Overview of Fusion Materials Research at PNNL

R. J. Kurtz

Materials Science Program Peer Review
August 27-28, 2001
Santa Barbara, CA

Outline

- People
- Facilities
- Tasks:
  - Damage Modeling/Helium Effects
  - Ceramic Composites
    - SiC/SiC
  - BCC Metals
    - Vanadium Alloys
    - Tempered Martensitic Steels
  - FCC Metals
    - Copper Alloys
    - Austenitic Steels & Ni-Base Alloys

People

Scientific Staff

Person	Role
RJ Kurtz	Project Manager, Vanadium Task Leader, He Effects Modeling
RH Jones	SiC Task Leader
DJ Edwards	Cu Alloys Task Leader, Electron Microscopy
JD Embury (Consultant)	Mechanical Properties, Nanolayered Materials
AR Ermi (Cogema)	JUPITER Coordination, Experimental Design
F Gao	Helium Effects Modeling
FA Garner	Senior Scientific Advisor, Swelling, Irradiation Creep
DS Gelles	Ferritic Steels Task Leader, ODS Steel Development,Electron Microscopy
LR Greenwood	Dosimetry, Experimental Design
HL Heinisch	Damage Modeling, Helium Effects Modeling, Transmutation Calculations
RG Hoagland (Consultant)	Helium Effects Modeling
DJ Senor	SiC Joining
MB Toloczko (post-doc)	Mechanical Properties, Shear Punch Test Development, Irradiation Creep
GE Youngblood	SiC Irradiation Effects, Thermal Conductivity Modeling

People Continued

Technical & Administrative Staff

Person	Role
BH Wardlow	Lead Project Secretary
SL Weber	Support Secretary
EM Dieffenbacher	Electron Microscopy Specimen Preparation
RM Ermi	Mechanical Property Testing, Hot Cell, Shipping/Receiving
LK Fetrow	Mechanical Properties, High-Vacuum Systems
JP Keavney	Mechanical Property Testing, Hot Cell
GK Whiting	Mechanical Property Testing, Density Measurements, Hot Cell

Facilities for Testing and Characterization of Activated and Non-Activated Materials

Materials Science Building

- Microstructure/chemistry: Electron Microscopy, Auger Spectroscopy
- Mechanical Properties, Corrosion/SCC
- Small-Specimen Testing: Shear Punch, Micro-hardness, Impact

Radiochemical Processing Laboratory

- High-sensitivity quadrupole mass spectrometry system for the determination of helium and hydrogen in irradiated materials (mg sample sizes)

High Temperature Testing Laboratory

- High-Temperature Mechanical Properties
- Small-Specimen Tensile Testing

Radioactive Materials Handling Building

- Activated Material Receiving, Shipping, Sorting, Sectioning
- Material Density Measurements

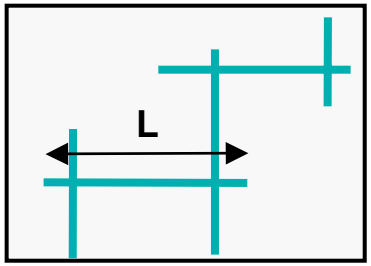
Damage Modeling & Helium Effects

- Task Leader: H. L. Heinisch
- Contributors: R. J. Kurtz, R. G. Hoagland, F. Gao, F. A Garner
- Recent Accomplishments:
  - Atomic scale kinetic Monte Carlo simulations of defect accumulation in metals under neutron irradiation
  - Computer studies of the effects of defect migration characteristics on defect reaction kinetics in irradiated metals
  - Working with University of Tokyo, developed a model for the strong flux sensitivity of the transient regime of void swelling. The effect appears to be universal, found so far in pure Ni, austenitics, F/M steels, vanadium and V-Cr.

New Defect Reaction Kinetics for 1-D Migrating Interstitial 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

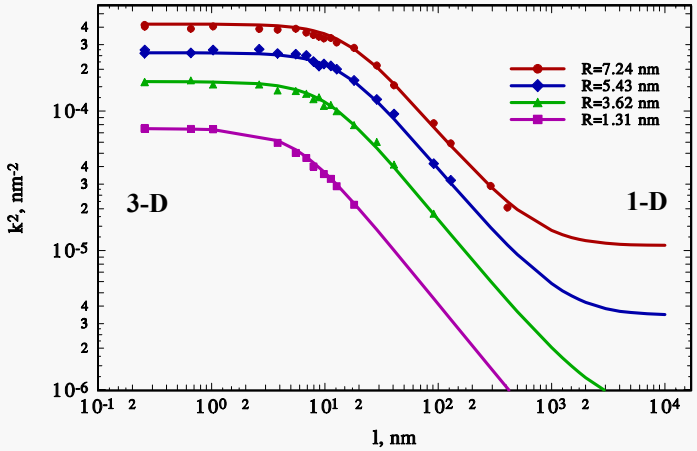


Mixed 1-D/3-D migration, average 1-D segment length L

KMC "thought experiments"

- Defects migrating by mixed 1-D/3-D with the same L, interact with …
- Random field of absorbers of radius R, number density N
- "Sink strengths" k^2 are determined from the defect lifetimes as a function of L

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



Sink strength as a function of 1-D segment length. Analytical expression compared to KMC results

KMC "thought experiments" are perfectly described by a new analytical theory for reaction kinetics from 1-D to 3-D.

The new reaction kinetics is incorporated into the new Production Bias Model of microstructure evolution (Singh, Woo, Trinkaus, Foreman, Golubov)

SiC/SiC Composites

- Task Leader: R. H. Jones
- Contributors: D. J. Senor, G. E. Youngblood, H. L. Heinisch
- Recent Accomplishments:
  - Measured the thermal creep rate for several SiC fibers using the bend stress relaxation (BSR) method
  - Initiated experiments to measure the irradiation creep rate of SiC fibers using the BSR method, completed preliminary evaluation of the fundamentals of irradiation creep of SiC
  - Modeled the irradiation creep behavior of SiC/SiC composites (in collaboration with BES and NERI)
  - Determined the thermal conductivity of SiC fibers, developed samples for irradiation in several reactors and compared results with thermal conductivity models (in collaboration with NERI)

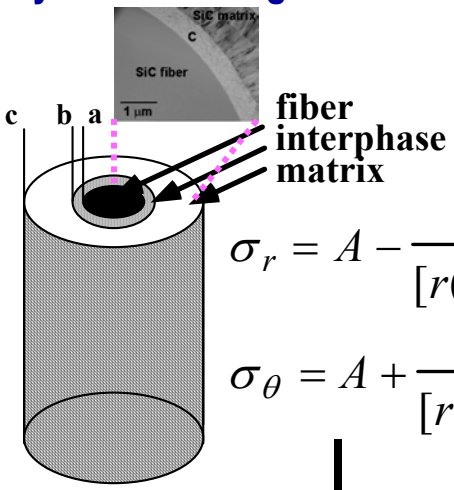
SiC/SiC Composites

- Recent Accomplishments:
  - Measured the bend strength as a function of temperature, dose and composite type of SiC/SiC composites
  - Selected test methods for measuring the shear and tensile strength of joints between SiC/SiC composites
  - Evaluated and modeled the shrinkage stresses in SiC/SiC joints produced with joints with polymer precursors
  - Reviewed the thermal shock data and models for continuous fiber ceramic composites

Crack Growth is a Potential Lifetime Limiting Mechanism Controlled by Microscale Phenomena

Analytical modeling of internal stresses

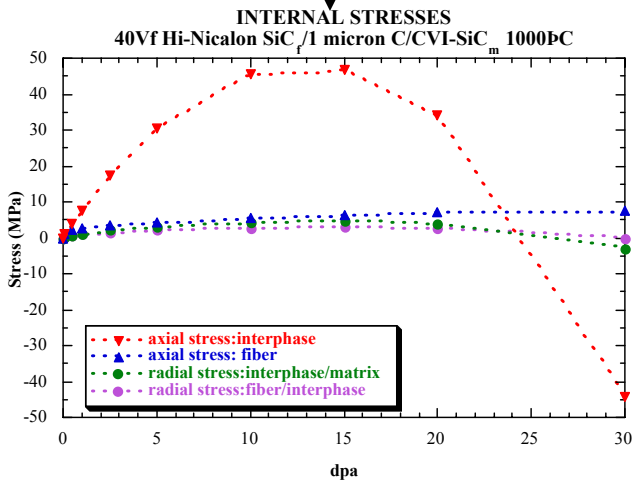
microscale



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

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

macroscale



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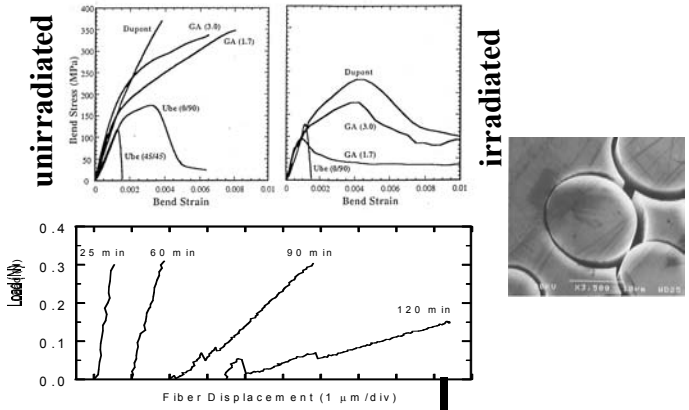
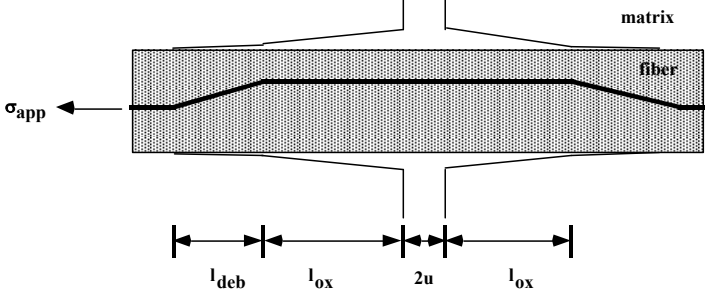
Experimentally determined, semi-empirical, bridging-compliance relations



$$u_f = \left(\Phi_f^l + P_f \Phi_f^n\right) P_f$$



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

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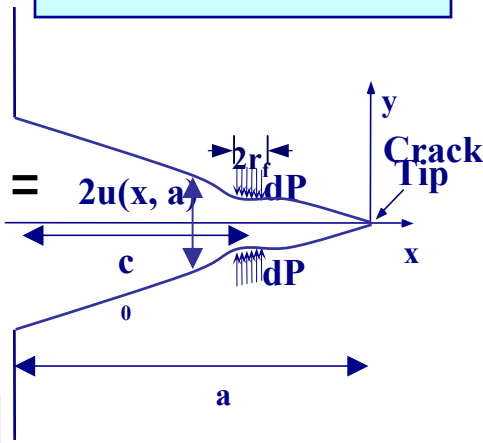
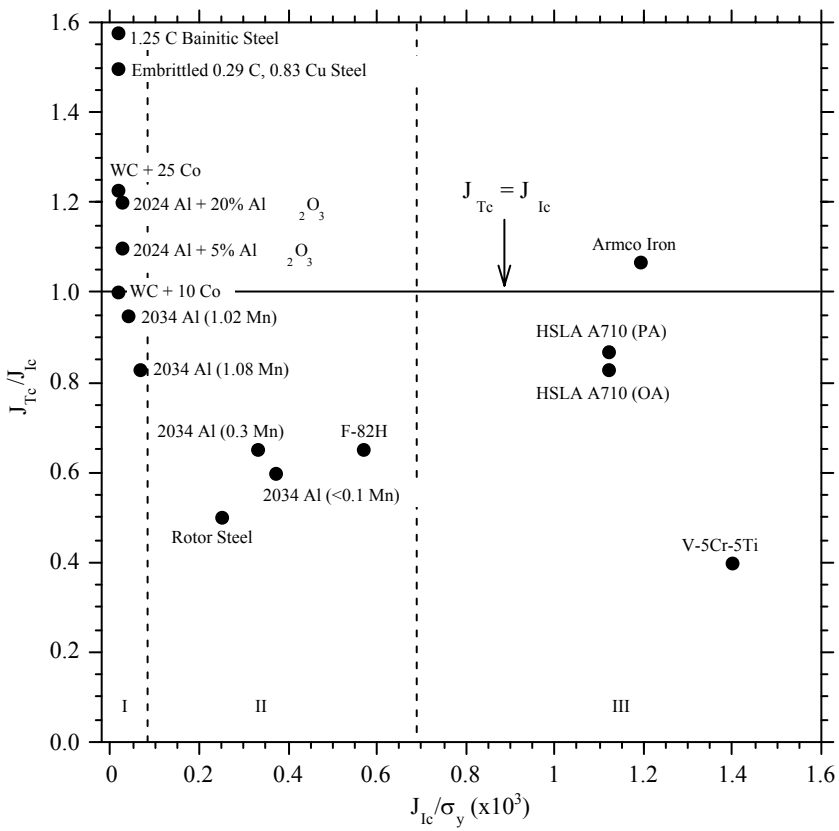


Vanadium Alloys

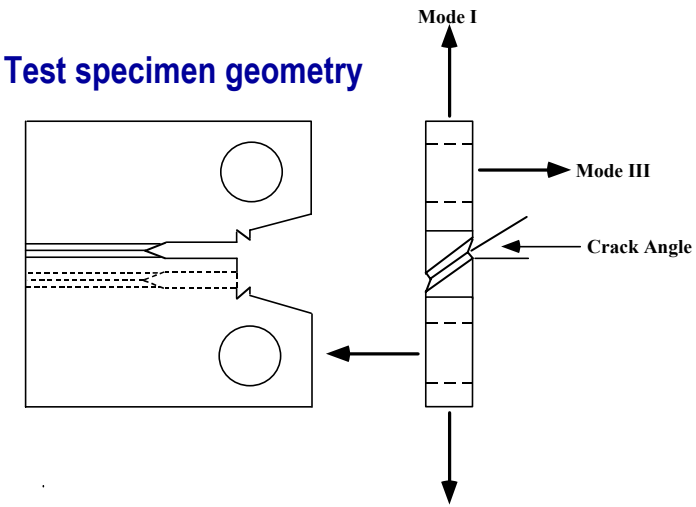
- Task Leader: R. J. Kurtz
- Contributors: D. S. Gelles, F. A. Garner
- Recent Accomplishments:
  - Explored the effect of loading mode and specimen thickness on fracture behavior of V-4Cr-4Ti
  - Performed dynamic finite element modeling of 1/3-scale Charpy specimens to determine effect of material variables
  - Investigated the effect of oxygen on subcritical crack growth and propensity for dynamic embrittlement of V-4Cr-4Ti
  - Characterized the high-temperature, biaxial creep response of vanadium-based alloys

Effect of Loading Mode on Fracture Toughness of V-5Cr-5Ti and F82H

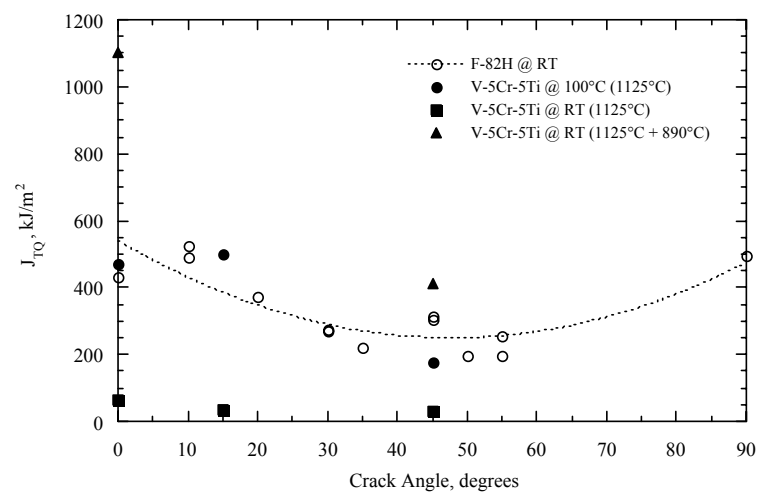
Ductile materials exhibit strongest effect



Test specimen geometry



Fracture toughness lowest under mixed mode loading



Tempered Martensitic Steels

- Task Leader: D. S. Gelles
- Contributors: F. A. Garner, M. B Toloczko, B. H. Sencer (New Mexico Tech)
- Recent Accomplishments:
  - Explored the post-irradiation deformation mechanisms in ferritic steels
  - Developed novel experimental techniques to determine mechanical property data, microchemistry, and microstructural information on irradiated metals from a single TEM disk
  - Quantified the relationship between thermal creep and irradiation creep in HT9 over the range 490-605°C

Tempered Martensitic Steels

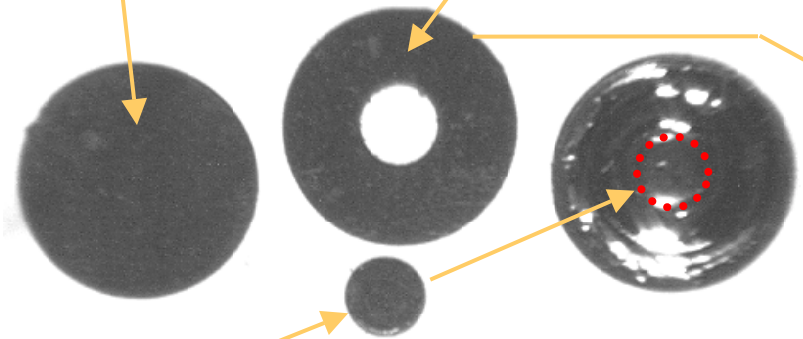
- Recent Accomplishments:
  - Measurement of irradiation creep coefficients for various F/M steels, showing that the creep compliance in absence of swelling is ~0.5×10^{-6} MPa^{-1} or ~1/2 of that of austenitic steels, but the creep swelling coupling coefficient is essentially the same at ~1×10^{-2} $(MPa\ dpa)^{-1}$
  - Demonstrated with simple Fe-Cr model alloys that swelling can occur for all temperatures between 400 and 593°C, with the transient regime being very long at high temperatures
  - Demonstrated that the transient regime of swelling is very sensitive to dpa rate, decreasing strongly with decreasing dpa rate

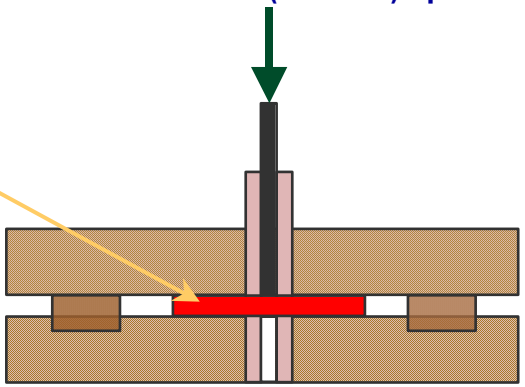
Newly Developed Techniques Allow Greater Materials Science Output From Smaller Irradiation Volumes

3 mm TEM disk is irradiated in fission reactor

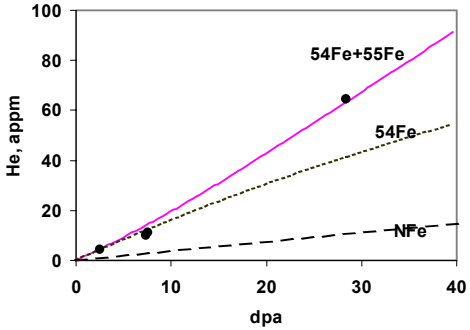
He and H analyses on outer rim

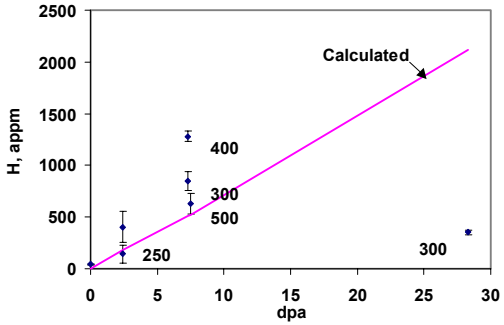
Shear punch test yields mechanical properties data that correlate with tensile data and can be correlated with data on conventional (full size) specimens



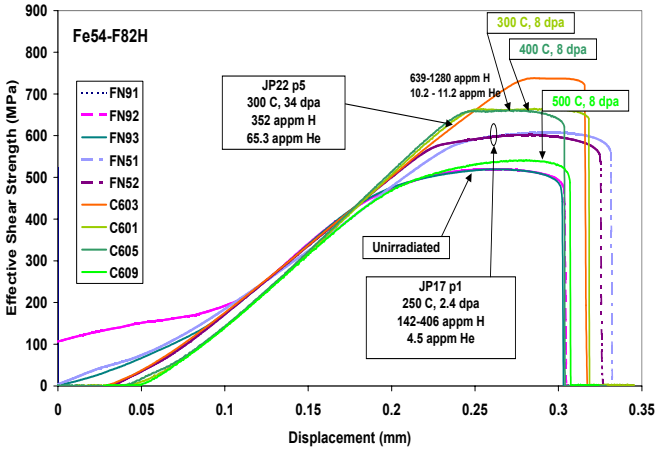


Bonded into unirradiated disk to reduce radioactivity levels and waste generation in evaluation of microchemistry and microstructures





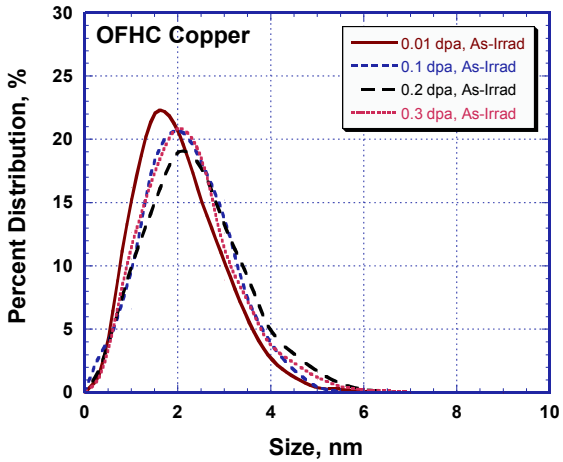
Hydrogen and Helium analysis results



Copper Alloys

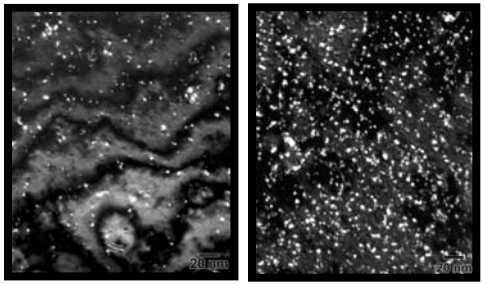
- Task Leader: D. J. Edwards
- Recent Accomplishments:
  - Investigation of the post-irradiation annealing behavior of copper alloys at low temperatures and doses
    - Investigation of yield point phenomenon and work hardening behavior in as-irradiated and post-irradiation annealed pure copper
  - Investigation of radiation effects in pure copper and copper alloys (T_{irr} 50 to 450°C, 0.01 dpa to 2 dpa)
    - Collaborations with Denmark (Risø National Laboratory, ORNL, Efremov Institute, SRIIAR)
  - Investigation of the strain-rate and test temperature sensitivity of unirradiated copper alloys
    - Collaboration with ORNL, Univ. of Illinois

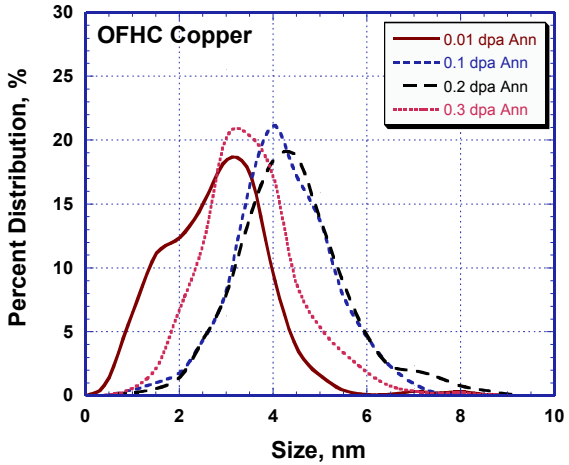
Microstructure of As-Irradiated and Post-Irradiation Annealed OFHC Copper (PNNL & Risø National Laboratory)



As-Irradiated

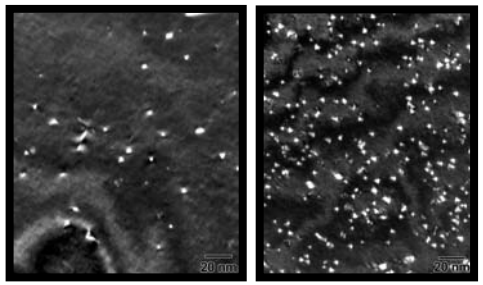
0.01 dpa **0.3 dpa**





Post-Irradiation Annealed

0.01 dpa **0.3 dpa**

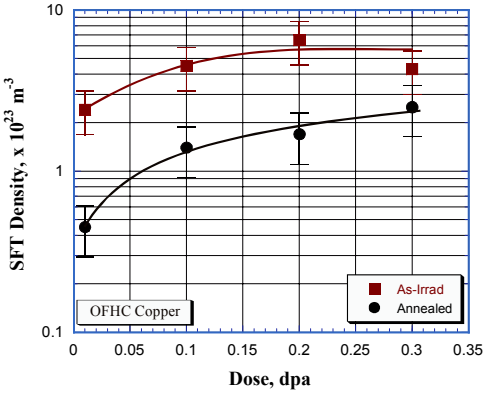


As-Irradiated

- High density of stacking fault tetrahedra that reaches saturation at ~0.1 dpa
- Small interstitial loops present 5 x 10^{21} m^{-3} at 0.01 dpa
- Network dislocations form at higher doses

Post-Irradiation Annealed (300°C for 50 hrs)

- SFT still present but in somewhat lower density
- Larger interstitial loops and network dislocations present in higher density than in as-irradiated specimens

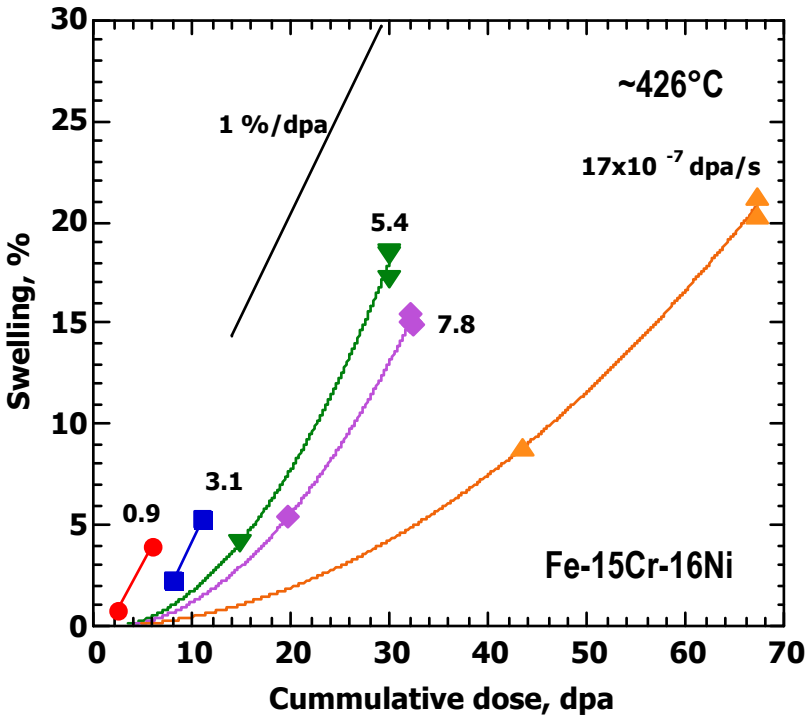
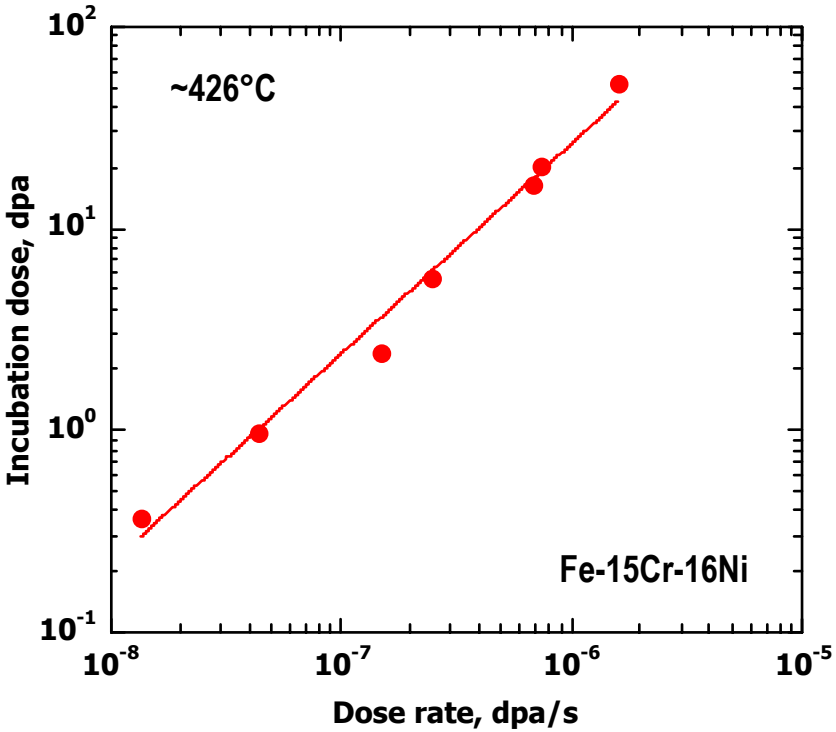


Austenitic Steels & Ni-Base Alloys

- Task Leader: F. A. Garner
- Contributors: M. B. Toloczko, B. H. Sencer, G. L. Hankin (Loughborough Univ.), G. M. Bond (NM Tech)
- Recent Accomplishments:
  - Demonstrated that the creep compliance and creep-swelling coupling coefficient are independent of composition over a wide range of Ni and solute contents
  - Demonstrated both experimentally and theoretically that the creep compliance of stainless steels appears to increase at higher He/dpa ratios, as a result of bubble formation
  - Demonstrated in a joint PNNL-Russian experiment that steady-state swelling of 1%/dpa can be reached at temperatures at least as low as ~335°C

Austenitic Steels & Ni-Base Alloys

- Recent Accomplishments:
  - Demonstrated that the incubation period of swelling is reduced strongly and progressively at lower dpa rates. These results were confirmed in ion irradiations as well
  - Developed completely general tensile shear punch correlations for 300 series stainless steels that are independent of starting microstructure, irradiation temperature, dpa level, He/dpa ratio, level of swelling and dislocation microstructure
  - Developed FIM models to explain the slope and intercept of the tensile-shear punch correlation.

Austenitic Steels & Ni-Base Alloys

Garner and Okita, 2001