Mesoscale Microstructural Phenomena: Void swelling, Effects of Helium, and Irradiation-Induced Stress Corrosion Cracking

Roger E. Stoller, Oak Ridge National Laboratory
Todd R. Allen, University of Wisconsin
Louis K. Mansur, Oak Ridge National Laboratory

SC-NE Workshop on:
Advanced Computational Materials Science:
Application to Fusion and Generation-IV Fission Reactors

Washington, DC
31 March - 2 April 2004

ornl

What is “mesoscale”?

- an intermediate size scale, lying between the atomistic and macroscopic
- relevant to many phenomena in materials science and radiation effects
  - grain growth
  - dislocation evolution, by thermo-mechanical or radiation-induced processes
  - void swelling
  - precipitation of additional phases, and solute segregation
  - stress corrosion cracking, and irradiation-assisted SCC
- dependent on fundamental atomistic processes, and controls macroscopic observables such as strength, ductility, creep, ...

Reaction rate theory: application to mesoscale modeling

- models based on the so-called reaction rate theory (by analogy to chemical reaction rates) are well suited to mesoscale problems in radiation effects
- the material is treated as a spatially-homogeneous effective medium with embedded effective sinks and sources for point defects
- time- and spatially-averaged point defect generation rates are also generally employed
- these assumptions have been relaxed in particular cases, e.g. to investigate cascade-induced fluctuations in point defect concentrations

Rate theory, con't

- the models are formulated as a series of differential equations describing the production and fate of point defects and the corresponding evolution of the microstructure

- e.g. the vacancy (C_v) and interstitial (C_i) concentrations are given by:

$$\frac{dC_{i,v}}{dt} = \langle \eta G_{dpa} + G_{i,v}^{em} \rangle - \alpha C_i C_v - D_{i,v} C_{i,v} S_{i,v}^{T}$$

where the $D_{i,v}$ are the point defect diffusivities, the $S_{i,v}$ are the extended defect (GB, dislocation, etc.) sink strengths, α is the recombination rate coefficient, ηG_{dpa} is the net point defect generation rate, and $G_{i,v}^{em}$ is the total rate of emission of point defects from sinks

Rate theory, con't

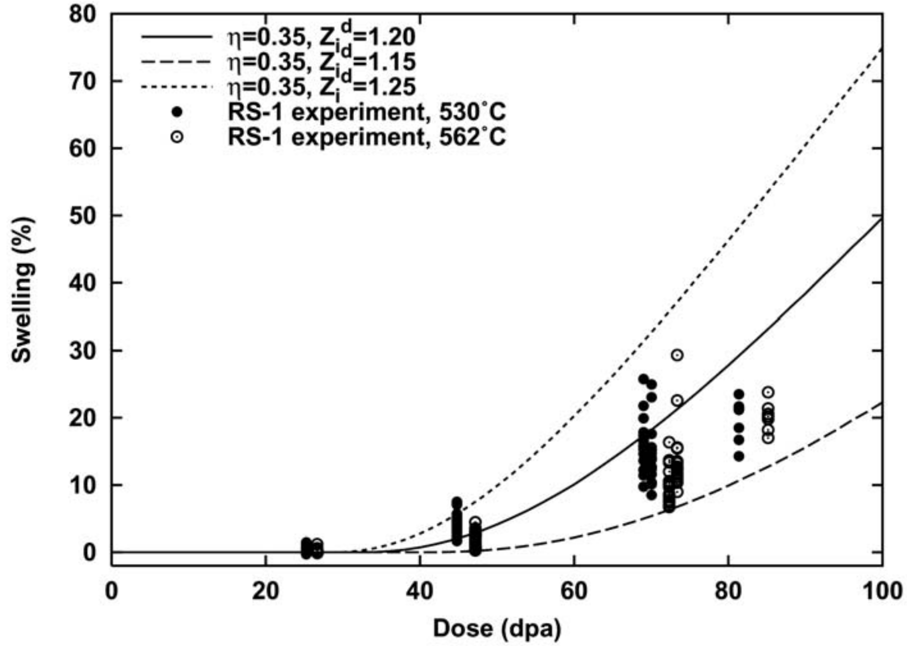
- and in a system with growing voids, the void growth rate is:

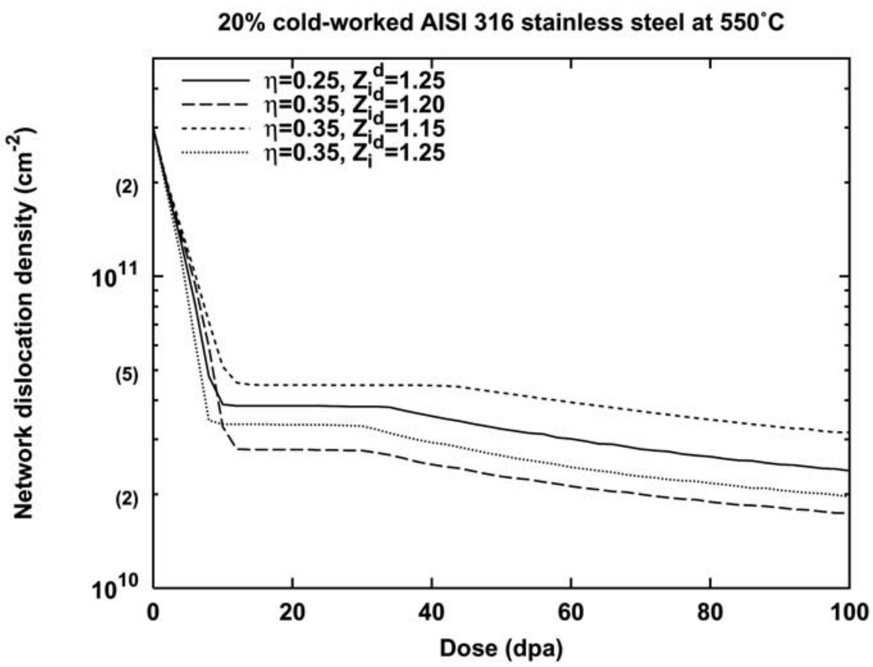
$$\frac{dr_v}{dt} = \frac{1}{r_v}\left(Z_v^v D_v\left(C_v - C_v^v\right) - Z_i^v D_i C_i\right)$$

- analogous equations can be written to describe an evolving point defect cluster population, for helium generation and distribution, the redistribution of solute species, and for the other microstructural components
- greater or lesser detail can be built in as needed to simulate a given phenomenon, e.g. nucleation vs. growth regimes
- model predictions are found by simultaneous integration of the equations included in a given model

Rate theory, con't

- model predictions can be compared with experimental data and parameter uncertainties evaluated





- when well calibrated with experimental data, such models have some predictive capability

ornl

However, devil is in the details ...

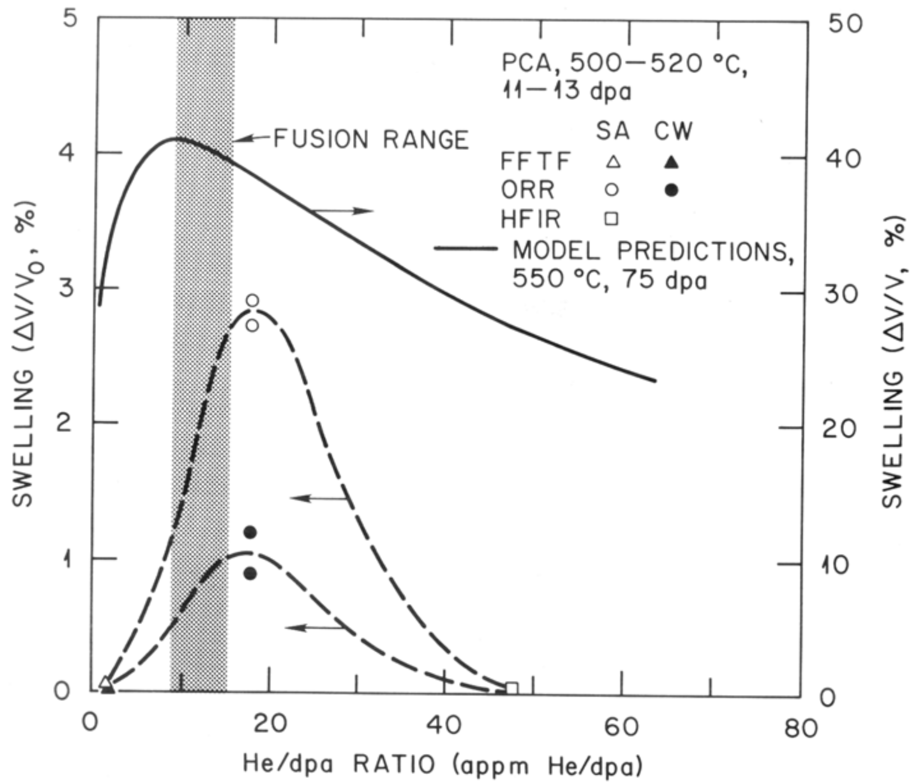
- data fitting with incomplete models leads to use of “effective” parameter values, limits confidence in model extrapolation
  - more complex models may be ‘stiffer’ with respect to arbitrary parameter choices, but,
  - more complex models introduce additional parameters
- *ab initio* methods and MD can provide improved estimates of material parameters, e.g. defect formation energies, primary radiation damage parameters
  - former is largely limited to pure materials and small atomic systems, e.g. limited information on diffusion and defect formation energy parameters
  - latter is limited by range of materials for which realistic interatomic potentials can be developed

Neutron energy spectrum differences are an issue for extrapolation of models calibrated using fission reactor data

- solid transmutations vary due to relatively high threshold energy (>5 MeV) for many reactions, 10 to 100s appm/dpa levels of new solute can be created - potentially significant for some materials

- most attention has been focused on gaseous transmutation products, He from (n,α) and H from (n,p) reactions
  - fission: ~0.2-0.5 appm He/dpa (higher for some elements with thermal neutrons
  - DT fusion: ~10-20 appm He/dpa
  - spallation (SNS): ~500 appm H/dpa, ~100 appm He/dpa

• previous modeling indicated that microstructural response may not be a monotonic function of He level

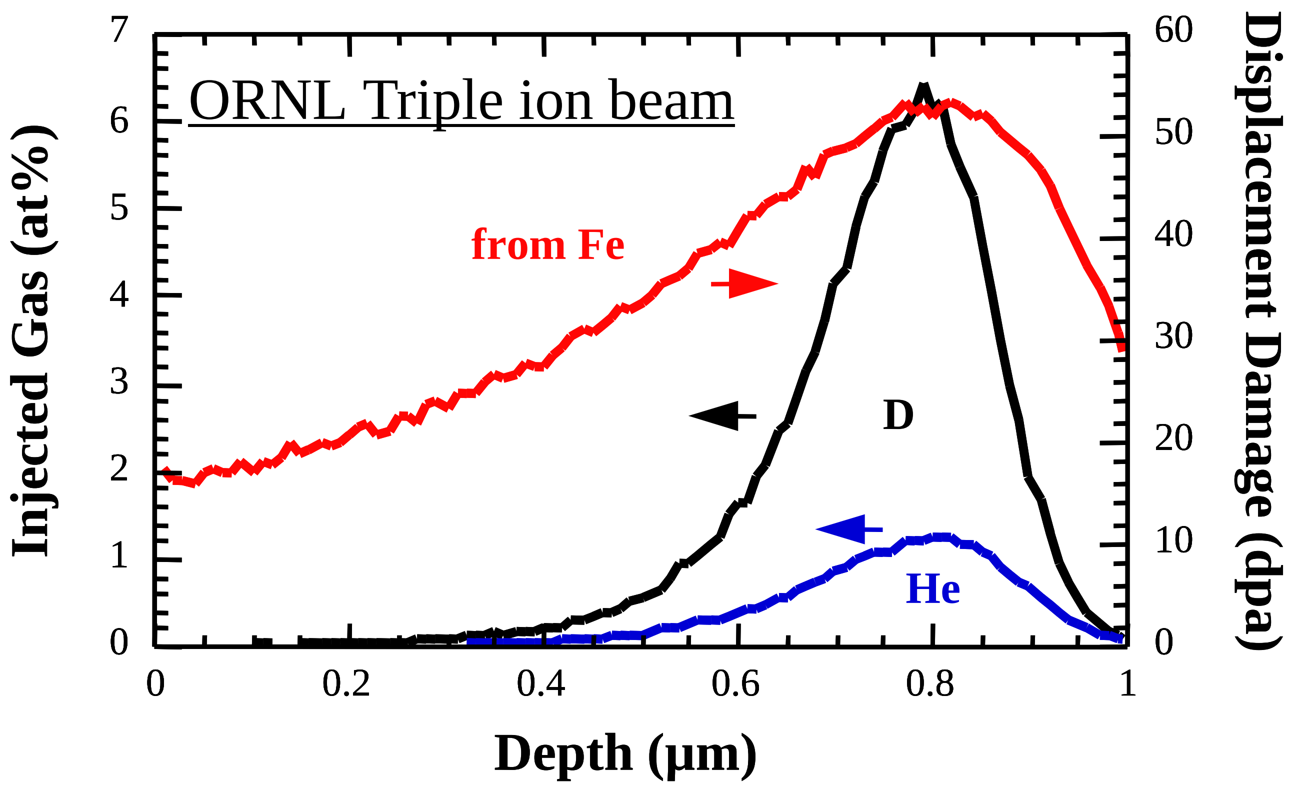


(Stoller, et. al., JNM 1988)

• caveats: overly simplistic cavity nucleation model, predictions very sensitive scaling of cavity density with He, accounting for differences in displacement rate

ornl

Considerable recent work on He and H effects related to SNS target R&D

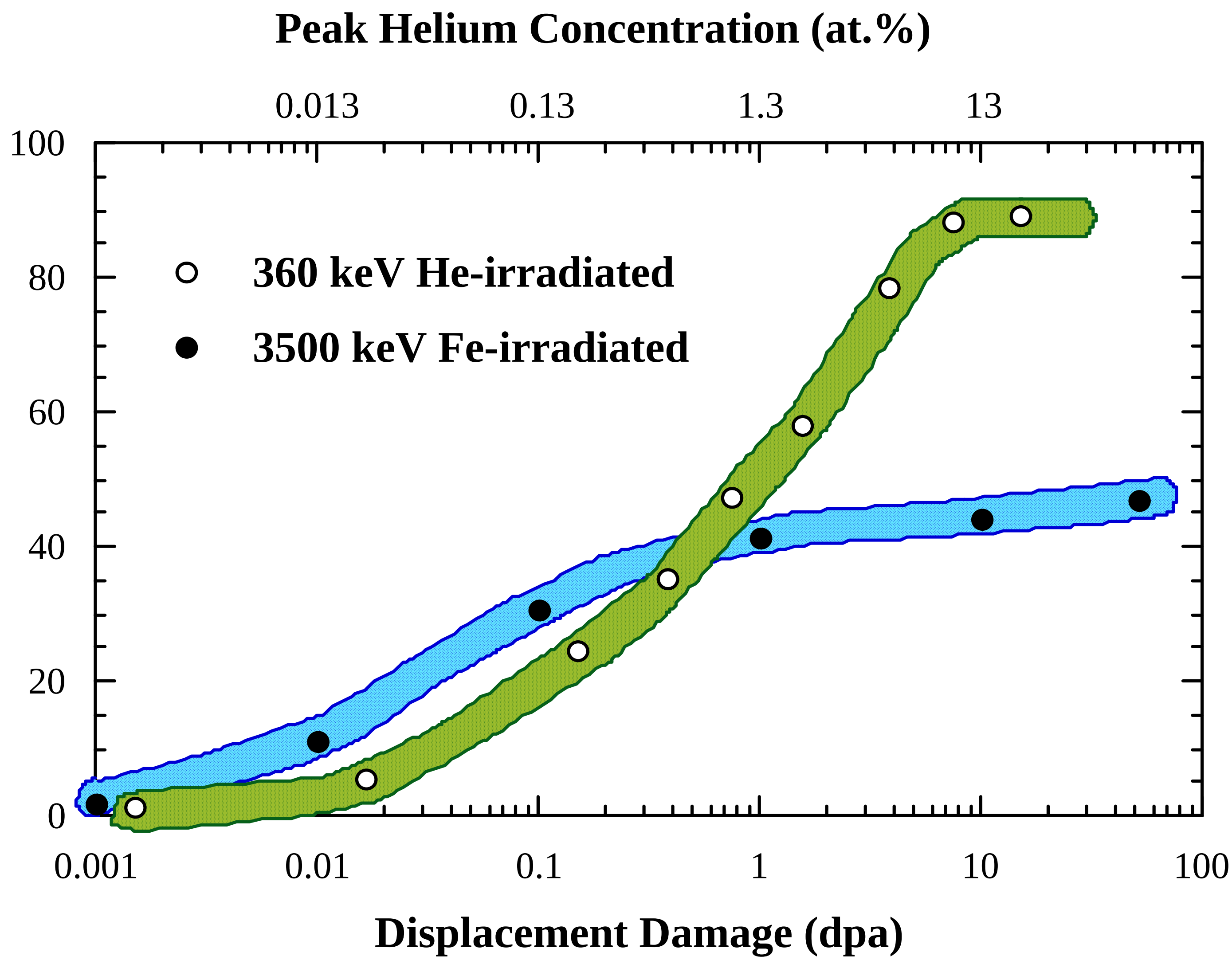


- Simultaneous injection of D, He, and Fe
- D analyzed by the nuclear reaction $^{3}He(D,^{4}He)p$
- He and Fe irradiation affect retention of D

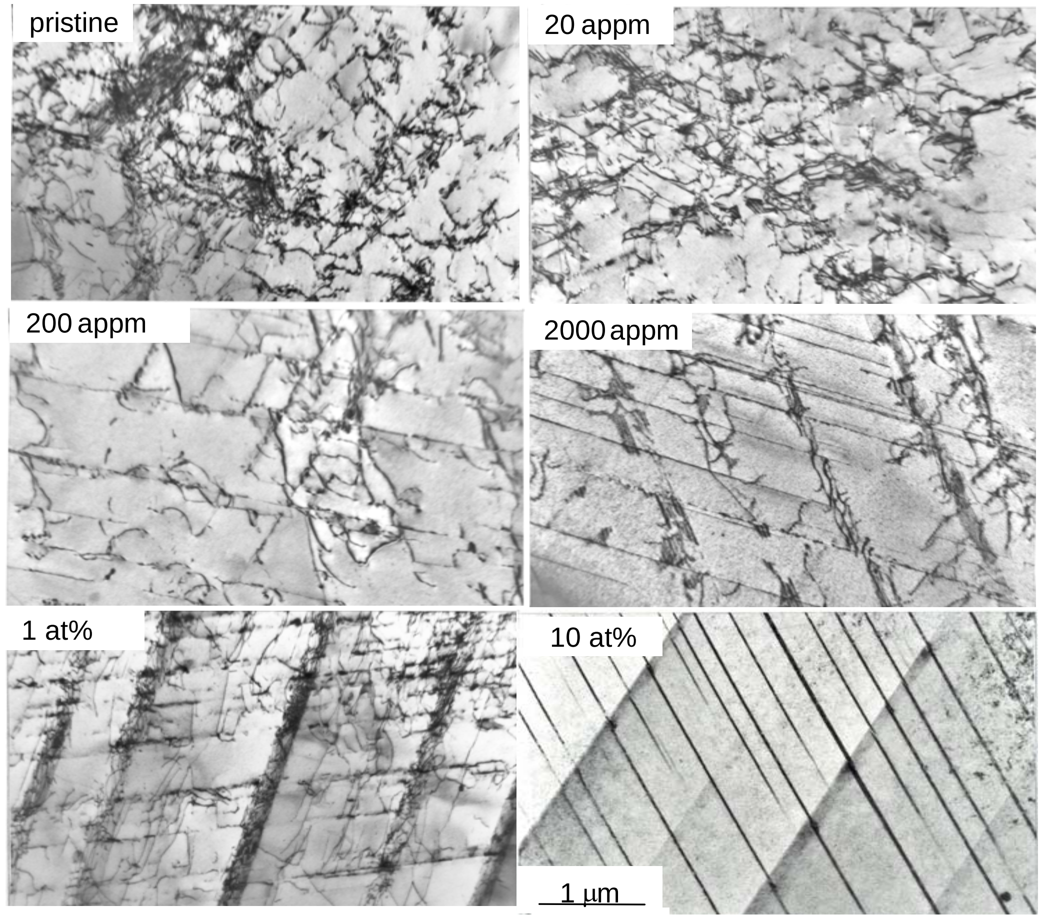
Key results of SNS studies

- High hardening and underlying defect structure caused by high He content
- Deformation mechanism changes, flow localization and dislocation channeling
- Retention of H in response to different radiation damage states (contrary to expectations), additional hardening observed from H

Hardening increment per dpa increased in He-implanted material

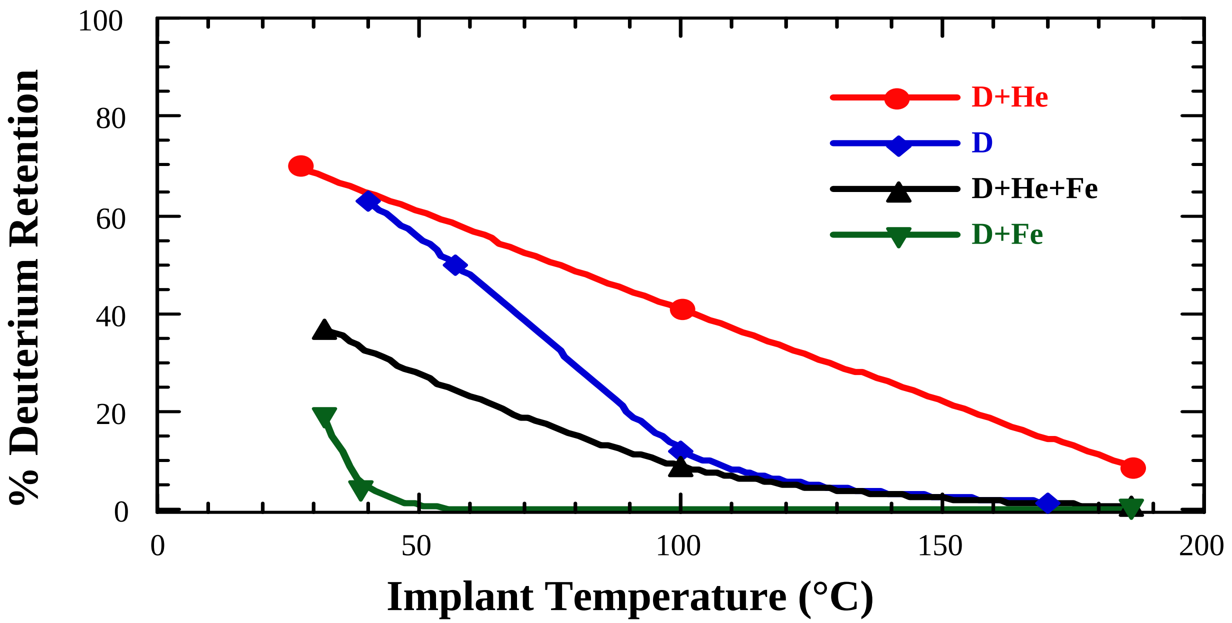


He (dose) effect on deformation mechanism

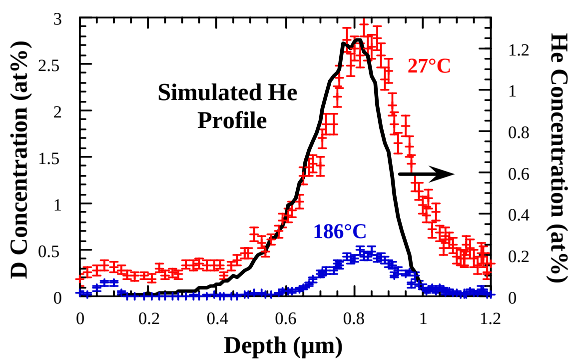


- 316 LN, 350 keV He implanted at 200 C to various levels and strained to 10% at RT
- associated with fine-scale He bubble formation

Influence of damage state on H retention

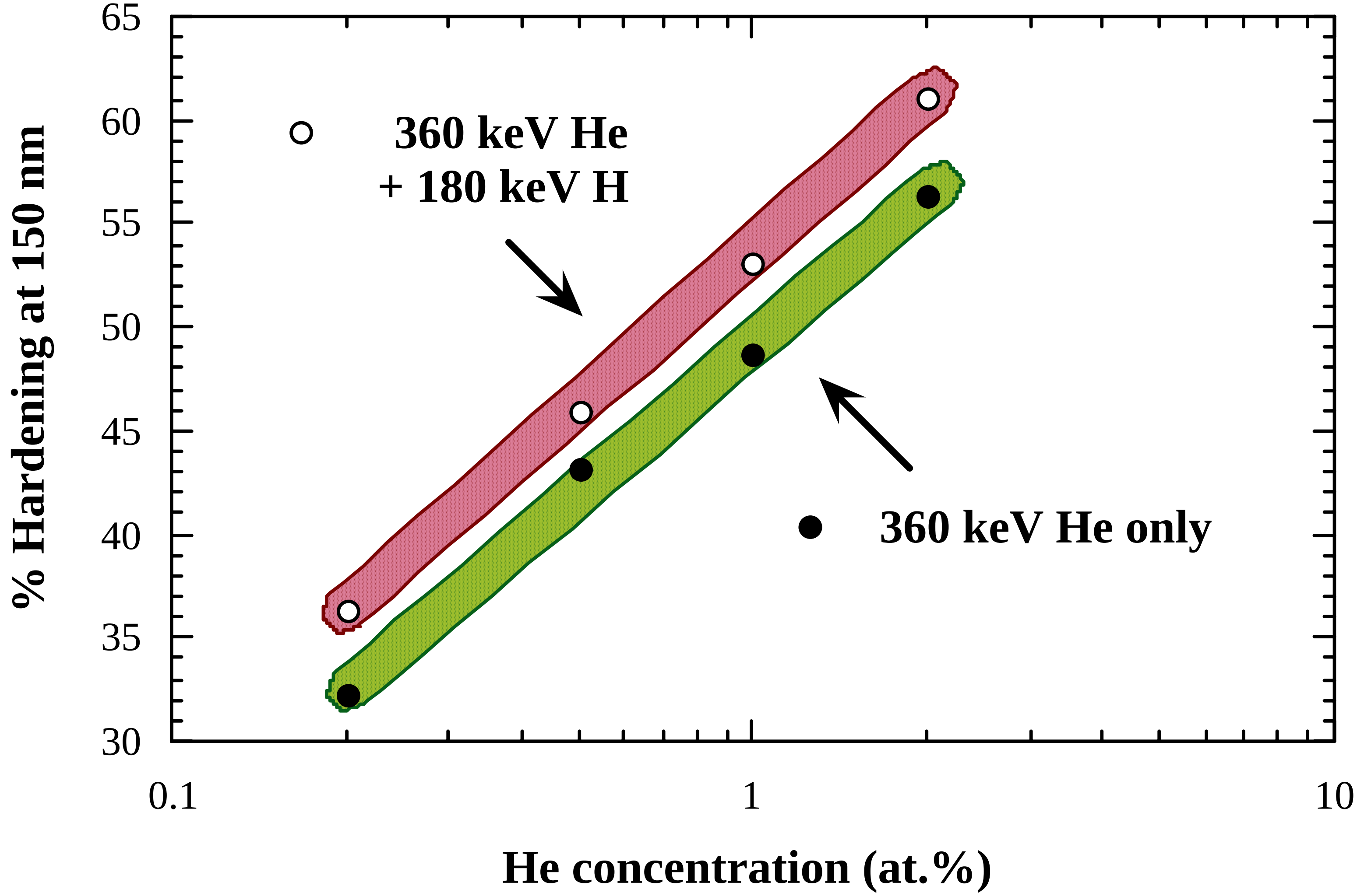


- Hydrogen retention in the irradiated specimens is high, especially in the presence of helium
- Hydrogen profile closely follows helium profile



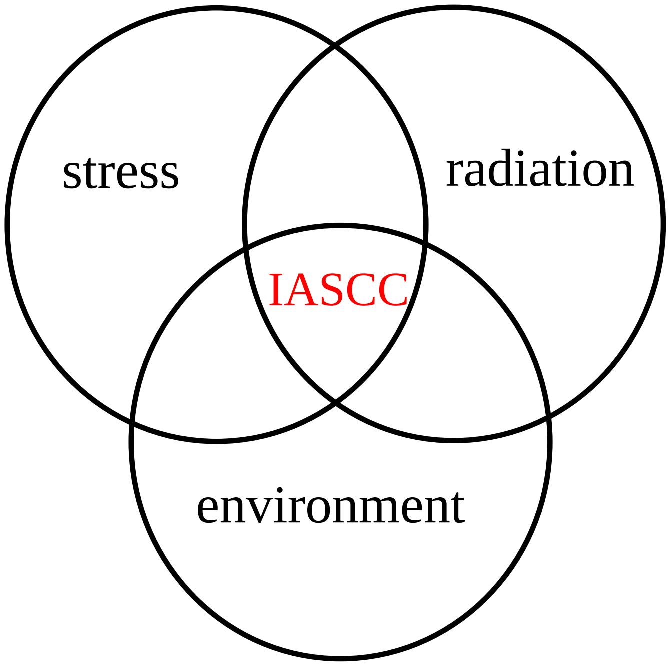
ornl

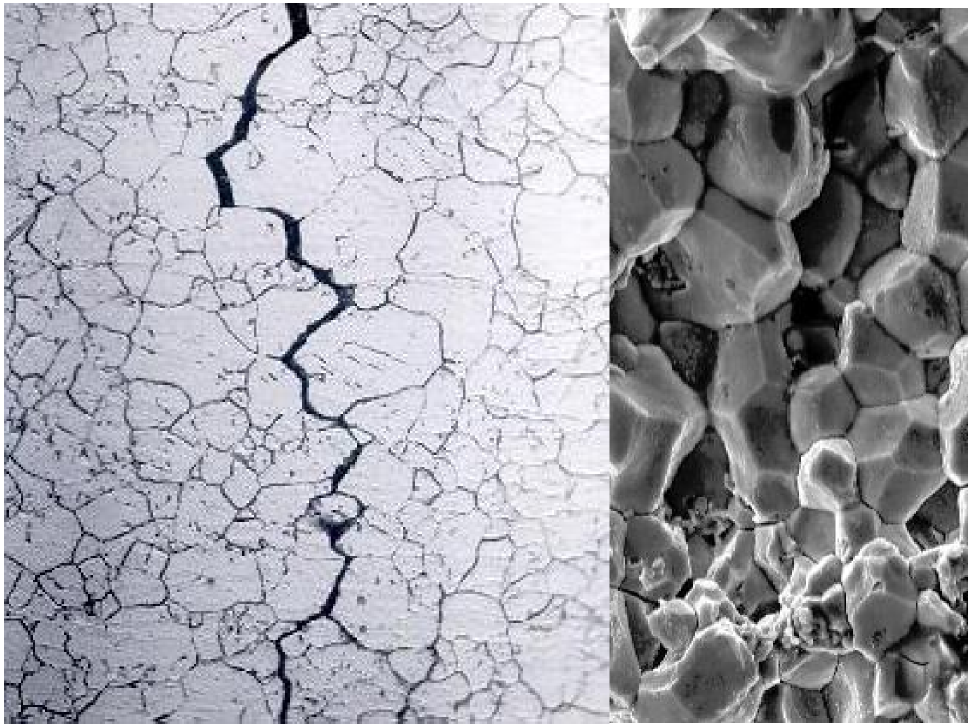
Additional hardening increment from H



Irradiation Assisted Stress Corrosion Cracking

- IASCC occurs in Fe, and Ni base austenitic reactor materials in LWRs
- Component cracking occurs at stress levels well below design stress



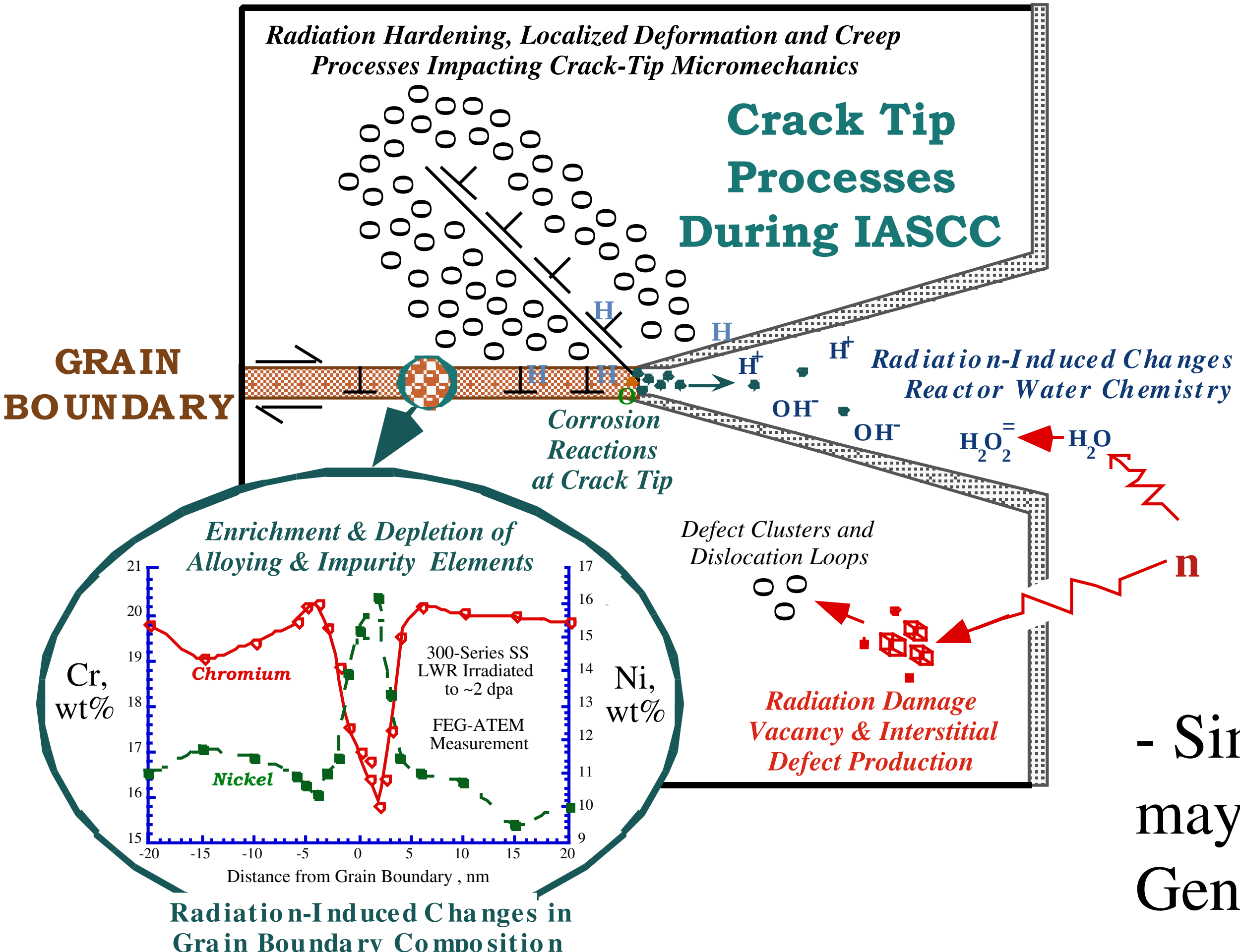


Intergranular cracking

S. M. Bruemmer, NERI 02-0110

Irradiation Assisted Stress Corrosion Cracking

DEPARTMENT OF
Engineering Physics
College of Engineering
University of Wisconsin-Madison

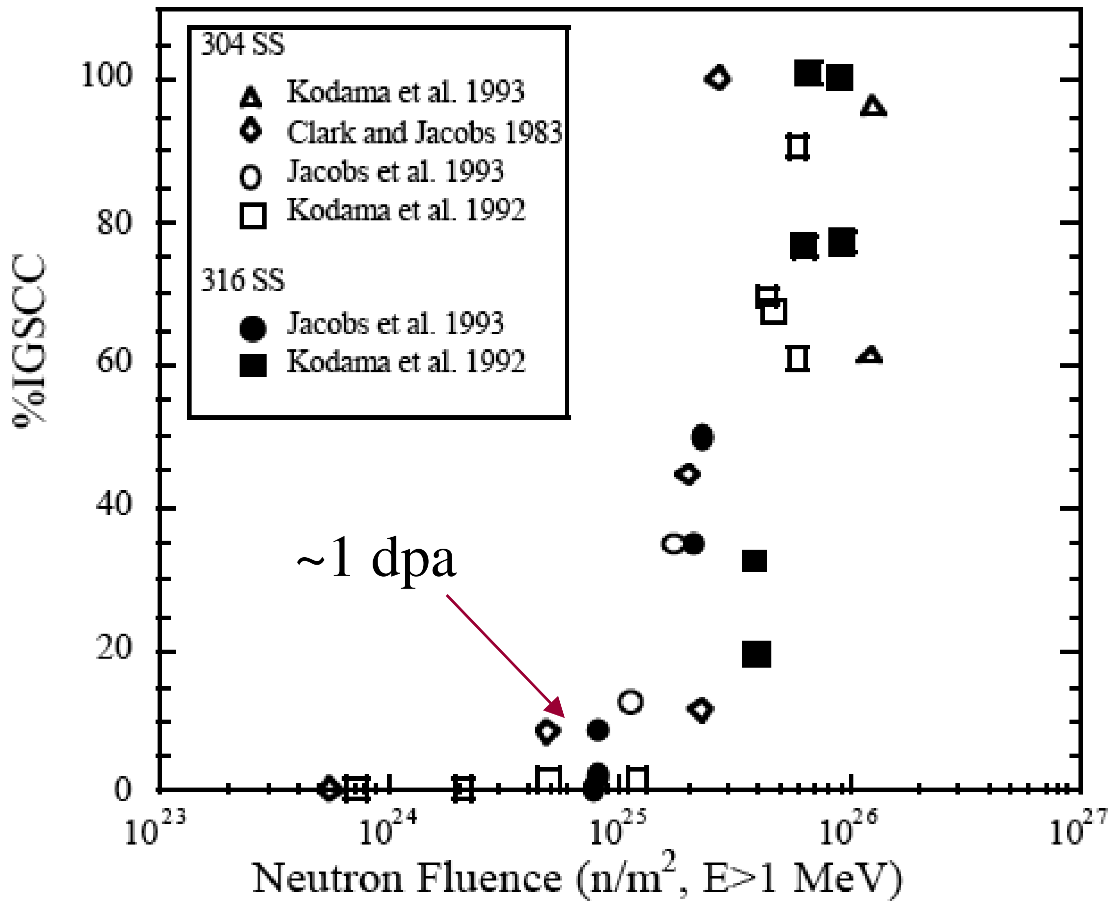


S. M. Bruemmer, 2001 Env. Deg. Conf

- EPRI believes improved IASCC predictive capability could save \$100K-\$500K per plant per year

- Similar mechanism may be present for Gen IV SCWR, LFR or water-cooled fusion

Dose Effect-BWR

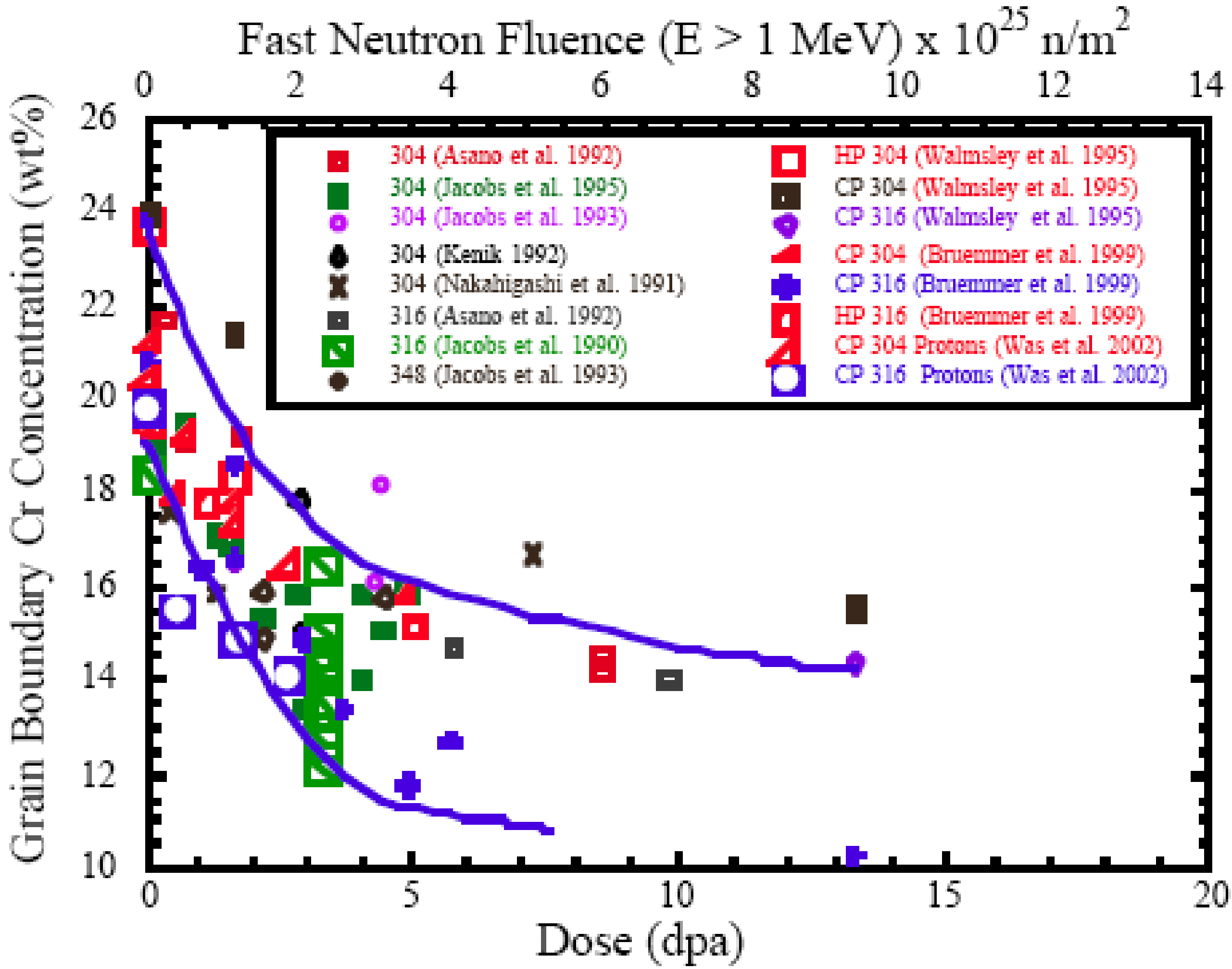


- IASCC susceptibility increases at higher fluence
- transition occurs at higher dose in PWR

G.S. Was, 2003 Env. Deg Conf

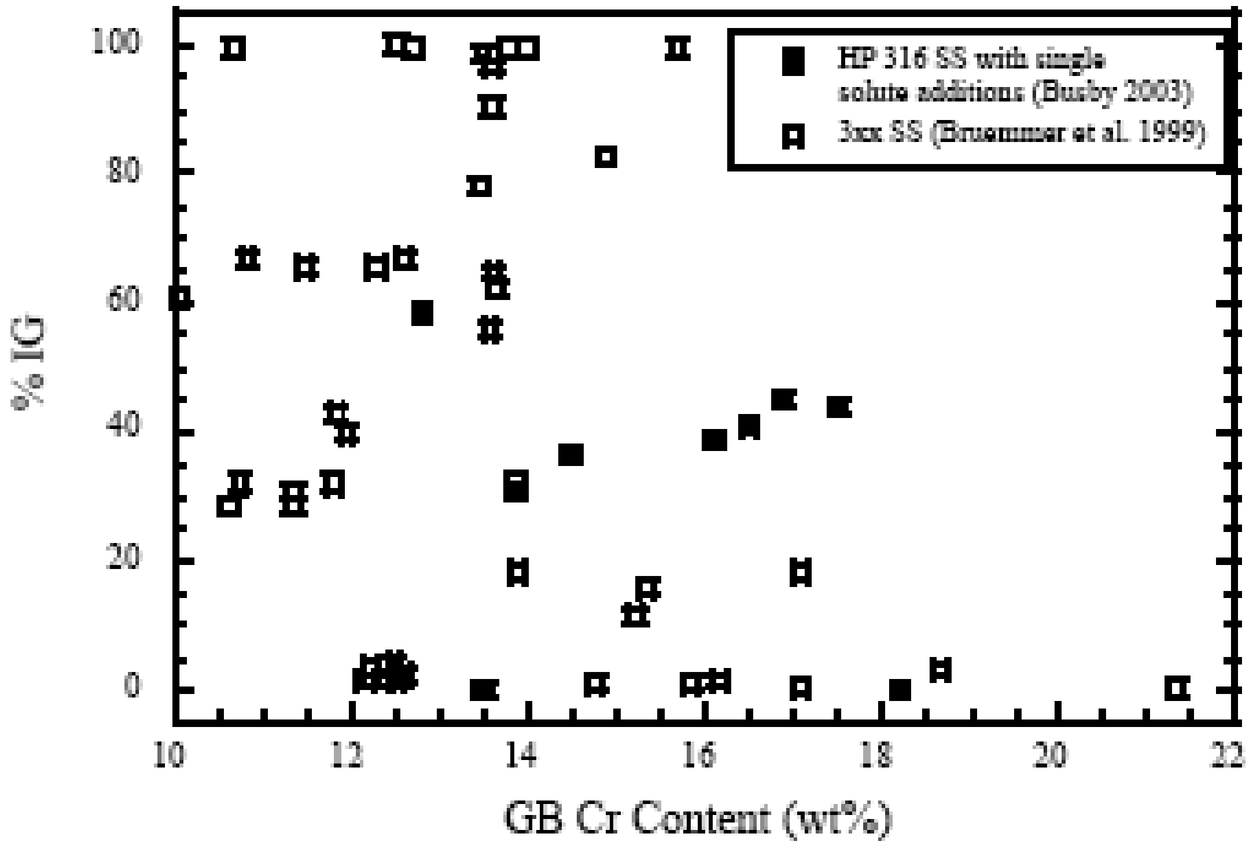
Grain Boundary Segregation

DEPARTMENT OF Engineering Physics
College of Engineering University of Wisconsin-Madison



G.S. Was, 2003 Env. Deg Conf

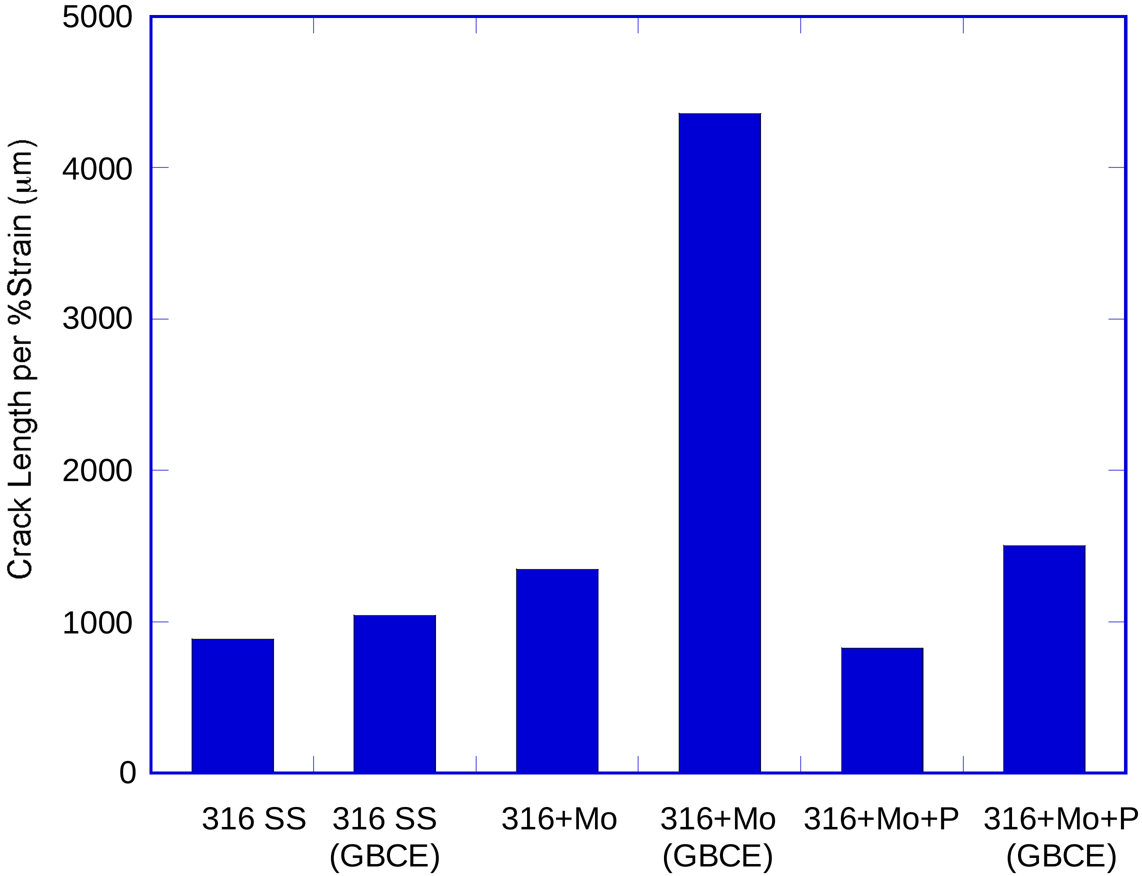
Grain Boundary Segregation



G.S. Was, 2003 Env. Deg Conf

Grain Boundary Cr Enrichment

Department of Engineering Physics
College of Engineering University of Wisconsin-Madison

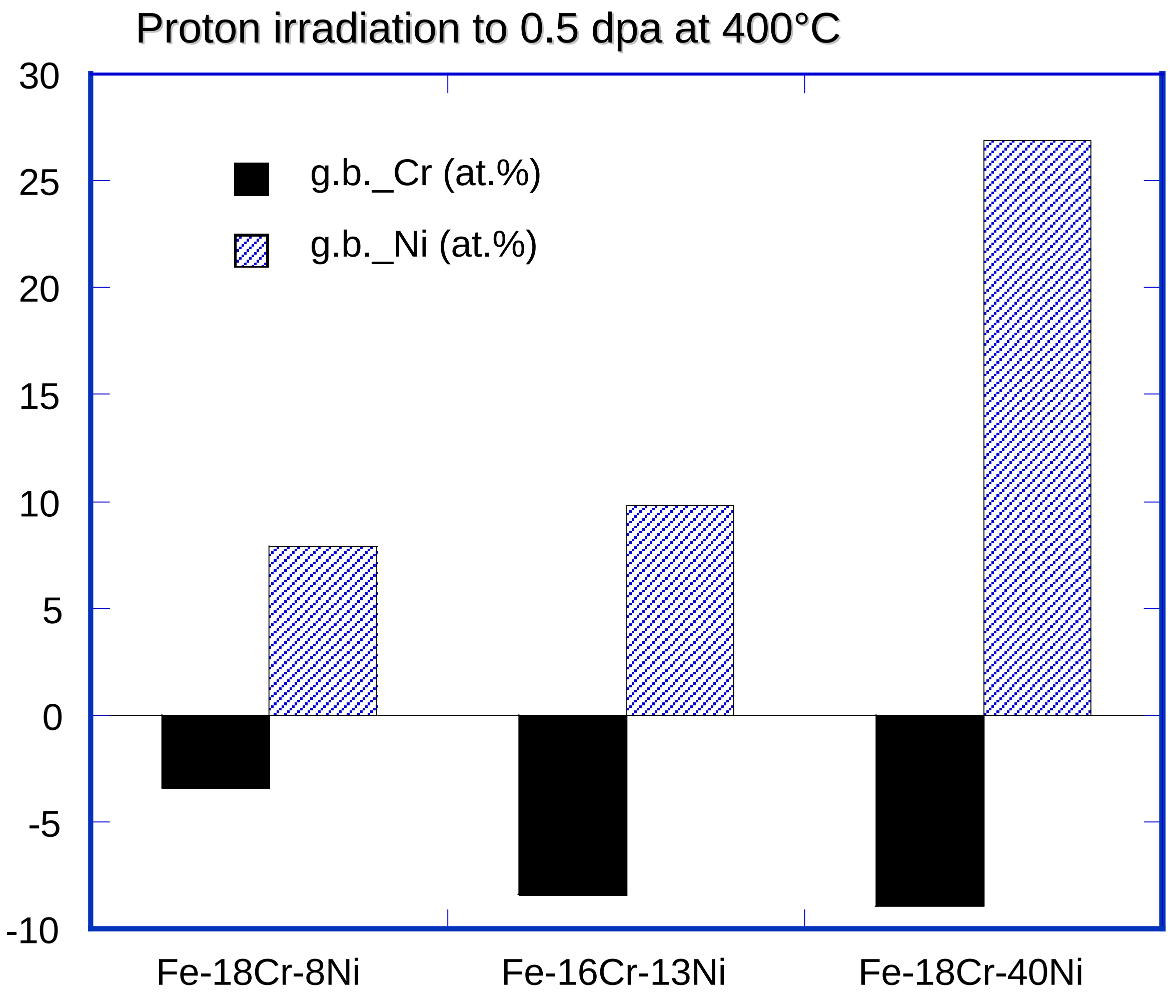


- GBCE=Cr pre-enrichment prior to irradiation

- In no case did Cr enrichment prior to irradiation reduce cracking

J. I. Cole & G.S. Was, NERI 02-0110

Effect of bulk Ni on RIS



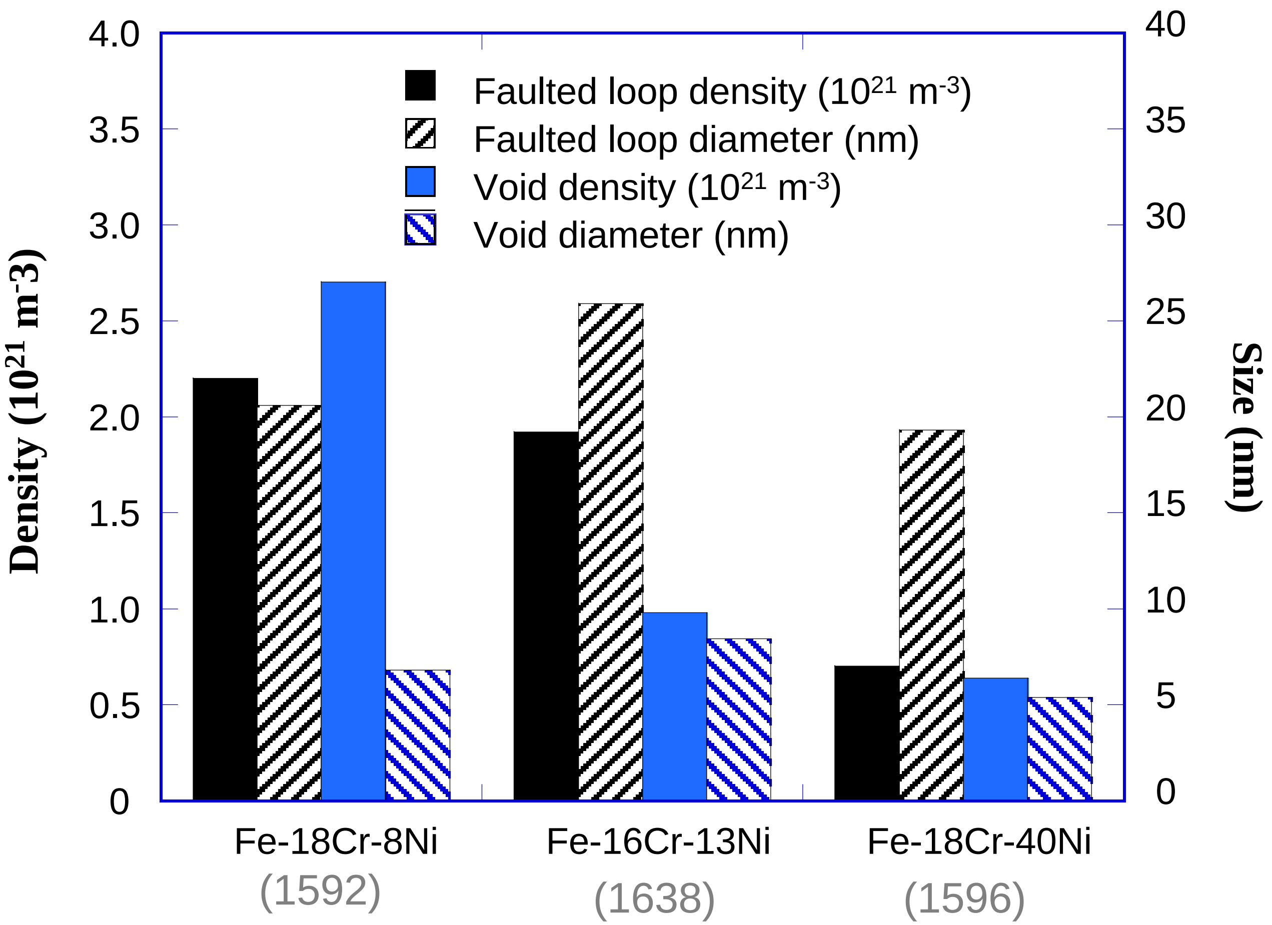
- RIS has a complex dependency on composition

- Current models just beginning to address compositional effects

T. R. Allen, NERI 02-0110

Effect of bulk Ni on microstructure

Proton irradiation to 0.5 dpa at 400°C

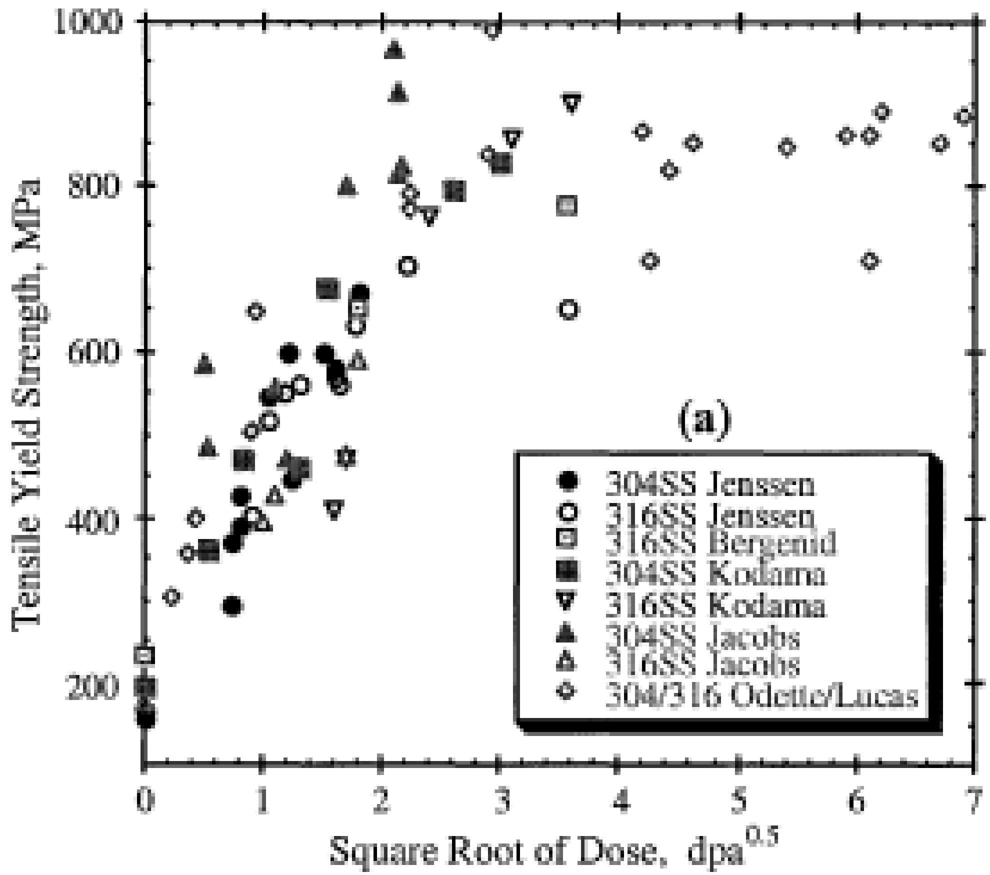


- Microstructural development has a complex dependency on composition

- Models need to address compositional effects

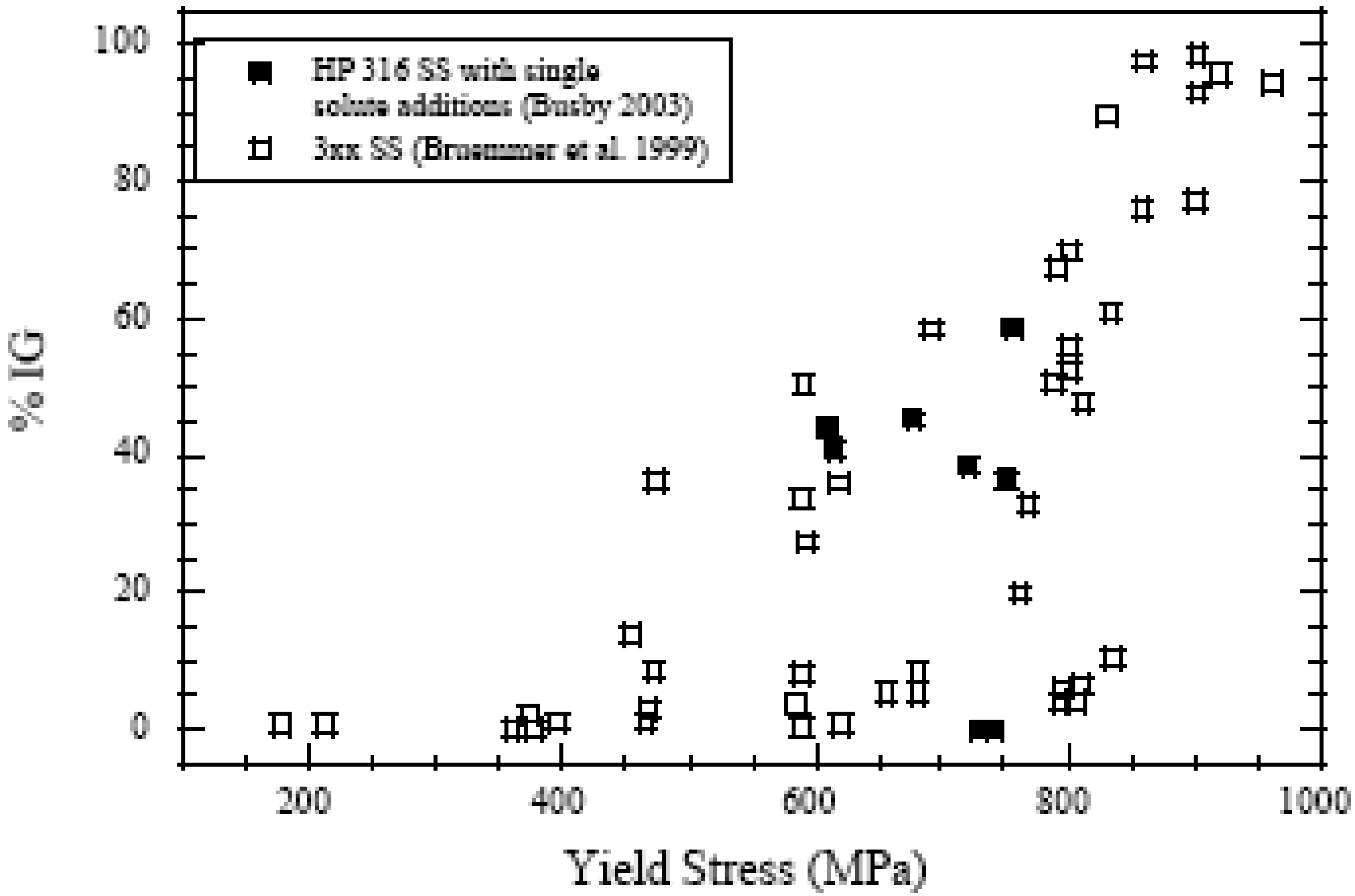
J. I. Cole and J. Gan, NERI 02-0110

Hardening



S. M. Bruemmer, 2001 Env. Deg Conf

Hardening

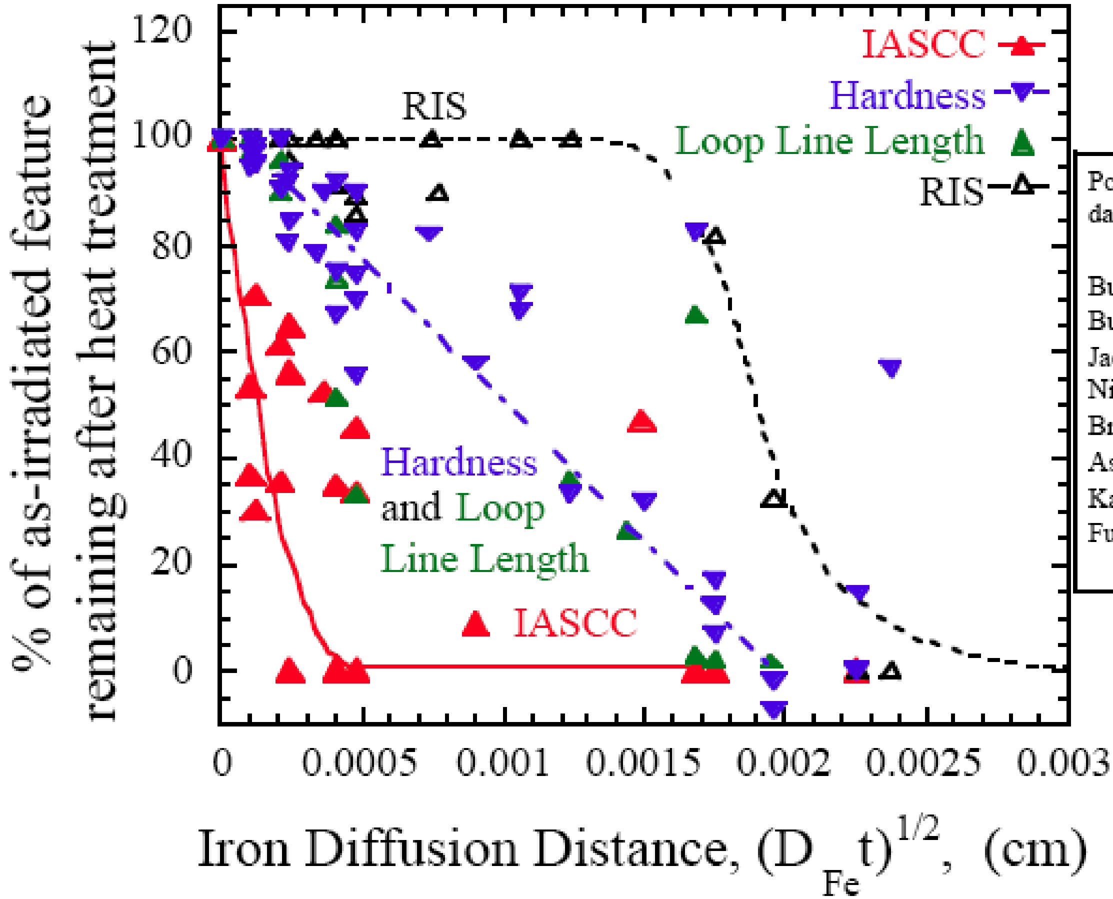


G.S. Was, 2003
Env. Deg Conf

- For a given corrosion potential, CGR is similar for materials with similar strength (cold-work or irradiation)

Annealing

Department of Engineering Physics
College of Engineering University of Wisconsin-Madison



Post-irradiation annealing data from

Busby: 304, p, 360°C, 1 dpa
Busby: 304, p, 360°C, 2.5 dpa
Jacobs: 304, n, 288°C, 2.5 dpa
Nishimura: 316, n, 288°C, ~11 dpa
Bruemmer 316, n, 288°C, 1.7 dpa
Asano: 304, n, 288°C, ~17 dpa
Katsura: 304, n, 288°C, ~11 dpa
Fukuya: 304, n, 320°C, ~25 dpa

G.S. Was, 2003 Env. Deg Conf

Summary

- rate theory models can be successfully applied to investigating radiation effects in materials at the mesoscale, intermediate link in multiscale chain
- relative success is qualified by knowledge that simplified models often hide an insufficient physical basis in their parameter choices
- extrapolation/interpolation of He, H-effects remains problematic, He partitioning and the influence of He on cavity density is critical
- resolving the complexity of IASCC involves synergistic effects of chemical (aqueous) environment, stress state, and irradiation on the microstructure
  - critical factors include radiation-induced hardening and solute segregation,