Potential Materials Science Benefits from a Burning Plasma Science Experiment

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Introduction

- The main materials science advances from a BPSX would occur during the R&D phase prior to construction
  - e.g., CIT/BPX, ITER
- Materials science opportunities during operation of a BPSX would likely occur in niche areas
  - Ceramic insulators (radiation-induced conductivity, tan δ degradation)
  - Optical materials (F center formation, absorption peaks, gamma ray vs. neutron effects)
  - Polymers (effect of irradiation spectrum on cross-linking and property changes)
  - Diagnostic components
  - Divertor materials

Desirable characteristics of a BPSX for materials science studies

- Well-defined temperatures, stresses, radiation fields
- Materials testing ports (cf. DIMES) or removable components (not necessarily complete blanket sectors)
- For more timely data acquisition, long reproducible pulse lengths and a high duty factor are desirable

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

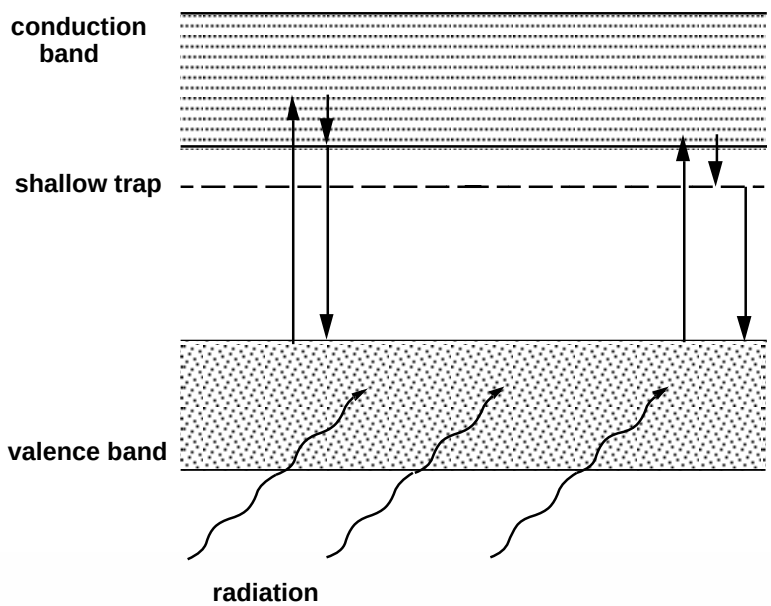
The R&D portfolio of the fusion materials science program has two general guiding features

- 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

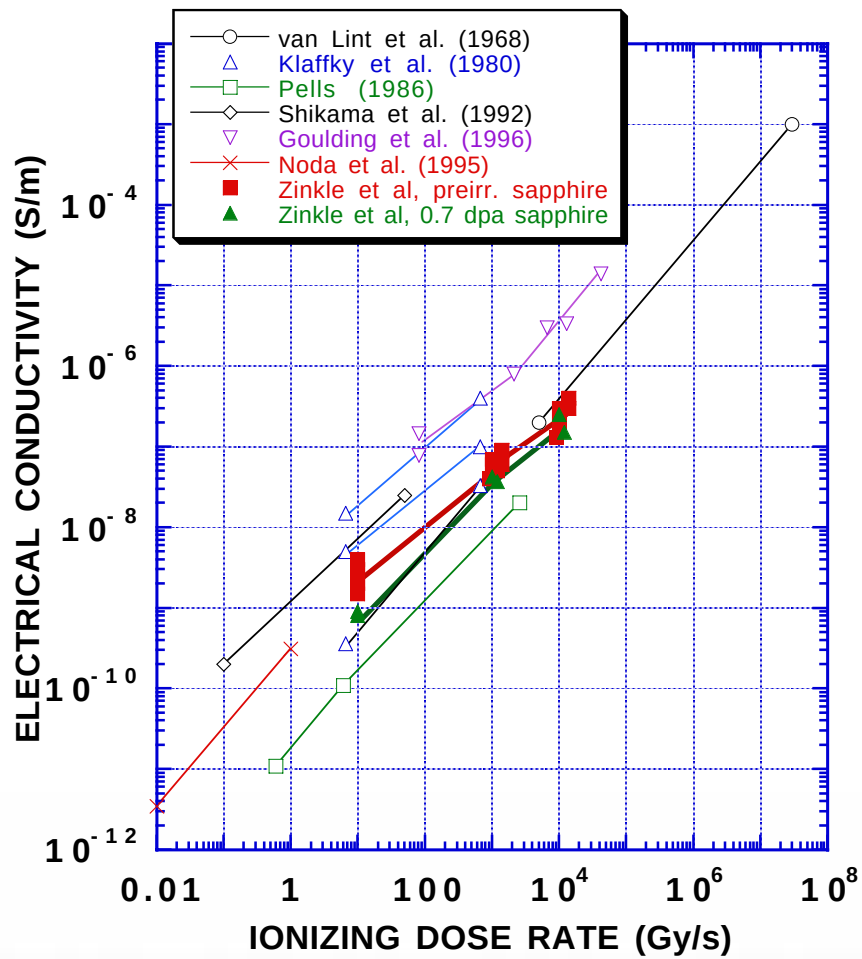
Topic	Fusion benefit	Science aspect
Displacement cascades	Quantification of displacement damage source term	• Is the concept of a liquid valid for time scales of only a few lattice vibrations • Transient (ps) electron-phonon coupling physics
Defect migration	Radiation damage accumulation kinetics	• 1D 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

Radiation-induced conductivity in Insulators

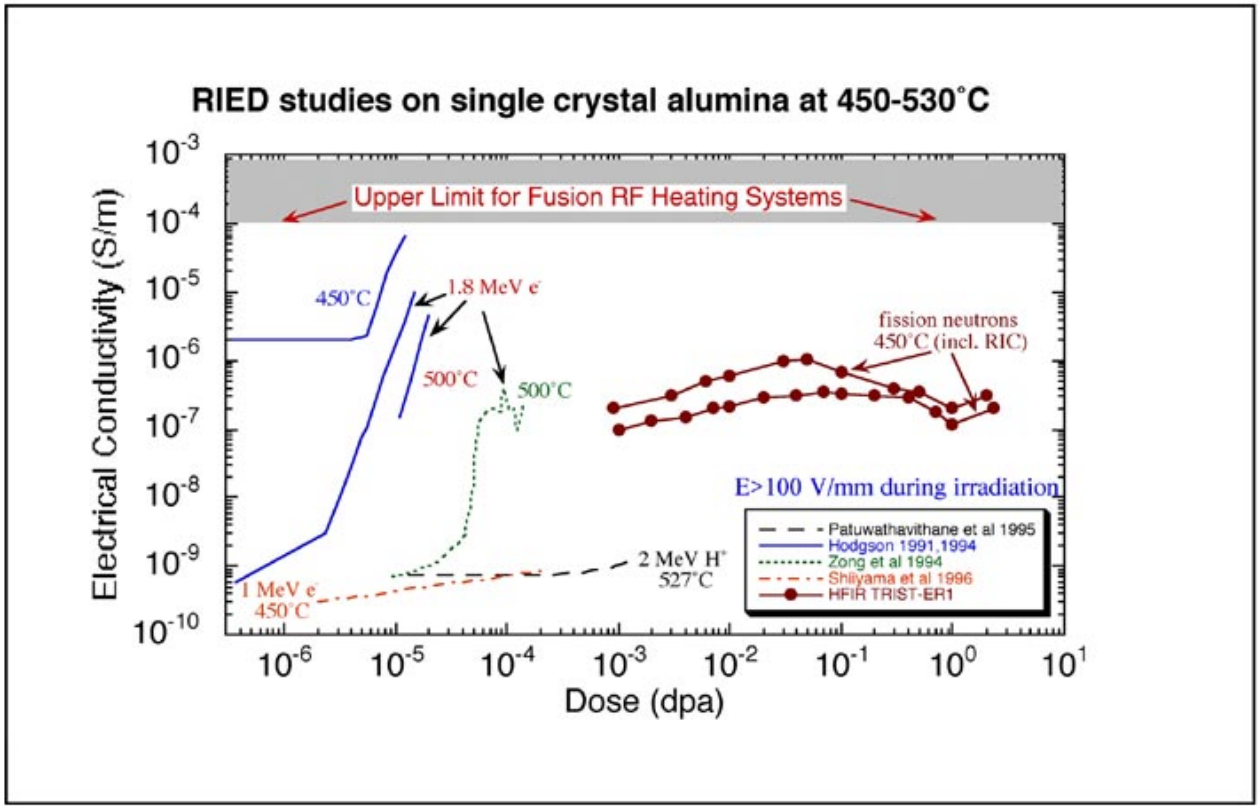
Radiation Induced Conductivity in Insulators



Summary of RIC data for alumina



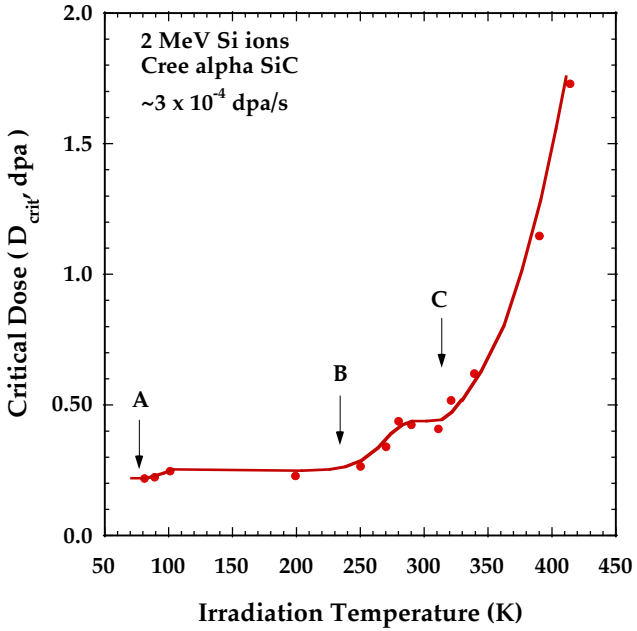
Permanent Radiation-Induced Electrical Degradation does not appear to be of concern for next-step machines

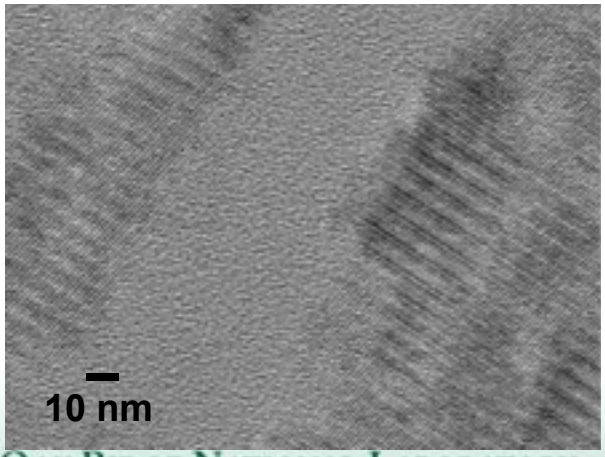


- Studies performed in the Early 1990's suggested that catastrophic RIED would occur in ceramic insulators irradiated with an applied electric field >100 V/mm
- Earlier reports of RIED are attributed to experimental artifacts (surface conduction and electron beam charging effects)

SiC Amorphization

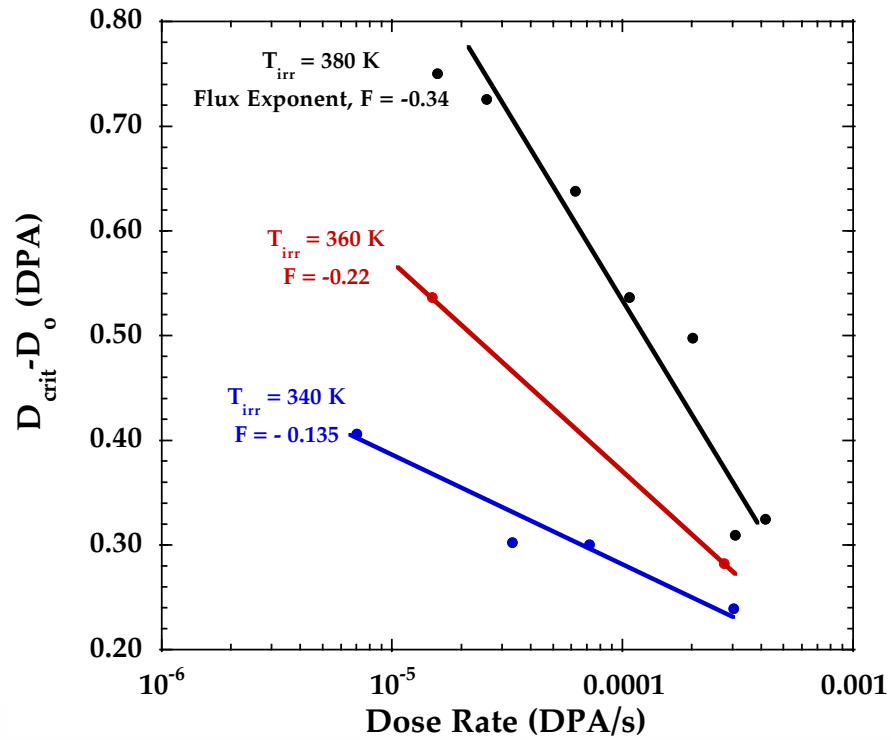
3 recovery substages are observed below 320 K





Analysis of flux dependence shows recovery substages are not associated with long range point defect migration (F<0.5 up to 380 K)

$$D_{crit}-D_o\ (DPA) = (A\Phi^F)e^{(-Em/2kT)}$$



Implies that both vacancies and interstitials are immobile in SiC up to 100˚C (interstitials are mobile in many other ceramics at room temperature)

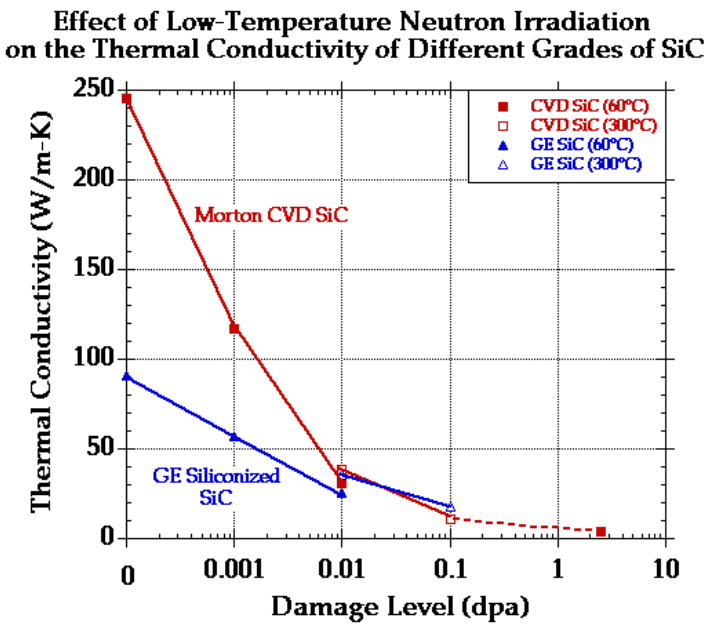
Physics of phonon transport & scattering are being investigated in neutron-irradiated ceramics

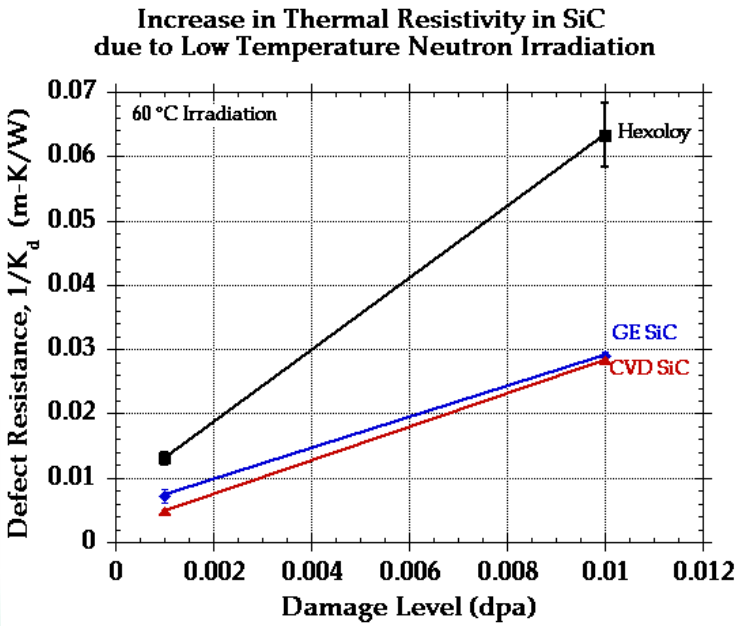
$$\left[K\,(T)\right]^{-1} = \left[\frac{1}{K_u(T)} + \frac{1}{K_{gb}(T)} + \frac{1}{K_{d0}} + \frac{1}{K_{rd}}\right]$$

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



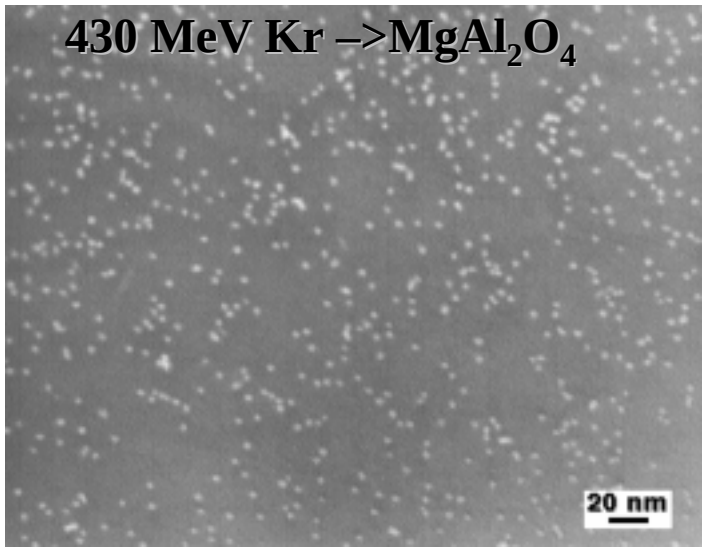


Ionizing Radiation can induce myriad effects in ceramics

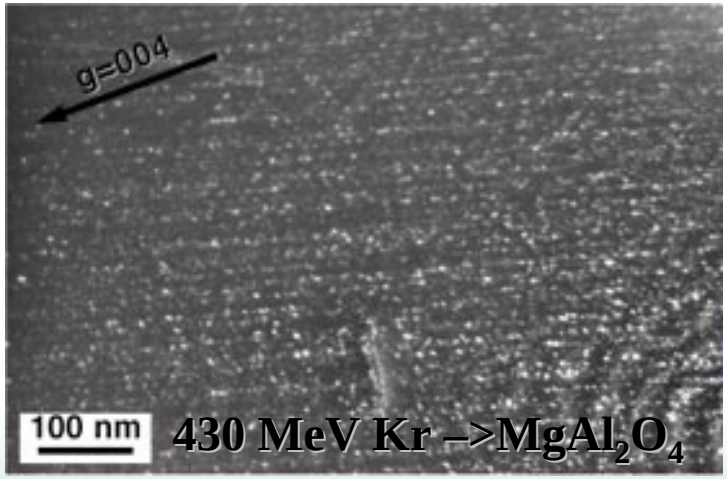
- **Defect production**
  - **Radiolysis (SiO_2, alkali halides)**
  - **Ion track damage (swift heavy ions)**

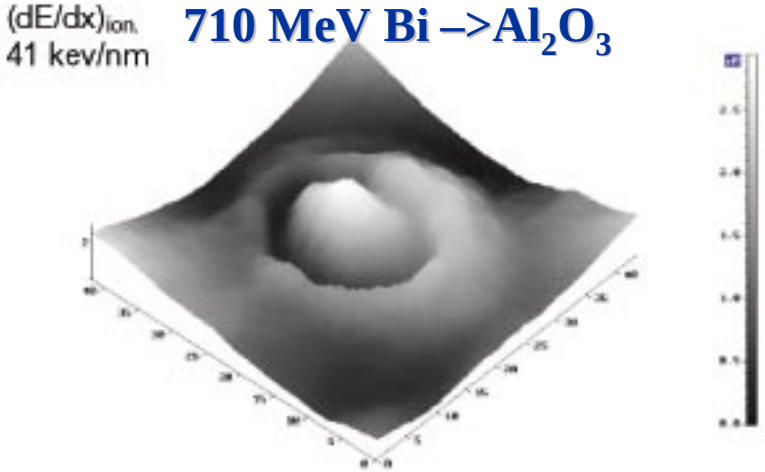
- **Defect annealing and coalescence (ionization-induced diffusion)**
  - **Athermal defect migration is possible in some materials**

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

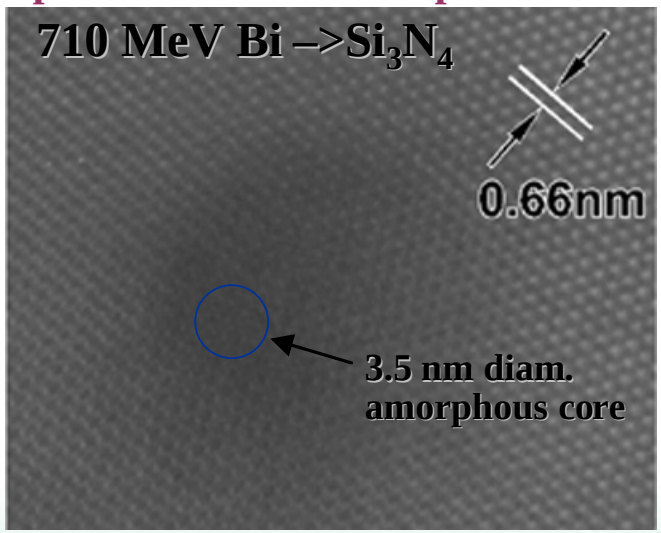


Ion tracks produce displacement damage via inelastic atomic events

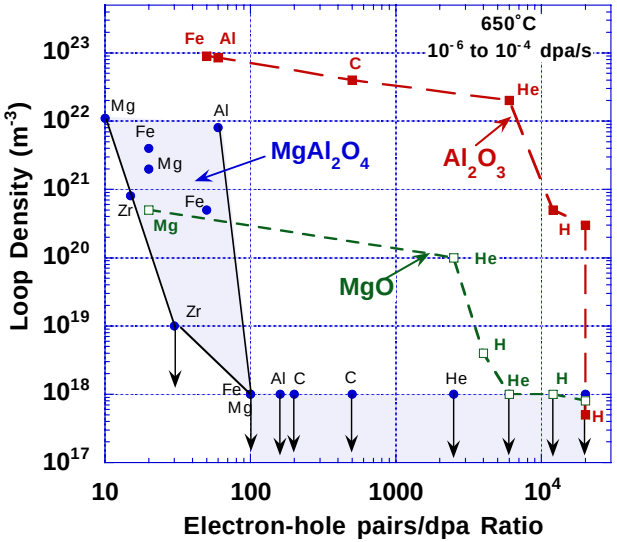


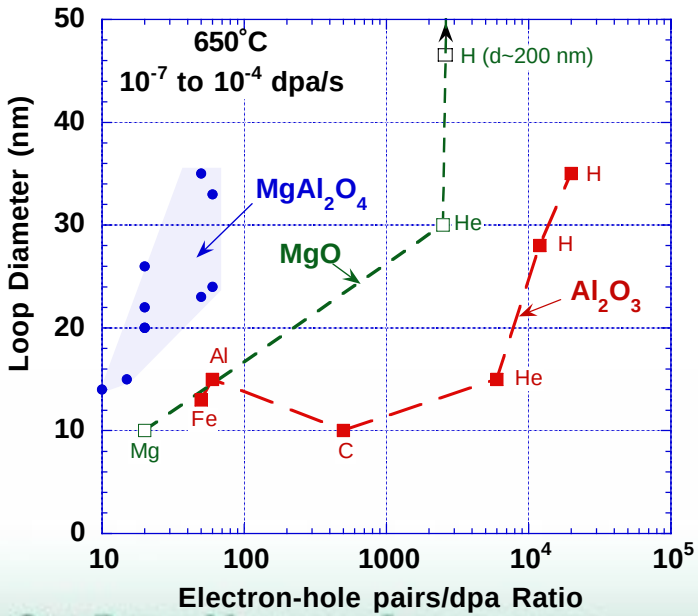


Swift heavy ions induce surface protrusions and amorphization

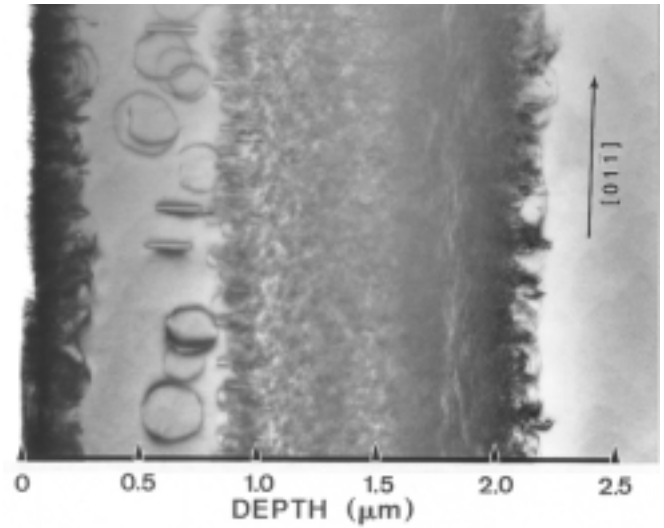


Investigation of ionization-induced diffusion in ceramics

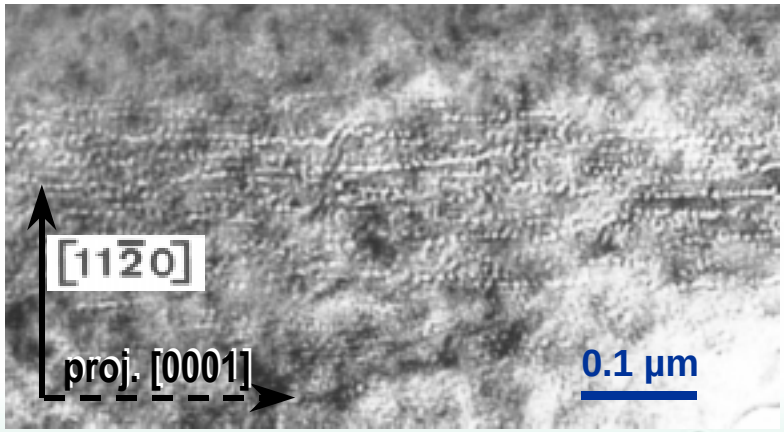




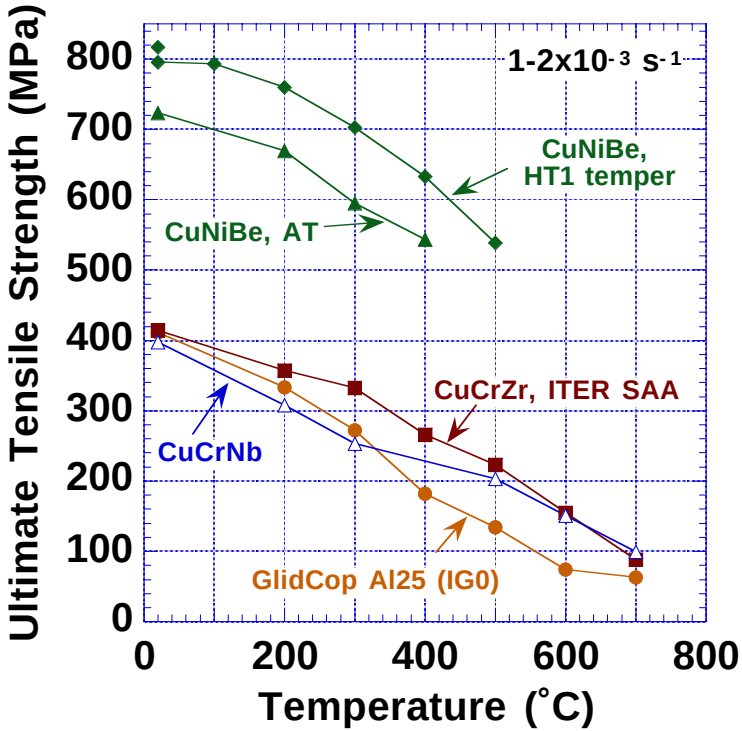
Large interstitial loops in $MgAl_2O_4$ ion-irradiated at 25˚C for regions with >100 eln.-hole pairs per dpa

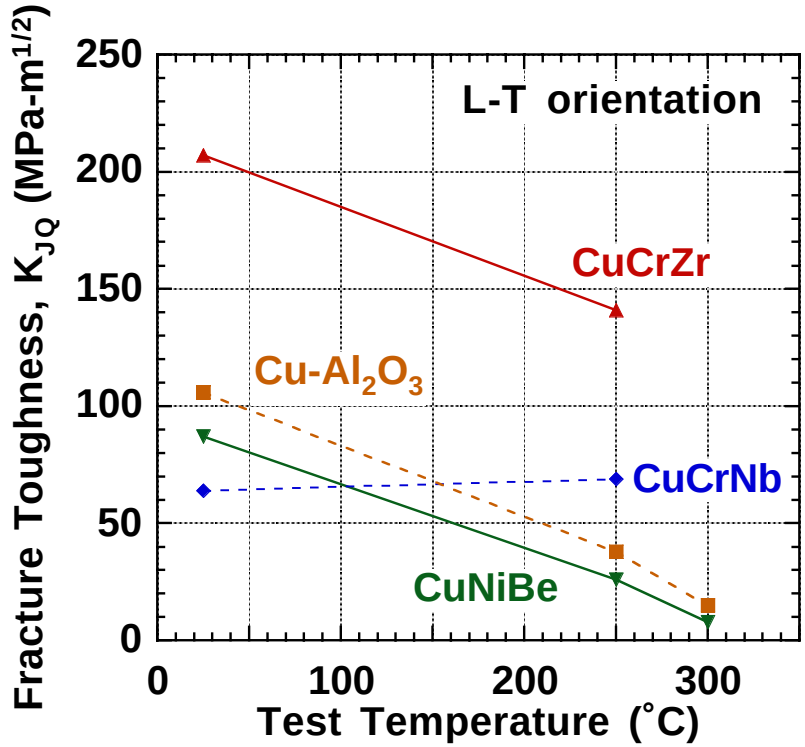


Aligned cavities in Al_2O_3 ion-irradiated at 25˚C (Al/O/He ion irradiation, >500 eln.-hole pairs per dpa)



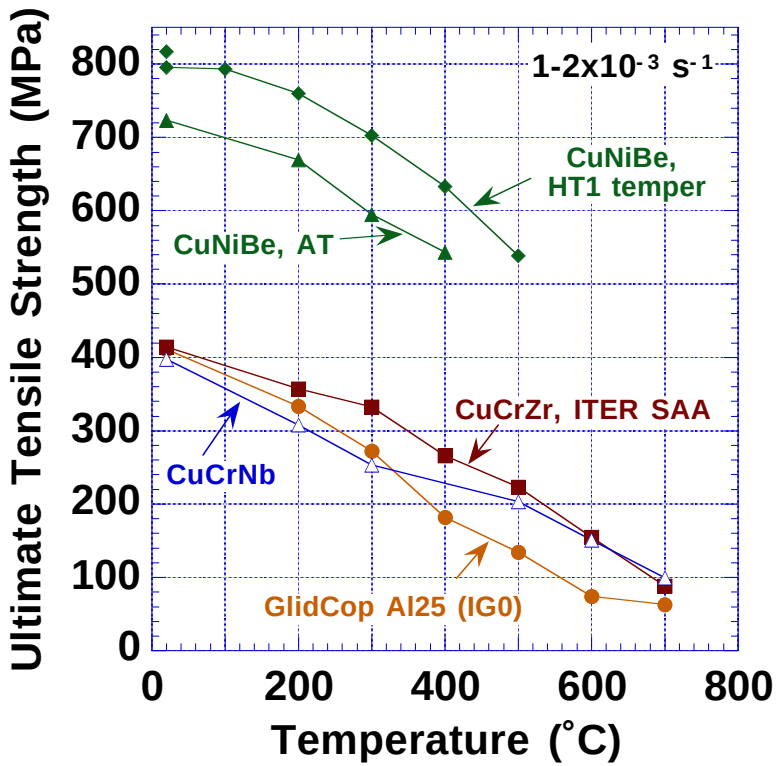
Mechanical behavior of a wide range of copper alloys has been investigated vs. strain rate and temperature (constitutive equations for deformation and fracture)



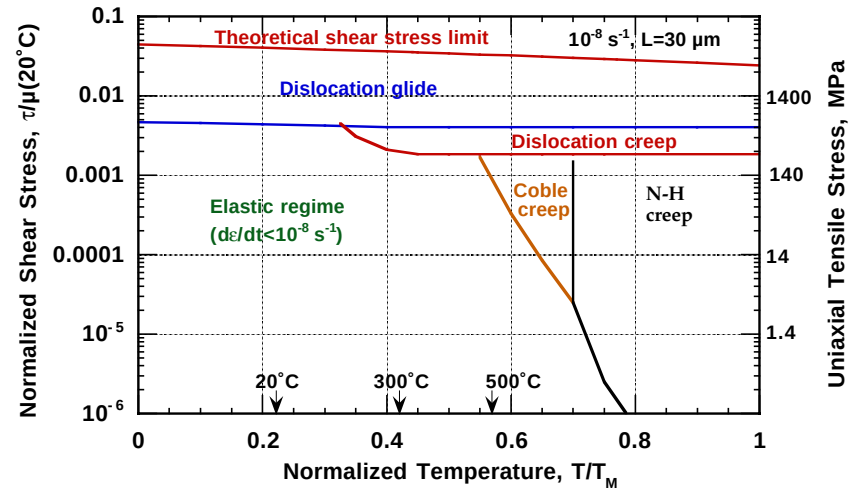


- CuNiBe has superior properties below 100˚C; CuCrZr and Cu-Al_2O_3 have best properties at intermediate temperatures
- high temperature limits in CuNiBe and Cu-Al_2O_3 alloys are associated with grain boundary phenomena

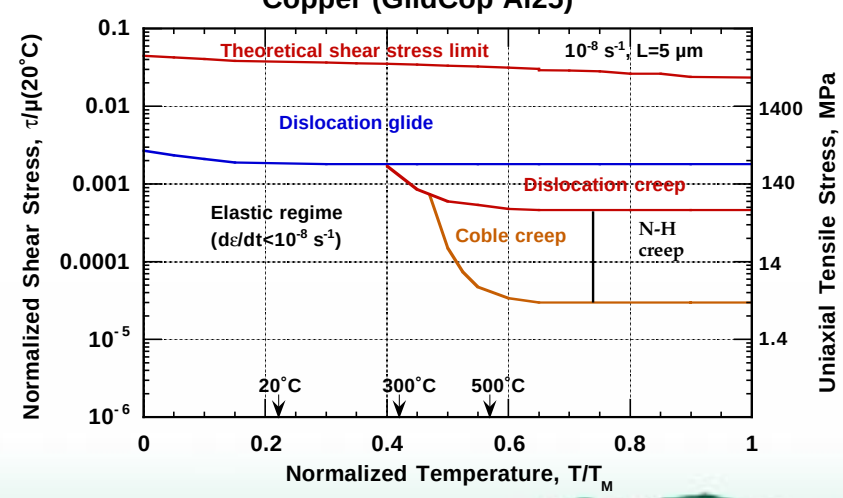
Mechanical behavior of copper alloys can be understood on the basis of current materials science models of deformation



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

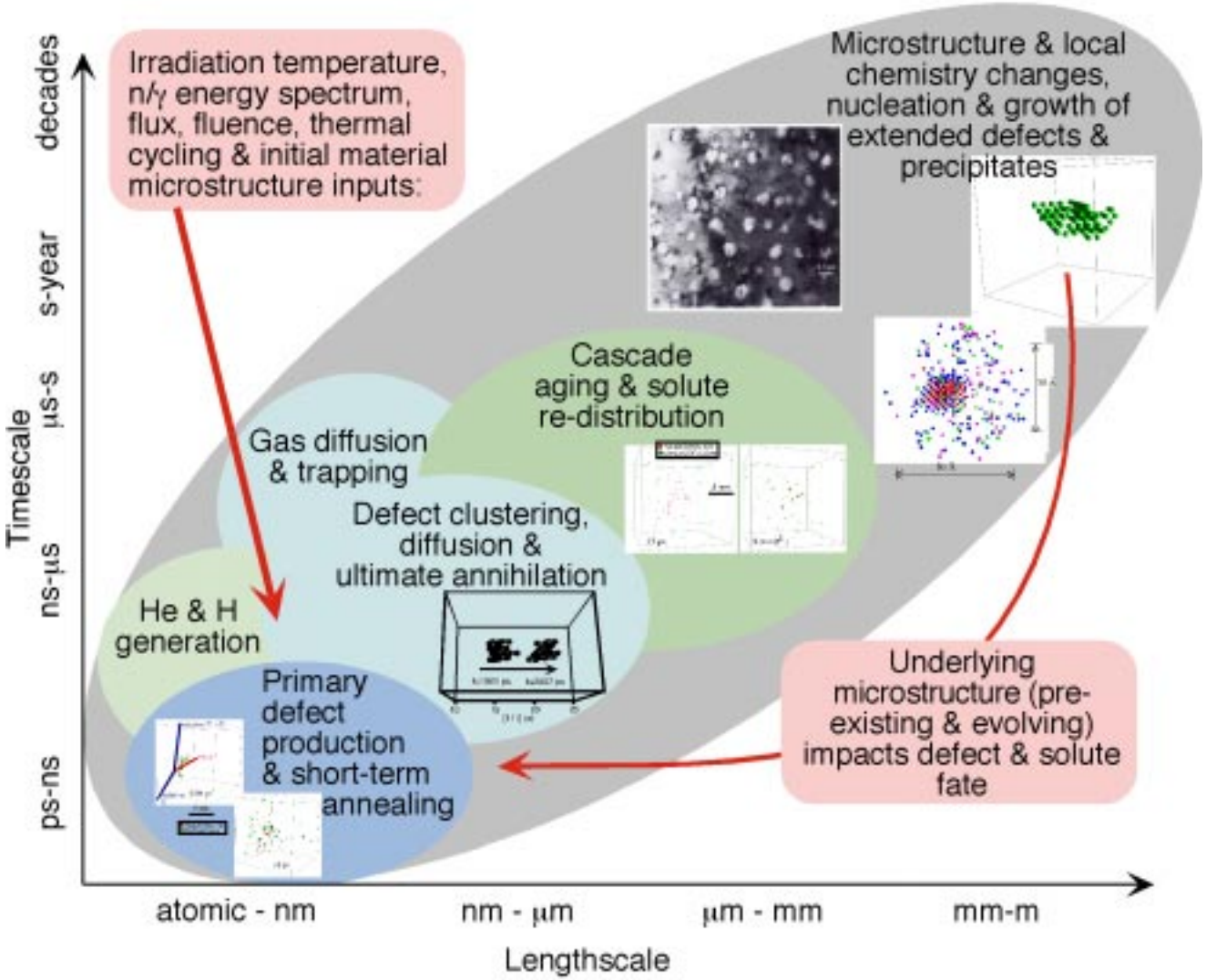


Deformation Map for Oxide Dispersion-strengthened Copper (GlidCop Al25)



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

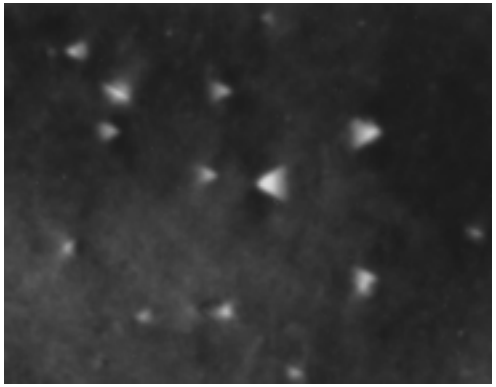
Radiation damage is inherently multiscale with interacting phenomena ranging from ps-decades and nm-m



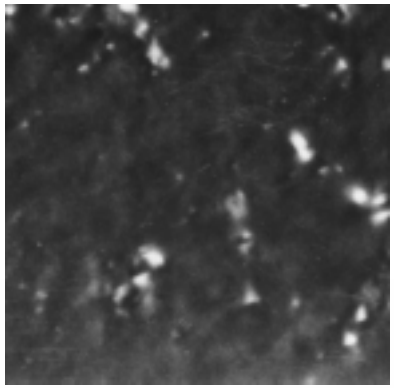
One of the Most Important Scientific Results From the US/Japan Collaborations on Fusion Materials has been the Demonstration of Equivalency of Displacement Damage Produced by Fission and Fusion Neutrons

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

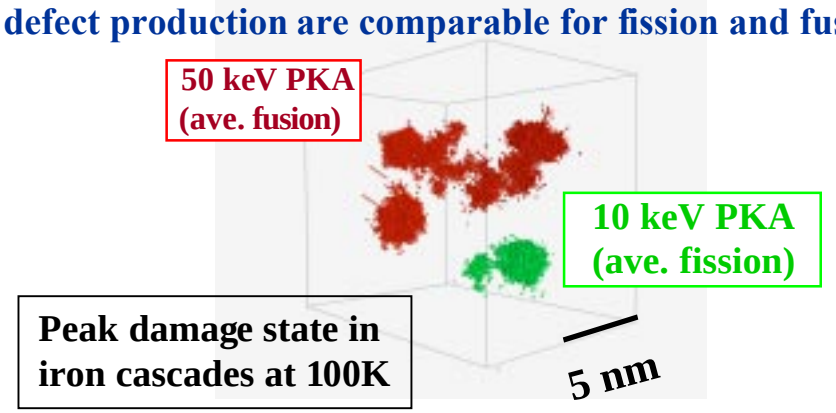
Fission (0.1 - 3 MeV)



Fusion (14 MeV)

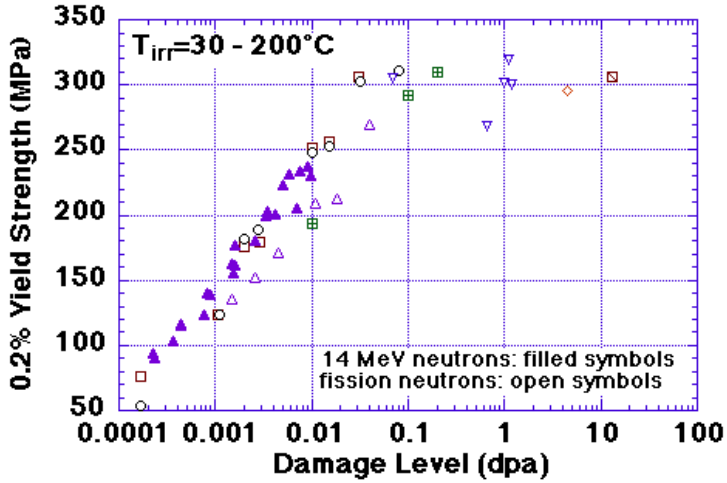


MD computer simulations show that subcascades and defect production are comparable for fission and fusion



Peak damage state in iron cascades at 100K

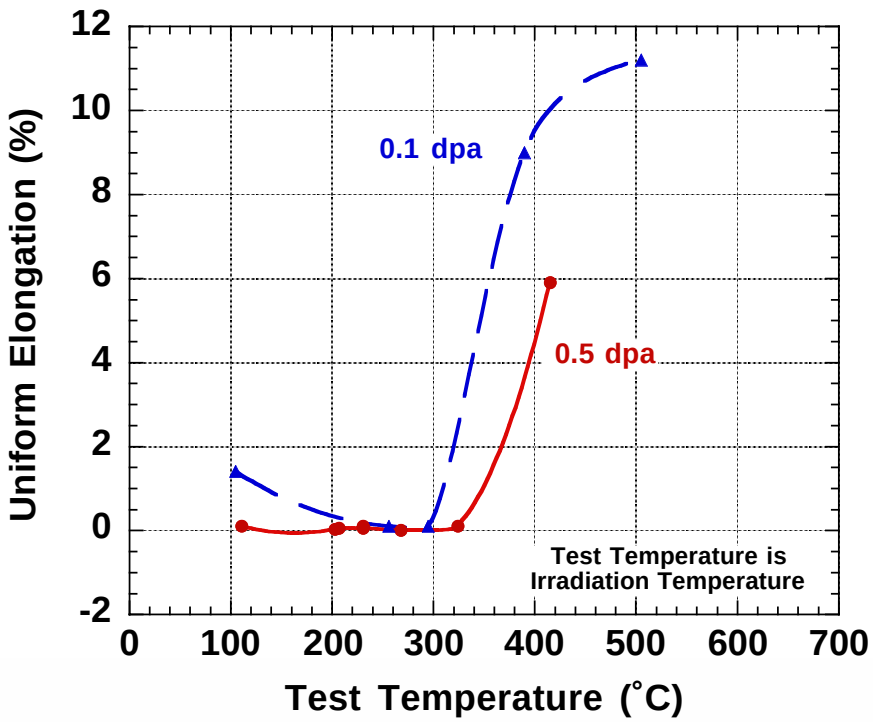
Similar hardening behavior confirms the equivalency



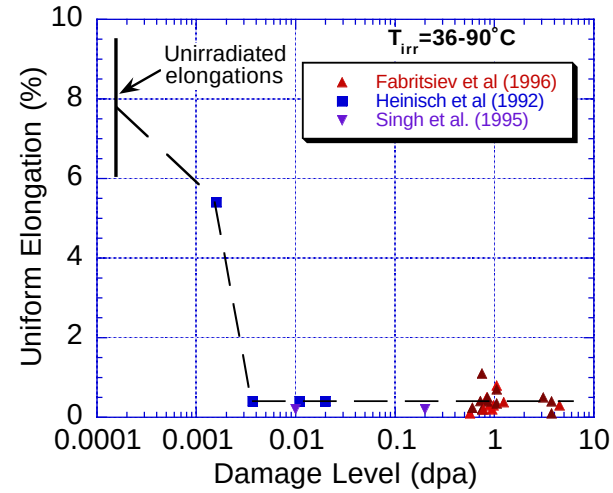
A critical unanswered question is the effect of higher transmutant H and He production in the fusion spectrum

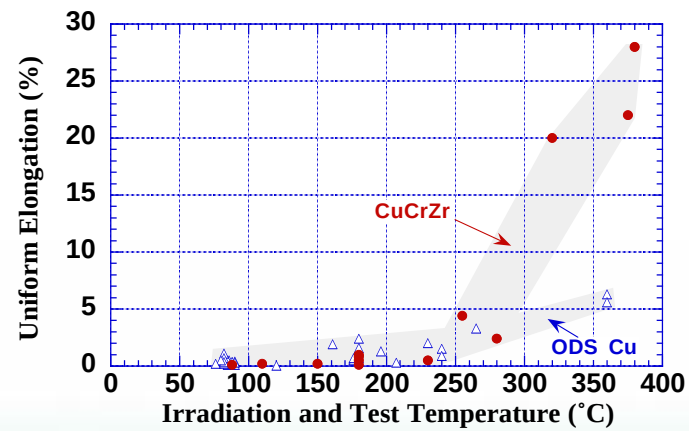
Low uniform elongations occur in many FCC and BCC metals after low-dose irradiation at low temperature

Uniform elongation of neutron-irradiated V-4Cr-4Ti

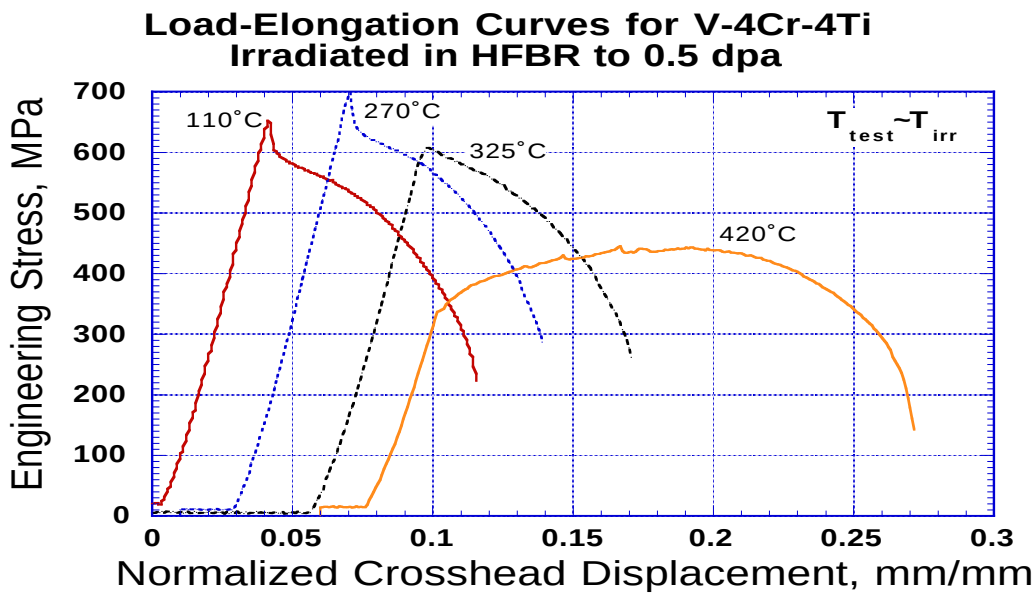


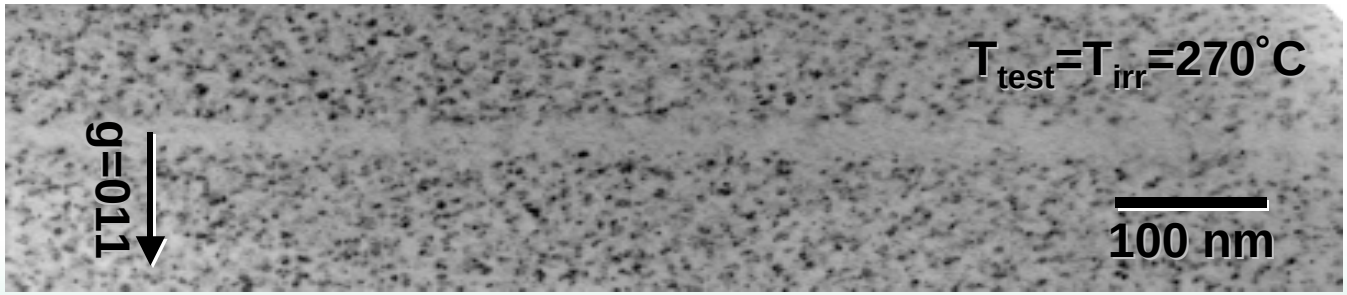
Uniform elongation of neutron-irradiated GlidCop Al25 and CuCrZr





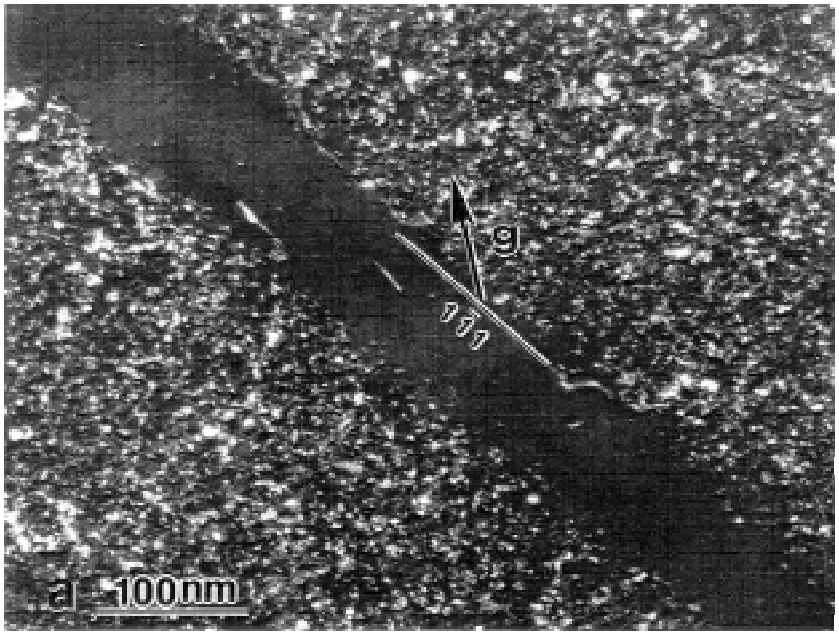
Irradiated Materials Suffer Plastic Instability due to Dislocation Channeling

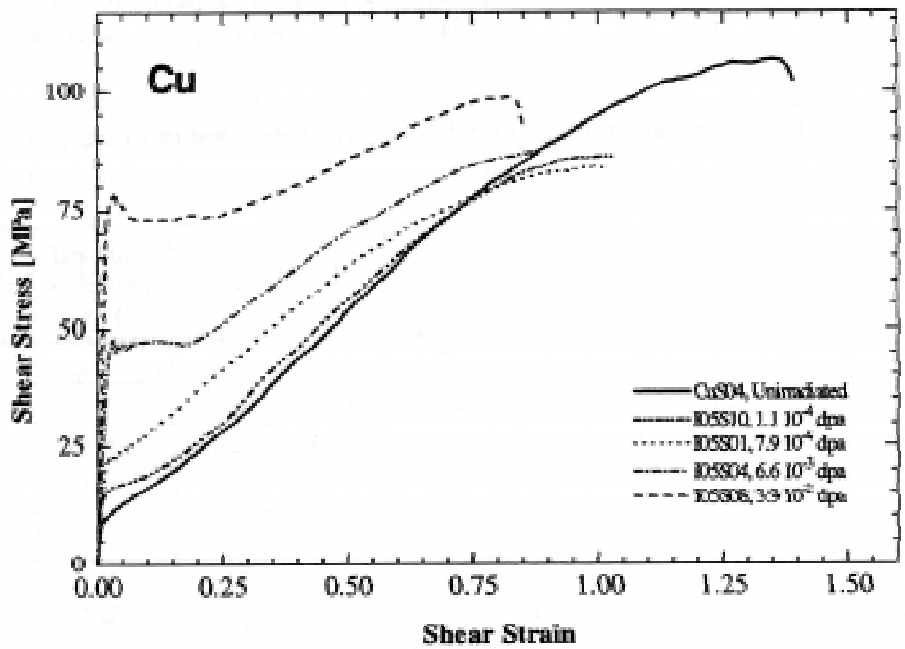




Irradiated materials undergo plastic instability and failure due to dislocation channel formation

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?**

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

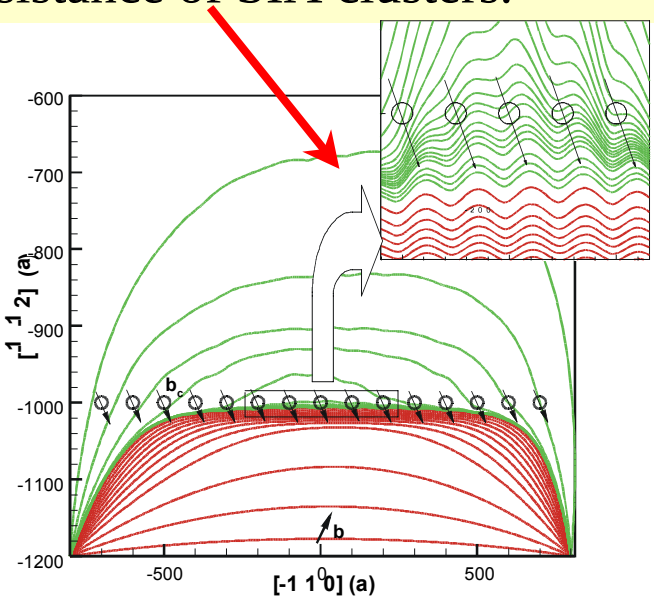
Broad Objectives of DD:

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.

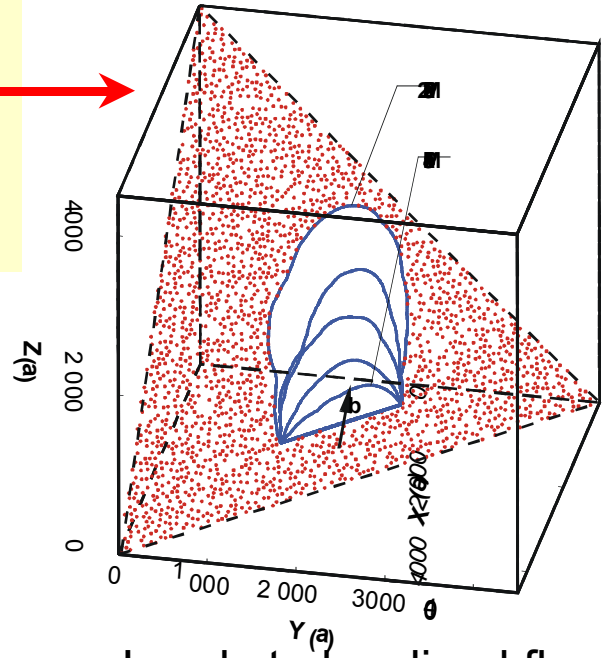
New Understanding (dislocation-defect interactions):

(a) Local heating destroys vacancy clusters;

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



Leads to yield drop

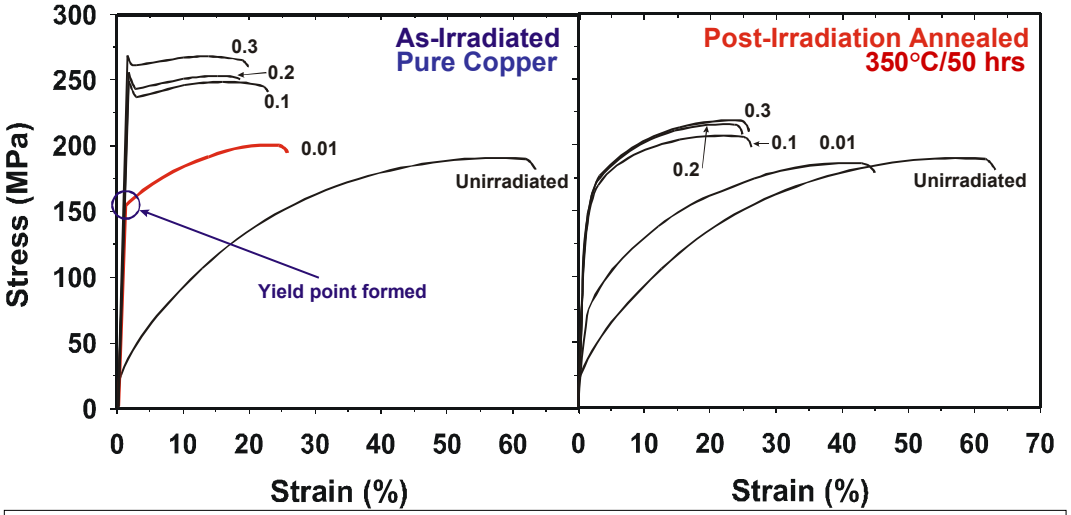


Leads to localized flow

(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

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

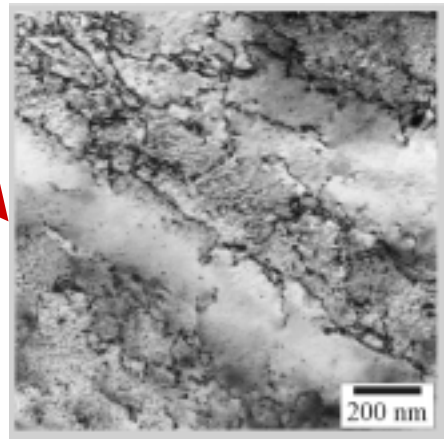


Post-Irradiation Annealed Condition

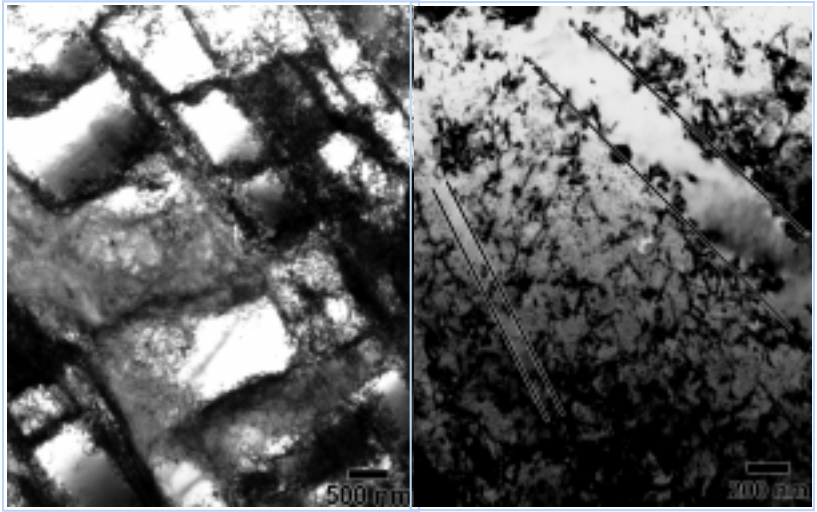
- Dislocation cell structure: material deforms homogeneously at 0.01 dpa
- Mixture of channeling and homogeneous deformation at 0.3 dpa

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



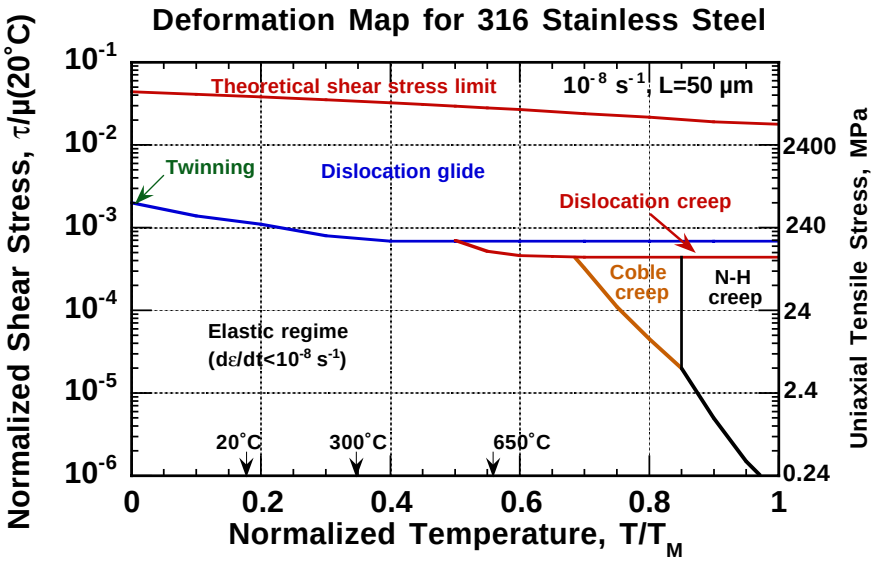
PI Annealed, 0.01 dpa **PI Annealed, 0.3 dpa**

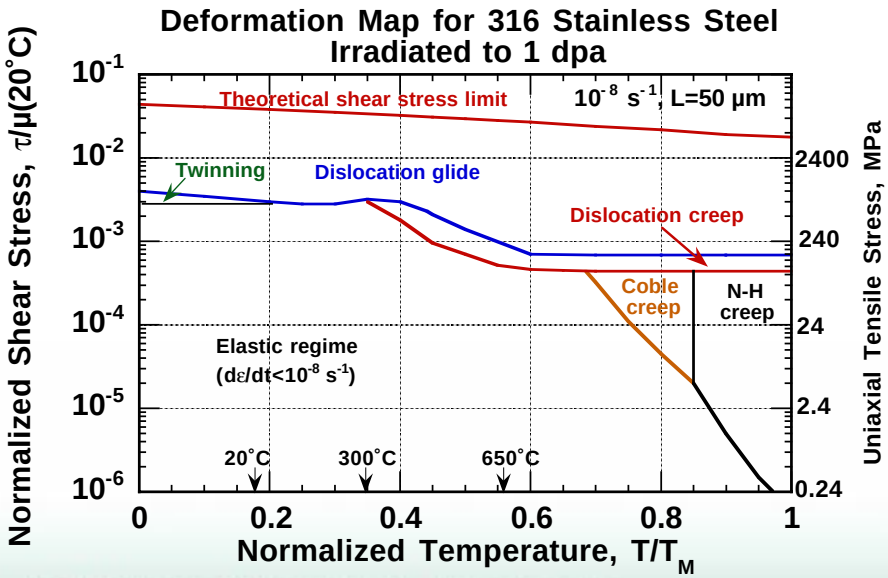


Battelle

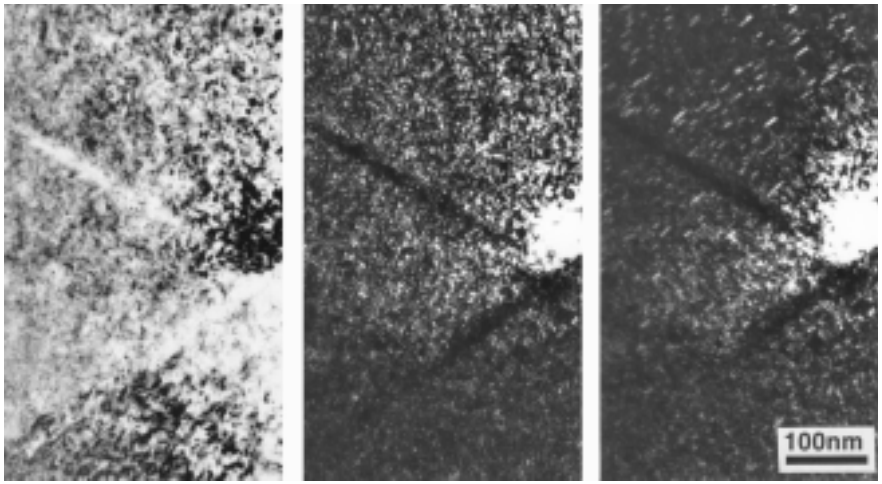
U.S. Department of Energy
Pacific Northwest National Laboratory

Deformation mechanisms in FCC metals

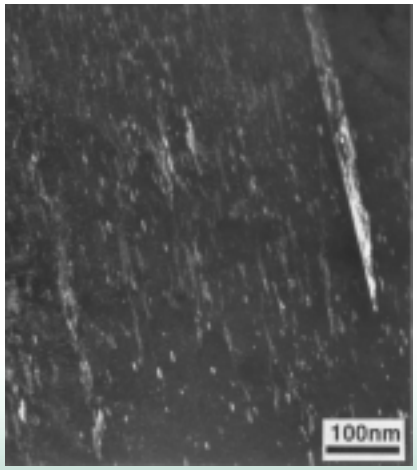




Irradiation is a useful tool to produce controlled microstructures for deformation mechanics studies



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

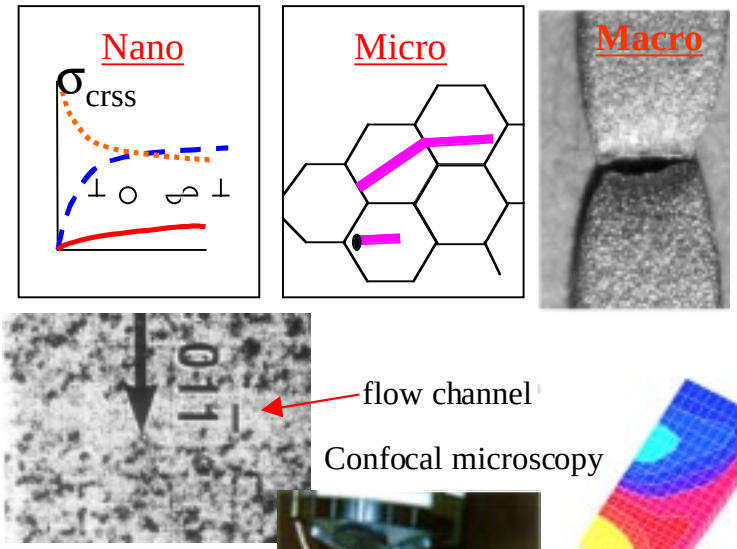


Twinning occurs at lower temperatures (<200˚C) and high strain rates

Deformation Flow Instability-Localization

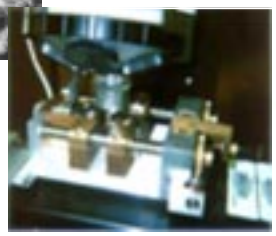
- **Understanding uniform strain loss-flow localization requires close integration of *multiscale models & experiments.* In many cases irradiation may enhance *functional* strength.**

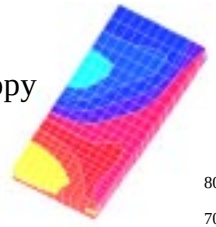
Multiscale Physics | **Engr s-e Instability Theory** | Hardness Pile-up/n | Beam Bend Tests

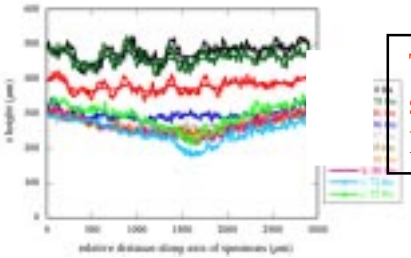


flow channel

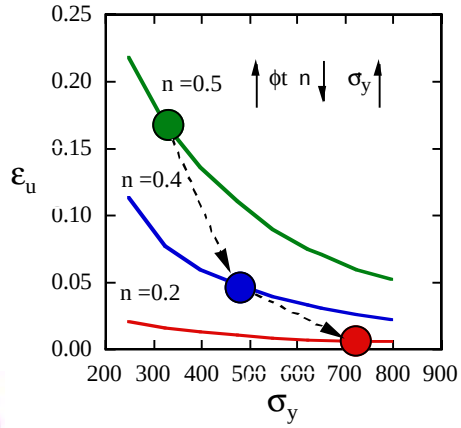
Confocal microscopy

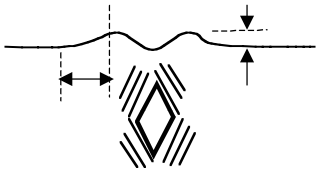


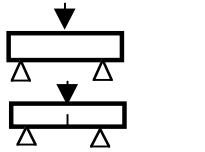


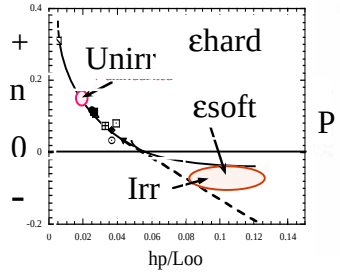


Tensile test 3-D shape imaging and FEA modeling









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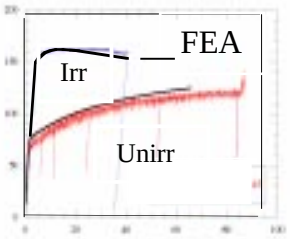
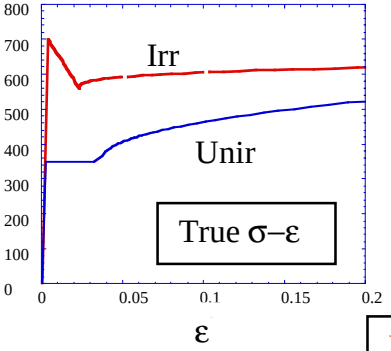


Δ



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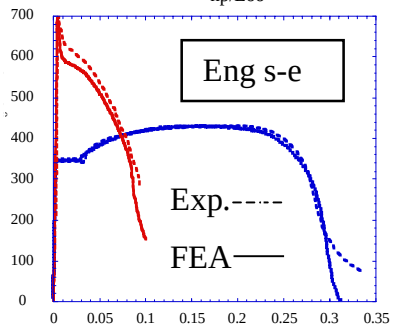
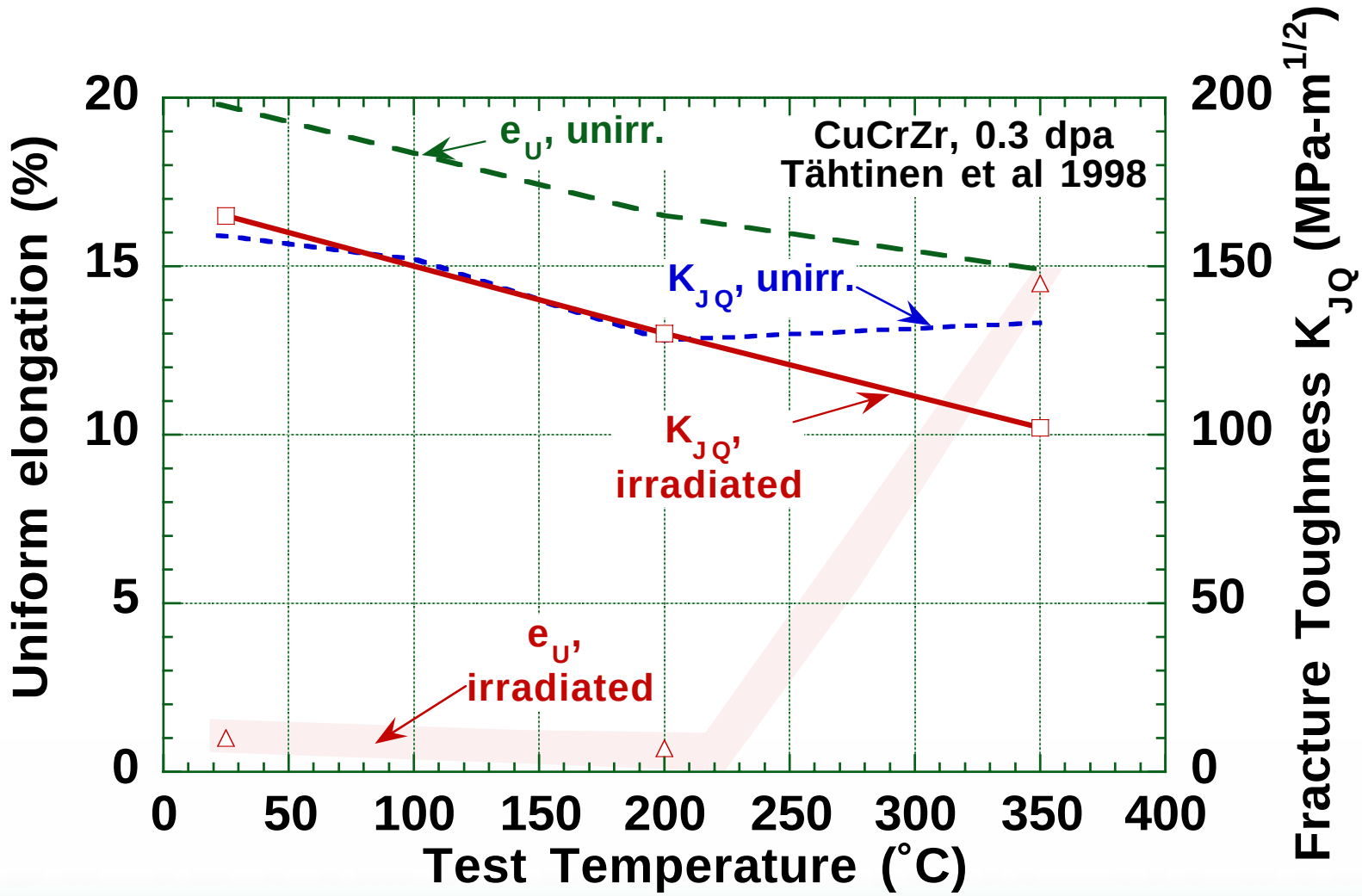


FEA

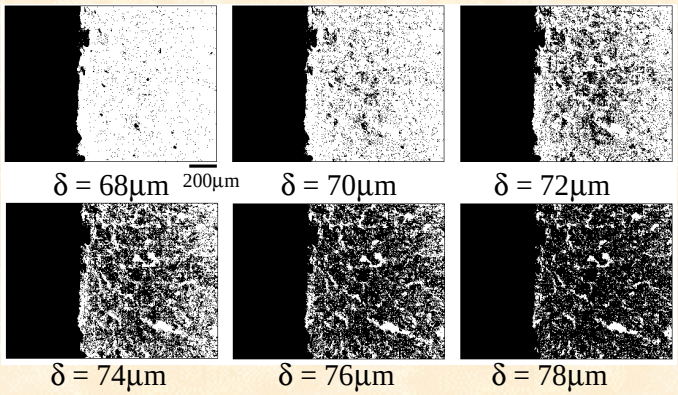
Radiation-induced Tensile "Embrittlement" does not Necessarily Produce Fracture Toughness Embrittlement



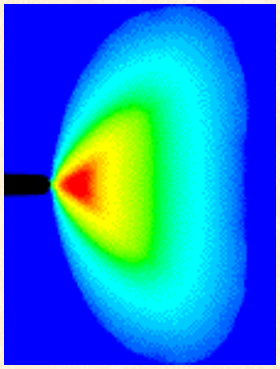
Multiscale Research on Fracture Mechanisms, Mechanics, Models and Structural Integrity Assessment Methods

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.

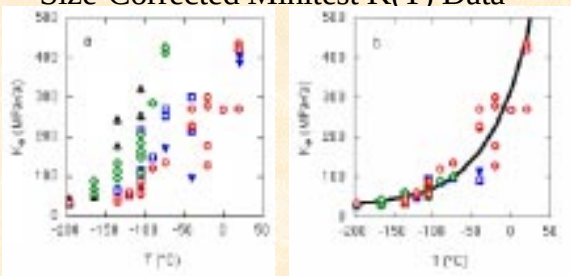
Tomographic Imaging of Cleavage



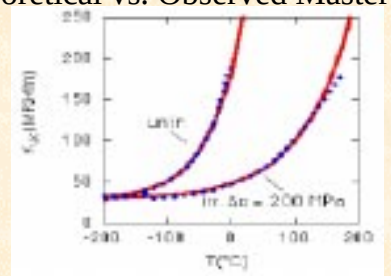
FEM Simulations of Crack Fields



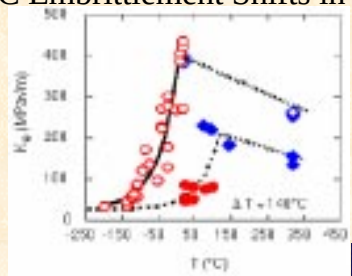
Size-Corrected Minitest K(T) Data



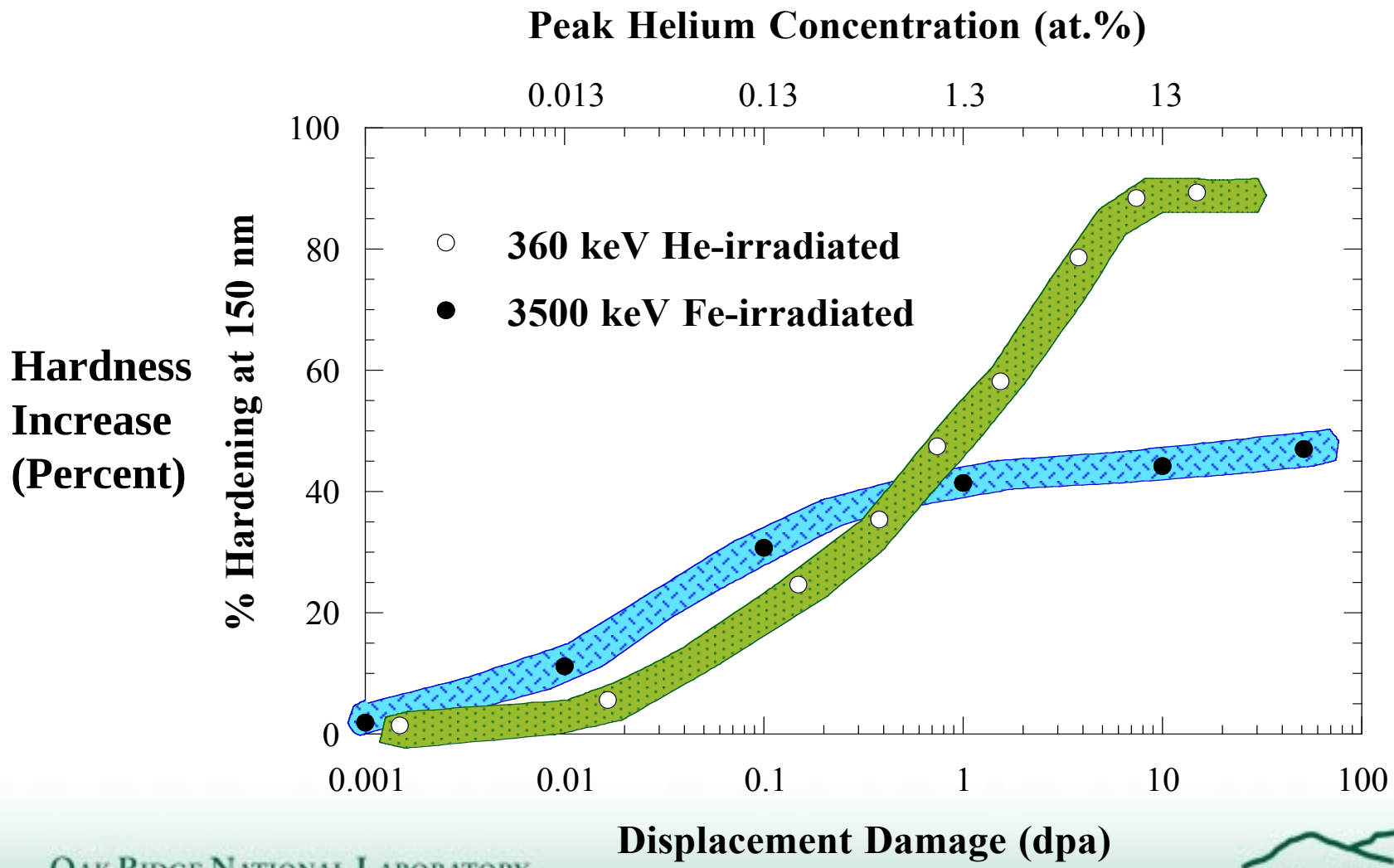
Theoretical vs. Observed Master Curve



MC Embrittlement Shifts in F82H

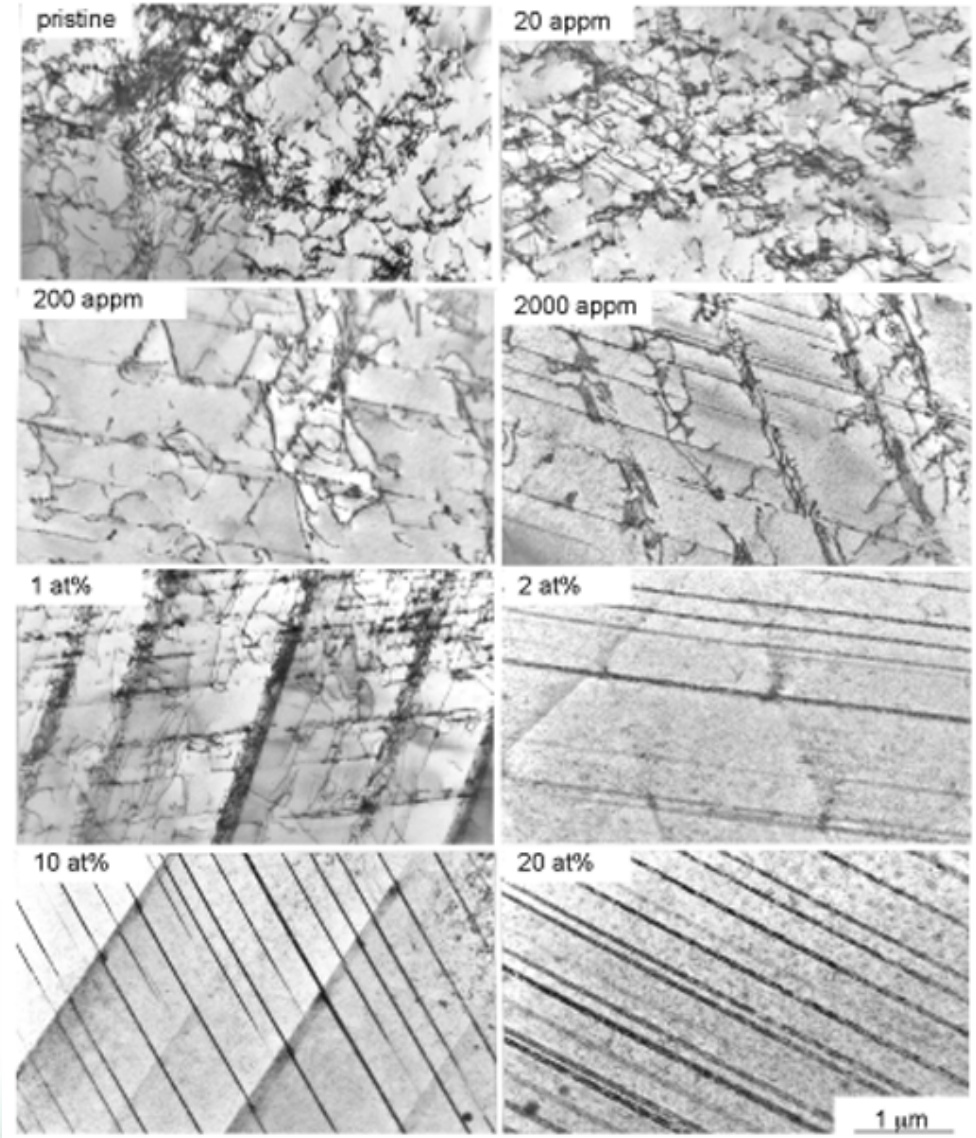


Hardening by Implanted He can be Substantially Higher than by DPA Alone



Deformation Microstructures: Helium Implantation

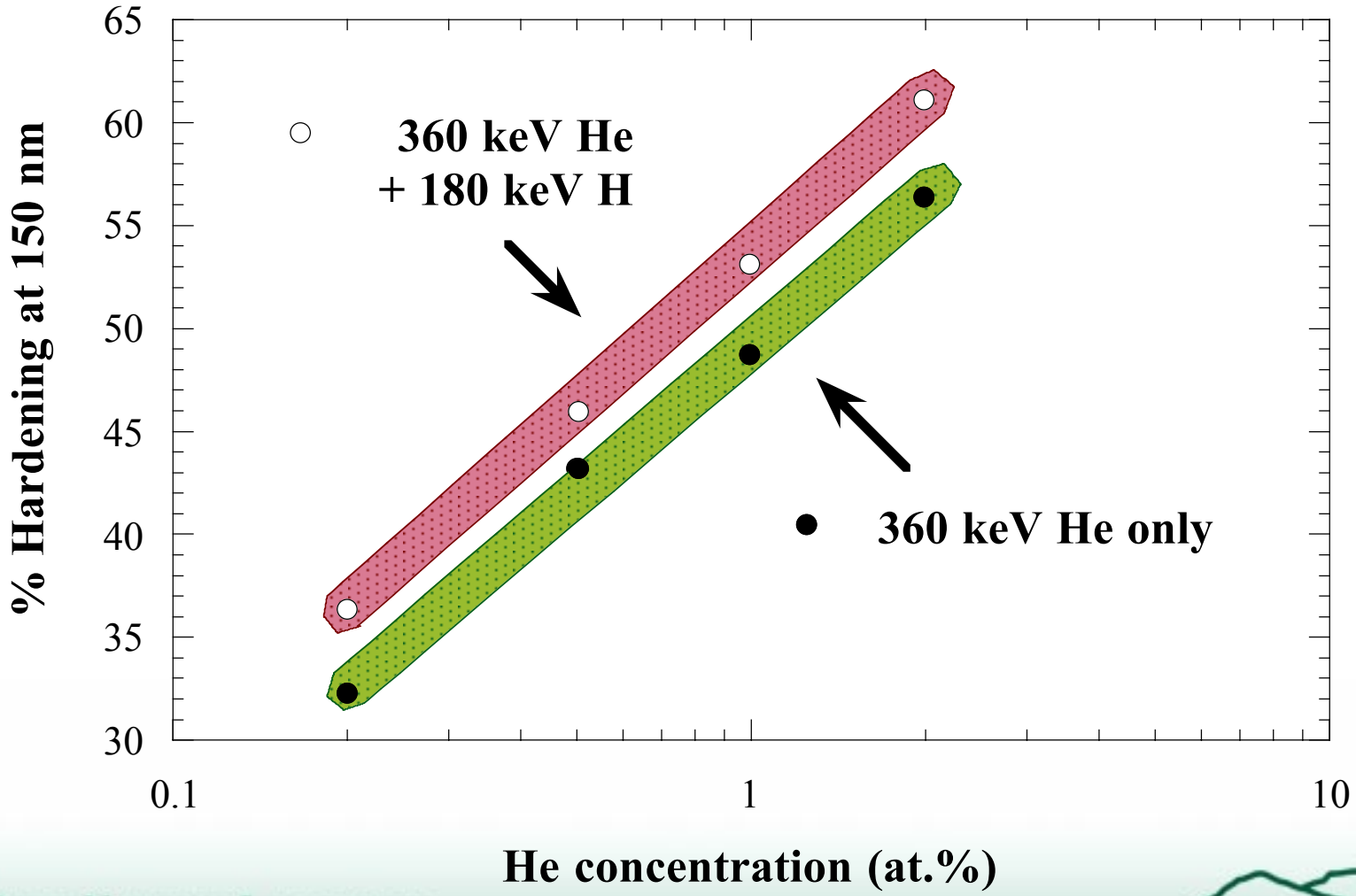
316 SS: He implanted at 200 C and strained to 10% at 20˚C



Channeling becomes significant for implanted He conditions of C_{He}>200 appm

(0.02 dpa)

H Causes Additional Hardening when Implanted with He

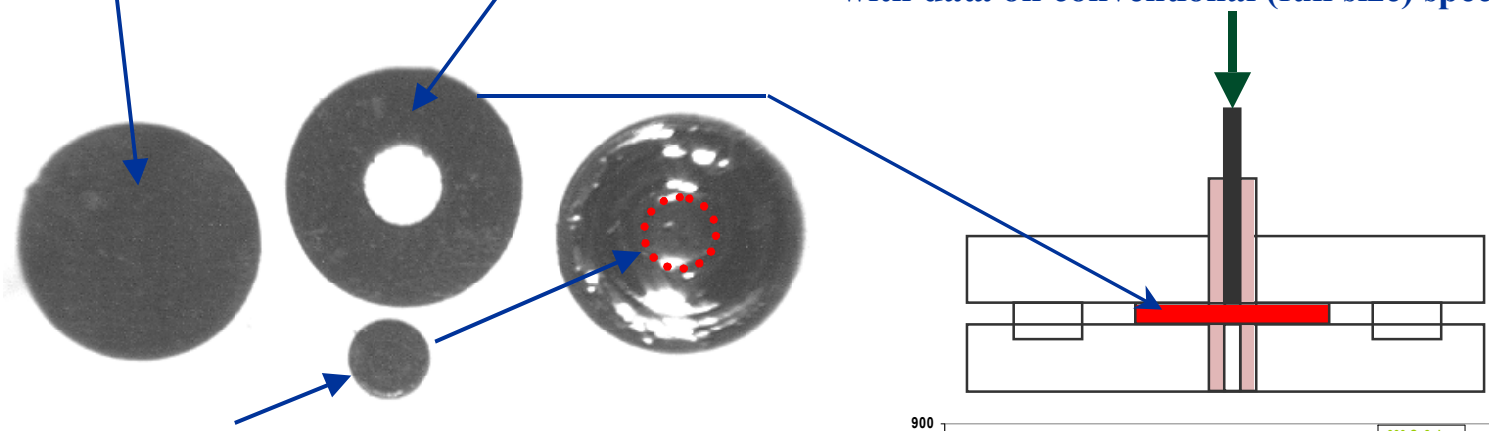


Newly Developed Techniques Allow Greater Materials Science Output From Smaller Irradiation Volumes

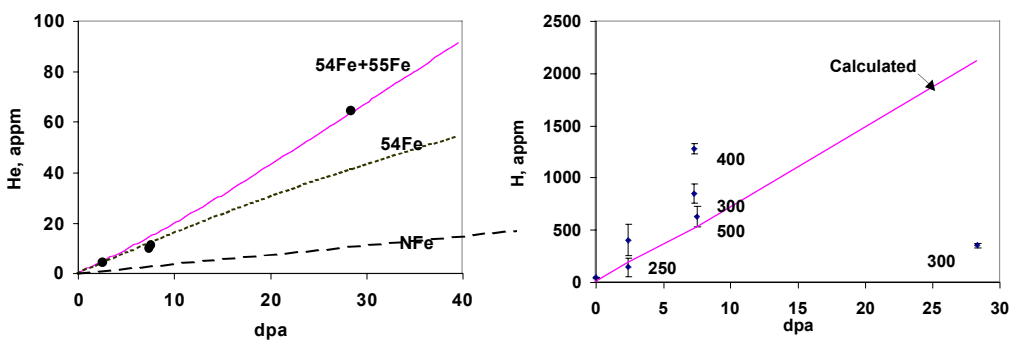
3 mm TEM disk is irradiated in fission reactor

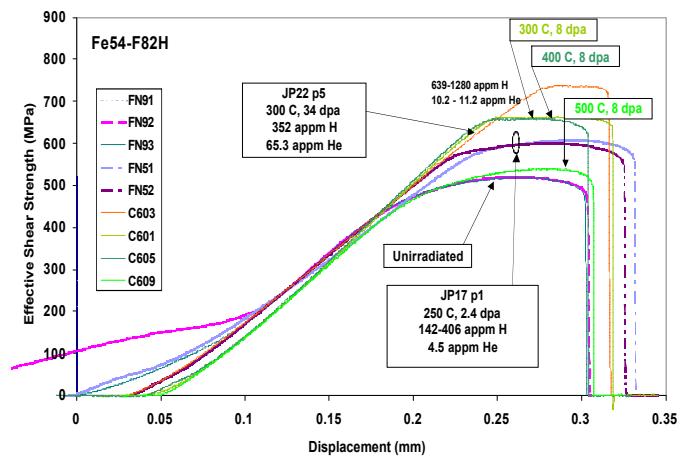
He and H analyses on outer rim

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



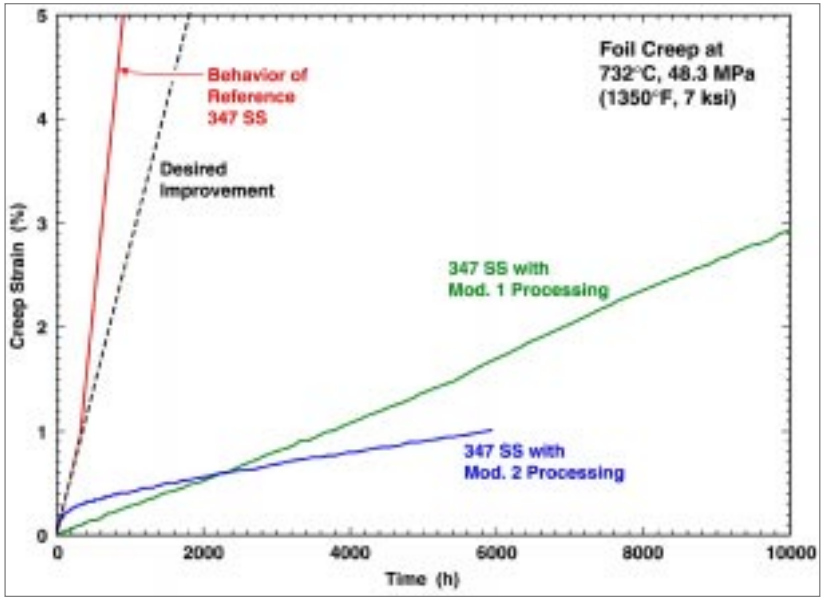
Bonded into unirradiated disk to reduce radioactivity levels and waste generation in evaluation of microchemistry and microstructures



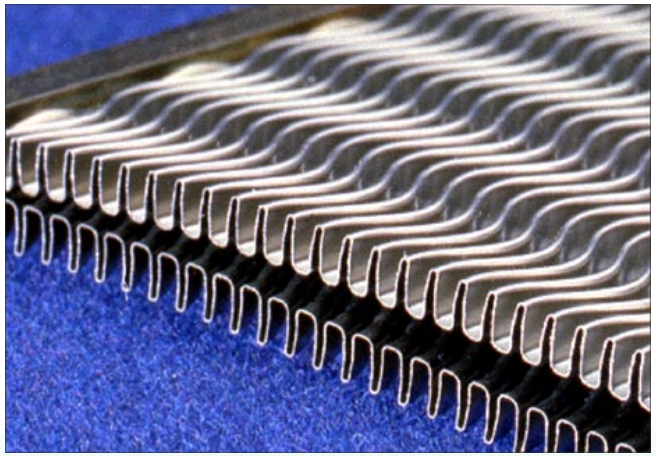


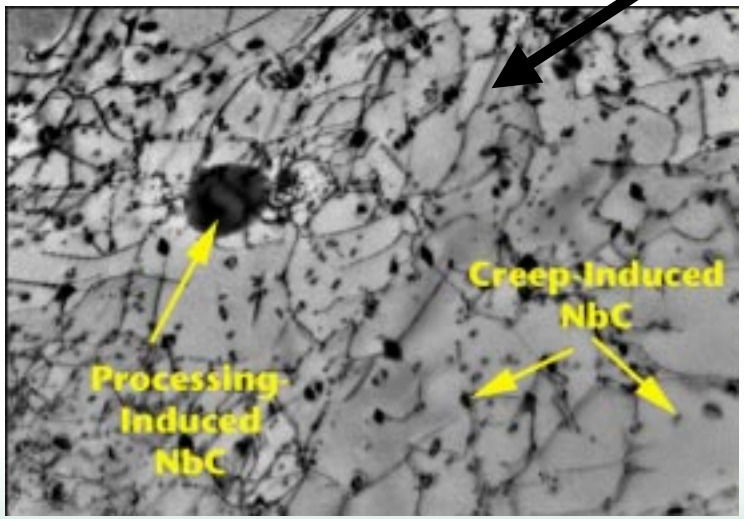
Hydrogen and Helium analysis results

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

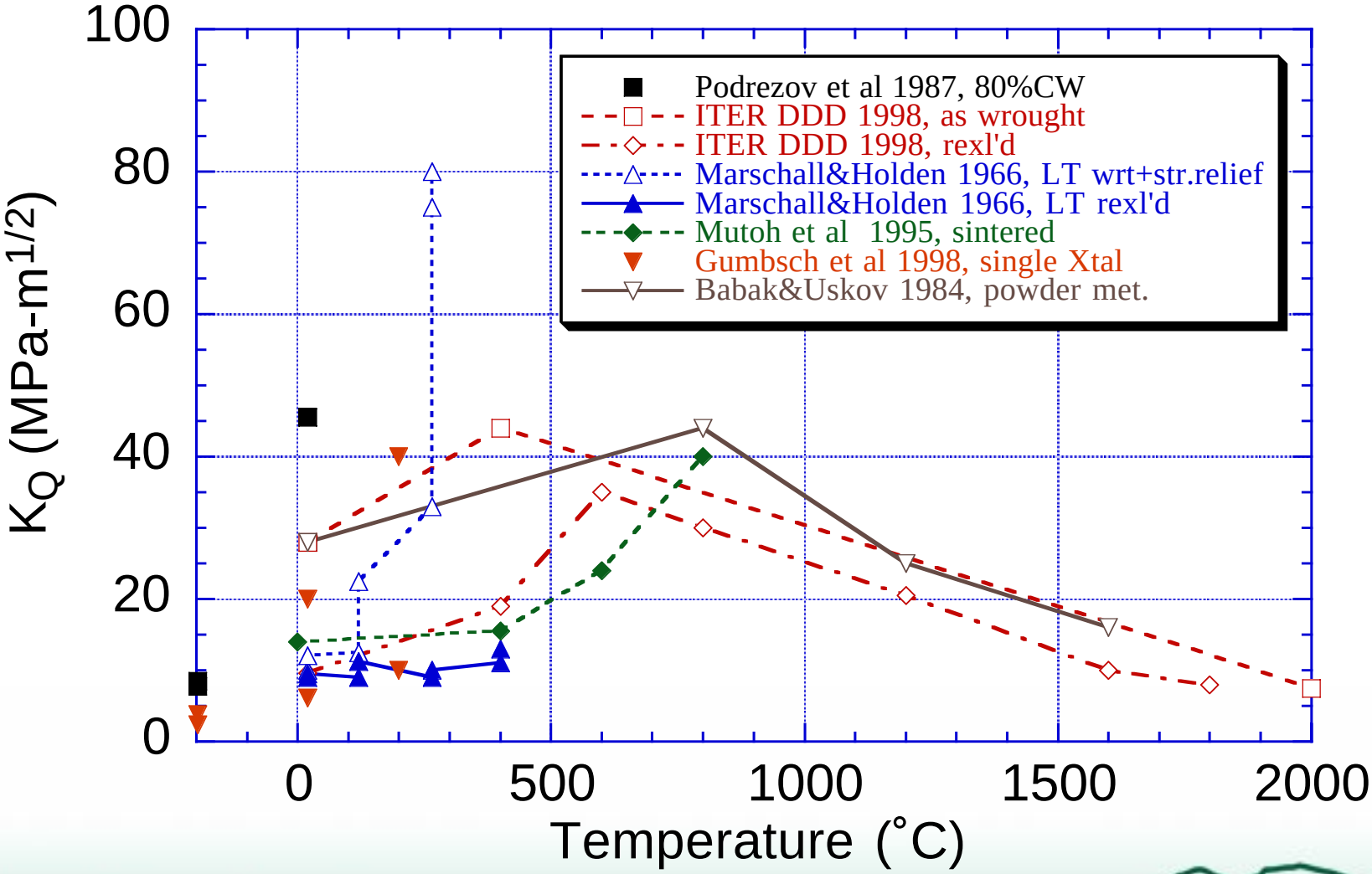


Precipitate stability knowledge derived from radiation effects studies can be used to develop highly creep resistant alloys (microturbine recuperator)

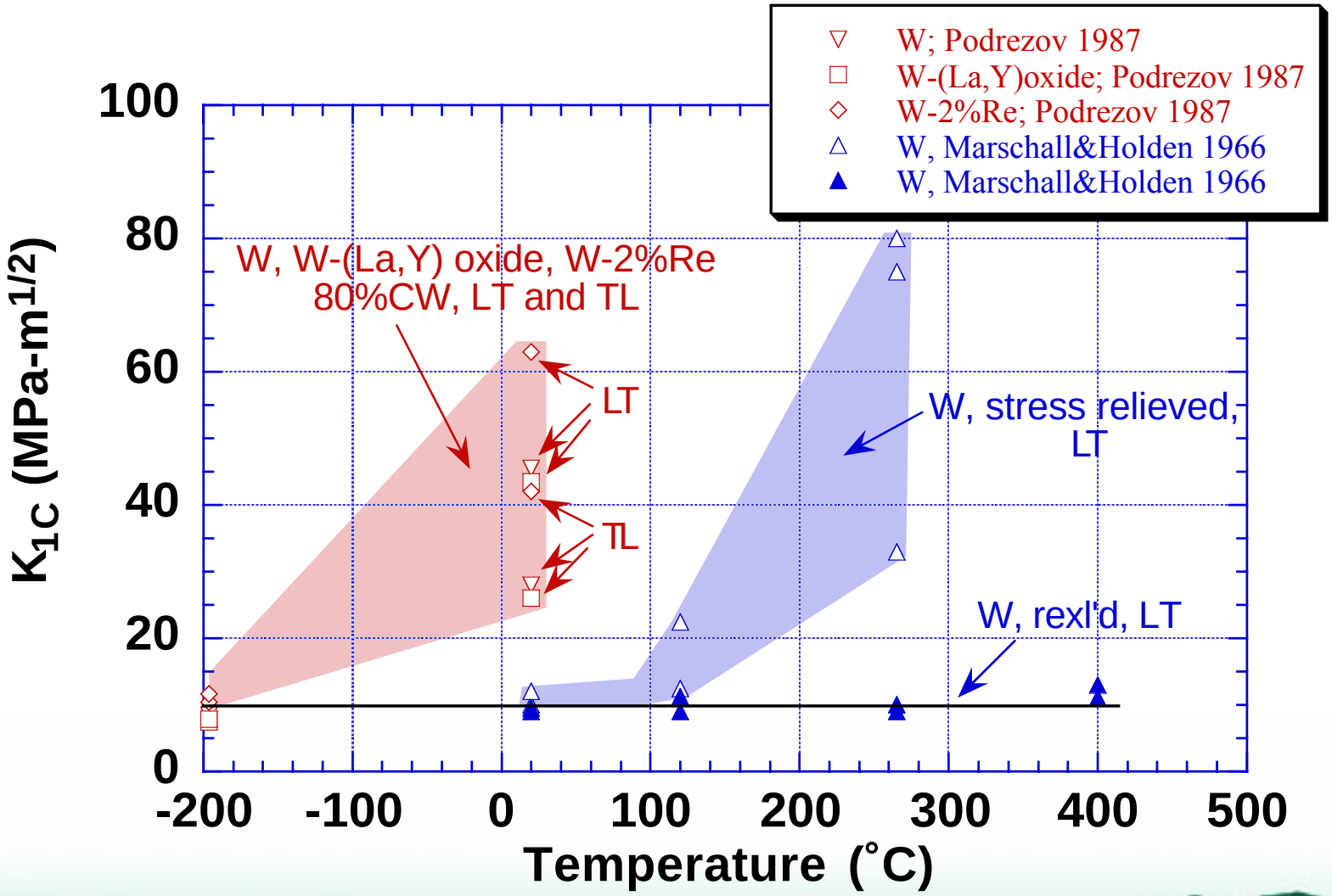




Fracture Toughness of Pure Tungsten



Effect of Thermomechanical Processing and Alloying Additions on the Fracture Toughness of Tungsten



Recent Fabrication Successes with Vacuum Arc Remelted Mo-Re Alloys May be Applicable to BPSX Refractory Components

Ingots of arc melted Mo-Re are routinely processed from powder

These ingots have been fabricated into precision components by extrusion, rolling, and machining

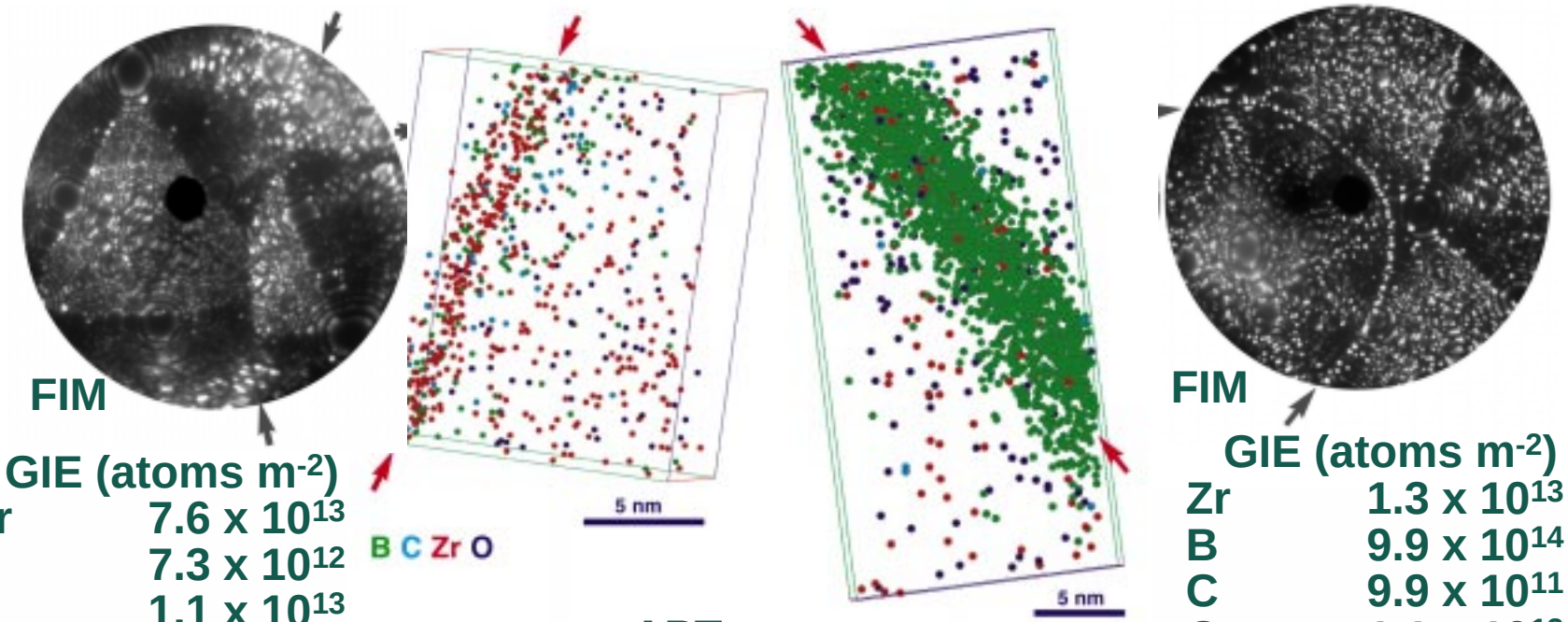
VAR Mo-Re has exhibited good weldability and weldment ductility

E.K. Ohriner and J.P. Moore
Radioisotope Power Program

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**



GIE (atoms m^{-2})

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

APT atom maps

GIE (atoms m^{-2})

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

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

Conclusions

- A BPSX could contribute in niche areas of materials science; larger contribution would be in the field of engineering technology
- Ongoing R&D may enable use of improved materials during BPSX maintenance/repair operations