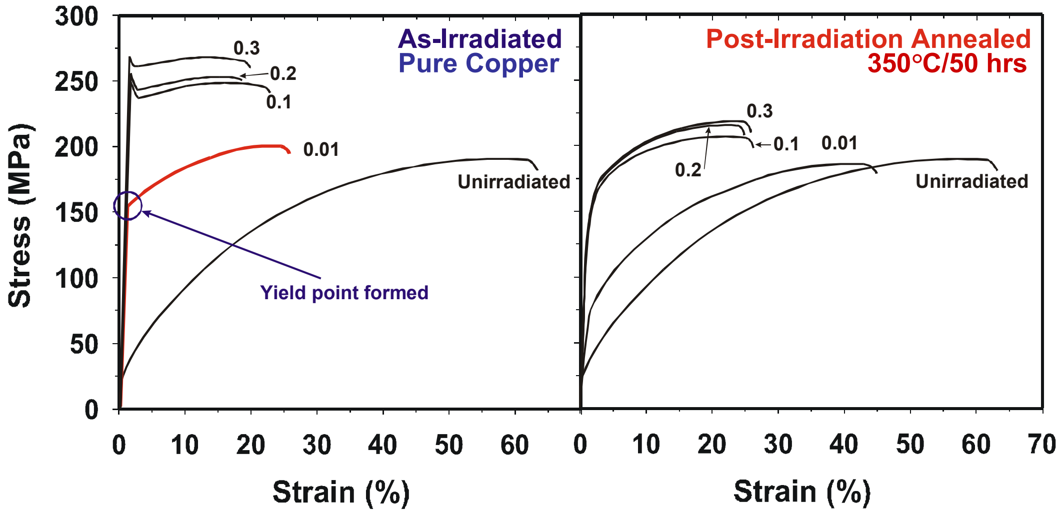
Experiments on Irradiated Cu

Irradiated Materials Suffer Plastic Instability due to Dislocation Channeling





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

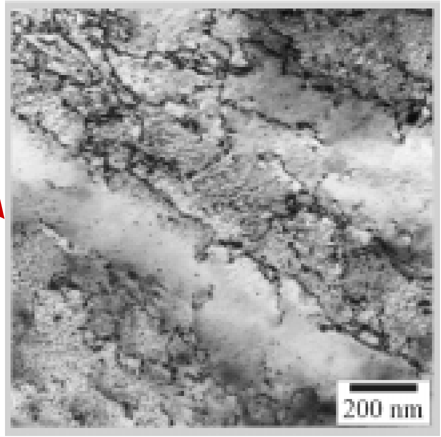


Post-Irradiation Annealed Condition

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

As-Irradiated, 0.3 dpa

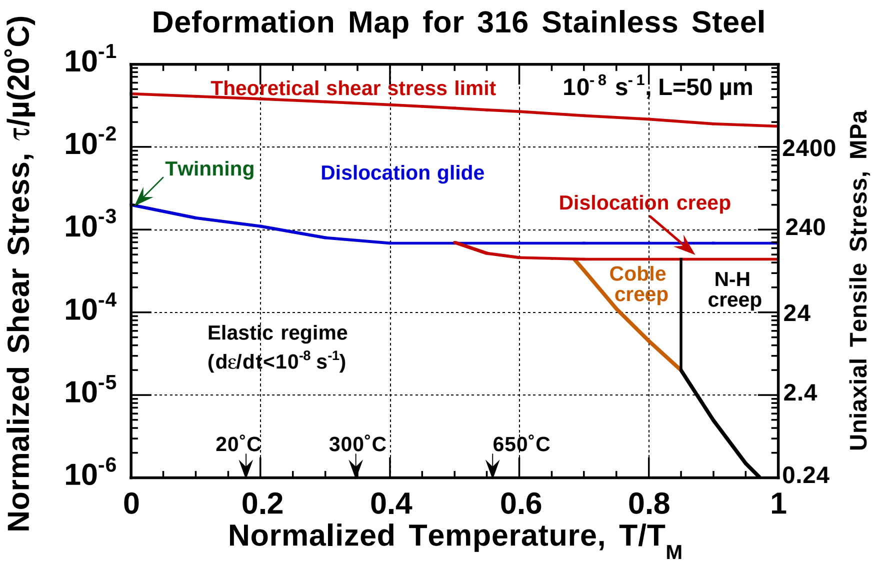
- Cleared channels with little to no dislocation movement between the channels; localized deformation
- Large increases in strength (6 to 8x)
- Loss of uniform elongation and work hardening capacity
- Formation of a clearly defined yield point

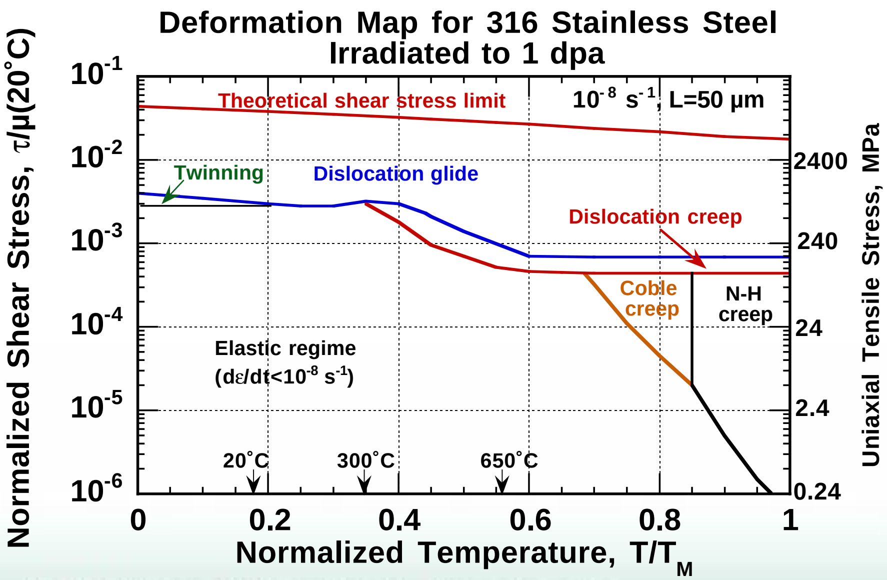


PI Annealed, 0.01 dpa

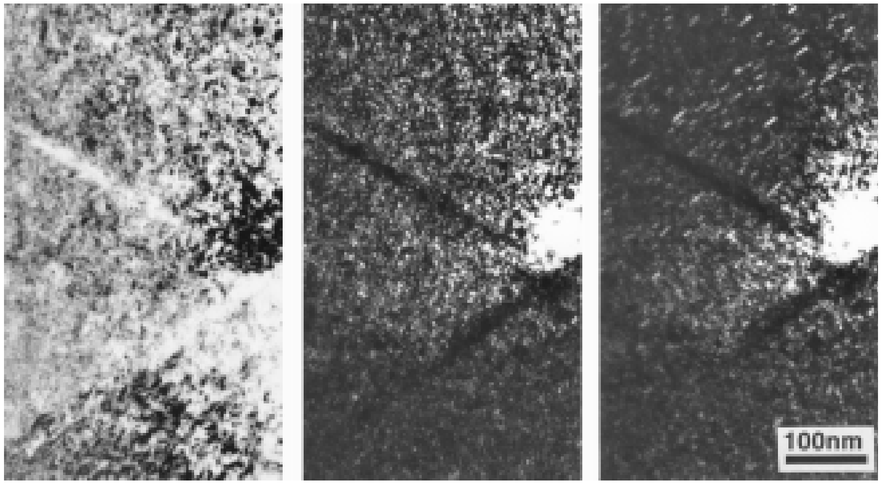
PI Annealed, 0.3 dpa

Deformation mechanisms in FCC metals

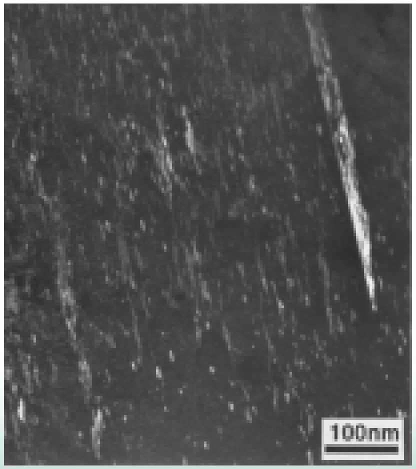




Irradiation is a useful tool to produce controlled microstructures for deformation mechanics studies



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



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

Deformation Flow Instability-Localization

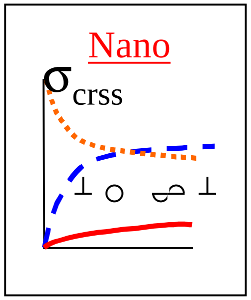
- Understanding uniform strain loss-flow localization requires close integration of ***multiscale models & experiments.*** In many cases irradiation may enhance *functional* strength.

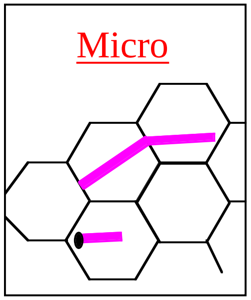
Multiscale Physics

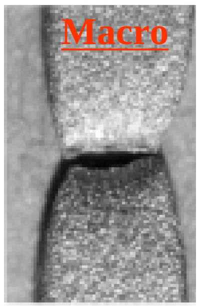
Engr s-e Instability Theory

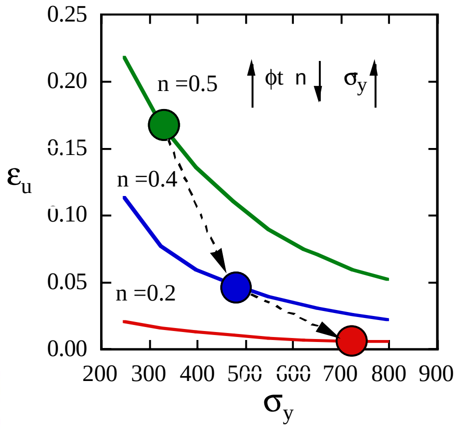
Hardness Pile-up/n

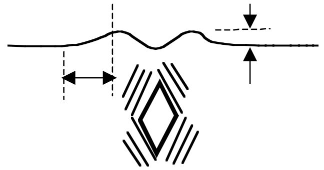
Beam Bend Tests

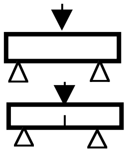


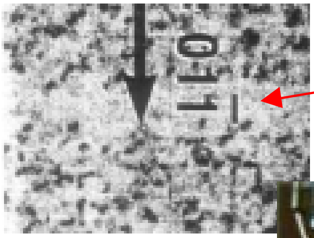






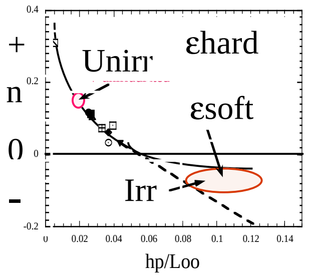


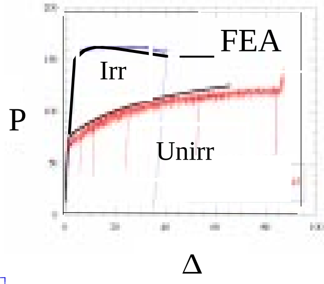


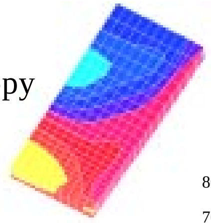


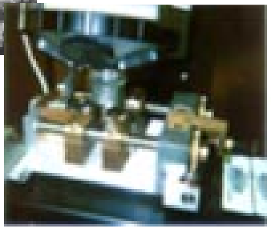
flow channel

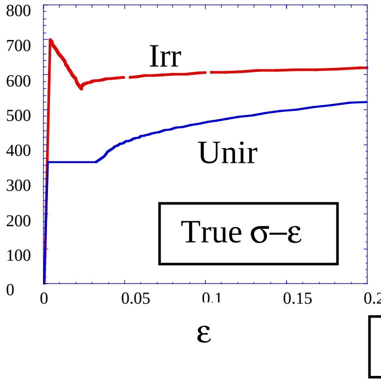
Confocal microscopy

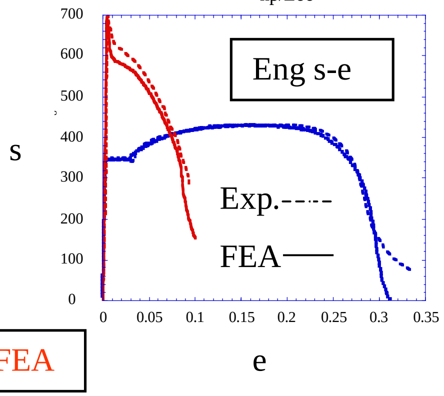


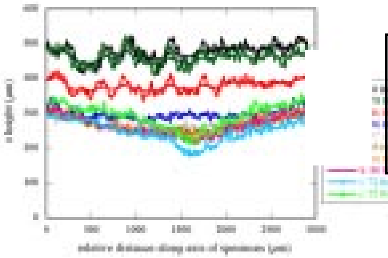








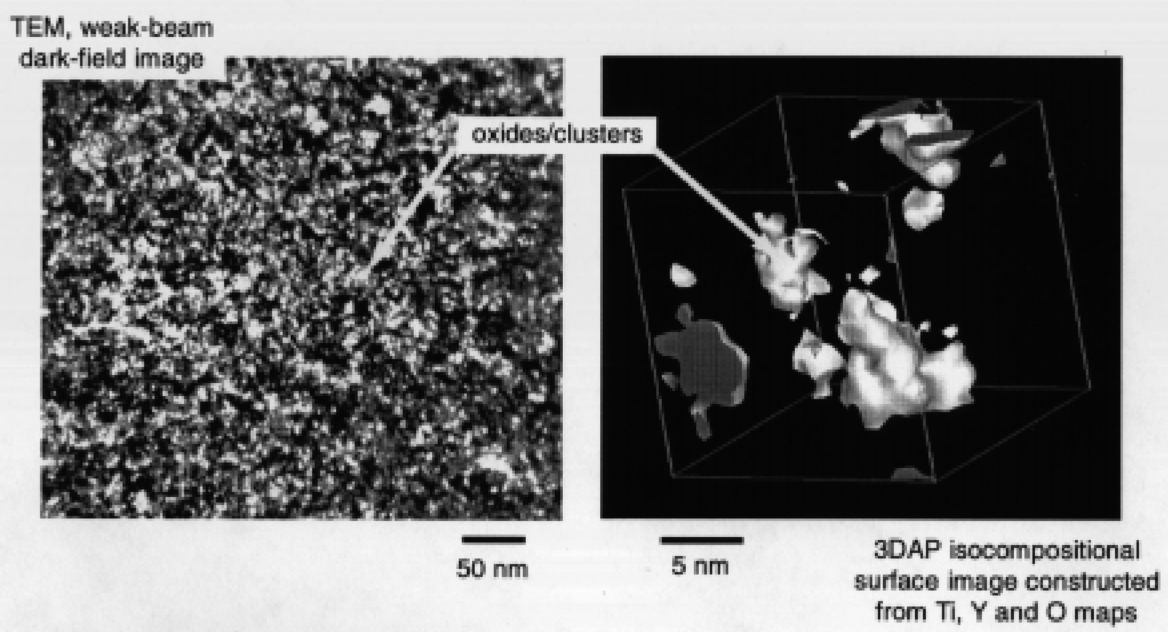




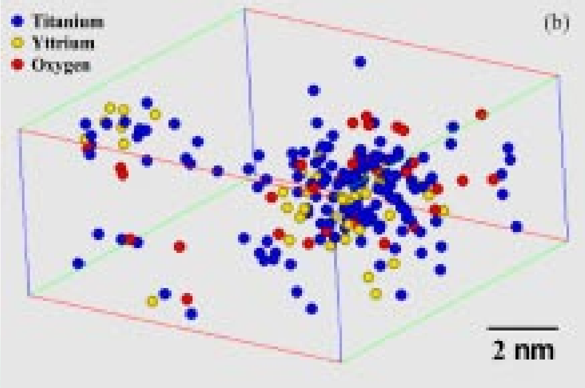
Tensile test 3-D shape imaging and FEA modeling

FEA

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

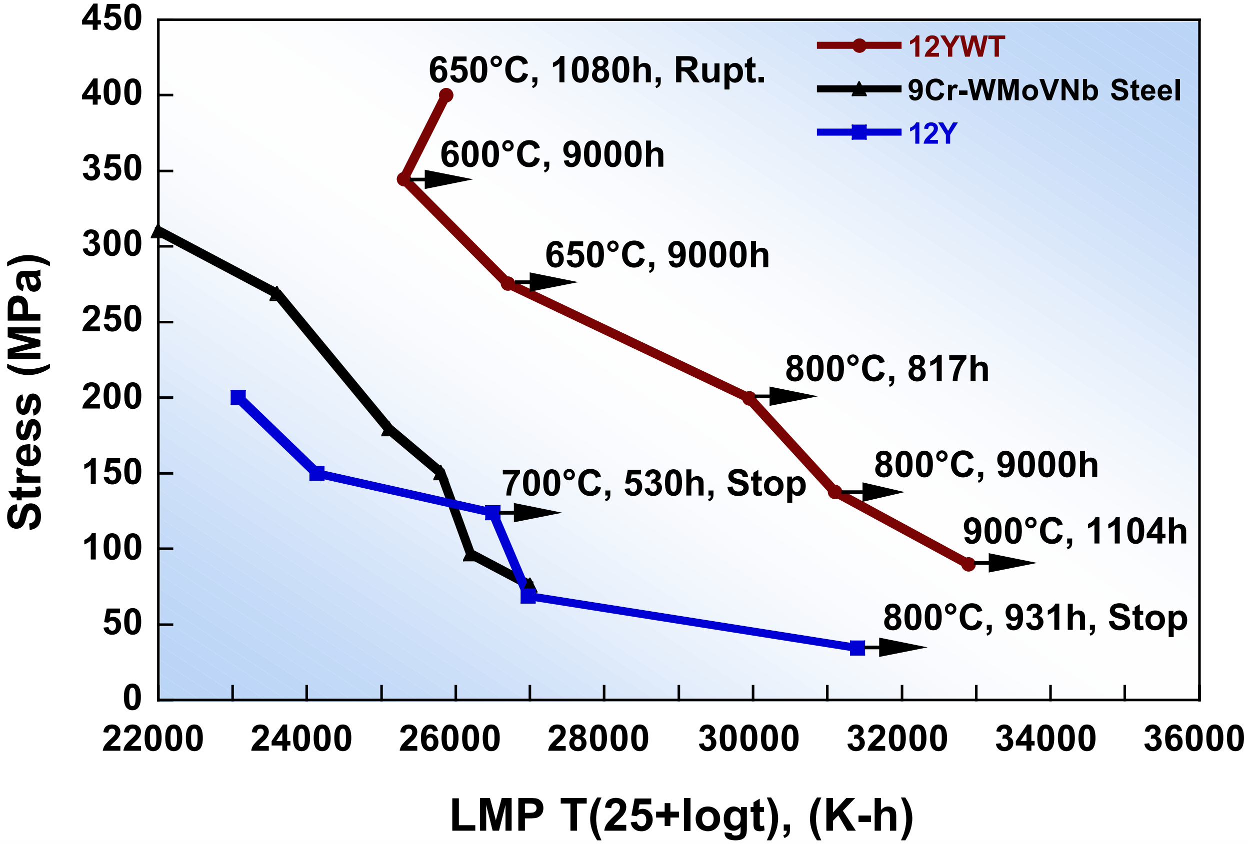


Atomic composition of nanoclusters



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

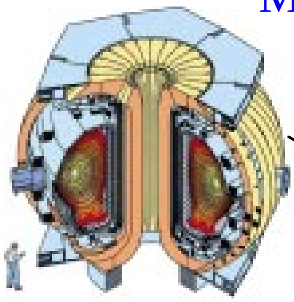


- **Time to failure is increased by several orders of magnitude**
- **Potential for increasing the upper operating temperature of iron based alloys by ~200°C**

Multiphysics - Multiscale Fracture Modeling - I

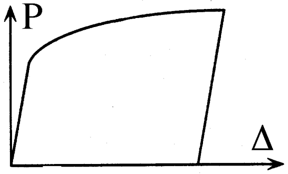
10 m

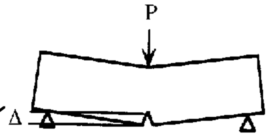
Macroscopic Scale



10^{-2} m

structure





specimen

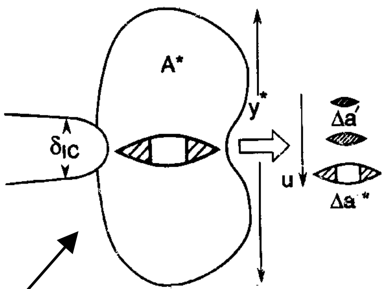
Elastic-plastic deformation and fracture of a cracked body as a function of temperature and loading rate as characterized by material macro constitutive and fracture toughness properties.

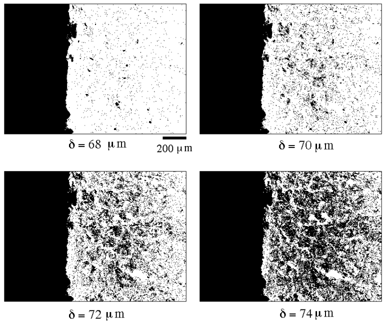
FEM: load-displacement

Large scale bridging

10^{-3} m

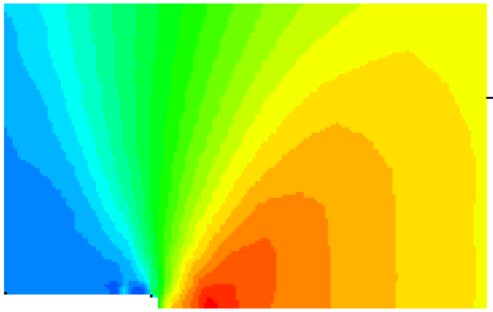
Mesoscopic Scale

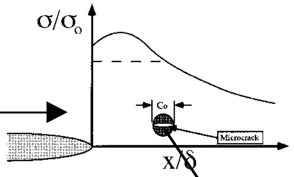


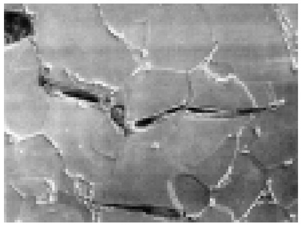


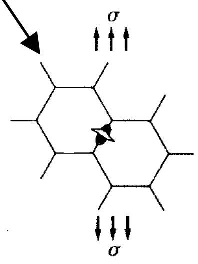
Local multiaxial plasticity at blunting macro-crack tip resulting in stress-strain field concentrations that crack mm-scale brittle trigger particles. Many micro-cracks arrest at particle-ferrite interfaces, lath packets, and grain boundaries. Ultimate process zone damage development and collective instability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

FEM: blunting fields









Trigger particle mechanics

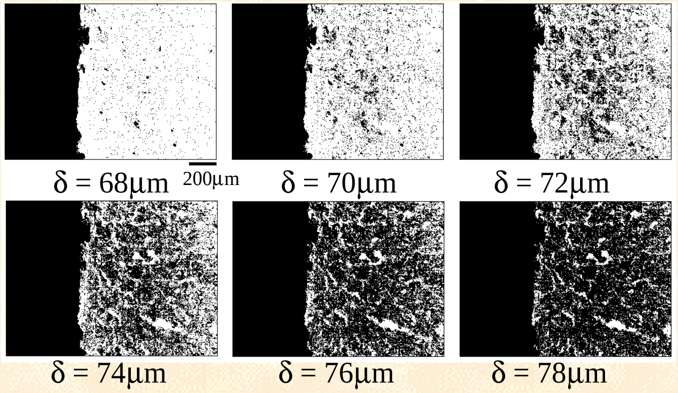
$\sigma^* = K_{micro}/C\sqrt{\pi a}$

10^{-10} m

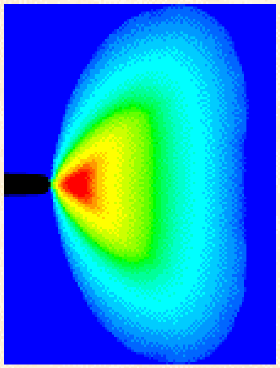
Multiscale Research on Fracture Mechanisms, Mechanics, Models and Structural Integrity Assessment Methods

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.

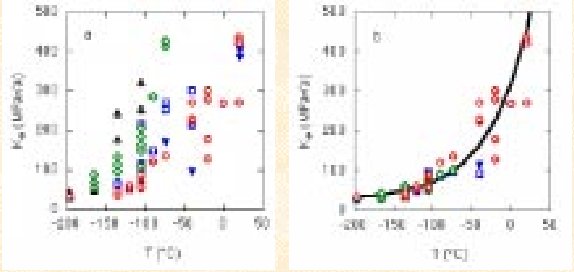
Tomographic Imaging of Cleavage



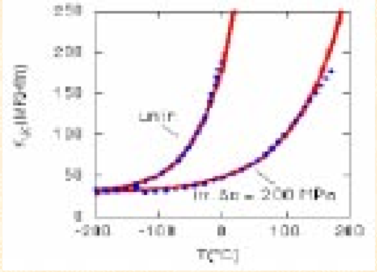
FEM Simulations of Crack Fields



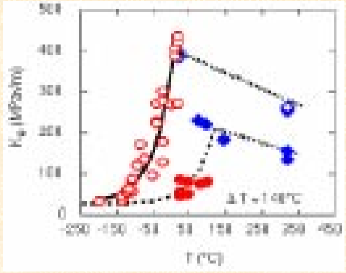
Size-Corrected Minitest K(T) Data



Theoretical vs. Observed Master Curve

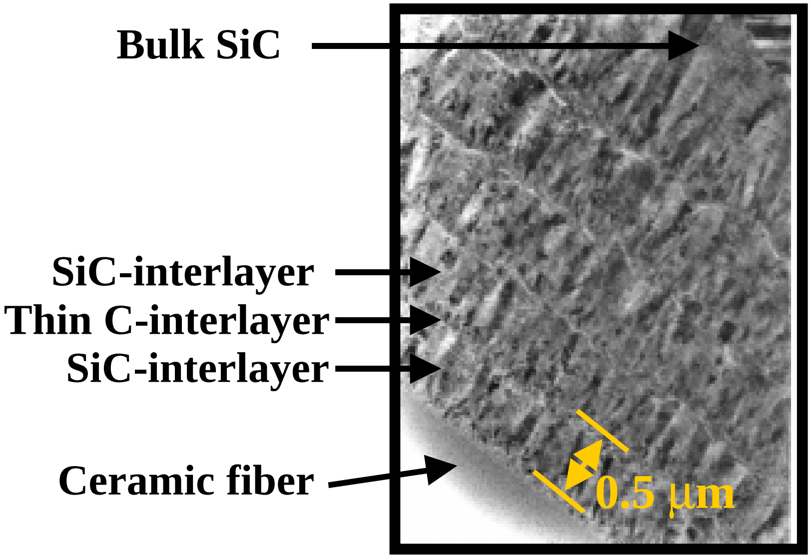


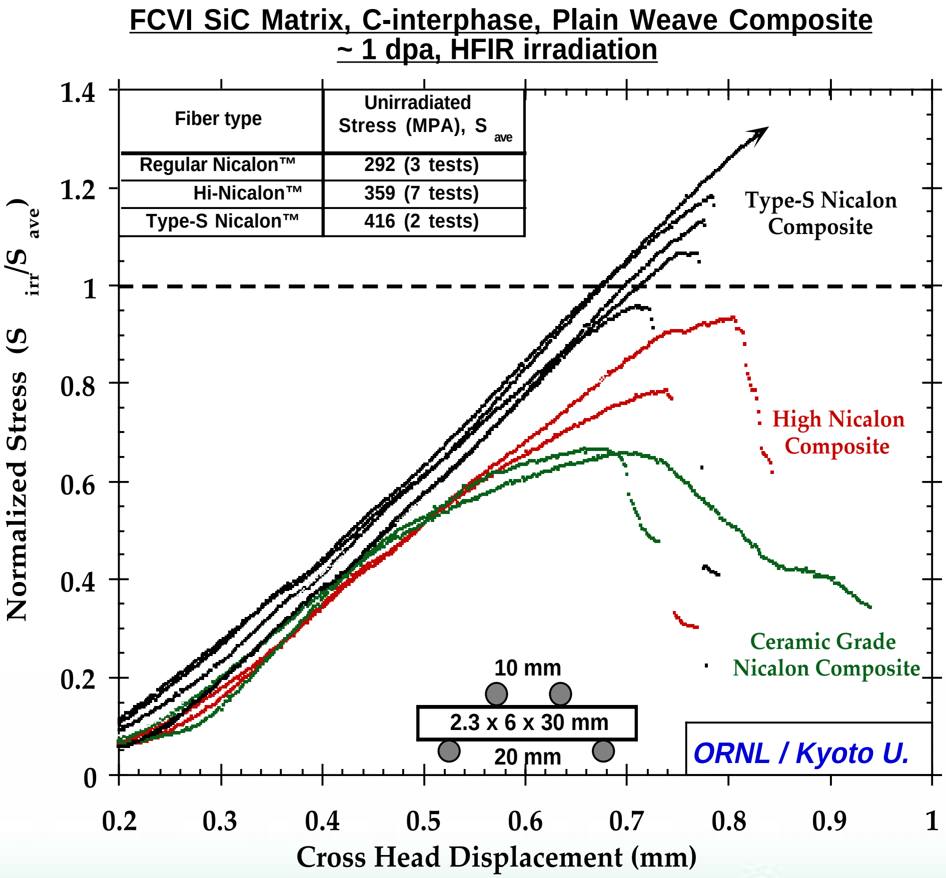
MC Embrittlement Shifts in F82H



UCSB

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





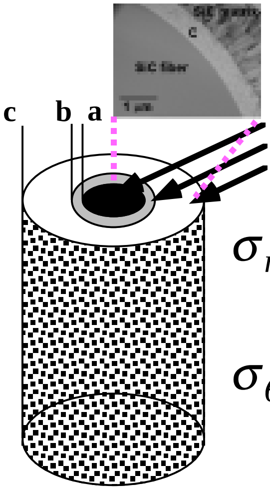
FCVI SiC Matrix, C-interphase, Plain Weave Composite
~ 1 dpa, HFIR irradiation

Fiber type	Unirradiated Stress (MPA), S_{ave}
Regular Nicalon™	292 (3 tests)
Hi-Nicalon™	359 (7 tests)
Type-S Nicalon™	416 (2 tests)

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

Analytical modeling of internal stresses

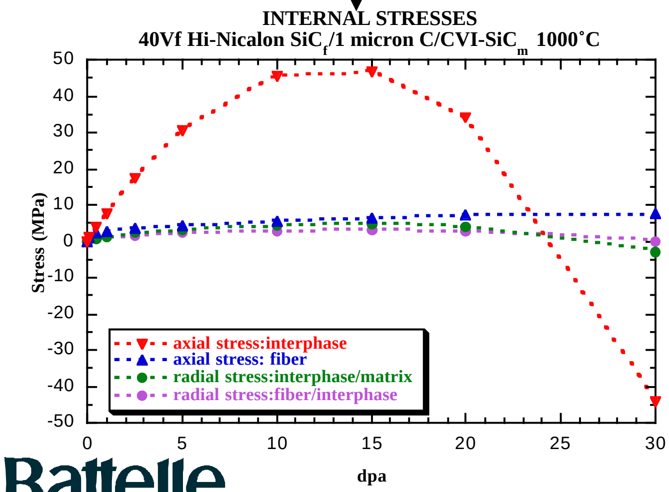
microscale



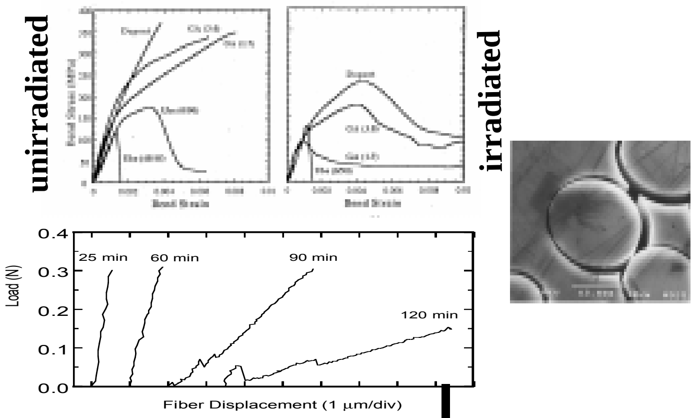
$$\sigma_r = A - \frac{B}{[r(dpa)]^2}$$

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

macroscale

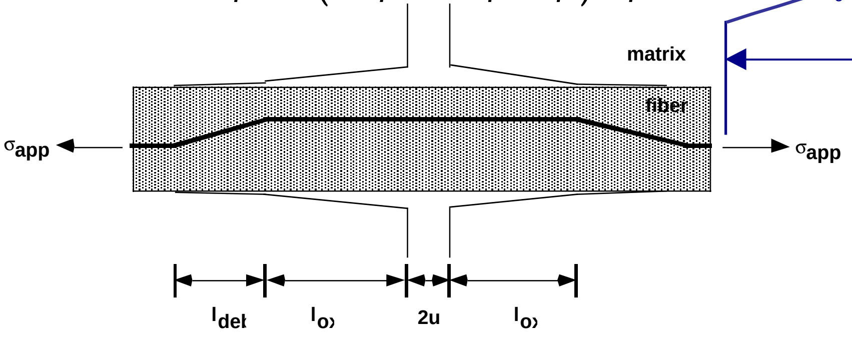


Experimentally determined, semi-empirical, bridging-compliance relations



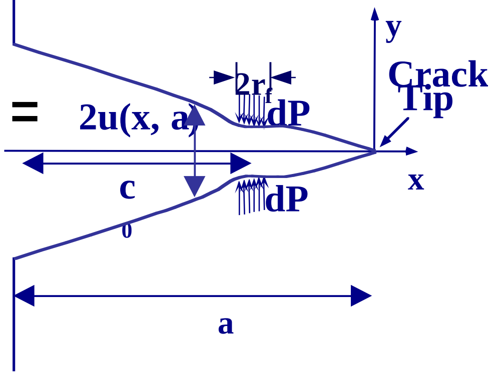
+

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



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

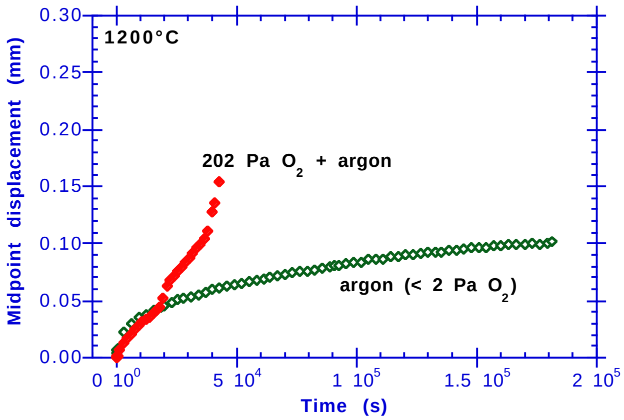
=



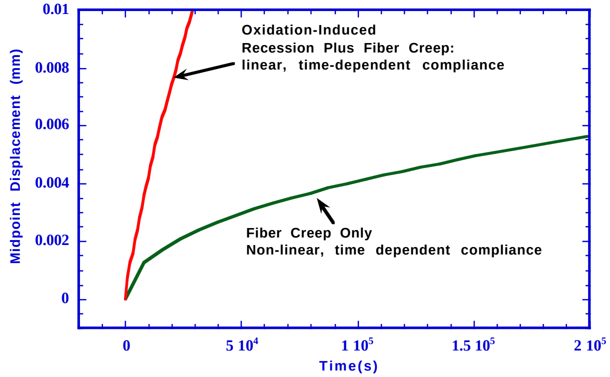
Micromechanical Modeling Allows Prediction of Component Lifetime of Ceramic Composites

Model verification

experiment



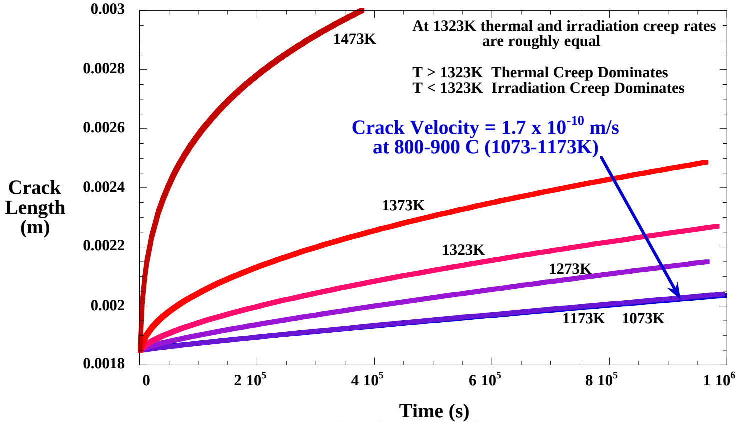
model



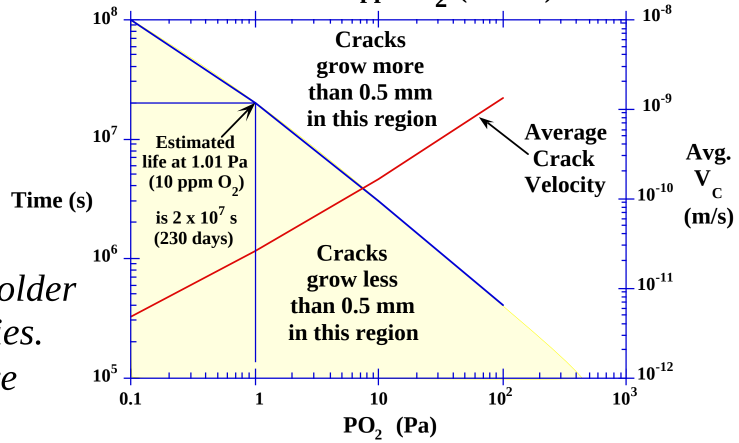
Oxygen atmosphere investigated in conjunction with DOE office of Basic Energy Science Program

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.

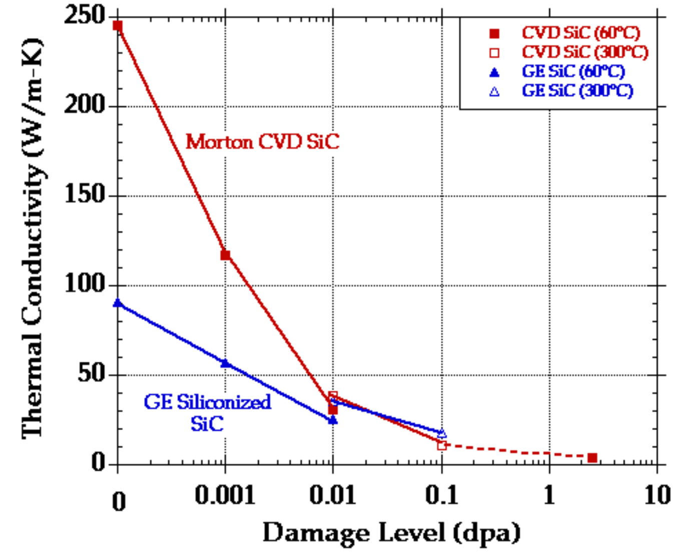
Physics of phonon transport & scattering are being investigated in neutron-irradiated ceramics

$$\left[K\,(T)\right]^{-1} = \left[\frac{1}{K_u(T)} + \frac{1}{K_{gb}(T)} + \frac{1}{K_{d0}} + \frac{1}{K_{rd}}\right]$$

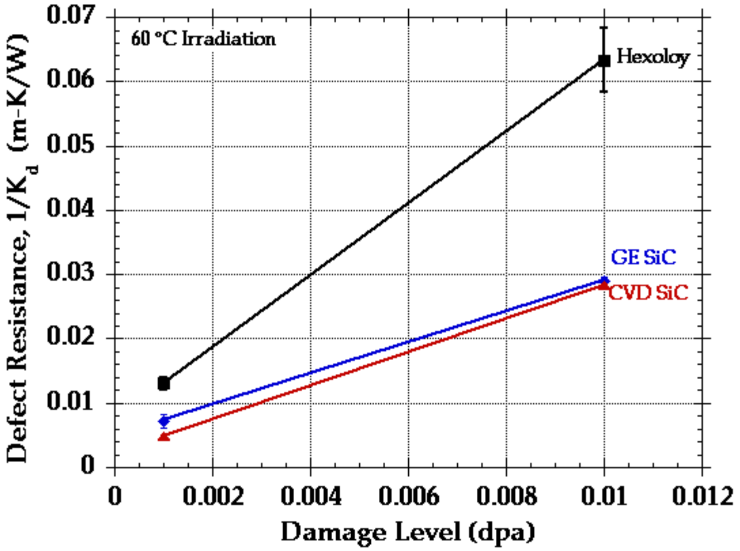
Thermal resistance of different phonon scattering centers can be simply added if their characteristic phonon interaction frequencies are well-separated from one another

$$\frac{K_{irr}}{K_{unirr}} = \left(\frac{2h\upsilon^2}{18\pi^2\Omega\Theta_D K_{unirr} C_v}\right)^{1/2} \tan^{-1}\left(\frac{2h\upsilon^2}{18\pi^2\Omega\Theta_D K_{unirr} C_v}\right)^{-1/2}$$

Thermal resistance due to radiation-induced defects (vacancies, dislocation loops, etc.) is proportional to their concentration



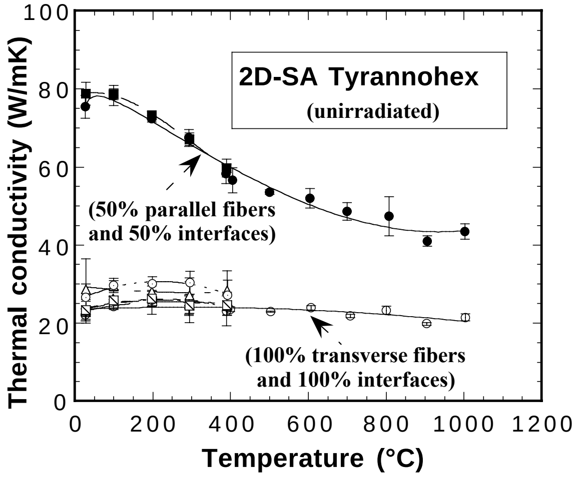
Effect of Low-Temperature Neutron Irradiation on the Thermal Conductivity of Different Grades of SiC



Increase in Thermal Resistivity in SiC due to Low Temperature Neutron Irradiation

Thermal Conductivity of 2D SiC/SiC Composites

Fusion Materials Program



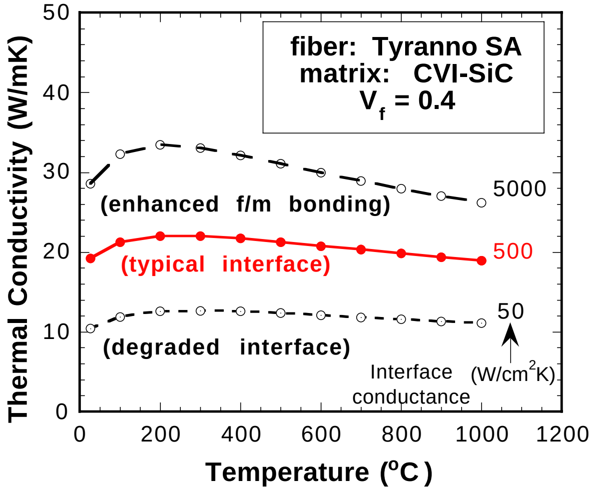
Experimental:

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

NERI Program

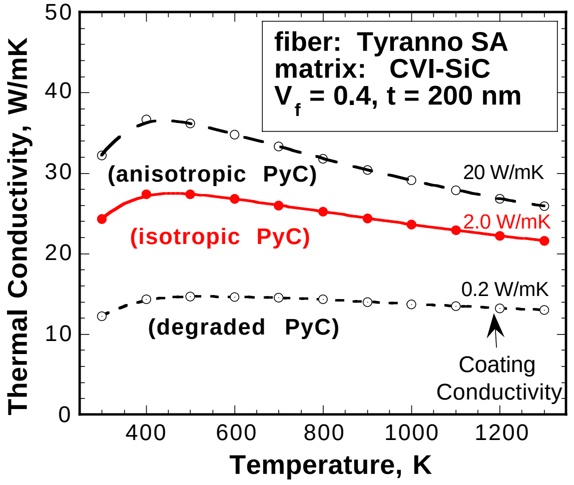
Model 1: Thin Interface Conductance

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

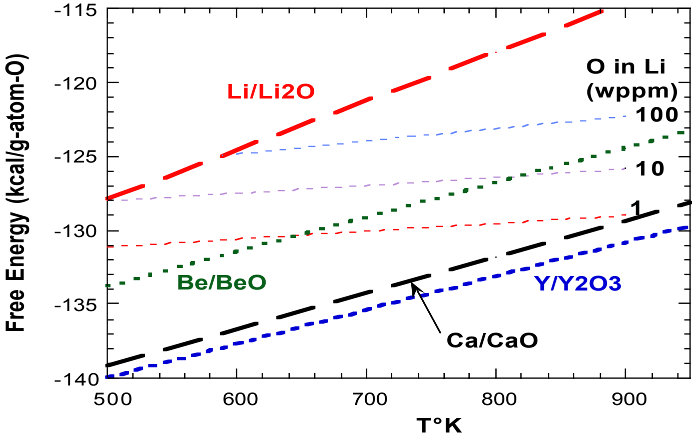


Model 2: Interphase Conductivity

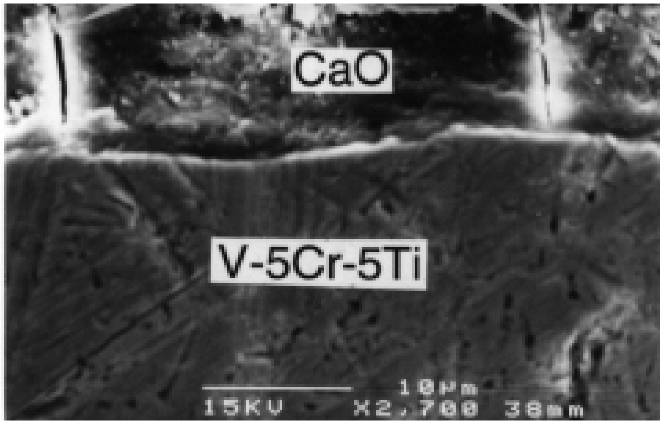
- Preferred orientation of graphitic crystallites
- Strong interface cohesion
- Degraded interphase due to irradiation or oxidation



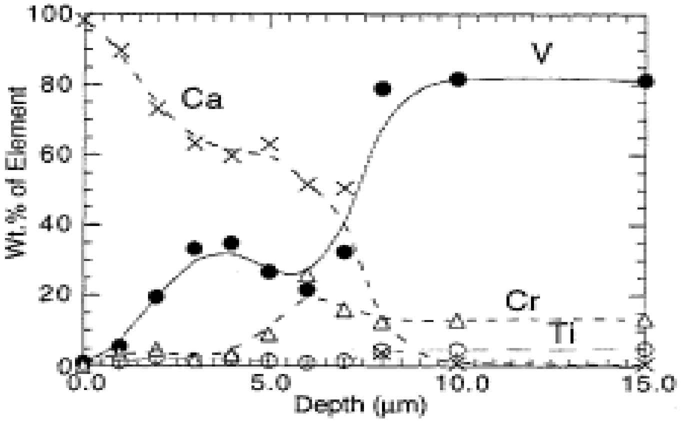
Thermodynamic Stability, Microstructure Characterization, and Property Evaluation of In-situ Formed “CaO” Insulating Coating on Vanadium Alloys



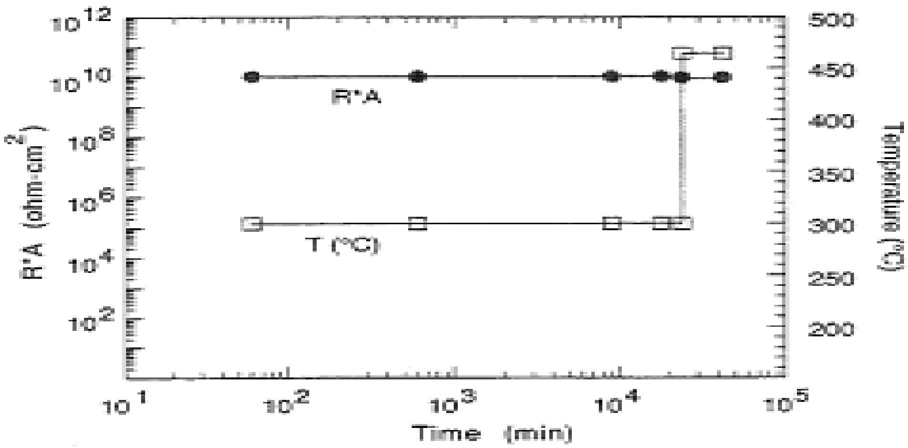
- Calculated thermodynamic stability of candidate oxides in lithium as function of oxygen content



- Microstructure of “CaO” coating on V-alloy



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



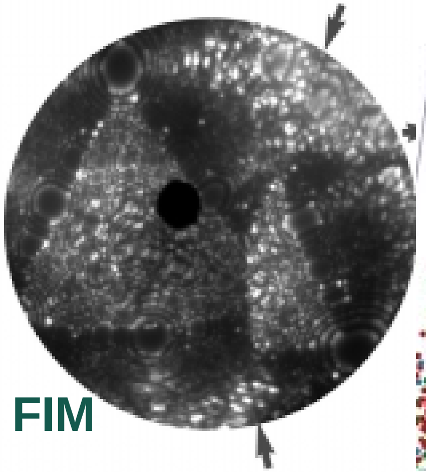
- In-situ resistance of “CaO’ coating in lithium

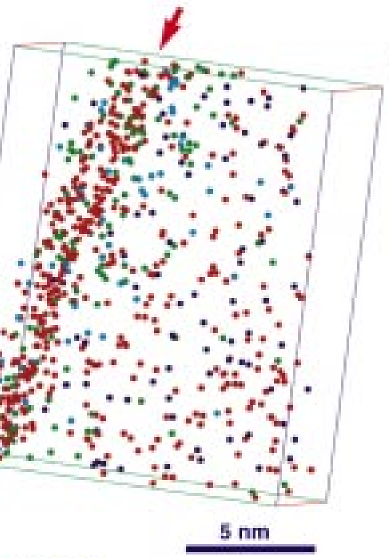
Argonne National Laboratory

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

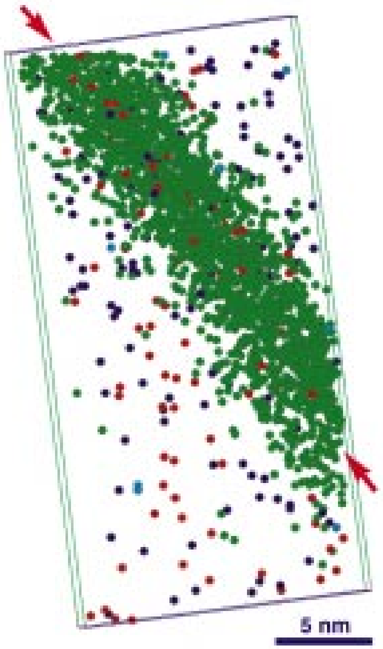

FIM



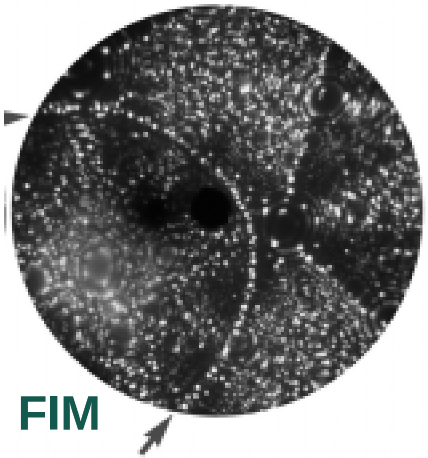
B C Zr O

GIE (atoms m^{-2})	
Zr	7.6×10^{13}
B	7.3×10^{12}
C	1.1×10^{13}
O	-3.9×10^{12}

HEAT AFFECTED ZONE



APT atom maps


FIM

GIE (atoms m^{-2})	
Zr	1.3×10^{13}
B	9.9×10^{14}
C	9.9×10^{11}
O	1.1×10^{13}

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

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

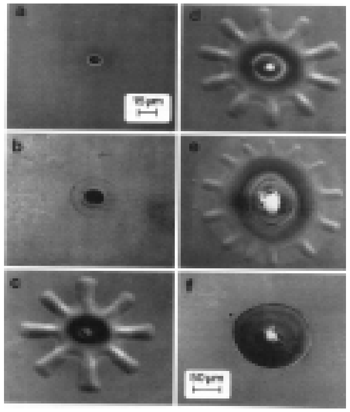
UT-BATTELLE

LASER-INDUCED SURFACE DEFORMATION MECHANISMS

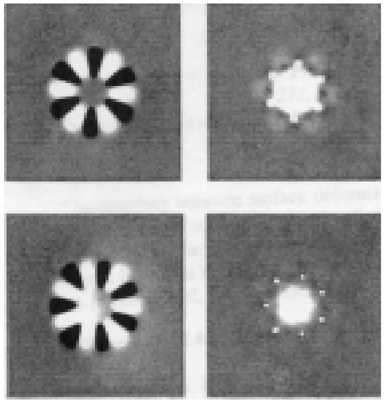
- **Single Shot Effects on LIDT:**
  - **Laser Heating Generates Point Defects**
  - **Coupling Between Diffusion and Elastic Fields Lead to Permanent Deformation**
- **Progressive Damage in Multiple Shots**
  - **Thermoelastic Stress Cycles Shear Atomic Planes Relative to one Another (Slip by Dislocations)**
  - **Extrusions & Intrusions are Formed when Dislocations Emerge to the Surface**

SINGLE-SHOT LASER DAMAGE EXPERIMENTS & MODELING

Focused Laser-induced Surface Deformation



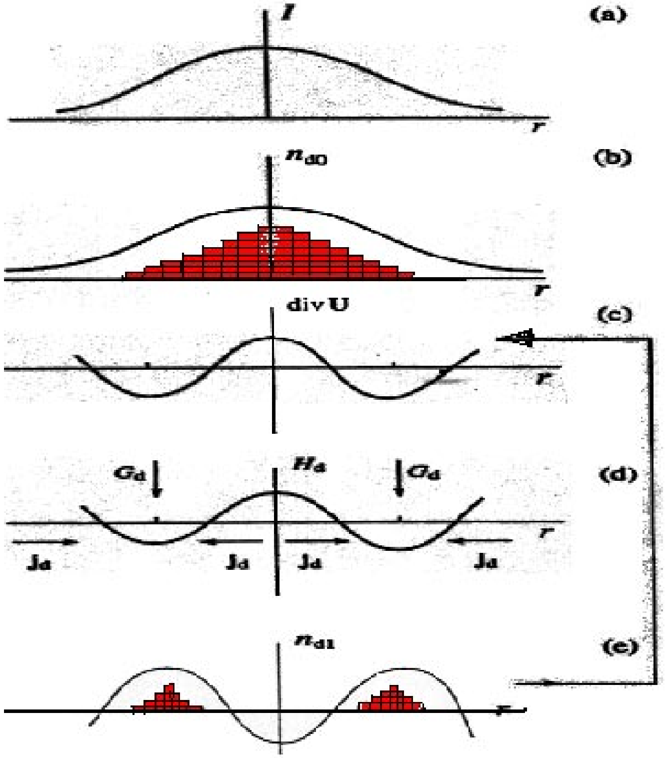
Experiment



Computer Simulation

Focused laser-induced surface deformation (Lauzeral, Walgraef & Ghoniem, **Phys. Rev. Lett. 79, 14 (1997) 2706**)

Physical Mechanism of Feedback in Point Defect GDDI: Laser Intensity Distribution

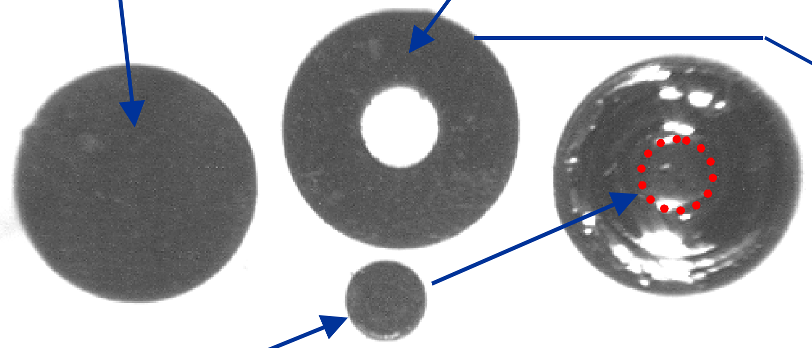


Deformation instability mechanisms

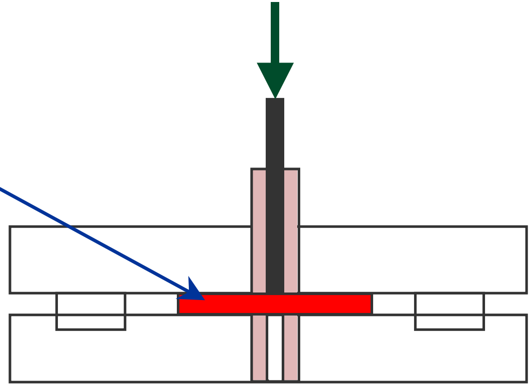
Newly Developed Techniques Allow Greater Materials Science Output From Smaller Irradiation Volumes

3 mm TEM disk is irradiated in fission reactor

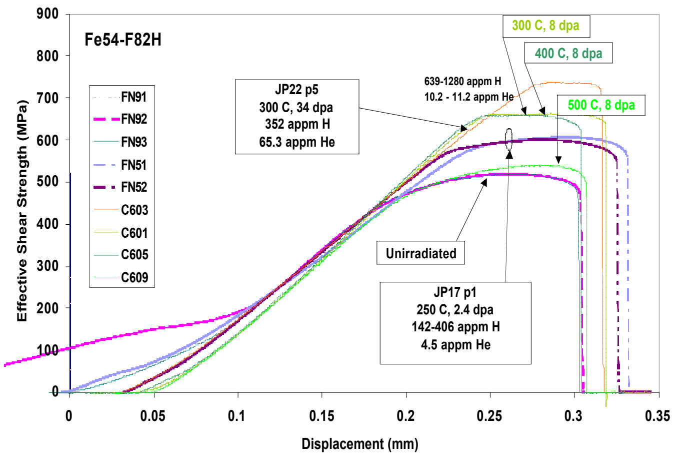
He and H analyses on outer rim

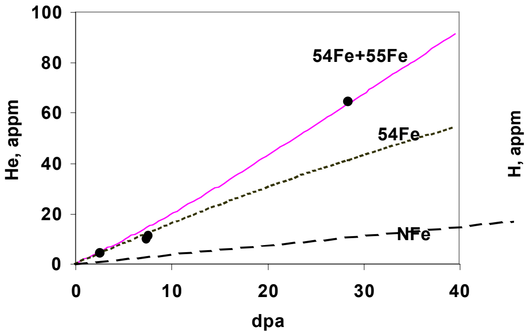


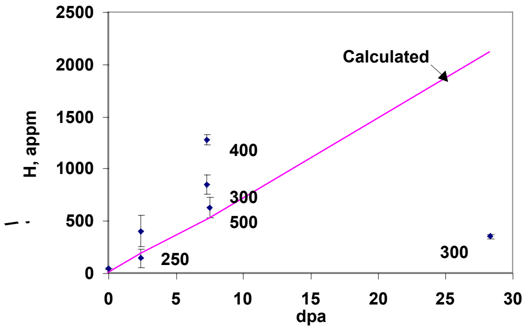
Shear punch test yields mechanical properties data that correlate with tensile data and can be correlated with data on conventional (full size) specimens



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







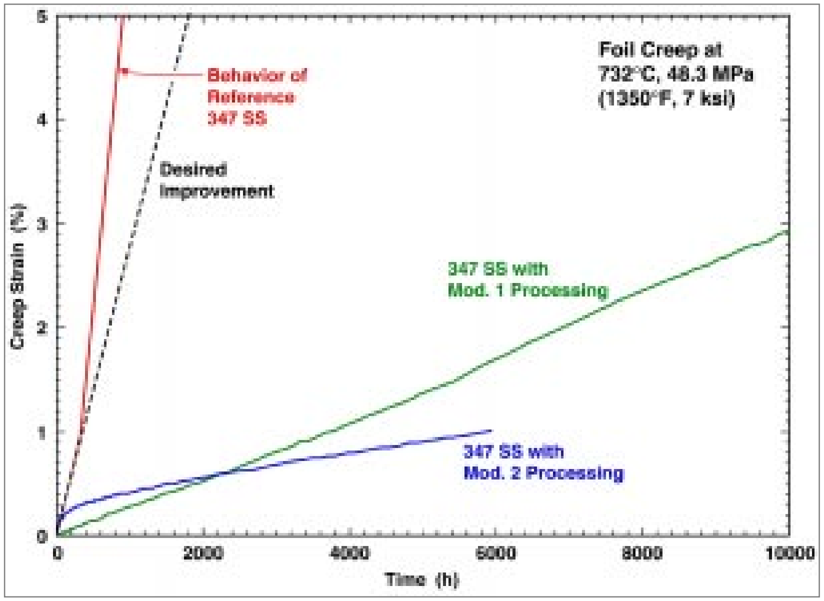
Hydrogen and Helium analysis results

The fusion materials program is participating in ground-breaking remote microscopy investigations

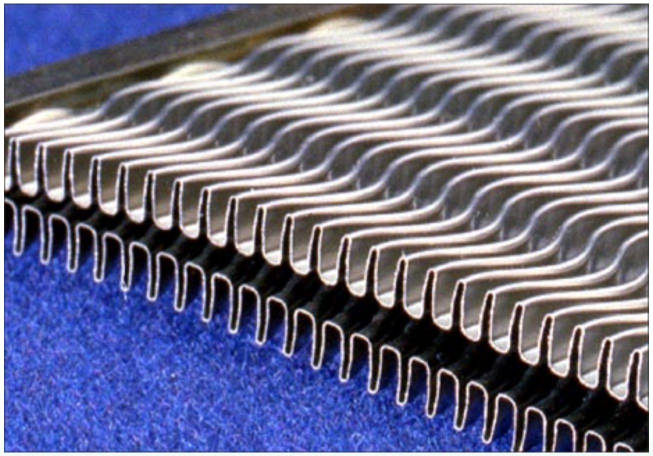
DOE/JAERI remote microscopy analysis of irradiated SiC/SiC composite, July, 2000

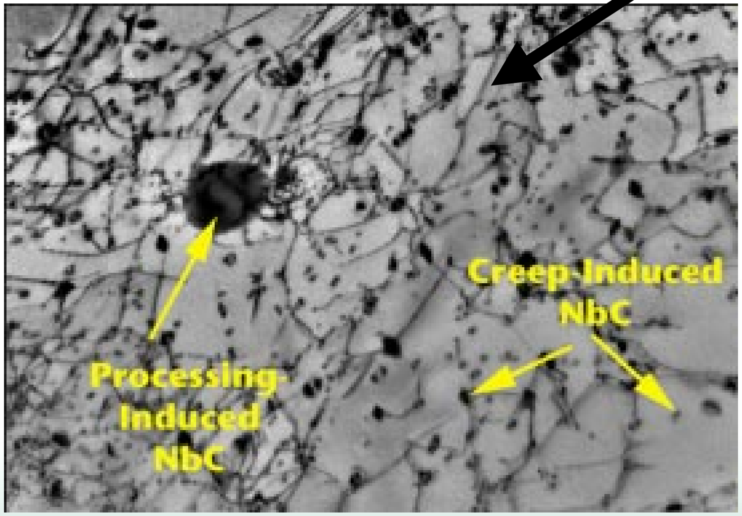
Groundwork laid by DOE 2000 Materials Microcharacterization Collaboratory initiative (OASCR)

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)



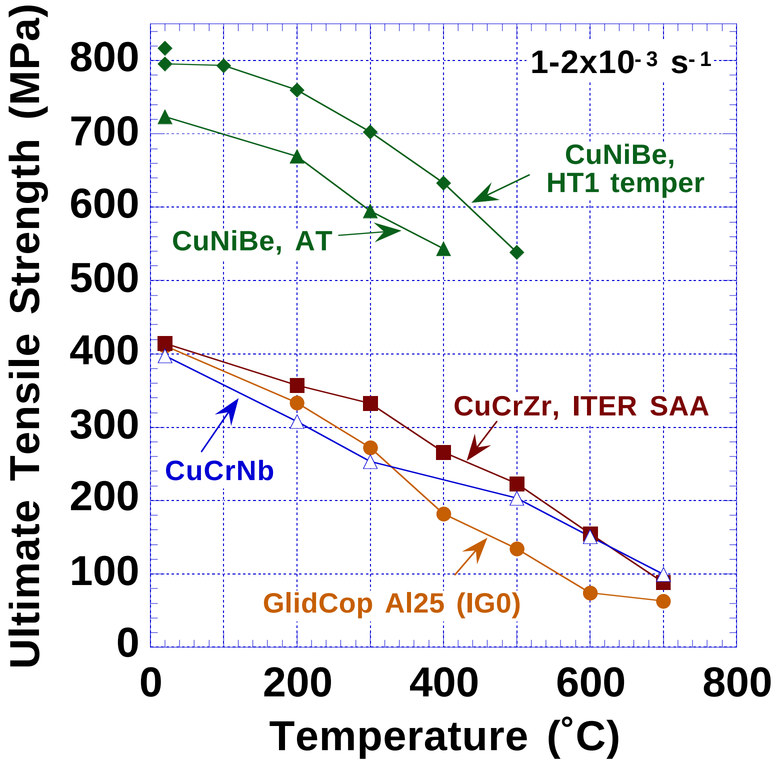


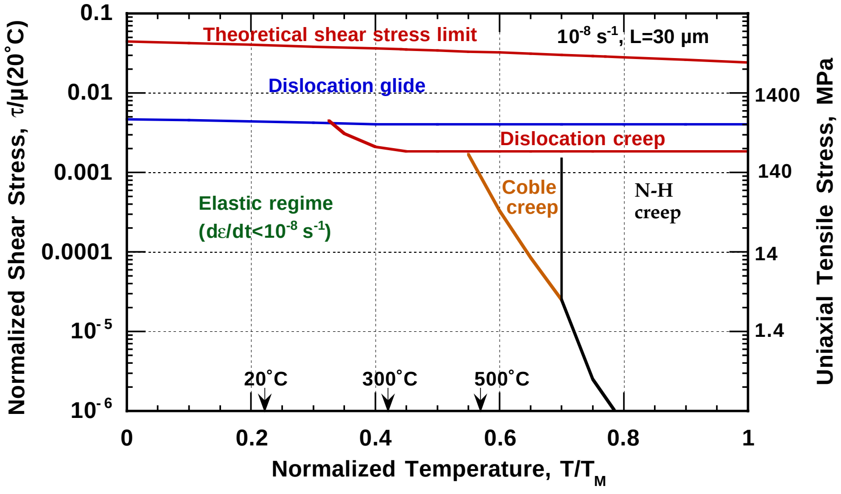
Conclusions

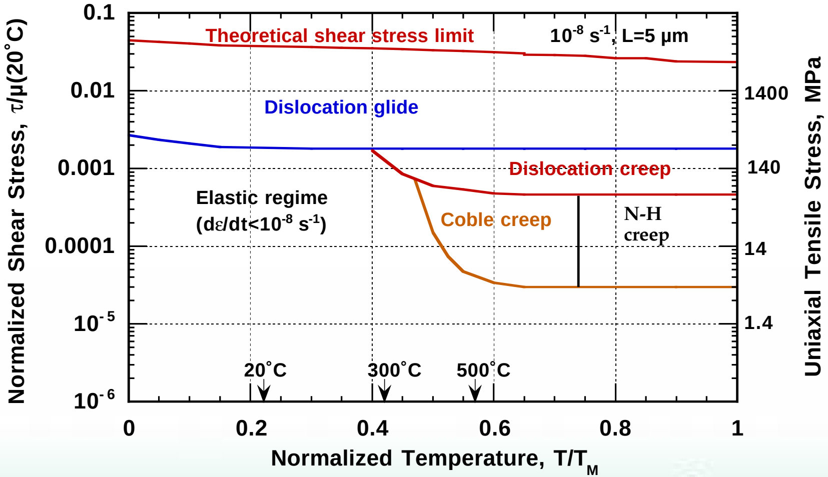
- **The Fusion Materials Sciences program is pursuing simultaneous scientific excellence (fusion energy and materials science)**
  - **Research portfolio is determined by fusion energy needs (guided by fusion materials roadmap key feasibility issues)**
  - **research results are of interest to broader materials science community**

Backup viewgraphs

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

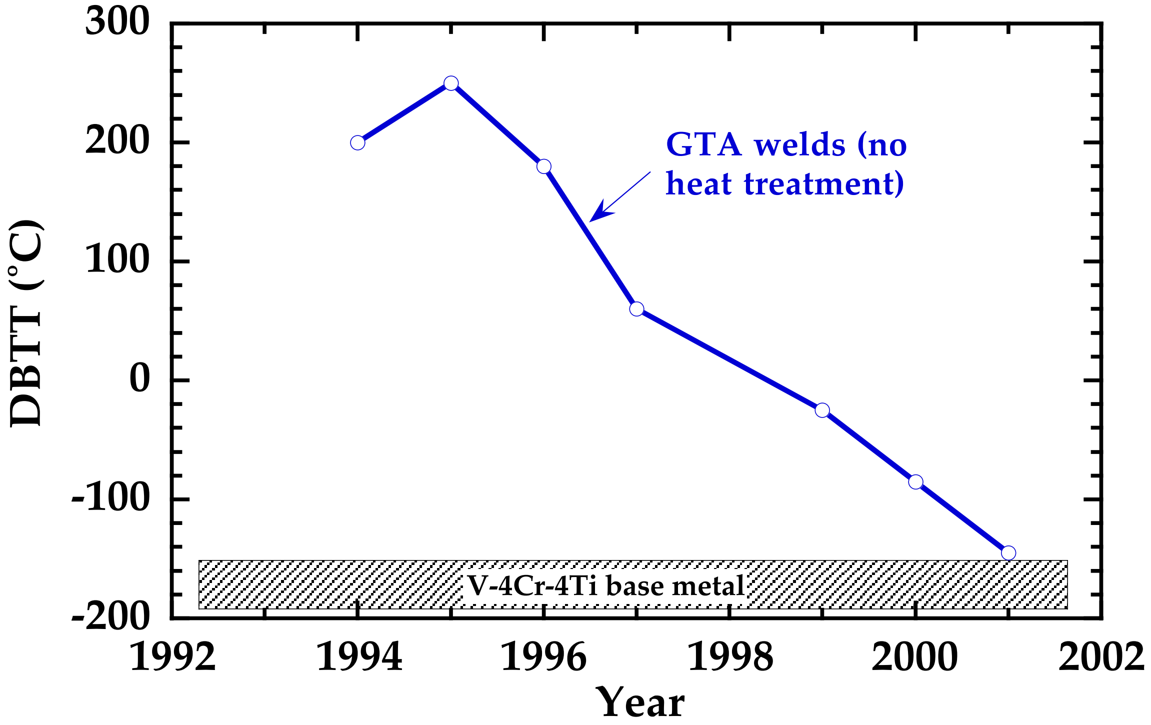


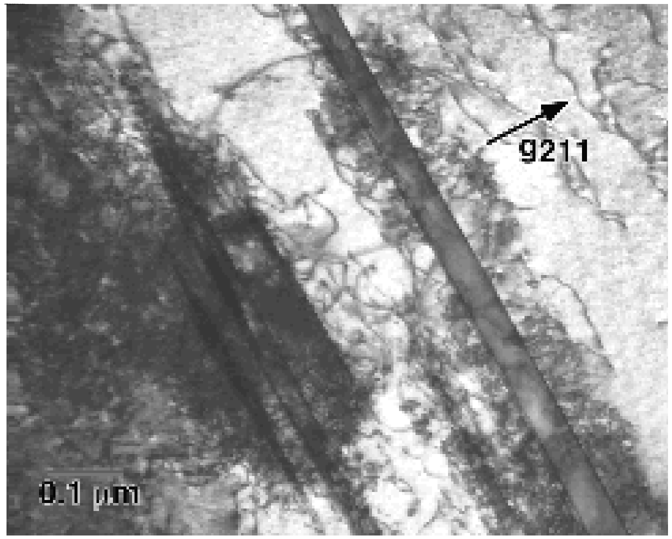

Deformation Map for CuNiBe (Brush-Wellman Hycon 3HP)


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

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

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





Success is due to simultaneous control of impurity pickup, grain size

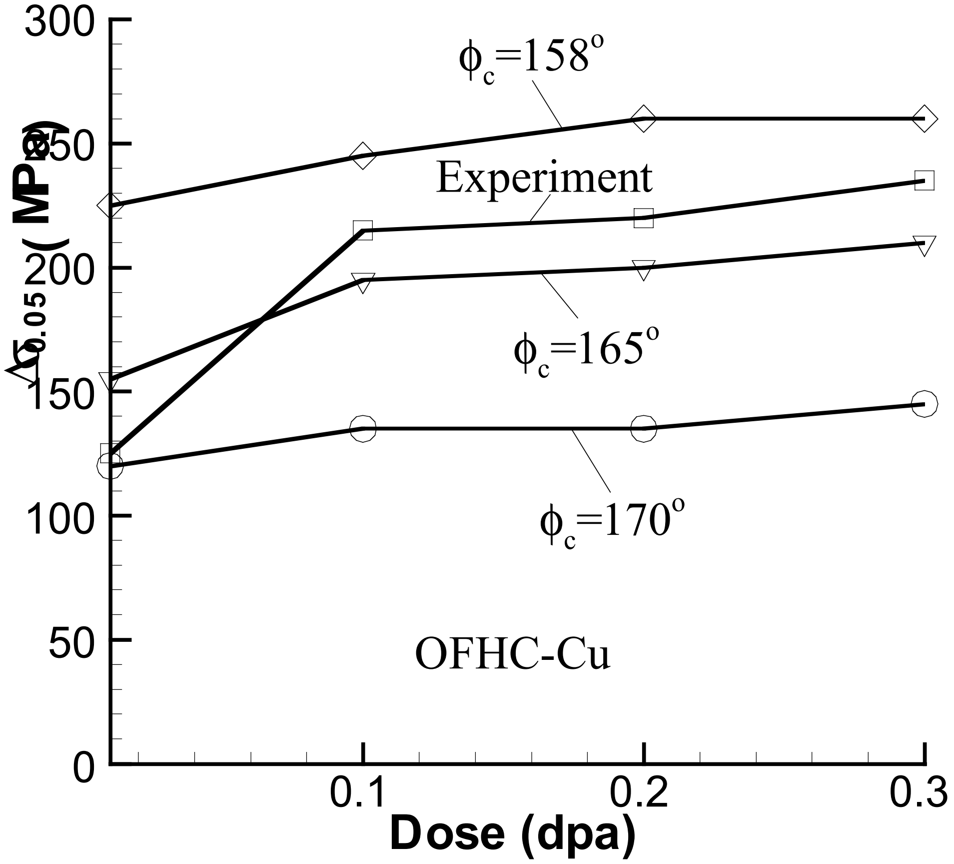
– Results are applicable to other Group V refractory alloys (Nb, Ta)

Successful Applications in Fusion Material Science (2)

Quantitative predictions of hardening with only one adjustable parameter

Measurements at PNNL& RISO

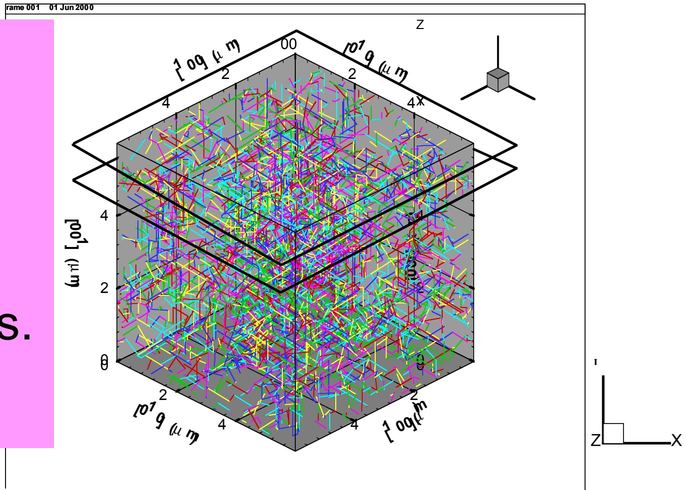
Simulations at UCLA.



Dislocation Dynamics (DD) is a new computer simulation method developed at UCLA for modeling fundamental microscopic mechanical properties

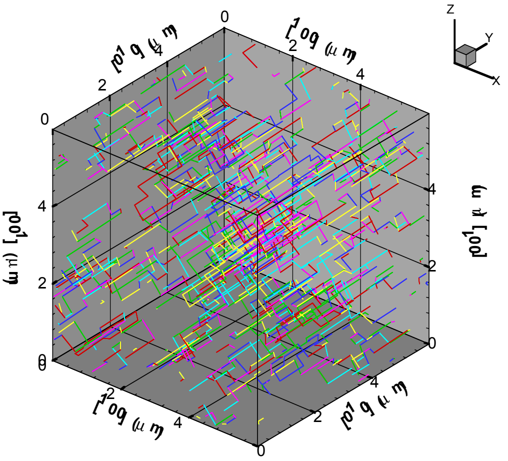
Broad Objectives of DD:

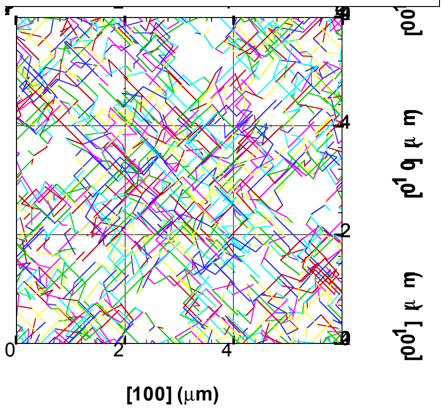
1. Understand fundamental deformation mechanisms
2. Provide a physical basis for plasticity
3. Determine stress-strain behavior without assumptions.
4. Design new ultra-strong and super-ductile materials.



(1) N. M. Ghoniem, L. Sun, ***Phys. Rev. B***, **60(1)**: 128-140 (1999).

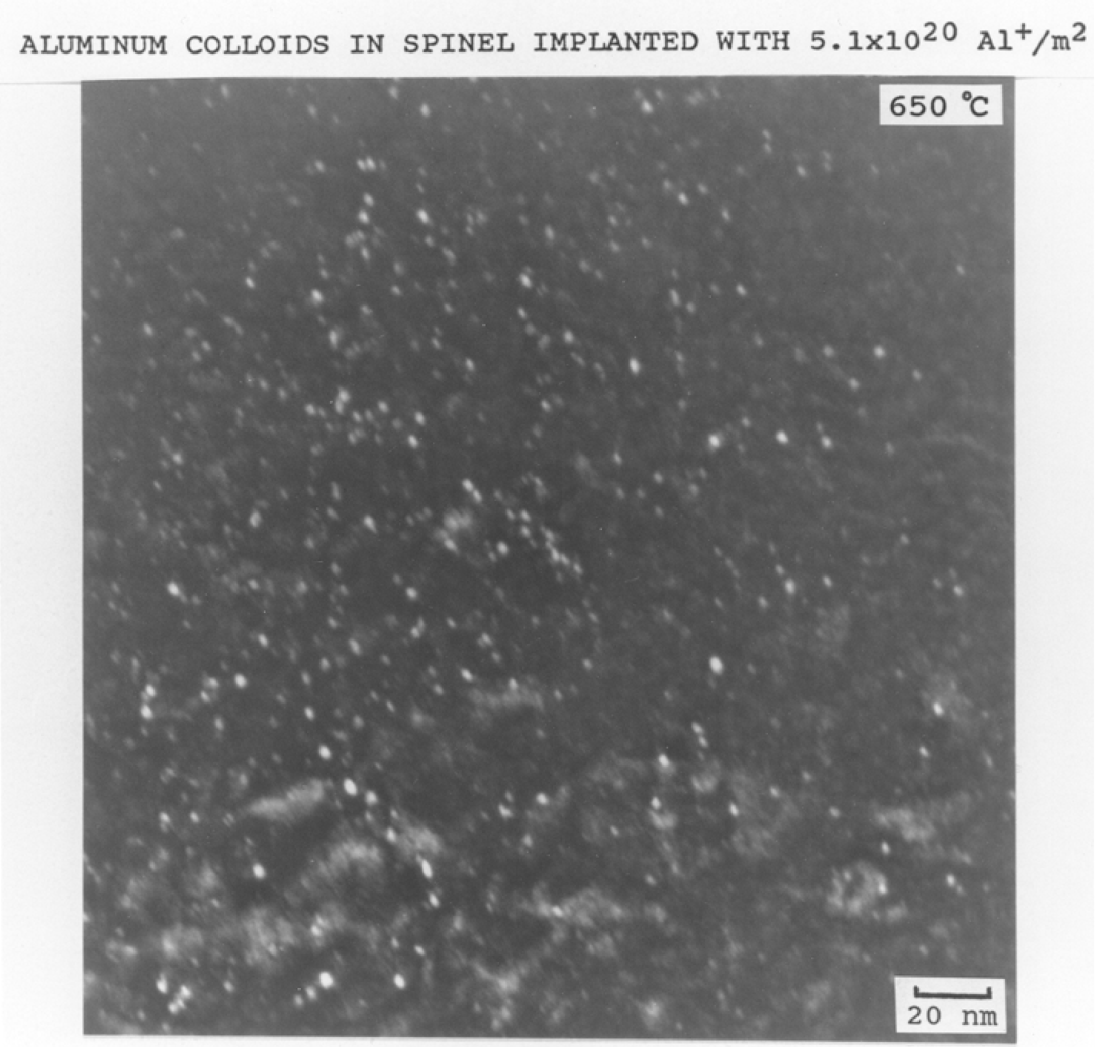
(2) N.M. Ghoniem, S.- H. Tong, and L. Z. Sun ***Phys. Rev. B***, **61(1):** 913-927 (2000).



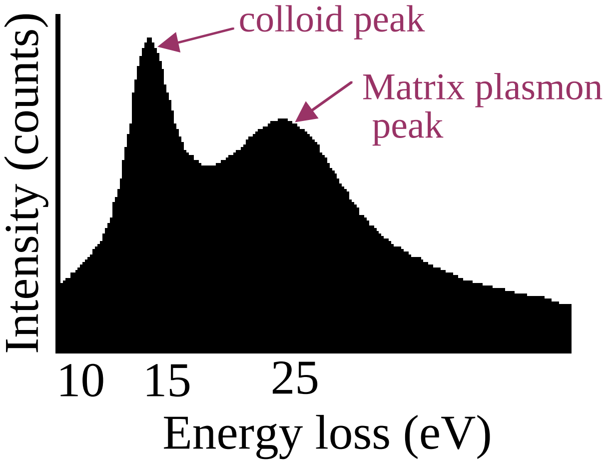


TEM-Slice

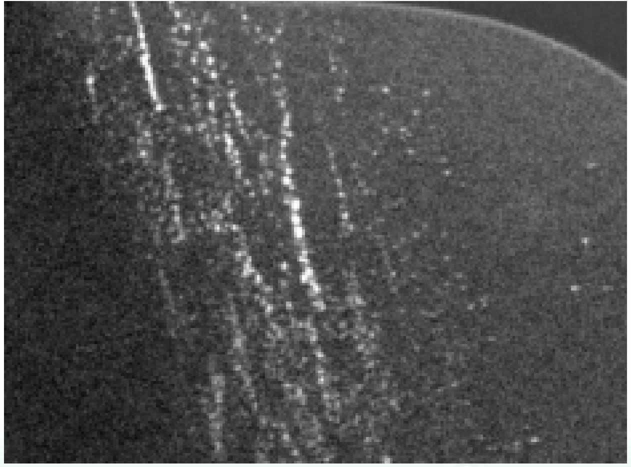
Colloidal metal nanoclusters can be created in $MgAl_2O_4$



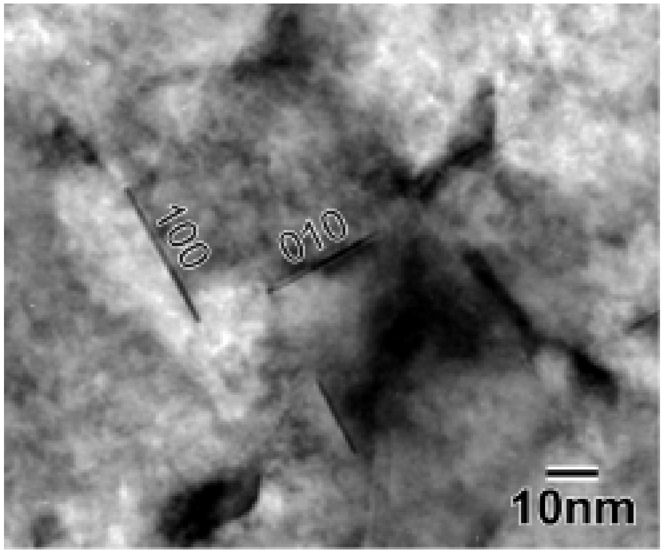
PEELS spectrum for implanted $MgAl_2O_4$

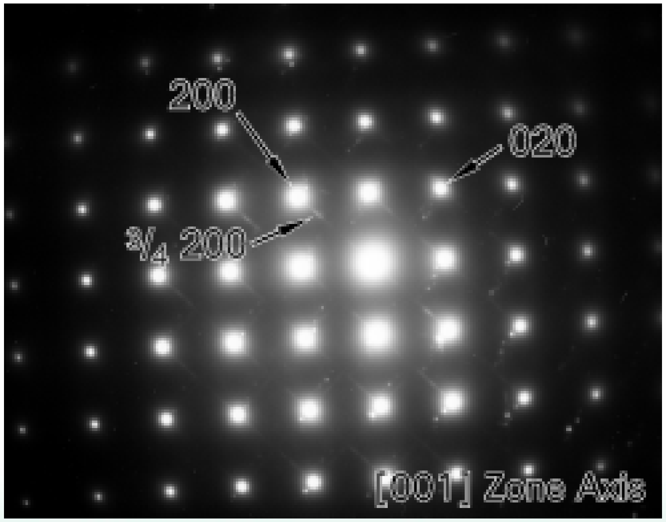


Energy-filtered TEM used to quantify colloid distribution

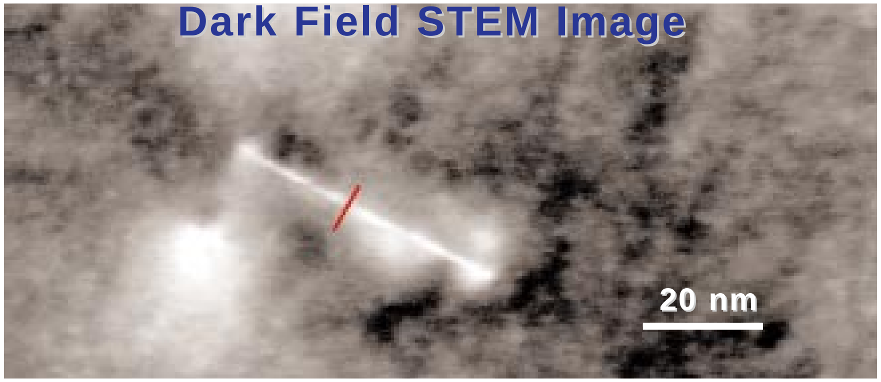


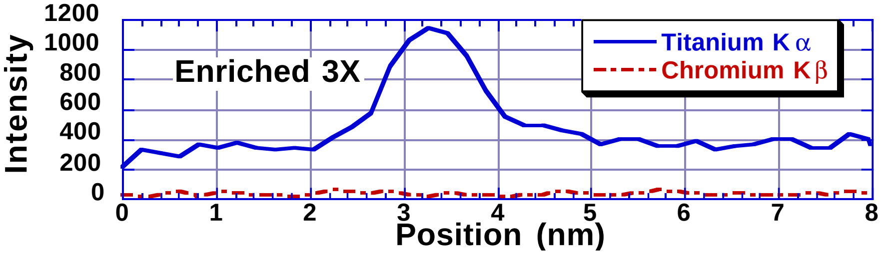
Advanced Analytical Electron Microscopy Techniques are being used to Examine Precipitates in V alloys

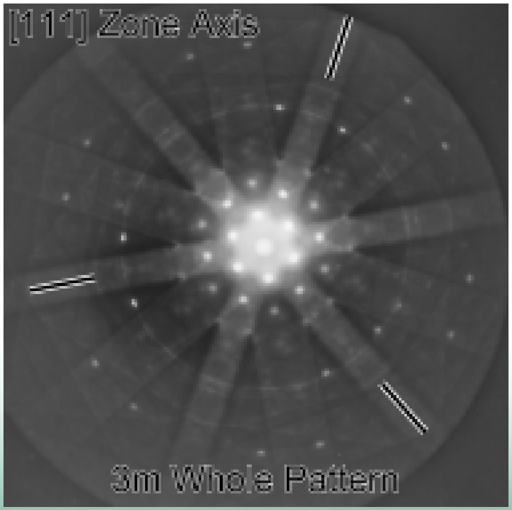




Solute Segregation Was Detected in V-4Cr-4Ti Following Neutron Irradiation to 0.5 dpa at Elevated Temperatures







Analytical microscopy reveals Ti-rich precipitates with Fm3m space group
(Baker-Nutting precipitate-matrix orientation)

Oak Ridge National Laboratory
U. S. Department of Energy

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