An Introduction to Materials, Properties and Microstructures:an Integrated Experiment-Modeling Paradigm

presented by

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Fusion Program Review

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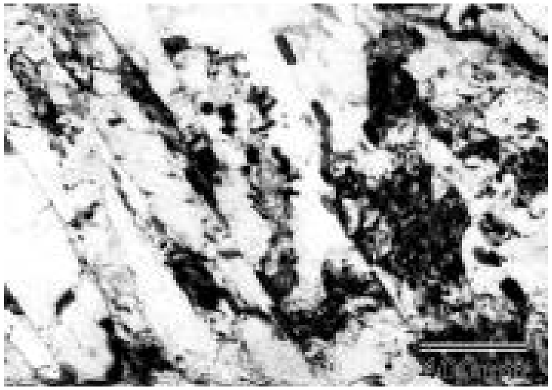
Microstructure Based Performance

- Fusion power will require knowledge of essentially all conventional material properties and then some -properties, in-service component failures controlled by combinations of many variables.
- An expose-test-extrapolate approach is not viable.
- The start-of-life(SOL) and service-evolved microstructure is the most practical unifying basis for:
    - selection of alloy systems
    - in-service performance and property predictions
    - development of improved high - performance materials
    - understanding
- The FMS program is committed to a microstructural underpinning in developing a long-term knowledge base.

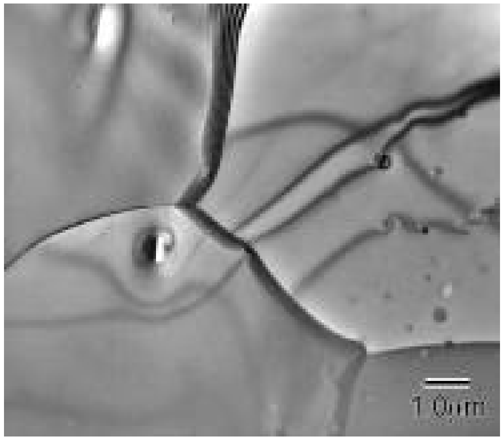
Tempered Martensitic (8Cr) Steels (TMS)

- Low activation (Mo to W), swelling resistant (high He?) F82H variants evolved from 12Cr (HT-9) and 9Cr (Klueh-T91) fossil-breeder steels.
- Lower Cr (≈ 8%) Q&T martensite reduces embrittlement by avoiding fine scale α’. Microalloying (e.g., Ta) for creep strength and grain size control.
- Medium strength tempered martensite - a high sink-density dislocated lath-packet-PAG & primary W, Cr-rich carbides.
- Low-T embrittlement limits and high-T by creep, corrosion, instabilities & brittle (e.g., Laves) phases.
- Large programs in Japan, Europe and coordinated IEA activity - US view as a complex heat treatable model alloy.



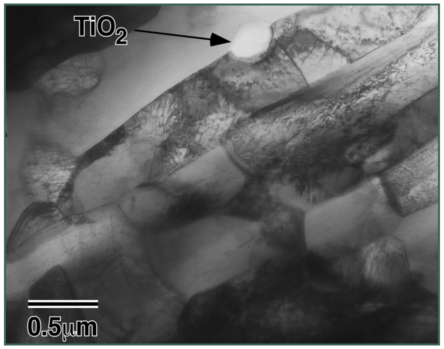
Solid Solution V-4Cr-4Ti (SSV)

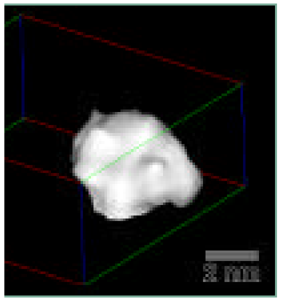
- A relatively low Cr-Ti solid solution ANL alloy balancing strength (≈ 325 MPa), *toughness* and swelling (high He?).
- High temperature extrusion, hot/cold rolled, recovered-recrystallized to approximately equiaxed, low dislocation, low sink density structures.
- Primary ‘phases’(inclusions) TiOCN with impurity O and N (100-1000 ppm).
- Limits - low T by embrittlement and at high T likely by He creep embrittlement. Requires Li coolant-O control and an an electrically insulating coating.
- Ongoing US focus, emerging interest in Japan - US view as a ‘simple’ model refractory.



Nanocomposited Fe-Based Alloys (NCF)

- High temperature, creep resistant Fe-based alloys evolved from powder processed MA956 & 957 breeder candidates.
- Typically master alloy (Fe-12-14Cr-2W-Ti) and Y_2O_3 powders high energy milled and hot extruded:
  - highly textured very fine grain structures, impurity inclusions, high recovery temperatures - hence, poor non-isotropic properties.
- High creep strength provided by fine scale Y_2O_3 dispersoids plus even finer nanoscale coherent transition phases-clusters.
- Advanced alloy focus worldwide with variants and alternatives





POSAP image of
Y-O-Ti-nanocluster

Fusion Environment & Performance Goals

- At 15 MW-yr/m^2 at first wall:

  ≈ 170 dpa; ≈ 800-1800 appm He; ≈ 4000-7500 appm H

  plus variety of solid transmutation products.
- High cyclic heat flux, primary and secondary loading and high rate disruption events.
- Large, complex, joined structures with thermal-stress-property gradients and ubiquitous dimensional instability by irradiation creep.
- Other material and system issues of corrosion, coatings, compatibility, magnetism ....
- No detailed and stable system design objectives - but reliability and safety paramount.

Rationale for Base ‘Model’ Systems

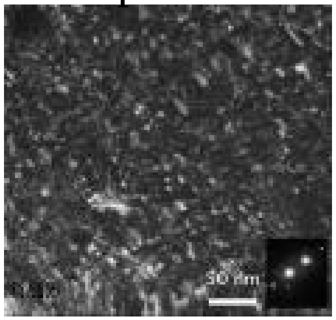
- No current, narrow near-term path for engineering alloy *development*.
- TMS - Low activation, good SOL toughness-strength combination, swelling resistant (He?), large technology base for processing-fabrication-joining, potential for optimization. Evolutionary-replacement approach leading to long-term power systems development that is initially tolerant of limited efficiency.
- SSV - Low activation, good SOL toughness, lower strength is compatible with better thermal properties (low stress), swelling resistant, high T creep strength,
- NCF - potential for optimized combination of properties and high temperature strength (also tailored mutliphase V-based alloys?)

Properties - Key Cross-Cutting Issues*

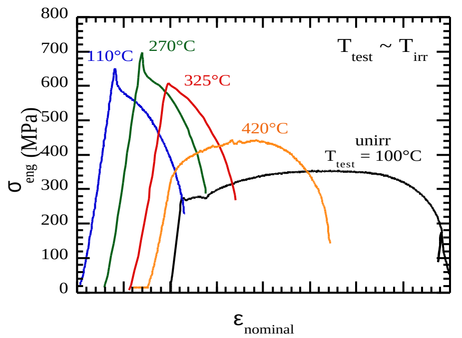
- Emphasis on some (not all) cross-cutting or viability issues
- SSV, TMS, NCF
  - *flow:* Low-T hardening, loss of uniform strain, softening at high T, irradiation creep and swelling (He?), thermal creep
  - *fracture*: Low-T irradiation embrittlement (impurity, thermal, He, H), high-T He creep embrittlement
- System
  - coatings (particularly SSV)
- Lower or deferred priority
  - corrosion, compatability
  - fatigue in its various horrible forms

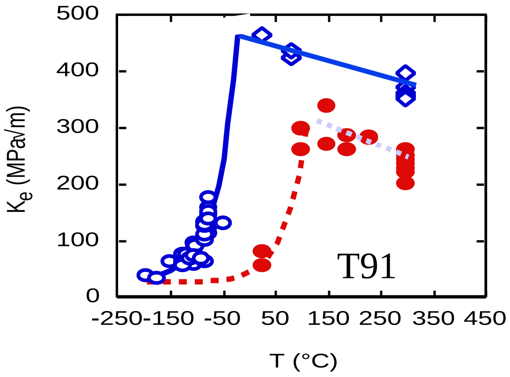
* See whitepaper proposing an integrated program of theoretical, experimental and database research

I-loops F82H



Effect of 0.4 dpa irradiation on σ(ε) curves





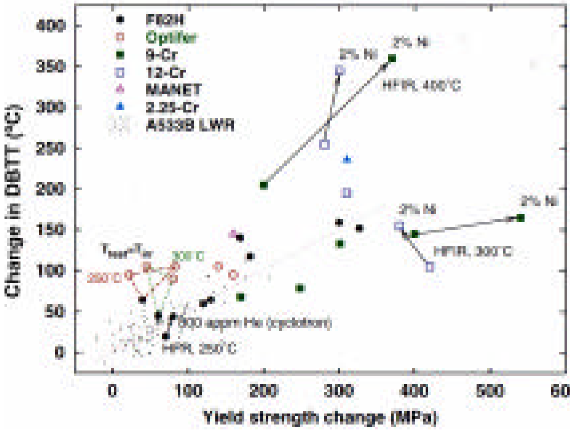
Irradiation Processes and Microstructures

Alloy	Dominant Features & Processes	Property Consequences	Issues*
TMS	**loop-complex, bubbles nano-ppts (?),voids (?)**	**harden, low e_u, embrittle, $\Delta V/V$(He)?**	**little control, can mitigate embrittlement?, $\sigma/\Delta\sigma$? He?**
	bubbles, coarser ppts, voids, some recovery	softening	$\sigma/\Delta\sigma$? He?
	structural instability, gb bubbles, brittle phases	softening & embrittle	$\sigma/\Delta\sigma$? He? not very pertinent
SSV	fine loop-complex & ppts (TiCON), bubbles	hardening, low e_u, embrittle, $\Delta V/V$(He)?	interstitial impurity effects? $\sigma/\Delta\sigma$? He? pertinent?
	bubbles, voids(?), O, N-pick-up and phases	T_{low}?, $\Delta V/V$ (He)? impurity embrittle	system
	gb bubbles, O, N-pick-up and phases	**creep rupture, impurity embrittle**	**system, require helium management?**
NCF	loop-complexes, bubbles α'-ppts, voids (?)	hardening, low e_u, embrittle, $\Delta V/V$(He)?	α' higher Cr, SOL K_e lower?, pertinent?
	bubbles, cluster irradiation stability?	soften?	??
	bubbles, gb bubbles? cluster stability	soften? poor creep rupture?	??

*** General issue: temperature-time history effects and irradiation creep.**

Low-Intermediate T He Effects

- Controversy regarding a possible effect of to date ‘modest’ He levels on hardening regime fast fracture will be resolved in upcoming US-JAERI experiments. Balance of data and understanding suggests the effect small to moderate.
- Possible effects on high He on void swelling. Innovative dynamic helium charging and isotopic tailoring experiments have shown enhanced bubble formation but no major effect on void swelling.
- The high dpa (> 30 dpa) and very high He (> 100 ppm) regime unexplored.
- Near term emphasis basic evaluation and mechanisms.



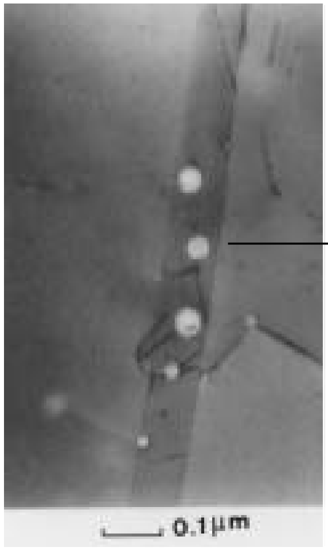
Producing High Helium

- Fission reactors (φ_{th}, φ_{epi}, φ_{fast}) with spectral tailoring and alloying-doping with isotopic tailored $^{10}\underline{\mathrm{B}}$ /$^{11}\mathrm{B}$, $^{58}\underline{\mathrm{Ni}}$/$^{60}\mathrm{Ni}$, $^{54}\underline{\mathrm{Fe}}$/Fe
- In-situ implantation (foils)
- Ion beams
- Spallation sources (p and n)
- High energy neutron sources
- Note - high helium effects of interest to advanced fission reactor and accelerator technologies

$^{58}\mathrm{Ni}(n_{th},\gamma)^{59}\mathrm{Ni}(n_{th},\alpha)$

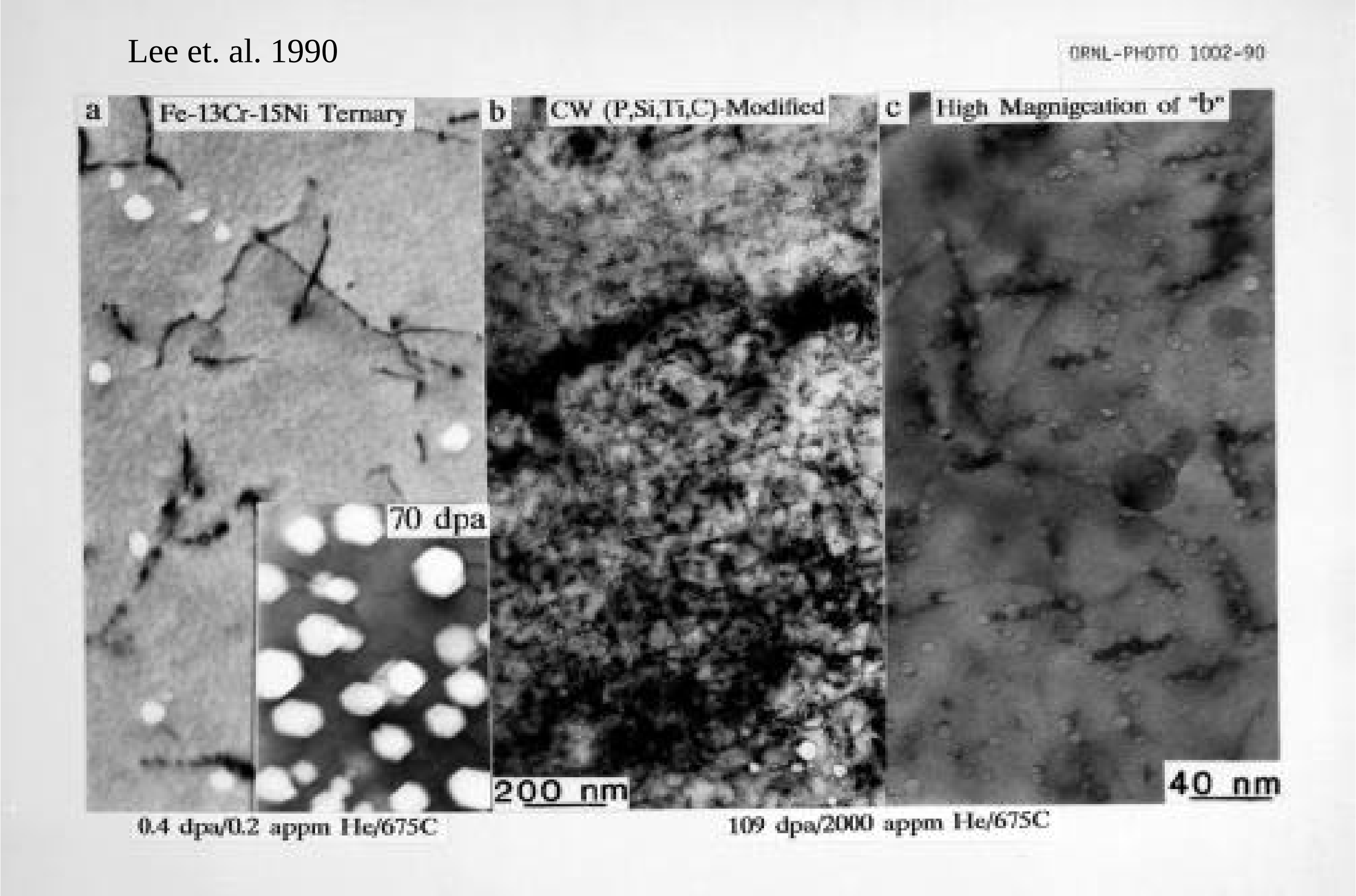
High T Helium Effects

- Potential for severe degradation of creep rupture (ductility and particularly life) at high He levels due to enhancement of GB cavitation. Thus He-management will be critical to developing high-performance high-T alloys.
- Based on austenitic alloy experience, best strategy is to sequester He in small-stable bubbles at interfaces of stable fine scale designer phases. High trap sink density necessary not sufficient. Careful balancing and optimization of the overall dislocation, grain-subgrain, matrix and grain boundary precipitate microstructures.



He bubbles

He Trapping on Phosphides



Lee et. al. 1990

A New Paradigm

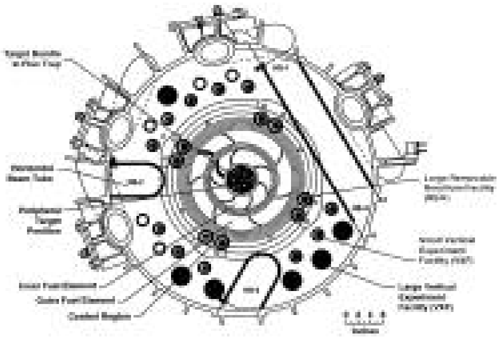
- Integrate modeling and designed single-variable (and combinations) and mechanism-type experiments (including characterization tools) based on sharply focused questions eminating from the underlying issues:

  - what processes control the transport, fate and consequences of helium, defects and solutes and how are these processes influenced by the SOL microstructure and alloy chemistry

  - best strategy to trap helium in fine stable matrix bubbles and recombine vacancies-interstitials, avoid segregation and maintain stable phases

Tools

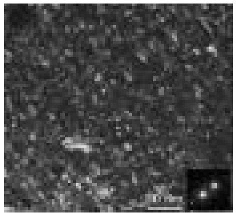
- Near term irradiations primarily in the ORNL High Flux Isotope Reactor (HFIR) using ‘tricks’ like spectral tailoring and elemental doping-isotopic tailoring to study He - lead up to a high energy neutron source.
- Specimens tailored to questions and PIE-characterization: mini to micro mechanical property, multipurpose coupons, diffusion-phase couples, simple model alloys with array of phases-interfaces, dislocation and grain structures (partly combinatorial approach?).
- Key is use of multiple complementary characterization techniques tied to multi-scale multi-physics modeling.



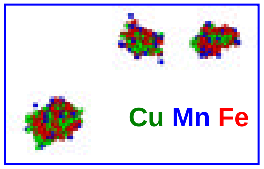
Key Underpinning Issue

- Focus on accounting for the transport and fate of defects, solutes and transmutation gases and the basic mediating processes.
- Combine various analytical & high resolution TEM, XRD, SANS, ASAXS, APT, PAS, ER/SC, PIA mechanical properties, MSMP modeling (a computational microscope).
- Proper preparation and pre-configuration of specimens is a key: examples are pre-thinned ASAXS foils and POSAT wires, ...

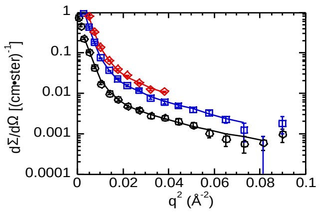
TEM



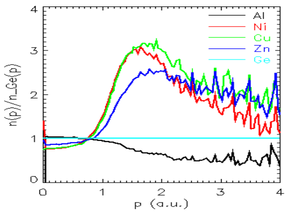
APT



SANS



PAS



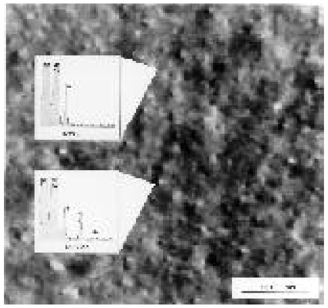
OTHER

$\Delta\rho$, ΔS

Tracking the Fate of a Species (Solute)

Matrix Solute

FEGTEM



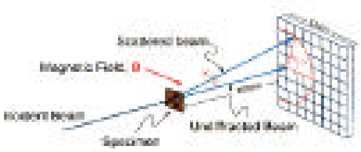
ATP

Δρ, ΔS

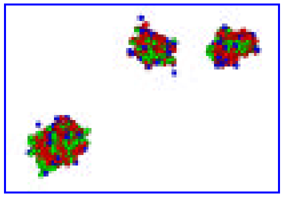
+

Precipitate Solute

SANS



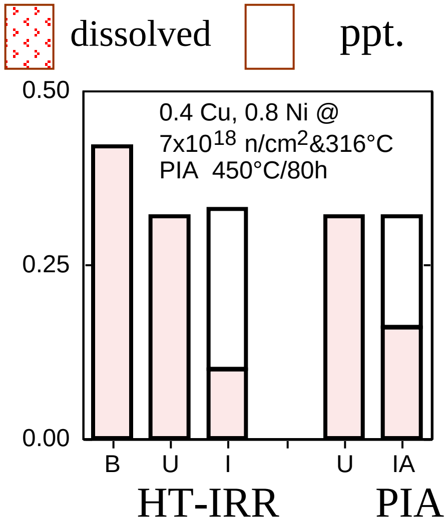
ATP



TEM

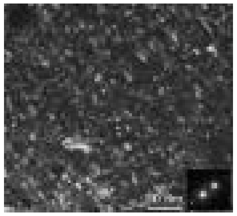
=

Total Solute

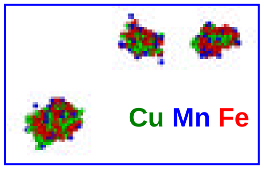


A Computational Microscope

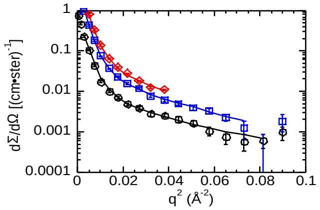
TEM



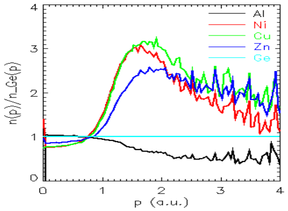
APT



SANS



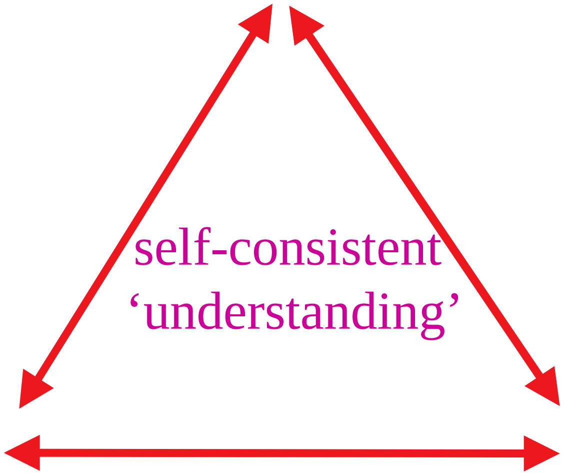
PAS



OTHER

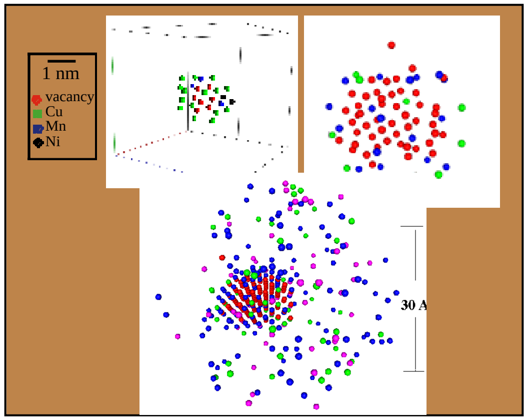
$\Delta\rho$, ΔS

feature
'signals'



self-consistent
'understanding'

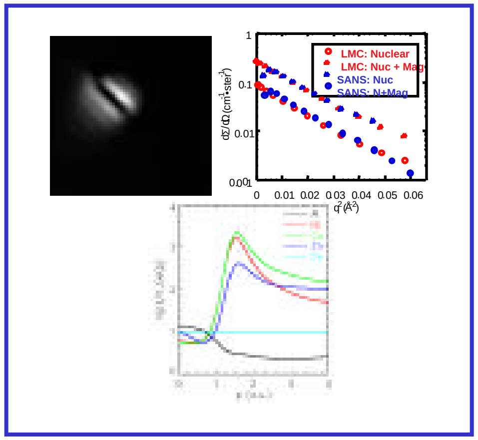
MSMP-LKLMC



predict
features

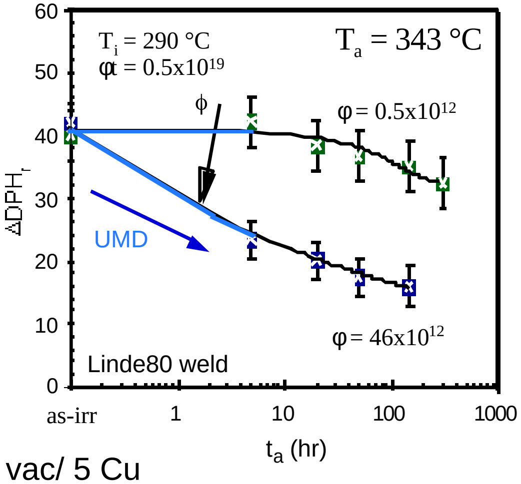
simulate
observables

TEM, SANS,
Positron theory

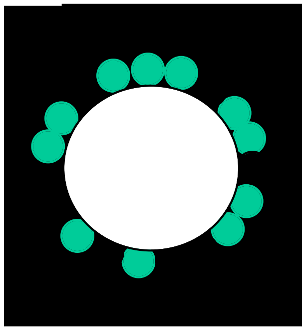


Cascade Vacancy Cluster-Complexes

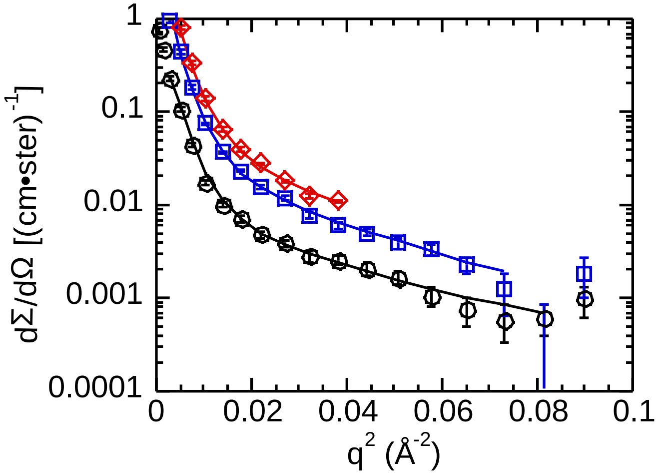
PIA



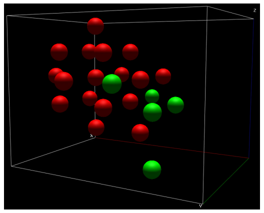
Cu-coated nanovoid



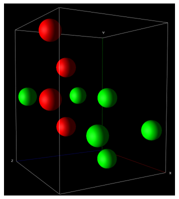
SANS + PIA



17 vac/ 5 Cu



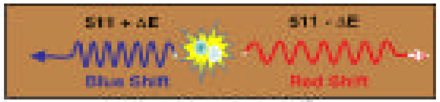
4 vac/ 6 Cu

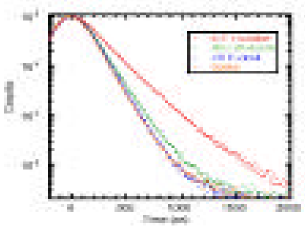


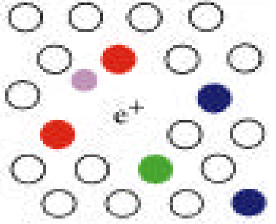
KLMC

Positron Annihilation Spectroscopy (PAS) + PIA

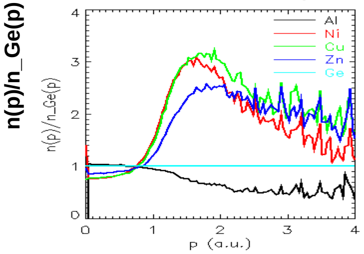
positron lifetime







Doppler broadening

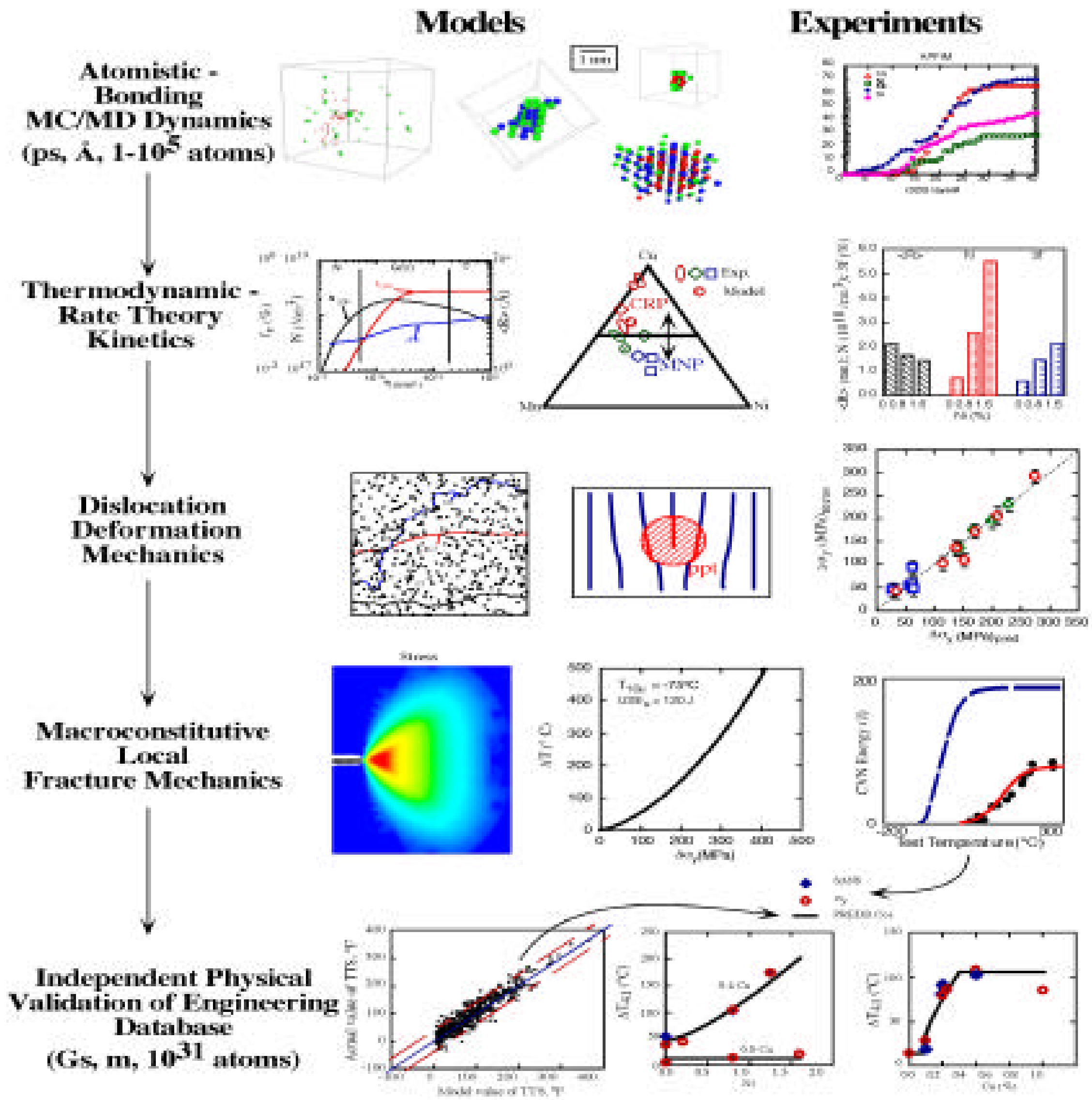


A MSMP Materials by Design Strategy

- Building a mechanistic physics base and knowledge fusion within the framework of MSMP models will be the basis for rational design of high performance materials - better to eliminate rather than predict degradation paths.
- MSMP philosophy based on integration of experiment and hierarchical physically based models to link:

  - structural evolutions to material/irradiation variables
  - basic properties to structural evolutions
  - complex properties to combinations of basic properties
  - structural integrity assessment to property predictions

MSMP Modeling: Embrittlement



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