Phase Stability & Material Design

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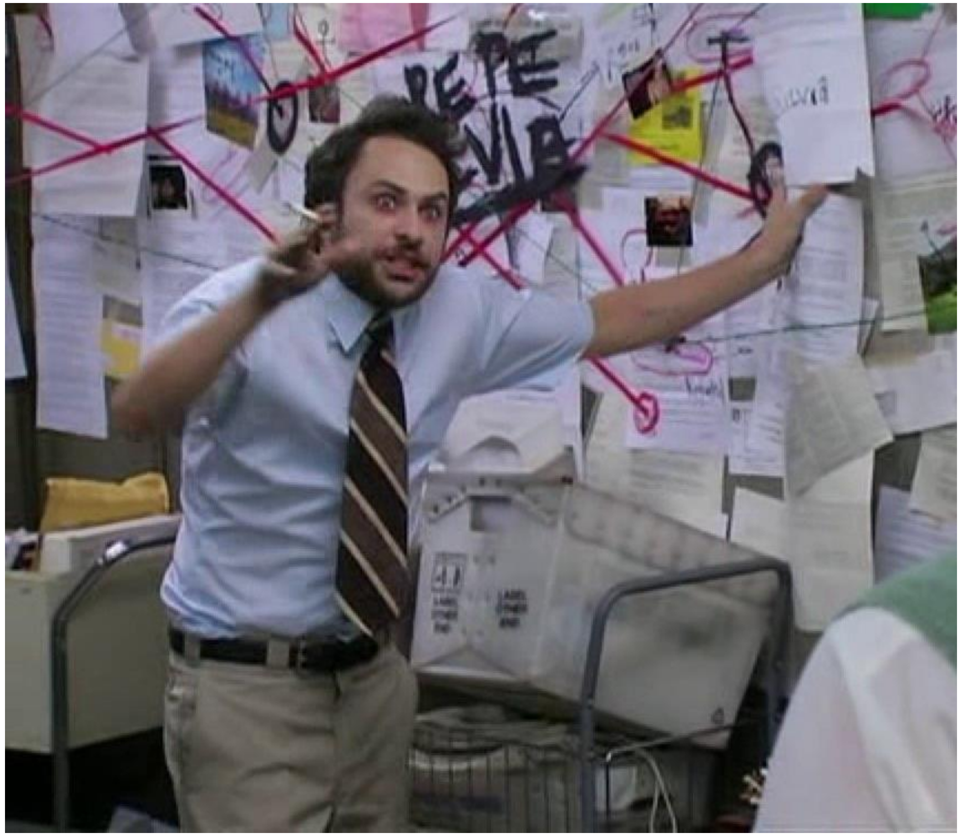
Don’t forget to submit HW5!

Final Exam Structure

- We will follow a similar format to the mid-term:
  - Non-cumulative: covers topics on previous slide

12/15 (Monday) from 10:30 am – 12:30 pm in Cooley 2918



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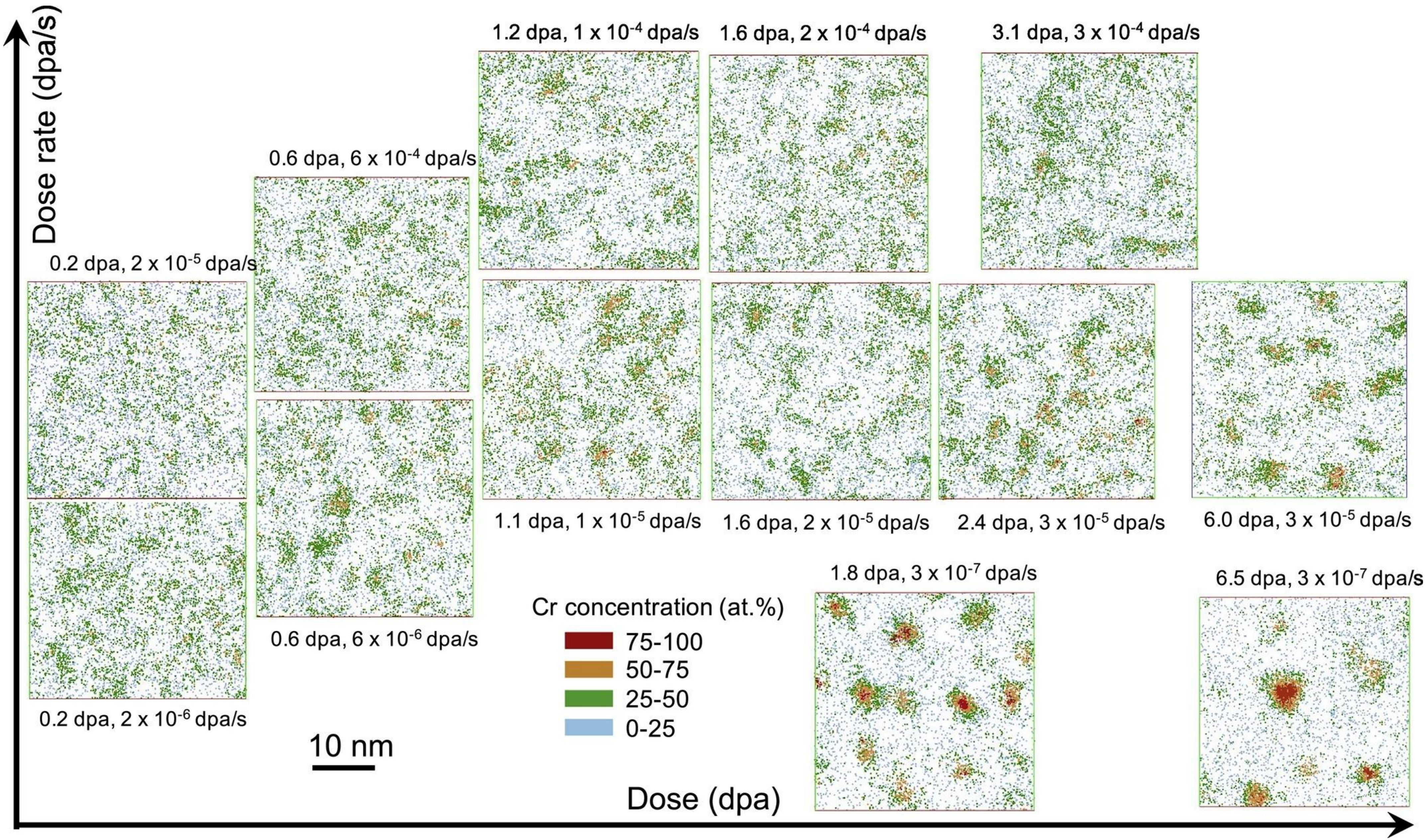

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Radiation-induced precipitate dissolution

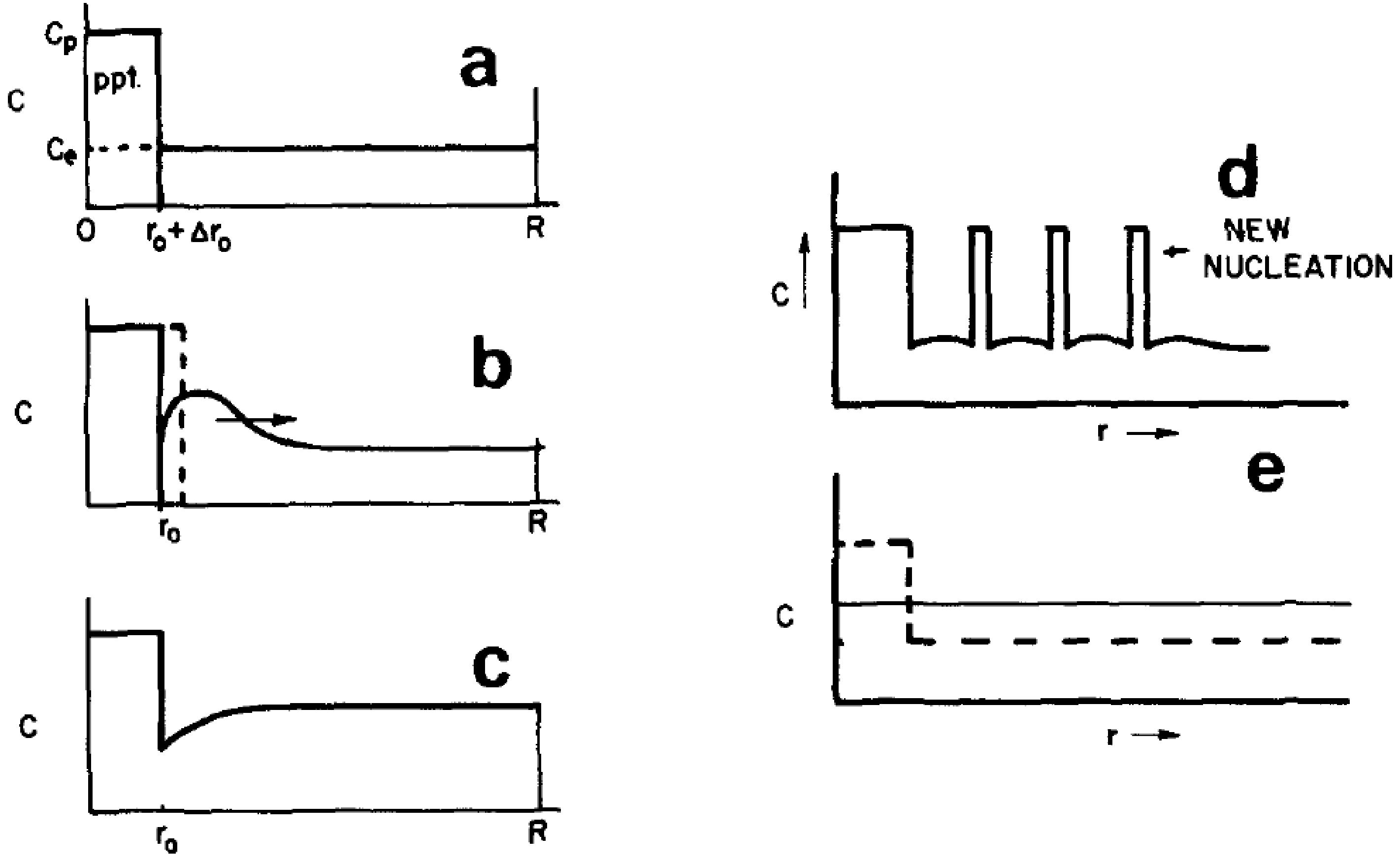
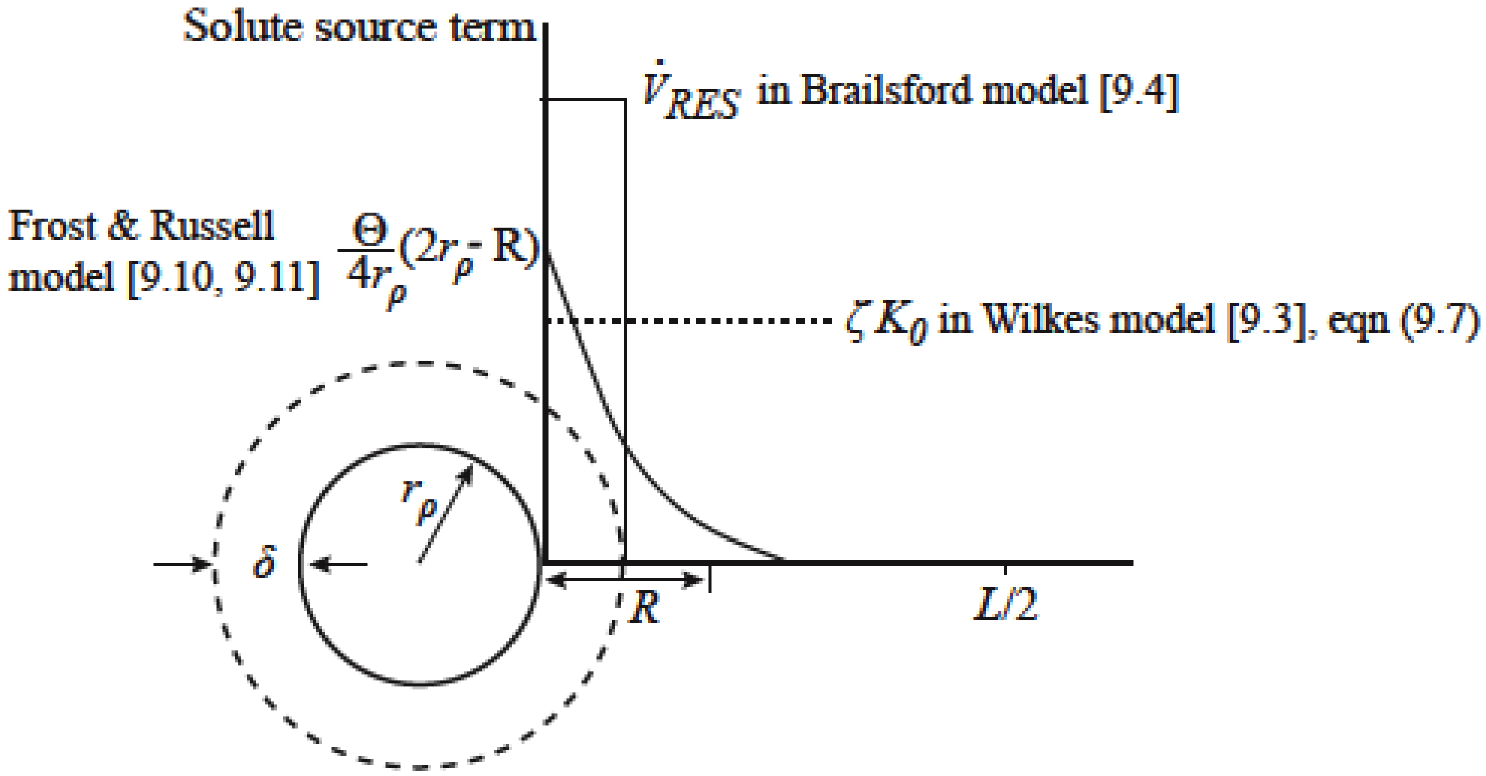


Fig. 3. A schematic diagram of concentration variations in a precipitate cell: (a) before irradiation with a precipitate of radius $r_0 + \Delta r$ in equilibrium with a uniform matrix concentration c_e; (b) when irradiation begins surface disssolution causes a local solute supersaturation some of which diffuses outwards down the gradient; (c) at steady-state, the matrix is now uniformly supersaturated and the precipitate dissolution is matched by the back diffusion into the precipitate; (d) if the local supersaturation around the precipitate exceeds that required for nucleation, new precipitates may nucleate; (e) if the precipitates are widely spaced, the matrix may not reach the steady-state value and all precipitates will then dissolve.

Radiation-induced precipitate dissolution

In reality, modeling recoil distribution is inherently complex. Models that try to take this into account:

- Nelson model (NHM) – pg. 488-489 in Was
- Wilkes model – pg. 489-492 in Was
- Frost and Russell – pg. 492-493 in Was



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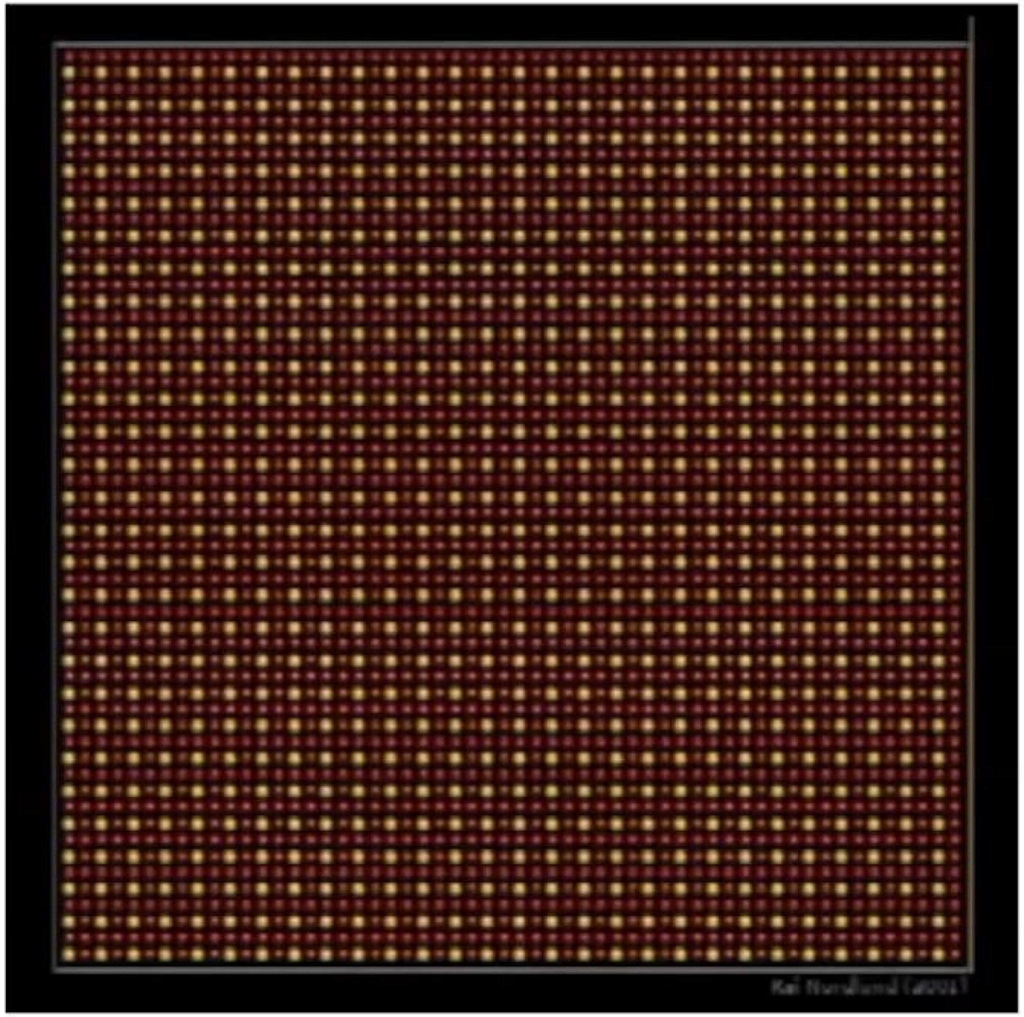
Phase transformations without changes in composition

Radiation Disordering

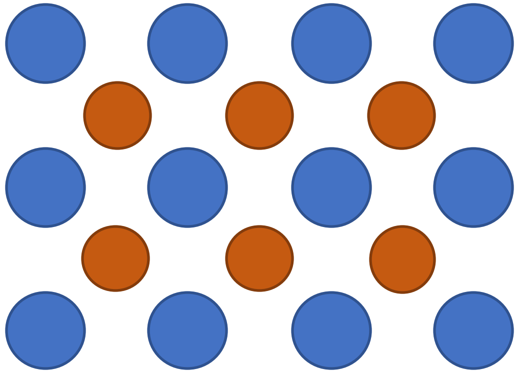
9.1 Irradiation-induced disordering.
Disordering of Cu_3Au (L12 structure)
by bombardment with 10 keV Au ions.
(courtesy K. Nordlund, University of Helsinki)

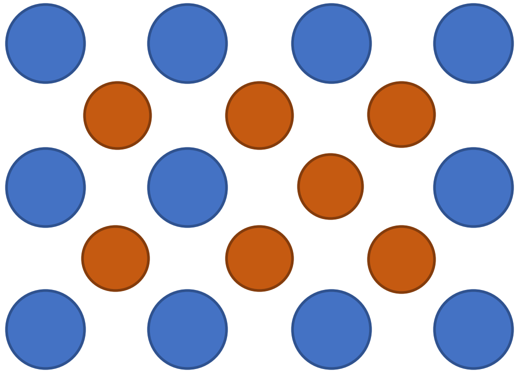


Radiation disordering: Loss of long-range order

Radiation Disordering

- Antisite defects:
  - Occur in an ordered alloy or compound when atoms of different type exchange position





  - We now need to consider random recombination so:

Radiation Disordering

- The steady state solution then becomes:

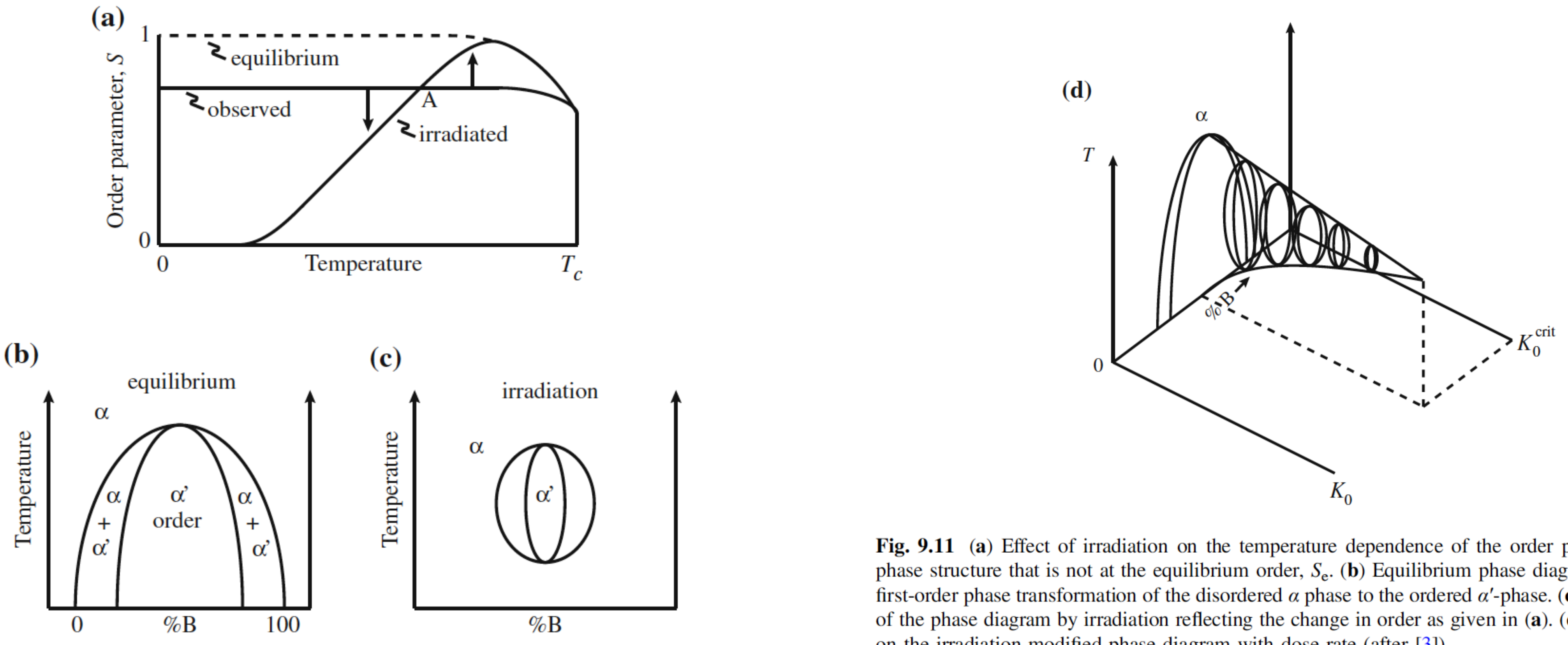
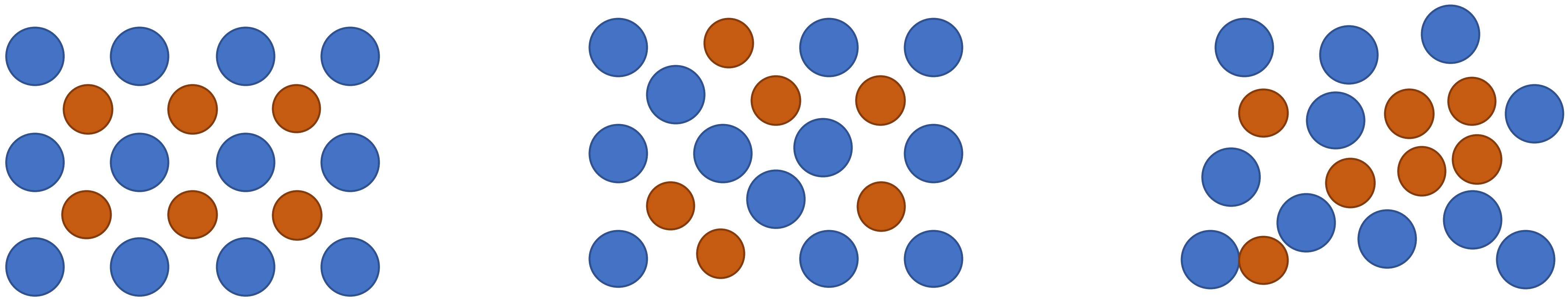


Fig. 9.11 (**a**) Effect of irradiation on the temperature dependence of the order parameter for a phase structure that is not at the equilibrium order, S_e. (**b**) Equilibrium phase diagram showing a first-order phase transformation of the disordered α phase to the ordered α'-phase. (**c**) Modification of the phase diagram by irradiation reflecting the change in order as given in (**a**). (**d**) Dependence on the irradiation-modified phase diagram with dose rate (after [3])

Temperature dependence of amorphization



- Disordering means the destruction of the sub-lattice patterns in ordered alloys (e.g., creation of anti-site defects)
- Amorphization by particle irradiation refers to the complete loss of long-range crystalline structure

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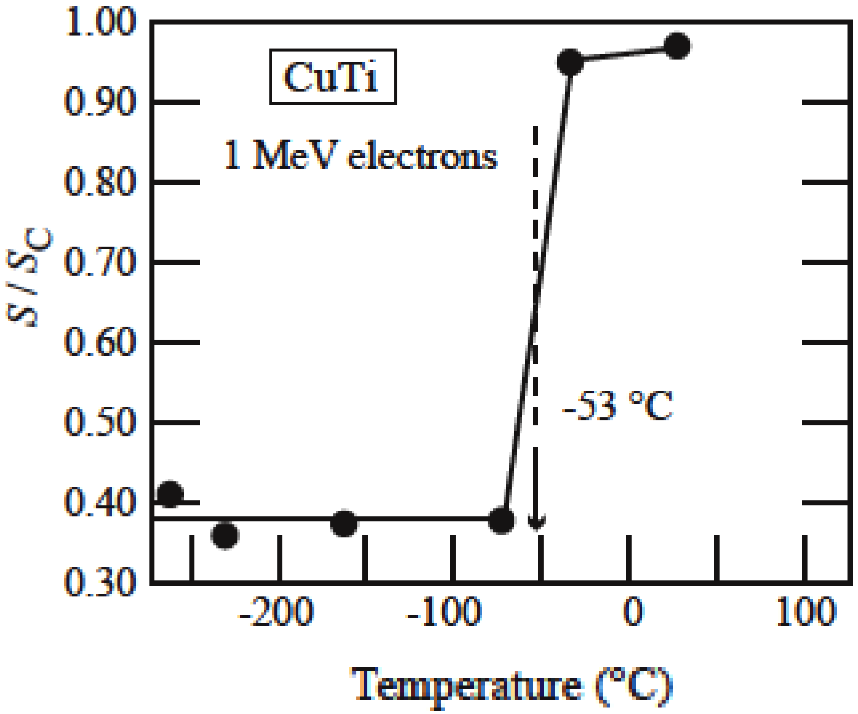
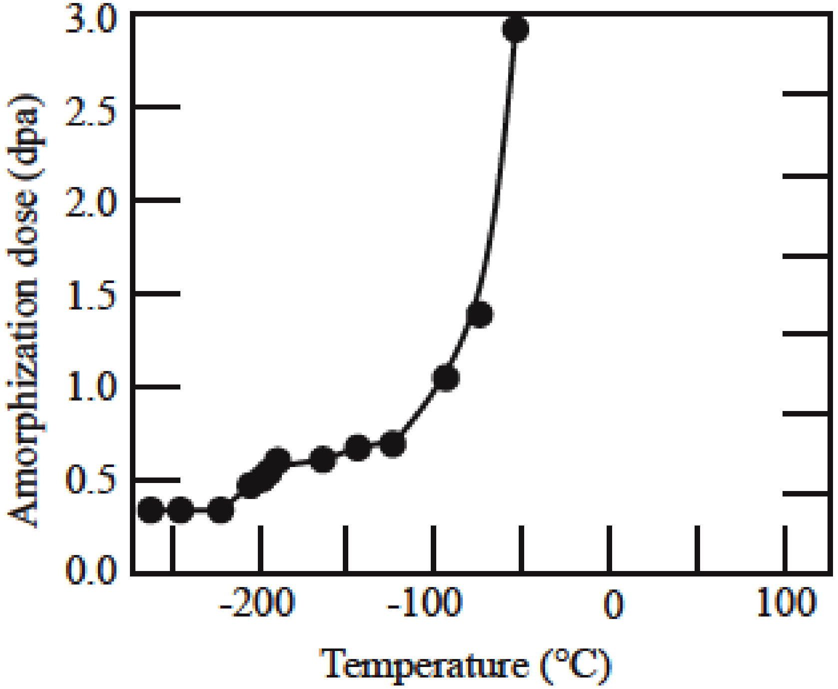
Temperature dependence of amorphization



a



b

Temperature dependence of a) the long-range order parameter S/S_C, and b) the critical amorphization dose for CuTi, irradiated with 1 MeV electrons

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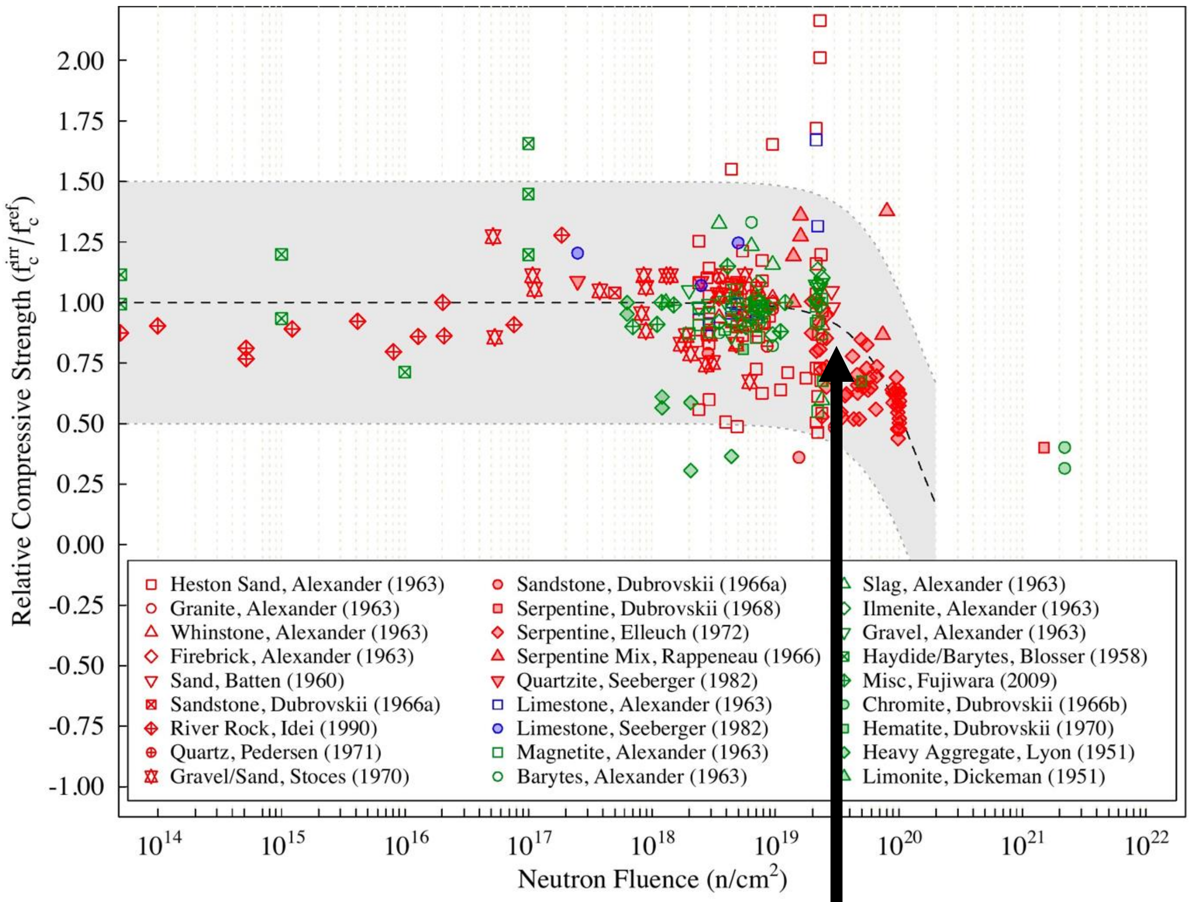
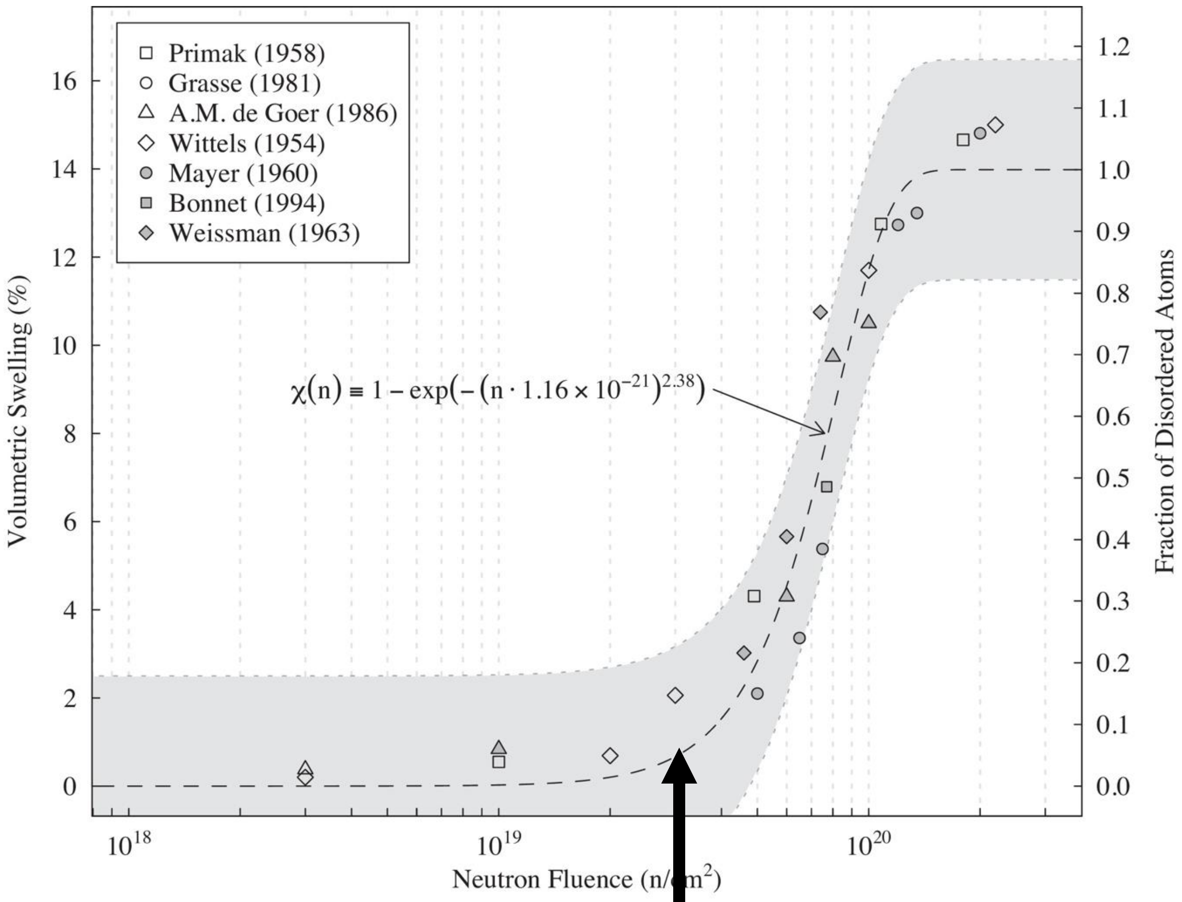
Irradiation-induced amorphization





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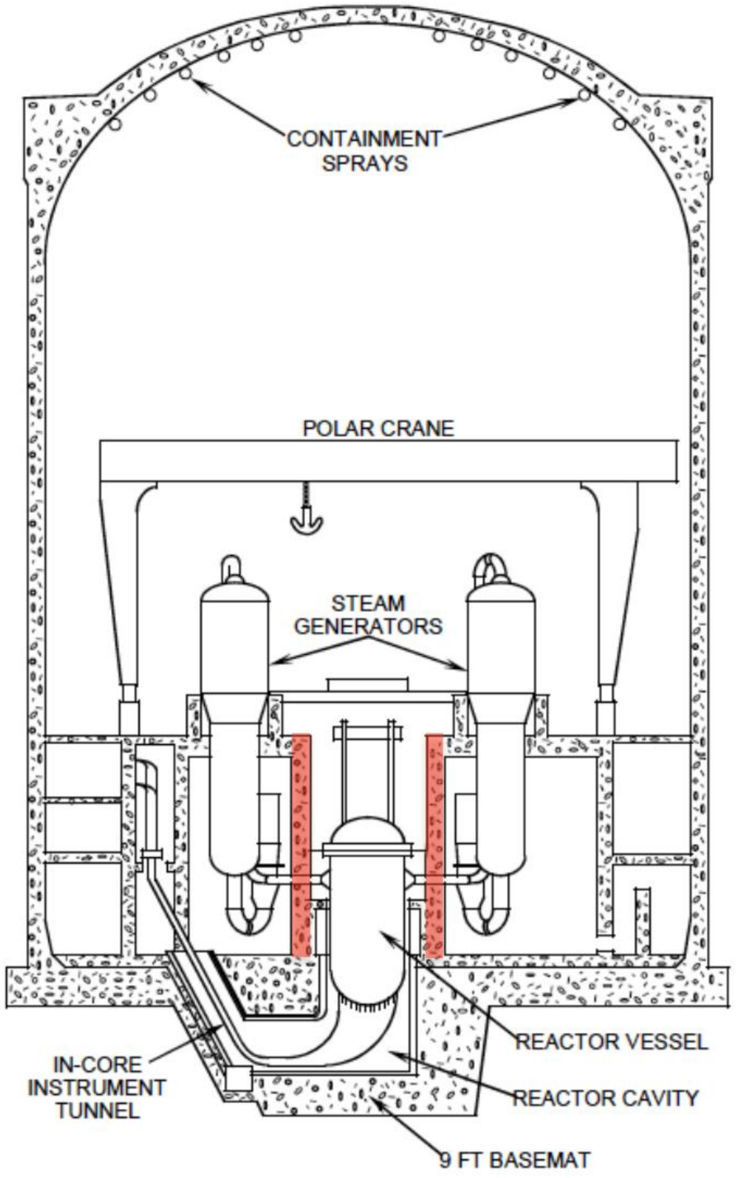
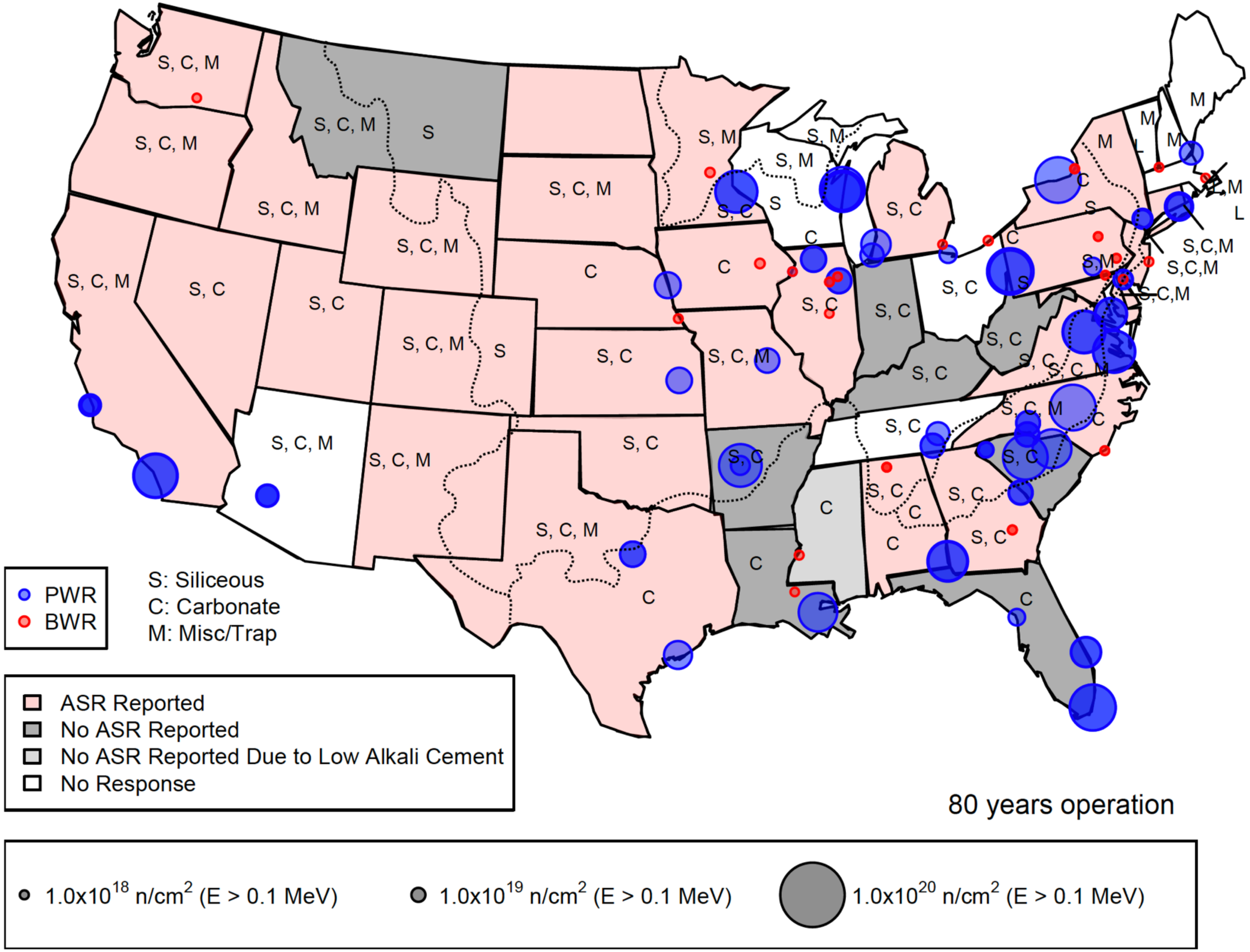
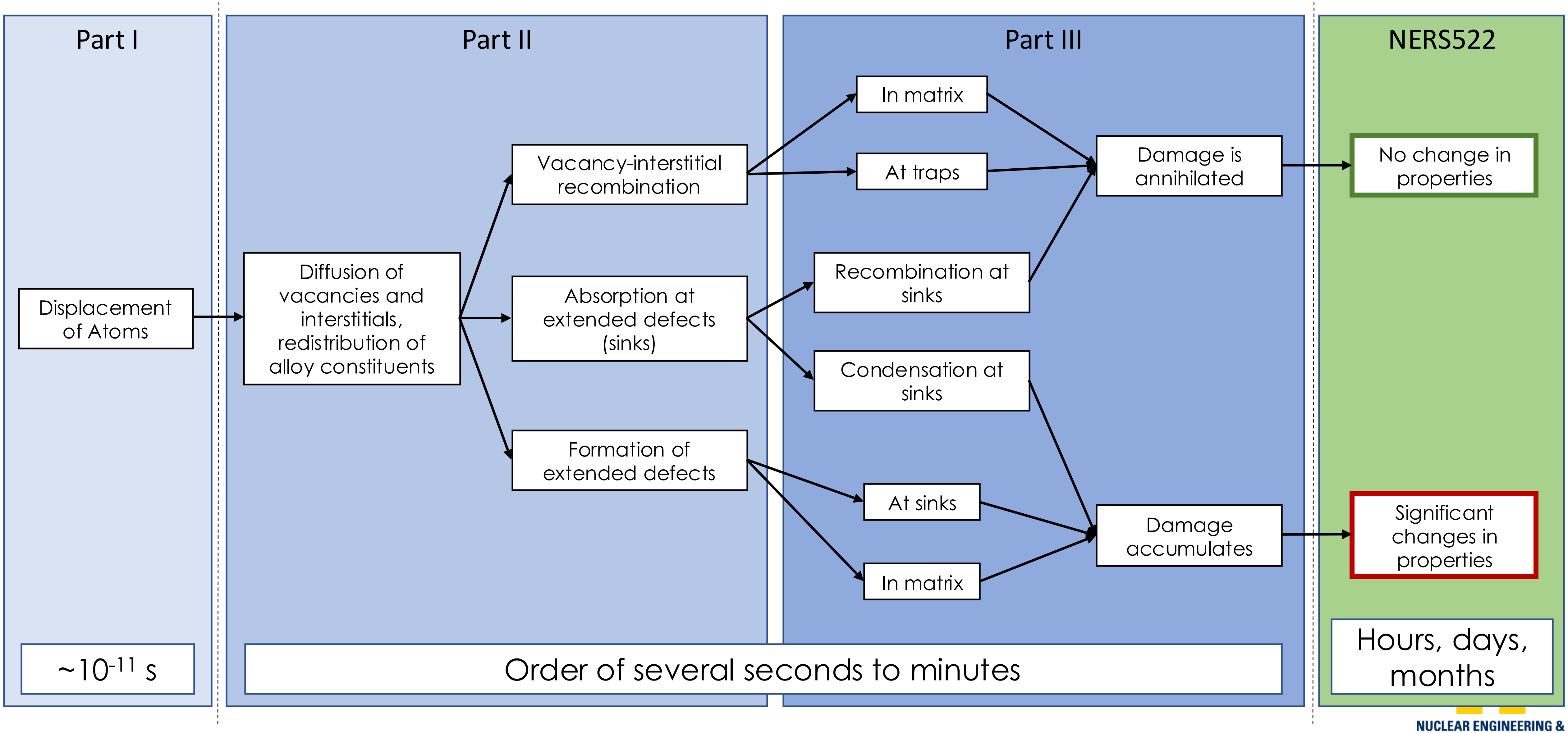
Irradiation-induced amorphization



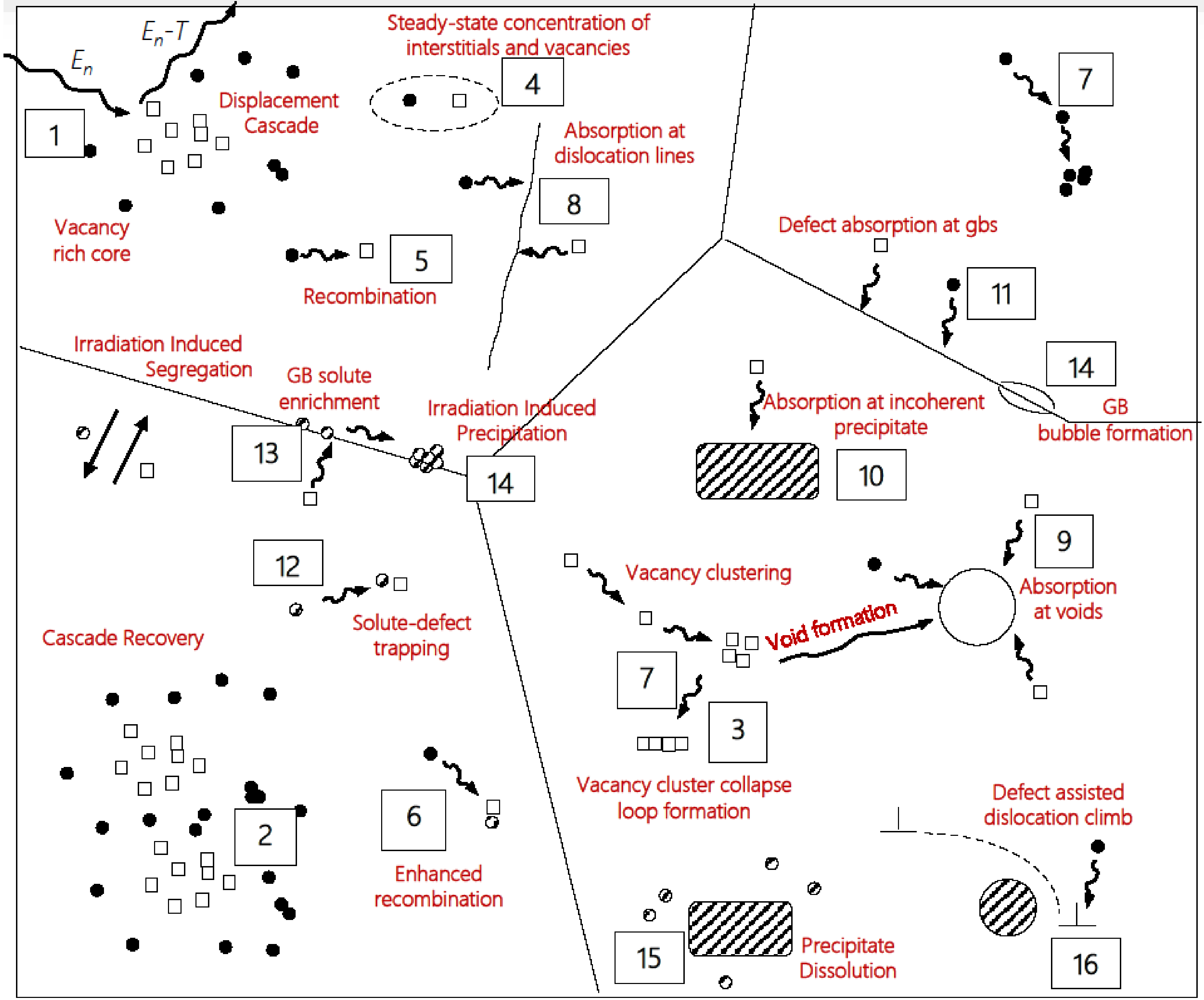


Flow chart for radiation damage



Louis Mansur, "Mechanisms & Kinetics of Radiation Effects in Metals and Alloys", in: Kinetics of Nonhomogeneous Processes, 1987

Putting it into a visual



What is the month, day, and year of the earliest recorded snowflakes in the state of Michigan history?

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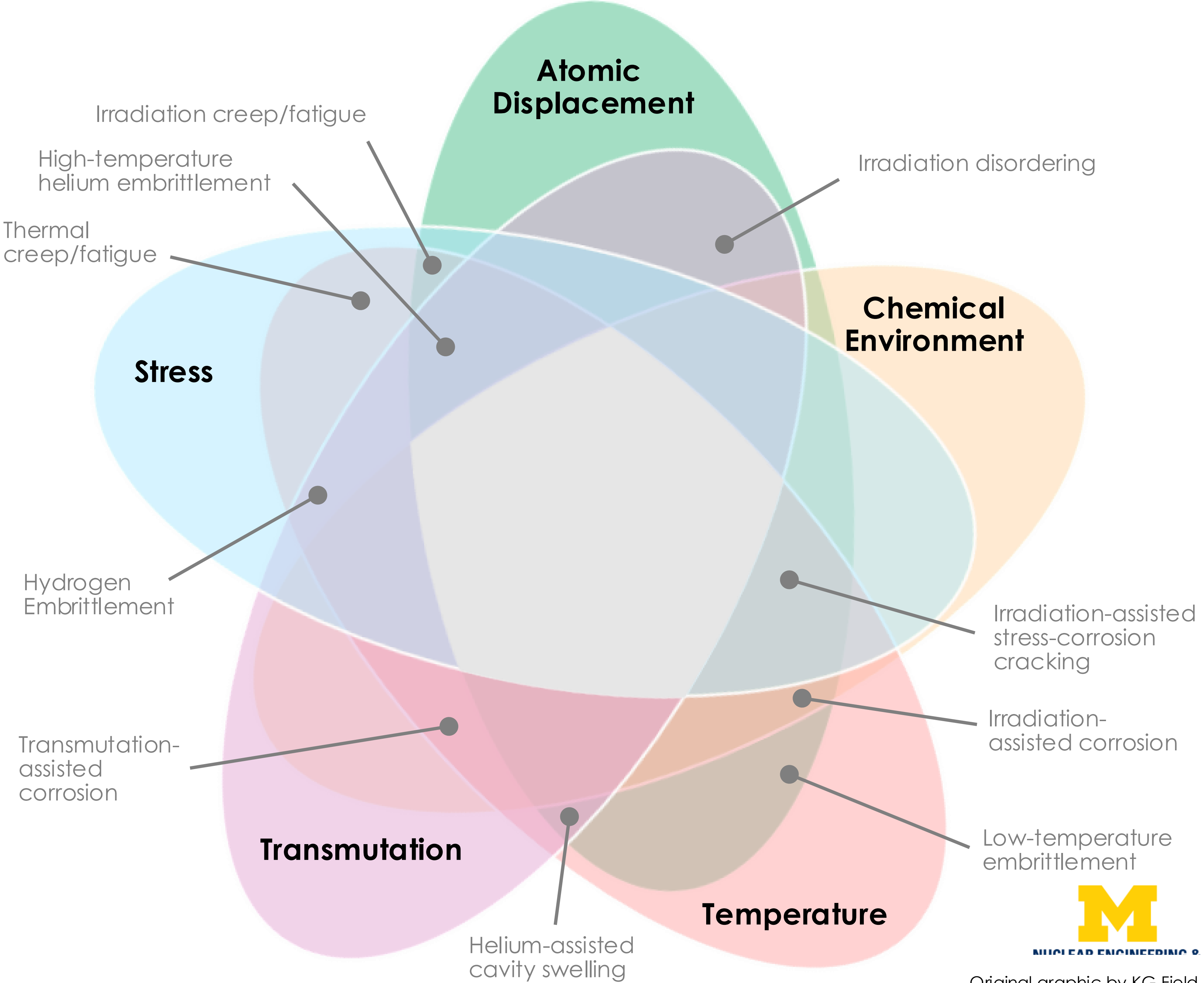
Applying the concepts of NERS521 to material design

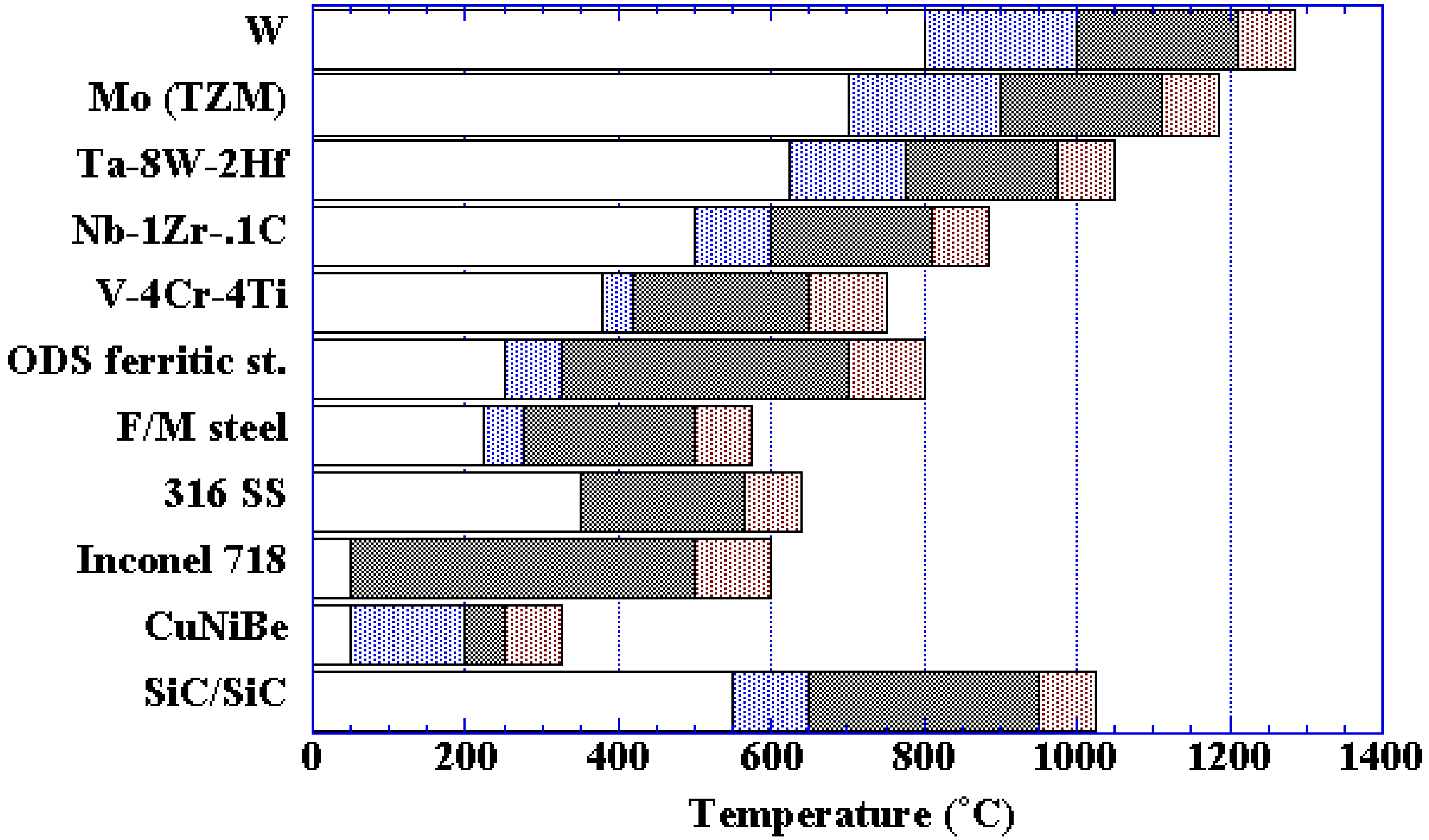
Materials degradation in a fusion and fission energy system can occur due to single- and ***combined-effects***

Listed degradation modes for structural materials



Original graphic by KG Field

Bringing it together: Radiation Materials Design



Zinkle and Ghoniem, Fusion Engr. Des. 49-50(2000) 709; S.J. Zinkle & J.T. Busby, Mater. Today 12(2009) 12

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Three options exist for designing radiation resistance materials

1. Use materials with negligible point defect mobility at desired operating temperatures
   - Slow down diffusion, but ideally want one defect type (e.g. vacancy/interstitial) mobile but the other not (to avoid amorphization/disordering)
2. Use materials with intrinsic resistance to radiation damage accumulation
   - Increased defect formation energies (e.g. stacking fault energies)
   - Examples: BCC alloys, high entropy/multicomponent alloys, nanocrystalline materials
3. Make materials with a high density of benign nanoscale recombination sites
   - Add microstructural features such as precipitates or nanolayered structures

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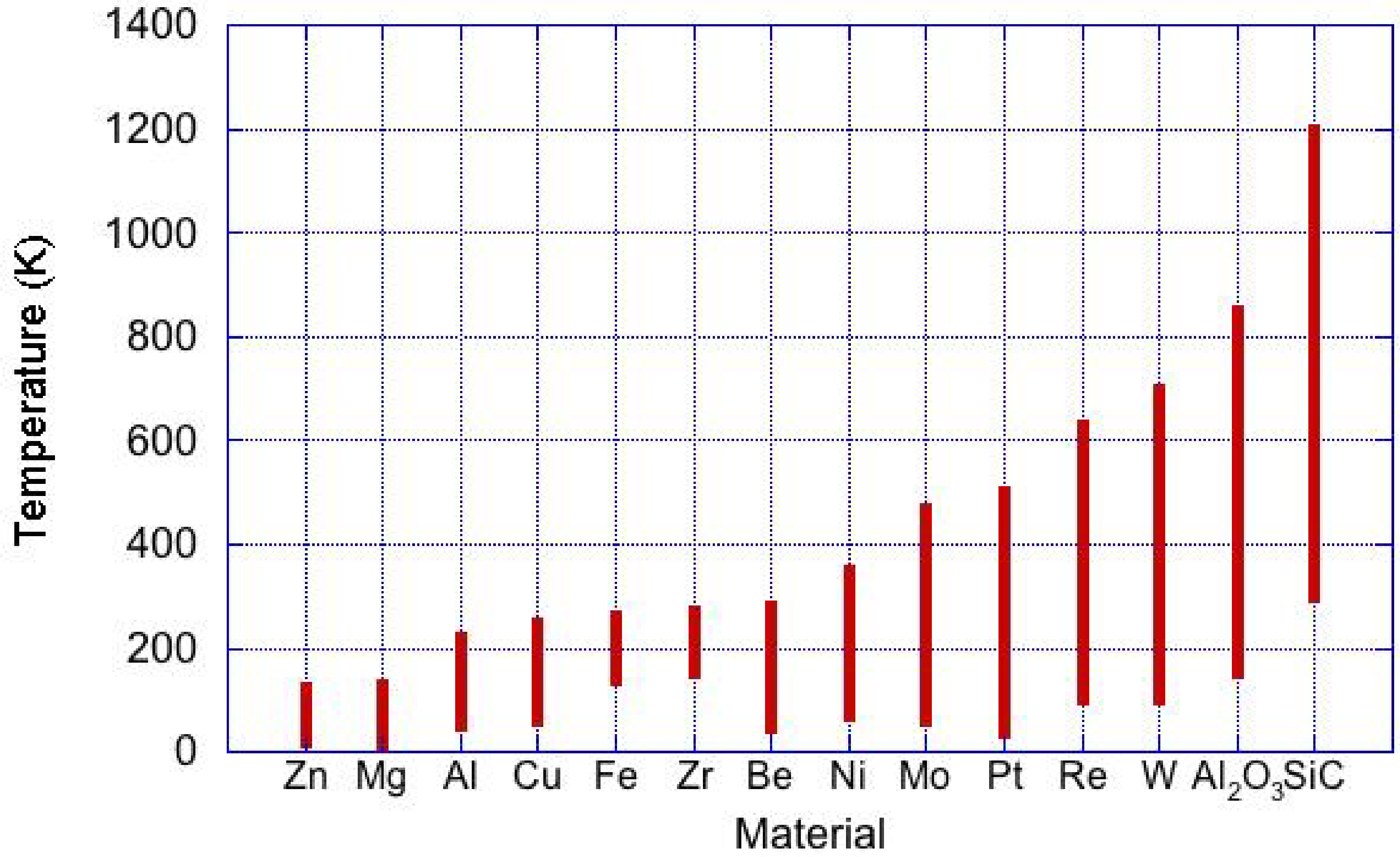
Design for Radiation Resistance I: Immobile point defects



Temperature regime where intrinsically high point defect recombination typically occurs

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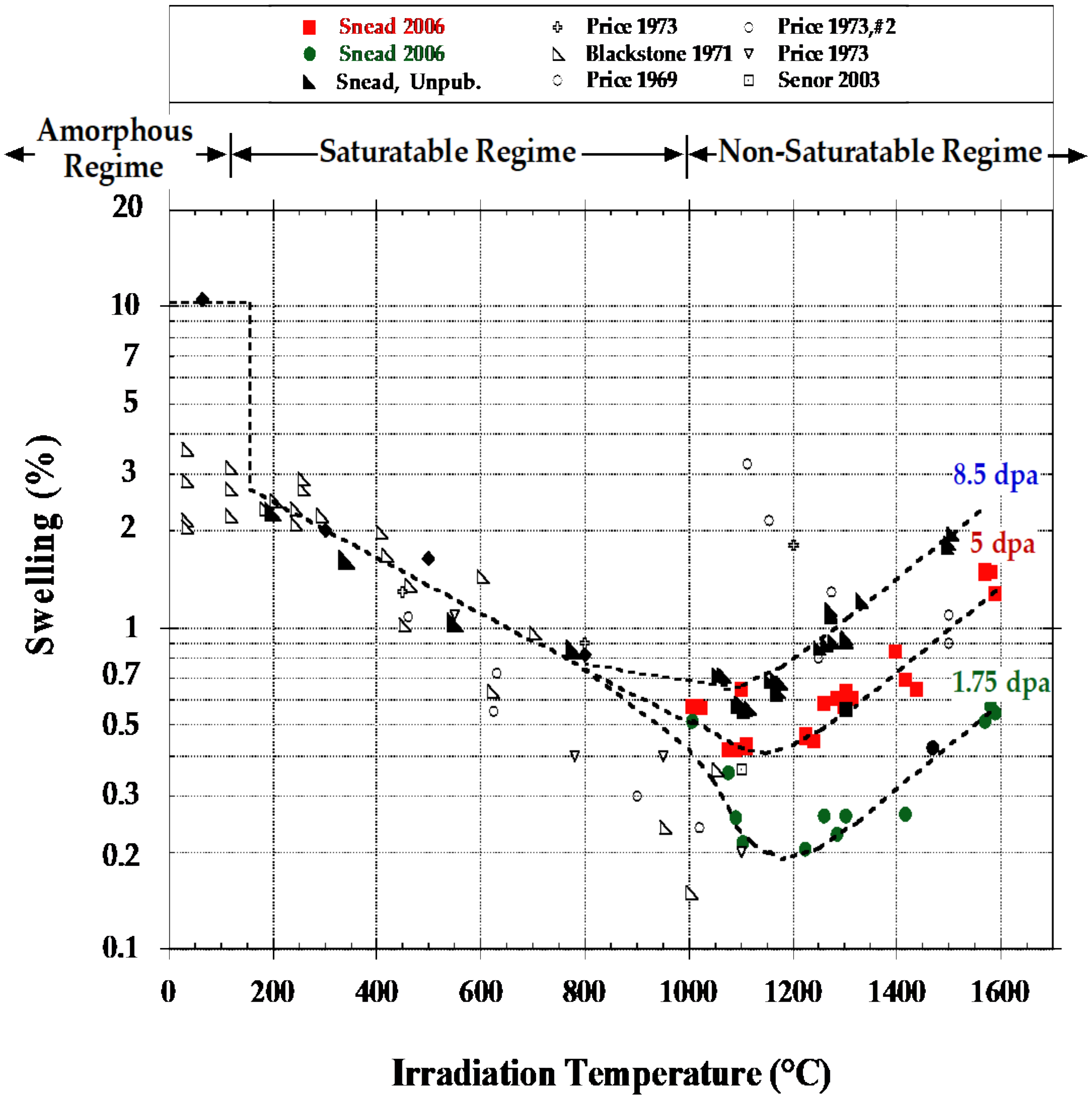

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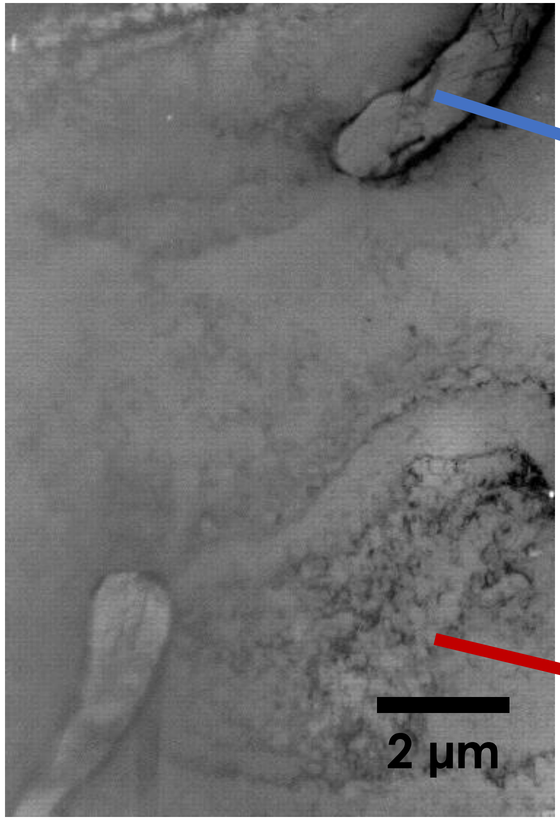
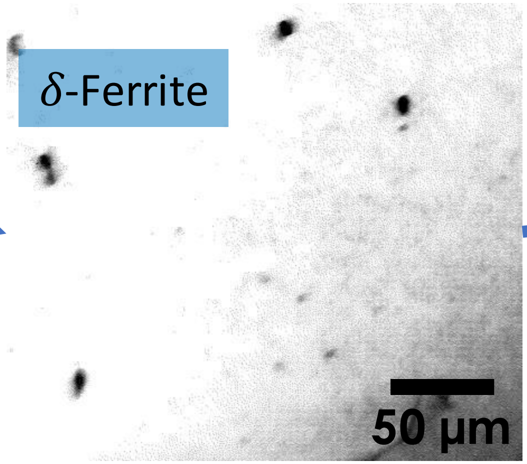
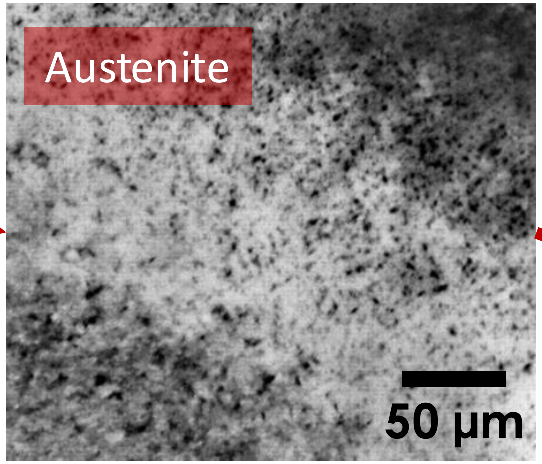
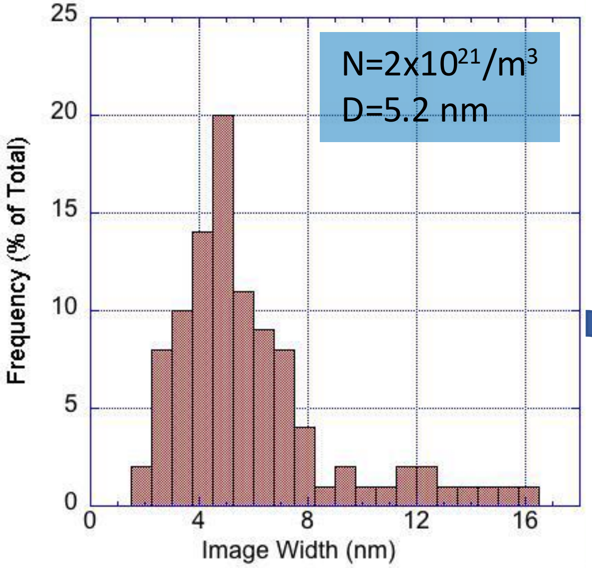
Design for Radiation Resistance II: Use radiation resistant phases

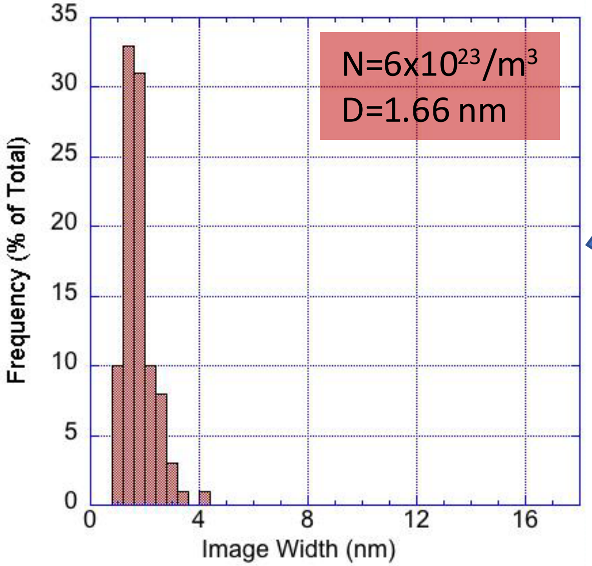


Type 308SS
0.065 dpa, 120°C









30x lower visible defect accumulation for BCC phase

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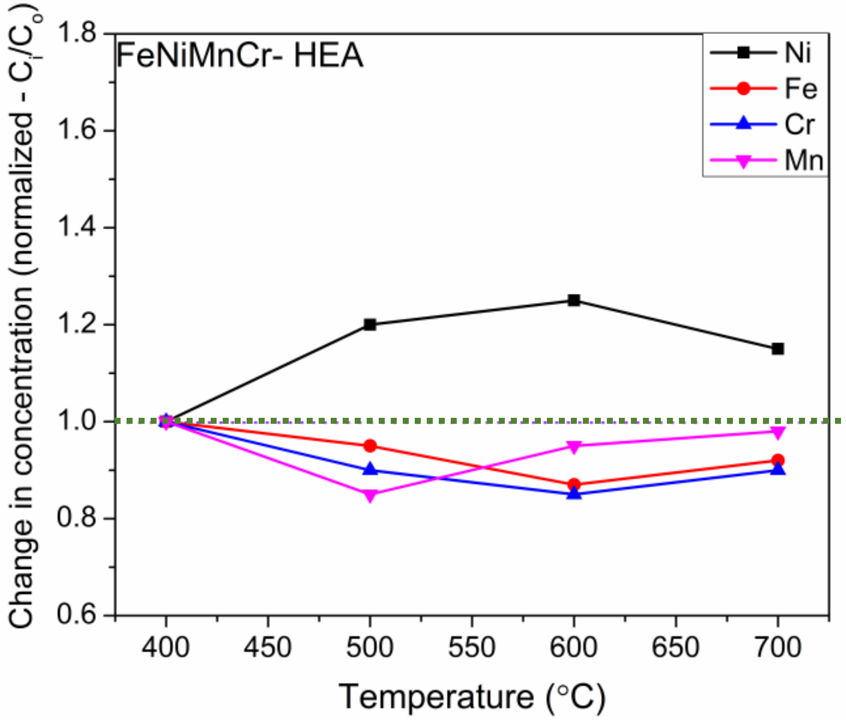
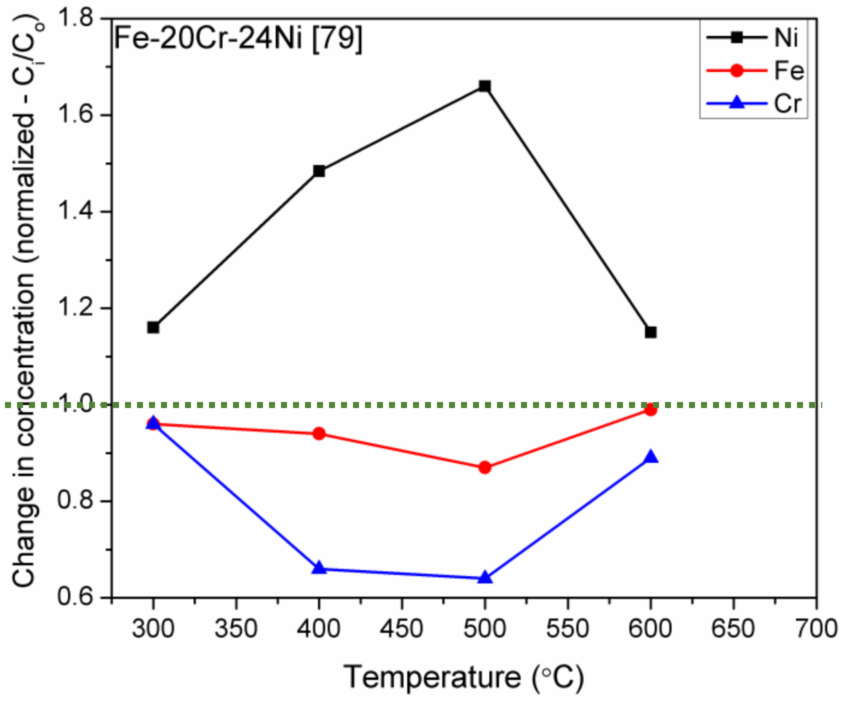
Design for Radiation Resistance II: Use radiation resistant phases





- RIS behavior for High Entropy Alloys is less pronounced than in traditional FCC FeCrNi(Mn) Alloys

=> HEA effect on solute diffusivities

N.A.P. KiranKumar et al., ActaMat. 113(2016) 230

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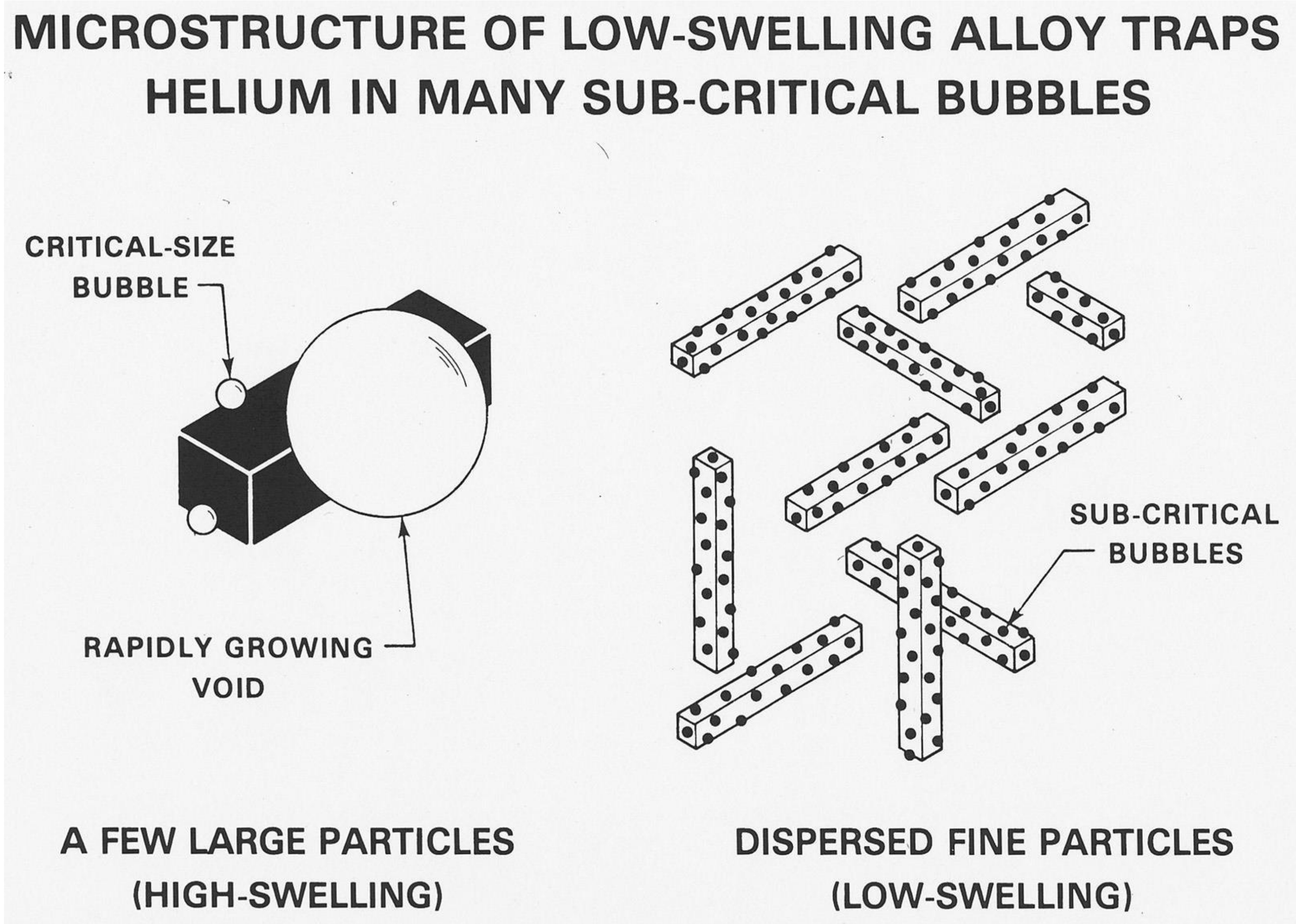
Design for Radiation Resistance III: High Sink Strength



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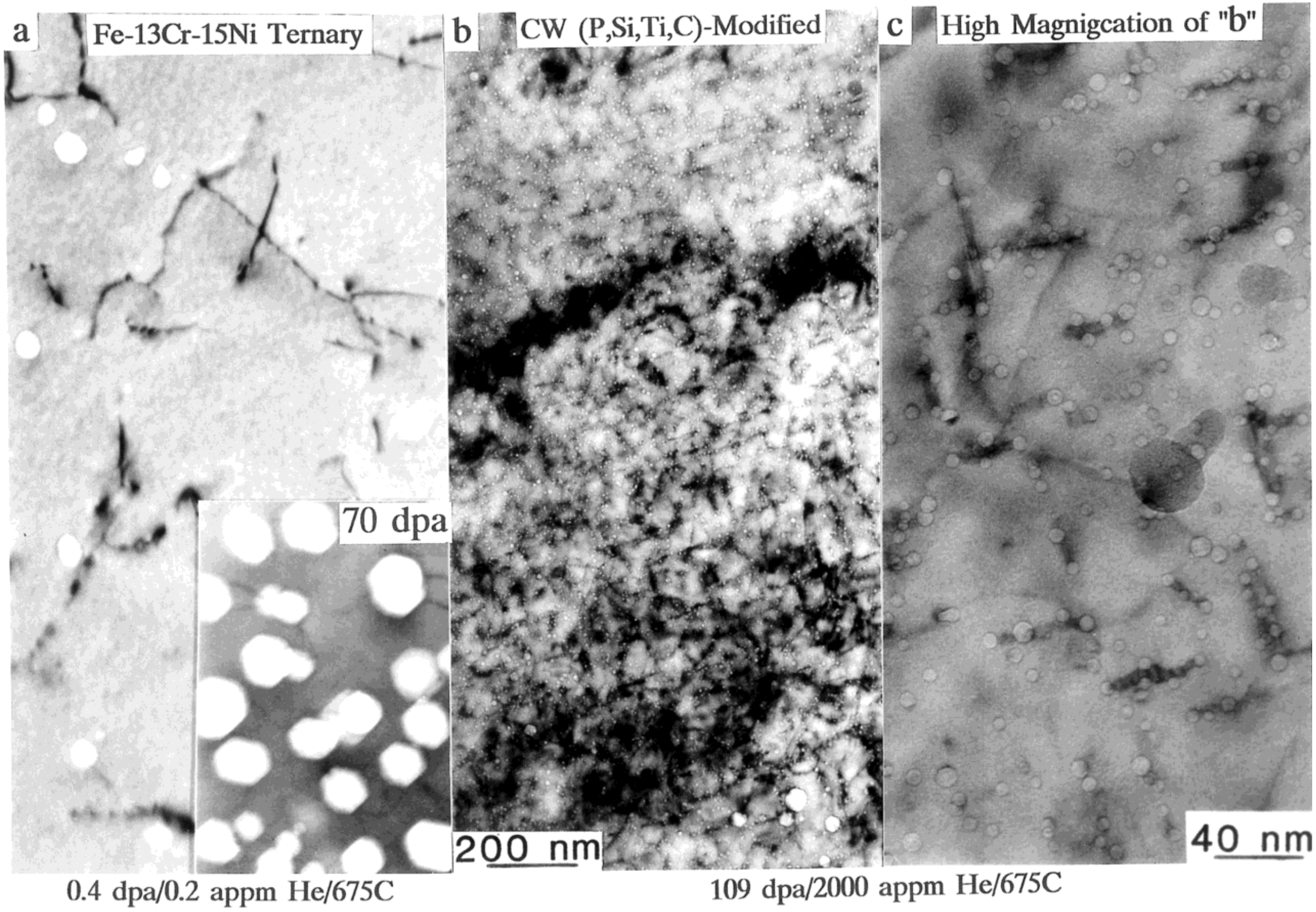

L.K. Mansur & E.H. Lee, J. Nucl. Mater. 179-181(1991) 105

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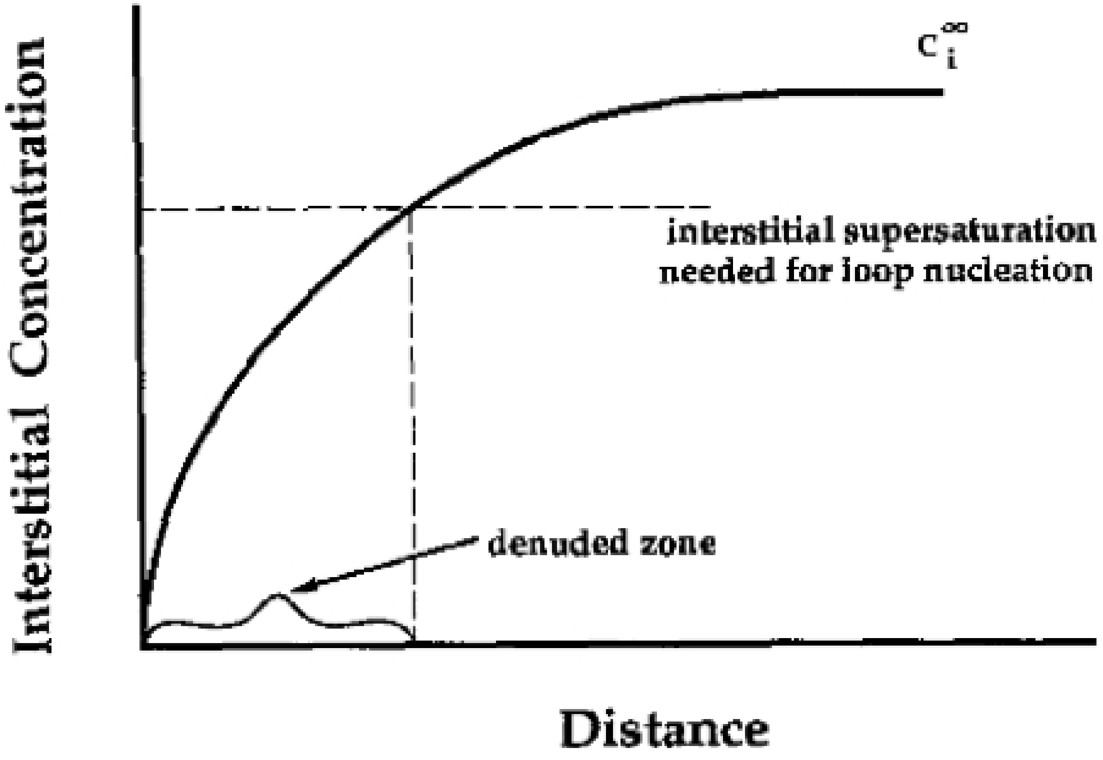
Design for Radiation Resistance III: High Sink Strength

- Early research also investigated fine grained architectures for radiation resistance, but sufficiently stable nanoscale grain boundaries were not discovered
  - Fine-grained materials are susceptible to radiation-enhanced grain growth



S.J. Zinkle, Nucl. Instr. Meth. B 91(1994)234

R. Yamada, S.J. Zinkle and G.P. Pells, J. Nucl. Mater. 209(1994) 191

L.K. Mansur & E.H. Lee, J. Nucl. Mater. 179-181(1991) 105

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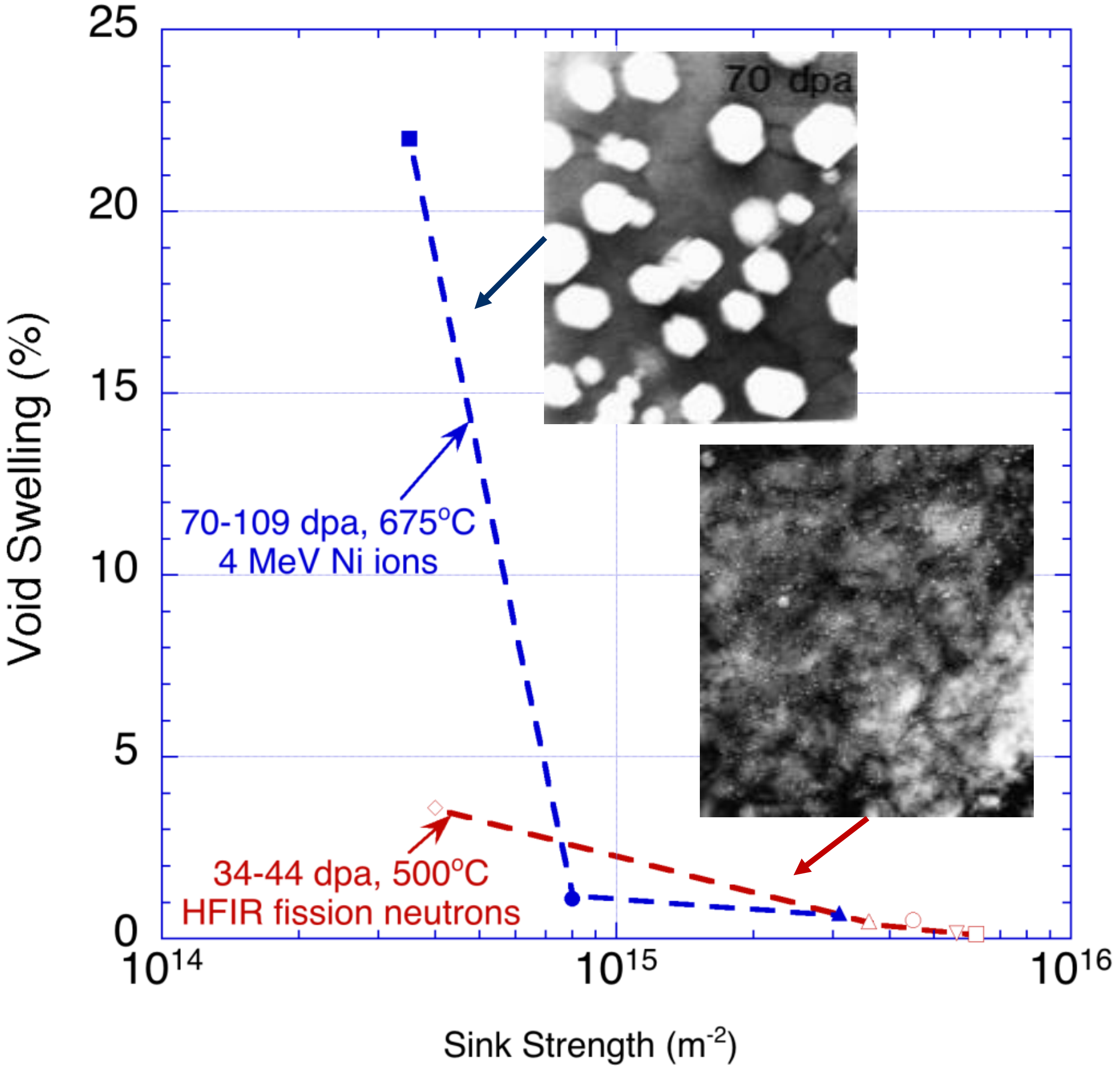
Design for Radiation Resistance III: High Sink Strength



Dramatic reduction in void swelling occurs when average spacing between voids is >10x average spacing between defect sinks

$$N_v^{-1/3} >> S_{tot}^{-1/2}$$

For void swelling resistance, sink strengths $>10^{15}/m^2$ are generally sufficient for fission reactors; fusion reactor irradiation may require even higher sink strengths ($>10^{16}/m^2$?) due to transmutant He production

S.J. Zinkle and L.L. Snead, Ann Rev. Mat. Res., 44(2014) 241; S.J. Zinkle et al., Nucl. Fusion (2017) 092005

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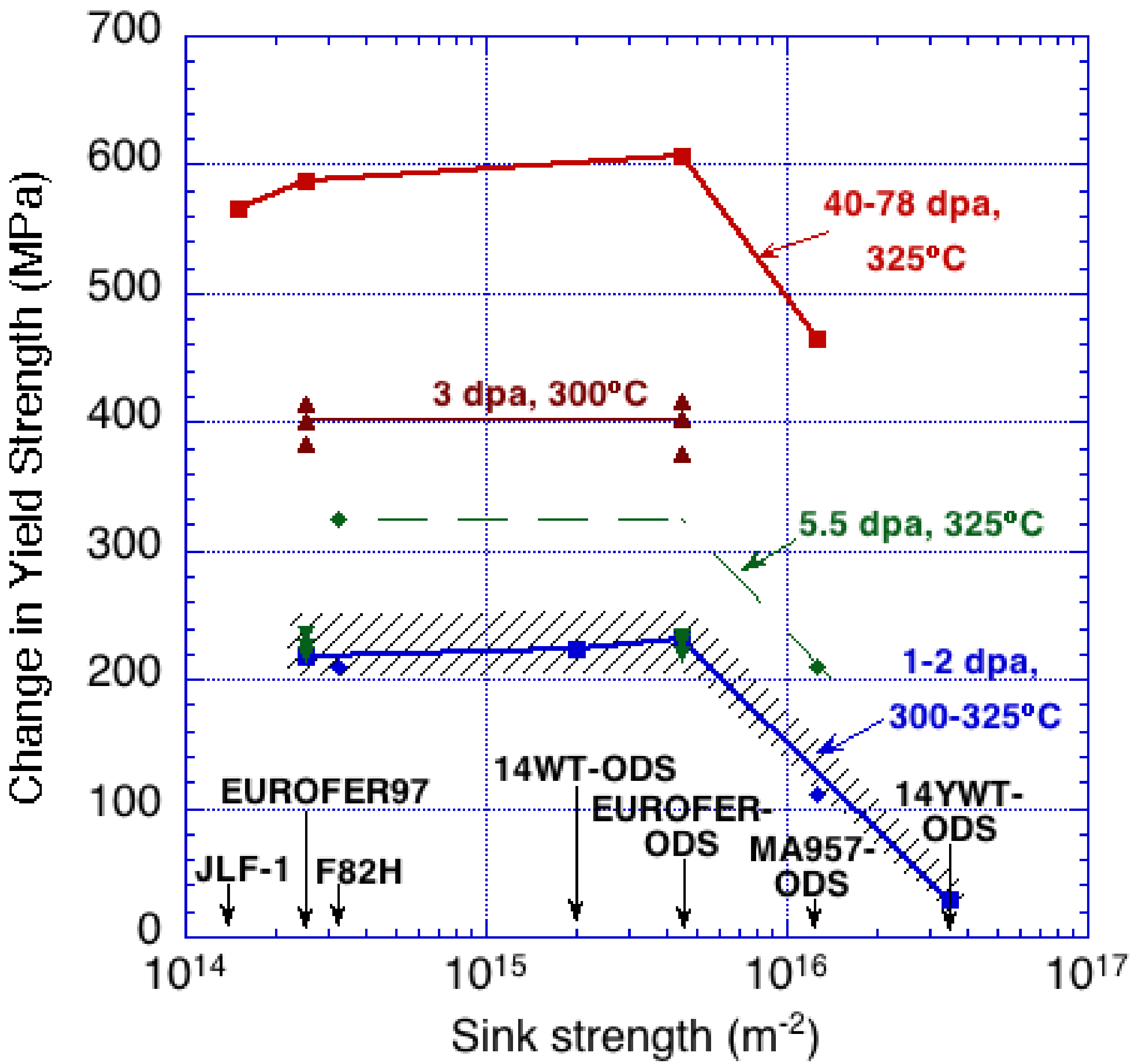
Design for Radiation Resistance III: High Sink Strength



Dramatic reduction in radiation hardening occurs when average spacing between defect cluster nuclei (dislocation loops, etc.) is much greater than average spacing between defect sinks

$N_{loop}^{-1/3} >> S_{tot}^{-1/2}$

-or-

$S_{tot} >> S_{rad\ defects}$

S.J. Zinkle and L.L. Snead, Ann Rev. Mat. Res., 44(2014) 241; S.J. Zinkle et al., Nucl. Fusion (2017) 092005

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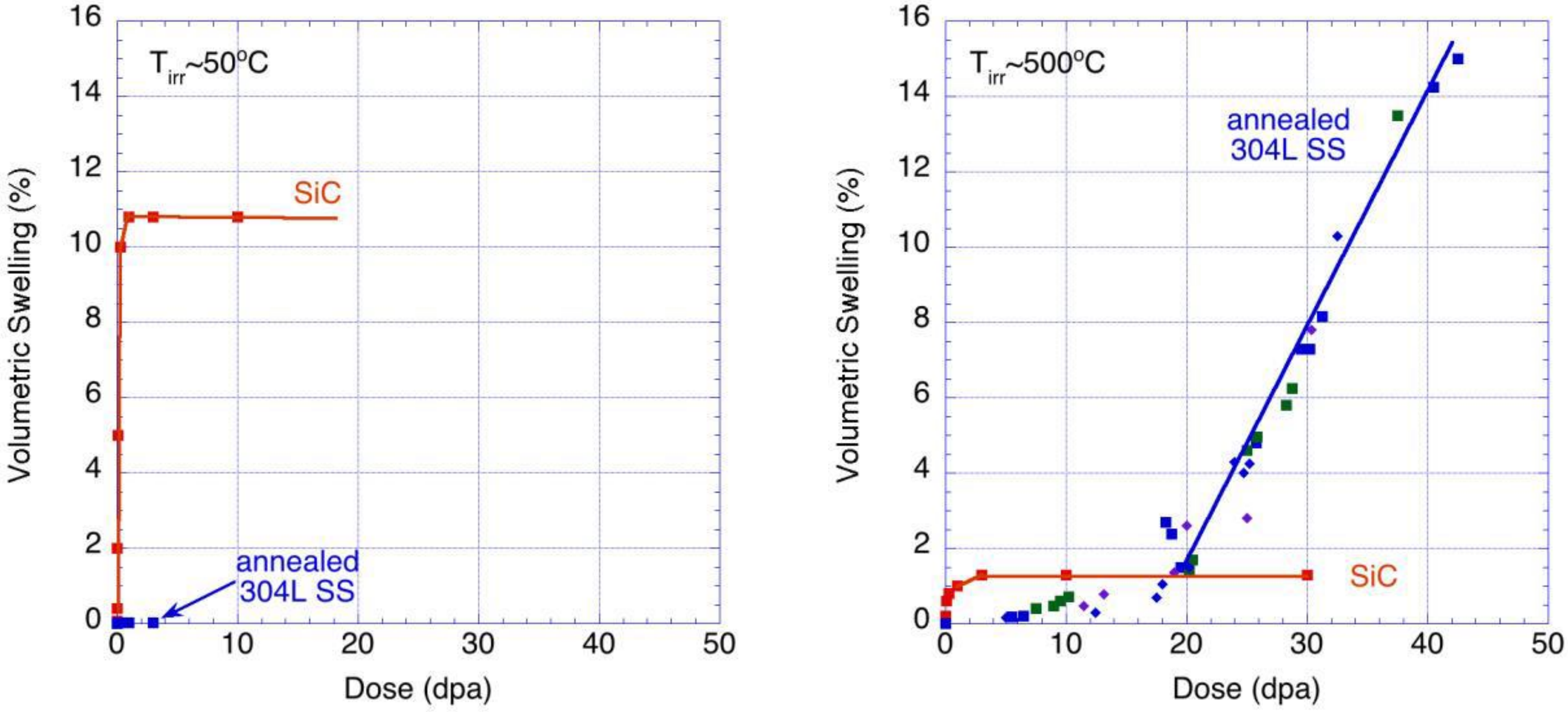
BUT, don't forget about irradiation regimes!



Swelling differences largely due to difference in melting temperatures (point defect mobility)

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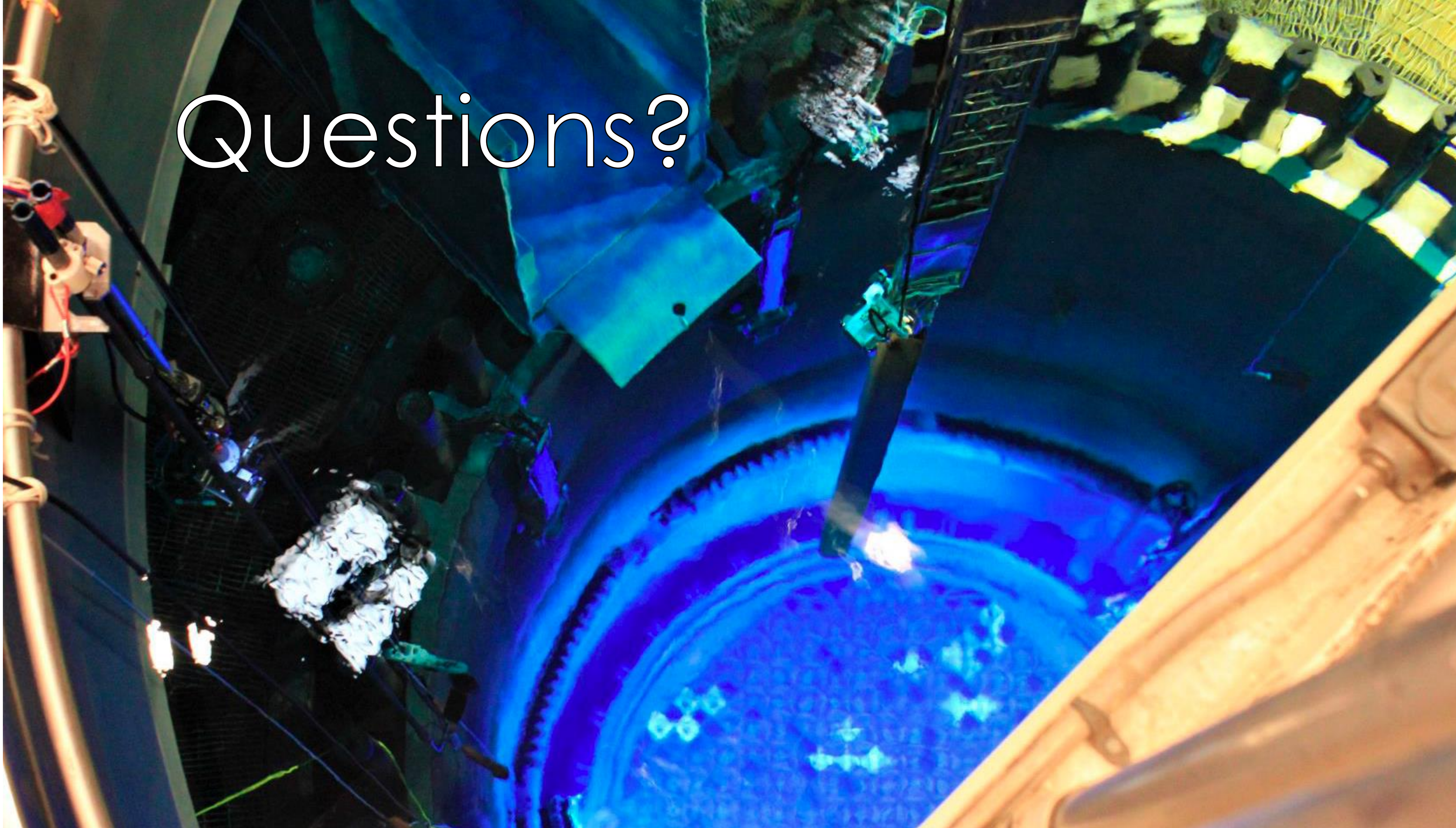
That's it!


Questions?