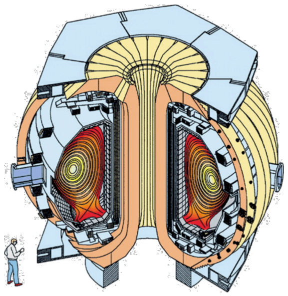
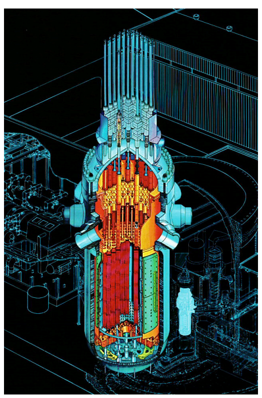
Materials Challenges in Advanced Nuclear Energy Systems: the Promise of Advanced High Performance Alloys

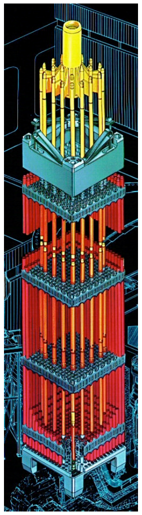
G. Robert Odette[1] and Brian D. Wirth[2]

[1]Materials and Mechanical Engineering Department
University of California, Santa Barbara

[2]Nuclear Engineering Department
University of California, Berkeley







Presented at
ICMR Summer Program on
Advanced Thermostructural Materials
UCSB, 9 August 2006

Outline

- Developing materials for nuclear fission and fusion presents many enormous materials challenges
  - severe thermomechanical/fatigue loading
  - aggressive chemical environments
  - inherent dimensional instabilities and stress re-distributions
  - severe transients and large safely margins
  - in-service property degradation of many performance sustaining properties that depend on the synergistic combination of many variables
- Overview of radiation damage and effects
- Introduction to the promise of a new high performance radiation tolerant alloy system - nanostructured ferritic alloys - more next week

Neutrons

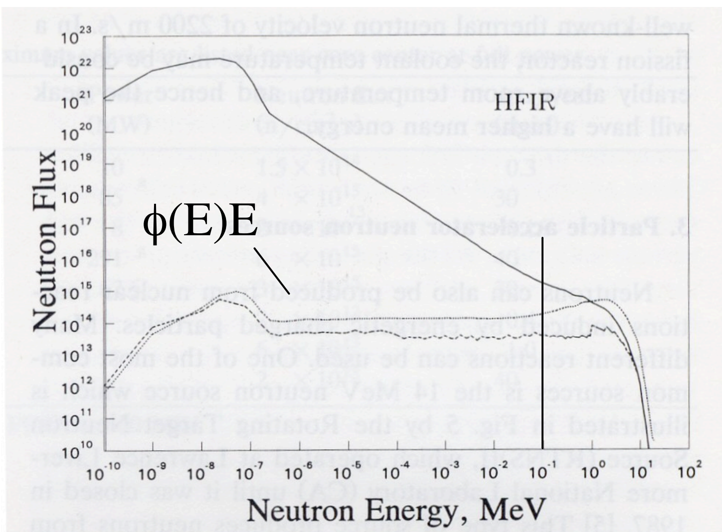
Fast neutrons > ≈ 0.1 MeV major source of *displacement damage*

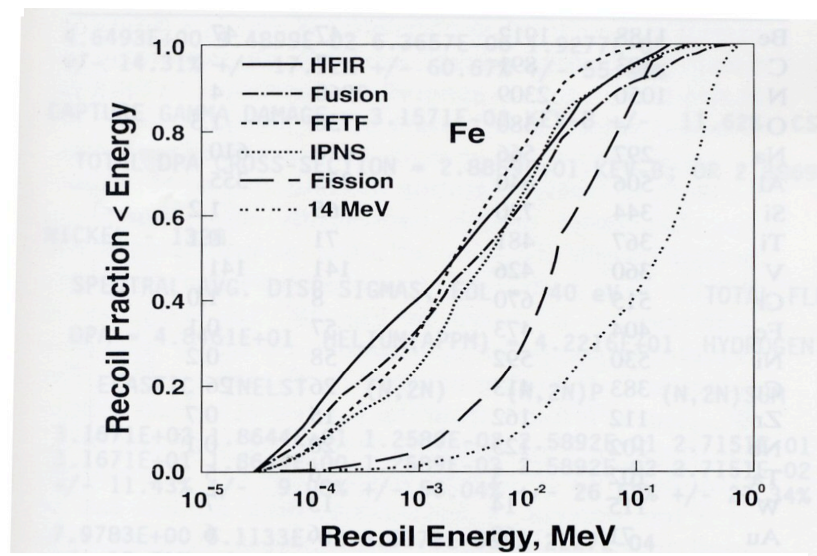
Fast neutrons > 1 MeV are the major source of *He and H transmutants*

Average fast fission neutron E ≈ 1 MeV

Average fast fusion neutron E ≈ 14 (20%) + 2 (80%) MeV

Neutron-nuclear interactions ->primary recoiling atoms (PRA)



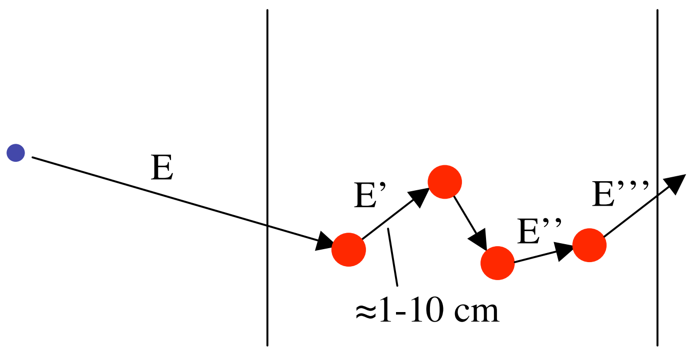


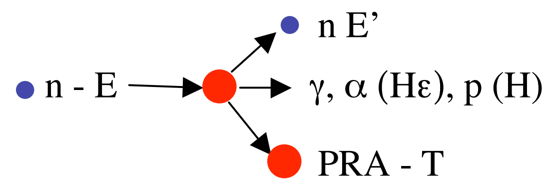
L. Greenwood

Neutron Processes

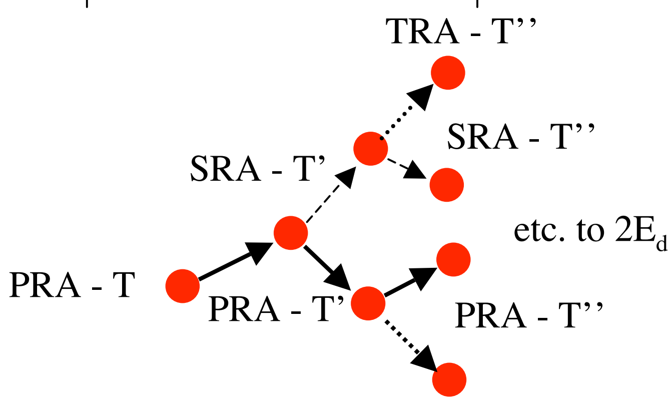
neutrons penetrate cms
between scattering & reactions

neutron scattering & reactions ->
primary recoil atoms (PRA)
PRA average T ≈ 10 keV fission
PRA average T ≈ 50 keV fusion

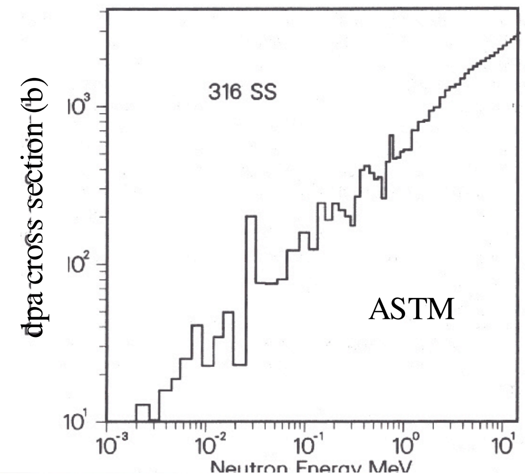




PRA -> displacement cascades
cascades -> ν_d displaced atoms -
> $\nu_d \approx T/2E_d$ +
excitation/ionization + heat
Ed displacement threshold energy



Neutron Damage Dose Units



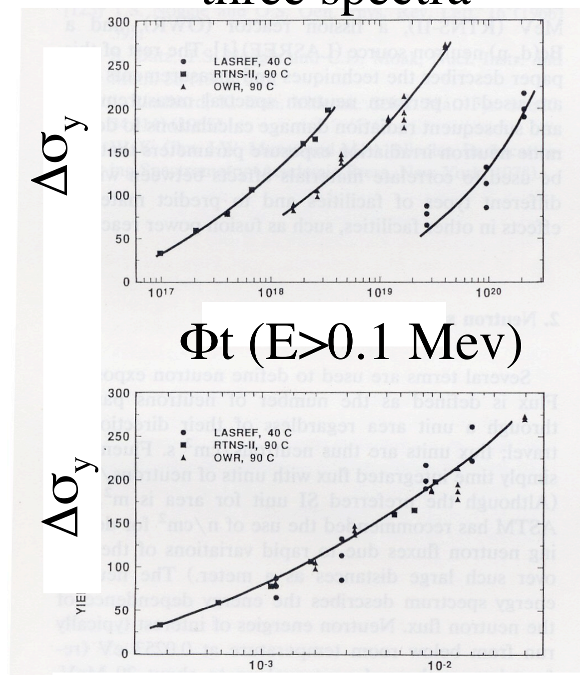
Damage Dose

displacements per atom (dpa) = $\phi t \sigma_{dpa}$

fluence - ϕt = (ϕ - flux) x (t - time)

σ_{dpa} = displacement cross section

three spectra



L. Greenwood

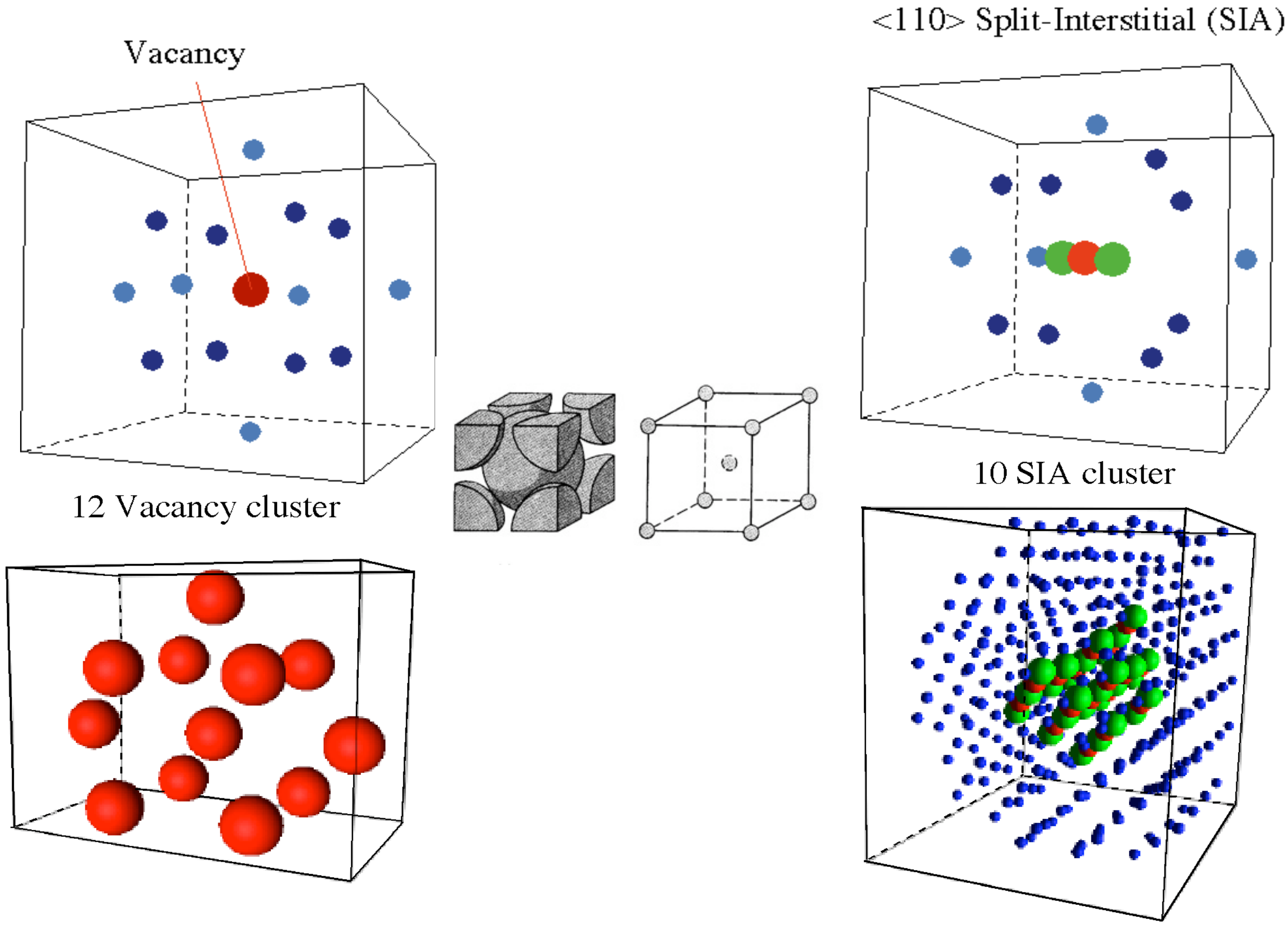
Primary Displacement Defects

vacancies = self-interstitial atoms (SIA)

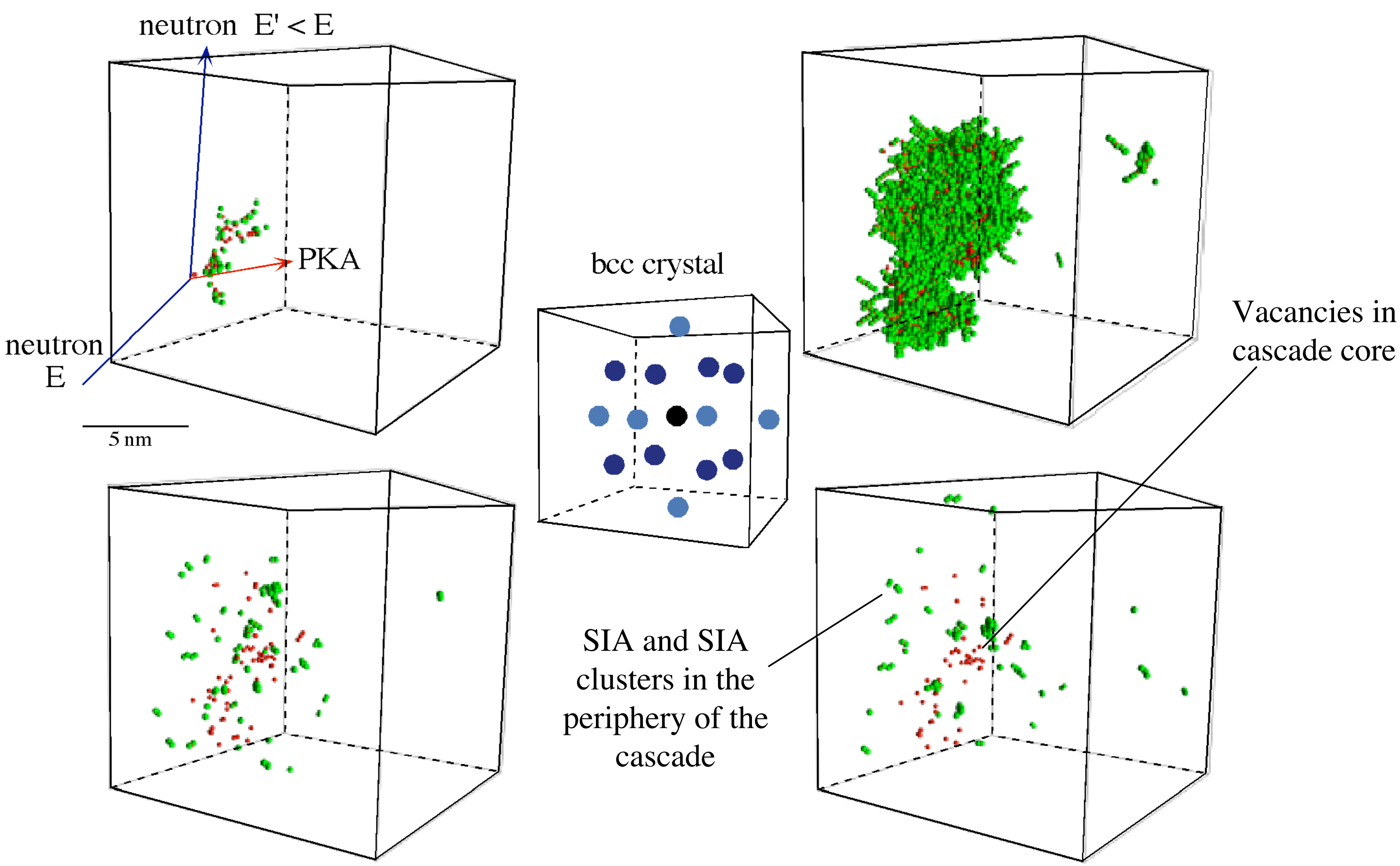
vacancy and SIA clusters

Also He, H and solid transmutants (appm)

Defects and Small Defect Clusters

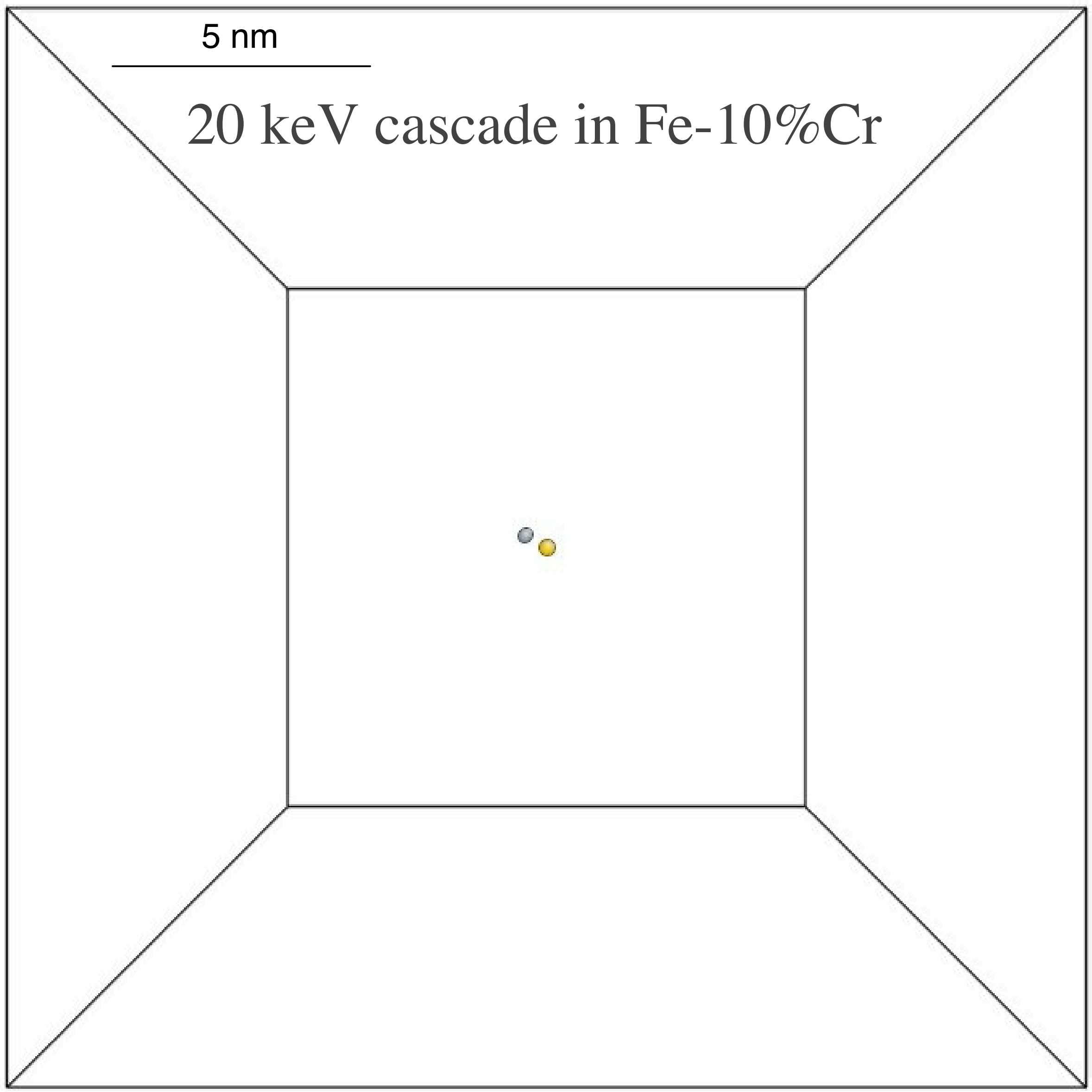


Molecular Dynamics Simulation of a Cascade



50 keV cascade in Fe

Molecular Dynamics Simulation of Cascade



Cascade Aging Phenomena

Vacancy-SIA recombination (self-healing)

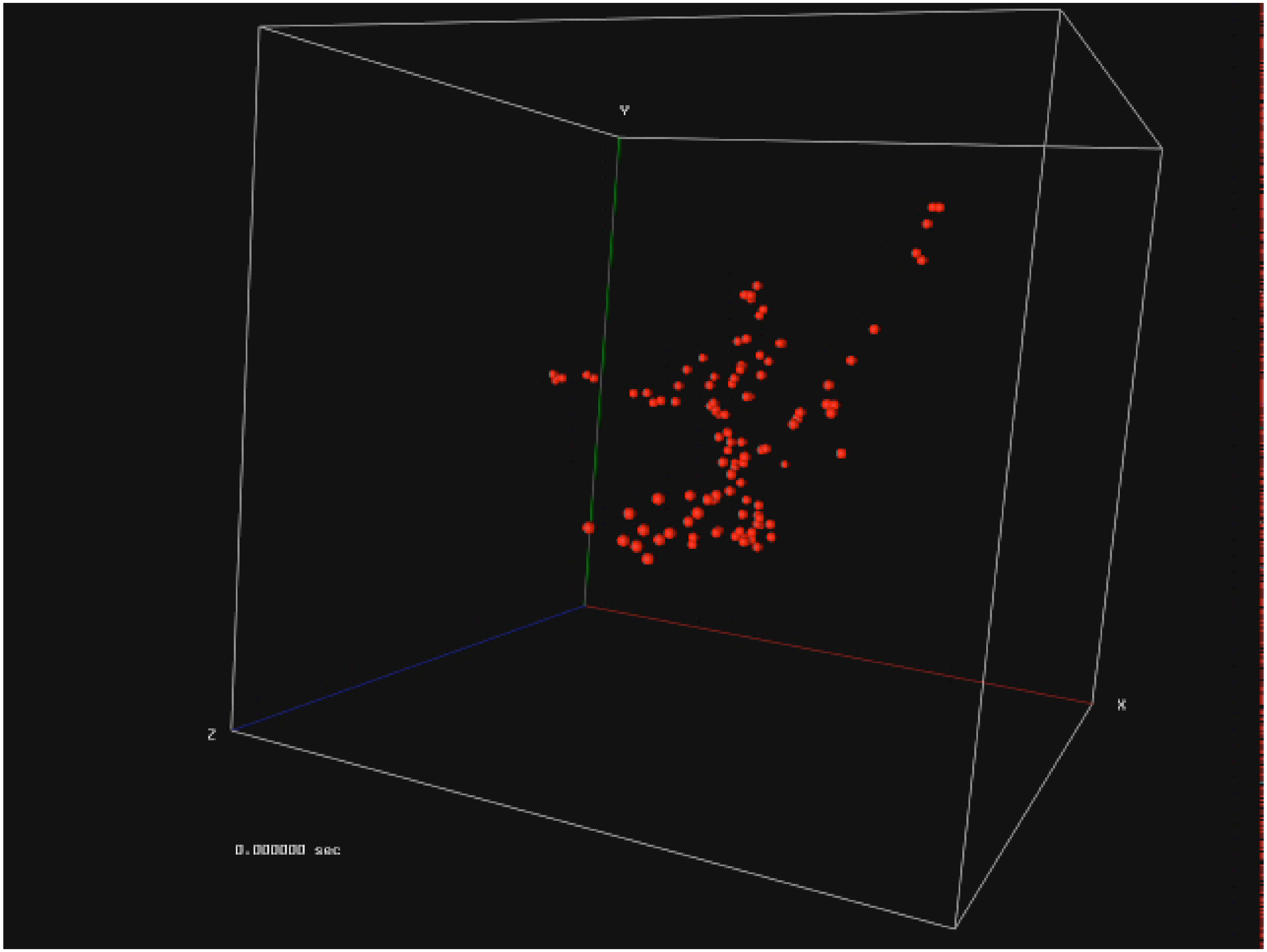
Additional SIA clustering and escape of mobile SIA and SIA clusters from cascade region-long range migration - < 1 ms

Vacancy-solute -> nanovoid cluster complexes - < 1 ms to s

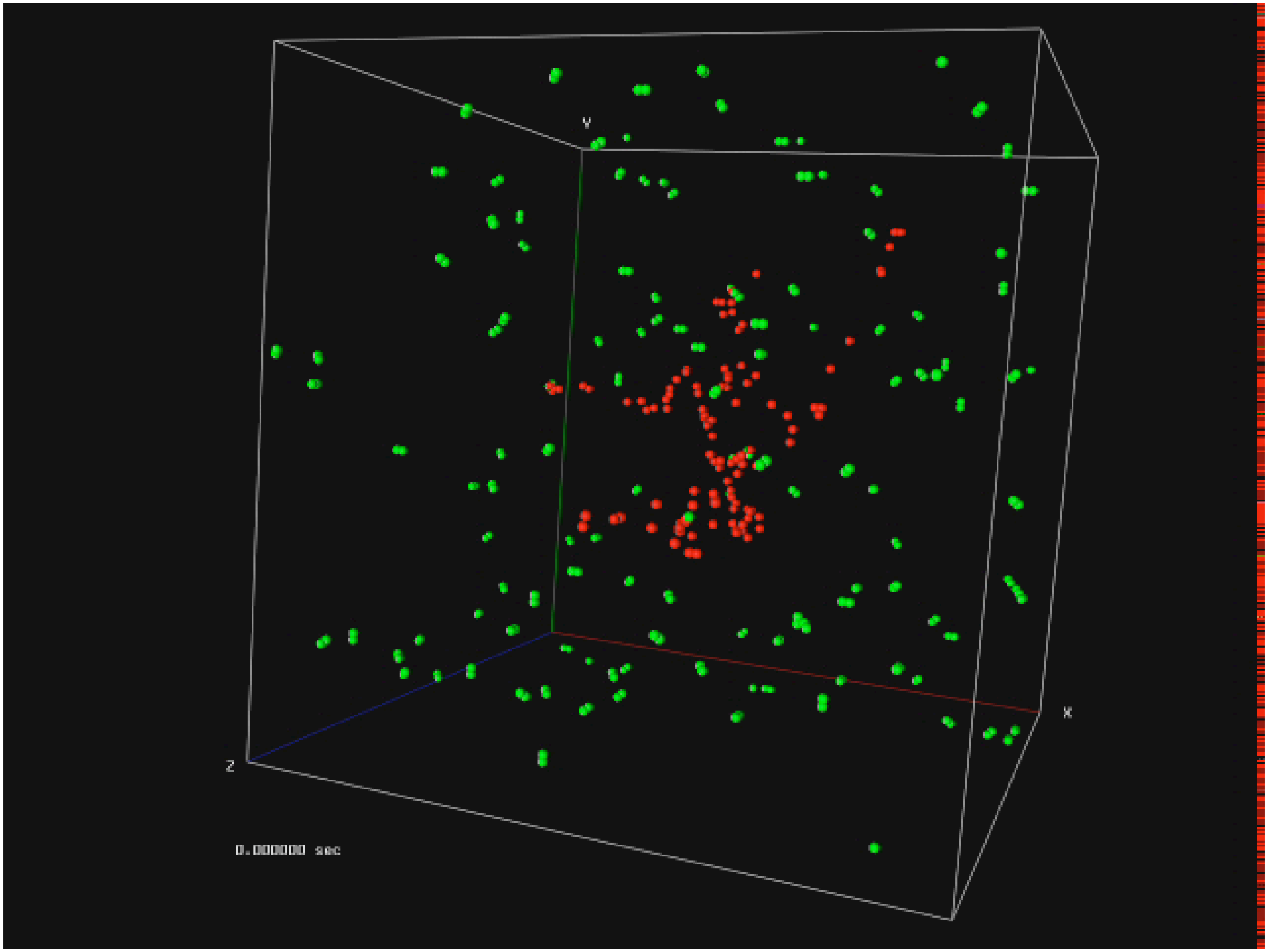
Vacancy cluster coarsening and ultimate dissolution escape from cascade region-long range migration - s to gs

Residual solute clusters and trapped SIA cluster dislocation loops

Aging of Cascade Vacancy Core in Fe

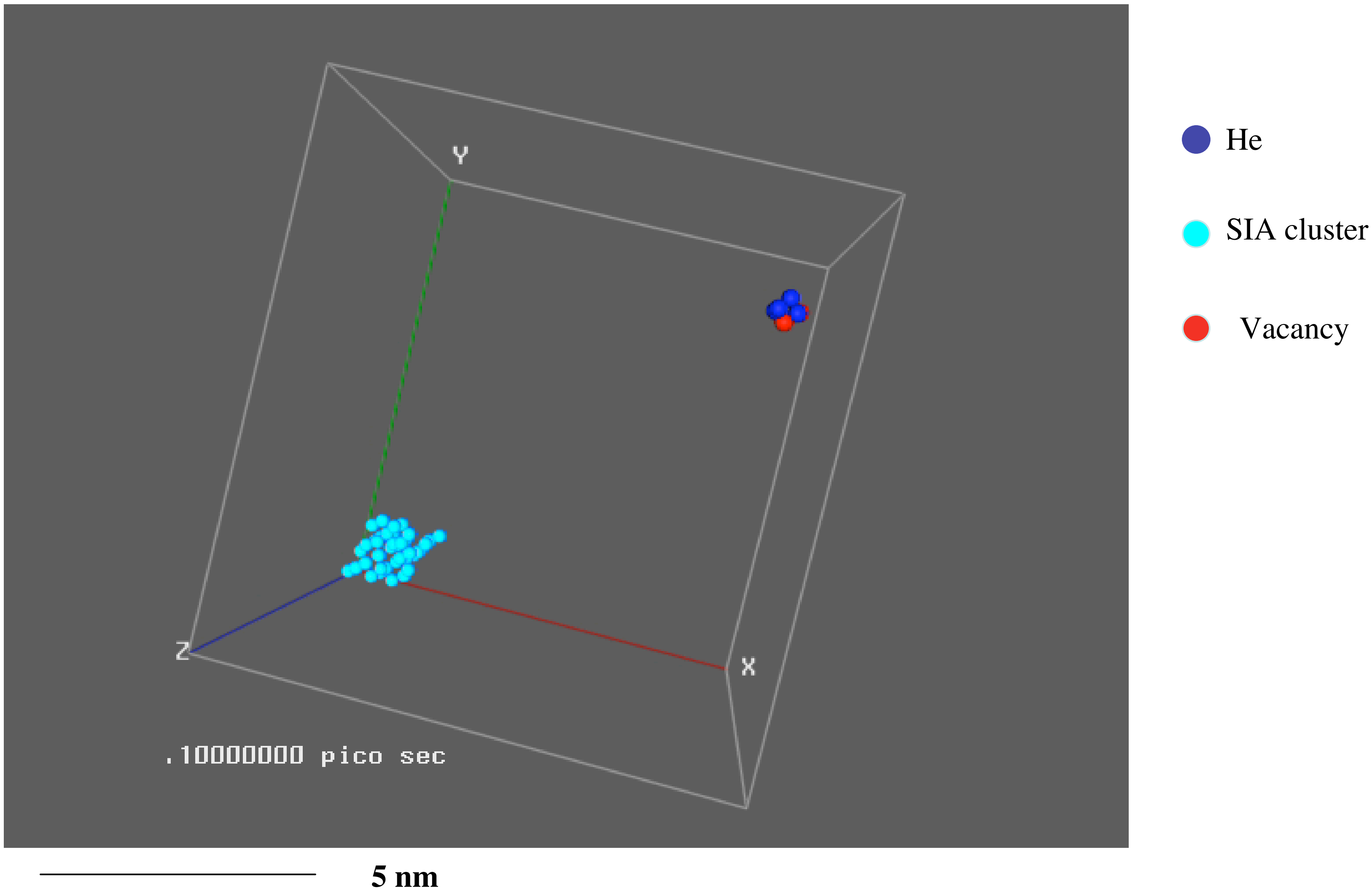


Aging of Cascade Vacancy Core in Fe-0.3%Cu



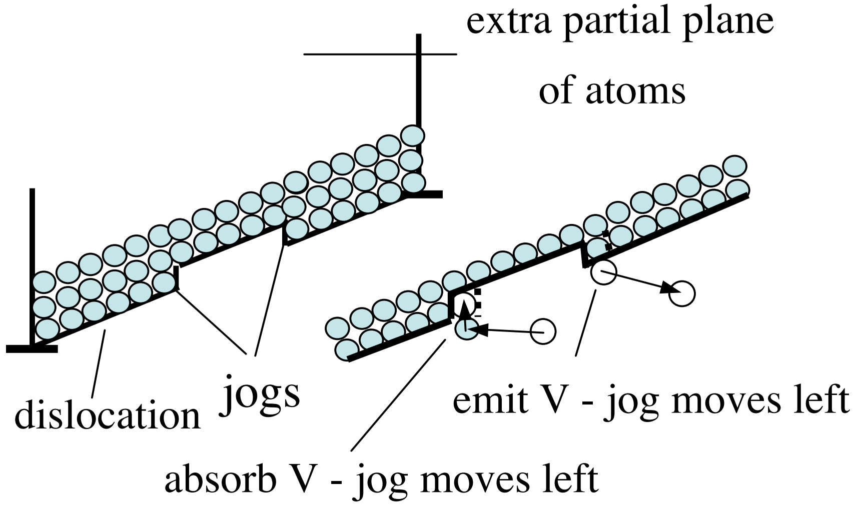
Example - Other Interactions

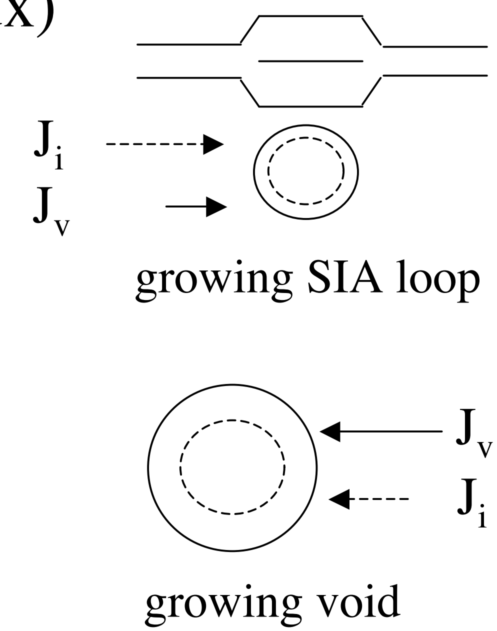
An 11 SIA cluster and a 4 He, 6 vacancy cluster at 1000 K



Long Range Defect Migration and Reactions

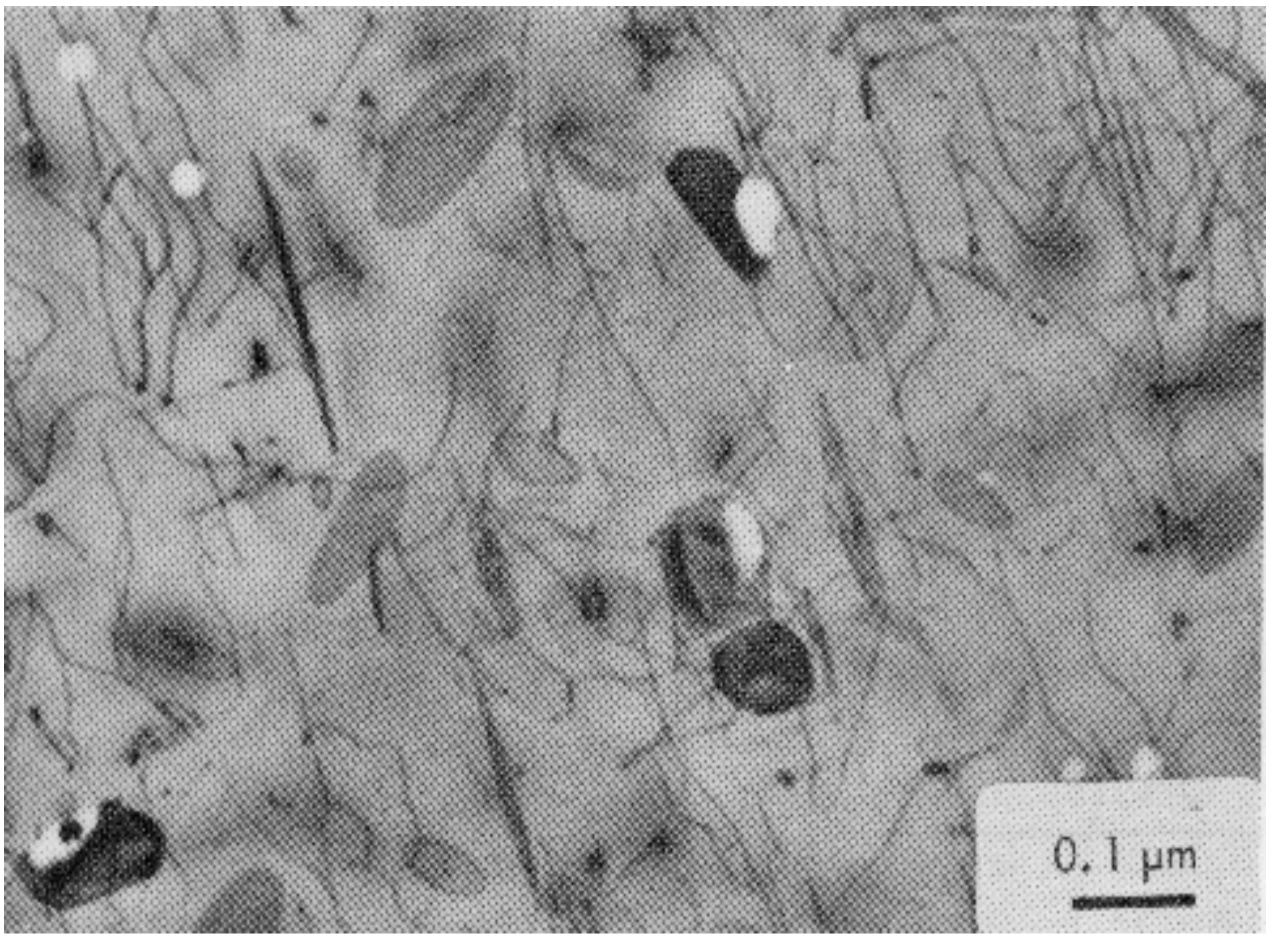
- Primary damage -> long range diffusion -> enormous SIA and vacancy supersaturation
- Additional vacancy-SIA recombination
- Annihilation at sinks (dislocations-grain boundaries-…)
- Sink bias driven clustering of vacancies (cavity growth by excess vacancy flux) and SIA (dislocation loops) as well as dislocation climb (by excess SIA flux)
- Coupled microstructual evolutions

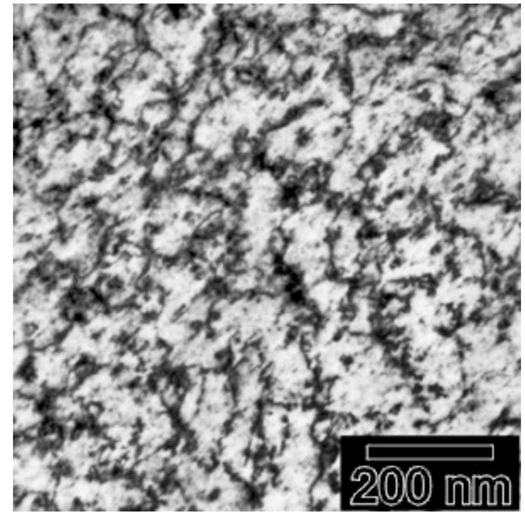


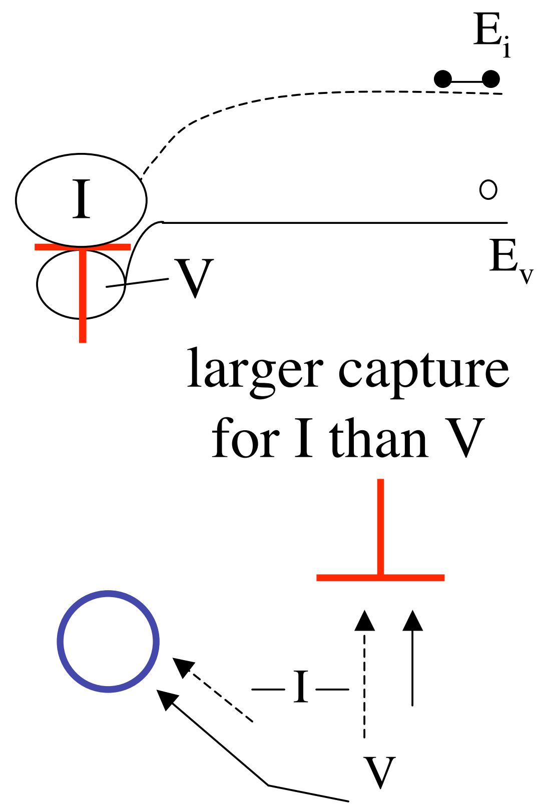


Microstructural Evolutions

J. Stiegler







Microchemical Evolutions

Significant microchemical changes accompany complex microstructural evolutions in multiconstituent-multiphase alloys - thermodmynics may be enhanced or induced (driven)

Vacancy/SIA supersaturations -> radiation enhanced diffusion (RED)

Coupled persistent solute defect fluxes to sinks -> radiation induced segregation (RIS) -> may drive alloys further from equilibrium

Ballistic mixing and amorphization

→

Accelerate low temperature precipitation

Grain boundary segregation-sensitization

Non-equilibrium precipitates

Destabilization of Fe-Cr-Ni austenite

Kinetically modified phase boundaries

…

Radiation Enhanced Diffusion (RED)

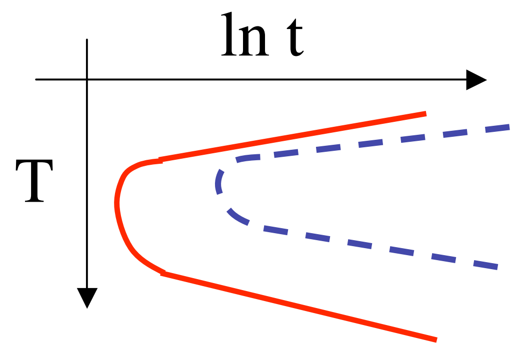
Simplest Case

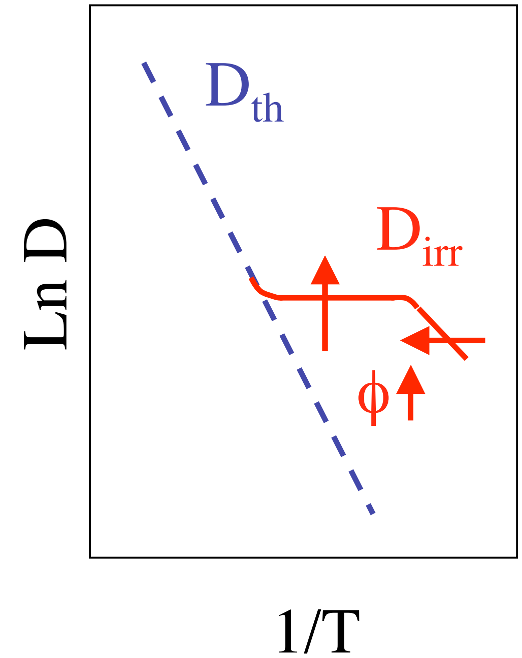
$D_{sirr}/D_{sth} \approx [G_v/S_v D_{sd}]$

G_v = vacancy gen. rate

S_v = sink strength

D_{sd} = self diff. coeff.

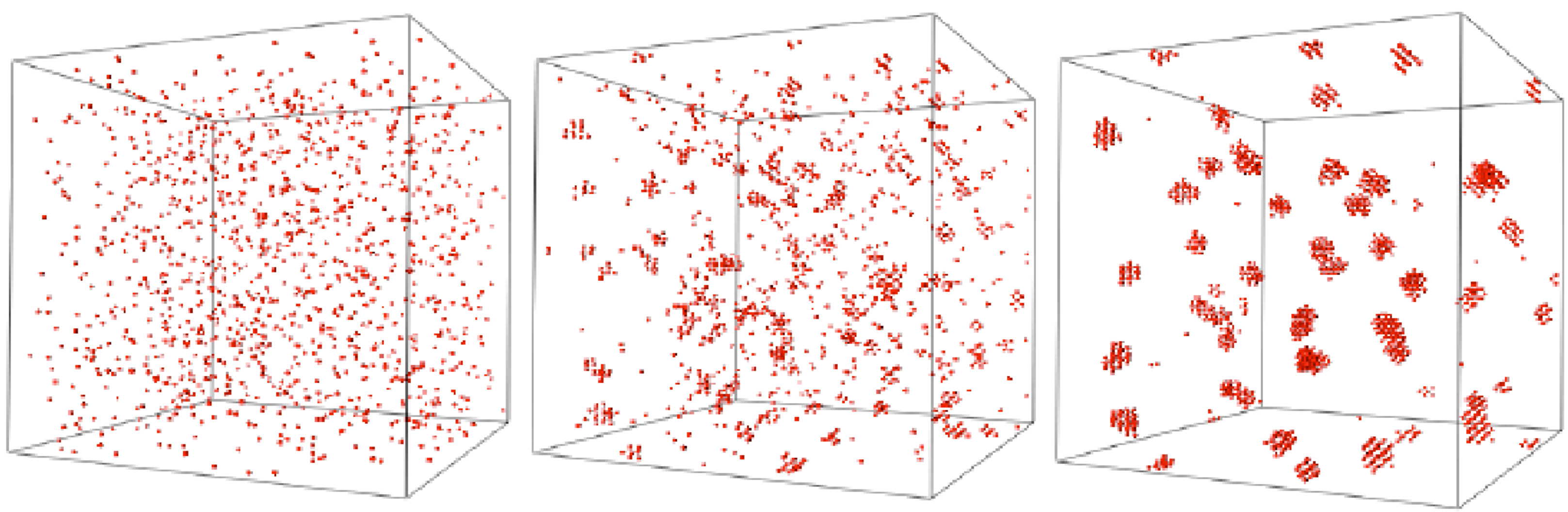




Cu in Fe at 300°C - $D_{cuth} \approx 10^{-23}$ cm^2/s and for $\phi = 10^{12}$ n/cm^2 and $S_v = \rho = 10^{10}$/cm^2 -

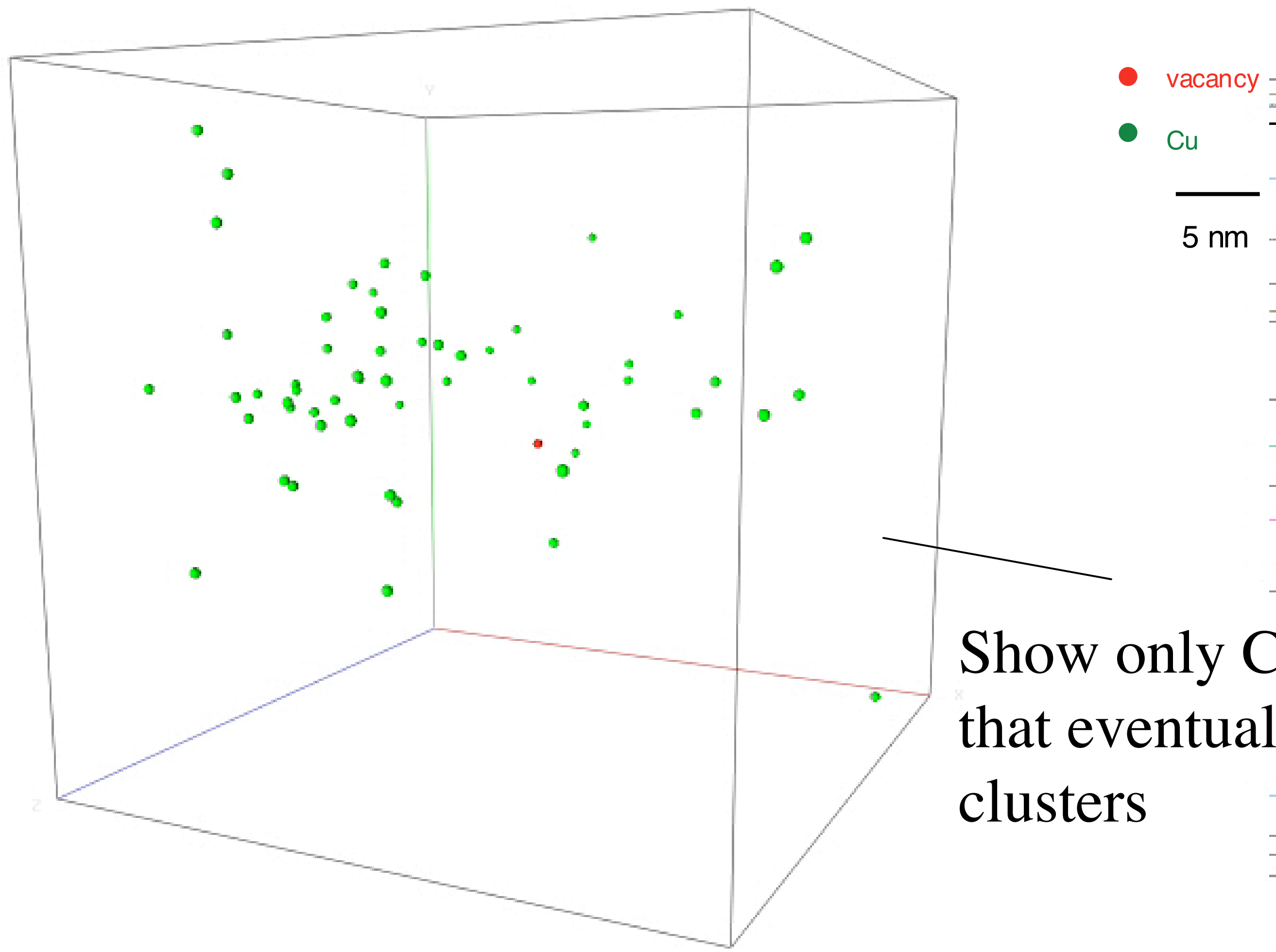
$D_{cuirr} = 6 \times 10^{-20}$ -

$D_{irr}/D_{th} \approx 6000$



KLMC Simulation of Cu Precipitation

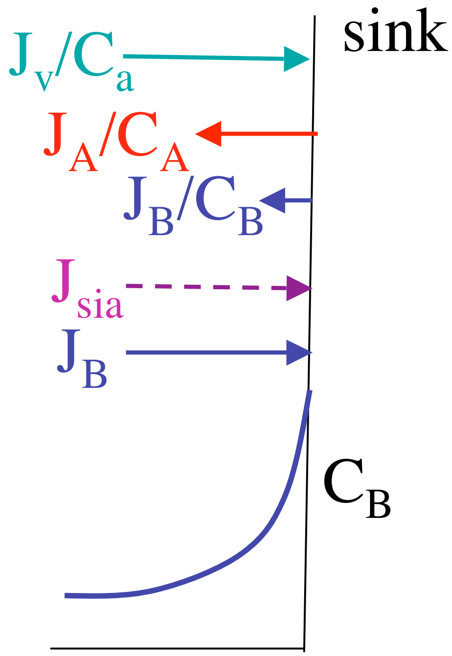
Kinetic lattice Monte Carlo simulation of diffusion and precipitation in Fe at 300°C for 0.3 at.%Cu

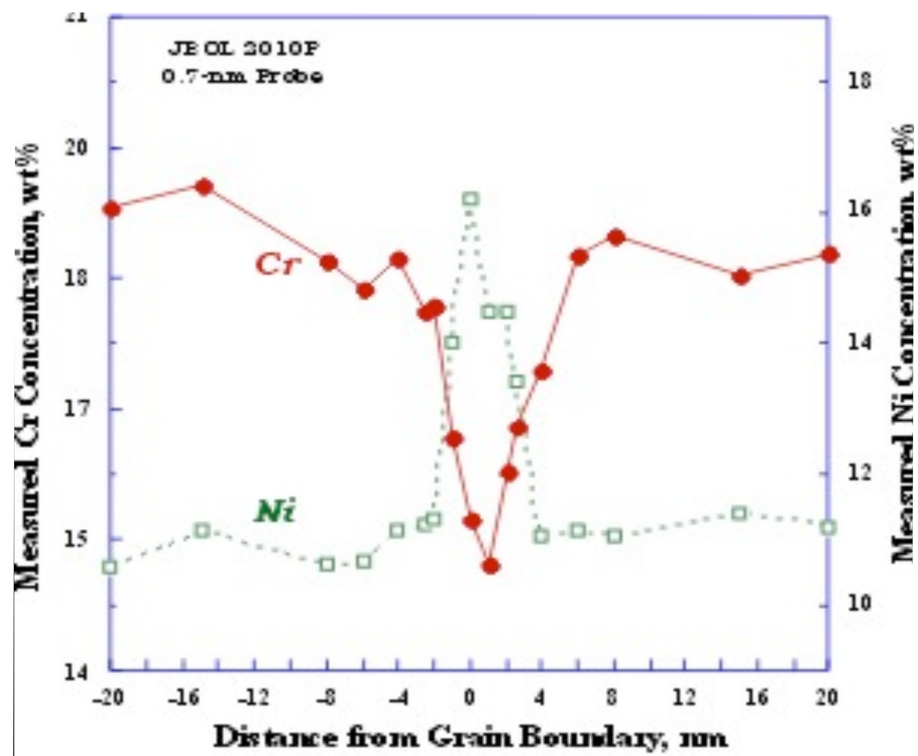


Show only Cu that eventually clusters

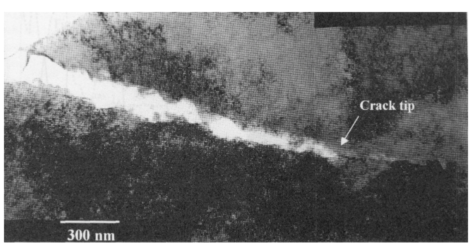
Radiation Induced Segregation (RIS)

Segregation driven by the inverse Kirkendall effect and SIA solute complex transport

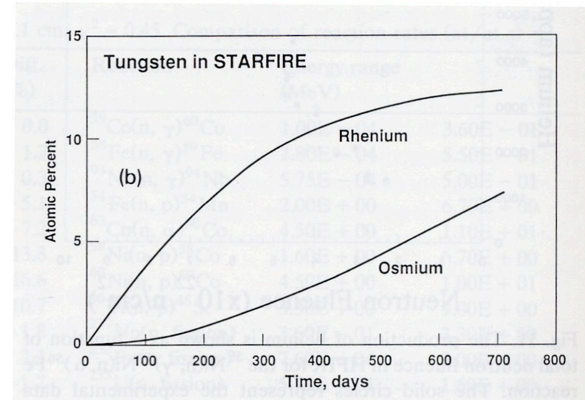




L. Thomas and S. Bruenner



Transmutations



L. Greenwood

At high doses transmutation reactions change elemental compositions but He and H gas are generally more significant

n + ^{54}Fe -> ^{51}Cr + α (He) and n + ^{54}Fe -> ^{54}Mn + p (H)

'Most' interstitial H diffuses out at high temperature

He is highly insoluble undergoing RED to precipitate as gas bubbles in the matrix as well as on both dislocations and various interfaces

He/dpa - <1 fission ≈10 fusion >50 spallation protons

He bubbles are excellent nucleation sites for stress and radiation driven growing cavities

Void Swelling and He Embrittlement

Helium bubbles become unstably growing voids and creep cavities without a nucleation barrier when -

bubble radius

$$\sigma_h + P_{He}(r_b) + \underline{[kT/V_a]\ln\{[D_v X_v - D_i X_i]/D_{sd}\}} > 2\gamma/r_b$$

mechanical stress

gas pressure

atomic volume

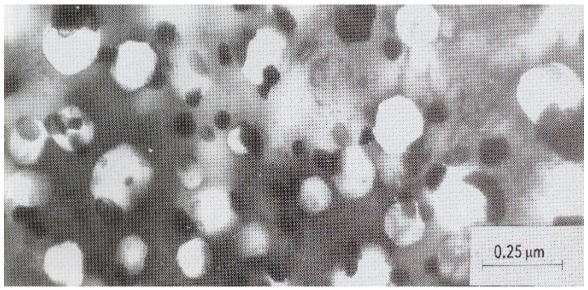
irradiation stress due to sink bias -> excess vacancy flux

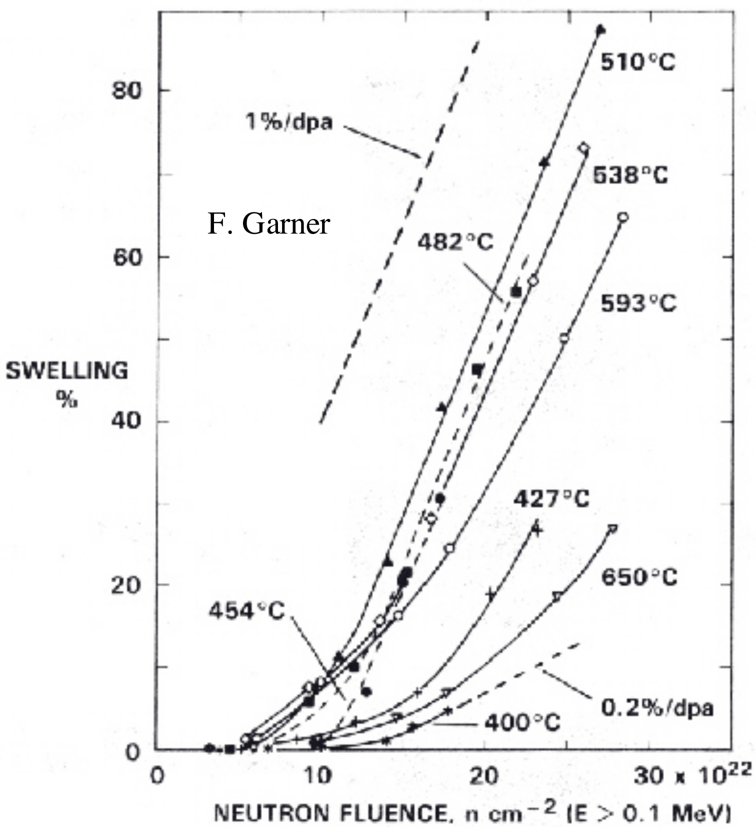
surface energy

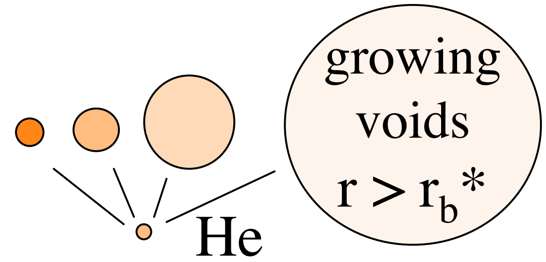
Instability at a critical bubble radius - r_b* and critical bubble He content - n_{He}* - functions of variables shown above

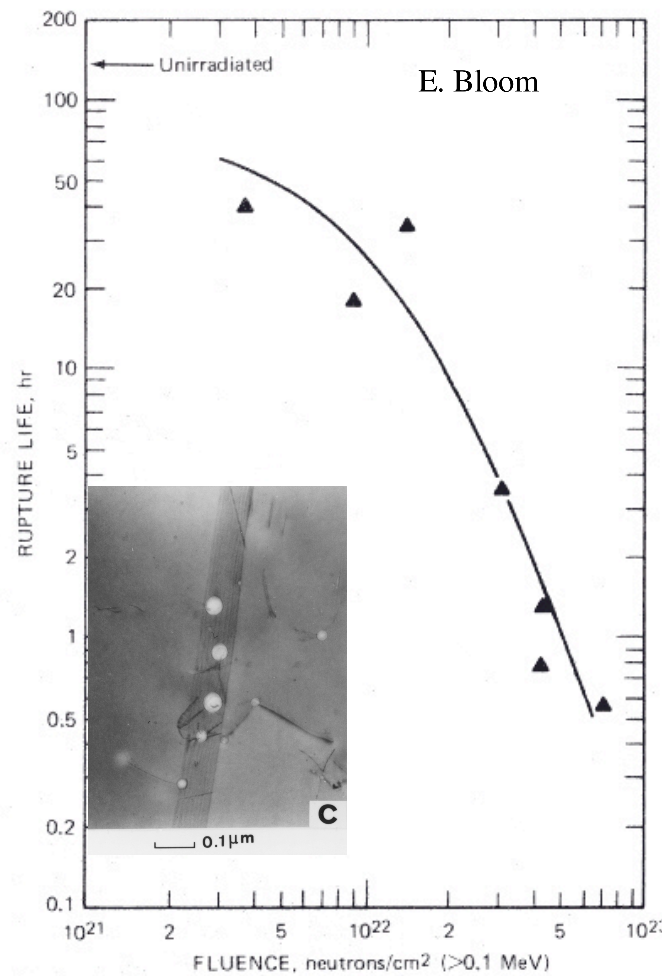
Helium accumulation in bubbles -> rapid void swelling and/or severe reductions in creep rupture life-ductility-subcritical creep-fatigue crack growth rates

Void Swelling and Helium Embrittlement

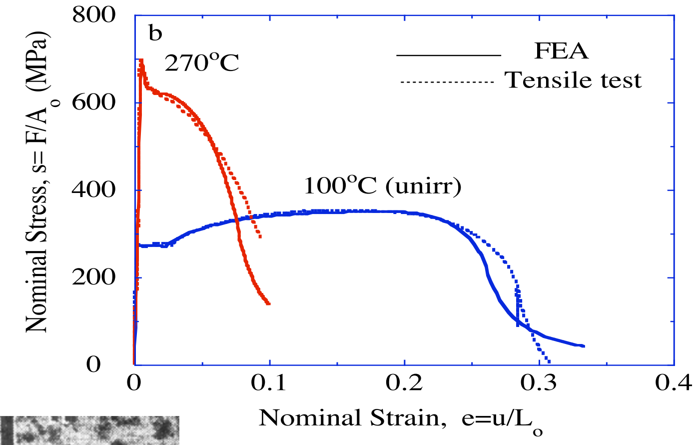


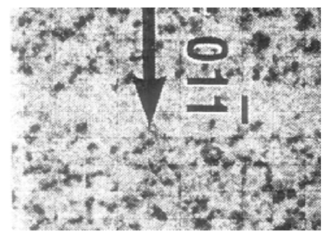






Other Irradiation Effects





S. Zinkle

Approximately athermal irradiation creep

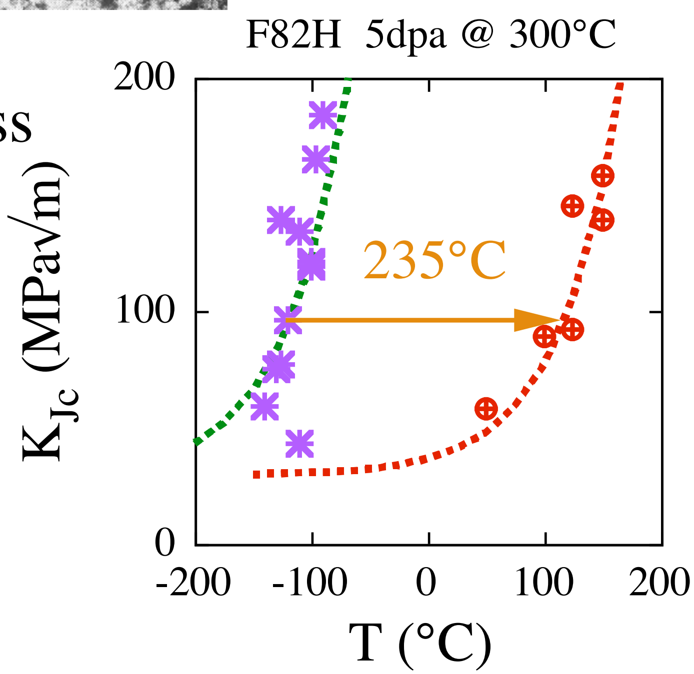
$\varepsilon \approx 10^{-5}\sigma$dpa -> 10% @100 MPa-100 dpa

Irradiation hardening at < ≈ $T_m/4$ -> loss of uniform strain ductility and flow localization-channeling

Hardening induced fast fracture embrittlement -> transition temperature shifts and reductions in tearing toughness

RED/RIS segregation and helium weakening of grain boundaries -> IGF

Non hardening fast fracture embrittlement by precipitation of brittle phases and microstructural instabilities



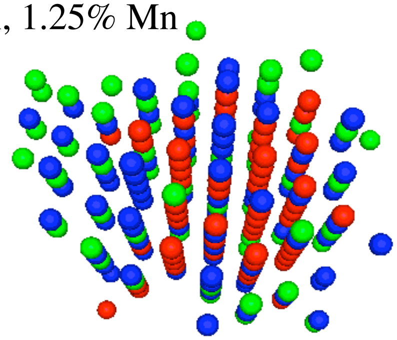
Nano-Precipitates in Irradiated RPV Steels

Not color change

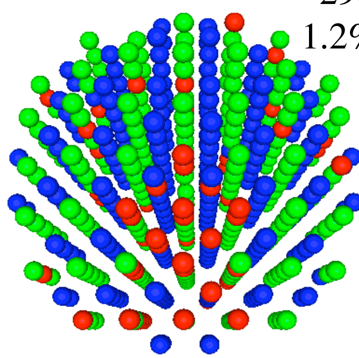
● Cu ● Mn ● Ni

Monte Carlo

260°C, 0.4% Cu
1.25% Ni, 1.25% Mn

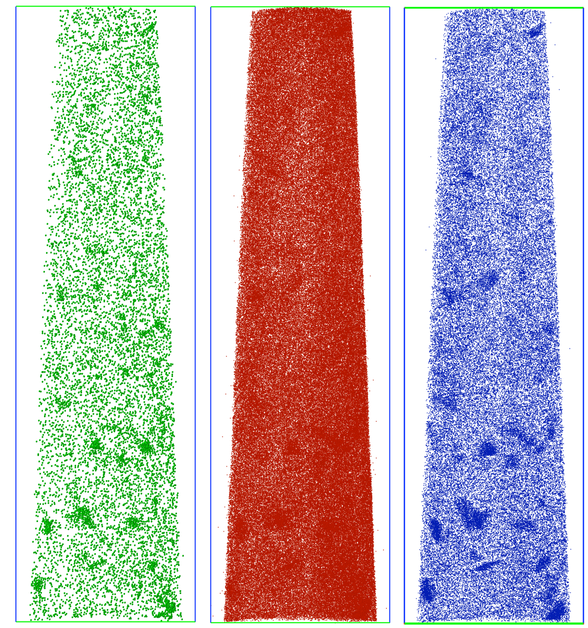


290°C, 0.15% Cu
1.2% Ni, 1.25% Mn



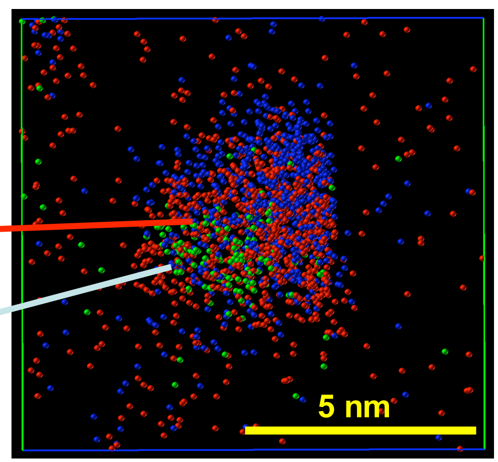
MNP

Cu Ni Mn



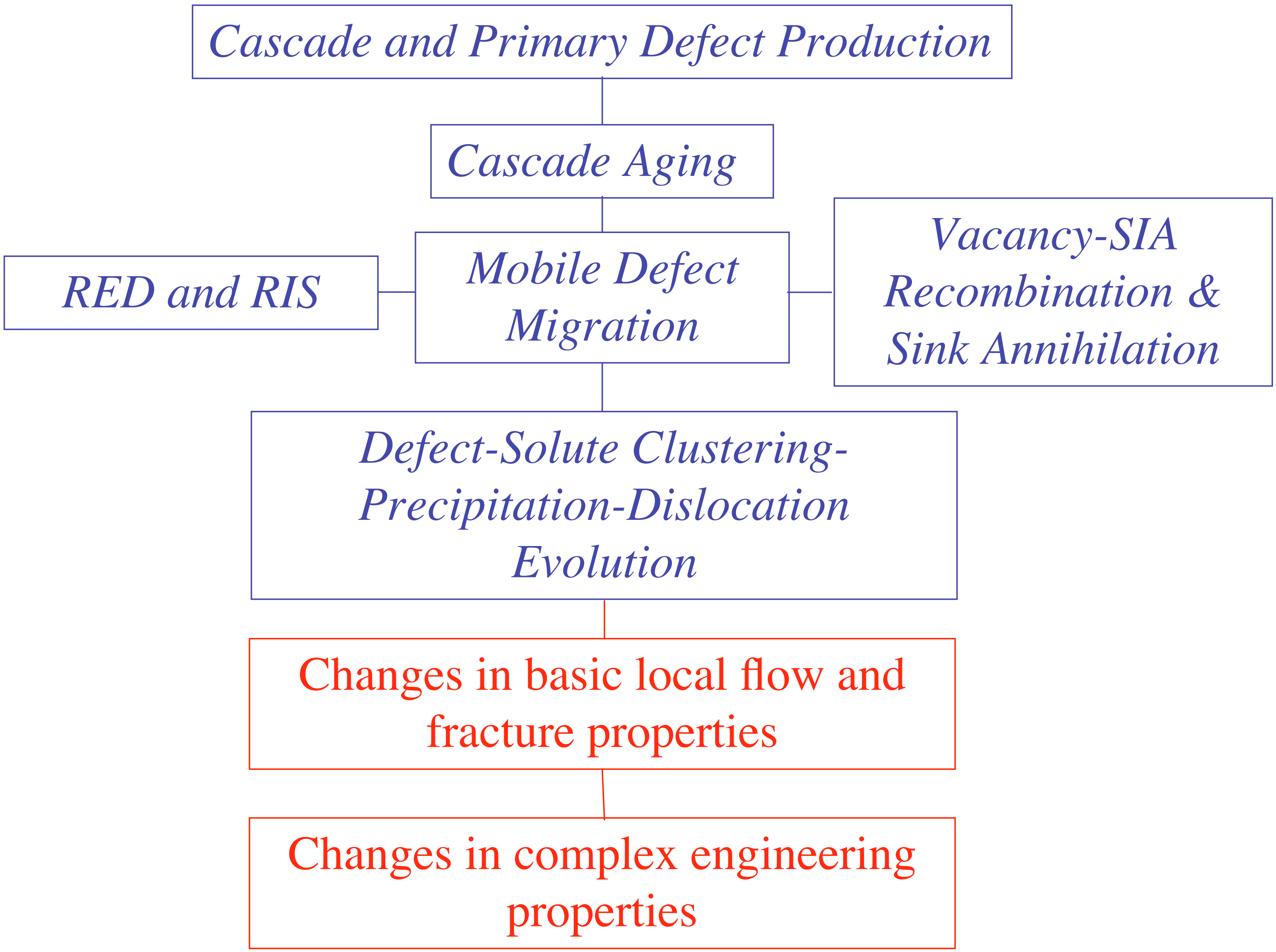
Ni + Mn

Cu



APT

Fe-0.2%Cu-1.6%Ni-1.6%Mn


Cascade and Primary Defect Production
Cascade Aging
RED and RIS
Mobile Defect Migration
Vacancy-SIA Recombination & Sink Annihilation
Defect-Solute Clustering-Precipitation-Dislocation Evolution
Changes in basic local flow and fracture properties
Changes in complex engineering properties

Design Strategy for Damage Resistant Alloys

Operate at high temperatures above displacement damage regime - other issues of creep strength-corrosion-…

High sink and trap densities to recombine (self-heal) vacancies and SIA

Protect grain boundaries and manage helium by trapping in fine nm-scale high pressure bubbles

Solution - nanostructured materials

Thermal and irradiation stability of far from equilibrium structures paramount

Kinetically constrain thermodynamically driven evolutions