Phase Transformations

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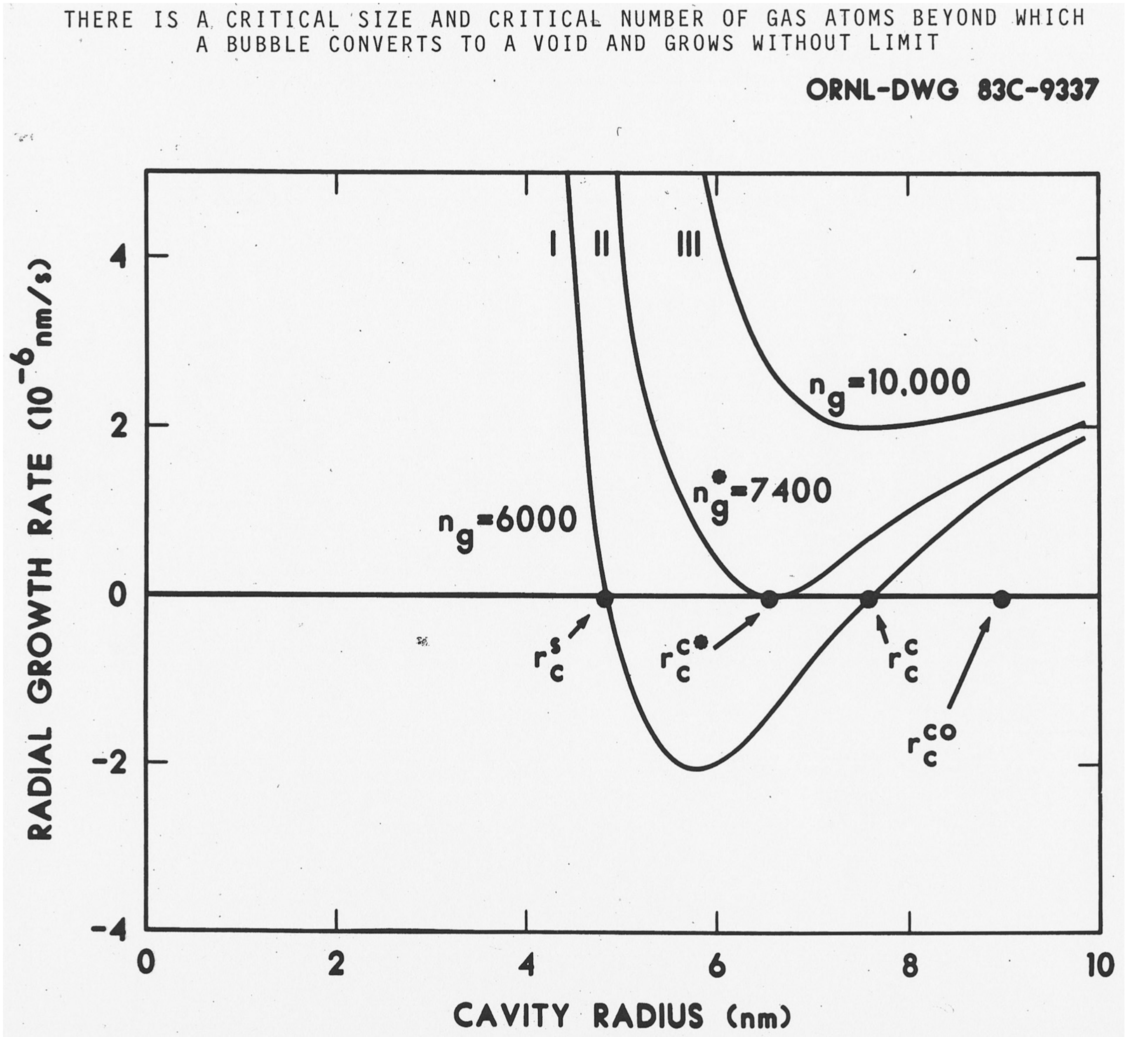
HW5

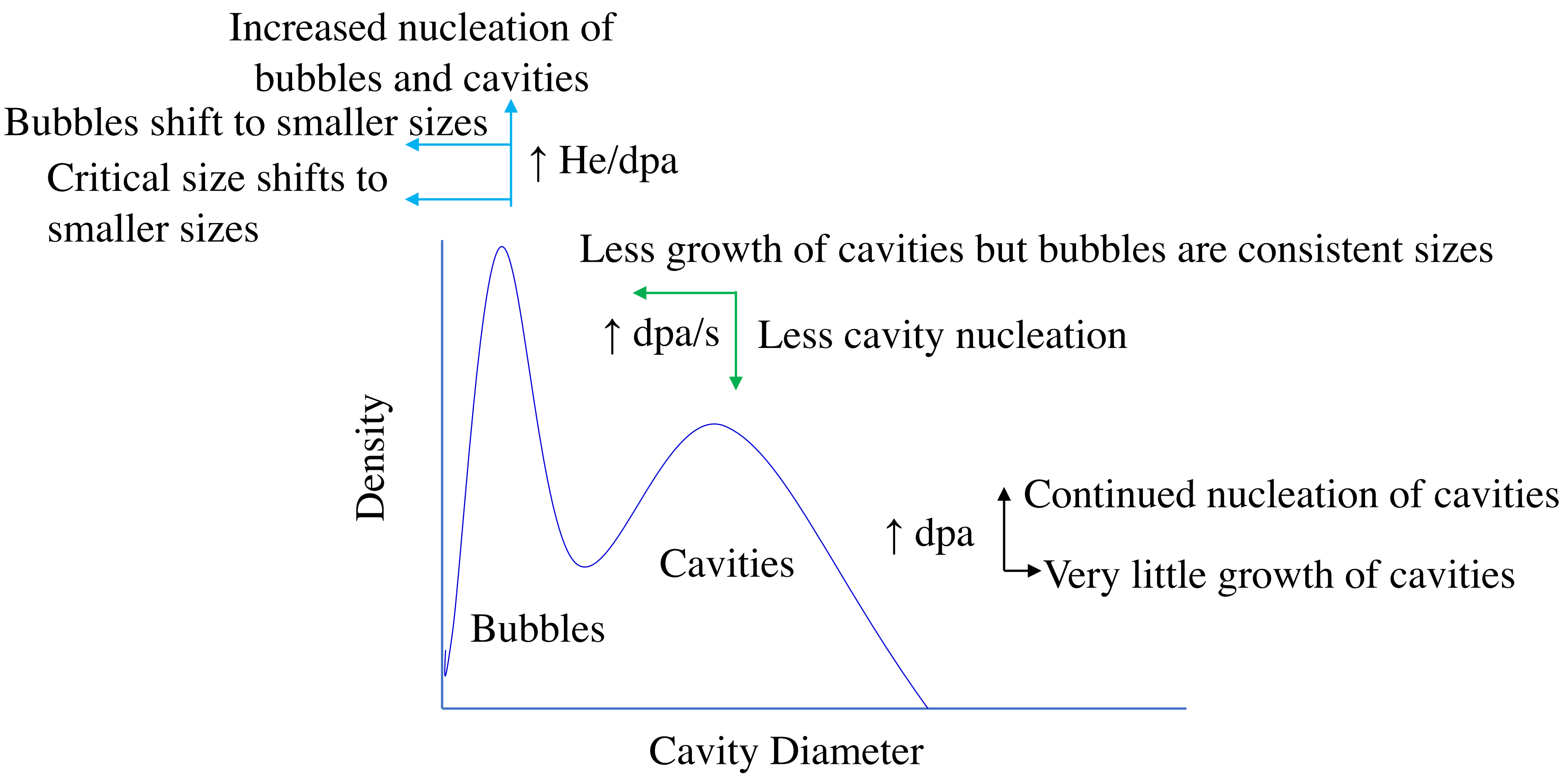
- Due tomorrow by 11:59 PM

Last Lecture

$$R\dot{R} = K_o\Omega\left(\frac{z_i - z_v}{z_v}\right)\frac{z_v\rho_d}{(4\pi R\rho_v + z_v\rho_d)^2}F(\eta) - \frac{D_v C_v^0 \Omega^2 z_v \rho_d}{kT(4\pi RN + z_v\rho_d)}\left(\frac{2\gamma}{R} - \frac{n_x kT}{{}^4\!/_3\,\pi R^3 - n_x B}\right)$$



Experimental examples



Fixed dpa/s – Variable He/dpa

Fixed He/dpa – Variable dpa/s

Increase in dpa for constant He/dpa and dpa/s

Taller (2019)

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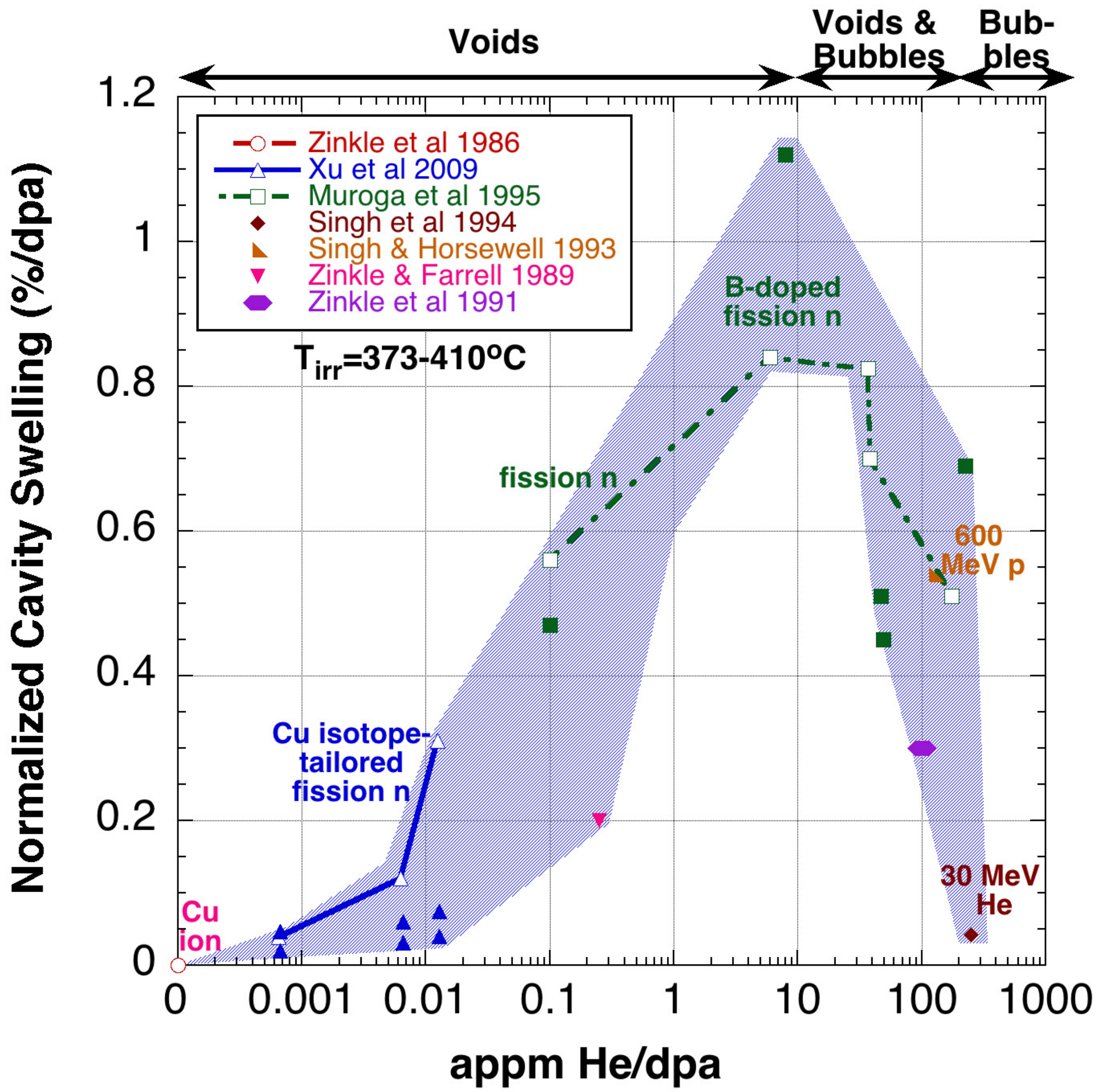
Cavity swelling vs. He/dpa ratio in irradiated copper



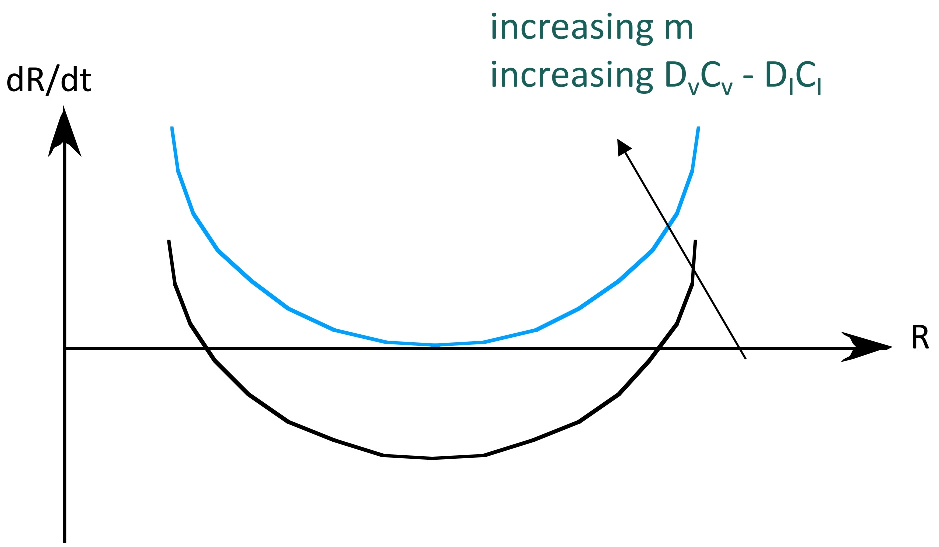
~1-10 dpa

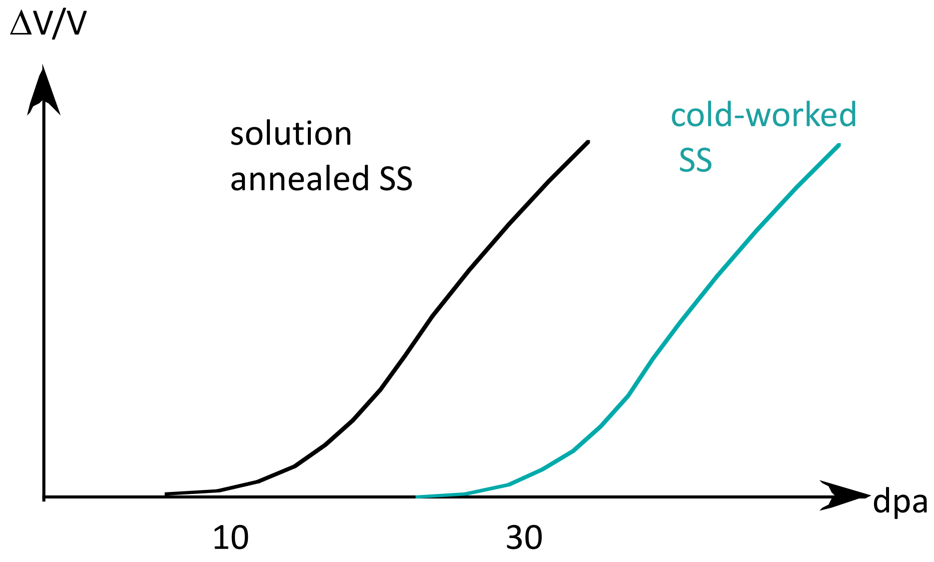
Remedies for void swelling?

Remedies for void swelling?

- Decrease D_vC_v - D_IC_I arriving at cavity;
- Eliminate He gas production (expensive or impractical)

- Reduce C_v, C_I:
  - increase recombination
    - add precipitates or dispersoids (TiC/TiO_2) to act as recombination sink, trap He and stabilize dislocations
  - increase other sink strengths
    - add dislocations (cold-work); generally only effective for low to moderate doses
    - introduce nanoscale grain boundaries





Why are we interested in phase transformations under irradiation?

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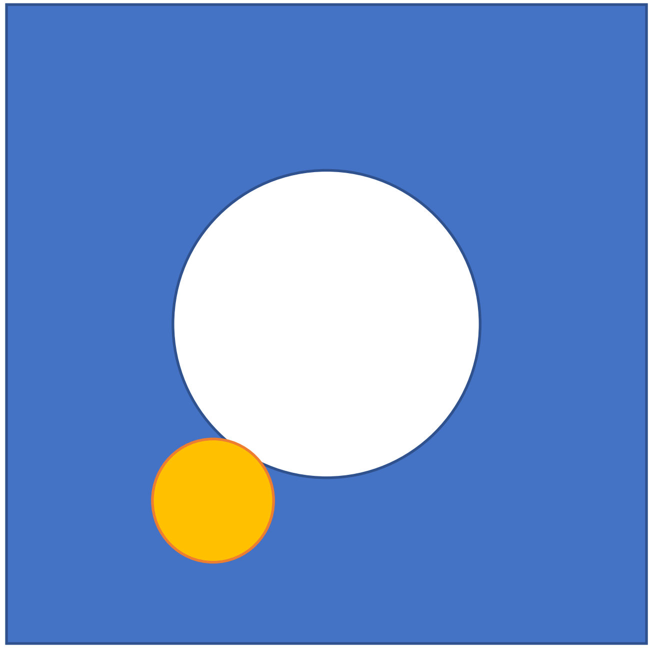
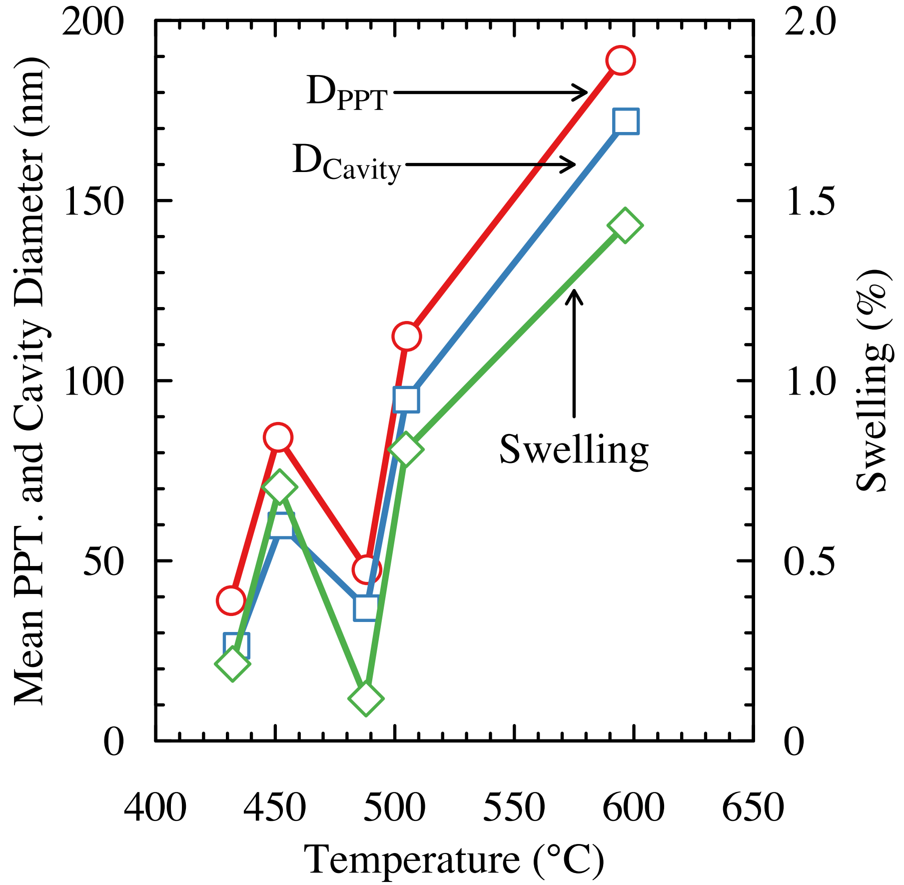
Influence of phase stability and cavity growth



If we account for cavity growth on a precipitate-matrix interface, then we can relate the **cavity growth to precipitate size** by:

$$\frac{dr_{cp}}{dr_c} = \frac{\left(r_{cp}^2 + r_p^2\right)^{1/2}}{r_{cp}^2} r_c$$



E.H. Lee et al. / Precipitation and cavity formation in austenitic stainless steels

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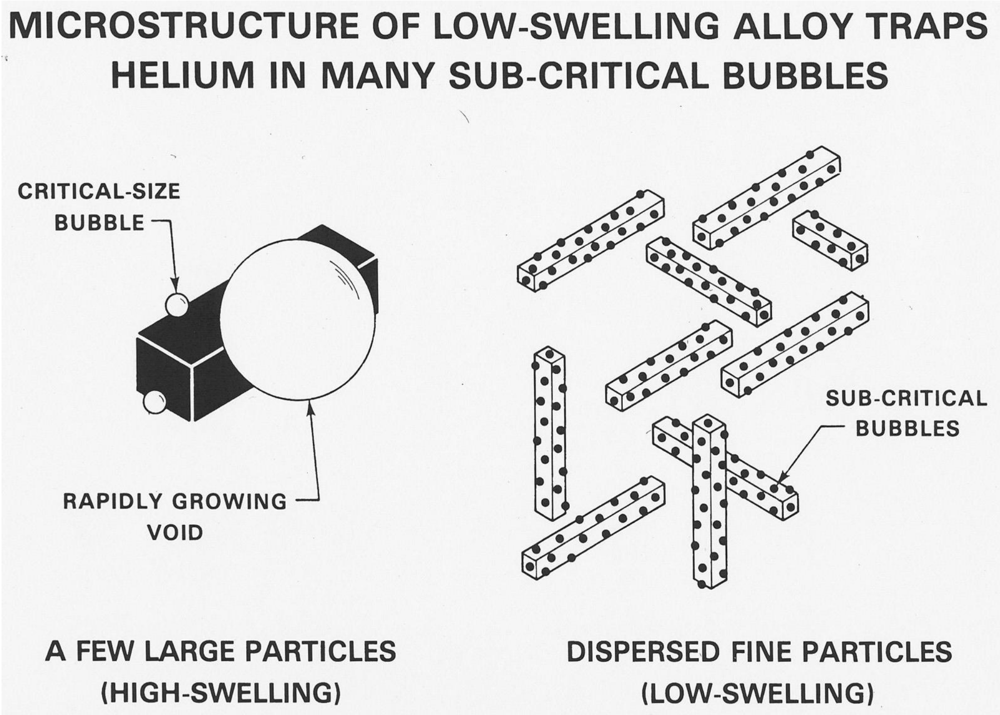
Influence of phase stability and cavity growth



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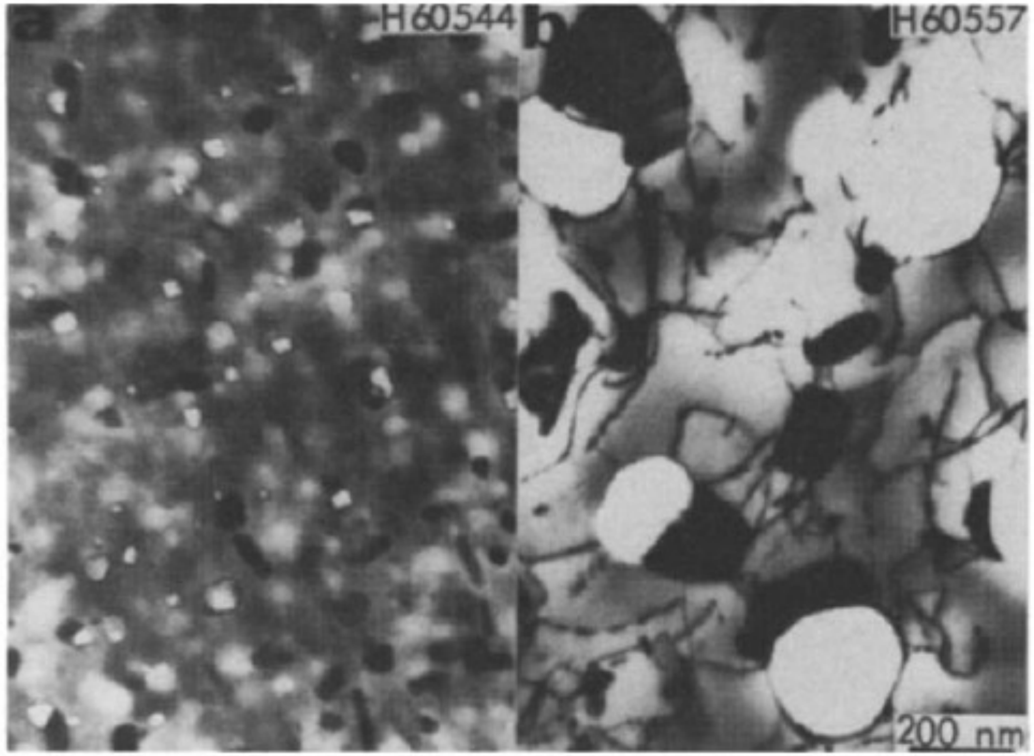

Fig. 2. Cavity-particle association in LS1C irradiated to ~35 dpa in EBR-II at (a) 425°C, (b) 600°C.

E.H. Lee et al. / Precipitation and cavity formation in austenitic stainless steels

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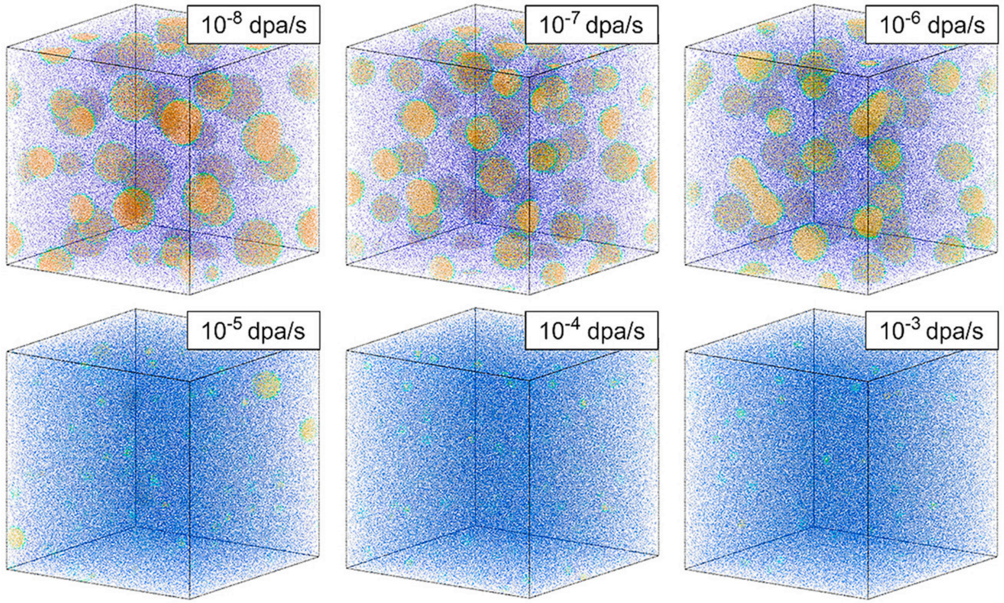
Lecture Break

- Beta carotene is a fat-soluble yellow pigment found in grass. When digested by cows, it ends up in the fat globules in the cow's milk and can be released during the cheesemaking process resulting in yellow cheese. How many C and how H atoms does a beta carotene molecule have?

Two primary irradiation induced phase transformation types:

1. Requires compositional changes
    1. Induced precipitation from solid solution
    2. Dissolution of precipitates
2. Constant composition
    - Allotropic or Polymorphic
        - Allotropic: change in the crystal structure of a single element
        - Polymorphic: change in the structure of an alloy or compound
    - Ordering/disordering
        - Loss of chemical order (disordering)
        - Loss of crystal structure, e.g. amorphization

Irradiation flux effect on α' precipitation in Fe-Cr



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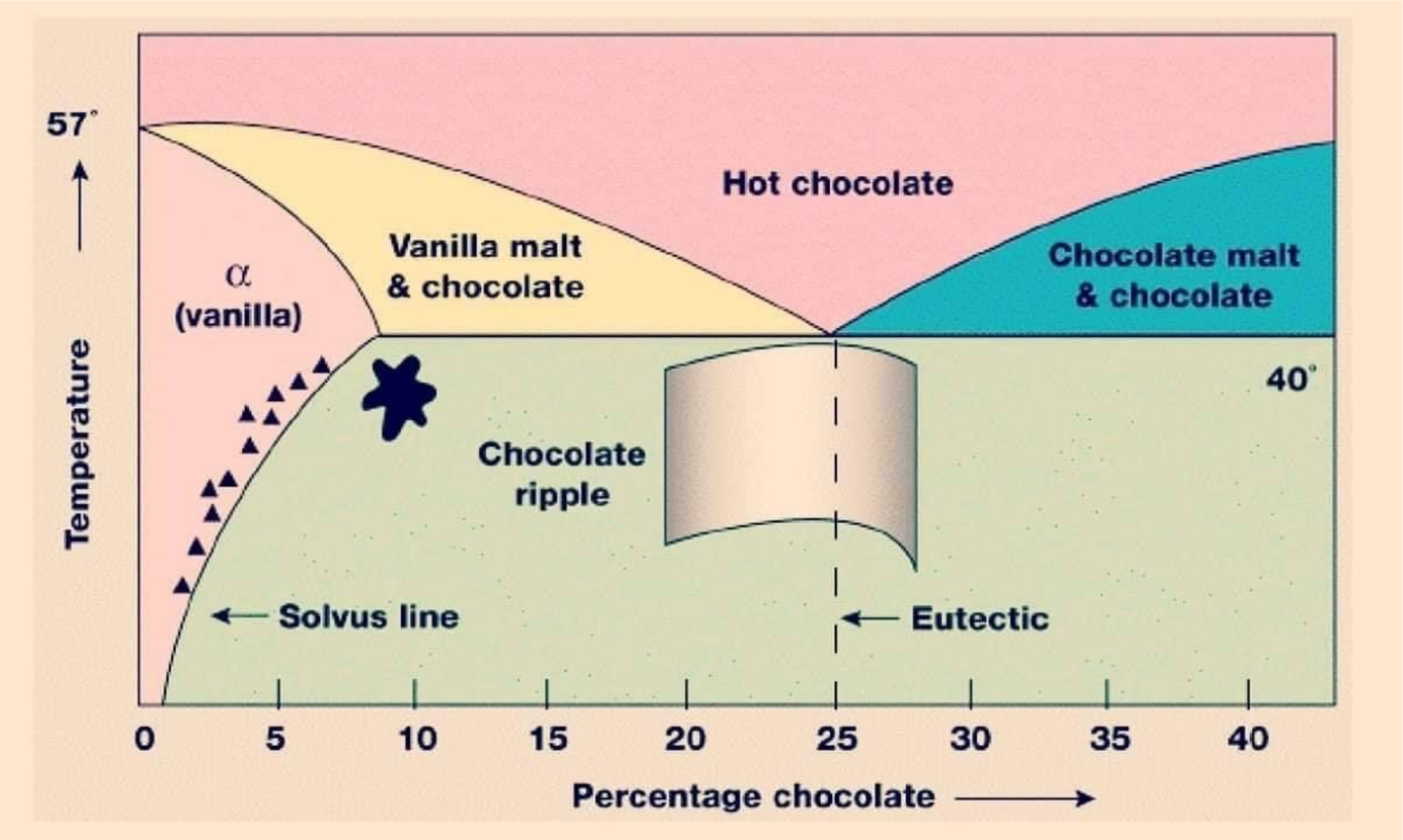
Phase transformations with changes in composition

Food for thought



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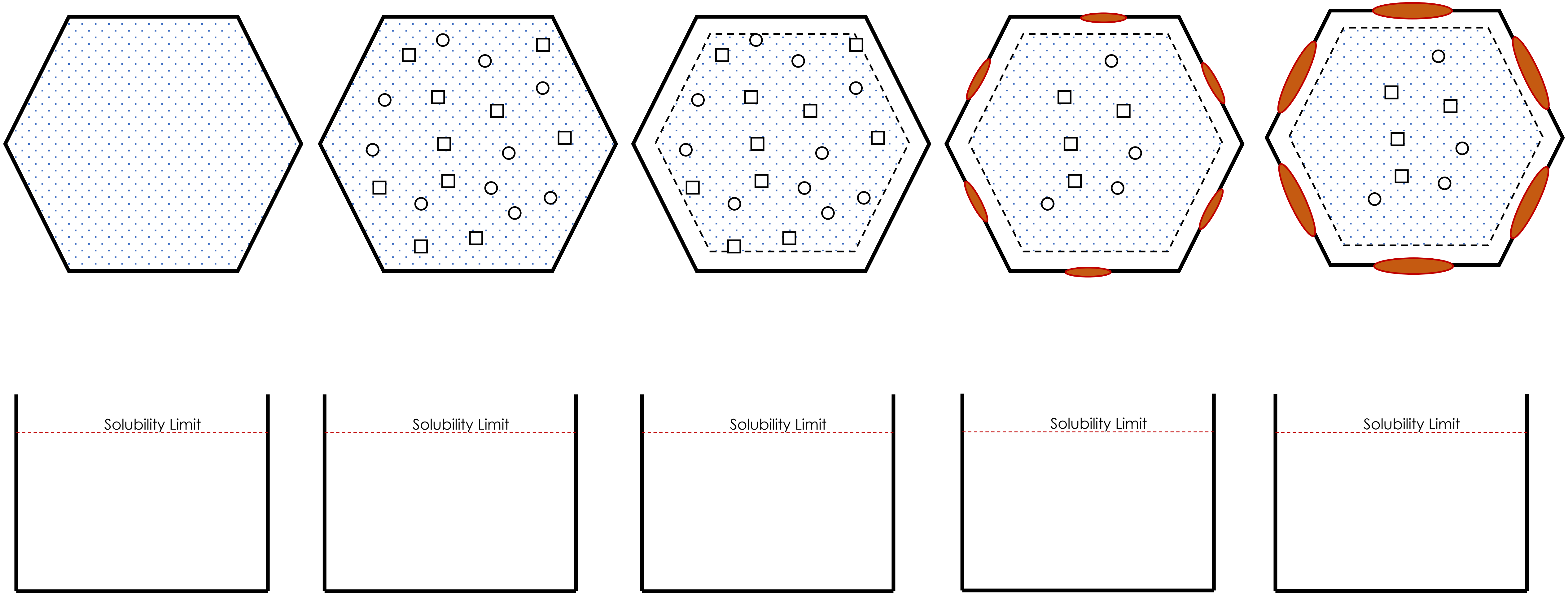
RIS and Radiation-induced precipitation



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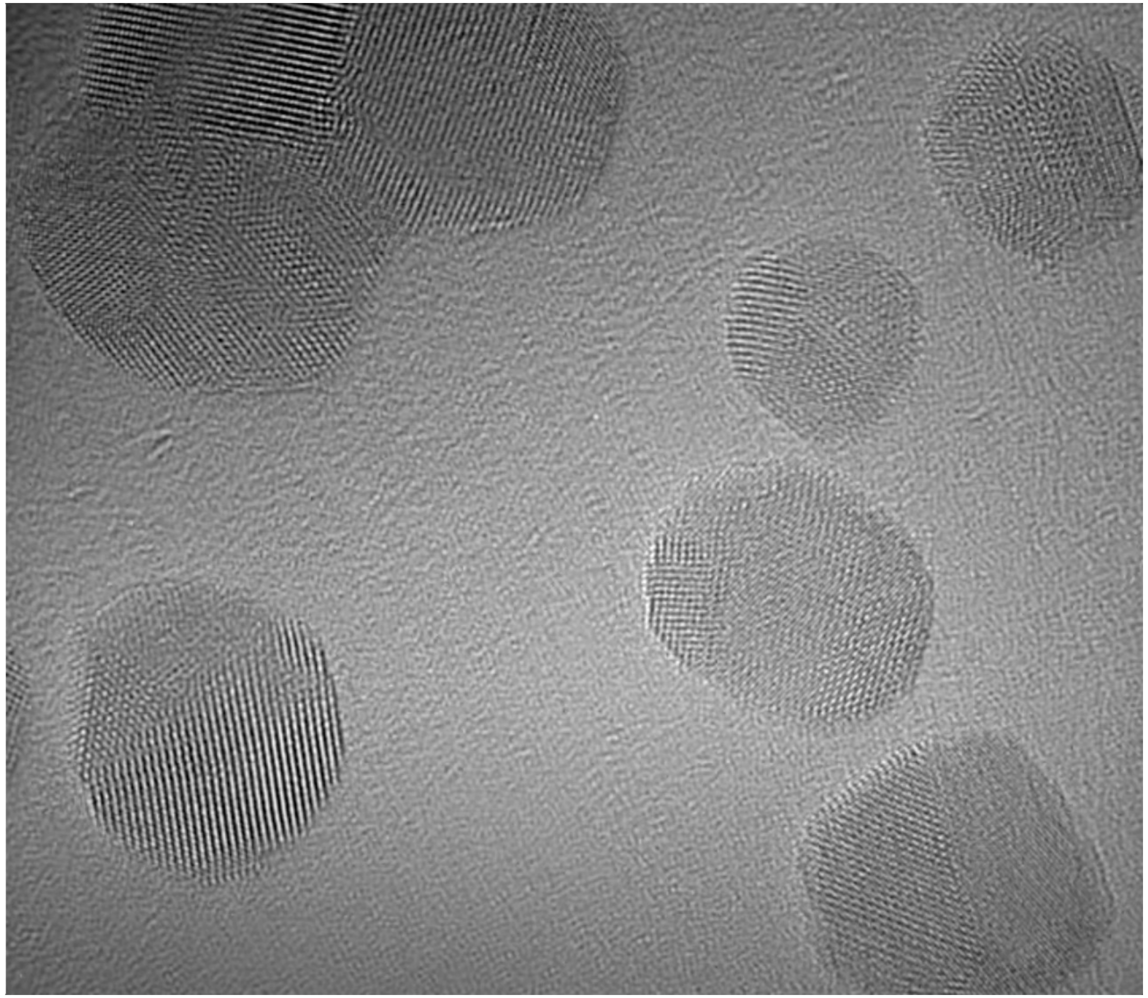
Ostwald Ripening

- Ostwald ripening is the spontaneous process of larger precipitates growing at the expense of small precipitates
- This is because:
  - Large precipitates have lower energy states
  - The formation of small precipitates is kinetically favored (in thermal systems)
  - Small precipitates have a larger surface area to volume ratio

→ **Small precipitates will attain a lower energy by being consumed by larger precipitates**



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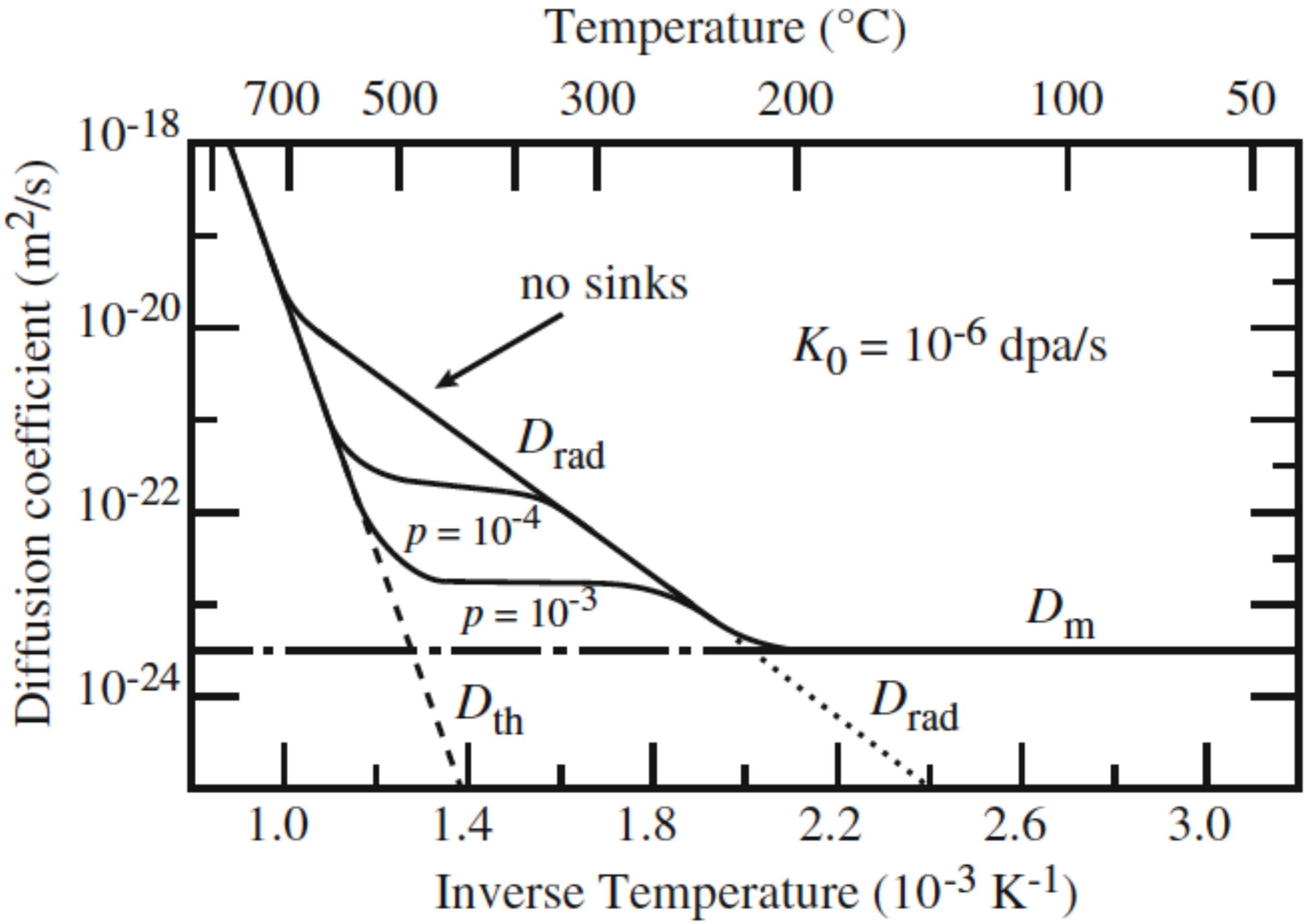
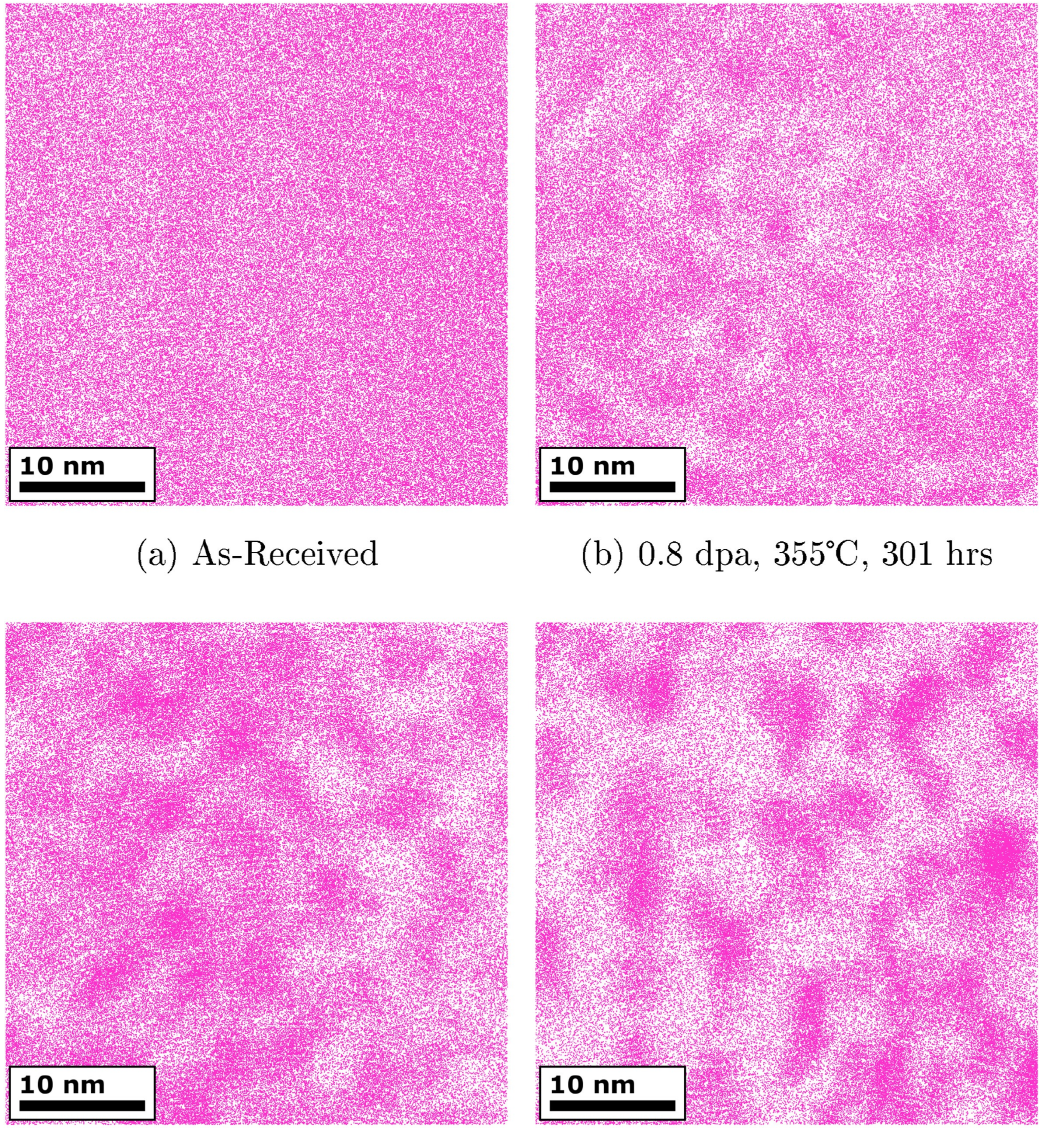
Radiation-enhanced effects on kinetics

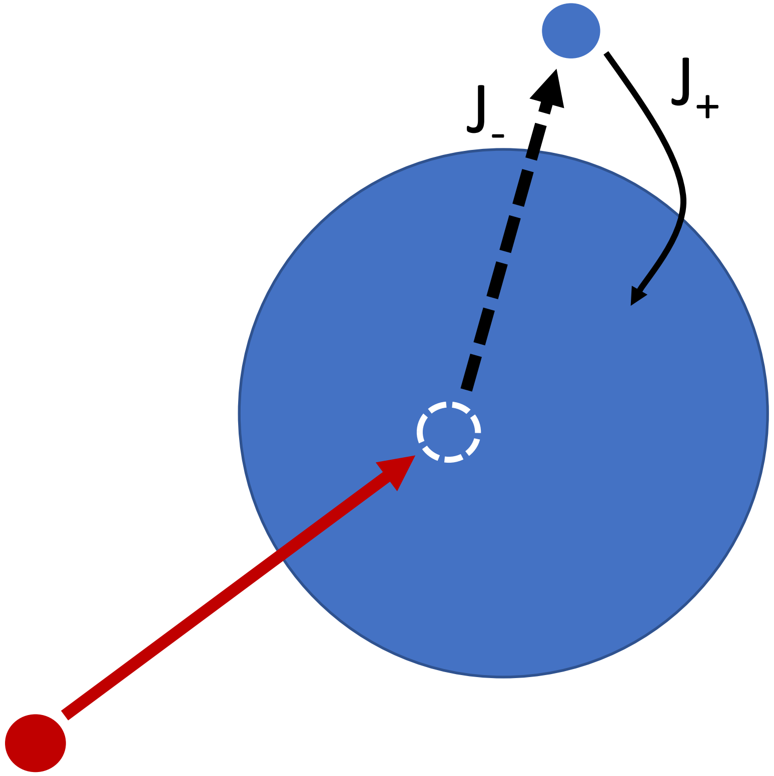




(a) As-Received (b) 0.8 dpa, 355°C, 301 hrs

(c) 1.8 dpa, 380°C, 614 hrs (d) 7.0 dpa, 320°C, 2456 hrs

Radiation-induced precipitate dissolution



Assumptions:

- Binary (simple) alloy
- Overall solute concentration: x_s
- Precipitates are evenly distributed
- Precipitates do not interact

Growth or dissolution of the precipitates will be governed by the solute flux at the precipitate interface:

$$dn/dt = J_+ - J_-$$

Radiation-induced precipitate dissolution

$$r_{eq}^3 = \frac{3}{4\pi N_p}\left(\frac{X_s}{C_p} - \frac{K_0\mu}{4}[1 - X_s]\frac{r_{eq}}{D_s}\right)$$

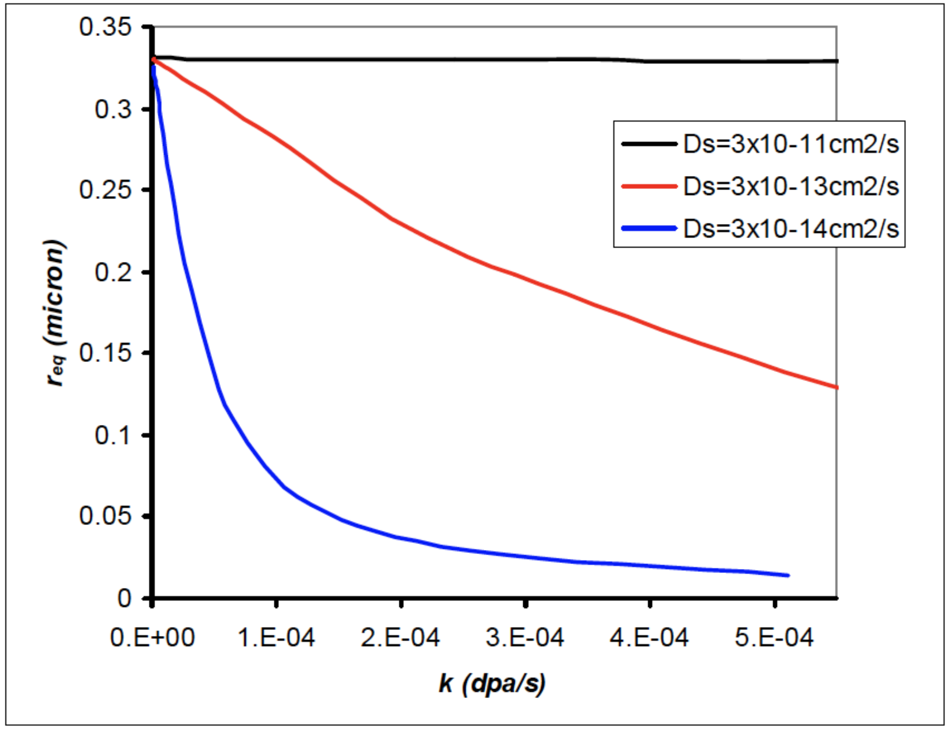


Figure 24.13: Equilibrium radius for a precipitate subjected to recoil dissolution as a function of displacement rate for three values of the solute diffusion coefficient. x_S=1% and C_p=66%.

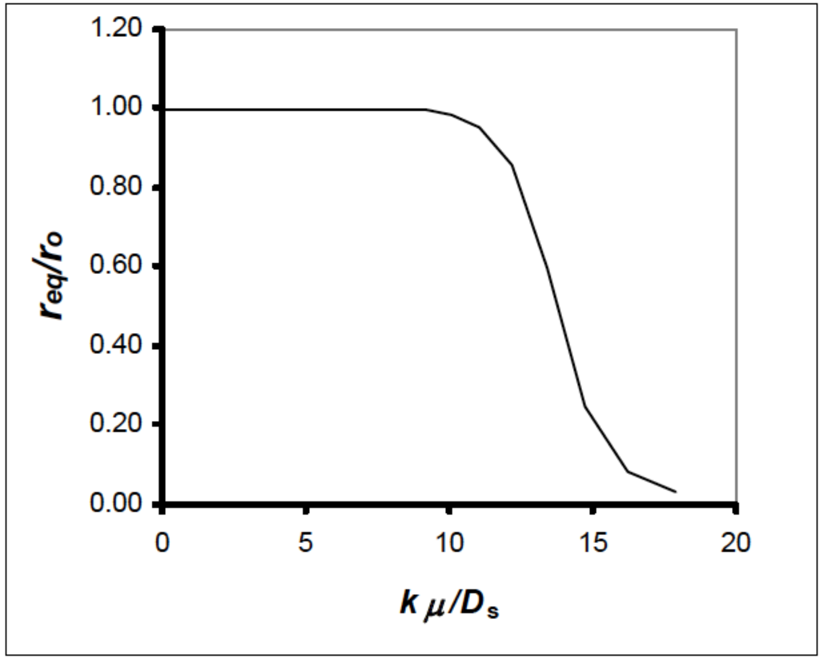
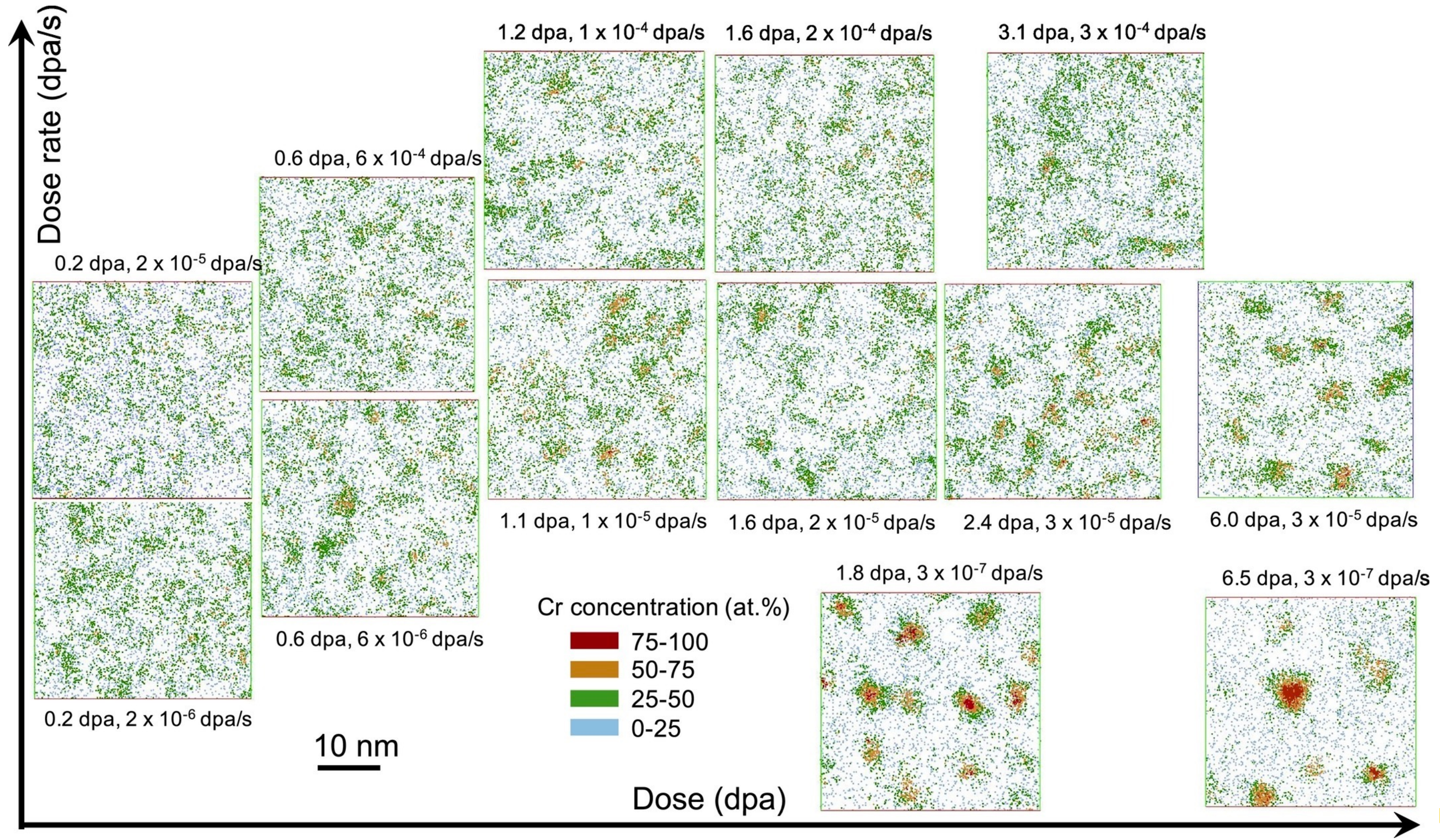


Figure 24.14: Ratio of equilibrium precipitate radius to radius in the absence of recoil dissolution, versus parameter $\frac{k\mu}{D_s}$.


Dose rate (dpa/s)
Dose (dpa)
0.2 dpa, 2 x 10^-5 dpa/s
0.2 dpa, 2 x 10^-6 dpa/s
0.6 dpa, 6 x 10^-4 dpa/s
0.6 dpa, 6 x 10^-6 dpa/s
1.2 dpa, 1 x 10^-4 dpa/s
1.1 dpa, 1 x 10^-5 dpa/s
1.6 dpa, 2 x 10^-4 dpa/s
1.6 dpa, 2 x 10^-5 dpa/s
3.1 dpa, 3 x 10^-4 dpa/s
2.4 dpa, 3 x 10^-5 dpa/s
6.0 dpa, 3 x 10^-5 dpa/s
1.8 dpa, 3 x 10^-7 dpa/s
6.5 dpa, 3 x 10^-7 dpa/s
Cr concentration (at.%)
75-100
50-75
25-50
0-25
10 nm

Radiation-induced precipitate dissolution

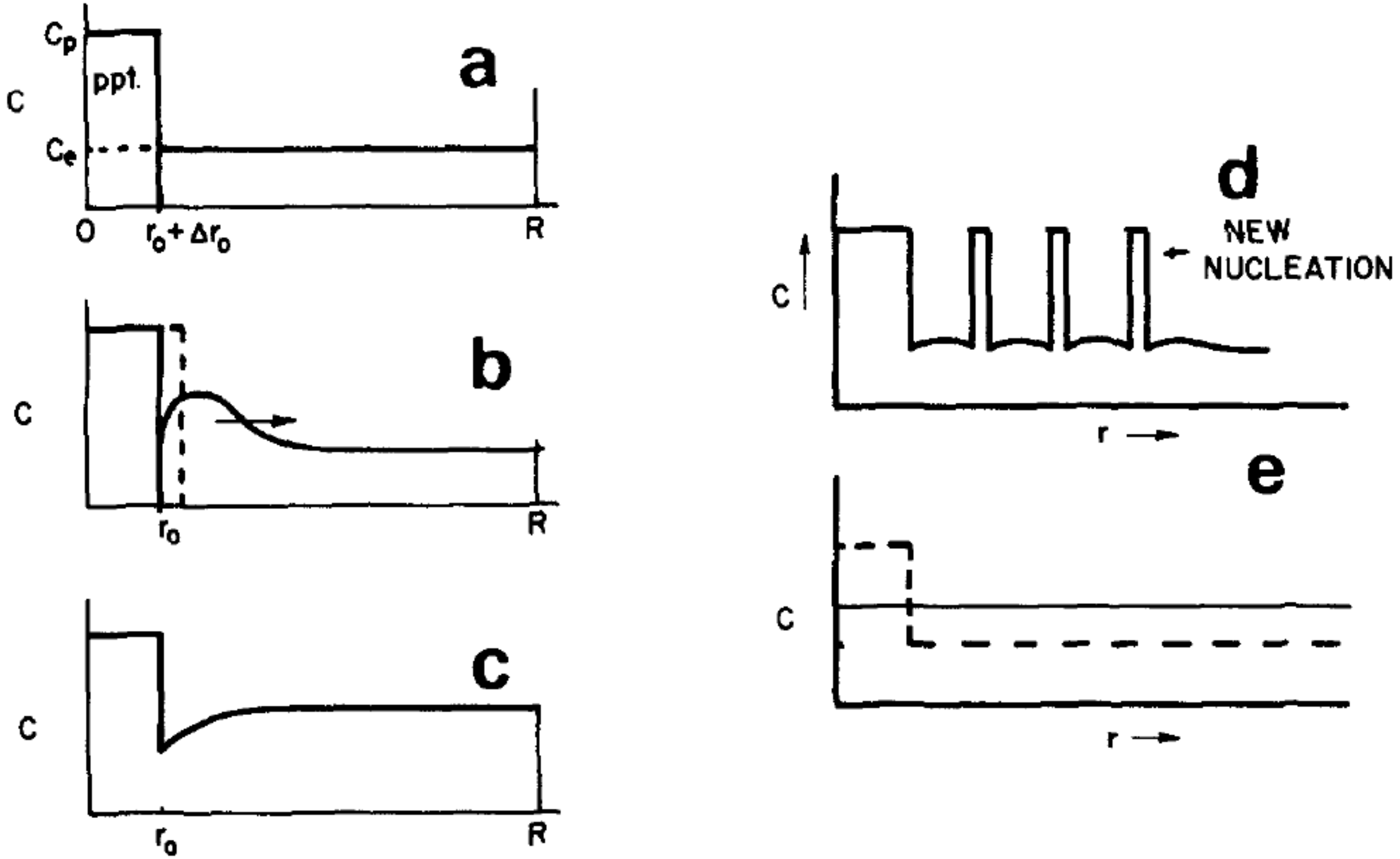
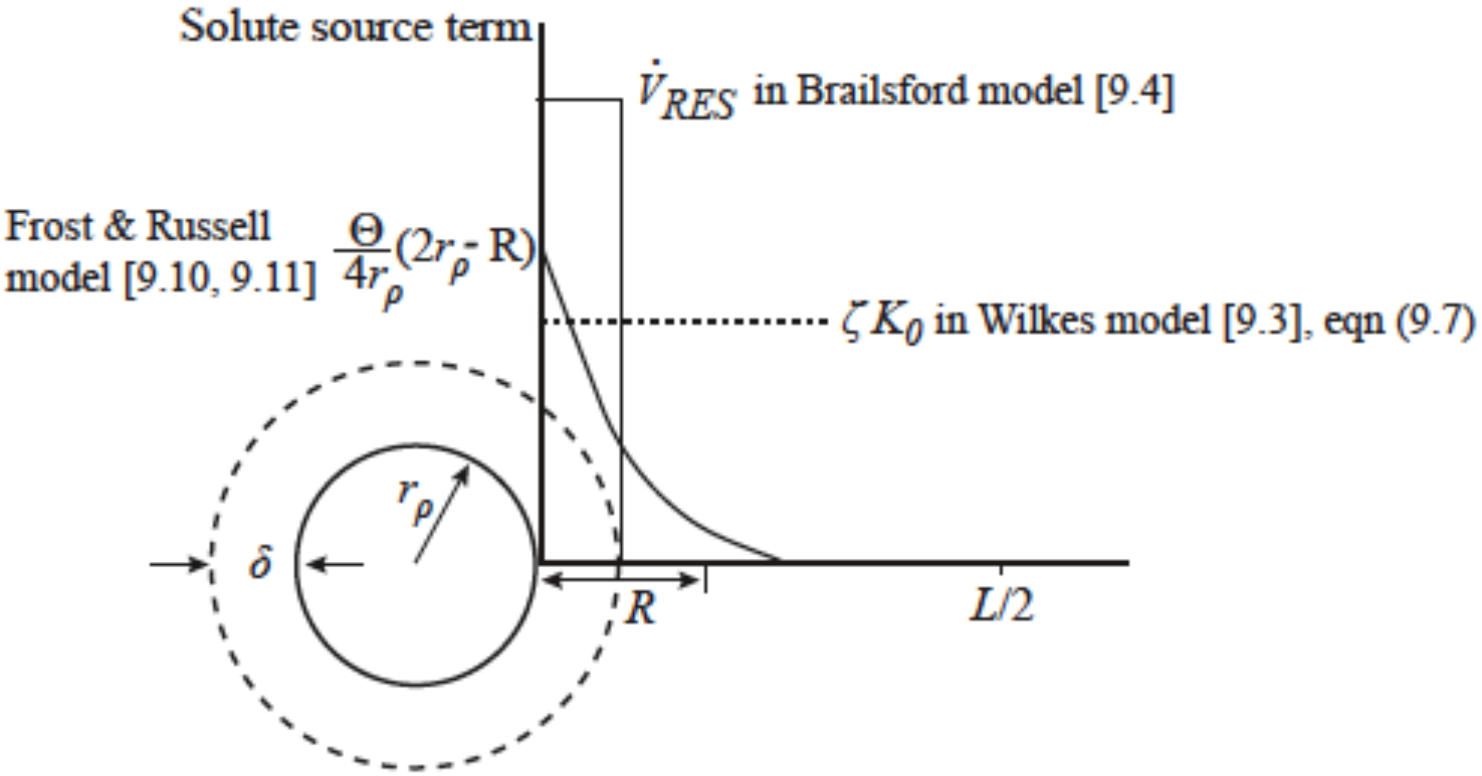


Fig. 3. A schematic diagram of concentration variations in a precipitate cell: (a) before irradiation with a precipitate of radius $r_0 + \Delta r$ in equilibrium with a uniform matrix concentration c_e; (b) when irradiation begins surface disssolution causes a local solute supersaturation some of which 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:

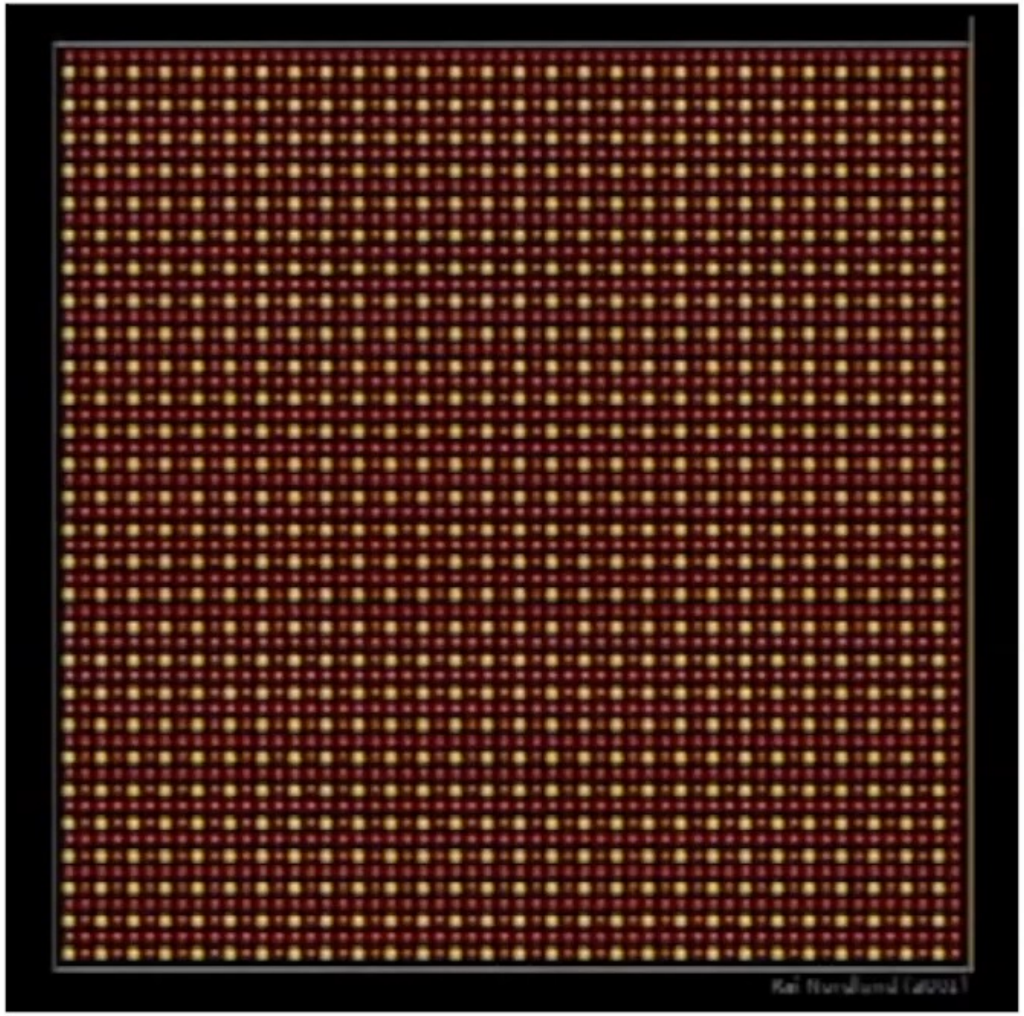
- Nelson model (NHM) – pg. 488-489 in Was
- Wilkes model – pg. 489-492 in Was
- Frost and Russell – pg. 492-493 in Was



Phase transformations without changes in composition

Radiation Disordering

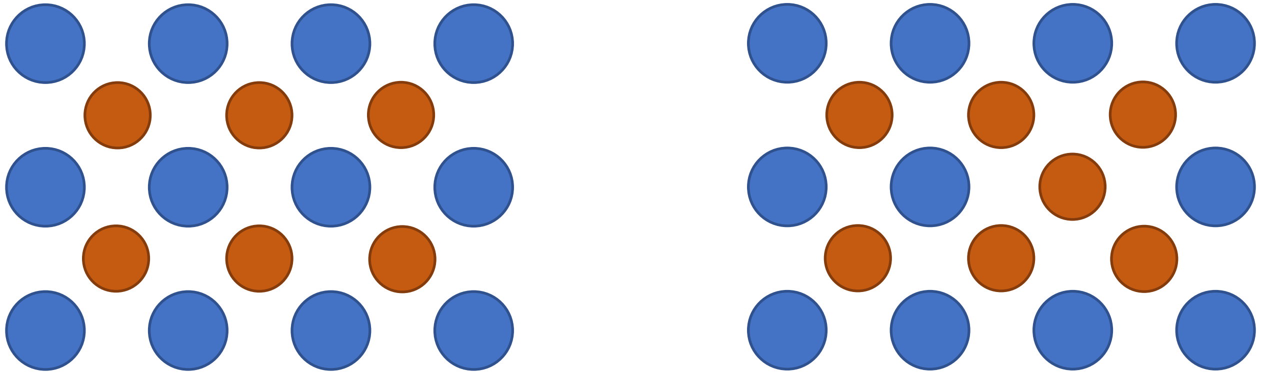
9.1 Irradiation-induced disordering.
Disordering of Cu_3Au (L12 structure)
by bombardment with 10 keV Au ions.
(courtesy K. Nordlund, University of Helsinki)



Radiation disordering: Loss of long-range order

Radiation Disordering

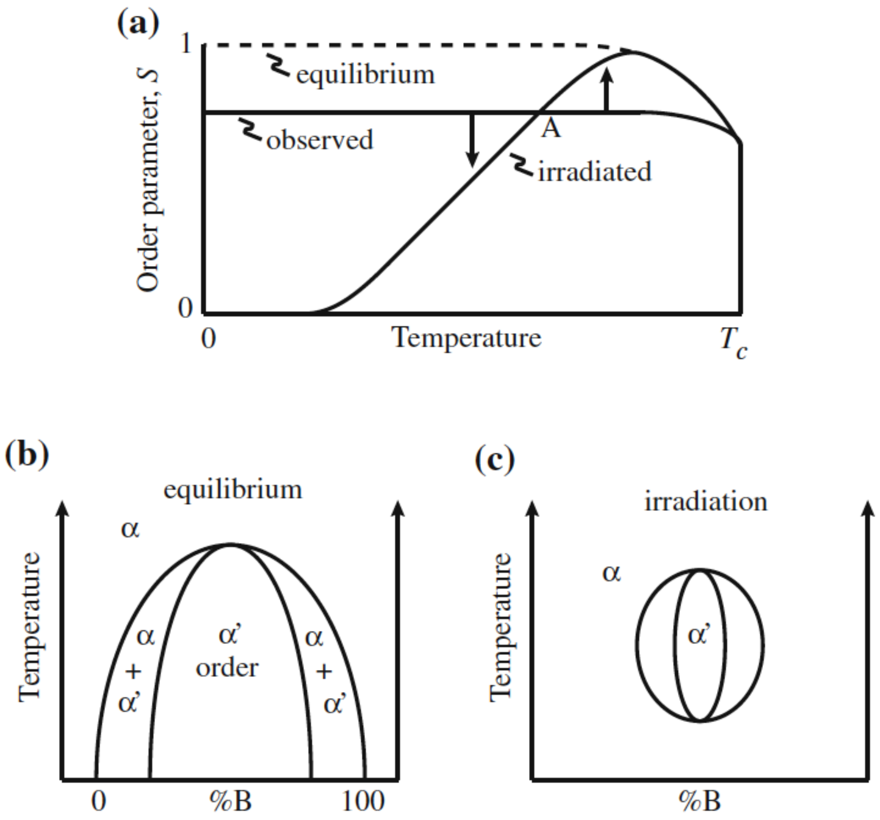
- Antisite defects:
  - Occur in an ordered alloy or compound when atoms of different type exchange position



  - We now need to consider random recombination so:

Radiation Disordering

- The steady state solution then becomes:



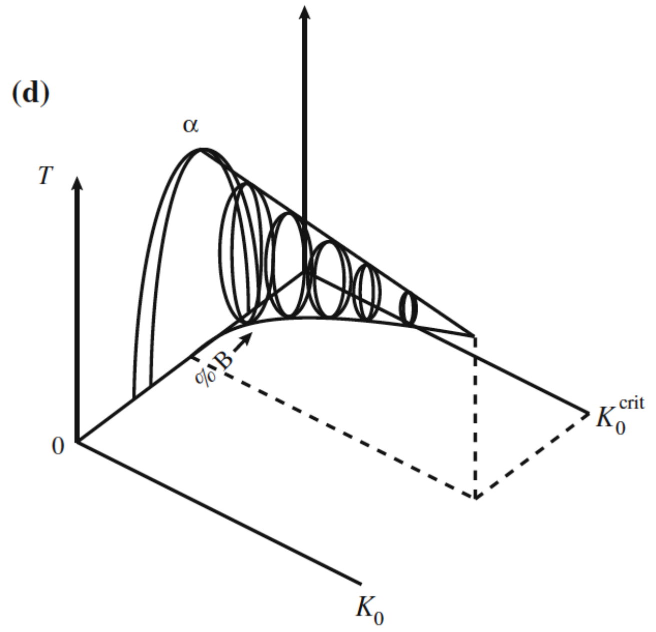
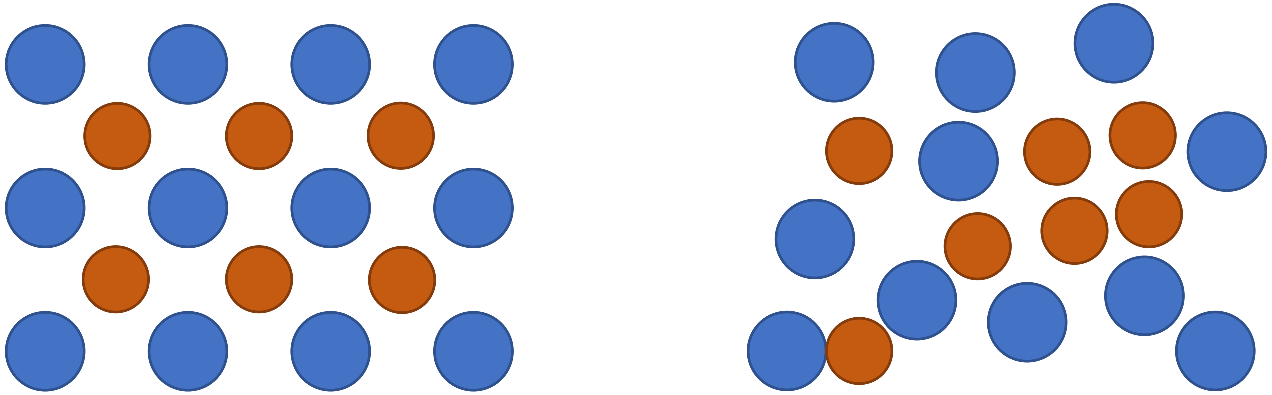


Fig. 9.11 (**a**) Effect of irradiation on the temperature dependence of the order parameter for a phase structure that is not at the equilibrium order, S_e. (**b**) Equilibrium phase diagram showing a first-order phase transformation of the disordered α phase to the ordered α'-phase. (**c**) Modification 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])

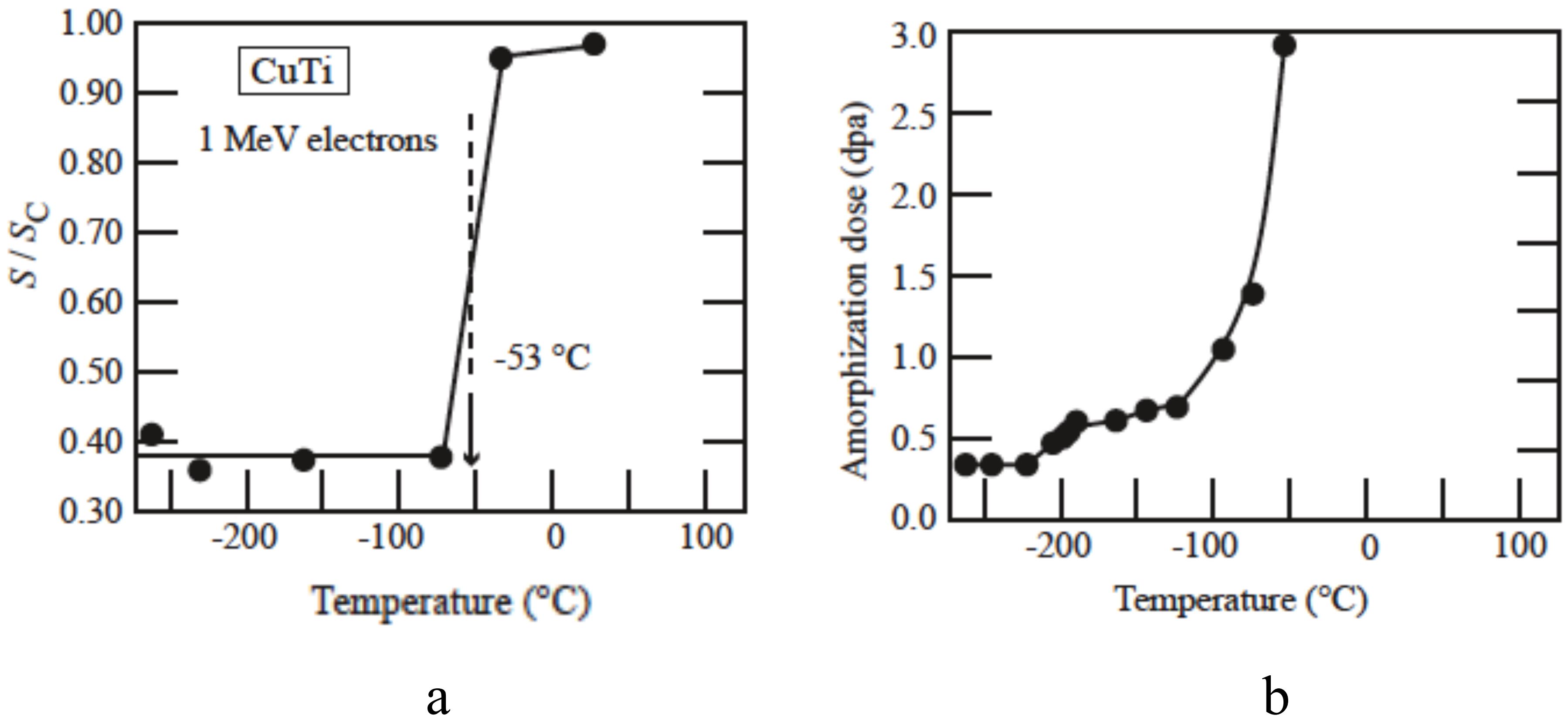
Temperature dependence of amorphization

- Amorphization by particle irradiation refers to the complete loss of long-range crystalline structure



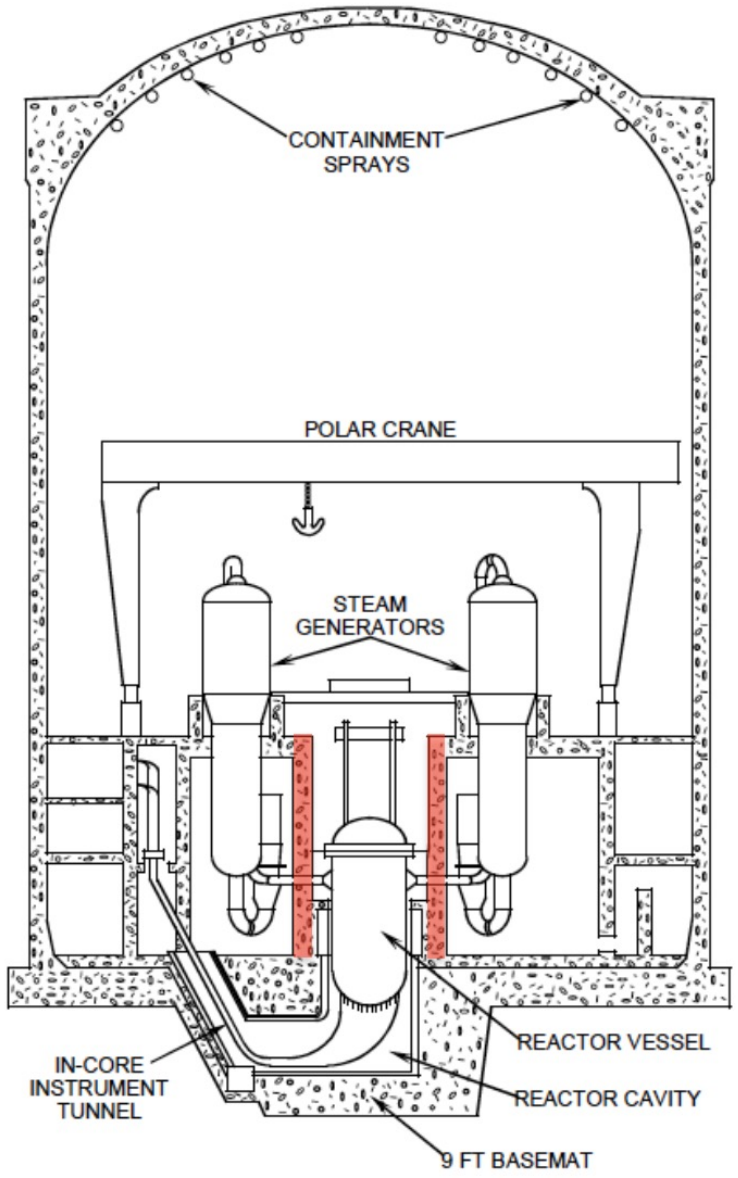
- Irradiation induced amorphization is difficult to describe (model) in a general basis
- Let's consider just describing the critical temperature and dose of amorphization for a simple system based on disordering

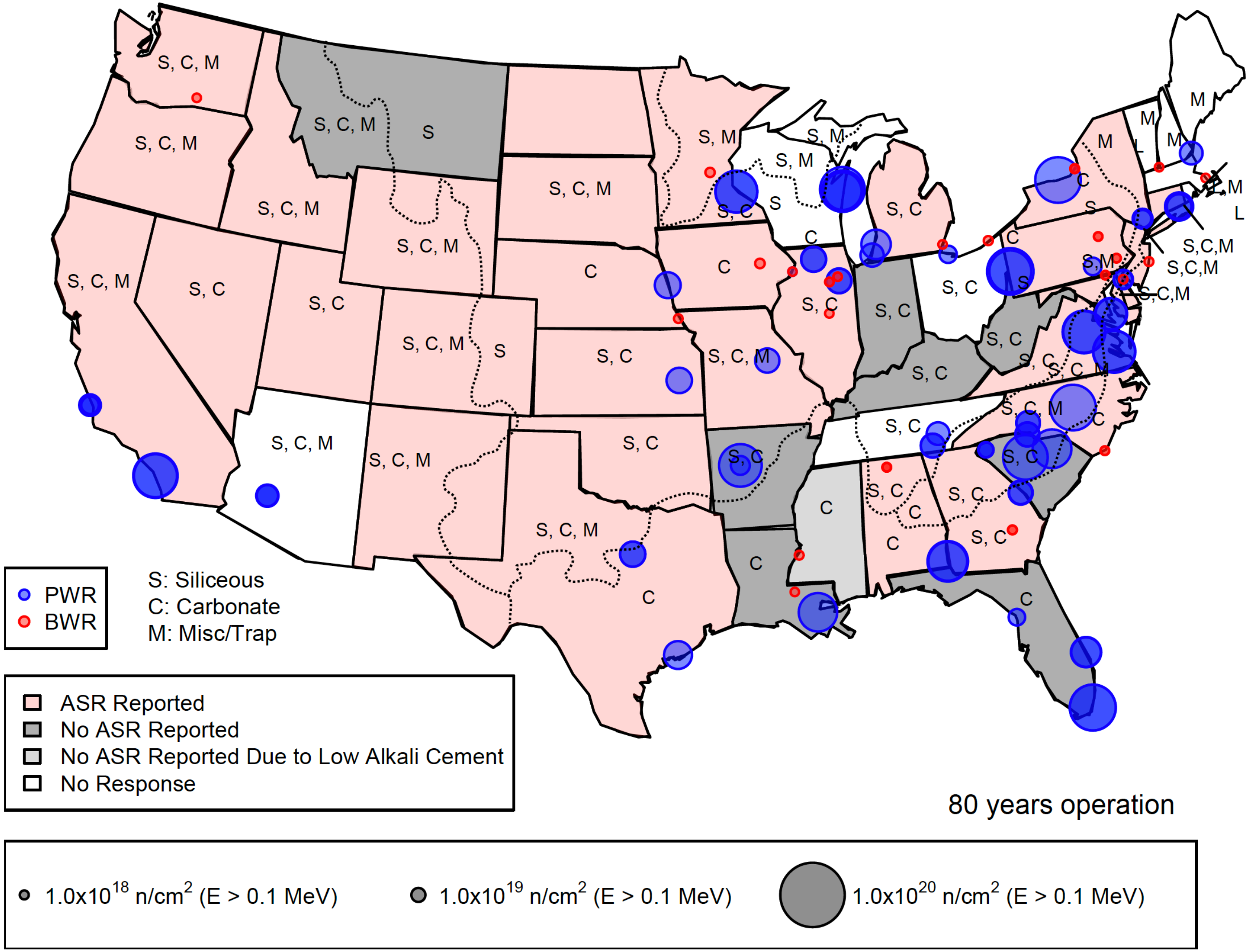
Temperature dependence of amorphization



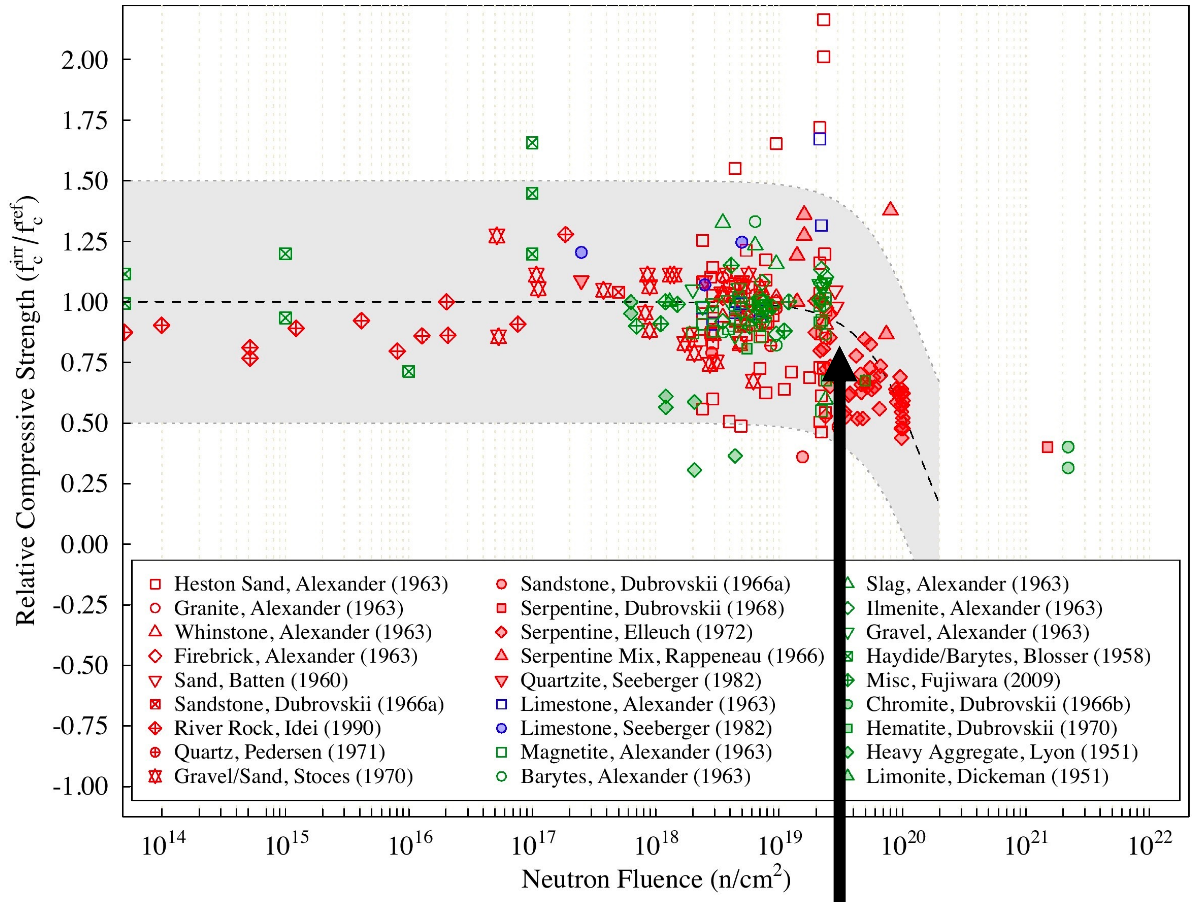
Temperature dependence of a) the long-range order parameter S/S_C, and b) the critical amorphization dose for CuTi, irradiated with 1 MeV electrons

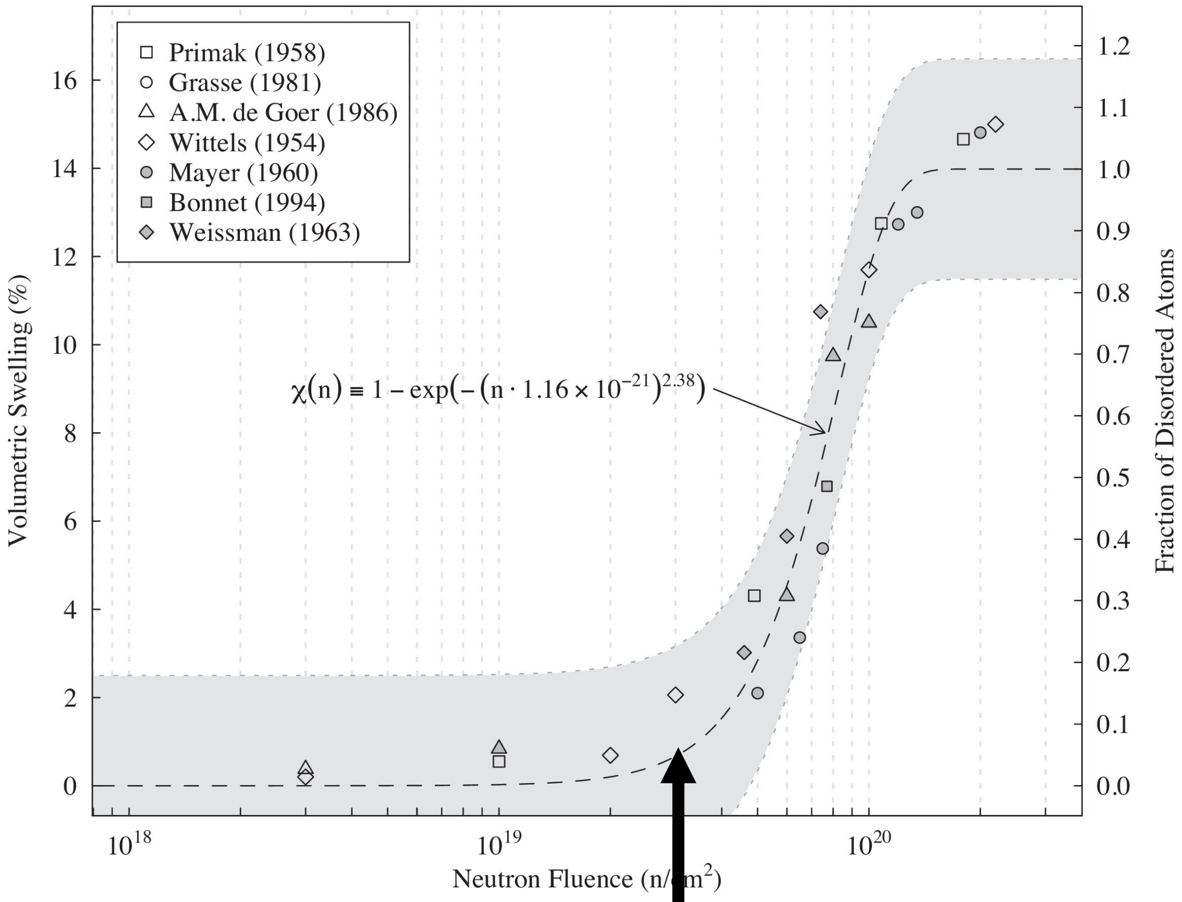
Irradiation-induced amorphization





Irradiation-induced amorphization





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That's it!

Questions?