Multiscale Modeling of Radiation Damage in Fusion Reactor Materials

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Presentation overview

- **Introduction to fusion reactor materials and radiation damage processes**
- **Multiscale modeling approach**
- **Microstructure evolution in bcc alloys under low to intermediate temperature (T < ~450°C) irradiation**
  - **Self-interstitial cluster properties, growth and accumulation of dislocation loops**
  - **Formation of sub-nanometer vacancy-solute clusters**
- **Impact of microstructure on mechanical property & performance**
  - **Dislocation - defect interactions**
  - **Constitutive & mechanical property modeling**
- **Summary & future directions**

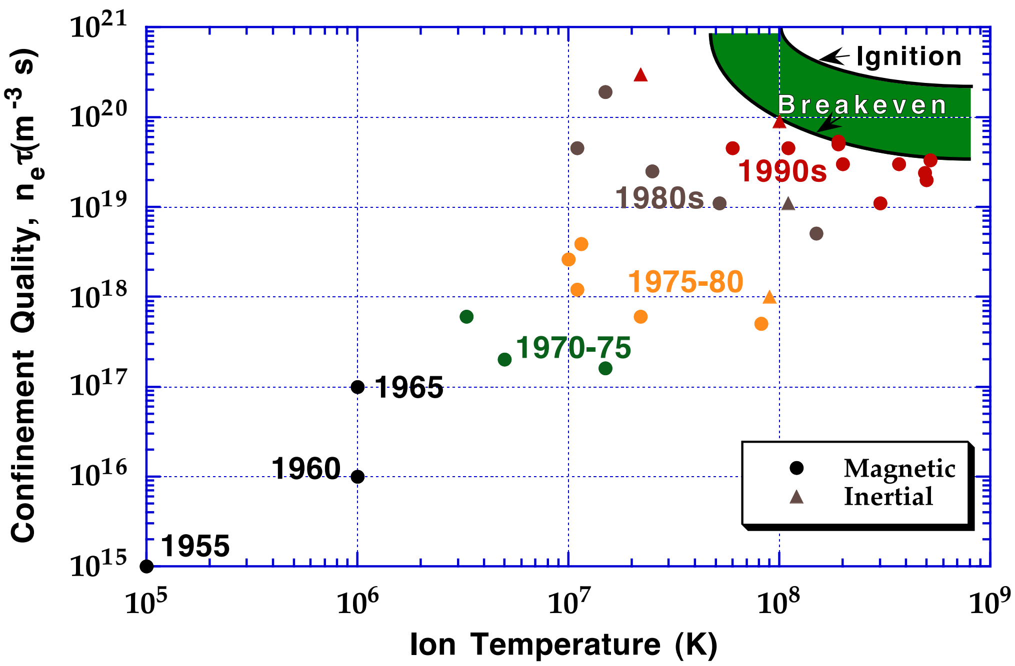
Fusion materials science program

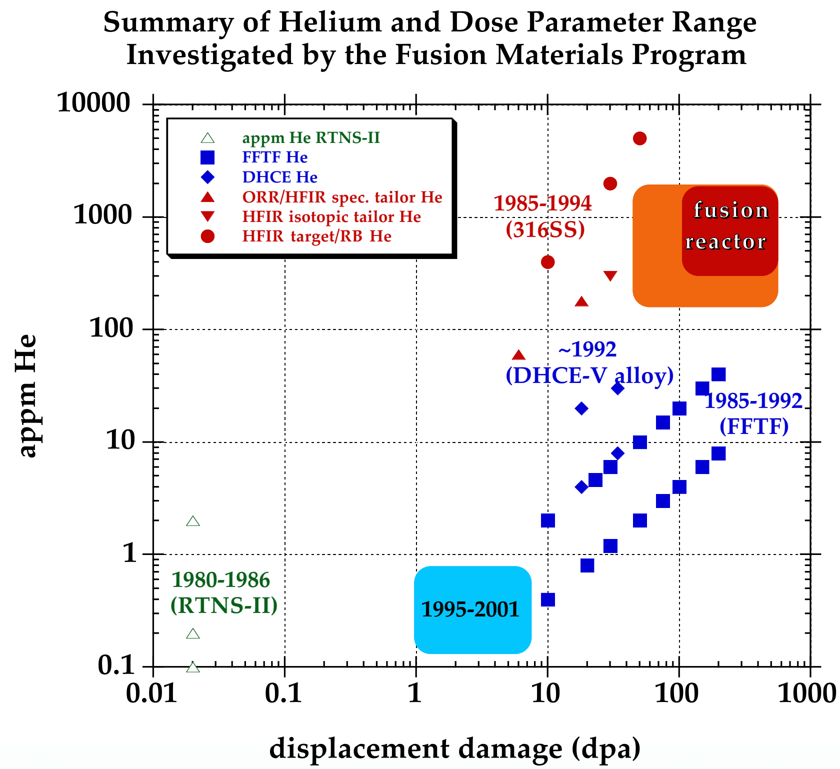
• **Similar philosophy for Fusion materials & plasma science programs**

	Fusion Plasma Science	**Fusion Materials Science**
Basic Goal	Understand 4th state of mater as it relates to fusion	Understand 1st state of matter as it relates to fusion
Key Issues		
• Basic properties and microscopic phenomena	-particle/energy confinement and transport	- defect properties, dislocation propagation, phonon transport - microstructural stability
• System properties and macroscopic phenomena	-MHD stability	- fracture and deformation
• Creation and sustainment	-plasma - wave interactions	- physical metallurgy and thermodynamics
• Interactions with environment	- plasma-wall interactions	-corrosion and compatibility; radiation effects on materials

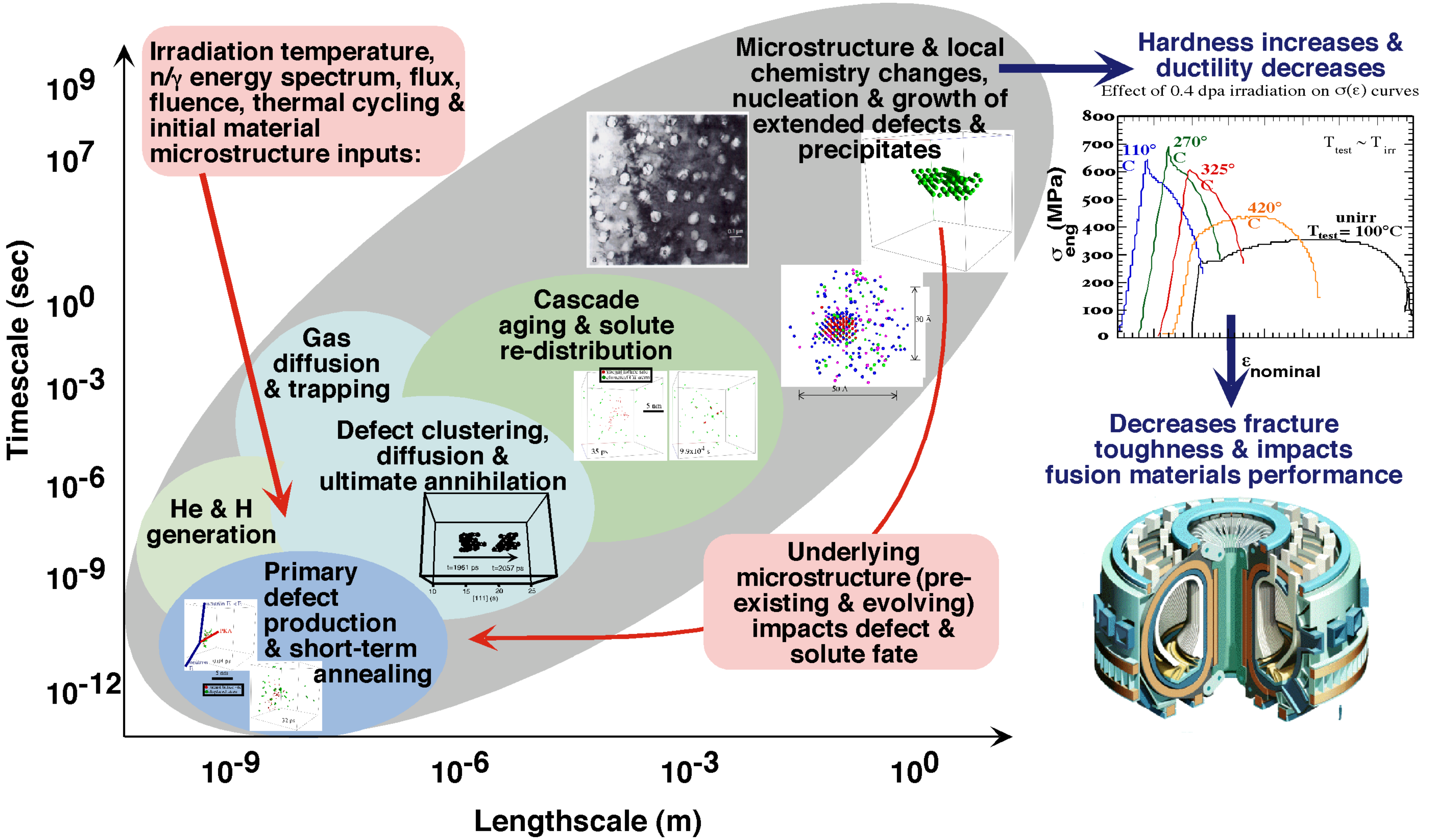
Fusion materials research must rely heavily on modeling due to inaccessibility of fusion-relevant operating regime

- **Extrapolation from currently available parameter space to fusion regime is much larger for fusion materials science than for plasma physics program**





Radiation damage processes



Lack of intense neutron source emphasizes the need for co-ordinated experiment, modeling & theory to develop fundamental understanding of radiation damage

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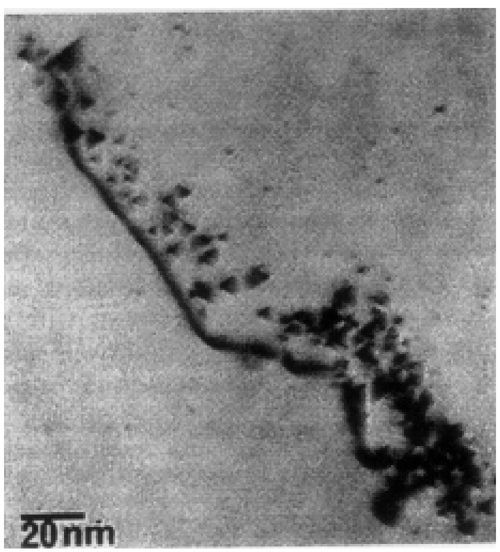
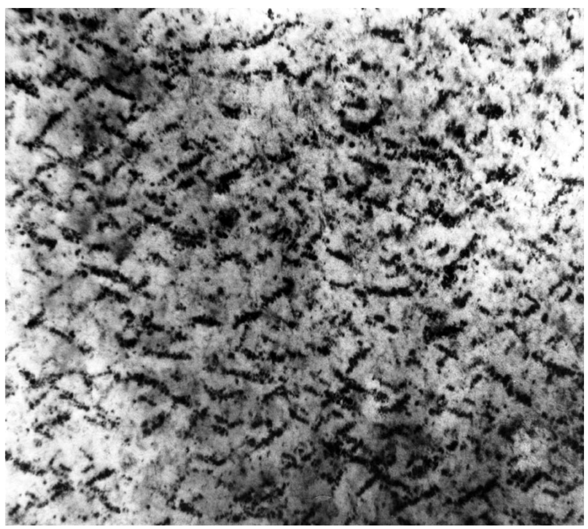
Low T (< ~450°C) irradiated microstructures

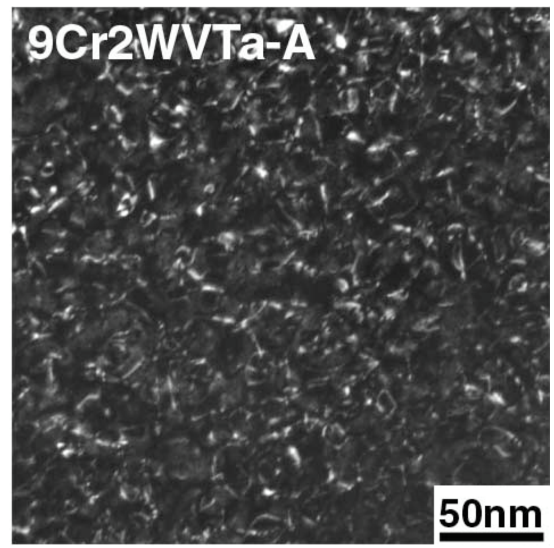
- **Dominant microstructural features in irradiated bcc (ferritic/ martensitic & Vanadium-based) alloys:**
  - **- nm dislocation loop-complexes**
  - **- nm precipitates**
  - **- sub-nm bubbles & voids, grow w/increasing radiation dose**

Loop decoration of dislocations & raft formation



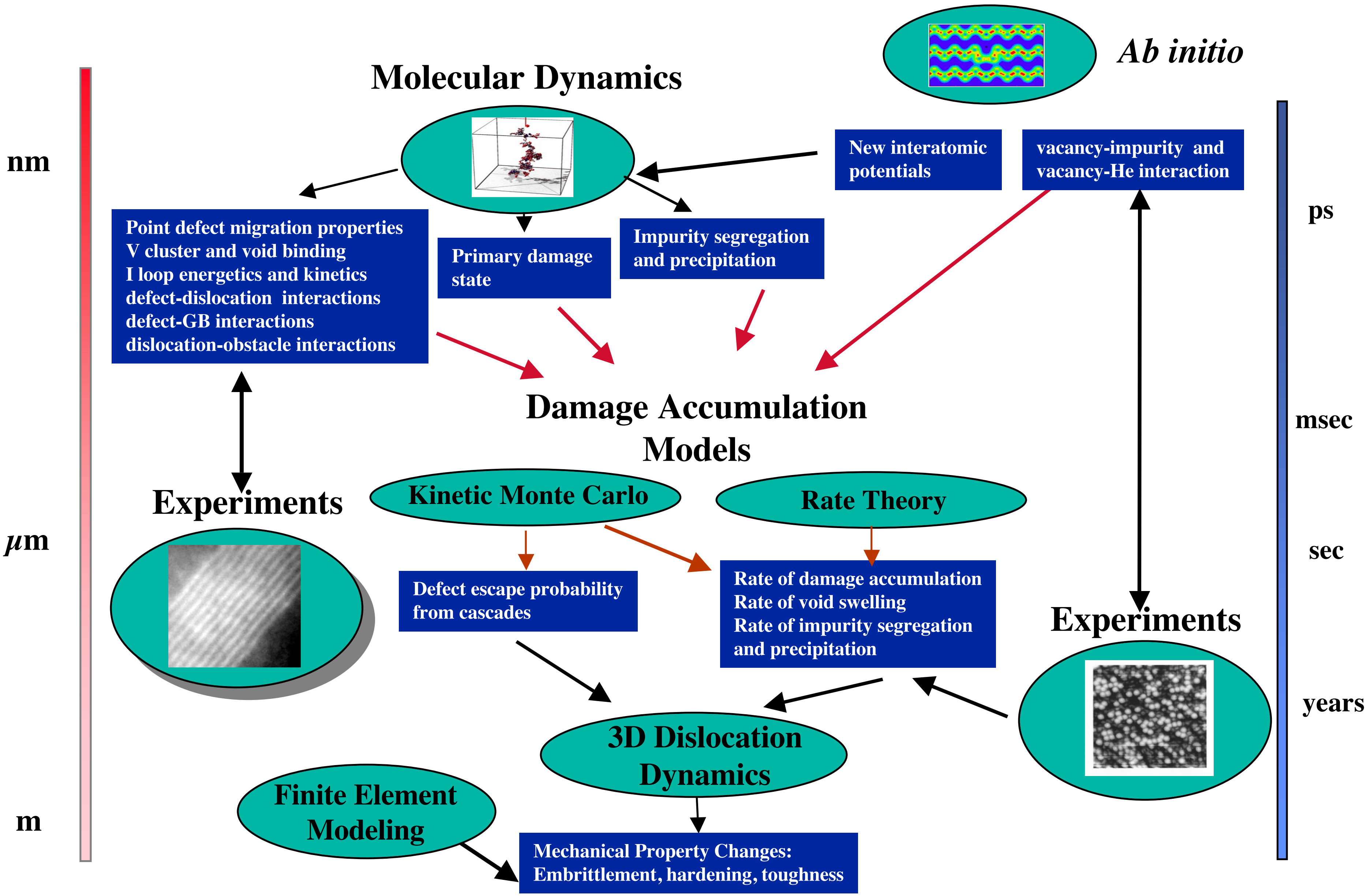


High density of <100> & <111> dislocation loops



	<d> (nm)	N (m^{-3})
<100>	20	$1x10^{22}$
<111>	30	$5x10^{21}$

Multiscale modeling approach

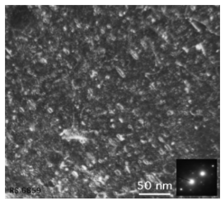


Computational microscope

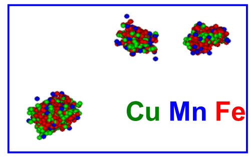
Experimental characterization

feature
'signals'

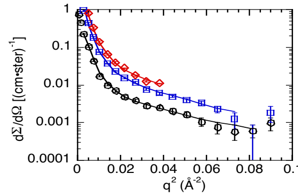
TEM



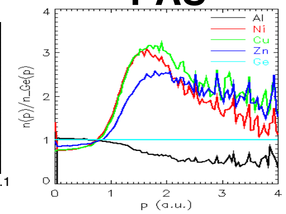
APT



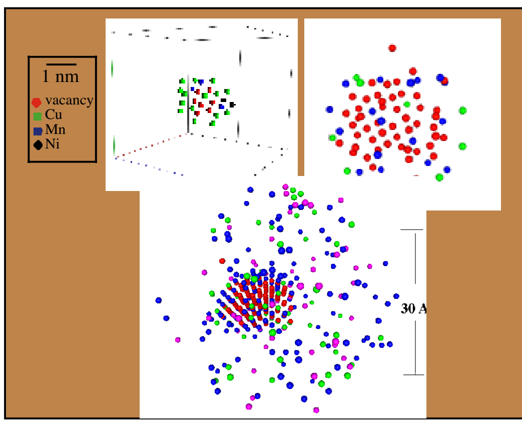
SANS



PAS



Multiscale modeling

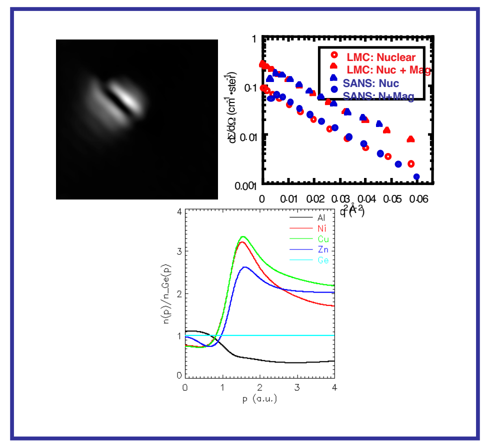


self-consistent
'understanding'

predict
features

simulate
observables

TEM, SANS, Positron theory



Apply complementary experimental measurements, closely coupled to modeling and positron theory

Ab-initio calculations lead to improved V potential

- Different EAM type potentials give very different predictions for Vanadium
- None of the EAM potentials correctly predict the stable form of the interstitial
- New interatomic Vanadium potential fit to experimental data and 1st principles calculations of: cohesive energy, bulk modulus, C_{11}, C_{12}, C_{44}, and vacancy formation energy

	vacancy	[100] split	[110] split	[111] split	[111] crowdion	Octa-hedral	Tetra-hedral
First Principles	2.60	3.57	3.48	3.14	3.15	3.62	3.69
Finnis-Sinclair	2.63	3.60	3.66	3.25	3.21	3.60	3.64

→ stable interstitial (orange shading: [111] split) Units: eV

- Very good agreement with 1st principles calculations
- Split [111] interstitial is most stable

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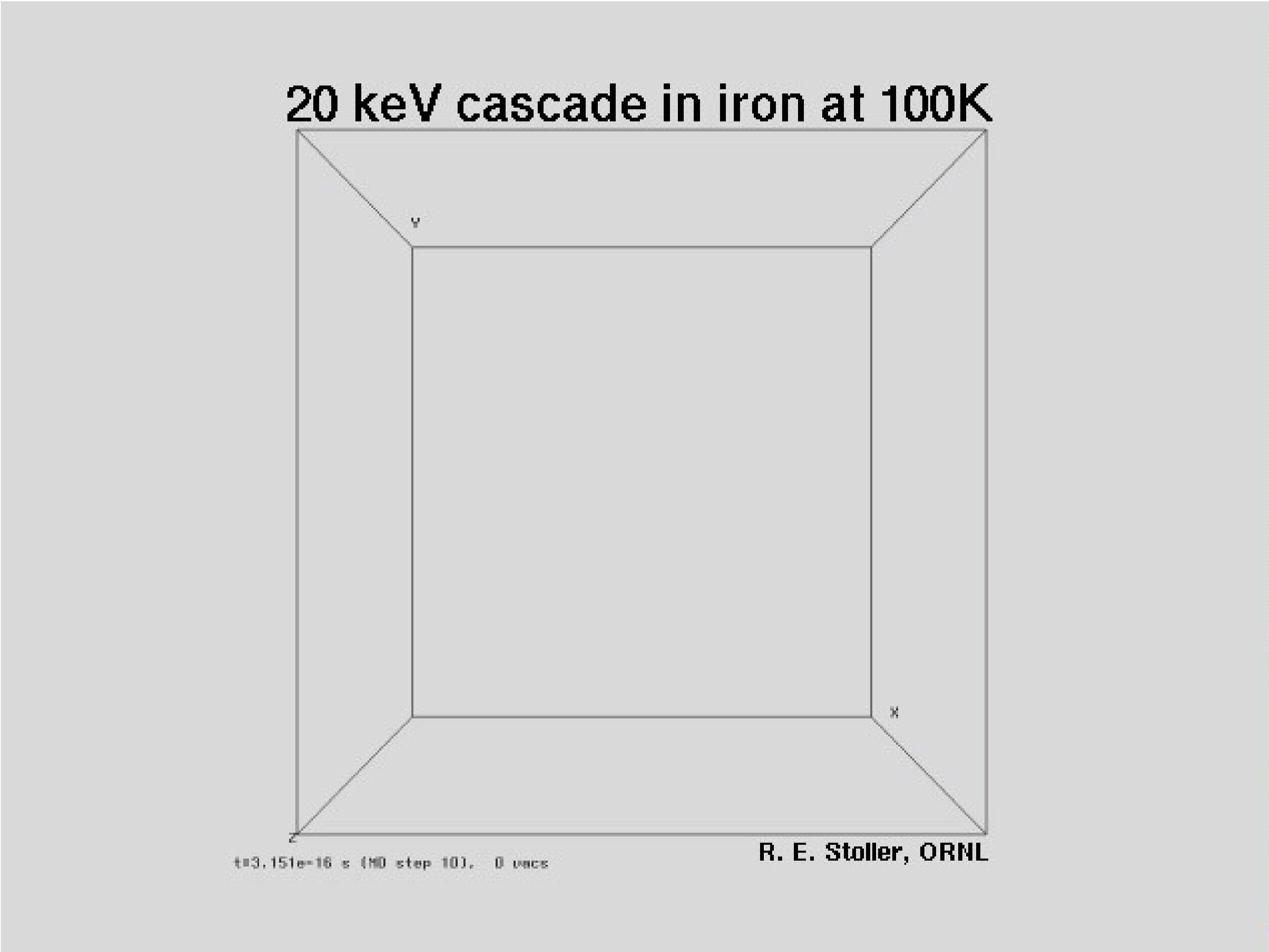
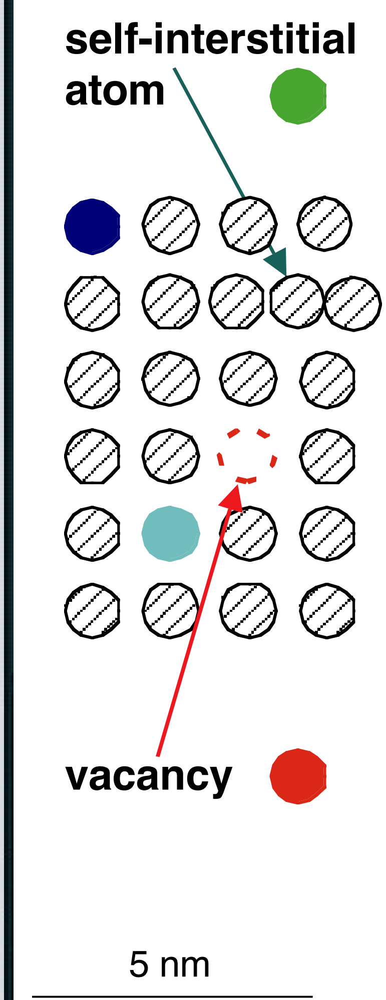
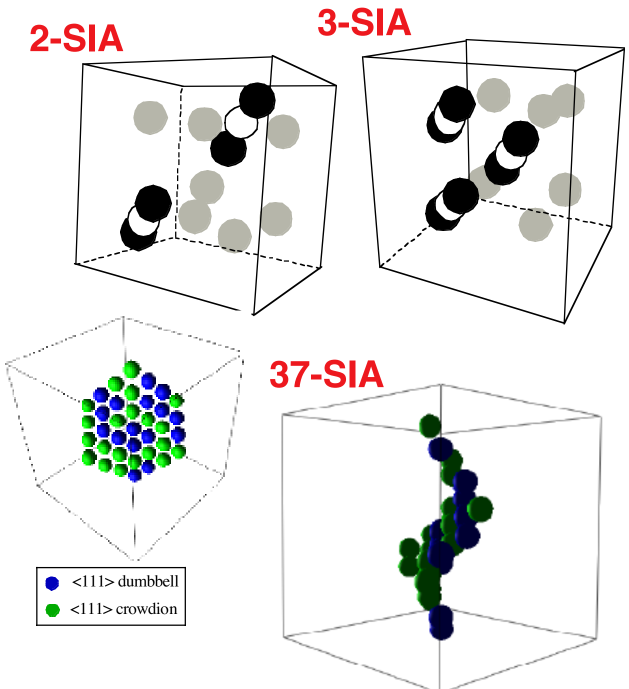
MD simulations of primary damage production



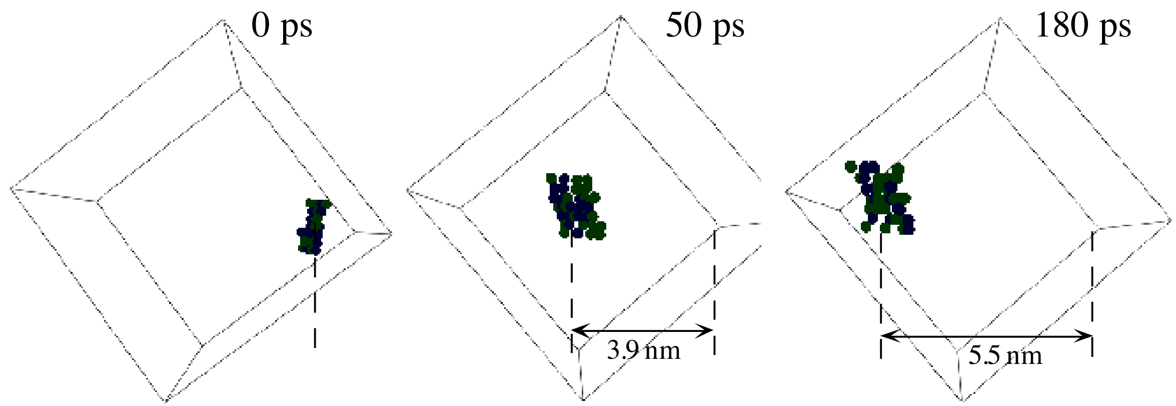


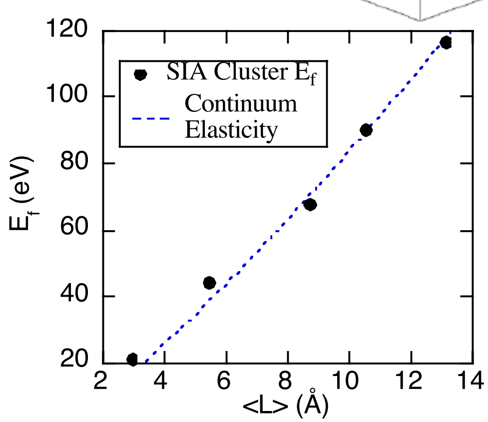
Self-interstitial clusters: <111> loops

- **Stability of <111> self-interstitial atom (SIA) clusters revealed by recent atomistic modeling (*Finnis-Sinclair and EAM-type interatomic potentials*)**



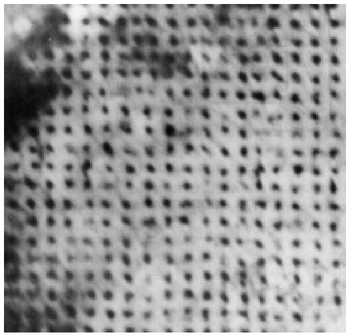
MD simulations at T=560 K reveal rapid (E^m < 0.1 eV) 1-D migration





- Form highly kinked, proto-<111> dislocation loops directly in cascades
- Migrate in 1-dimension with high mobility

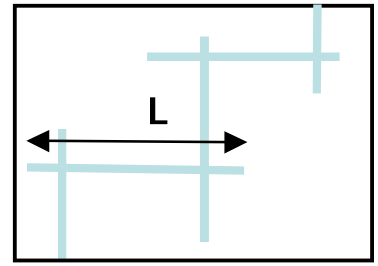
Reaction Kinetics of Interstitial Clusters and Void Lattice Formation



Void lattice in Mo, Evans et al., 1971

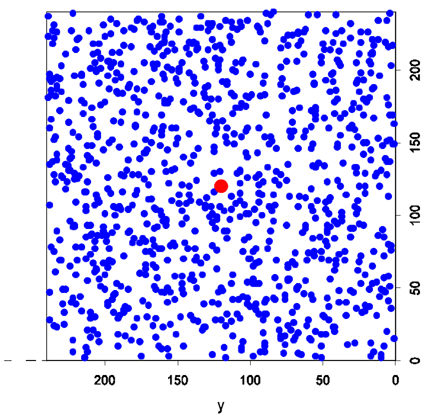
Void lattices form under high doses of cascade-producing irradiation.

Clusters of self-interstitial atoms (SIA) formed in cascades have 1D/3D defect reaction kinetics.



Extremely mobile interstitial clusters diffuse by 1D/3D migration, with average 1D path length L

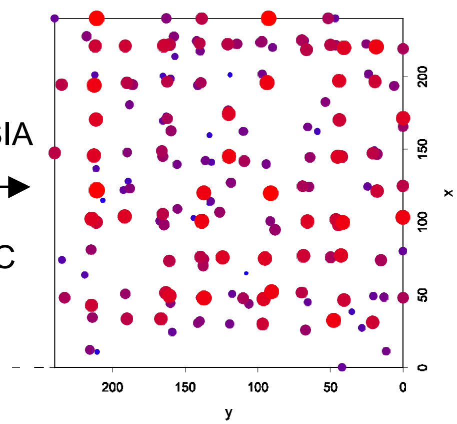
Kinetic Monte Carlo computer simulations demonstrate that irradiation producing 1D/3D SIA clusters can lead to void ordering.



Random Voids

1D/3D SIA →

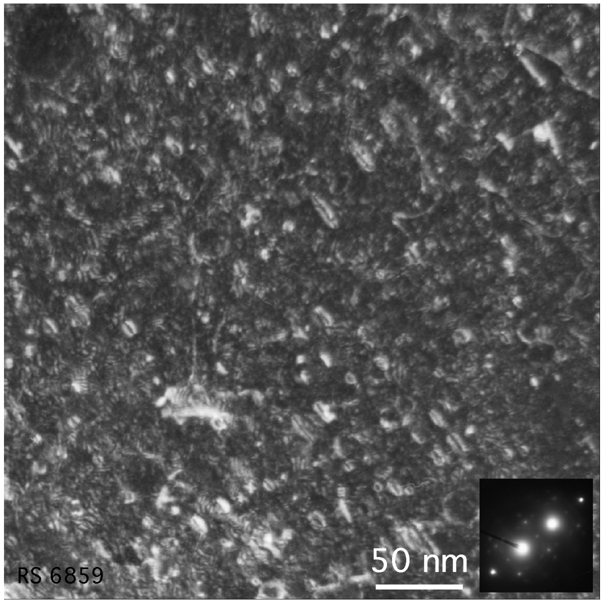
3D VAC



Ordered Voids

- **SIA clusters having 1D/3D reaction kinetics are a primary ingredient of the Production Bias Model rate theory that links atomistic defect production to microstructure evolution under irradiation.**
- **Modeling studies show that the 1D/3D kinetics of SIA clusters are essential for void lattice formation and stability.**

Dislocation loop formation in ferritic steels

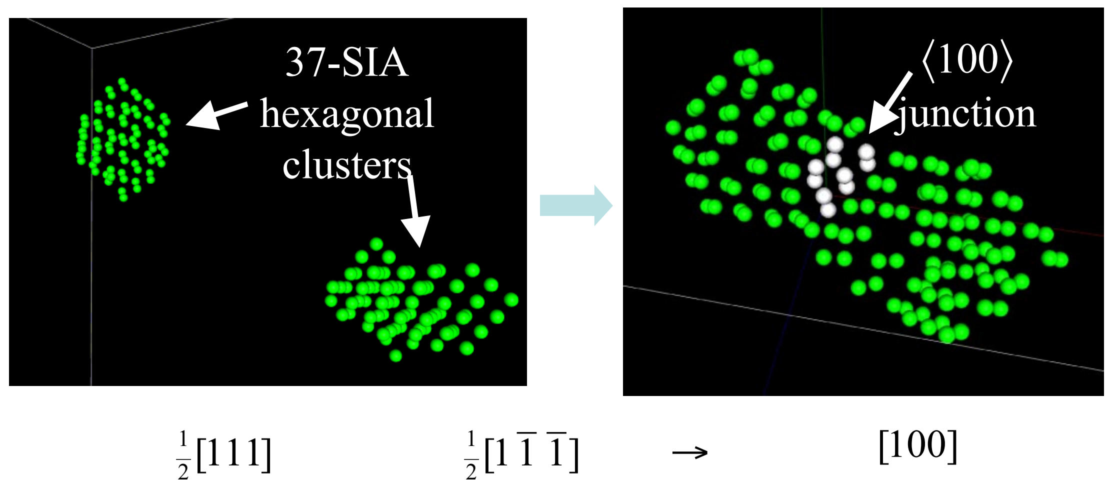


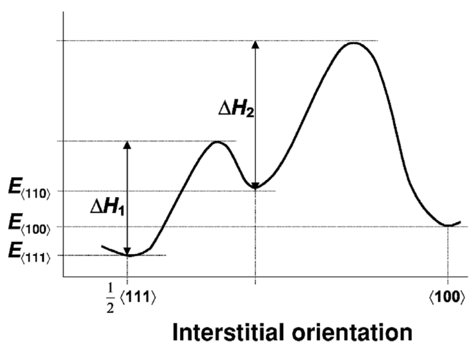
Irradiated ferritic steel (Fe-8Cr)

- **Large density of <100> loops observed (TEM) at high dose**

- New insight: <100> junctions form through interaction of highly mobile, <111> loops:

$$\frac{a_o}{2}\left[111\right] + \frac{a_o}{2}\left[1\bar{1}\bar{1}\right] \rightarrow a_o\left[100\right]$$





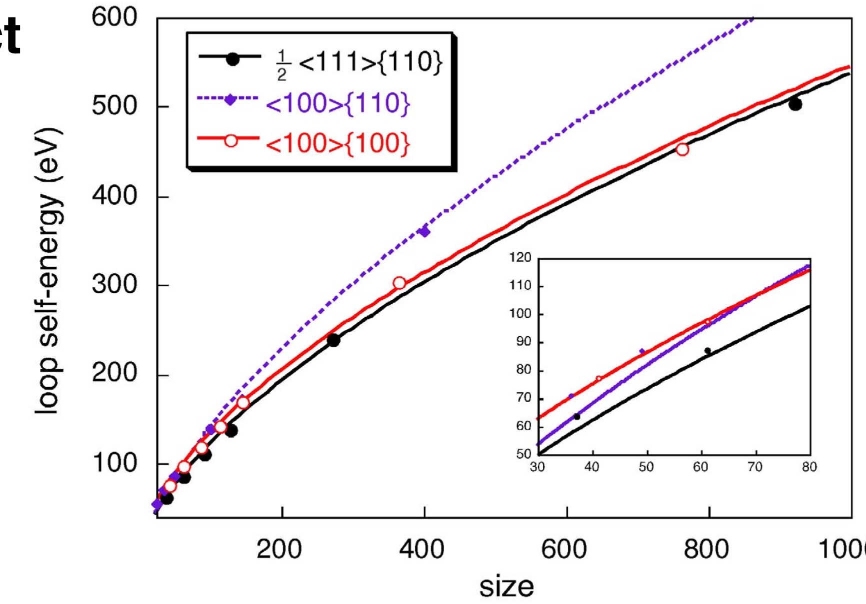
- Junction propagates or dissolves by 2-step mechanism

Energy landscape favors <100> growth

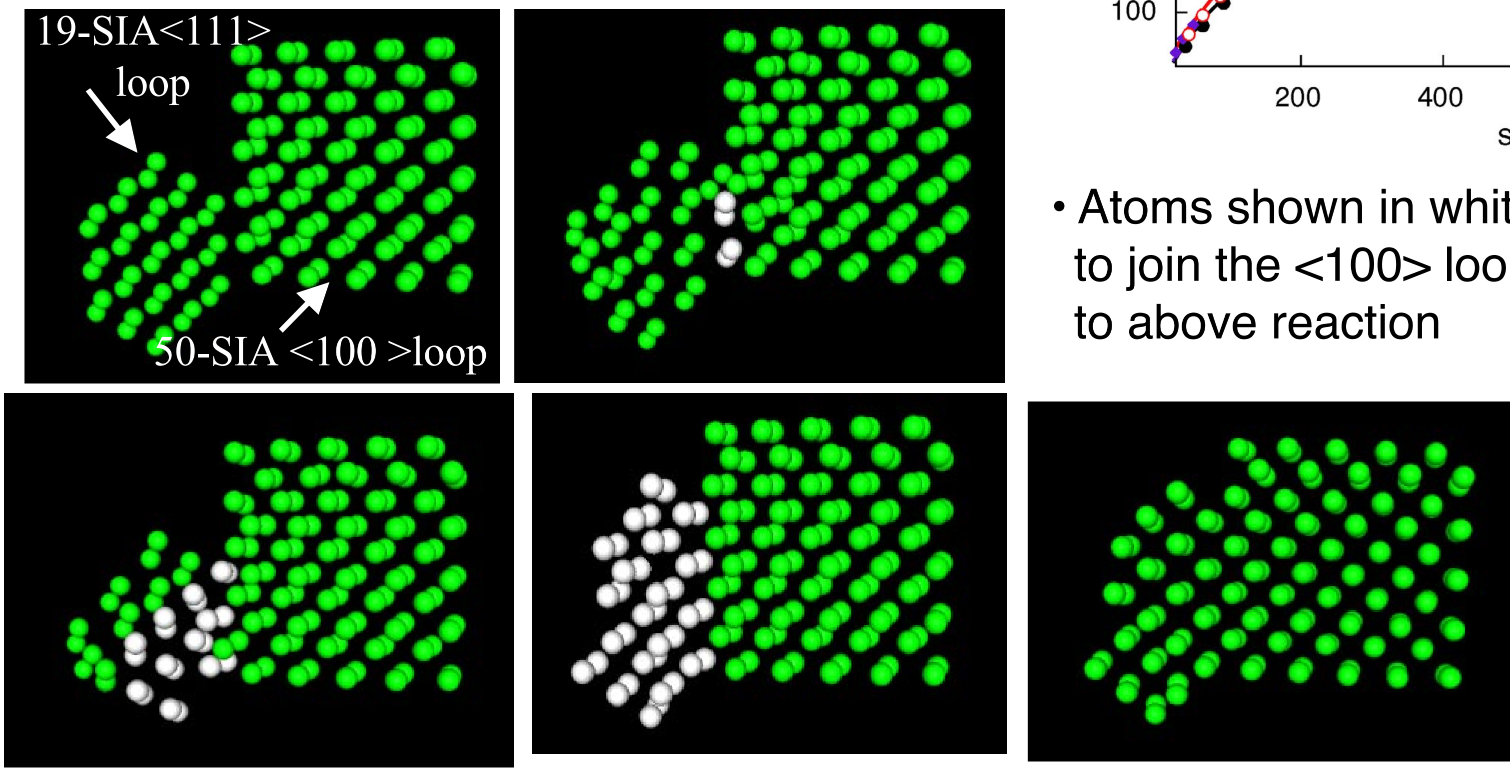
Growth mechanisms of <100> loops

- **Despite being metastable with respect to <111> loops, <100> loops grow by absorption of smaller <111> loops**

$$\langle 100\rangle + 2\,\frac{1}{2}\langle 111\rangle \rightarrow \langle 211\rangle \rightarrow \langle 100\rangle$$

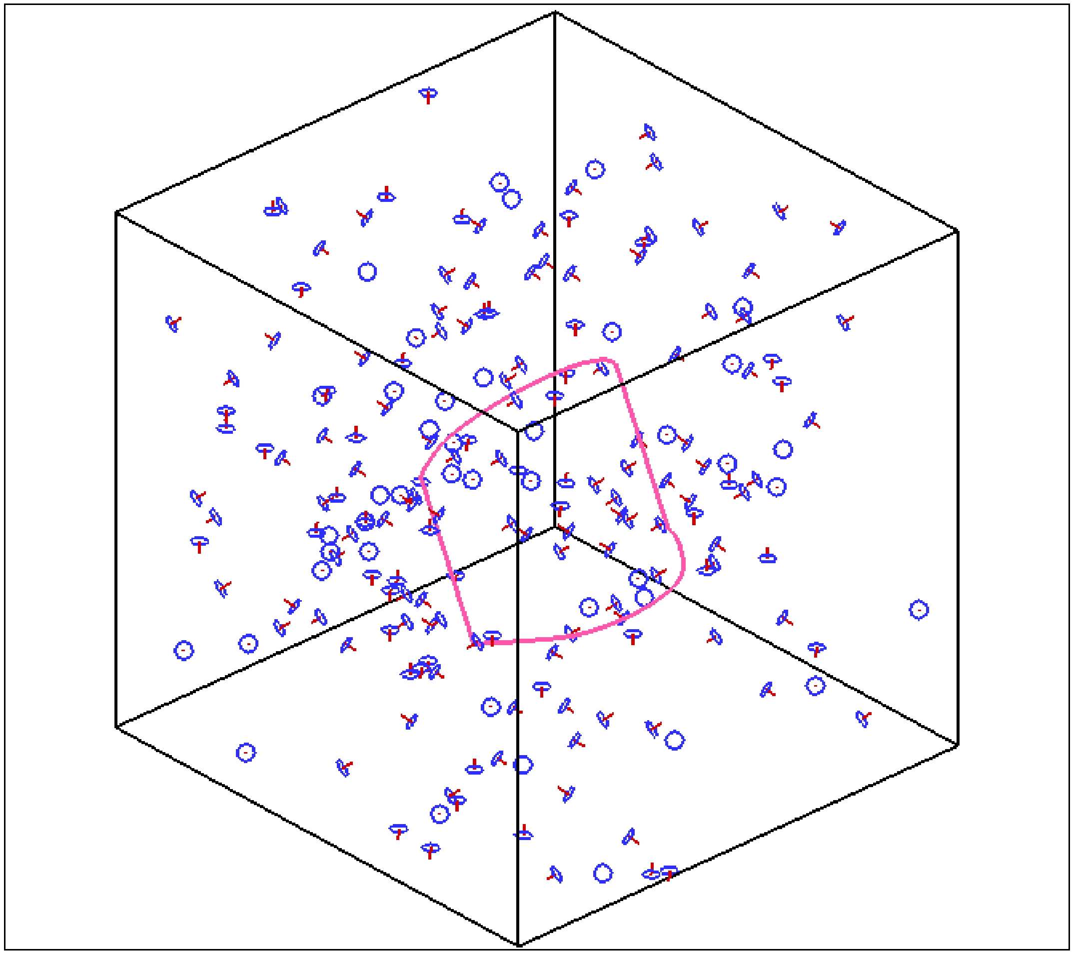


- Atoms shown in white, are rotating to join the <100> loop according to above reaction



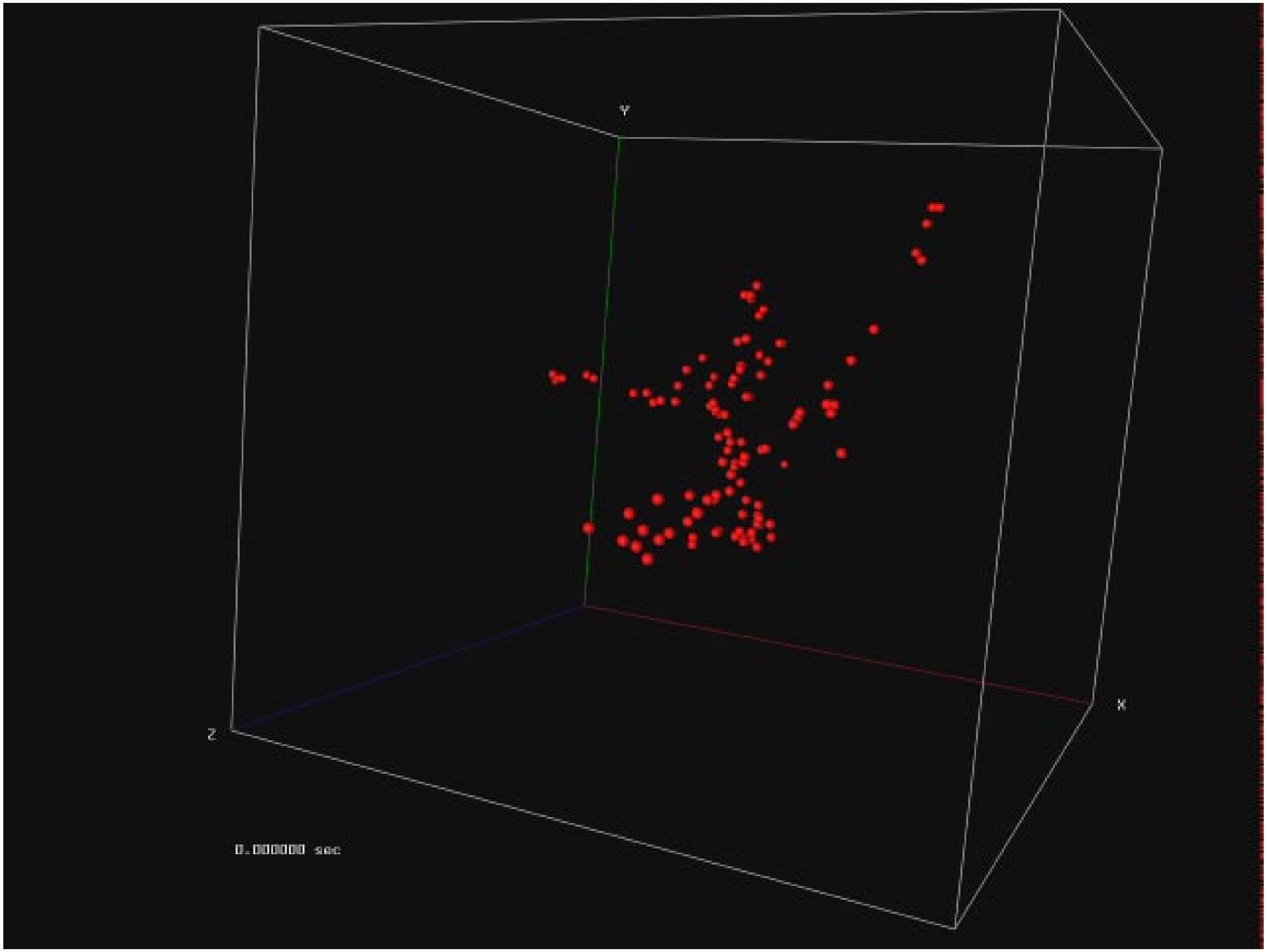
Dislocation decoration & rafting

Decoration



SIA Cluster Interaction with Dislocation Demonstrating the Importance of Cluster Rotation on Dislocation Decoration

50 keV cascade aging in Fe at 563 K



Vacancy cluster evolution movie

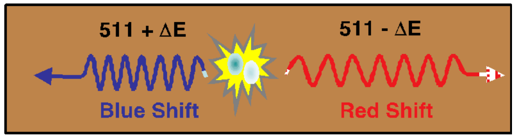
5 nm

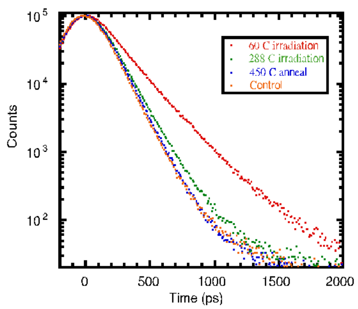
- Rapid formation of sub-nanometer 3-D clusters
- Small clusters are mobile and cluster growth often involves coalescence

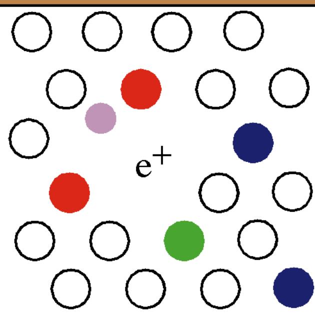
vacancy

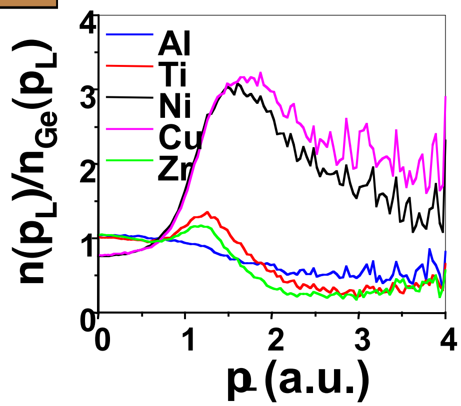
Validation of sub-nm vacancy-solute clusters

Positron annihilation spectroscopy

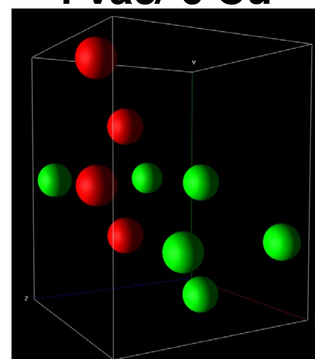






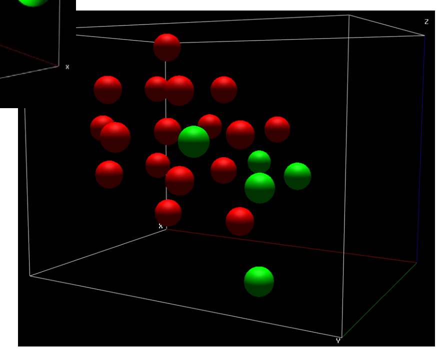


4 vac/ 6 Cu



KMC predicts vacancy-Cu clusters

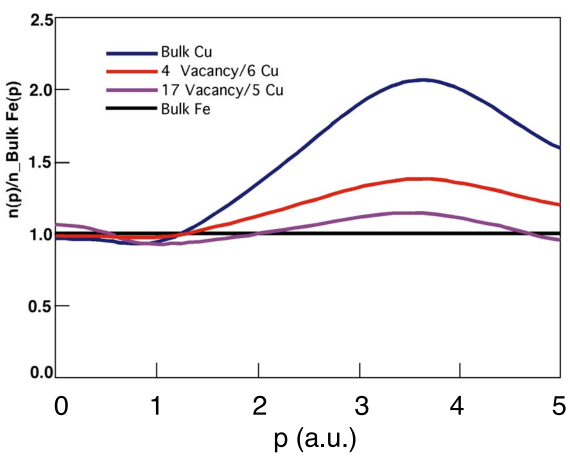
17 vac/ 5 Cu



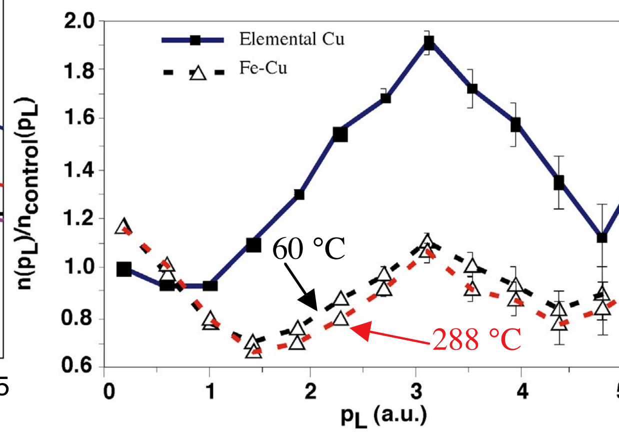
Predicted positron lifetimes

Vac/Cu	τ (ps)
3/6	173
4/6	216
17/5	350
>50/x	520

Predicted OEMS



Measured OEMS



Measured positron lifetimes

τ (ps) - 60°C
178
355

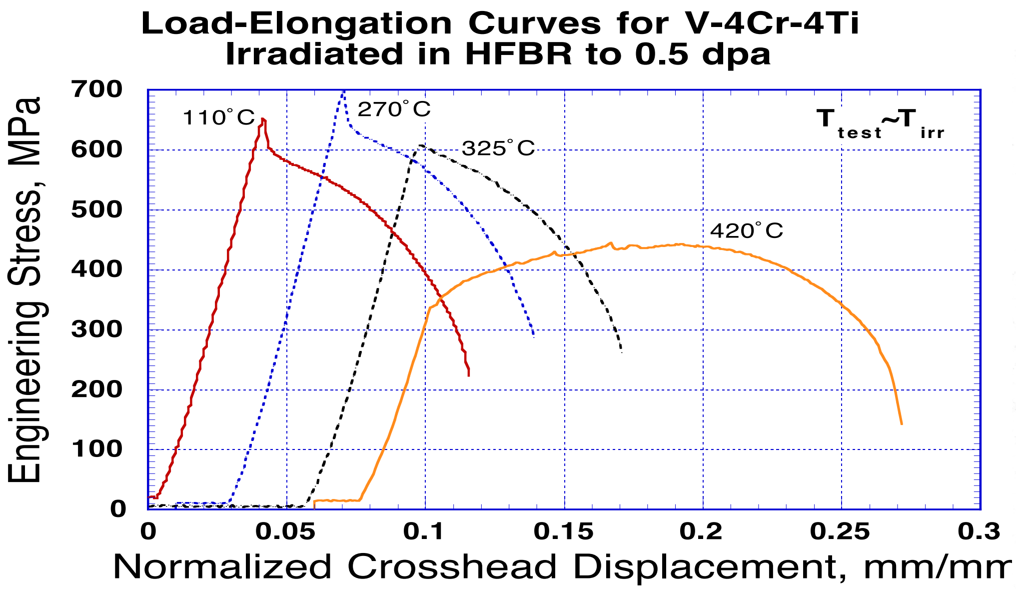
τ (ps) - 288°C
222
520

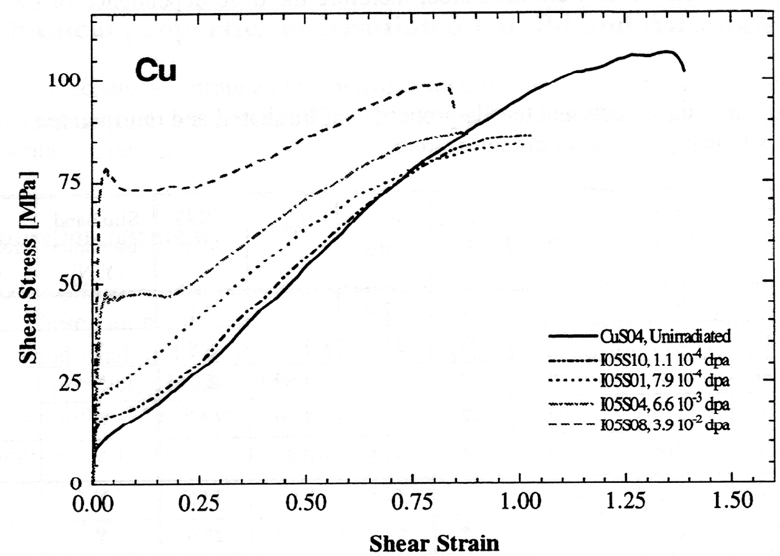
Summary of nanostructural evolution

- Radiation damage produces primary defects (vacancies & self-interstitials) in highly non-equilibrium, spatially correlated process
- Self-interstitial clusters in Fe-alloys formed with a/2<111> Burgers vector, undergo easy 1-dimensional glide
- At high dose (> ~0.1 dpa) in Fe-alloys, collisions between <111> loops result in the formation of dislocation loops with Burgers vector a<100>
- <111> loops which escape collision migrate to dislocations forming loop rafts which decorate dislocations
- Remaining vacancies cluster to form small 3-dimensional nanovoids

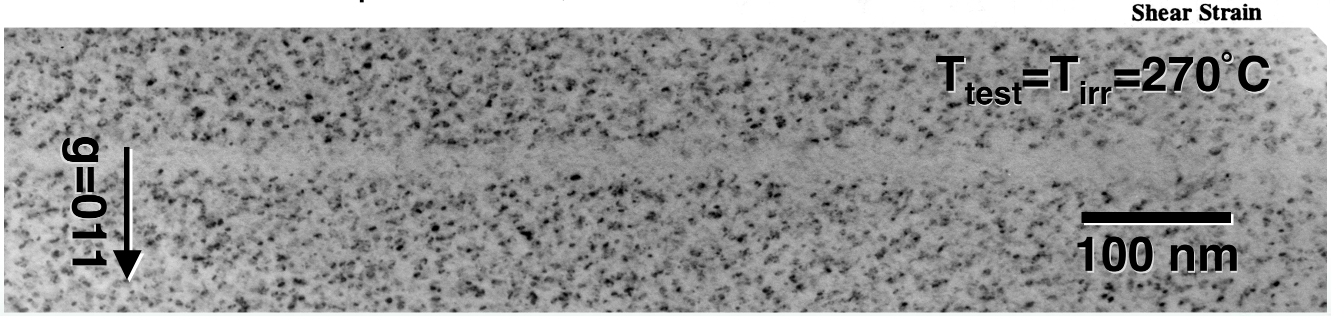
Impact on mechanical properties

- **Irradiation-produced nanostructures impede dislocation motion & significantly impact mechanical properties & structure performance**
  - hardening, decreased ductility, yield drops and dislocation channeling



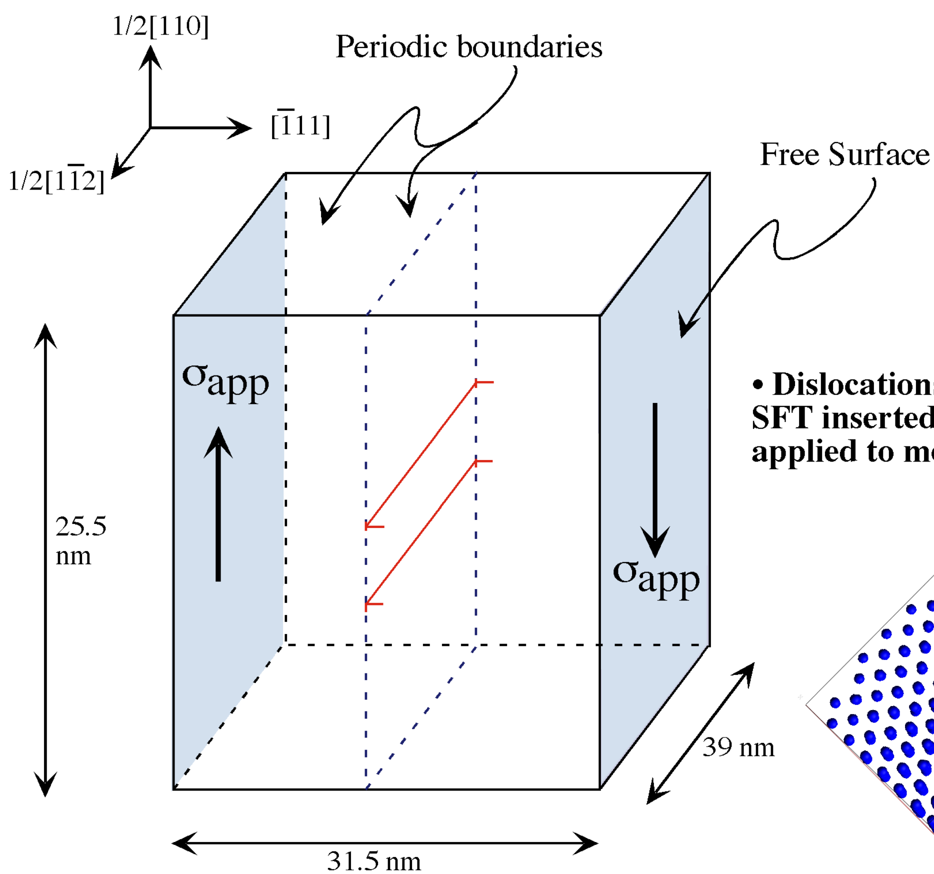


Dislocation channeling in V-4Cr-4Ti



Edge dislocation - SFT interaction (Cu)

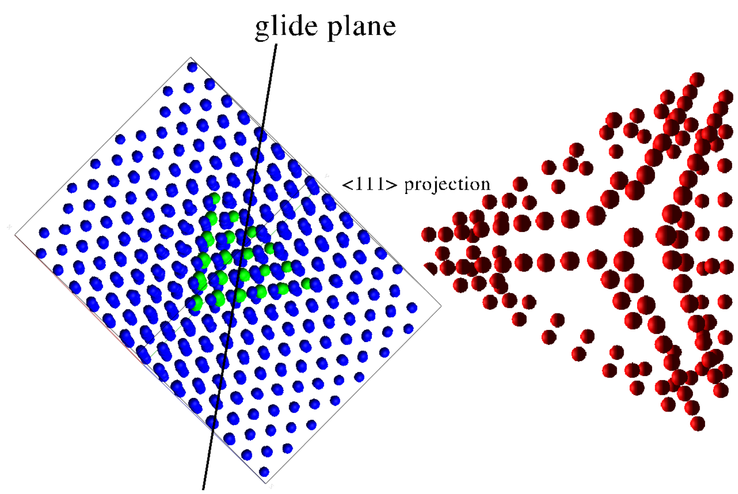
- **Atomistic (MD) simulations of individual dislocation - obstacle interactions provide fundamental understanding of radiation hardening and flow localization phenomena**



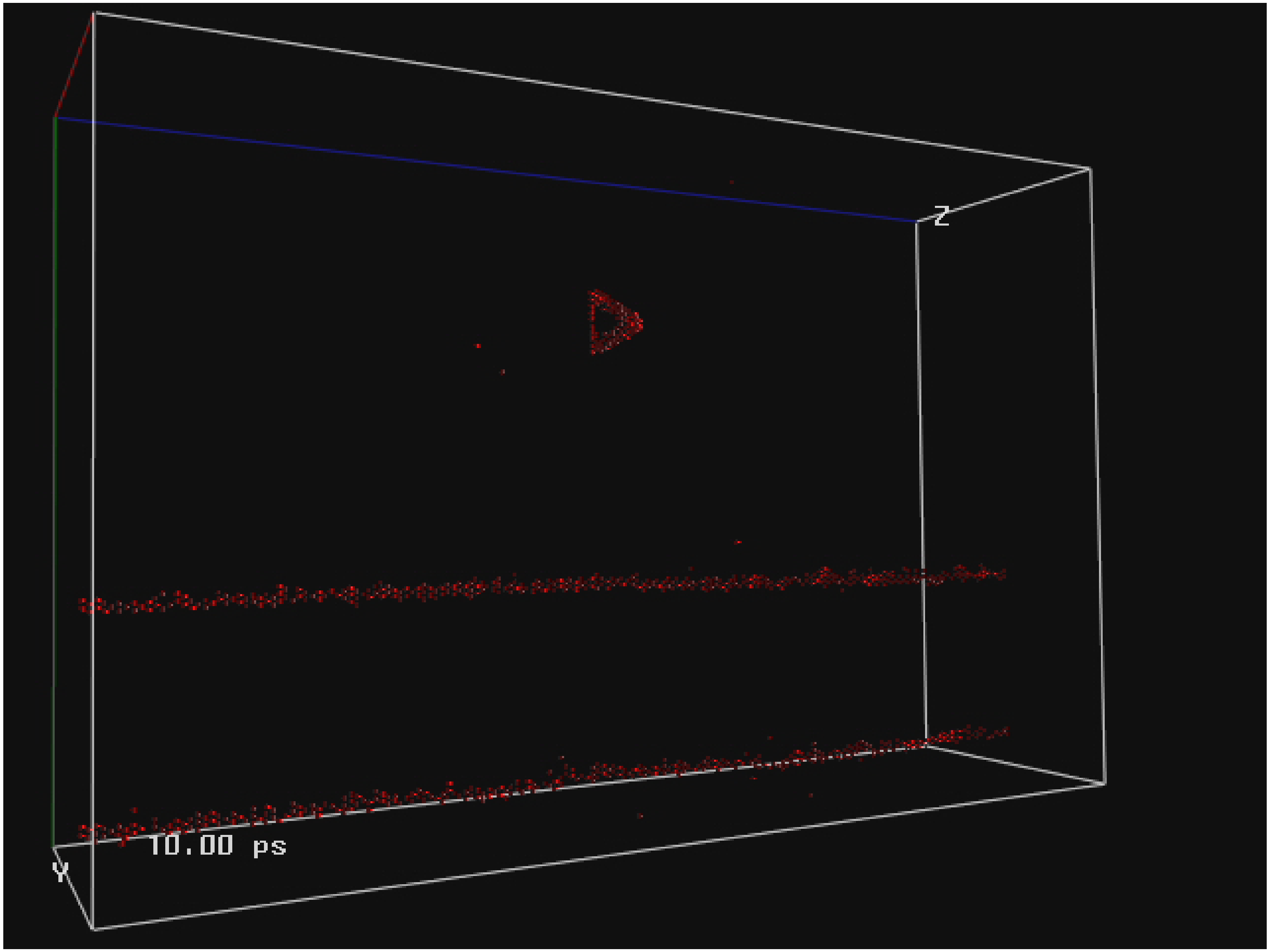
EAM Cu:

	(10^{10} Pa)
c_{11}:	17.6
c_{12}:	12.9
c_{44}:	8.23
μ:	5.88
γ_{SFE}:	11.40 mJ/m^2

- **Dislocations inserted and equilibrated at 100 K, SFT inserted across the glide plane and shear stress applied to move the dislocation**



Dislocation - SFT interaction (300 MPa)



Dislocation - SFT interaction movie

near - <111> projection

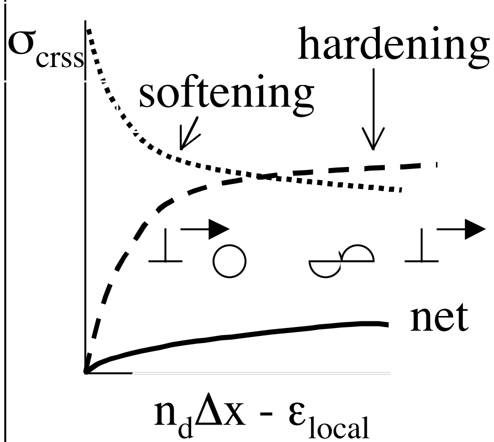
- SFT is a relatively strong obstacle $\phi \sim 80°$
- SFT sheared but neither absorbed or destroyed

Decouple Multiscale Localization Mechanisms

- Isolate and properly integrate *multiscale* parts - and determine what controls observables

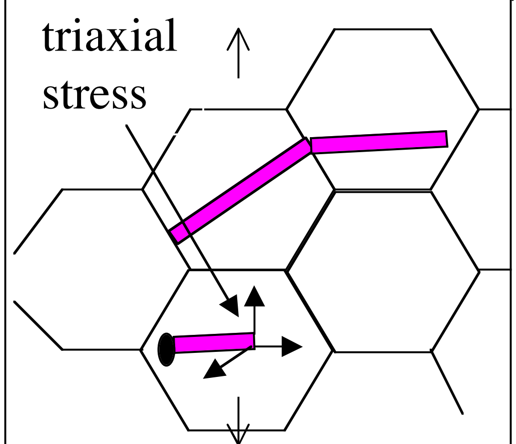
Microconstitutive

dislocation-obstacle interactions and processes controlling local $\sigma_{crss}(\varepsilon_{local})$



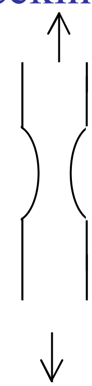
Micromechanics

deformation patterns and localization-depend on σ, σ-state redistribution



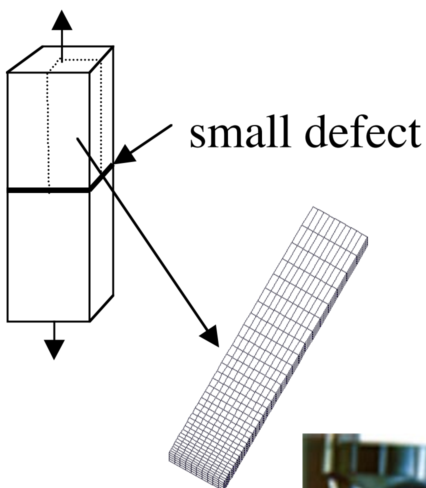
Continuum Mechanics

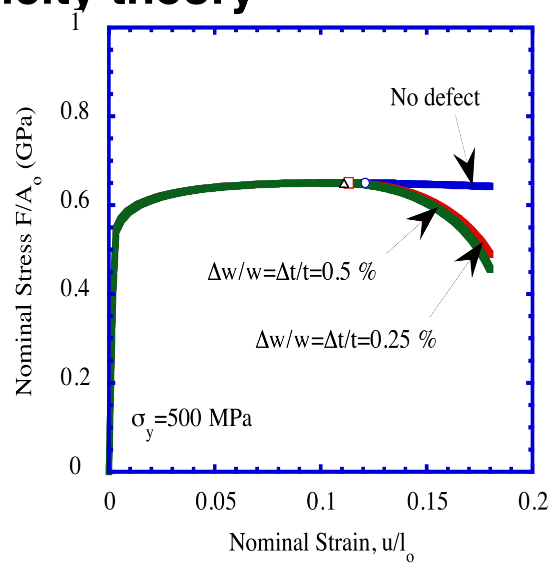
large geometry-change deformation & load- instability-necking

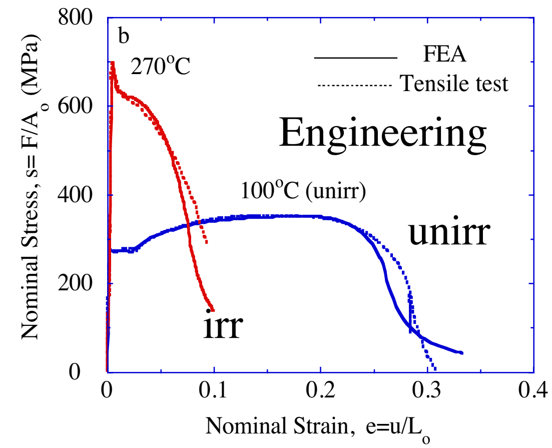


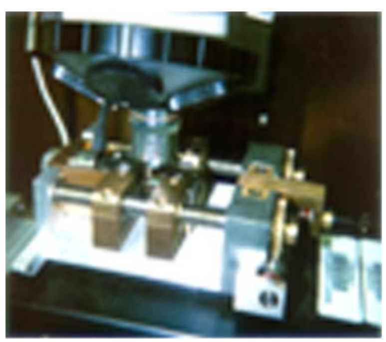
Understanding Loss of Uniform Strain Capacity

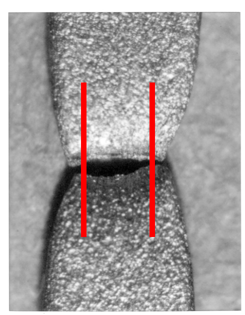
- **Assessment of engineering tensile data to demonstrate a modest true-strain softening, persistence of irradiation hardening and applicability of J_2 incremental plasticity theory**

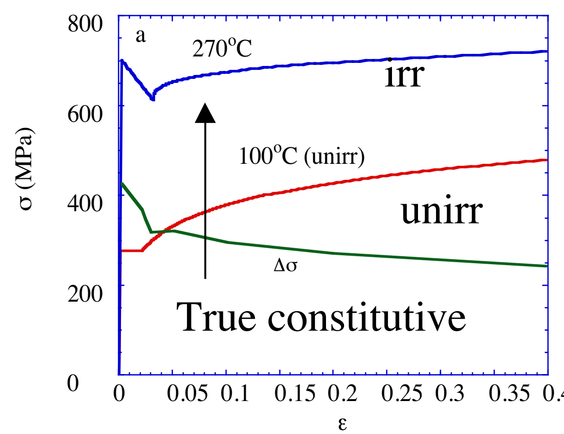












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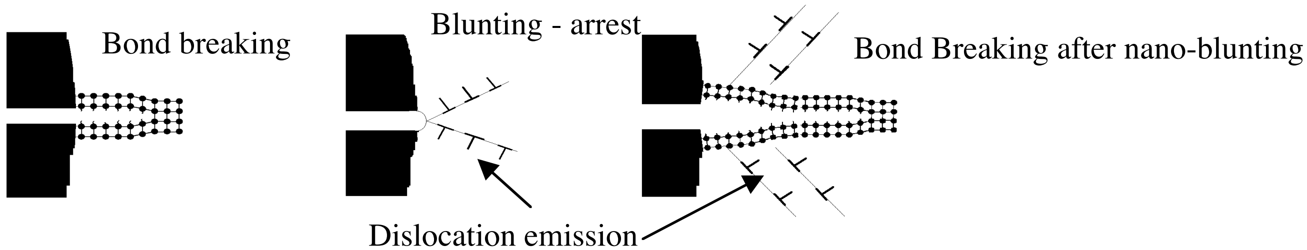
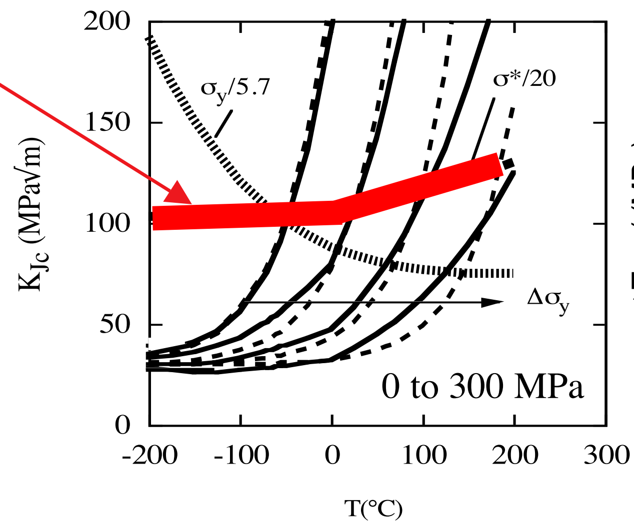
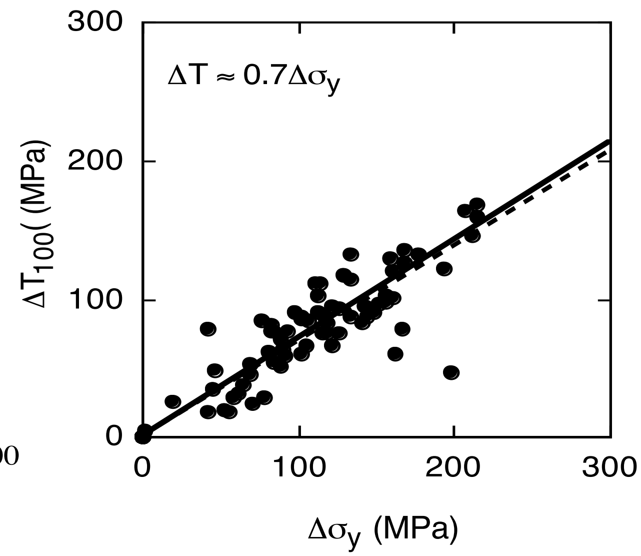
Micromechanics of Universal MC Shape & Shifts

Atomic scale dislocation-bond breaking processes modeled as the basis for the existence of a universal master toughness-temperature shape and magnitude of the shift due to irradiation hardening



New intrinsic property of bcc structures?





UCSB

Summary & future focus

- Radiation damage is inherently multiscale phenomena - US Fusion Materials program applying multiscale modeling, closely coupled with theory & experiments to develop *fundamental understanding of radiation damage in structural alloys*

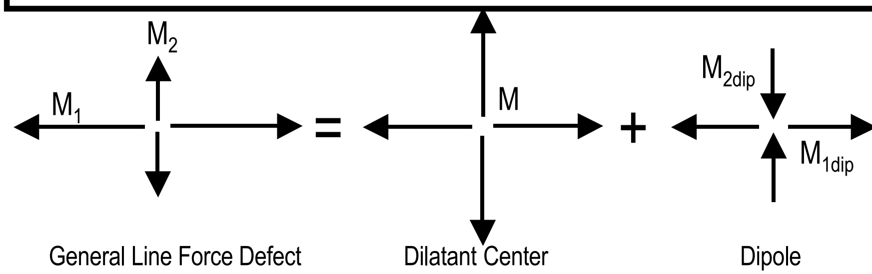
- Examples of radiation damage in bcc alloys at T <~450°C
  - nanostructural dislocation loop evolution
  - sub-nanometer vacancy cluster formation
  - effect of nanometer defect clusters on dislocation motion (hardening)
  - impact of radiation hardening on deformation & failure

- Future focus -> Investigate the impact of high He production rates on bcc alloy material evolution, properties and performance

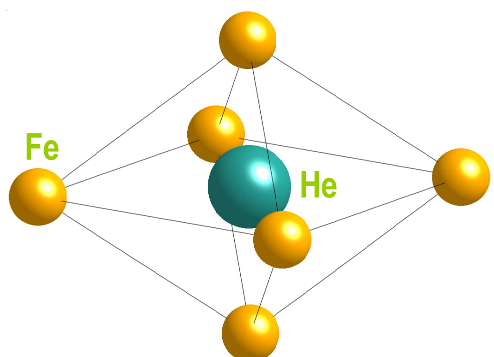
Displacement Fields of Helium in Iron

Point defect displacement fields are well approximated by line force dipoles. Fits of atomistic He displacement fields to dipole equations enables calculation of interaction energies and forces between helium atoms and other microstructural features at higher length and time scales.

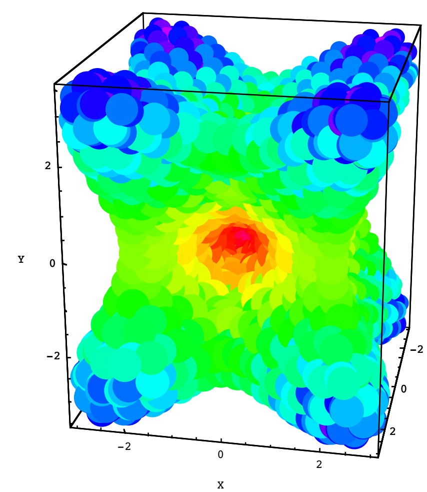
Schematic of displacement field represented by a line force defect (unequal force dipoles) and separation into dilatant center (equal force dipoles) and dipole part (equal but opposite force dipoles).



Atomic Model of Octahedral Interstitial He in Fe

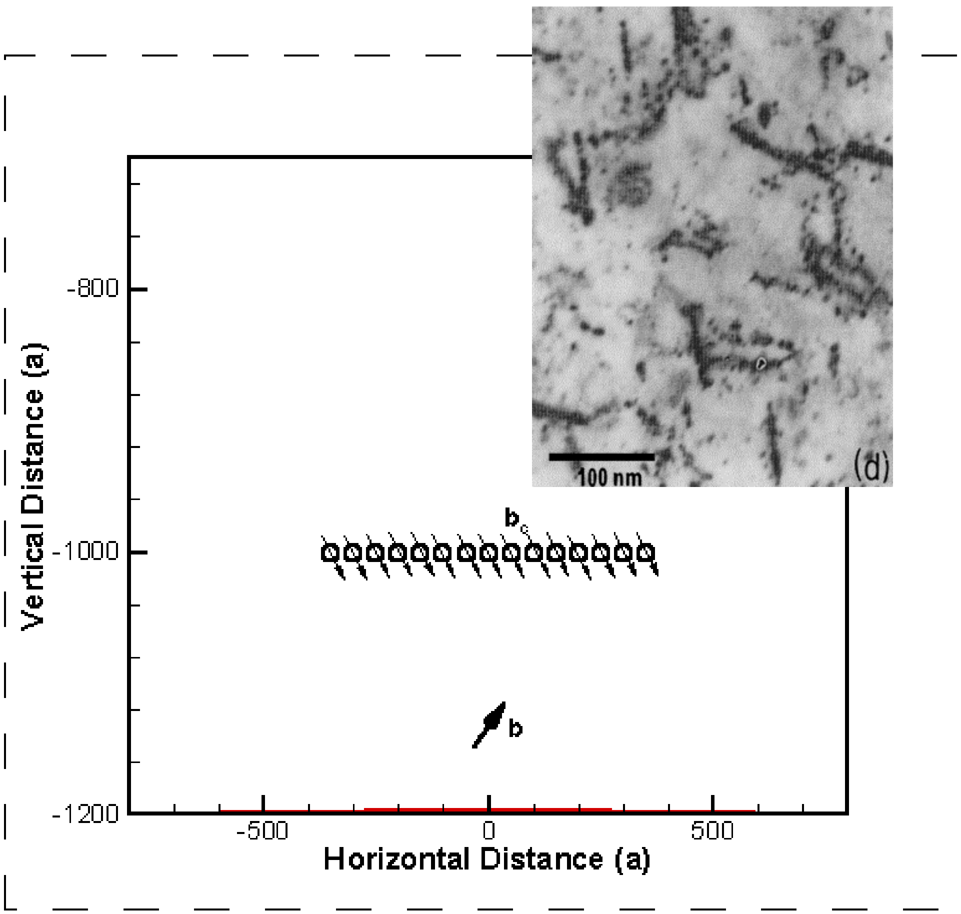


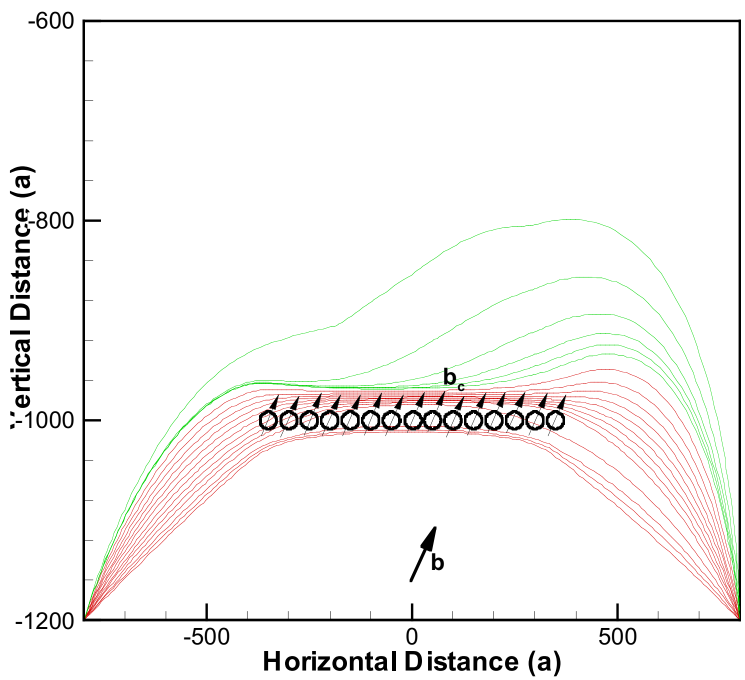
3D view of He interstitial displacement field showing a multi-lobed shape that is a characteristic of the octahedral site and the elastic anisotropy of Fe



Battelle

Mechanisms of Dislocation Unlocking from Cluster Atmospheres





Z=D=40, L=50,b=1/2(-101),Stress = 200 MPa, Attractive Clusters