Modeling Deformation and Fracture

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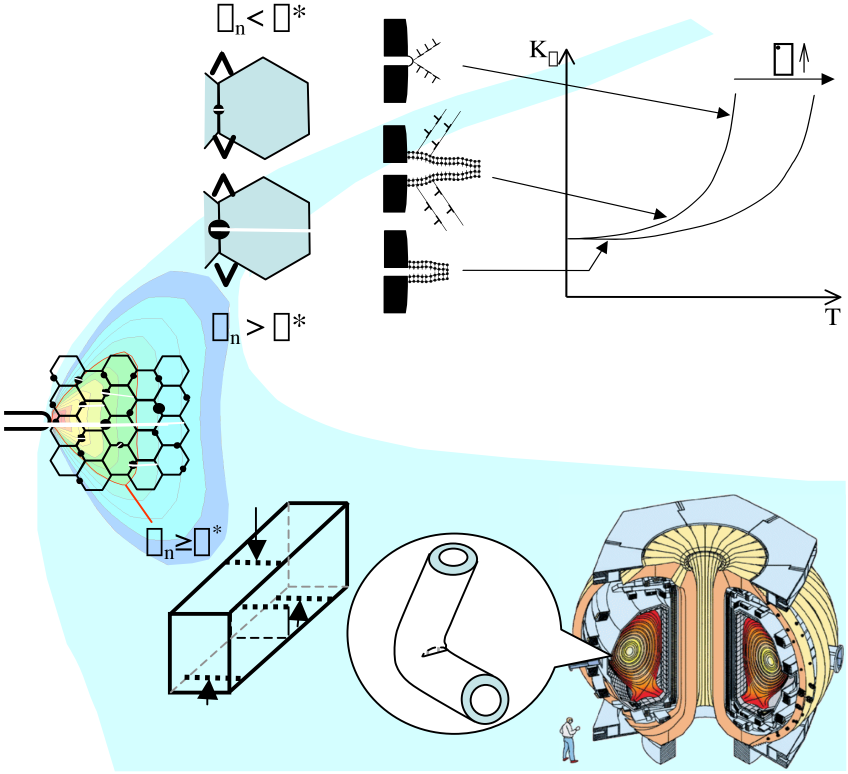
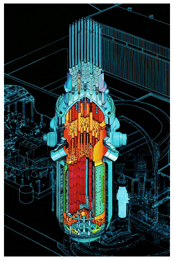
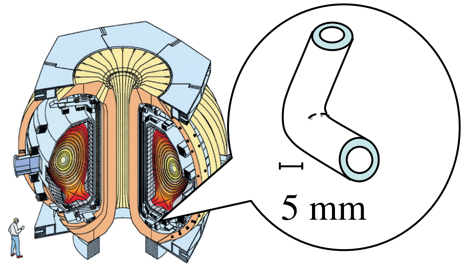


DOE SC-NE Workshop on Advanced Computational Materials Science:
Application to fusion and Generation-IV Fission Reactors
March 31 - April 2
Washington DC

The Challenge

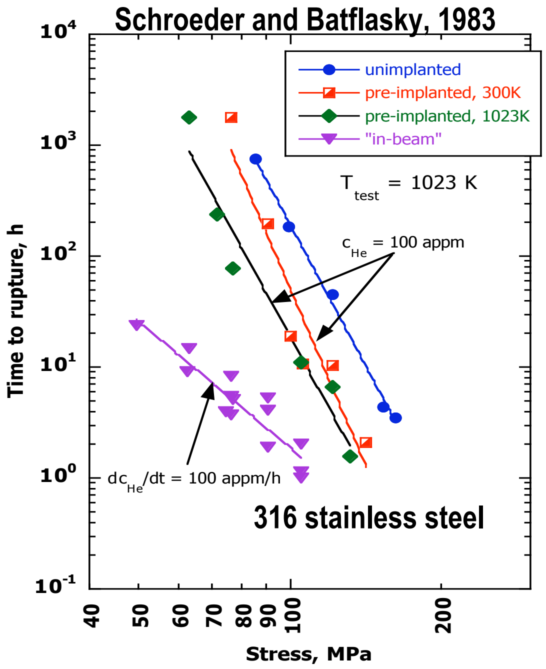
- Development of reliable and long-lived fusion structures may be the greatest engineering challenge of all time due to unprecedented demands on materials related to:
  - high heat fluxes and time varying thermal-mechanical loads on heat transfer structures with large, complex, interconnected geometries involving intricate materials systems
  - in-service degradation of a host of performance sustaining mechanical properties, internal damage development, macroscopic cracking, corrosion and dimensional instabilities.
  - numerous synergistic and hard to predict potential failure paths
  - requirements for high reliability, long life and large demonstrable safety margins.
- Many issues shared with advanced fission/accelerator based technologies
- Need to reliably predict in-service properties

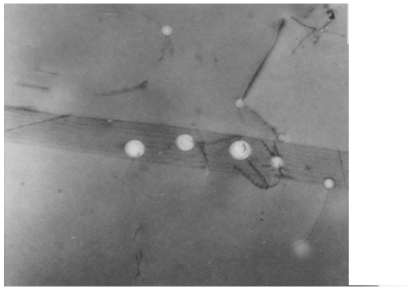




‘Properties’

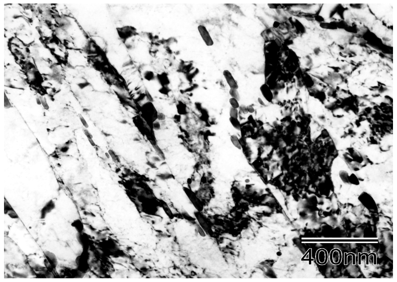
- Static (but rate dependent) constitutive & fracture ‘properties’ controlled by the evolved in-service microstructure
  - yield strength and strain hardening, ‘ductility’, fatigue crack growth rates & fracture toughness
- Time/history dependent properties where stresses, displacement defects, He, ... control the microevolutions & macro-damage
  - thermal and irradiation creep & rupture, thermo-mechanical fatigue, creep crack growth, creep-fatigue, environmentally assisted cracking, …
- ‘Properties’ often influenced by extrinsic factors in both coupon tests & structures and properties interact in complex materials systems.

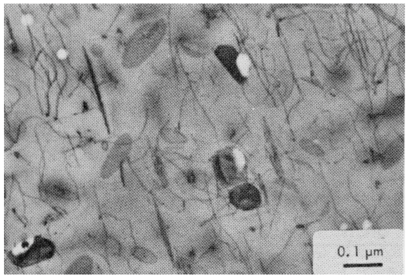




In-Service Property Changes

- Structural materials have very complex, multi-constituent, multi-phase, highly defected, non-equilibrium micro-structures that mediate an array of complex mechanical properties.
- Combinations of many environmental and material variables control microstructural and property evolutions
- Governing processes involve enormous degrees of freedom, are inherently □ multi-scale (time/ length) with many mechanisms (multi-physics) that act in parallel, series and in opposition - critical outcomes often depend on small differences between large competing effects (e.g., void swelling)


Unirradiated F82H


Radiation Damaged SS

Physically Based Property Change Models

- Objective - develop physically based property change (□P) models accounting for the combination of material and environmental variables statistically fit to high quality databases to provide *reliable interpolation and extrapolation*.

  □P = f_{model}[T_i, dpa, dpa rate, He, H, stress, .. , alloy,
  composition, microstructure/microchemistry, ..]

- Need *iterative cycles* of modeling and various kinds of experiments to build *understanding* and a *knowledge base*.

Experiments ↔ Multiscale Phenomena ↔ Models

Mechanisms Controlled single-combined variable Integrated (verification)	Atomic properties Mechanisms and processes Functional properties

The Good News

- Challenges cross cut technologies/materials
- Depend on 'common' microstructures.
- Enormous opportunity to integrate models and experiments - not only for 'validation' but to build understanding.
- Models can most often be hierarchical.
- Hierarchical, physics-based atomic to structural scale *model designs* will be critical to success.
- Useful knowledge and models can be developed <u>without</u> perfect theory.
- Strategy - roadmap answers to well-posed questions

Multiscale Fracture Models

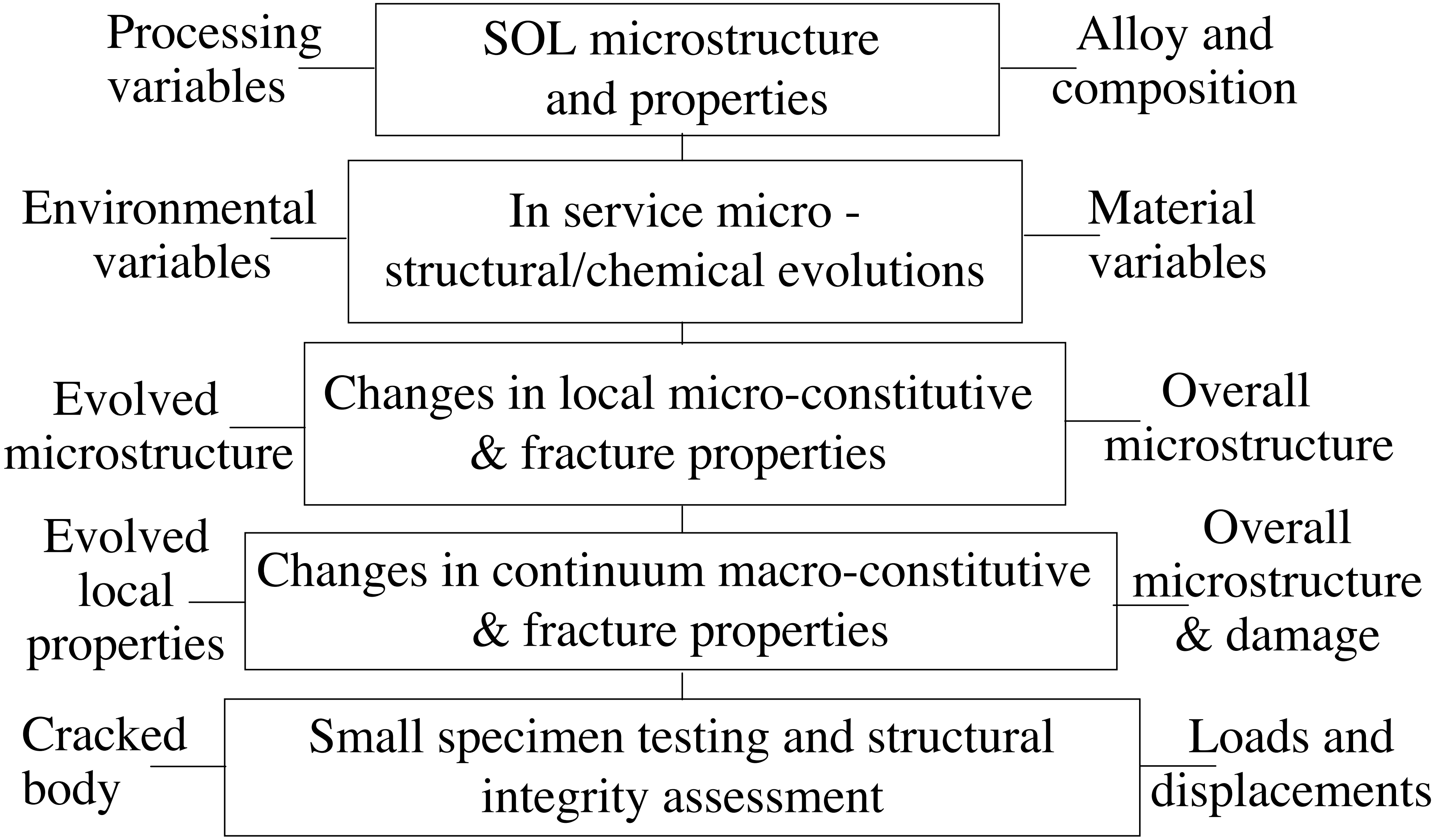
Critical structural fracture loads & displacements controlled by □(□), K_{Je}
FE models

Crack tip stress & strain fields controlled by □(□), K_J & cracked-body size & geometry
FE models

Critical crack tip stress fields controlled by □□-V* - hence by microstructure & microcrack arrest toughness
FE & dislocation models

Microcrack arrest toughness controlled by intrinsic shear strength of the bcc ferrite lattice
FE, dislocation and molecular dynamics models

Hierarchical Modeling Approach



Processing variables

SOL microstructure and properties

Alloy and composition

Environmental variables

In service micro - structural/chemical evolutions

Material variables

Evolved microstructure

Changes in local micro-constitutive & fracture properties

Overall microstructure

Evolved local properties

Changes in continuum macro-constitutive & fracture properties

Overall microstructure & damage

Cracked body

Small specimen testing and structural integrity assessment

Loads and displacements

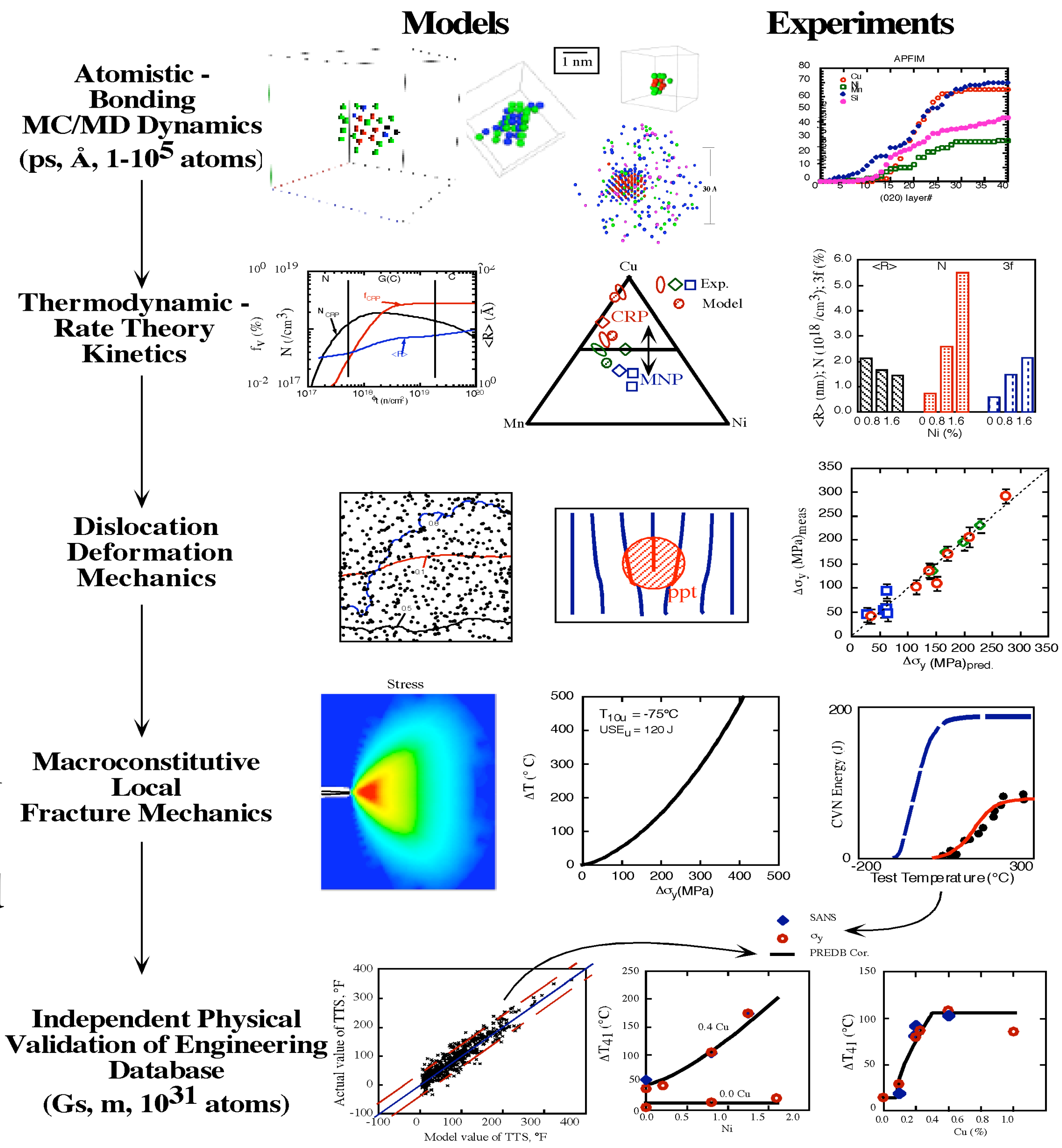
Modeling-Experiment Integration

Processing models	SOL microstructure and properties	Comprehensive characterization
Electronic, MD, MC, rate theory	In service micro - structural/chemical evolutions	TEM, PAS, APT SANS, ASAXS
MD, DD, micromechanics	Changes in local micro-constitutive & fracture properties	In-situ TEM, CM, micromechanics
FE models of fields/tests	Changes in continuum macro-constitutive & fracture properties	Innovative testing
VISTA, new methods	Small specimen testing and structural integrity assessment	Semi-scale testing

MS-MP Modeling of RPV Steel Embrittlement

Multiscale Multiphysics Modeling of Irradiation Damaged Materials:Embrittlement of Pressure Vessel Steels, R. Odette, B. Wirth,, N. Ghoniem and D. Bacon, *MRS Bulletin*, March 2001

Developing more formal integrated MS-MP models in the REVE and PERFECT projects



Models

Experiments

Atomistic - Bonding MC/MD Dynamics (ps, Å, 1-10^5 atoms)

Thermodynamic - Rate Theory Kinetics

Dislocation Deformation Mechanics

Macroconstitutive Local Fracture Mechanics

Independent Physical Validation of Engineering Database (Gs, m, 10^{31} atoms)

Key Nearer Term Crosscutting Issues

- Irradiation effects on true-stress strain constitutive laws, the causes & consequences of flow localization and their combined implications to effective ‘ductility’.
- Validity & physical basis for the Master Curve (MC)-Shifts (ΔT_o) method for measuring/applying fracture toughness:
  - a universal fracture toughness temperature MC shape
  - size and geometry effects on effective fracture toughness
  - embrittlement - MC ΔT_o shifts due to synergistic hardening and non-hardening mechanisms including He & H effect.
- Model based design of high performance radiation resistant alloys managing displacement and transmutant gas damage.

Key Nearer Term Crosscutting Issues

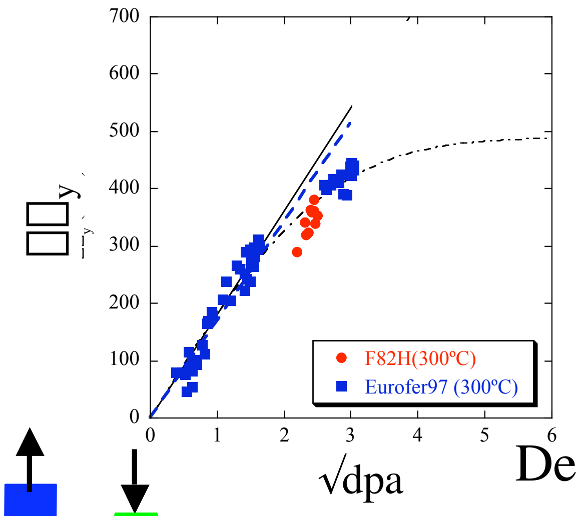
- High temperature creep/creep rupture including He effects.
- Dimensional instabilities due to possible void swelling and *irradiation creep* including He and H effects.
- Multiphysics models of time-dependent structural loading /deformation based on advanced constitutive-failure - models and integrity assessment methods -- Virtual International Structural Test Assembly (VISTA).
- Development of models for high performance, high temperature materials (alloys, ceramics and composites) with good balance of properties including processing, manufacturing and joining.
- Other very important but more complex properties later - tackle modeling later?

Irradiation Effects on Constitutive Properties

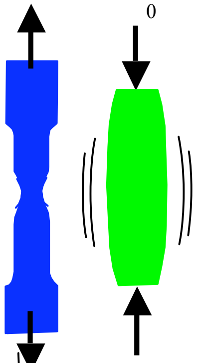
- Continuum true stress-strain hardening □(T_t, □) constitutive and plasticity (J_2?) laws linked to microstructural evolution models (T_i, dpa, …).

$$\square = \square_{yt}(\square,T) + \square_{ya} + \square_{sh}(\square,\square,T)$$

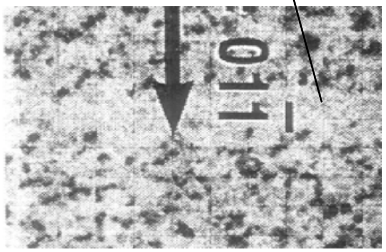
- Harmonization of continuum, crystal plasticity, dislocation dynamics and obstacle interaction views on the causes and consequences (‘ductility’ for various geometries) of micro-flow localization and relations to experimental observables.

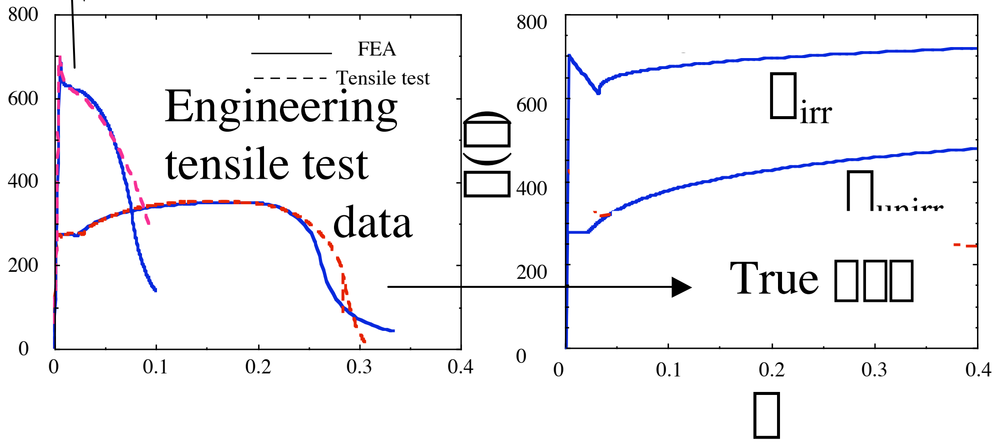


500MPa for
$T_i = T_t = 300°C$



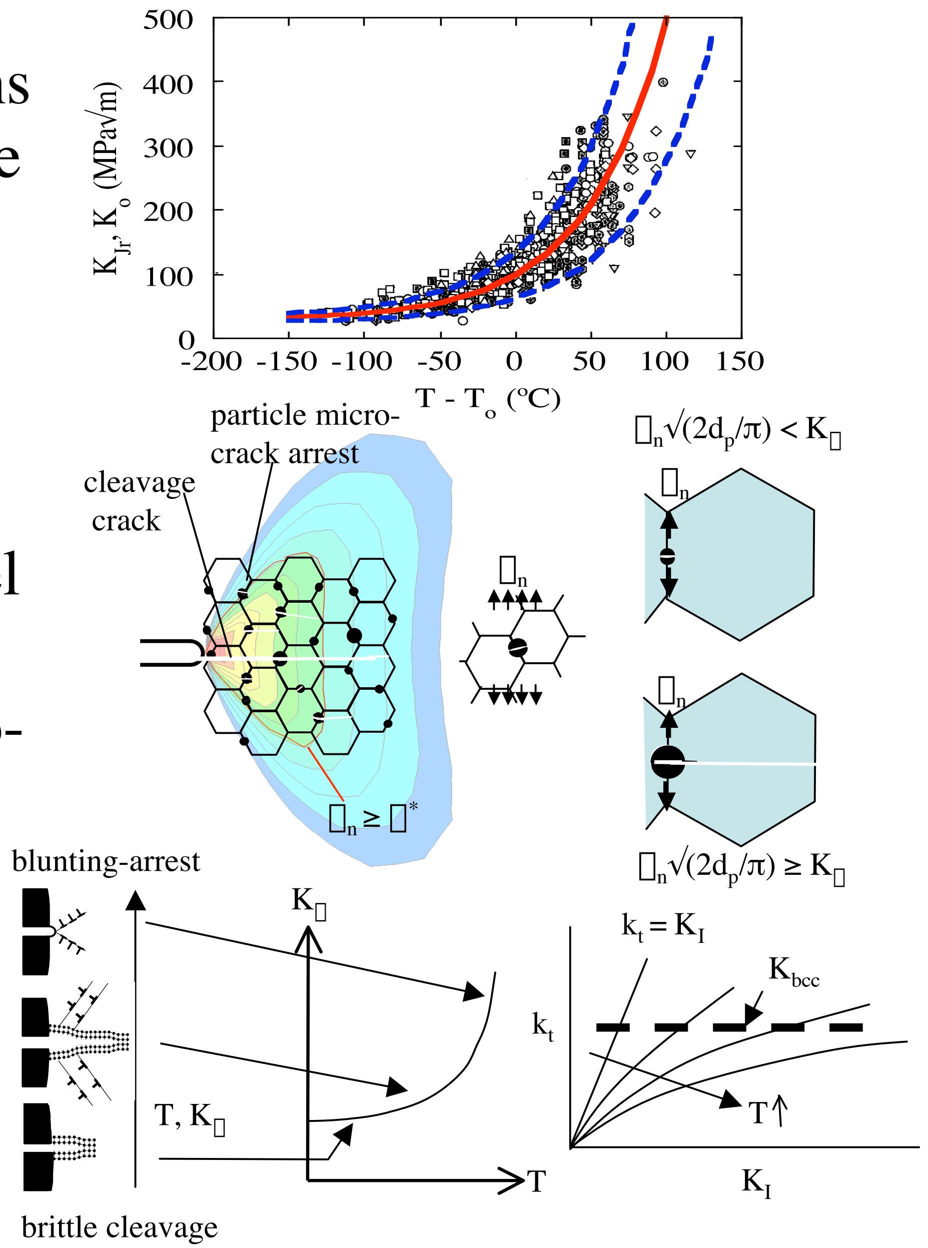
Defect free channel





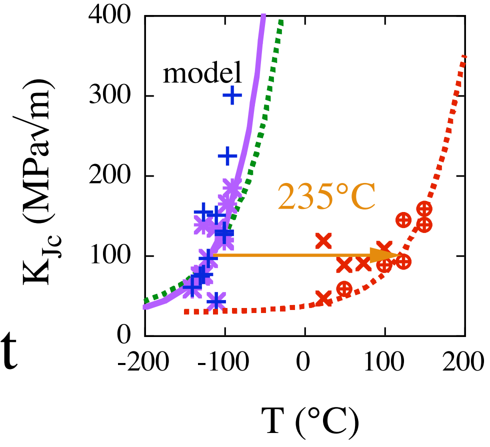
Physical Basis for a Master Toughness Curve

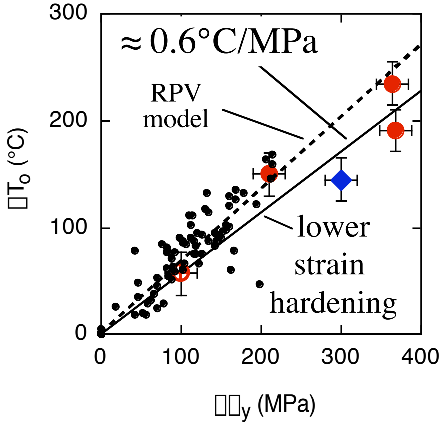
- MC method uses small specimens and ΔT models to predict fracture in large/complex structures.
- The universal (?) shape of the fracture toughness-temperature $K_{Jc}(T)$ curve is not understood.
- Need integrated multiscale model including atomic scale processes that valve the much larger macro-continuum $K_{Jc}(T)$ toughness.
- Key is experiments & MD + DD models of intrinsic BCC micro-arrest toughness at a nanoscale tip of a dynamic microcrack?

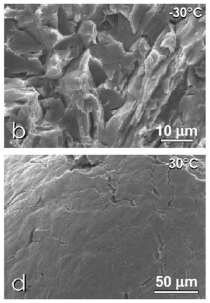


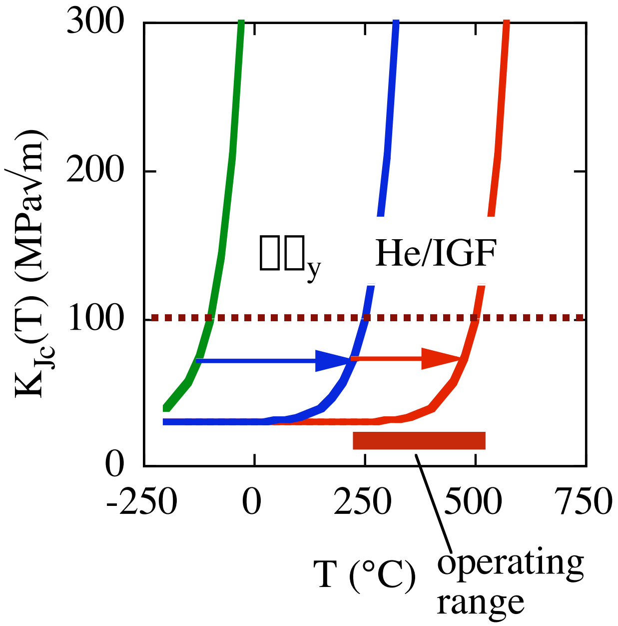
Master Curve Shifts (ΔT_o) and He Effects

- Modeled irradiation hardening ($\Delta\sigma_y$) induced $\Delta T_o \approx 0.6$°C/MPa.
- Peak hardening up to ≈ 600 MPa => large ΔT_o => $T_o \geq 250$°C.
- Spallation proton data suggests at > 600-800 appm He weakens grain boundaries producing very brittle intergranular facture that interacts synergistically with $\Delta\sigma_y$.
- Estimates of combined effects suggest $T_o > 500$°C possible - clearly a show stopper!
- High concentrations of H may also be damaging



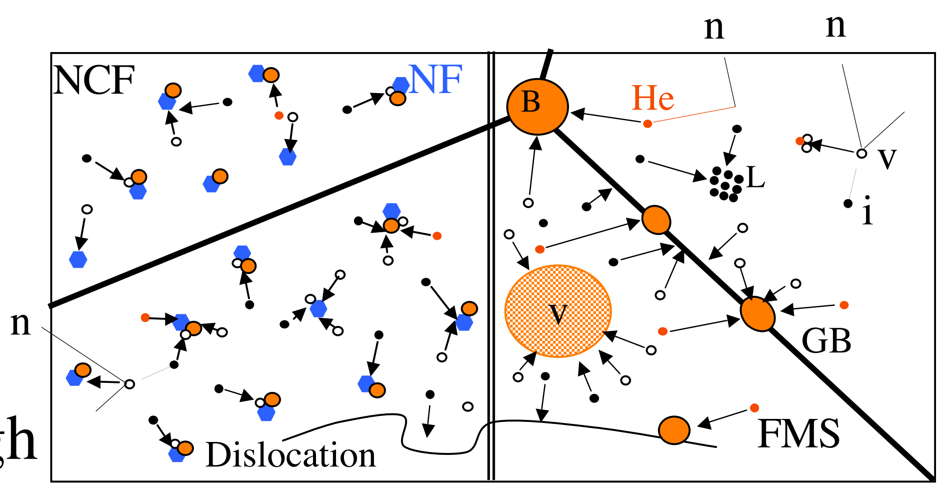


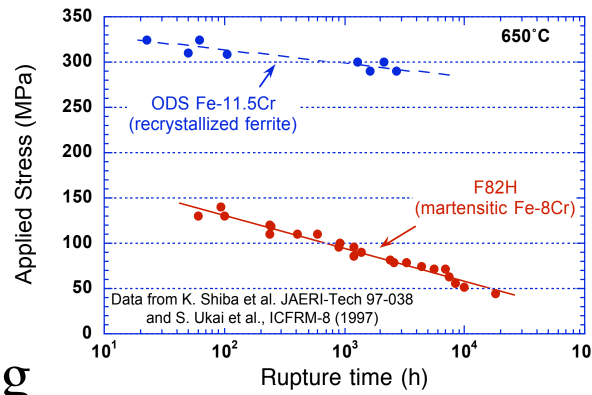




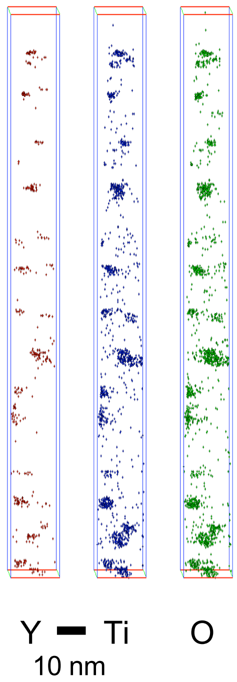
Model Based Design of Advanced Alloys

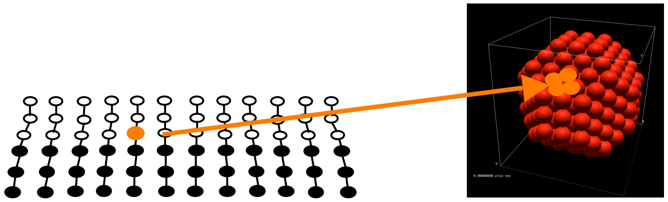
- Minimize displacement defect accumulation and protect grain boundaries from helium at both low and high temperature.
- Ultrahigh density of nanoscale solute clusters may provide high temperature creep strength while trapping helium in fine harmless bubbles as well as recombining vacancies and self-interstitials.
- Irradiation/thermal stability of the nanoclusters and interface trapping properties are critical.
- Balance of properties?





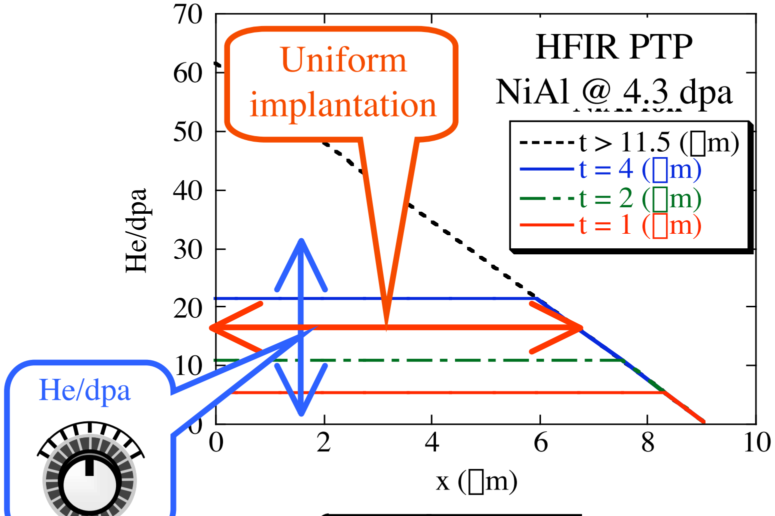
Data from K. Shiba et al. JAERI-Tech 97-038
and S. Ukai et al., ICFRM-8 (1997)

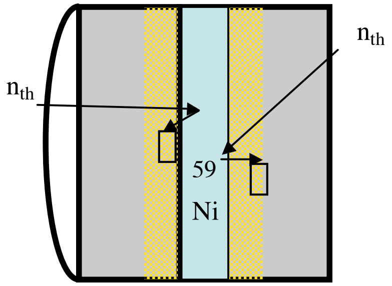




Transport, Fate and Consequences

- Overarching challenge is to understand model the *transport & fate* of alloy and radiation produced species and their *consequences* to properties - especially He (fusion).
- A comprehensive He fate model is under development but requires a large library of sub-models and material properties to be enabled.
- This model is being closely integrated with experiments, including an in-situ He implantation method providing controlled He/dpa ratios.





Basic He & He/dpa Mechanisms

- Diffusion & clustering kinetics with dpa.
- Trapping@dislocations/interfaces/boundaries,
- Sink strength effects and partitioning.
- Cluster/bubble sizes and stability
- Reaction to stress.
- He management.
- Model, FM and NCF alloys

Summary and Conclusions

- There are enormous opportunities to develop physically based models for better predictions of in-service properties of reactor materials.
- Developing such models is not an option -- it is an imperative.
- Advanced simulation tools will make important contributions.
- But, there are *no magic bullet* even with ‘perfect’ potentials and access to enormous numbers of computer cycles.
- We must embed *understanding* of complex physics in hierarchical models based on carefully planned development of sub-models and close integration with experiment.
- Efforts to develop such a *knowledge base* are on the cutting edge of materials science and will have a wide impact.