Fusion Materials Science
Overview of Challenges and Recent Progress

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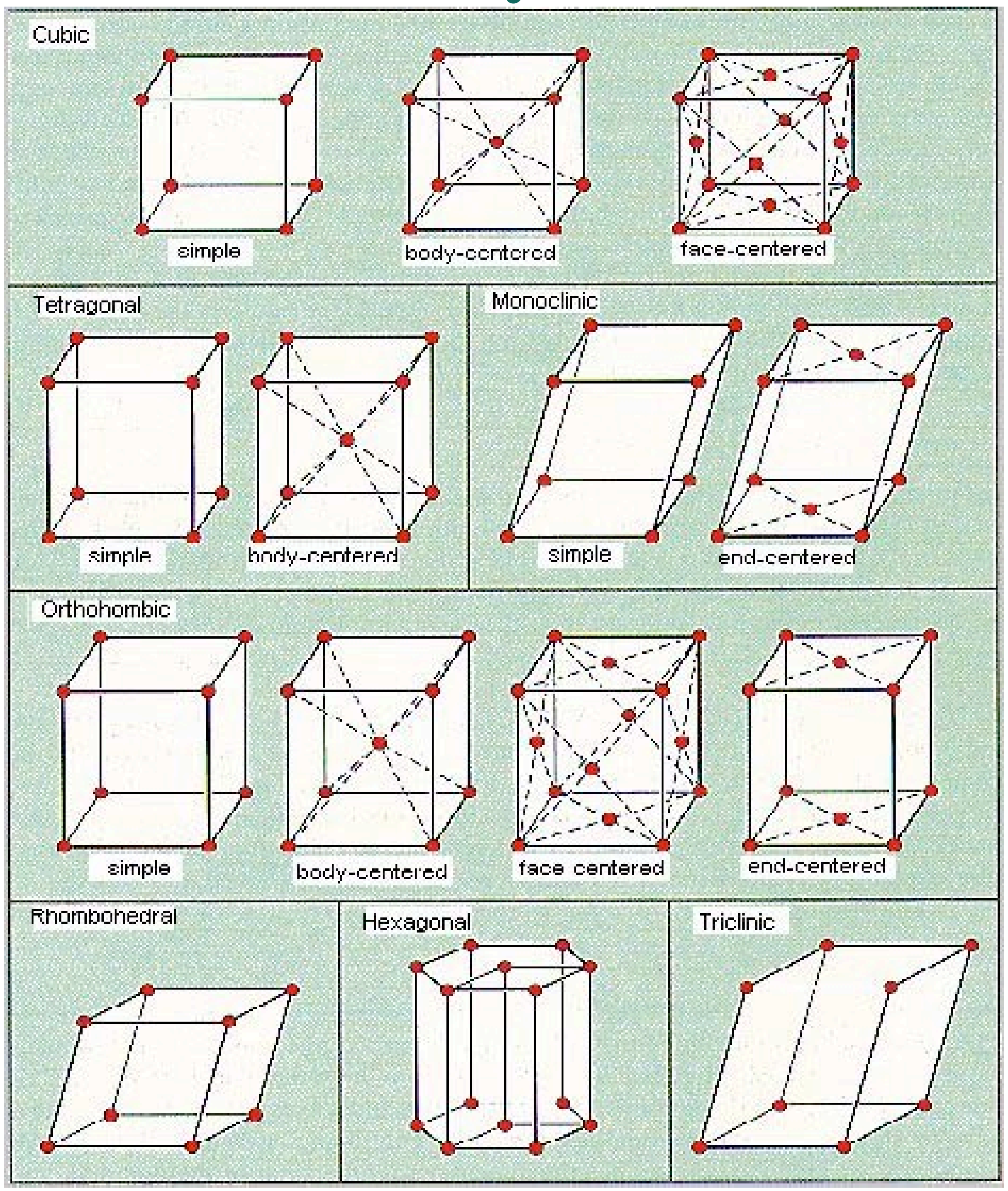
Introduction

- Large increases in worldwide energy needs are projected to occur over the next 40 years
  - China is planning to install 900 GW_e of new power by 2020 (will surpass US as leading energy consumer)
  - Nuclear power (fission) currently provides 24% of world electricity (20% in US)
- Historical paradigm: Development of new materials for structural applications is historically a long process
  - Ni_3Al intermetallic alloys commercialization
  - Superalloy turbine blade development
  - Cladding and duct materials for fast breeder fission reactors
- The hostile fusion environment (thermomechanical stress, high temperatures, high fusion neutron flux) arguably makes fusion materials development the greatest challenge ever undertaken by materials scientists
  - Requirement to restrict consideration to "reduced activation" elements produces further constraint
- This talk reviews operating environment challenges and multiscale modeling approach used to develop candidate materials for fusion reactors
  - Materials with high neutron radiation resistance generally have very good high temperature capability (high thermal creep resistance) due to high density of nanoscale precipitates

Outline

- Materials Science primer
- Overview of fusion reactor environment: radiation damage issues
- Multiscale materials modeling examples from U.S. fusion materials program
  - Close coupling with experimental studies
  - Main current emphasis is on radiation hardening and embrittlement of irradiated materials
- Examples of improved materials developed by fusion
  - Time frame for developing new materials

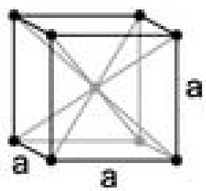
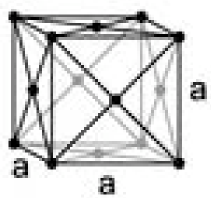
All crystalline solids can be described by one of 14 Bravais lattices



Cubic lattices are most important for structural materials

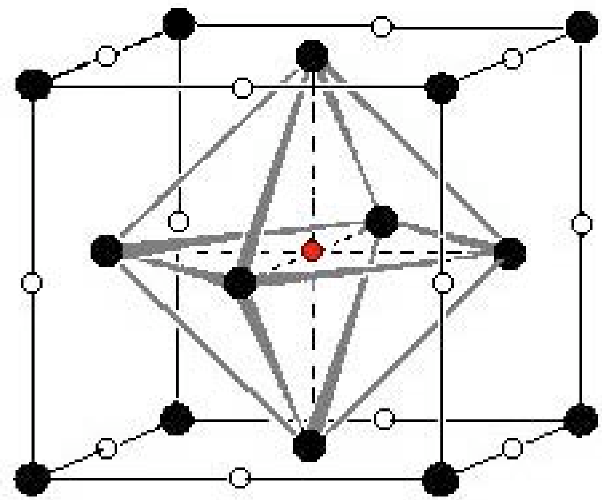
Metals are approximately equally divided among three Bravais lattices:
Body centered cubic (BCC)
Face centered cubic (FCC)
Hexagonal close packed (HCP)

Metals are approximately equally divided among three Bravais lattices

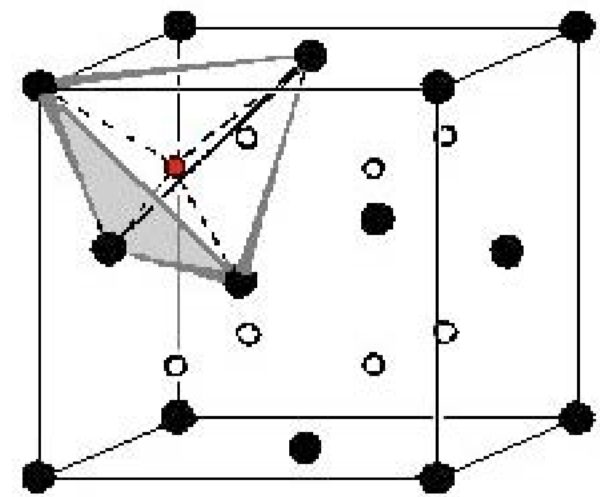
Bravais lattice	Coordination number	Packing density	Independent slip systems	Comments
Body centered cubic (BCC) 	8	68%	12	High strength
Face centered cubic (FCC) 	12	74%	12	High ductility
Hexagonal close packed (HCP)	12	74%	3	Low ductility

General plastic strain requires 5 independent slip systems

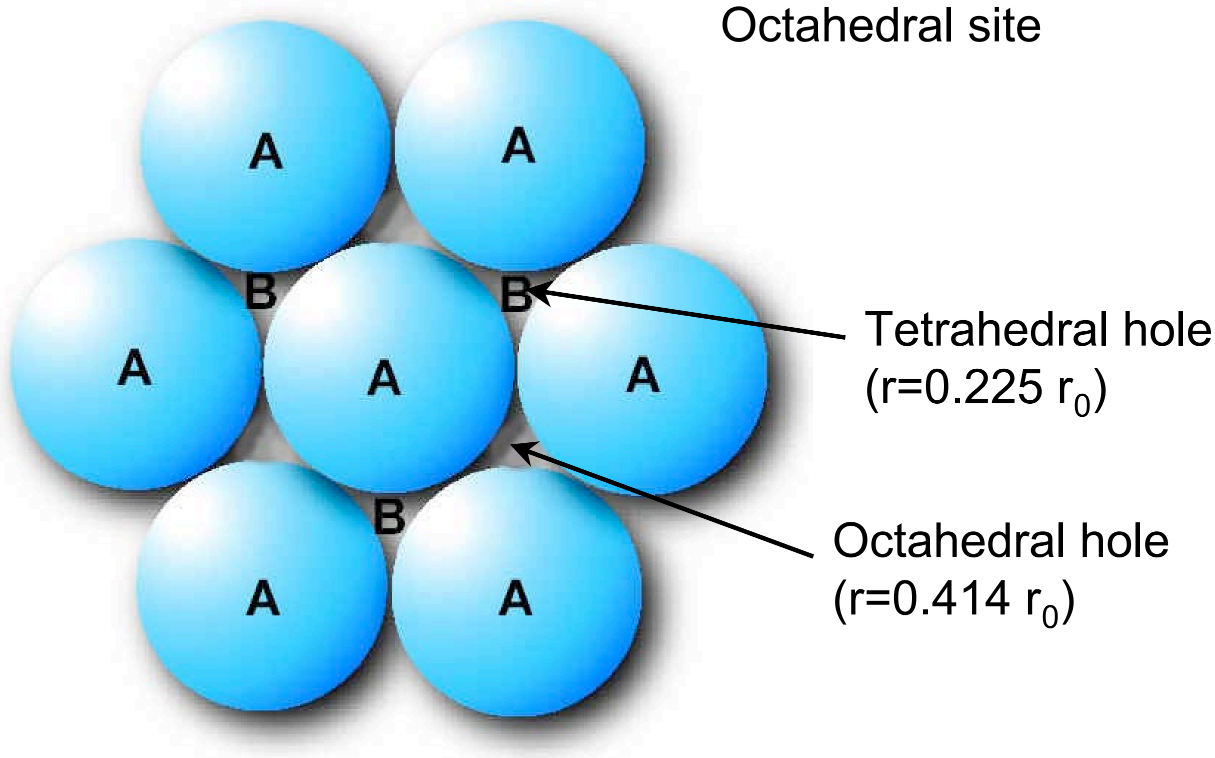
Octrahedral and tetrahedral lattice sites in FCC crystal



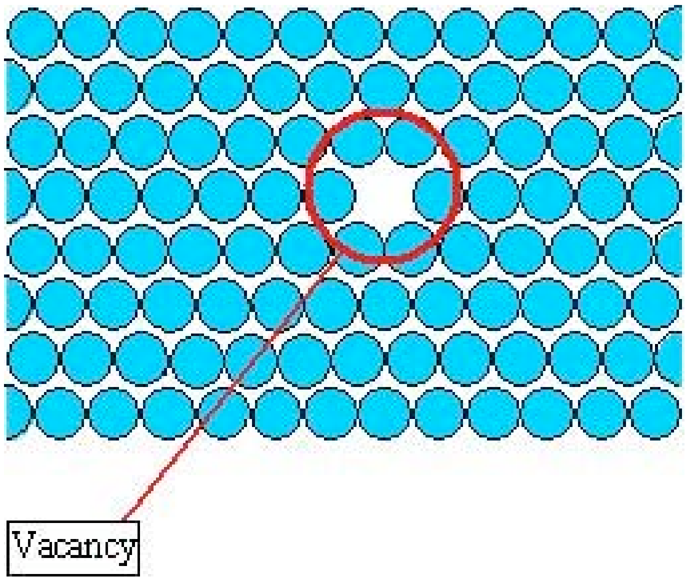
Octahedral site

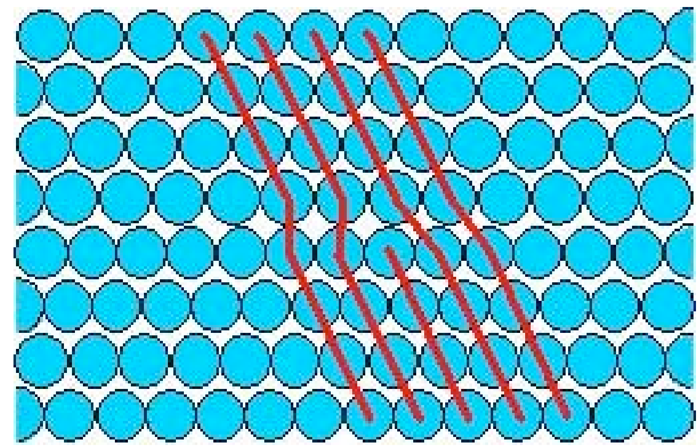


Tetrahedral site

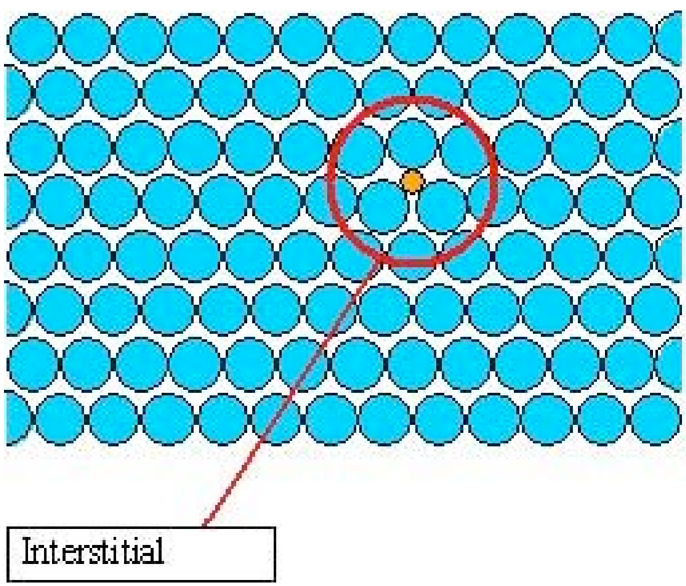


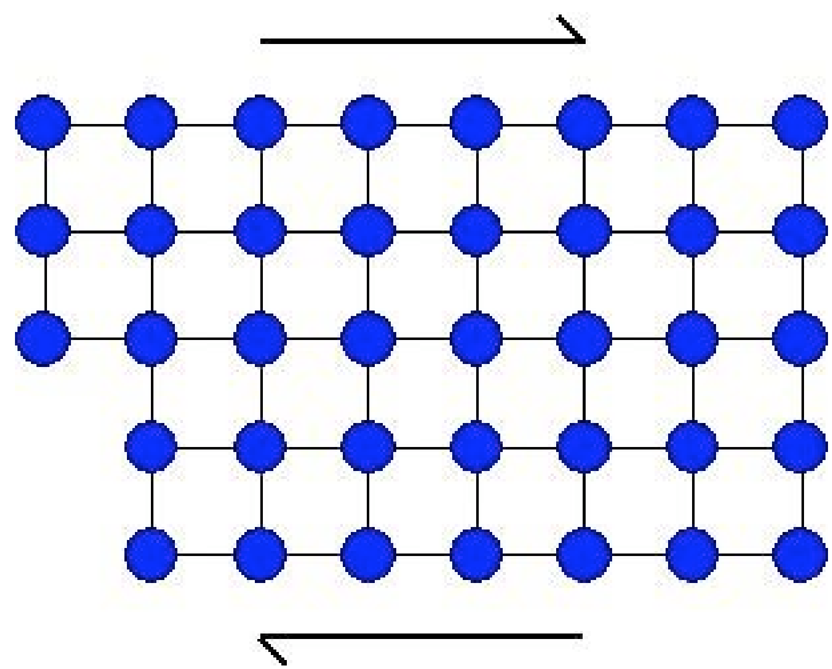
Defects in crystals





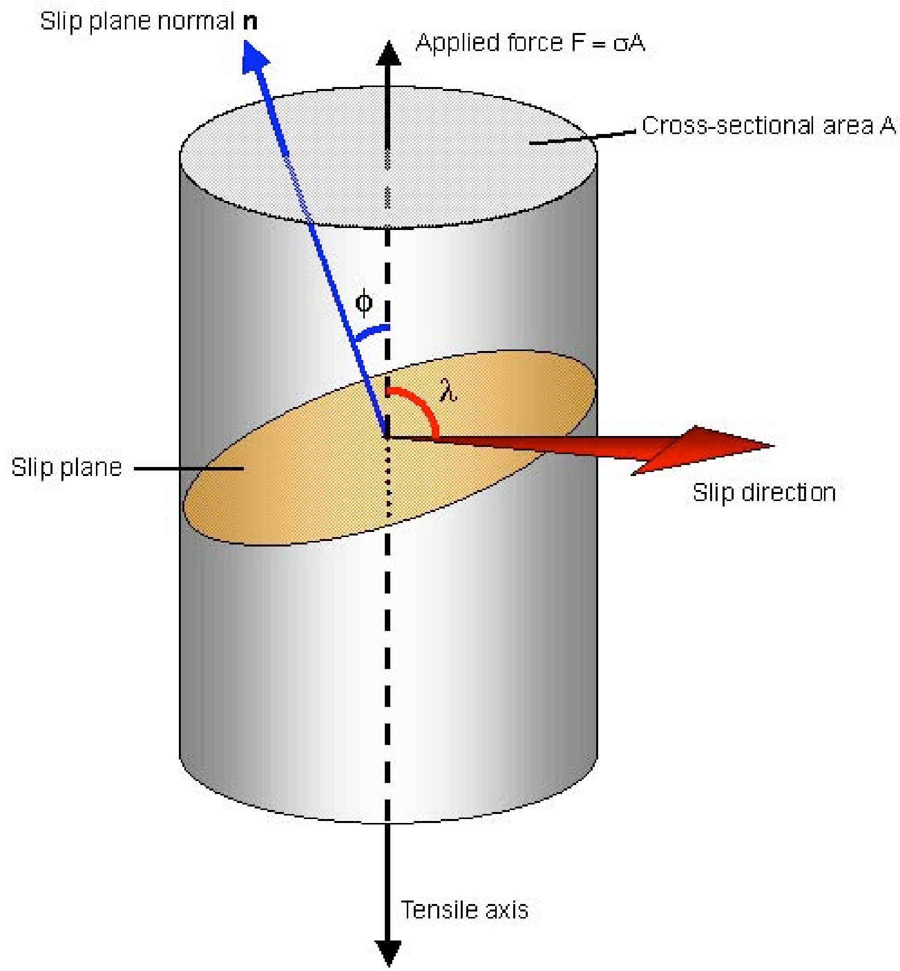
Dislocation



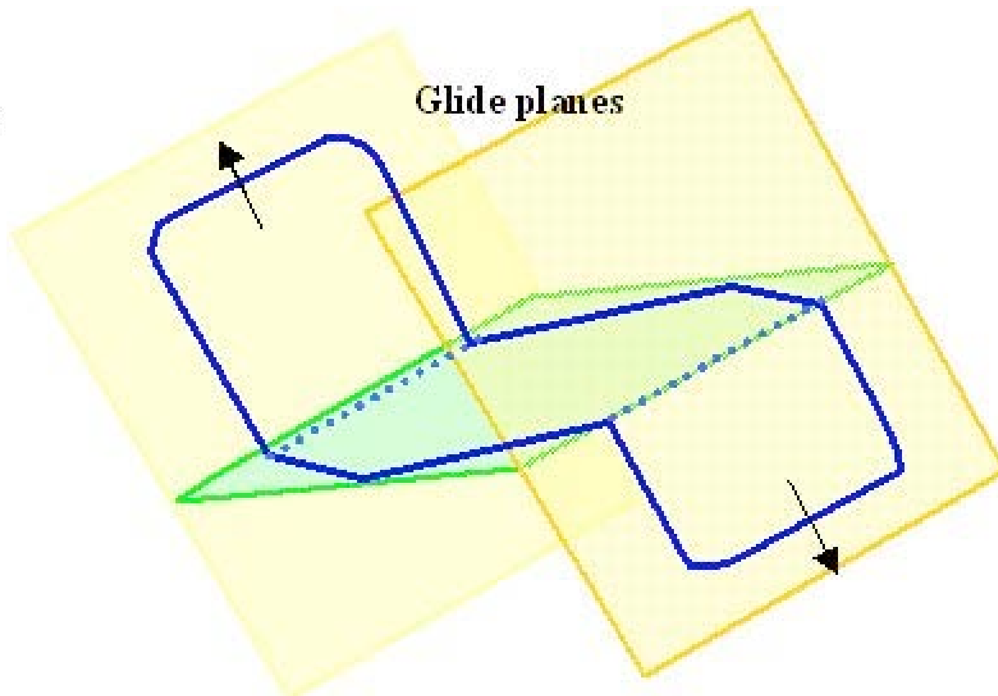


Deformation fundamentals

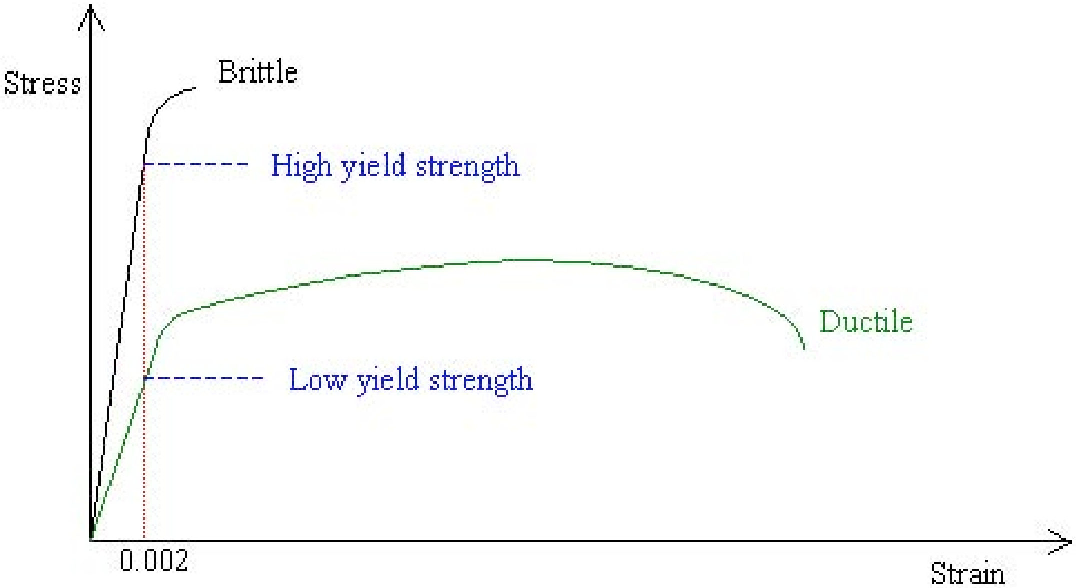
Resolved stress in slip direction is
σ=F/A cosϕ cosλ



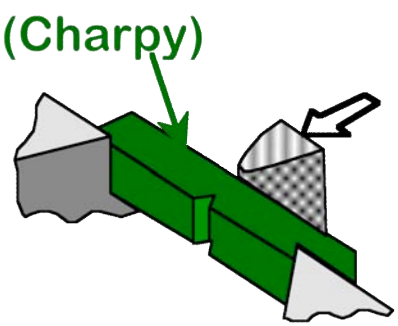
Dislocation cross slip occurs if obstacles impede motion

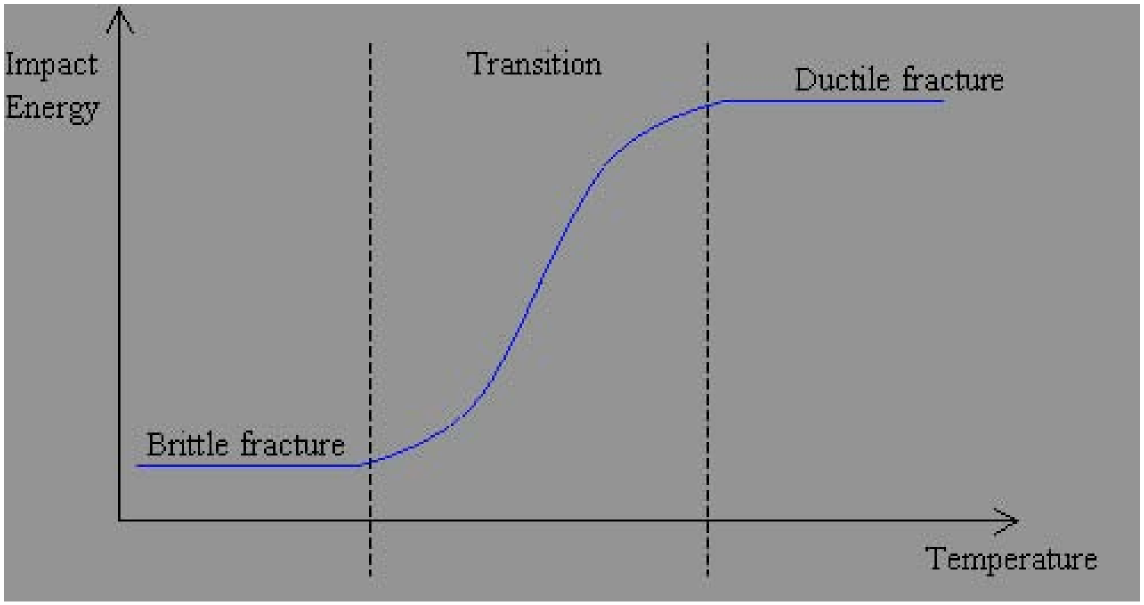


Structural materials involve compromise between strength and ductility



Schenectady Liberty ship, 1943

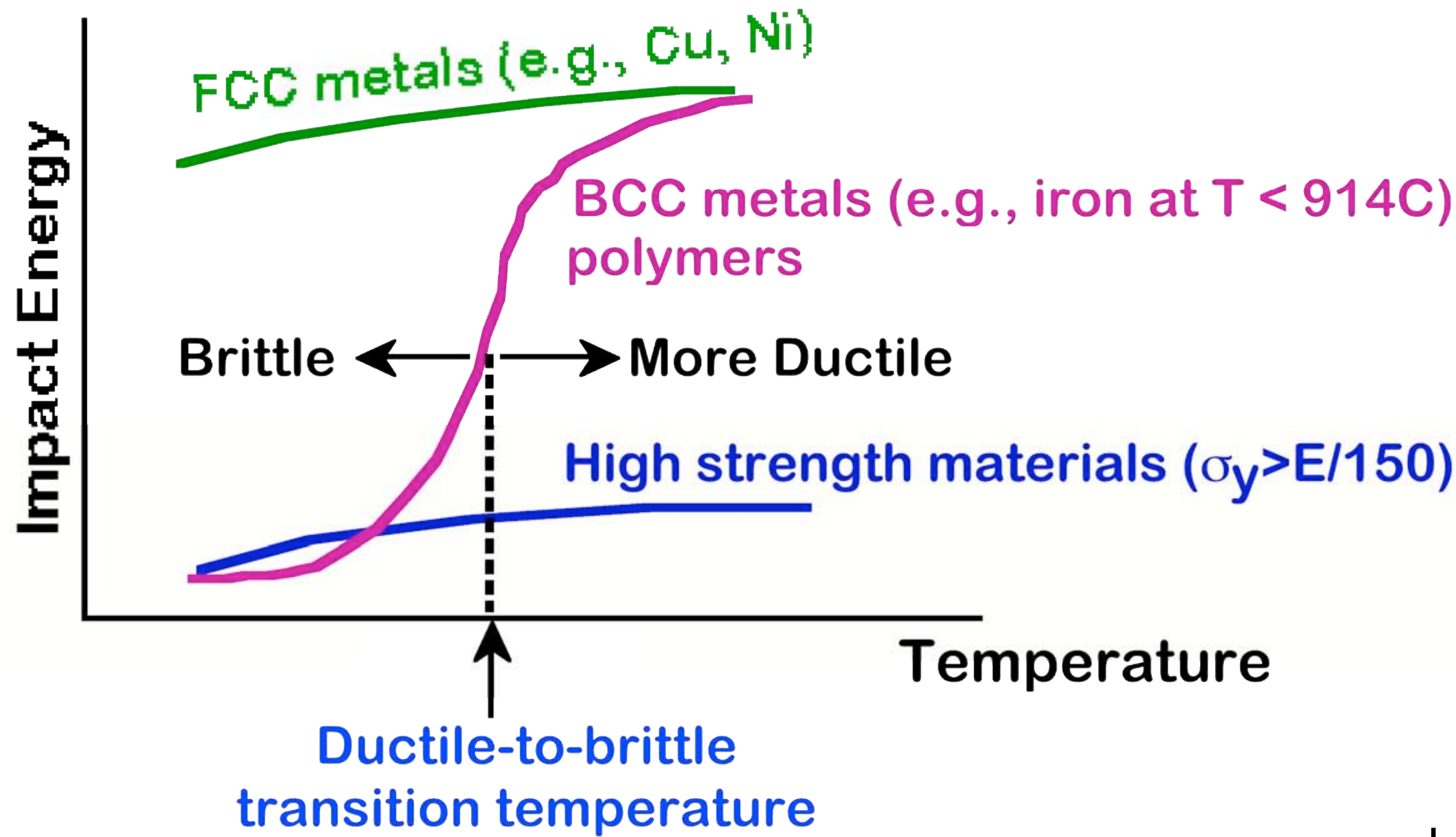




A simple measure of the resistance to brittle cleavage failure is the Charpy notched impact test

Brittle behavior at low temperature is of greatest concern for BCC metals (due to Peierls barriers)

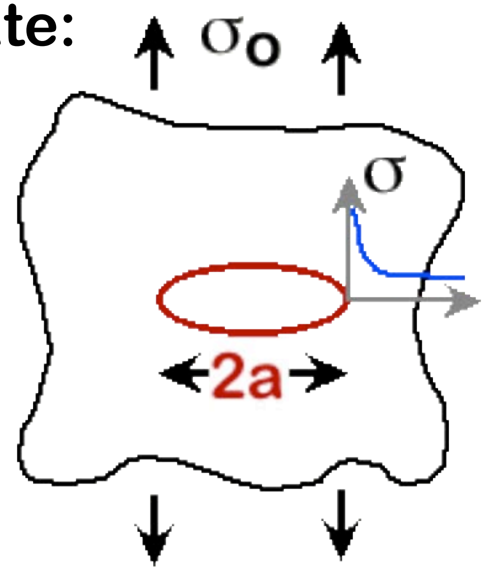
Design strategy: Stay above the DBTT whenever stress is applied



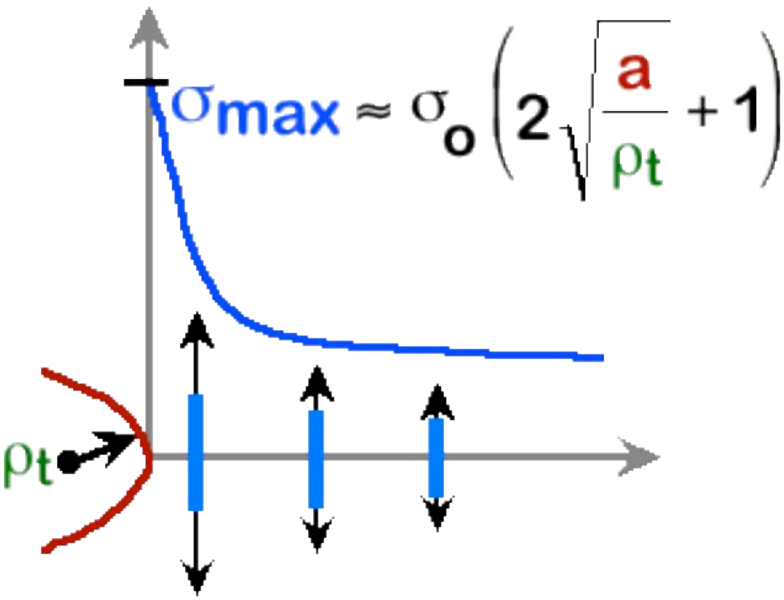
J. Hayton

FLAWS ARE STRESS CONCENTRATORS!

- Elliptical hole in a plate:

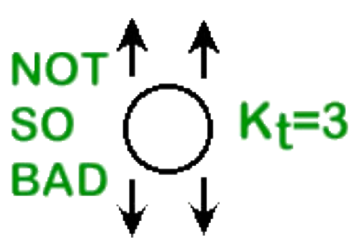


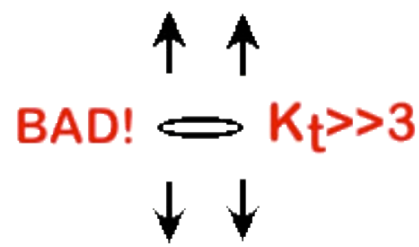
- Stress distrib. in front of a hole:



- Stress conc. factor: $K_t = \sigma_{max} / \sigma_o$

- Large K_t promotes failure:

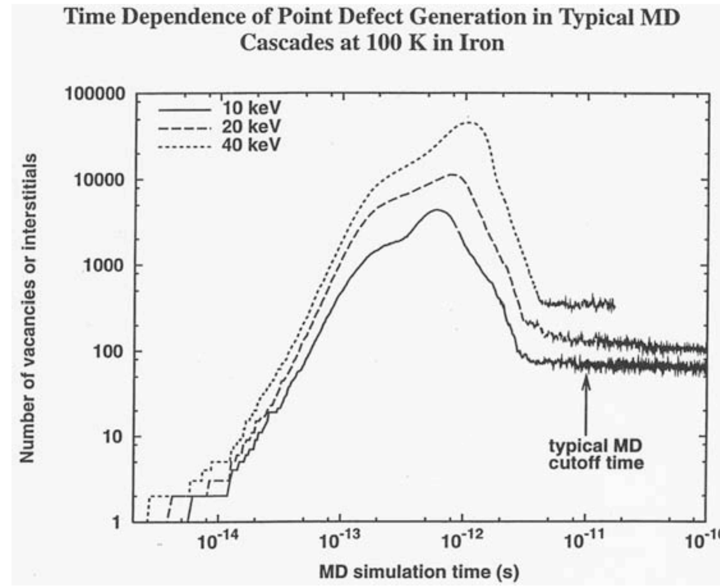




J. Hayton

Radiation damage: What is "dpa"?

- 1 displacement per atom (dpa) corresponds to stable displacement from their lattice site of all atoms in the material during irradiation near absolute zero (no thermally-activated point defect diffusion)
  - Initial number of atoms knocked off their lattice site during neutron irradiation is ~100 times the dpa value
    - Most of these originally displaced atoms hop onto another lattice site during "thermal spike" phase of the displacement cascade (~1 ps)



R.E. Stoller

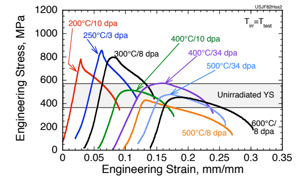
- At non-zero temperatures, many of the created defects recombine so that the net surviving defect fraction is low (<10% NRT dpa)
- Requirement for advanced structural materials in fusion and Gen IV fission reactors (~100 dpa exposure):
  - ~99.9% of "stable" displacement damage must recombine
  - "off-the-shelf" materials typically exhibit 90-99% recombination of "stable" damage

Comparison of fission and fusion structural materials requirements

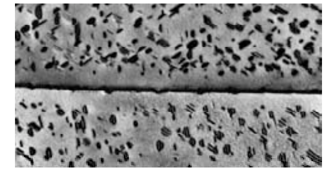
	Fission (Gen. I)	Fission (Gen. IV)	Fusion (Demo)	JIMO space react.
Structural alloy maximum temperature	<300˚C	500-1000˚C	550-1000˚C	~1000˚C
Max dose for core internal structures	~1 dpa	~30-100 dpa	~150 dpa	~10 dpa
Max transmutation helium concentration	~0.1 appm	~3-10 appm	~1500 appm (~10000 appm for SiC)	~1 appm
Coolants	H_2O	He, H_2O, Pb-Bi, Na	He, Pb-Li, Li	Li, Na, or He-Xe
Structural Materials	Zircaloy, stainless steel	Ferritic steel, SS, superalloys, C- composite	Ferritic/ martensitic steel, V alloy, SiC composite	Nb-1Zr, Ta alloy, Mo alloy

- Common theme for fusion,Gen IV fission and space reactors is the need to develop higher temperature materials with adequate radiation resistance

Radiation Damage can Produce Large Changes in Structural Materials

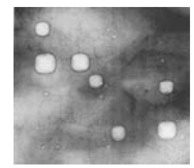


- Radiation hardening and embrittlement ($<0.4\ T_M$, >0.1 dpa)

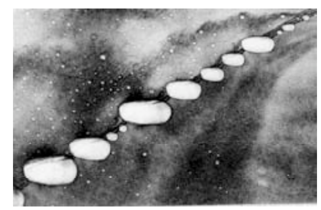


- Phase instabilities from radiation-induced precipitation (0.3-$0.6\ T_M$, >10 dpa)

- Irradiation creep ($<0.45\ T_M$, >10 dpa)



- Volumetric swelling from void formation (0.3-$0.6\ T_M$, >10 dpa)

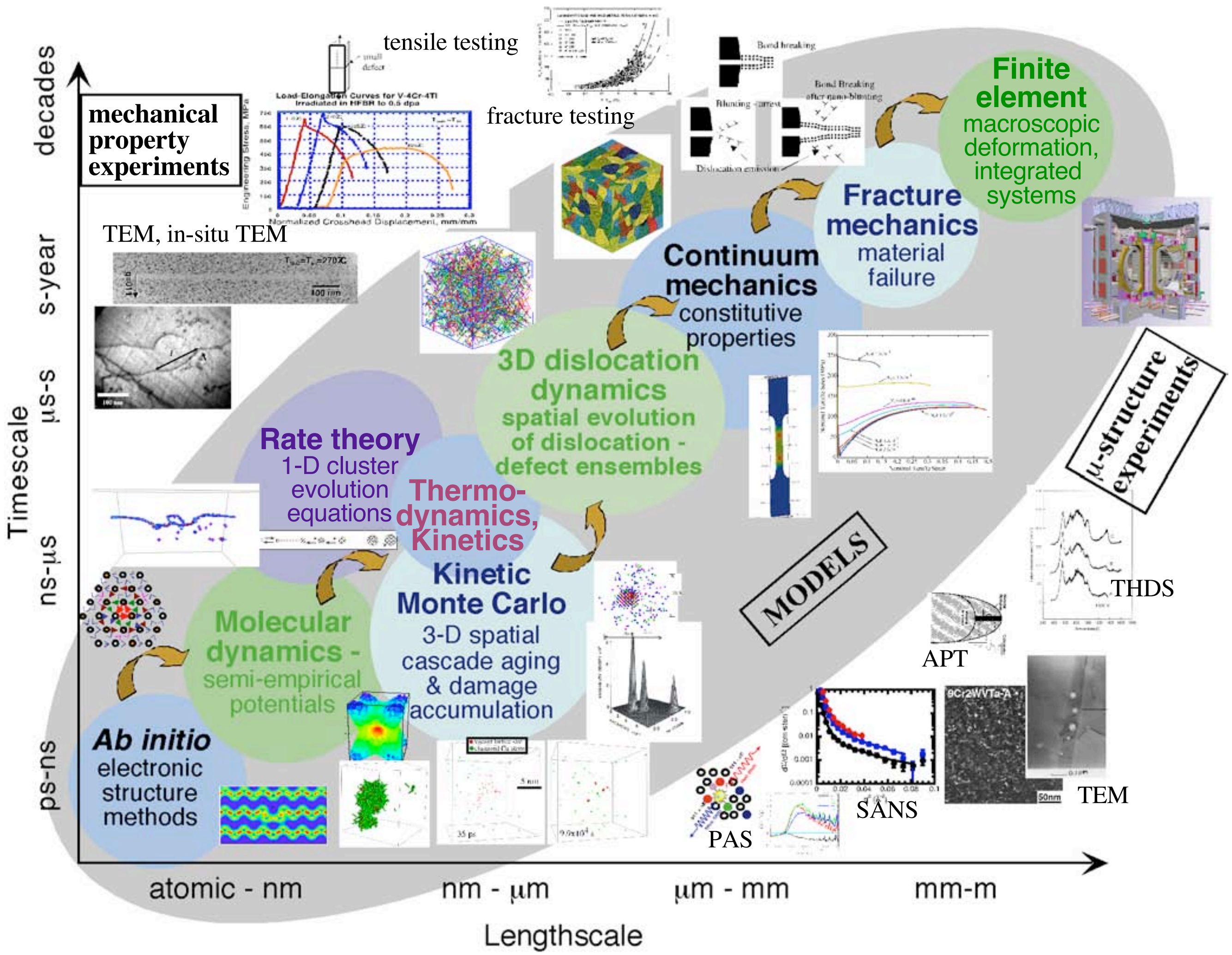


- High temperature He embrittlement ($>0.5\ T_M$, >10 dpa)

In addition…

- The irradiation environment associated with a D-T fusion reactor is more severe than in existing fission reactors
  - Higher lifetime dose requirements for structure
  - Higher He generation rates (promotes He embrittlement of grain boundaries, void swelling)

Radiation damage is inherently multiscale with interacting phenomena ranging from ps to decades and nm to m



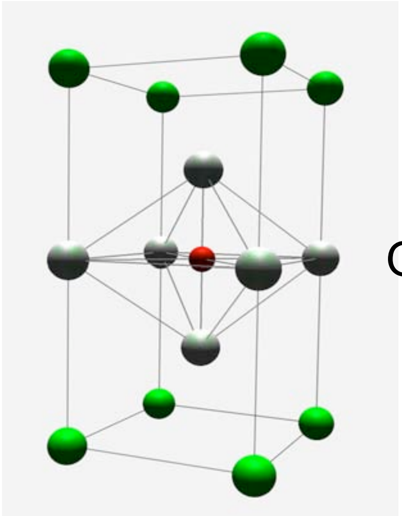
B.D. Wirth, UC-Berkeley

New interatomic potentials have been developed for vanadium and Fe-He, based on first-principles simulations

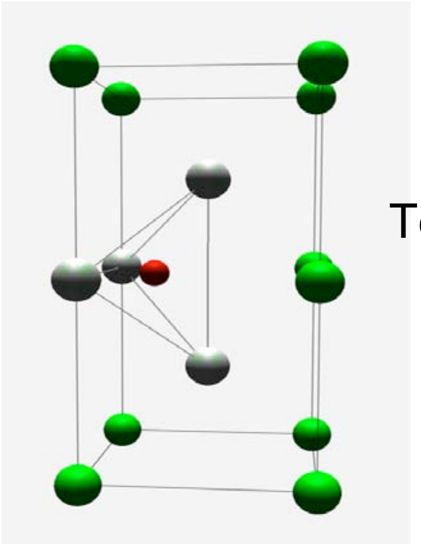
Vanadium calculations: Improved potential established split [111] interstitial as most stable configuration (Han, Srolovitz & Car, Princeton)
Fe-He Calculations: Unexpected stability of tetrahedral site arises from magnetic interaction

magnetic moment of He defect and surrounding Fe atoms (magnetic moment of pure *bcc* Fe=2.15 Bohr magneton)

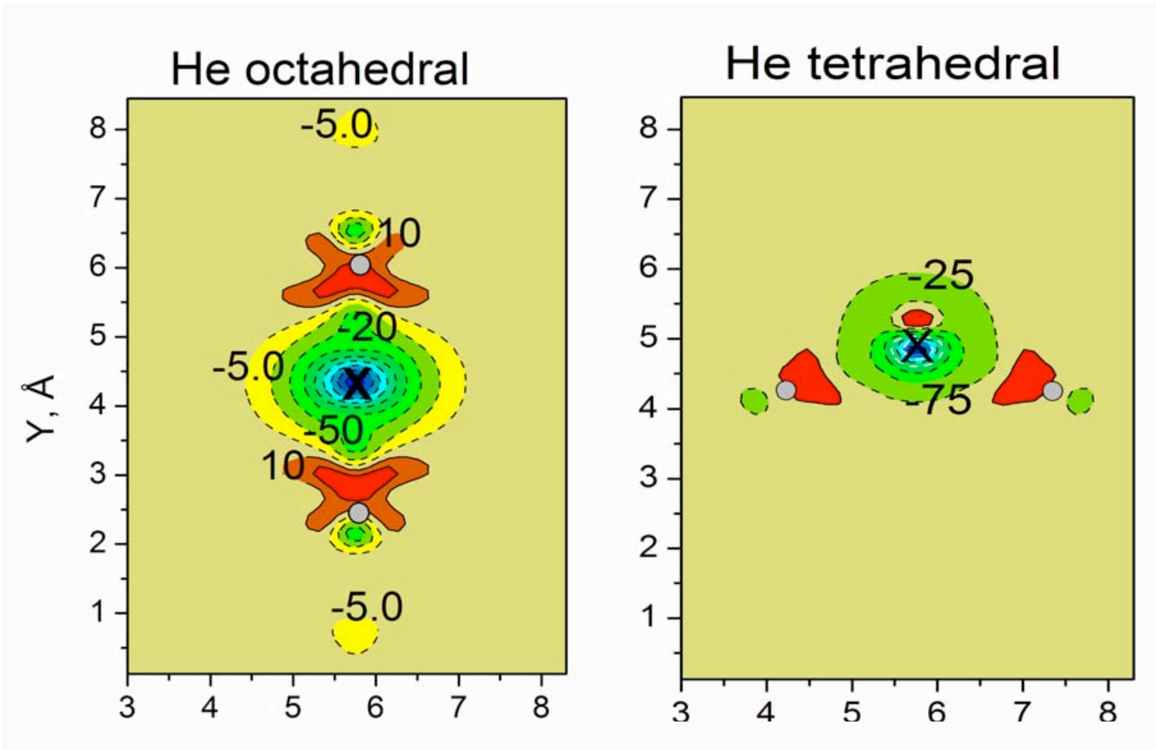
	He	Fe, 1st neighbor	Fe, 2nd neighbor
He octa , unrelaxed	0.012	1.67	2.17
He octa, relaxed	0.015	2.01	2.24
He tetra , unrelaxed	0.007	1.99	
He tetra, relaxed	0.012	2.15	



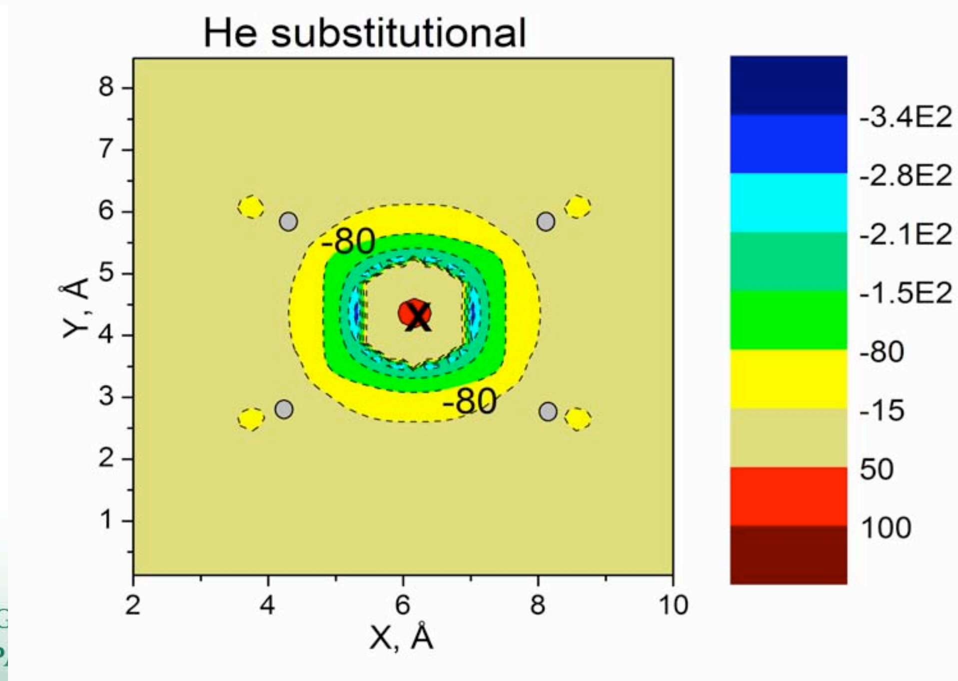
Octa.



Tetra.



Tetrahedral site provides least change in the charge density of Fe due to the He defect



Charge density (elns/Å^3)

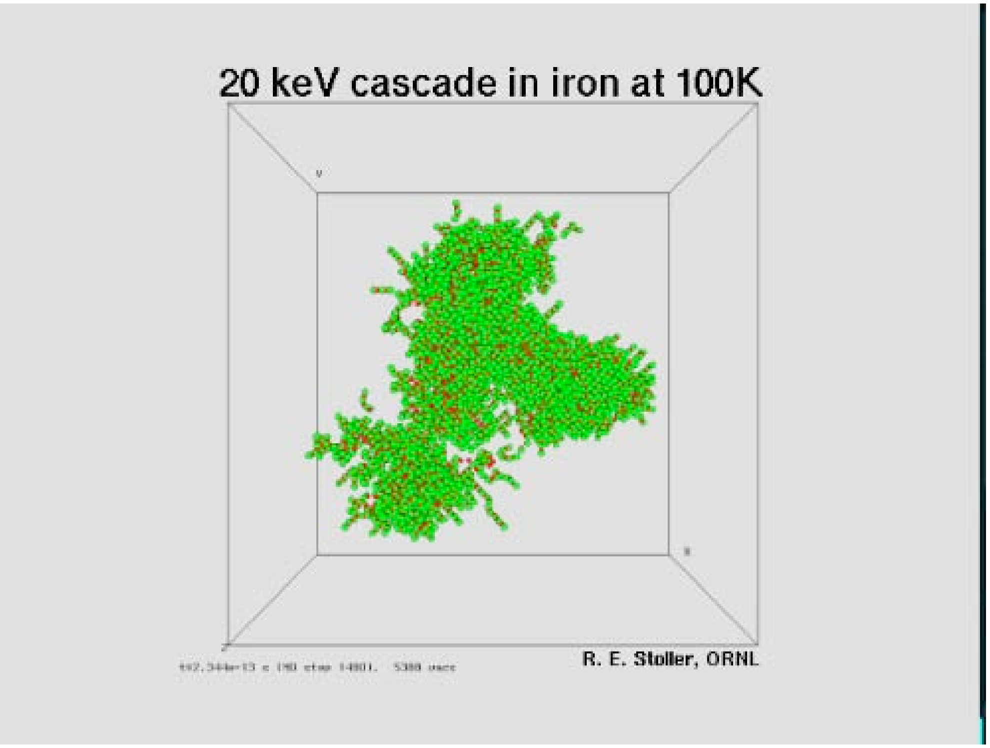
T. Seletskaia et al., PRL (in review, 2004)

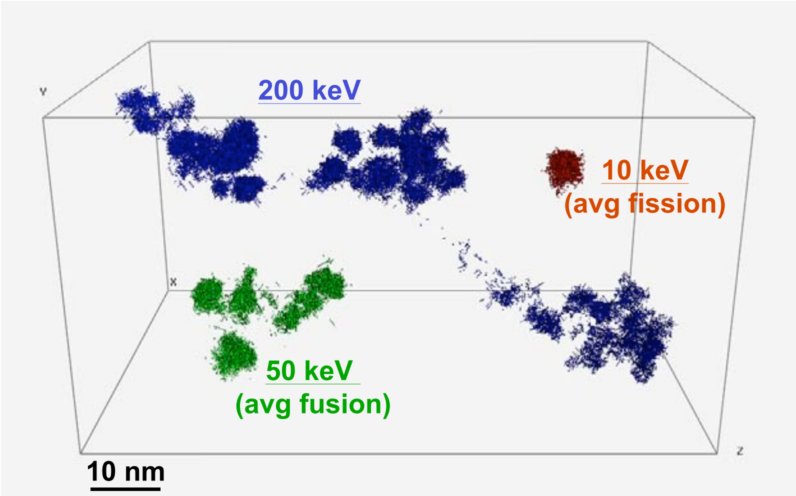
Current status of 1st principles computational materials science

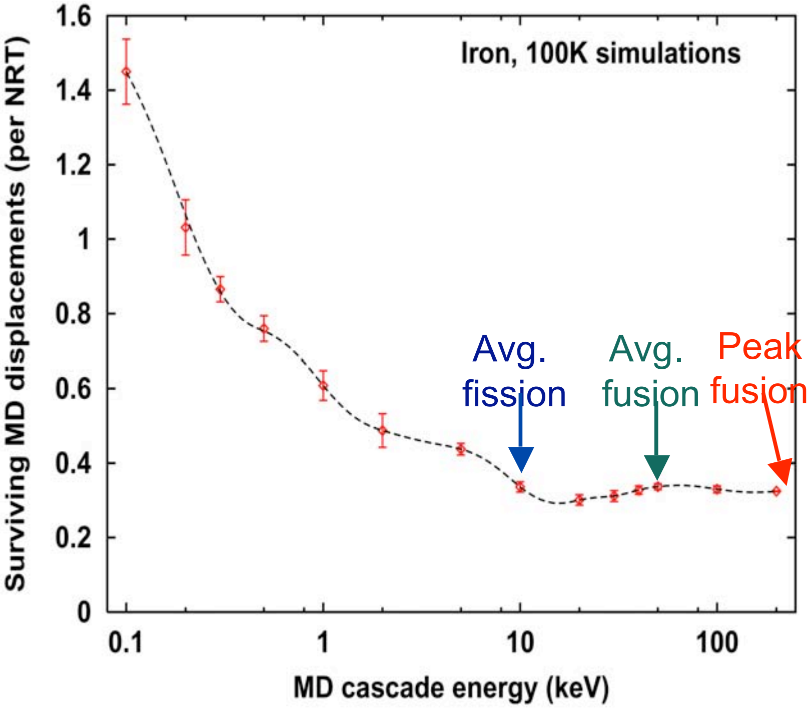
- Goal is to solve the Schrödinger equation (or Dirac eqn, if relativistic effects are important)
  - Trivial for hydrogen; very complex for higher mass systems due to many-body effects in the Hamiltonian
  - Electrons can be decoupled from ions using adiabatic approximation
  - Reducing the many-electron problem to an effective one-electron system requires approximations that can introduce significant errors
- Current "standard model" for condensed mater physics is Density Functional Theory (DFT) using Local Density Approximation (LDA)
  - Currently limited to 100-1000 atoms (n^3 scaling)
    - Largest MD-DFT simulation to date is 1080 B atoms (n=3840 electrons) on LLNL's 2000 CPU Linux cluster
    - Need to accurately model behavior of ~10^{12} to 10^{15} atoms (Z~25) to simulate behavior occurring within one individual grain
  - Generally successful in predicting structures and macroscopic properties
  - Underpredicts band gap energies, overpredicts lattice parameters, predicts wrong ground state for some magnetic systems (e.g., Fe)
  - Generalized gradient approximation (GGA) in DFT fixes some of these errors but introduces other errors
- Quantum chemistry models provide best accuracy, but are computationally expensive (e.g., n^6 scaling)

Molecular Dynamics simulations have found the primary damage formation is similar for fission and fusion neutrons

- subcascade formation leads to asymptotic behavior at high energies
- Agrees with experimental data (TEM, etc.)







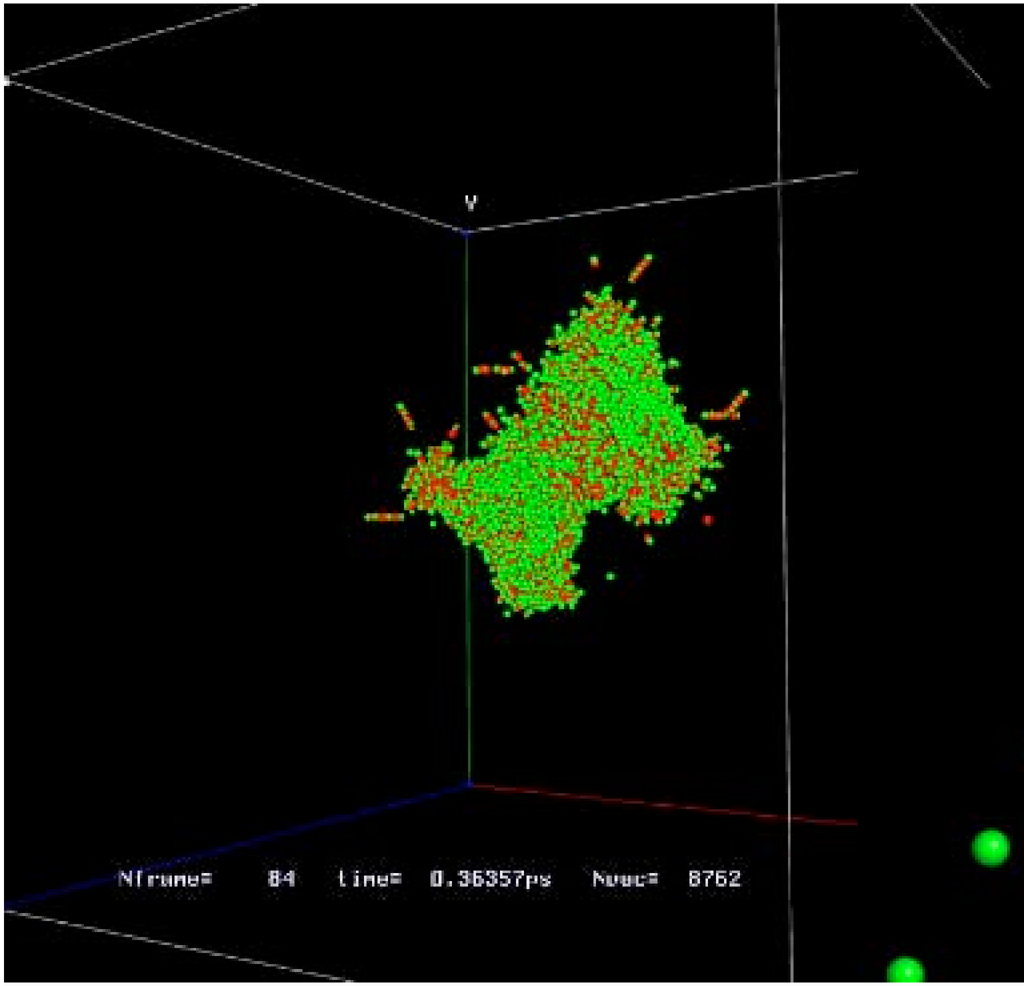
MD results have been confirmed by 14 MeV and spallation neutron experimental studies

A critical unanswered question is the effect of higher transmutant H and He production in the fusion spectrum

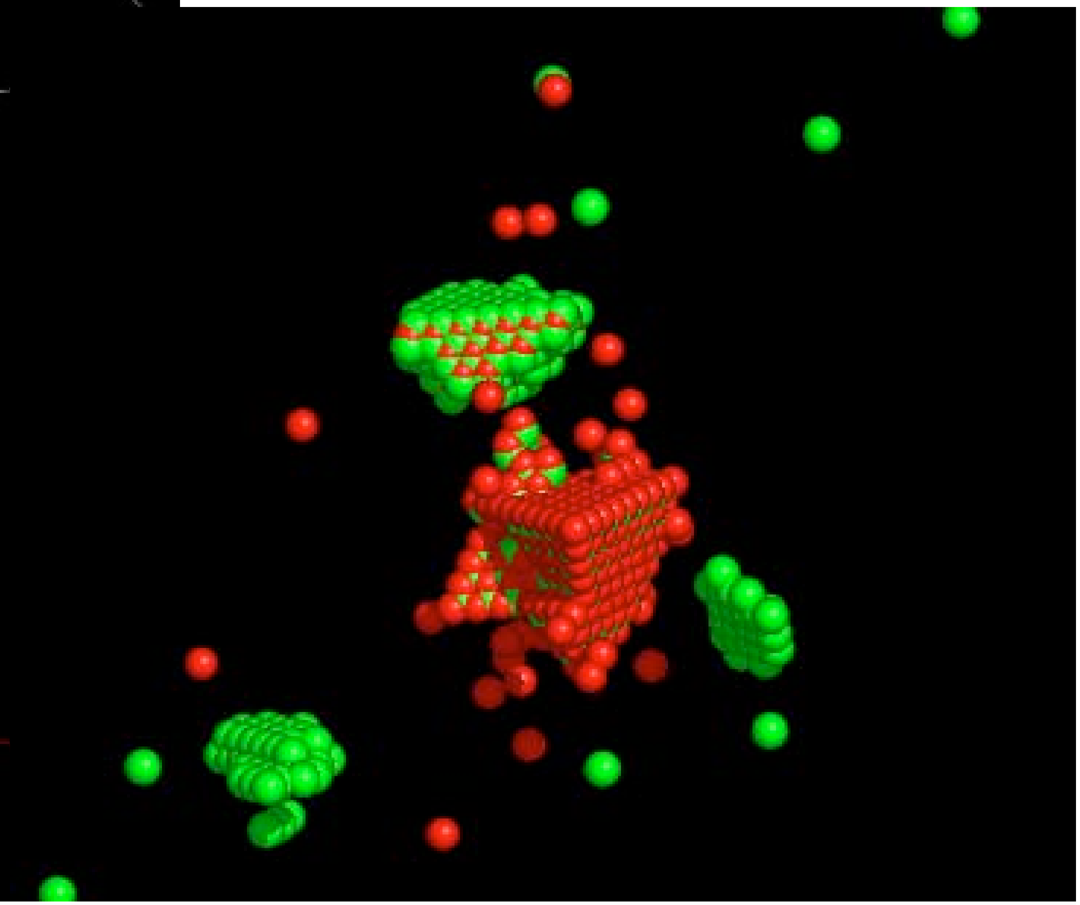
R.E. Stoller, 2004

Direct formation of SFTs in Cu displacement cascades based on molecular dynamics simulations

L=1.3 nm



L=2.3 nm

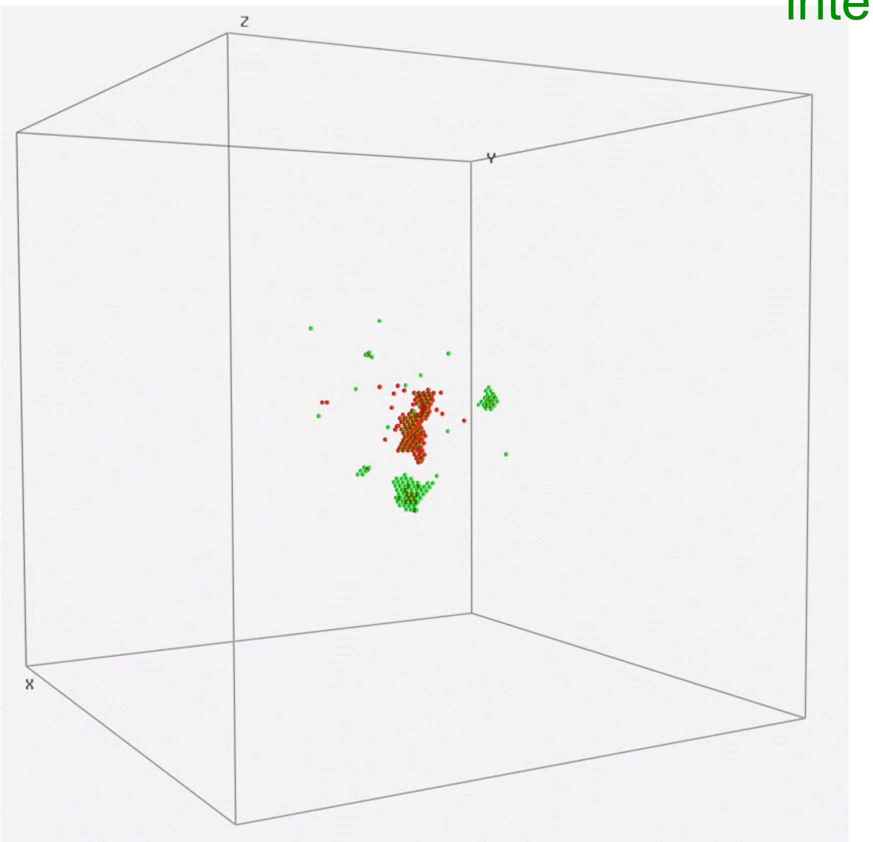


- Nearly perfect SFTs are formed in cascades within ~50 ps

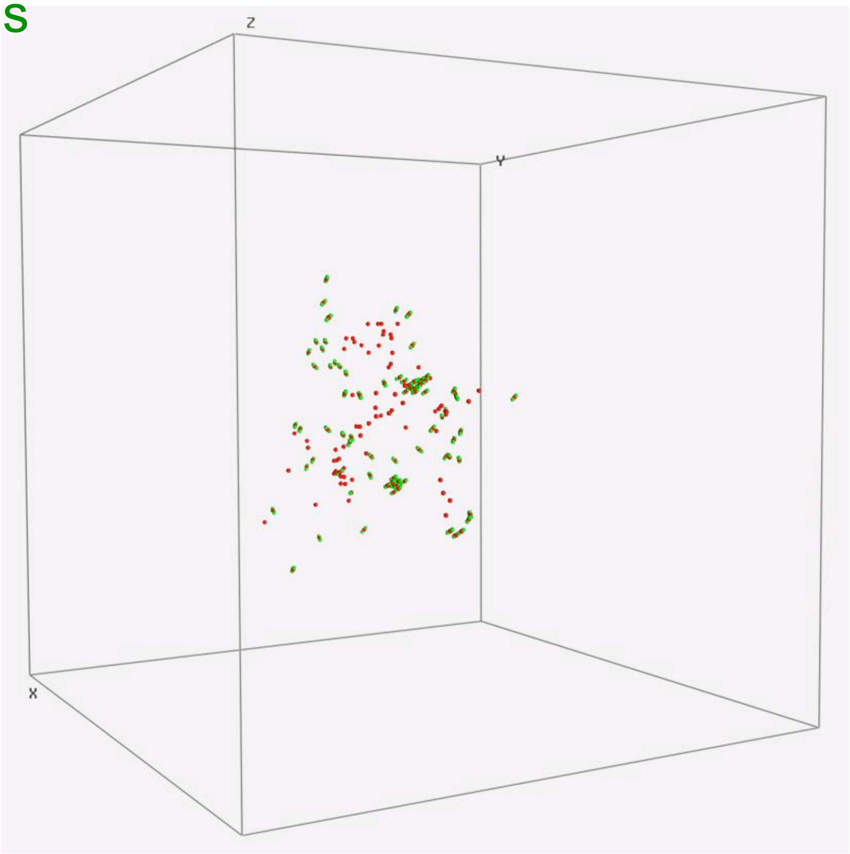
Yu. N. Osetsky

Comparison of surviving defects in a 25 keV displacement cascade in FCC (Cu) and BCC (Fe) metals

Vacancies
interstitials



Cu



Fe

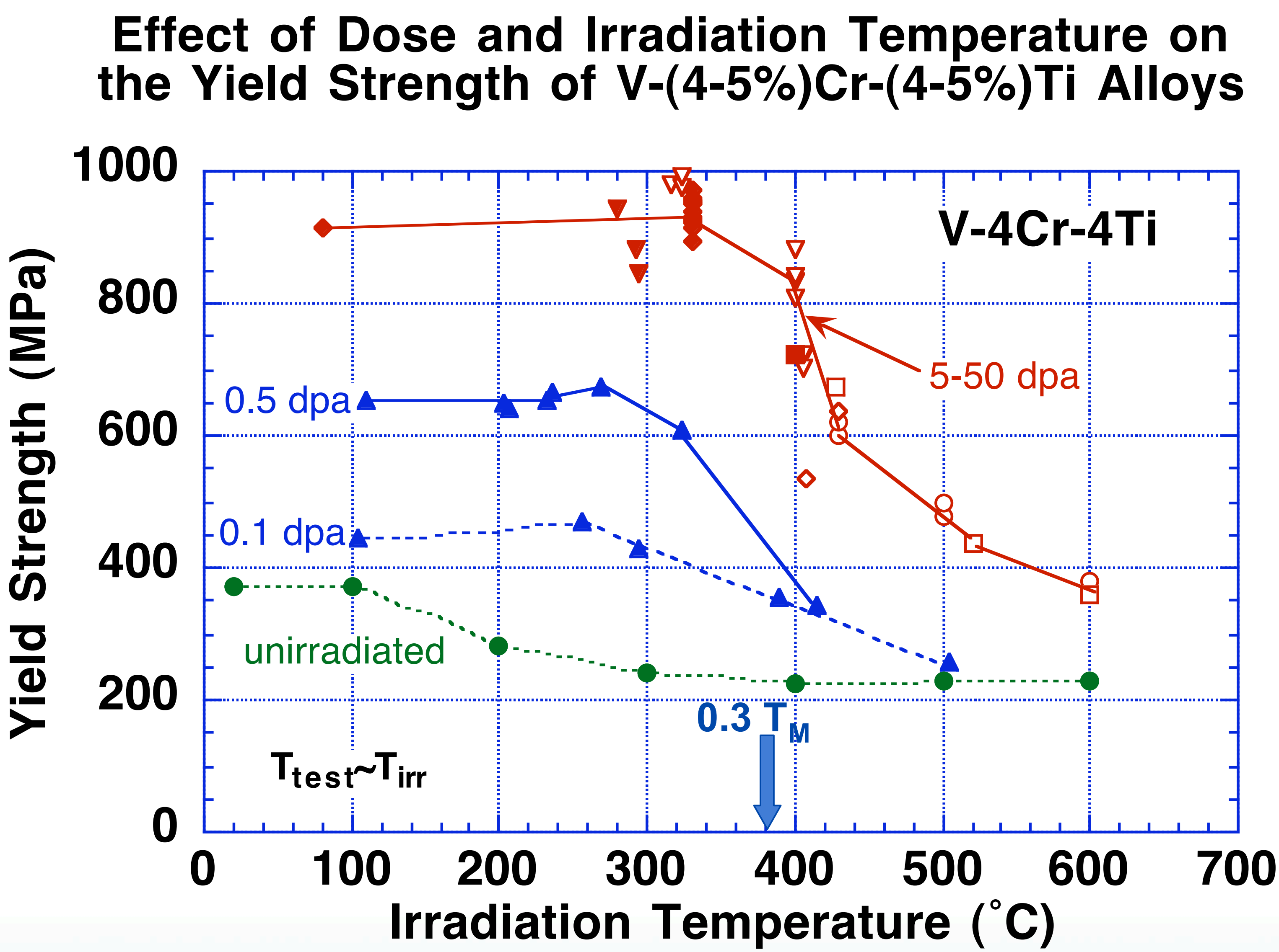
• Large vacancy clusters are not directly formed in BCC metal displacement cascades

Yu. N. Osetsky and R.E. Stoller

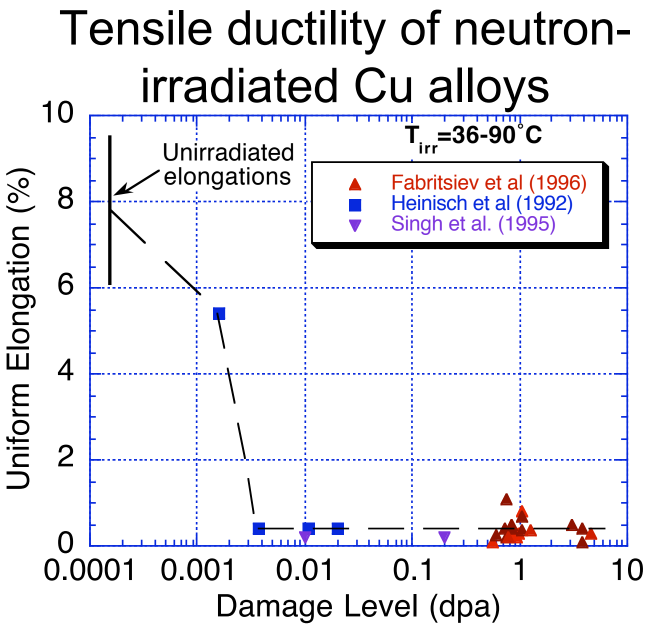
What are the consequences of radiation hardening?

- Increased strength (good!)
- Decreased tensile elongation (bad!)
  - Practical impact/consequences: need to use more conservative structural design rules for uniform elongation <2%
- For BCC metals, increase in the ductile-brittle transition temperature and decrease of toughness in the “ductile” regime (can be catastrophic!)
  - Radiation hardening also tends to reduce the fracture toughness of FCC metals
- Pronounced radiation hardening and embrittlement effects can occur for doses as low as 0.01 dpa in non-optimized materials

Radiation hardening in V-4Cr-4Ti



Low tensile ductility in FCC and BCC metals after irradiation at low temperature is due to formation of nanoscale defect clusters

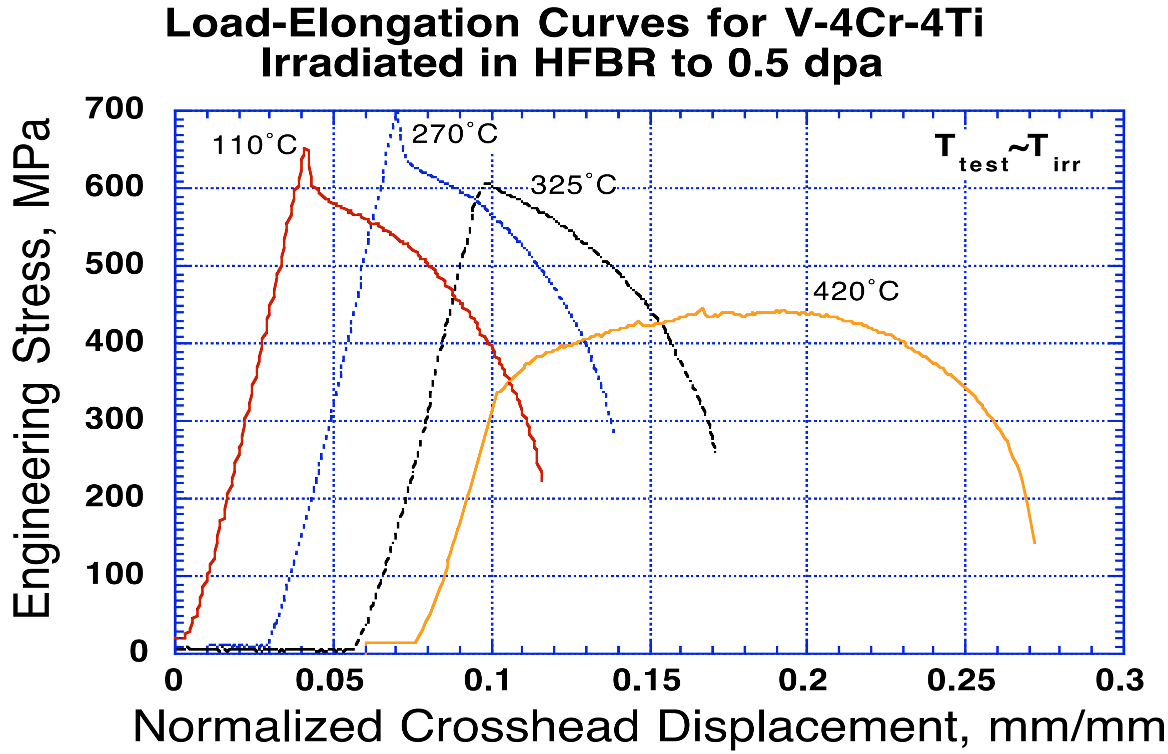


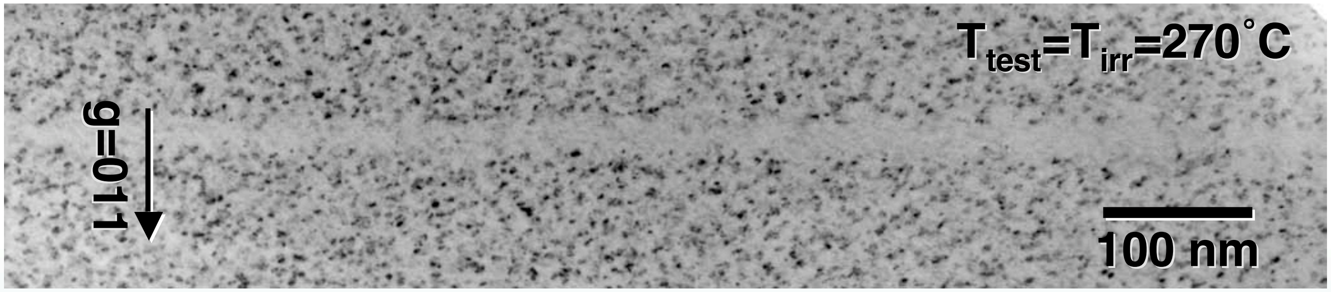
Outstanding questions to be resolved include:

- Can the defect cluster formation be modified by appropriate use of nanoscale 2nd phase features or solute additions?
- Can the poor ductility of the irradiated materials be mitigated by altering the predominant deformation mode? (e.g., twinning vs. dislocation glide)

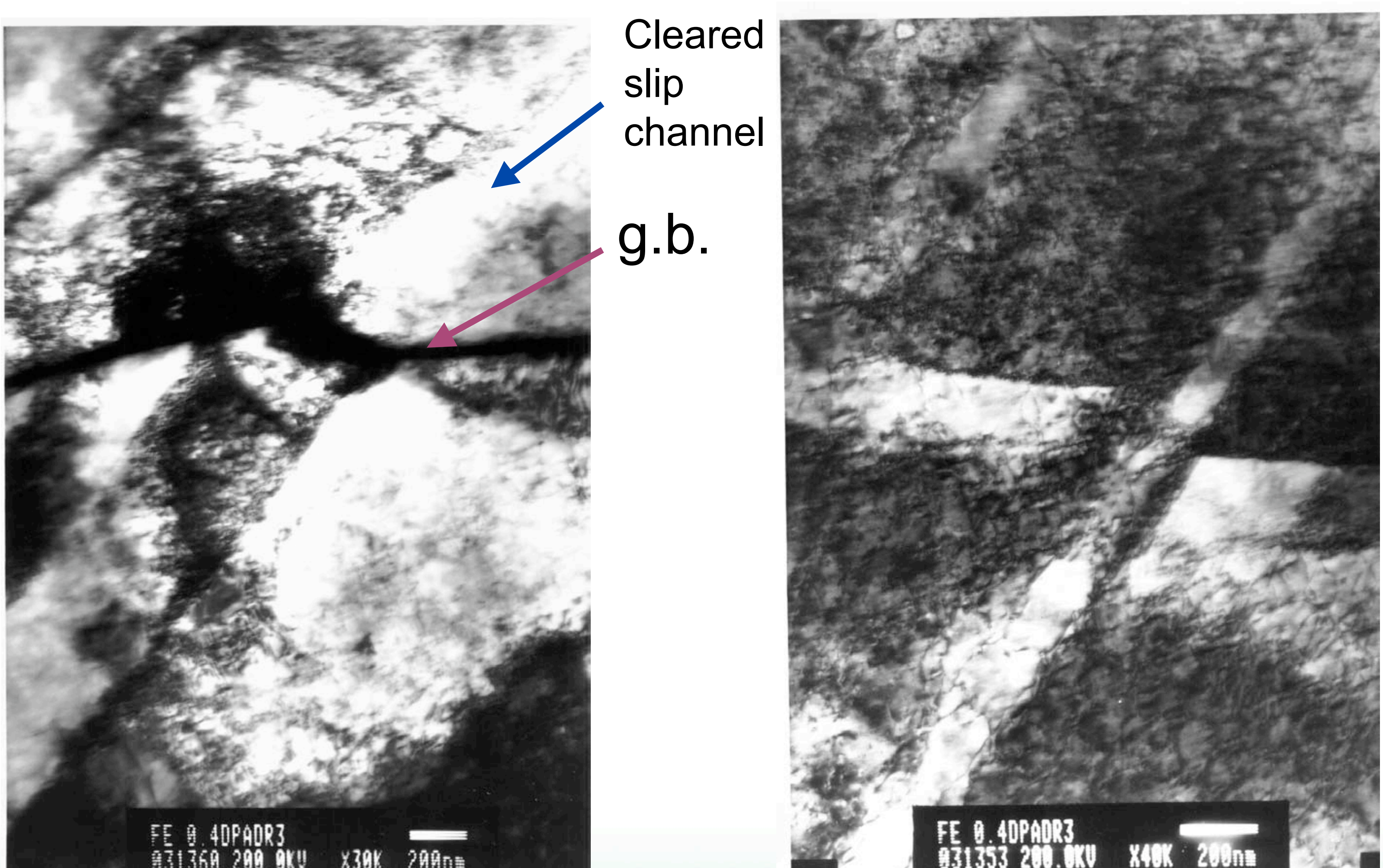
UT-BATTELLE

Irradiated Materials Suffer Plastic Instability (due to Dislocation Channeling?)





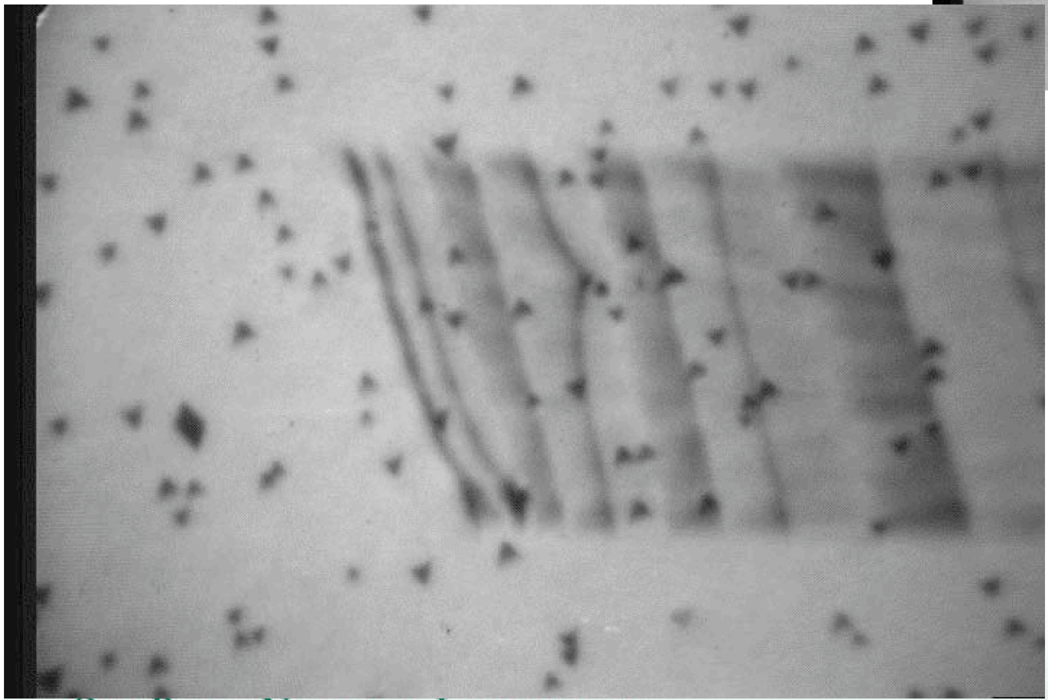
Dislocation channel interactions in Fe deformed following neutron irradiation at 70˚C to 0.8 dpa



Need well-engineered materials to mitigate neutron radiation effects

TEM In-situ deformation: dislocation/defect cluster interactions

SFT annihilation by a single dislocation

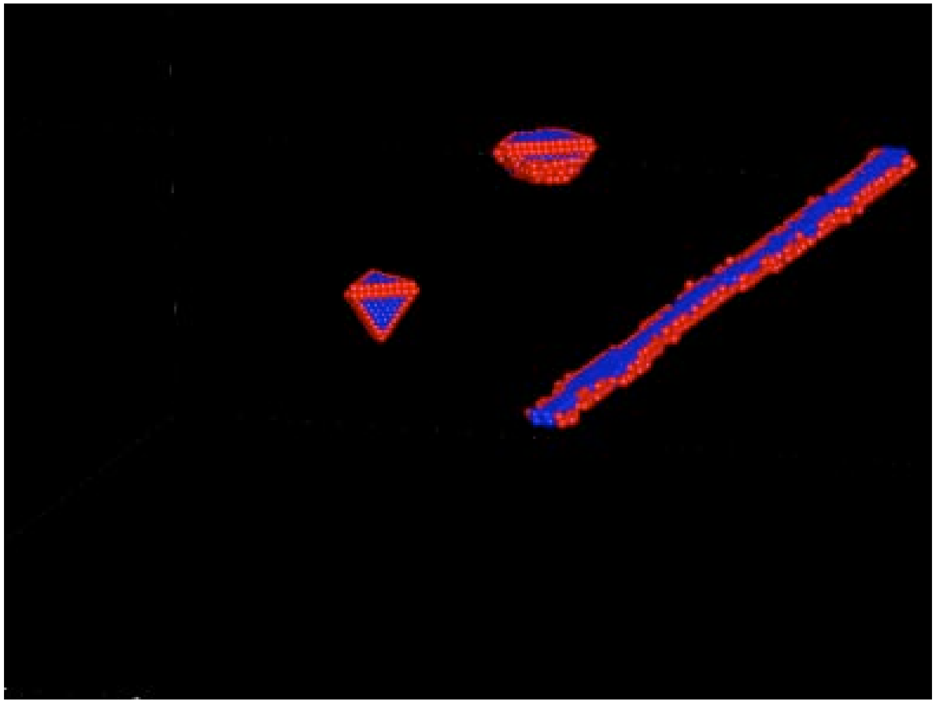


Dislocation pinning by small SFTs (no annihilation)

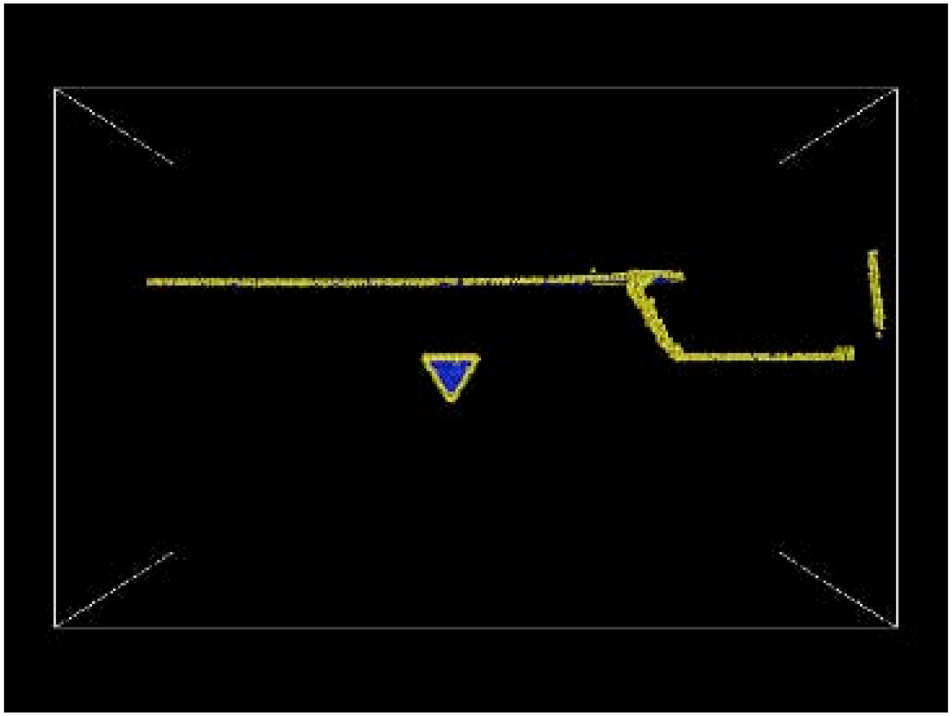
Understanding why annihilation sometimes does not occur is key for developing improved fusion and fission materials

Effect of cluster size on screw dislocation interaction with Cu SFT

3 nm



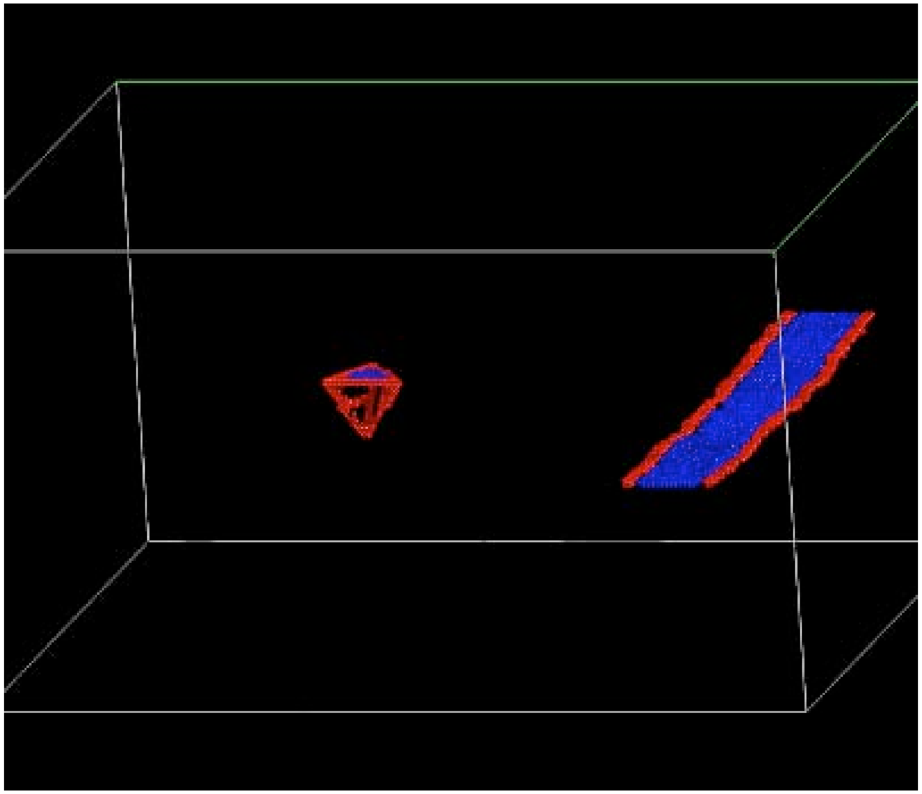
12 nm



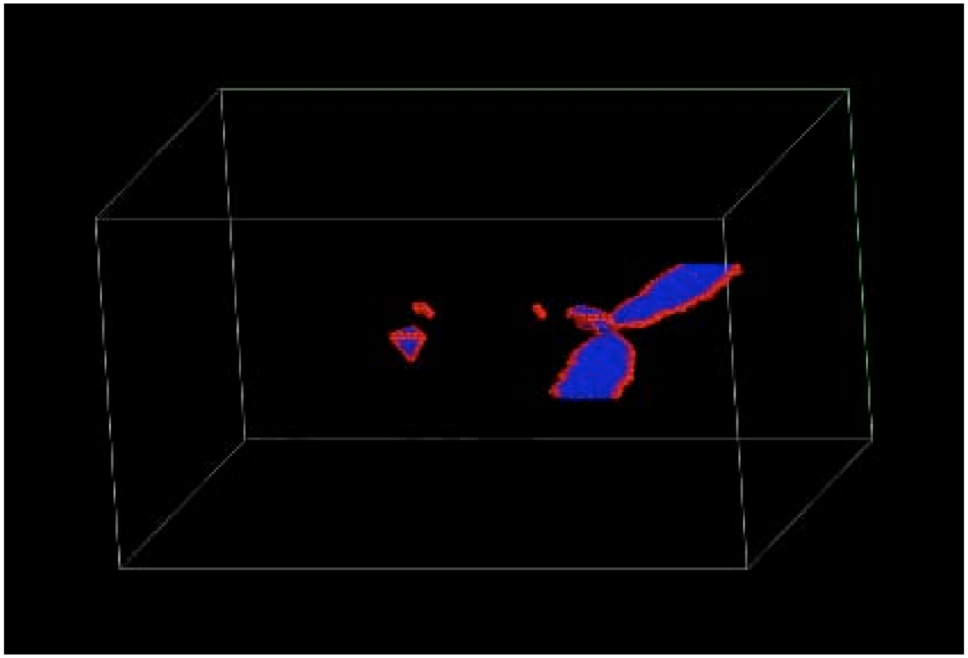
Defect cluster partial annihilation occurs over a wide range of defect cluster sizes

Effect of temperature on edge dislocation interaction with 136 vacancy SFT in Cu

300 K



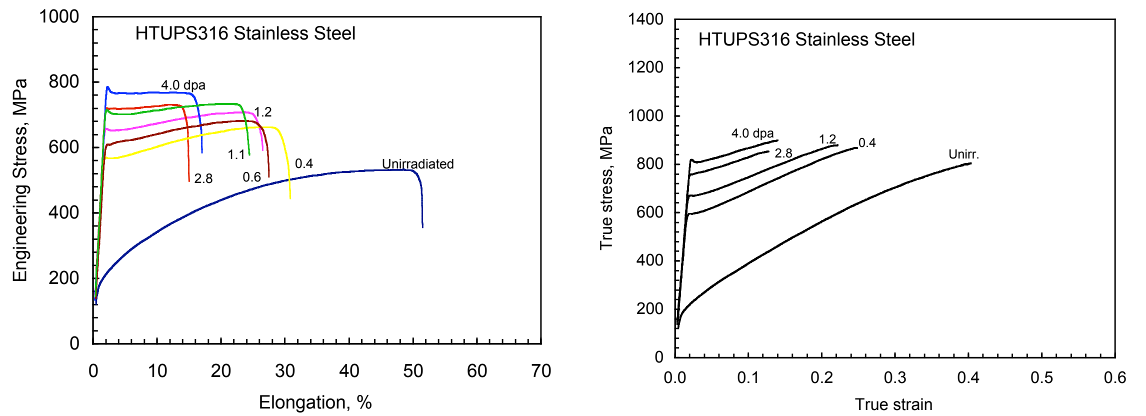
450 K



Defect cluster annihilation is enhanced at higher temperatures and slower strain rates (strain rate effect not shown)

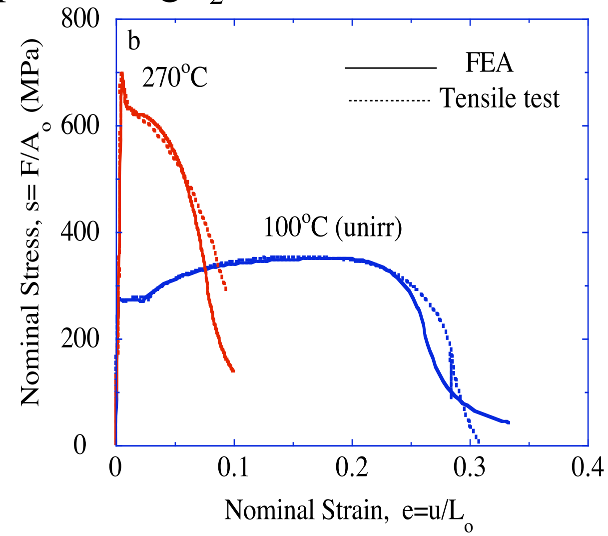
- agrees with experimental results

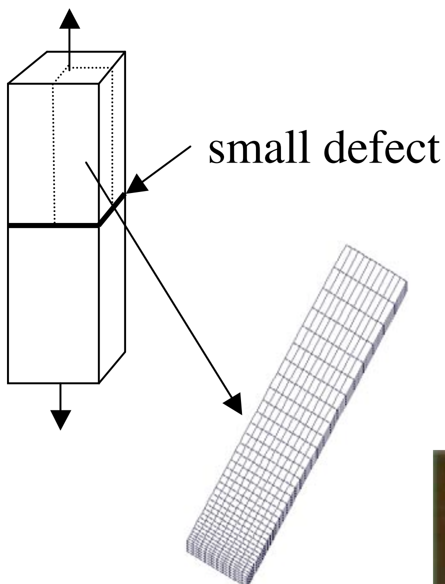
Understanding Loss of Uniform Strain Capacity

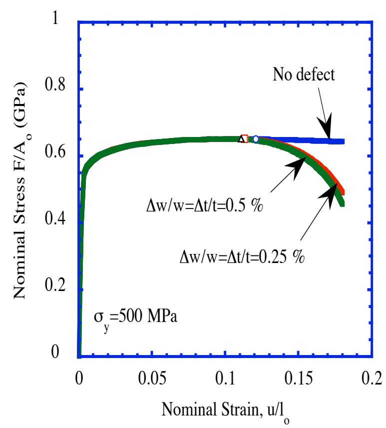


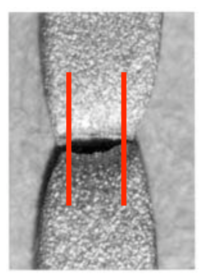
T.S. Byun et al., J. Nucl. Mater. 298 (2001) 269

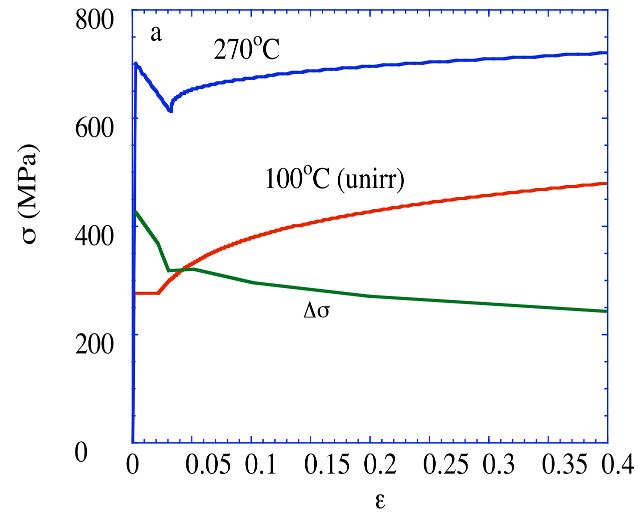
ABAQUS 1320 8-noded brick elements on 4x1x0.2 1/8 symmetry plate using J_2 incremental flow theory





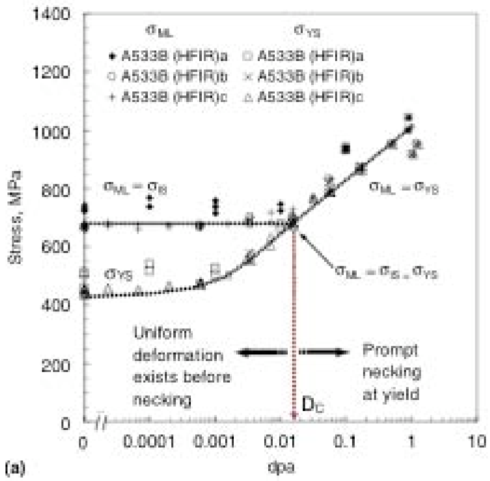


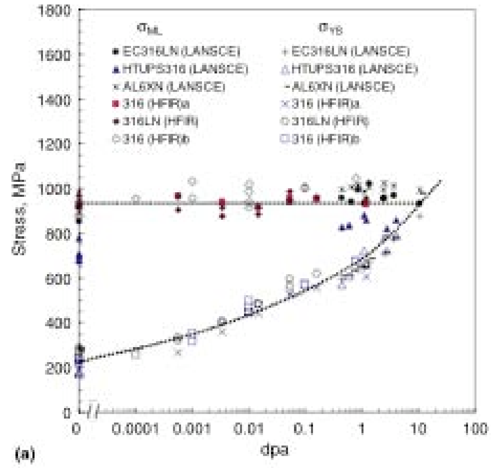


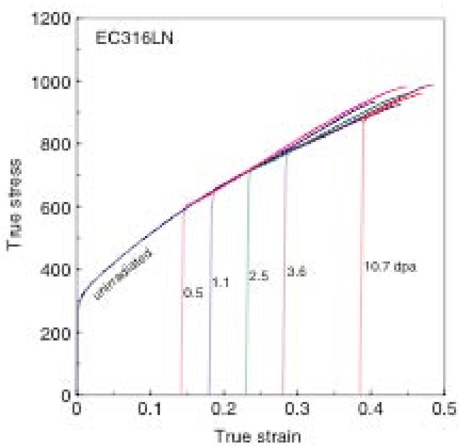


G.R. Odette et al., J. Nucl. Mater.307-311 (2002) 171

Dose to plastic instability (necking) at yield







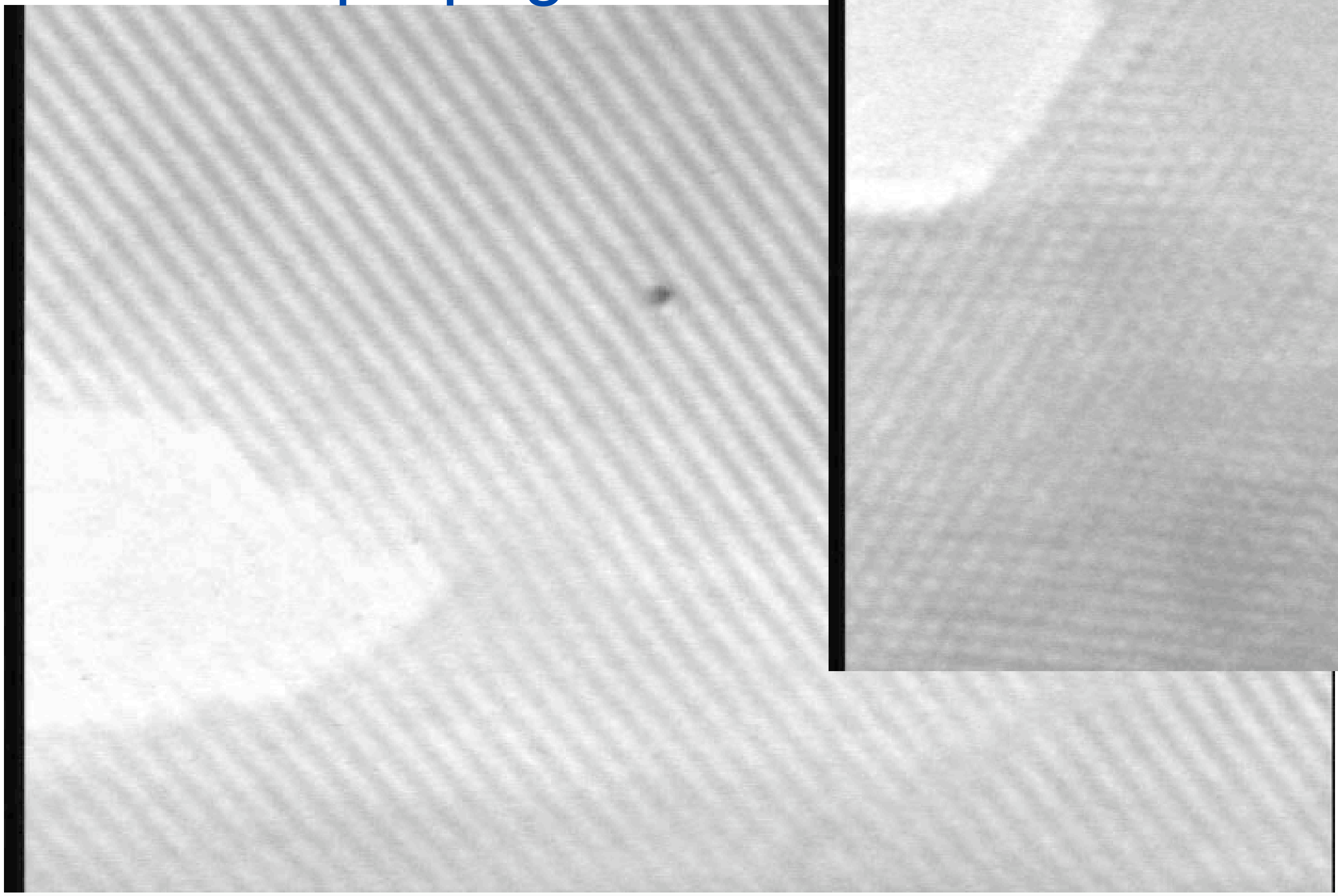
When the yield stress exceeds the instability stress, prompt necking or plastic instability will occur at yield.

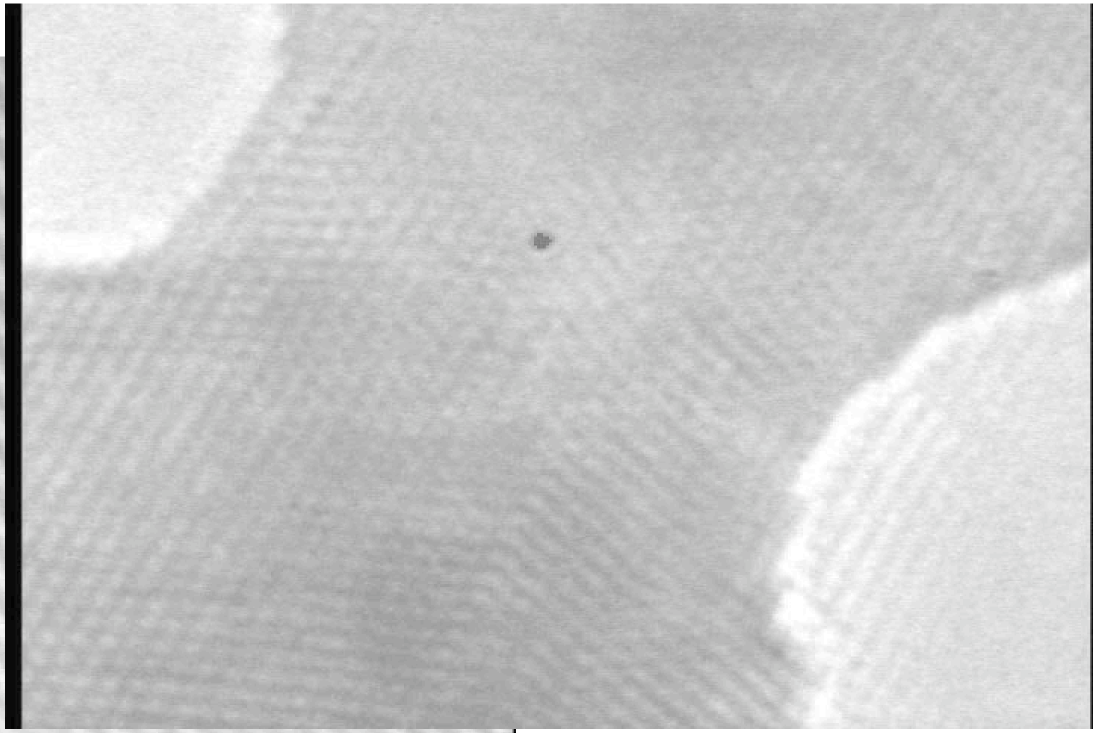
Radiation hardening effect can be treated by shifting by an equivalent work hardening strain in the true stress-strain curve

T.S. Byun and K. Farrell, Acta Mat. 52 (2004) 1597

TEM in-situ deformation studies are providing important insight on fundamental fracture processes

Atomic resolution imaging of crack propagation



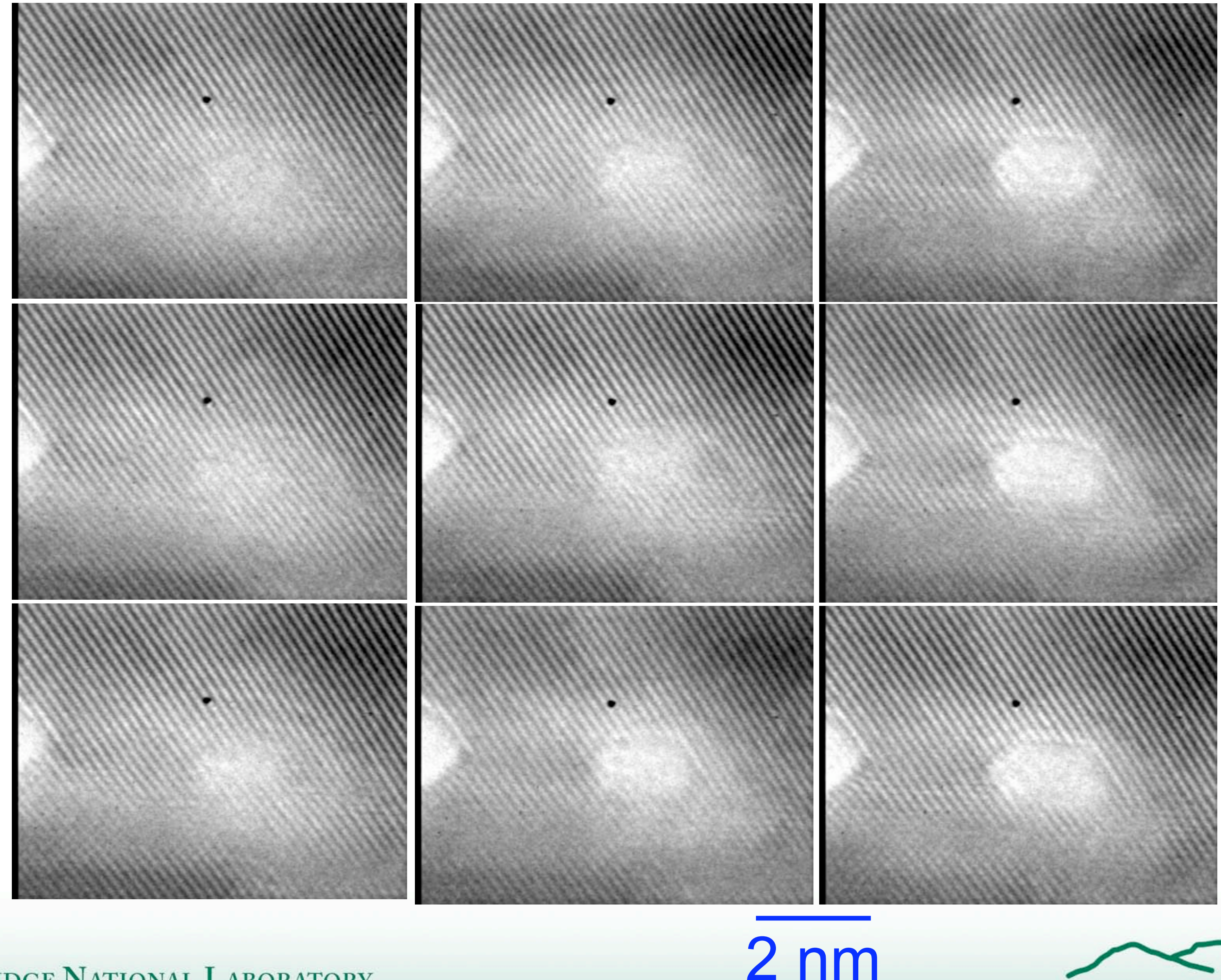


Nanoscale slip deformation

2 nm

Y. Matsukawa, ORNL

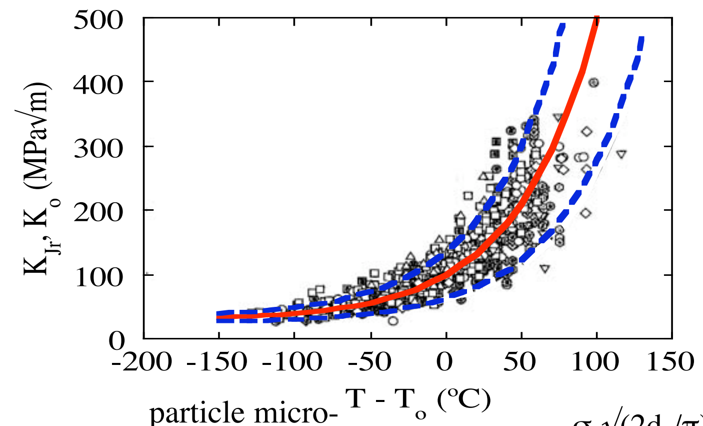
Formation of a nanocavity in front of a crack tip during TEM in-situ deformation

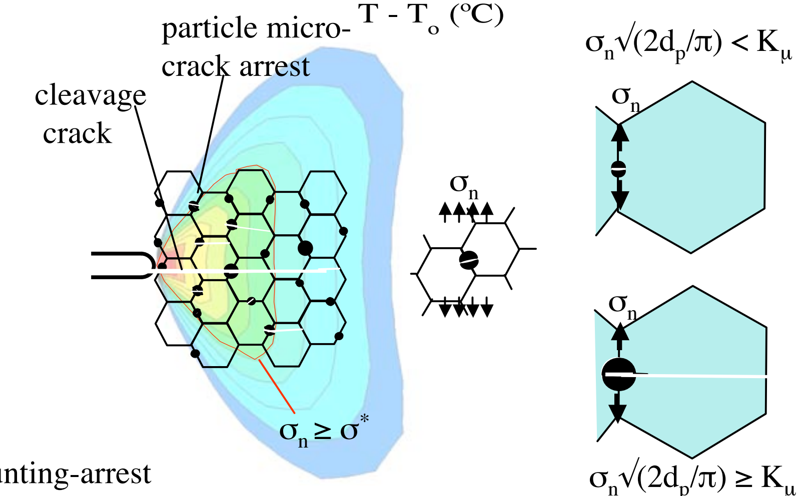


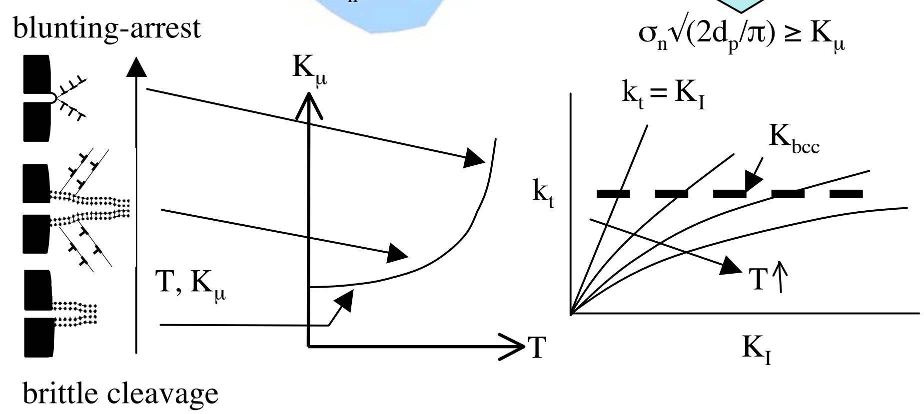
Y. Matsukawa, ORNL

Physical Basis for a Master Toughness Curve

- Master Curve 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 for atomic scale processes that determine the macro-continuum $K_{Jc}(T)$ toughness
- Key? - experiments & Molecular Dynamics + Dislocation Dynamics models of intrinsic BCC micro-arrest toughness at nanoscale tip of a dynamic microcrack

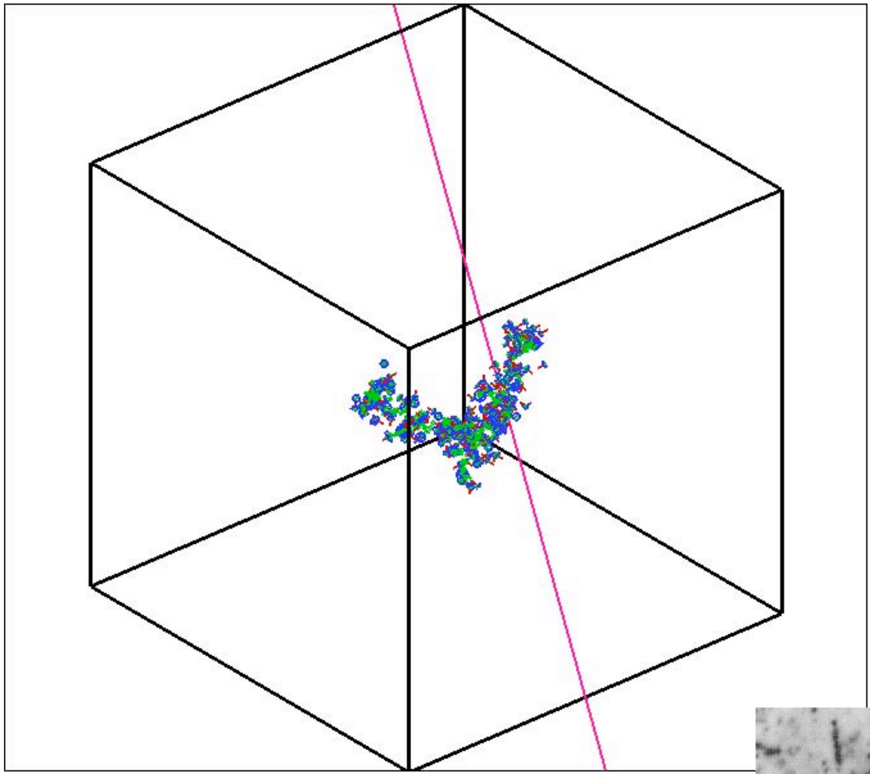


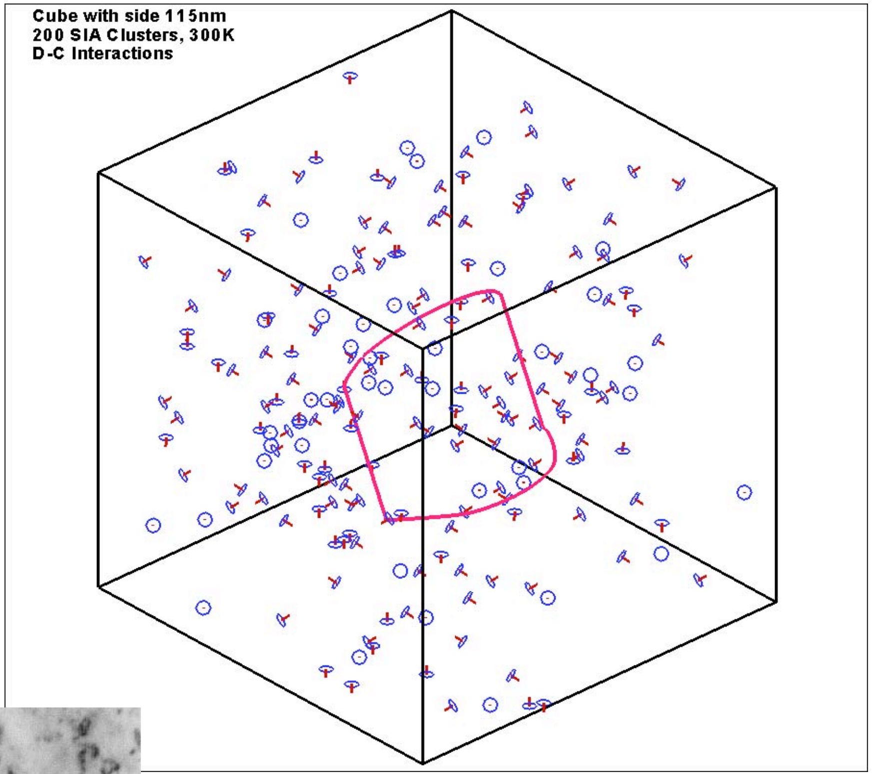


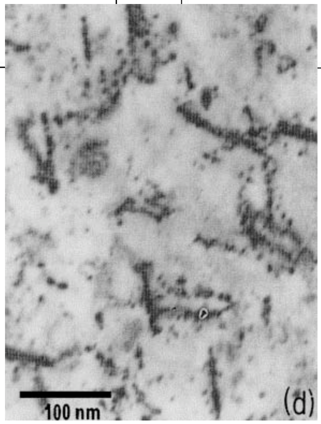


G.R. Odette, UCSB

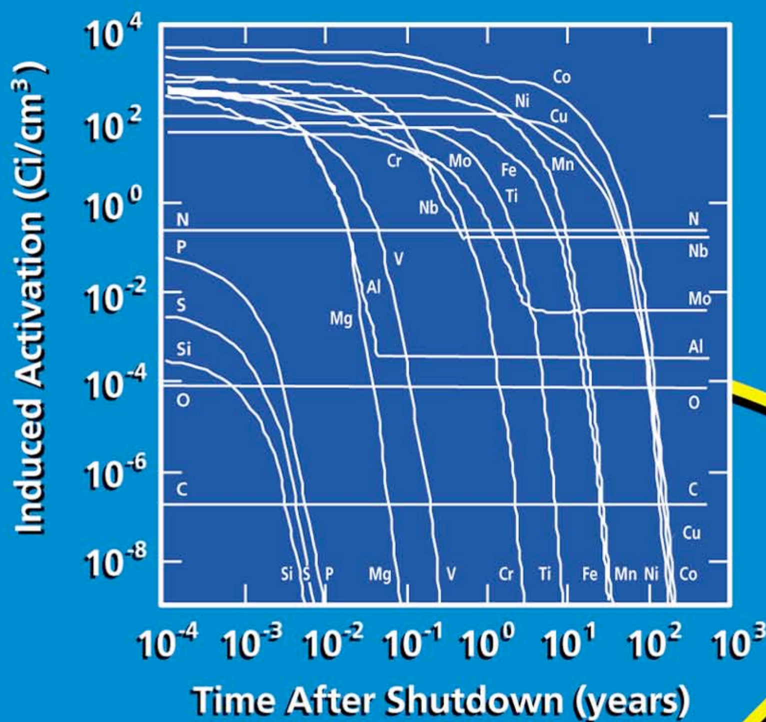
Design of Radiation-Resistant Materials: KMC Modeling of Pinning and Rafting

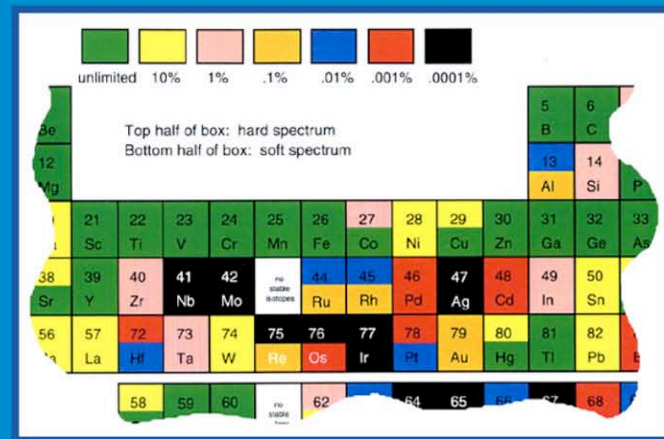




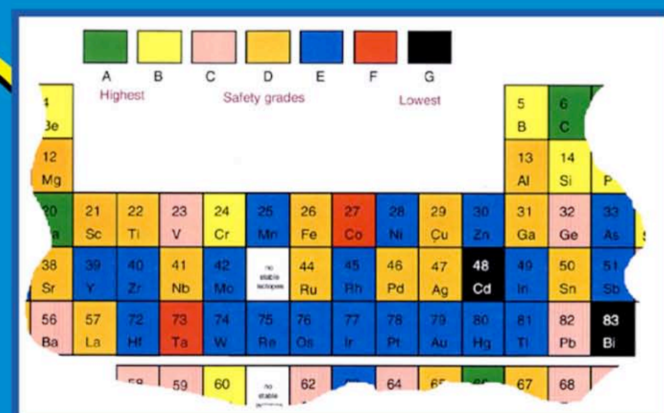


Structural Materials





Class C Waste Disposal



Safety

SiC

V Cr Ti Si

Fe Cr W V Ta

Leading candidate fusion blanket structural materials

- Of all blanket materials, structural materials most strongly impact economic and environmental attractiveness potential of fusion power
- Key issues include thermal stress capacity, coolant compatibility, safety, waste disposal, radiation damage effects, and safe lifetime limits
- Ti alloys, Ni base superalloys, and most refractory alloys have been shown to be unacceptable for various technical reasons
- Based on safety, waste disposal, and performance considerations, the 3 leading candidate blanket structural materials are:

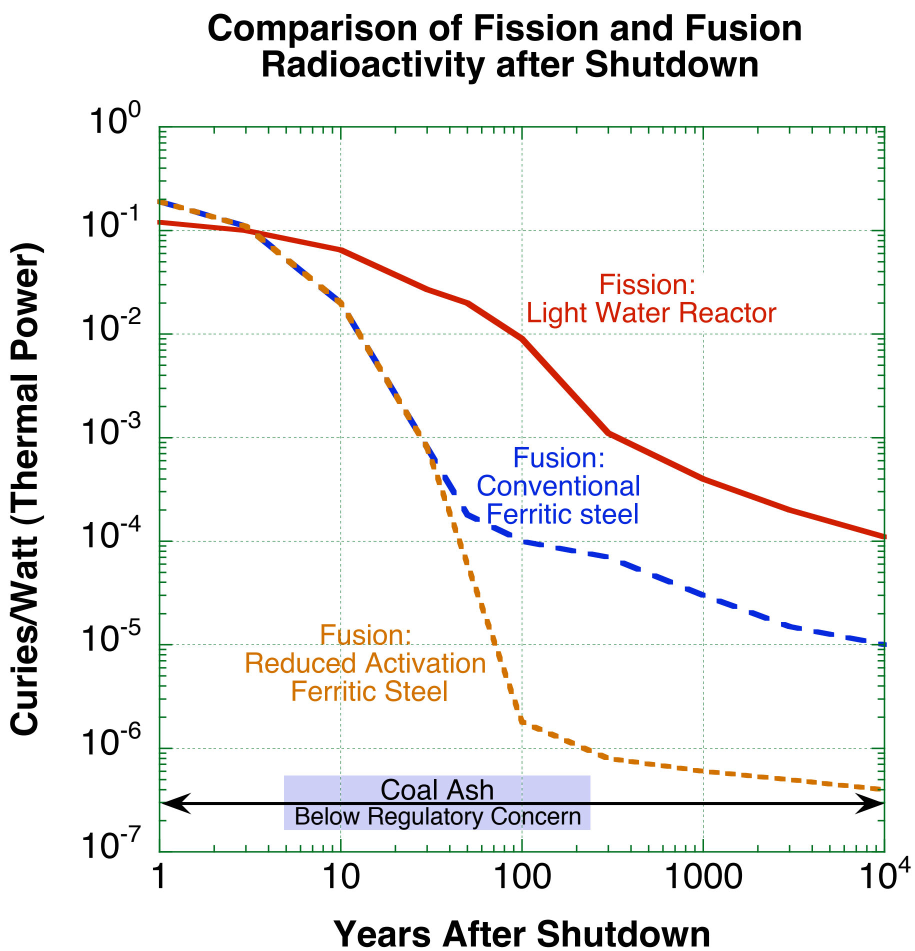
- Ferritic/martensitic steels

- Vanadium alloys

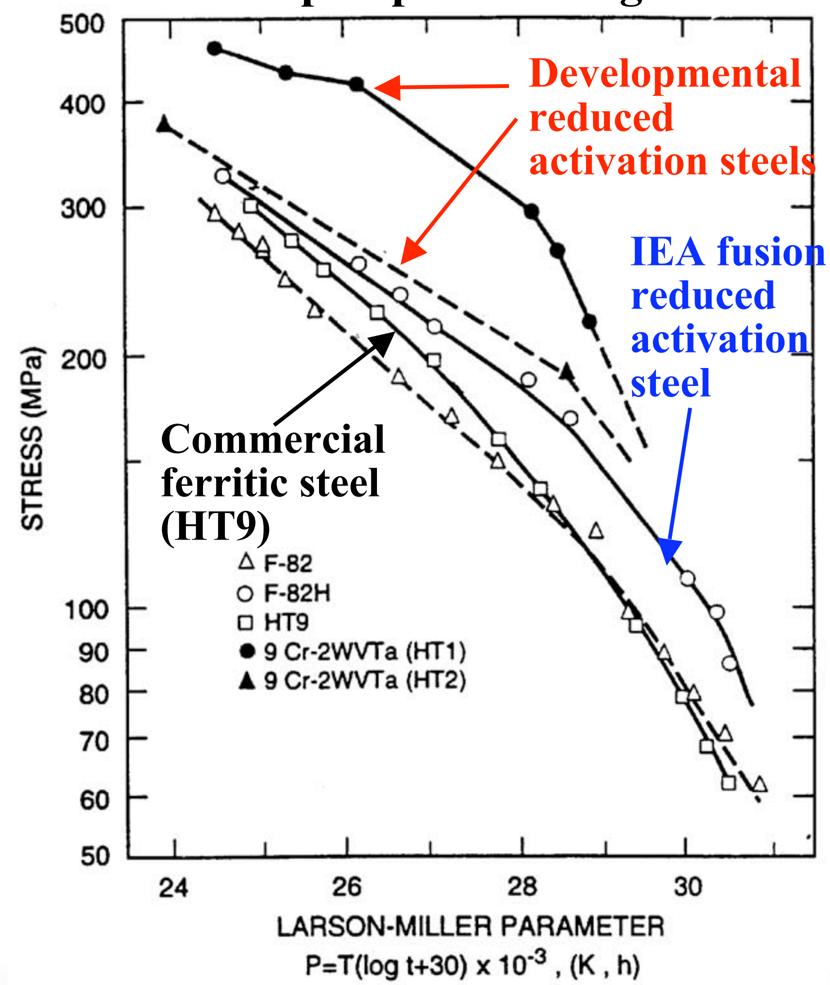
- SiC/SiC composites

None of the current reduced activation fusion materials existed 15 years ago

Ferritic/martensitic Steels with Reduced Radioactivity and Superior Properties Compared to Commercial Steels have been Developed by Fusion



Comparison of thermal creep-rupture strengths

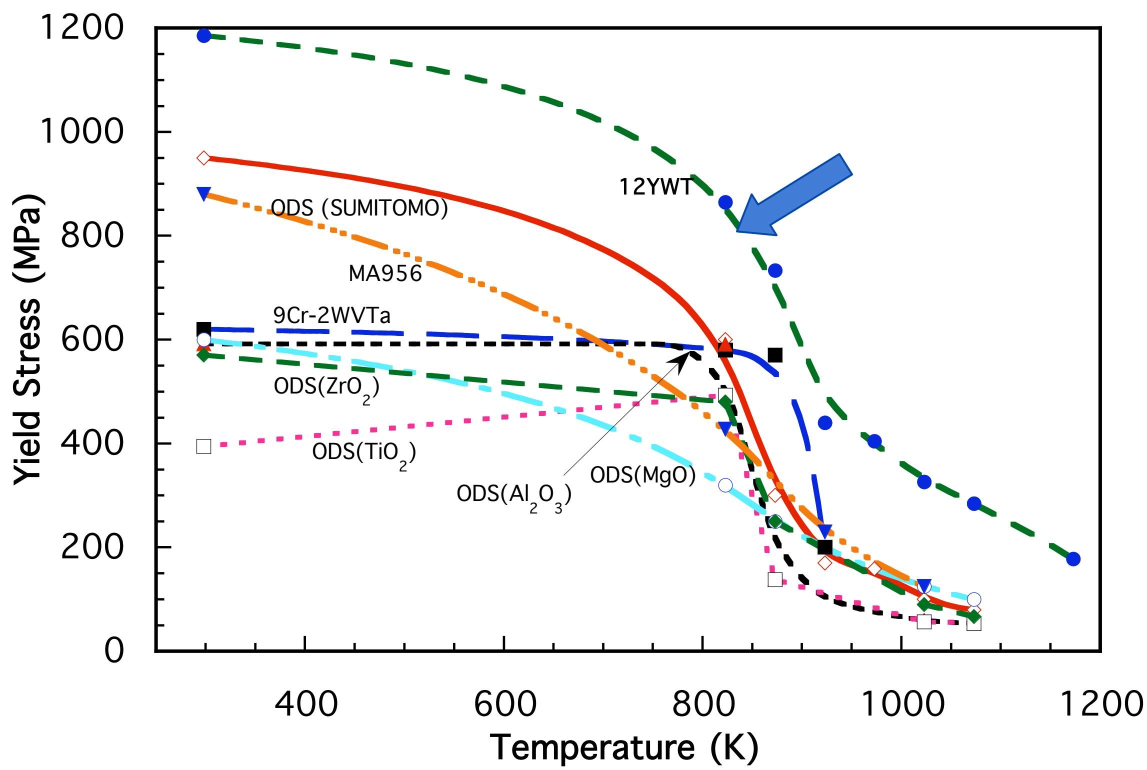


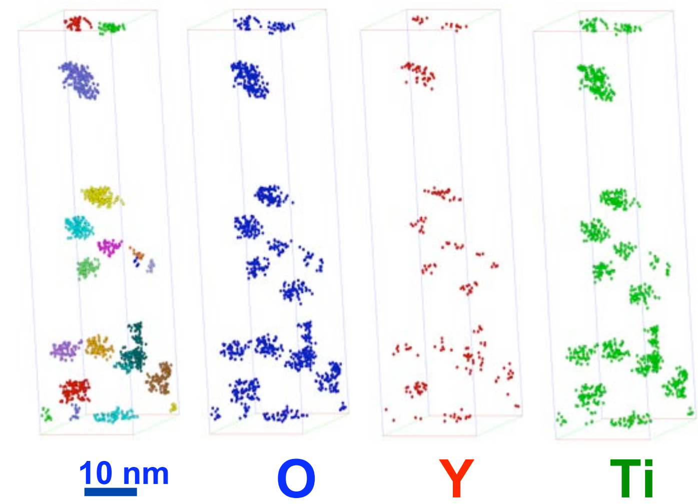
Fusion-developed steels also have superior tensile strength, irradiated fracture toughness, and thermal conductivity

Underlying alloy development philosophy for radiation environments

- Produce high density of uniformly distributed nanoscale particles that are highly stable (thermal and neutron exposures)
  - Avoid solutes and precipitate phases that are known to be susceptible to radiation induced dissolution or coarsening effects
  - Avoid phases that are known to cause embrittlement (e.g., δ-ferrite, chi and $M_{23}C_6$ phases in ferritic/martensitic steels)
- Employ a suite of computational tools to guide experimental studies
  - Thermodynamic codes for identifying intrinsic equilibrium structures in the absence of irradiation
  - Multiscale codes (atomistic, molecular dynamics, kinetic/lattice Monte Carlo, chemical rate theory, etc.) to probe radiation effects behavior
- Use targeted experiments to validate computational results and to probe conditions unsuitable for quantitative computational analysis
  - Numerous experiments use model alloy systems as well as complex engineering alloys

New 12YWT Nanocomposited Ferritic Steel has Superior Strength compared to conventional ODS steels

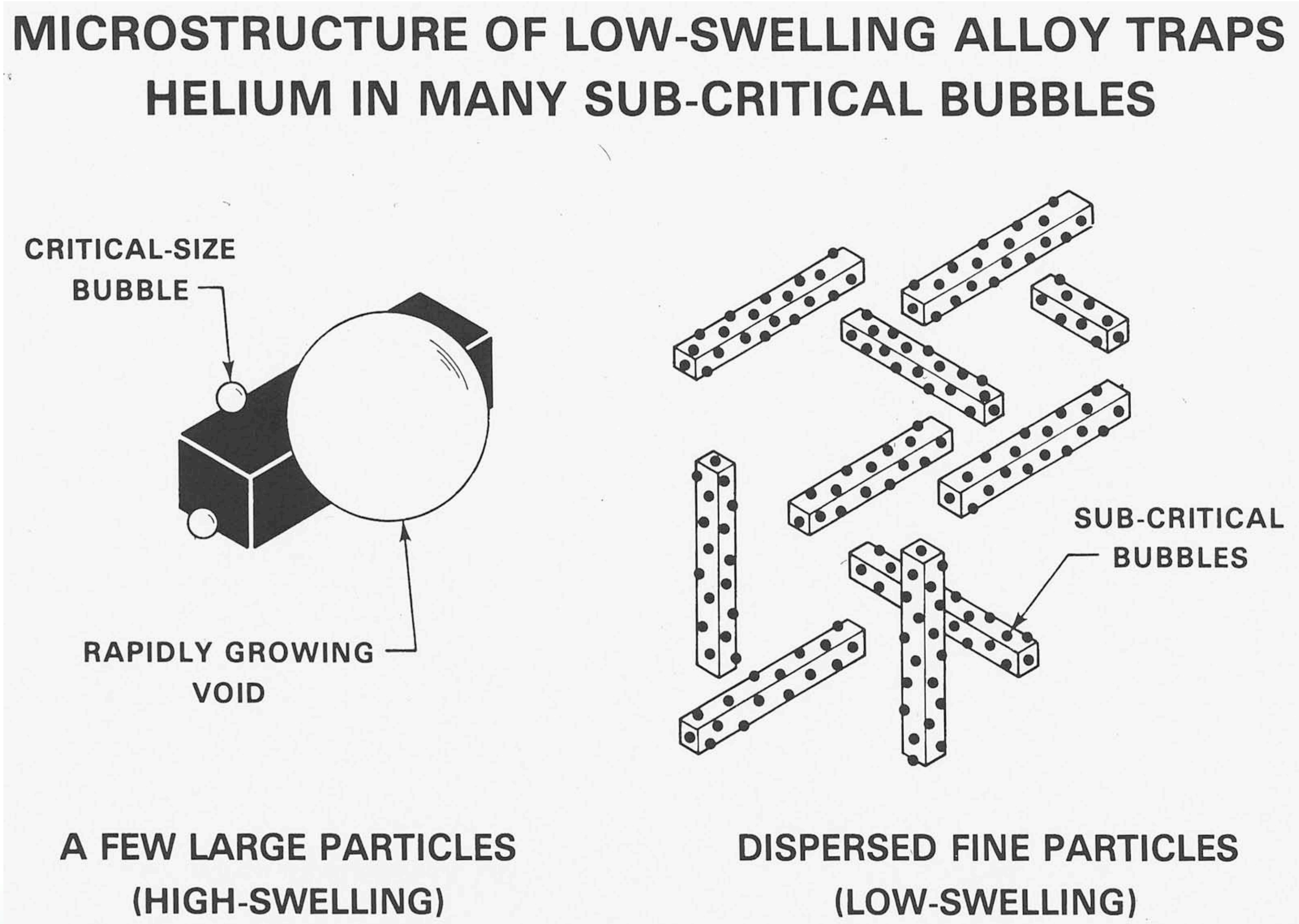




- Thermal creep time to failure is increased by several orders of magnitude at 800˚C compared to ferritic/martensitic steels
- Potential for increasing the upper operating temperature of iron based alloys by ~200°C
- Acceptable fracture toughness near room temperature

- Atom Probe reveals nanoscale clusters to be source of superior strength
  - Enriched in O(24 at%), Ti(20%), Y (9%)
  - Size : $r_g = 2.0 \pm 0.8$ nm
  - Number Density : $n_v = 1.4 \times 10^{24}/m^3$
- Original Y_2O_3 particles convert to thermally stable nanoscale (Ti,Y,Cr,O) particles during processing
- Nanoclusters not present in ODS Fe-13Cr + $0.25Y_2O_3$ alloy

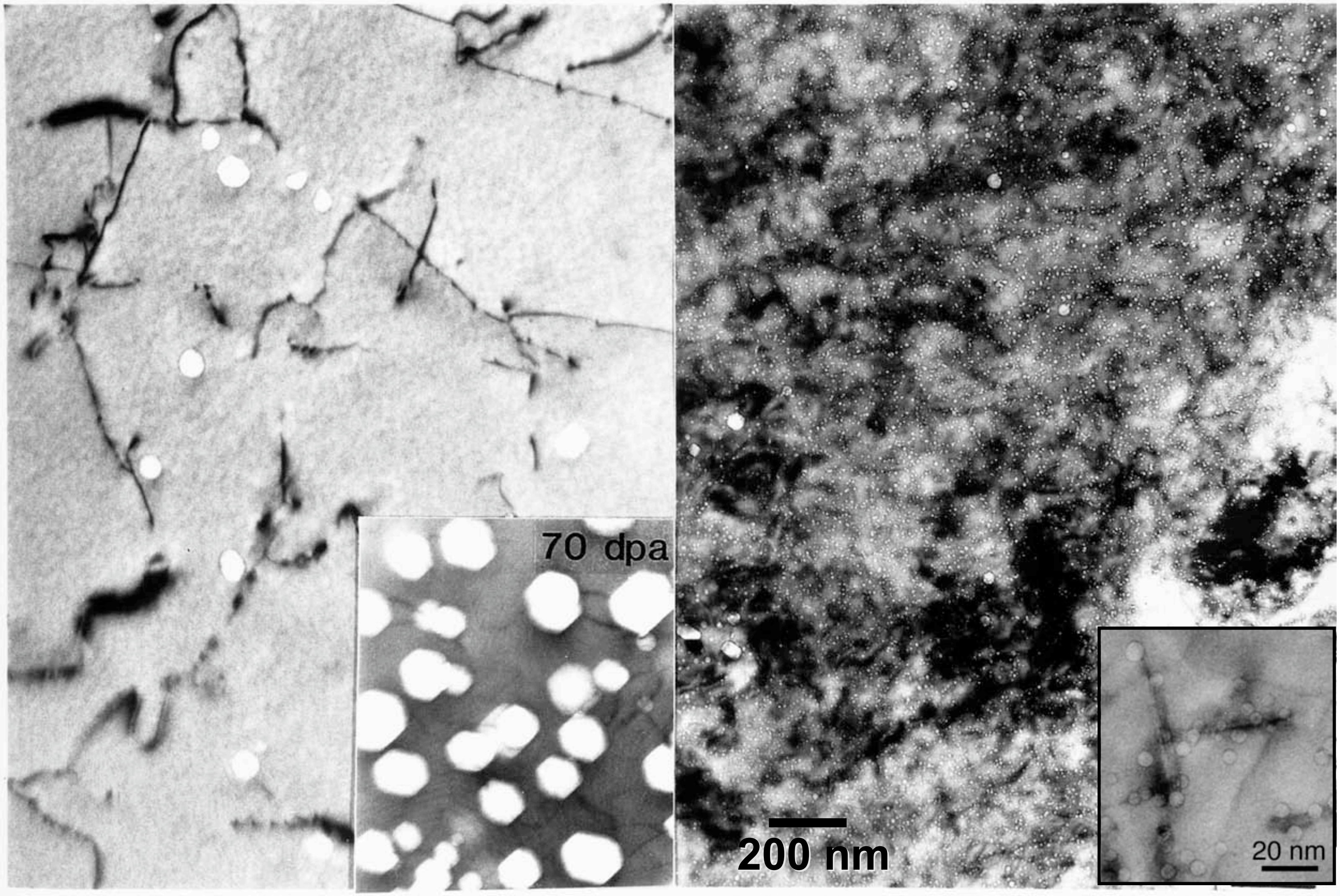
A high density of precipitates is essential for swelling resistance



Swelling Resistant Alloys can be developed by Controlling the He Cavity Trapping at Precipitates

Fe-13Cr-15Ni Ternary

(P,Si,Ti,C)-Modified



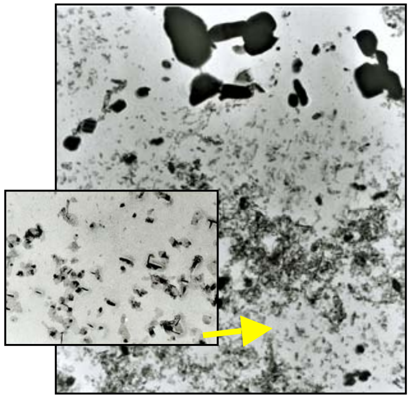
0.4 dpa/0.2 appm He/675C

109 dpa/2000 appm He/675C

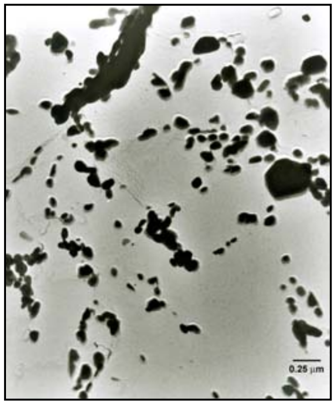
New Alloys Developed in the 1980's are finding advanced Manufacturing Applications: Example for 2 1/4 Cr alloys

Fusion Energy Project Led to Alloys with Exceptional Microstructure/Properties

New Microstructure Design - finer and more stable

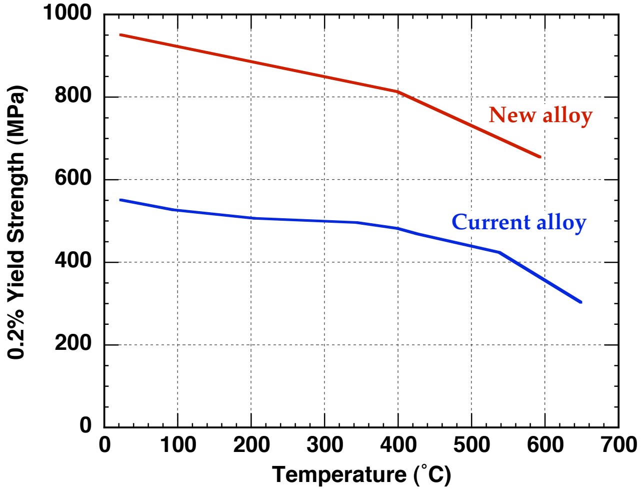


NEW: 2 1/4 Cr-2WV



Previous; 2 1/4 Cr-1Mo

Dramatic Property Improvements



1000 h creep strength is also improved by >50%

New Industrial Materials for the Future Project Focuses on Chemical Industry Applications

Planned Work:

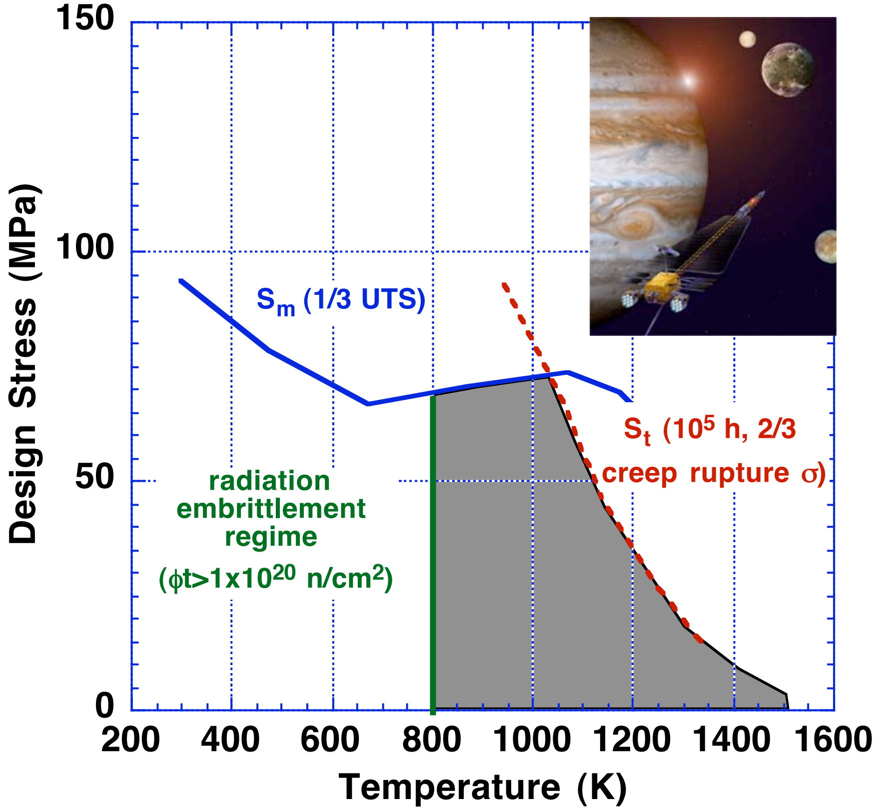
•Develop more advanced alloy compositions

•Scale up processing and fabrication

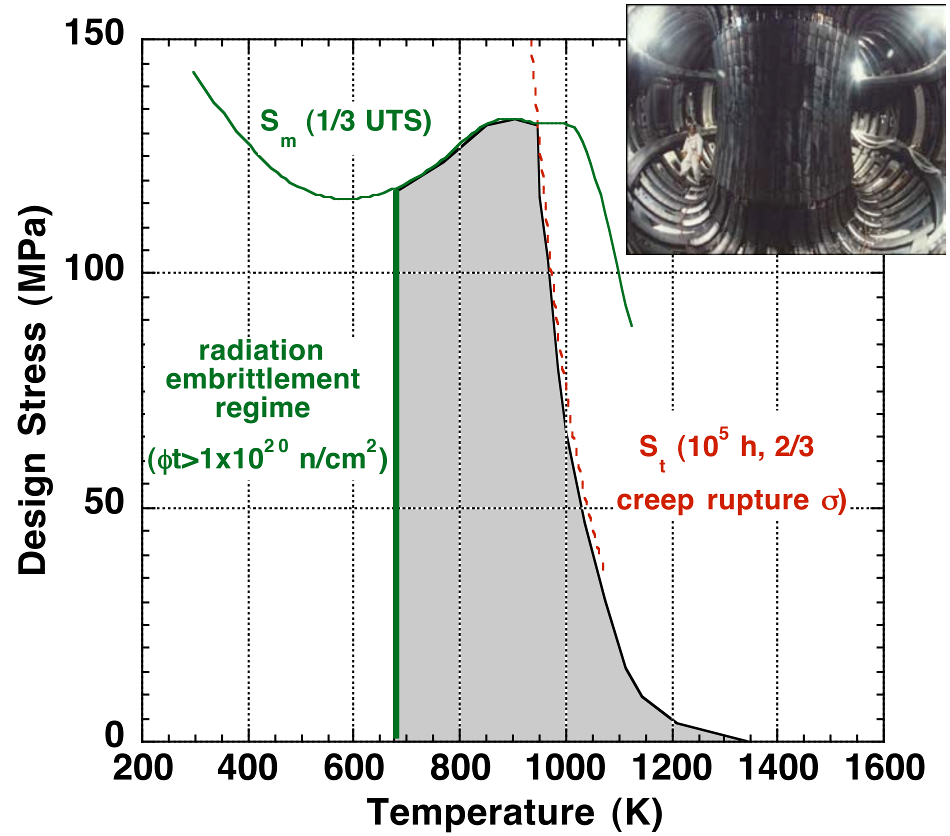
•Develop case-specific materials properties and welding technology

Comparison of the Design Window for Nb1Zr and V4Cr4Ti

Design Window for Nb-1Zr



Design Window for V-4Cr-4Ti

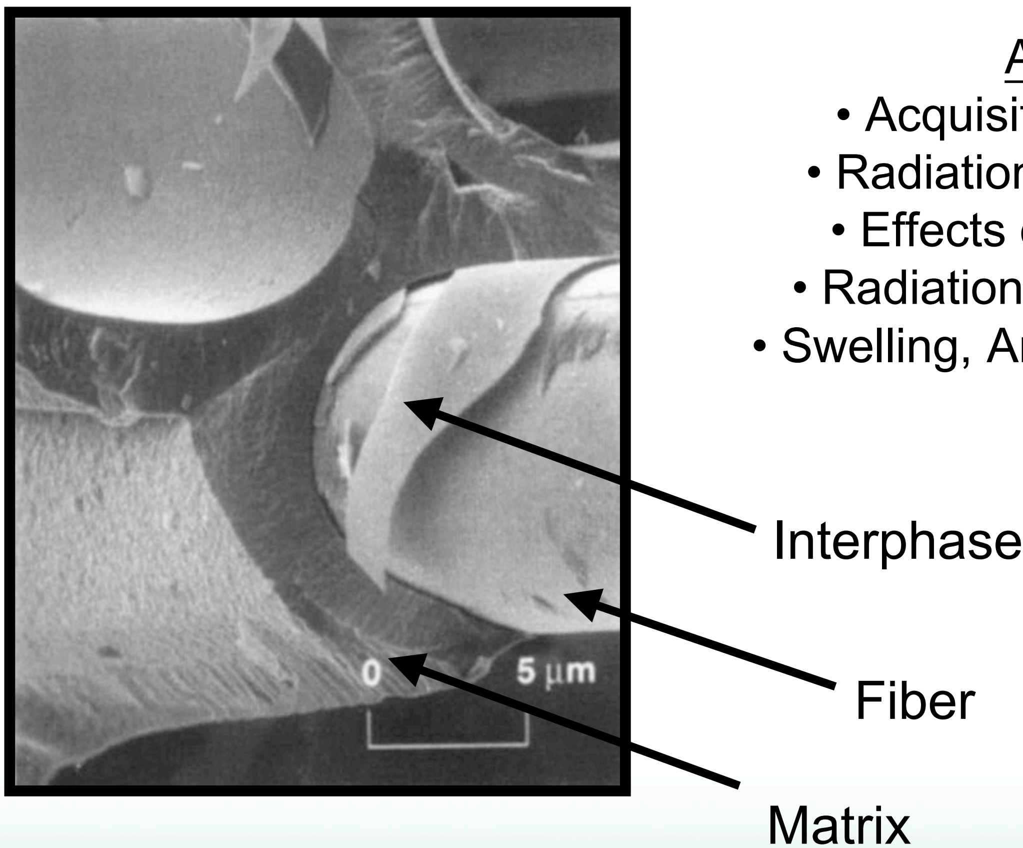


- V4Cr4Ti offers ~factor of two higher stress capability than Nb1Zr

Silicon Carbide Composite Development

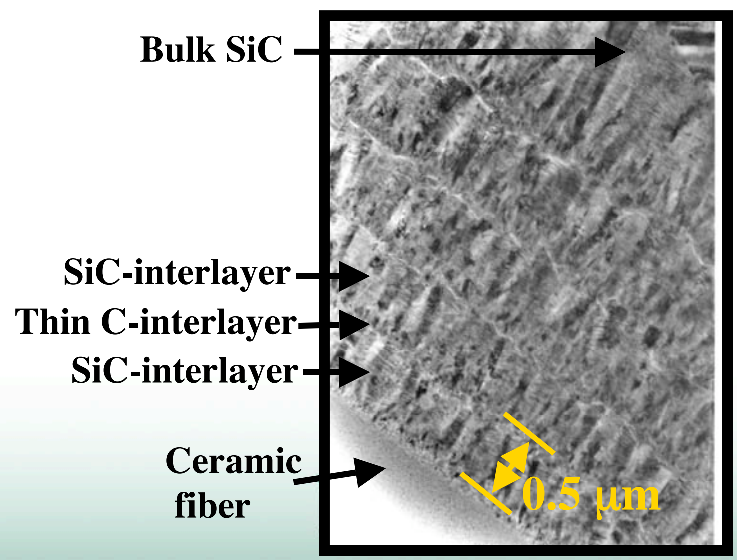
Silicon carbide composite is the least-developed of the 3 main structural materials being studied in the Fusion Materials Program, but it has the **greatest potential**

Very Low Radioactivation - Very High Temperature Use



<u>Areas being actively studied</u>

- Acquisition of structural material properties
- Radiation Hardened Composite Development
- Effects of Helium on Mechanical Properties
- Radiation Degradation of Thermal Conductivity
- Swelling, Amorphization and Defect Fundamentals

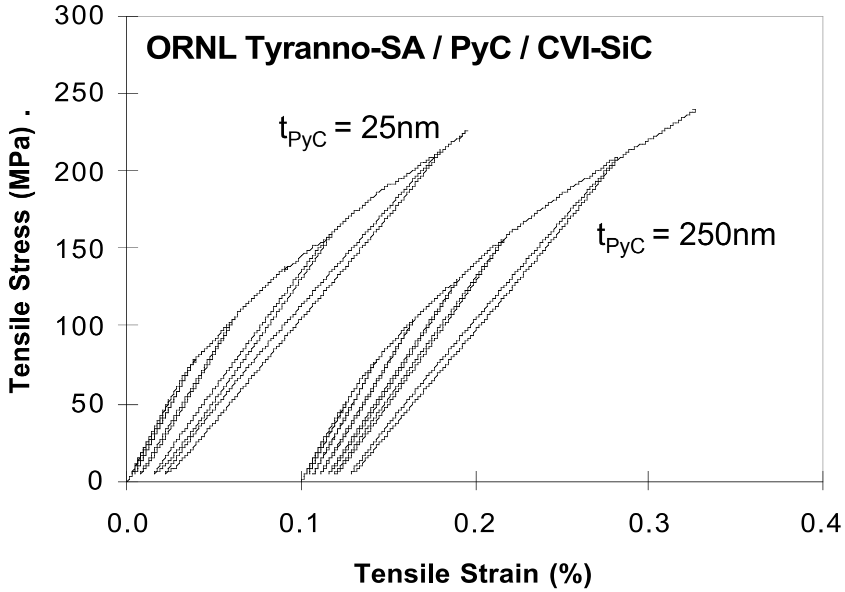


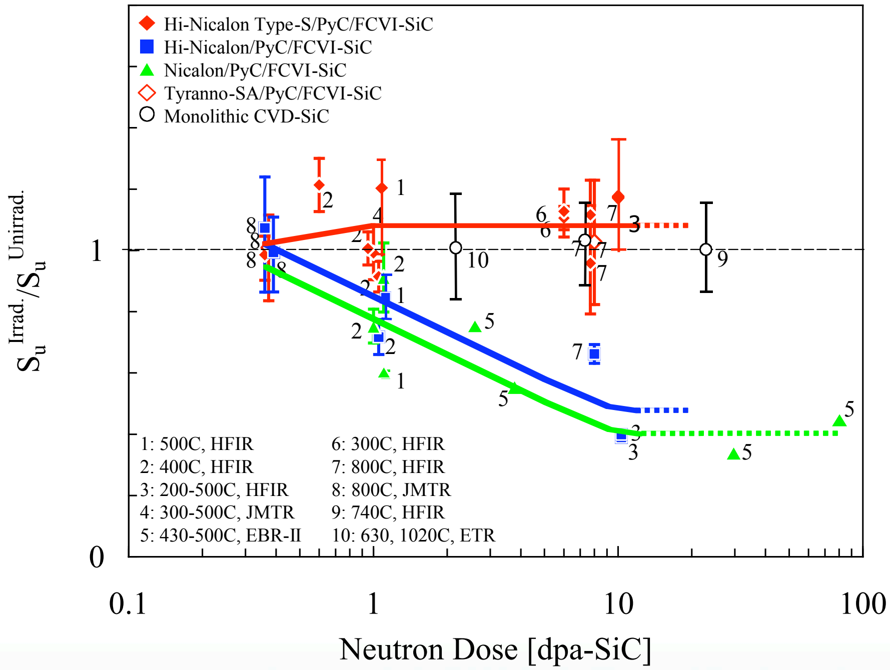
SiC/SiC Composites Development

Reference Chemical Vapor Infiltrated (CVI) Composites for Irradiation Studies

- Hi-Nicalon™ Type-S or Tyranno™-SA3 / PyC(50–150nm^t) / CVI-SiC composites have been selected as the reference materials
- Materials are under fabrication in US/Japan collaboration
- Extensive engineering data generation for irradiated properties (including statistical strength) is planned (prior studies utilized simple qualitative screening tests)

Bend strengths of irradiated "3rd generation" composites show **no degradation** up to 10 dpa

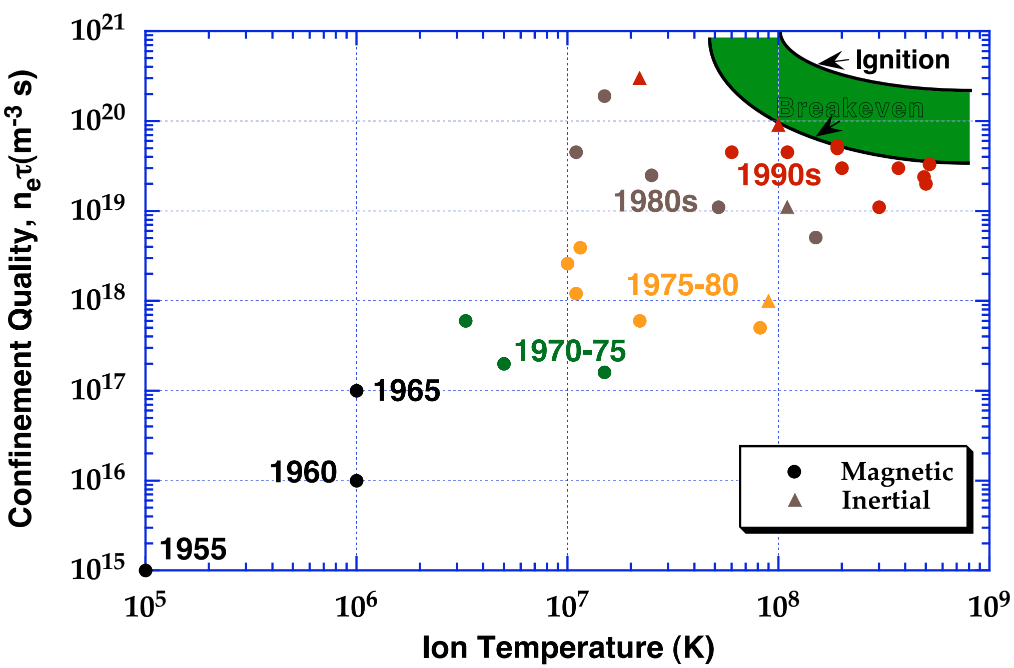




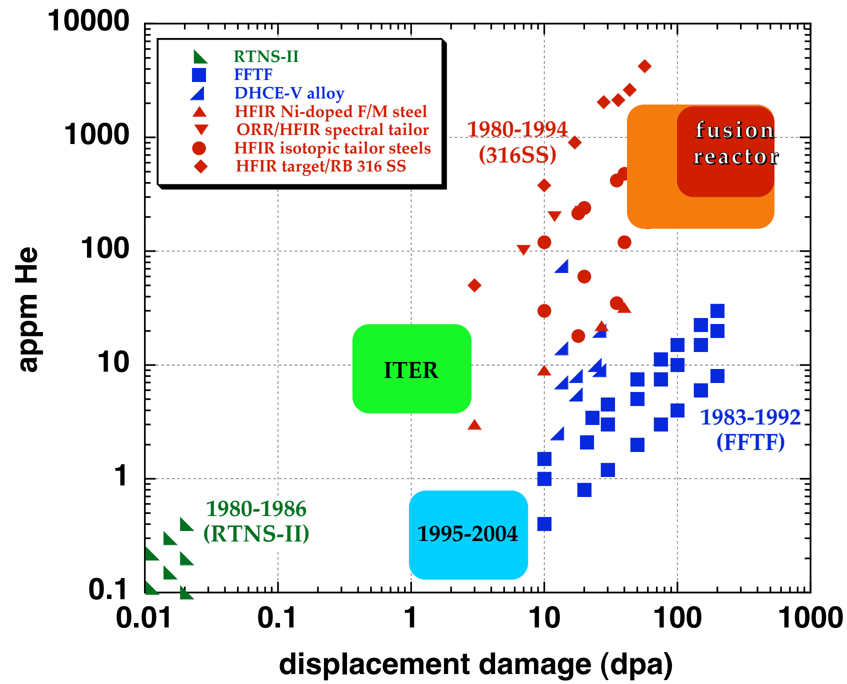
Improved performance is due to development of stoichiometric crystalline SiC fibers and advanced fiber/matrix interphases

The knowledge base on materials exposed to fusion-relevant operating conditions is very limited

- Extrapolation from currently available parameter space to fusion regime is much larger for fusion materials than for plasma physics program
- An intense neutron source such as IFMIF is needed to develop and qualify fusion structural materials
- Theory and modeling will accelerate the development of fusion materials, but does not replace the need for a dedicated neutron source such as IFMIF
  - R.E. Stoller et al., ORNL/TM-2004/132 (June 2004), Workshop on Advanced Computational Materials Science: Application to Fusion and Generation IV Fission Reactors (http://www.csm.ornl.gov/meetings/SCNEworkshop/)



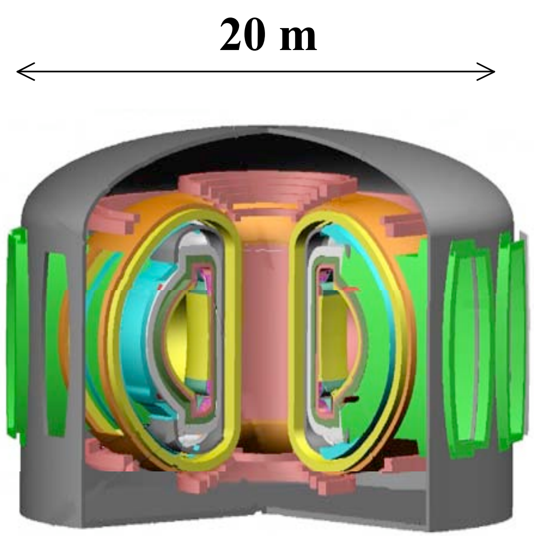
Summary of Helium and Dose Parameter Range Investigated by the Fusion Materials Program



Conclusions

- Development of structural materials for demanding environments such as fusion and fission reactors requires utilization of coordinated modeling and focused experimental studies
  - Must be based on advanced materials science principles
  - Alloying strategy based on precipitate or dispersion hardening generally improves both thermal creep strength and radiation resistance
    - 2nd phase must be stable under neutron irradiation!
- Materials science-based alloy development strategy is utilized to design improved materials once the underlying physical mechanisms responsible for property degradation are understood
  - Multiscale modeling is a key tool for investigating fundamental physical phenomena in irradiated materials

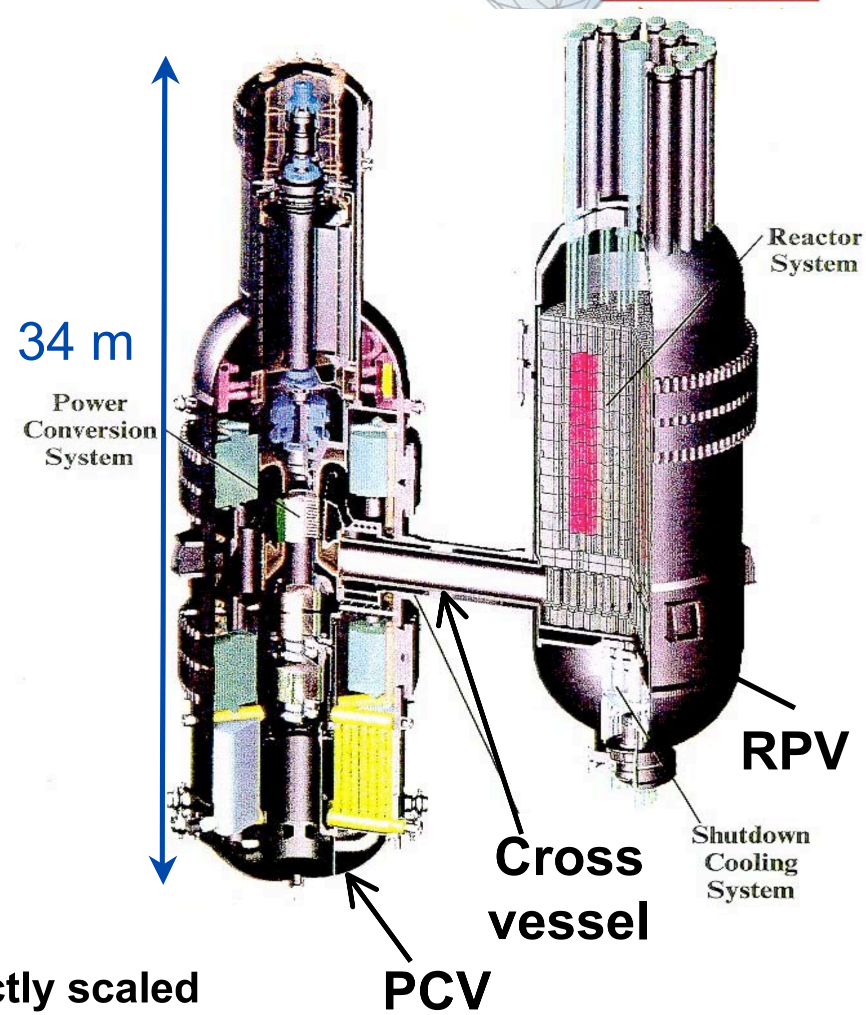
The ARIES-AT fusion reactor design is similar size as proposed Gen-IV fission Next Generation Nuclear Plant (NGNP)



Correctly scaled size of ARIES AT fusion reactor

Correctly scaled size of typical PWR RPV

NGNP



- Improved safety and performance (e.g., H_2 production) offset higher capital costs for future reactors