Phase Transformations

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Course evaluations:

https://umich.bluera.com/umich/

Open until Dec. 10

Your help in making this course better is greatly appreciated!

HW5

- Due tomorrow by noon (so I can grade them quickly)

Influence of phase stability and cavity growth

- Remember, our cavity growth rate equation in simple terms:

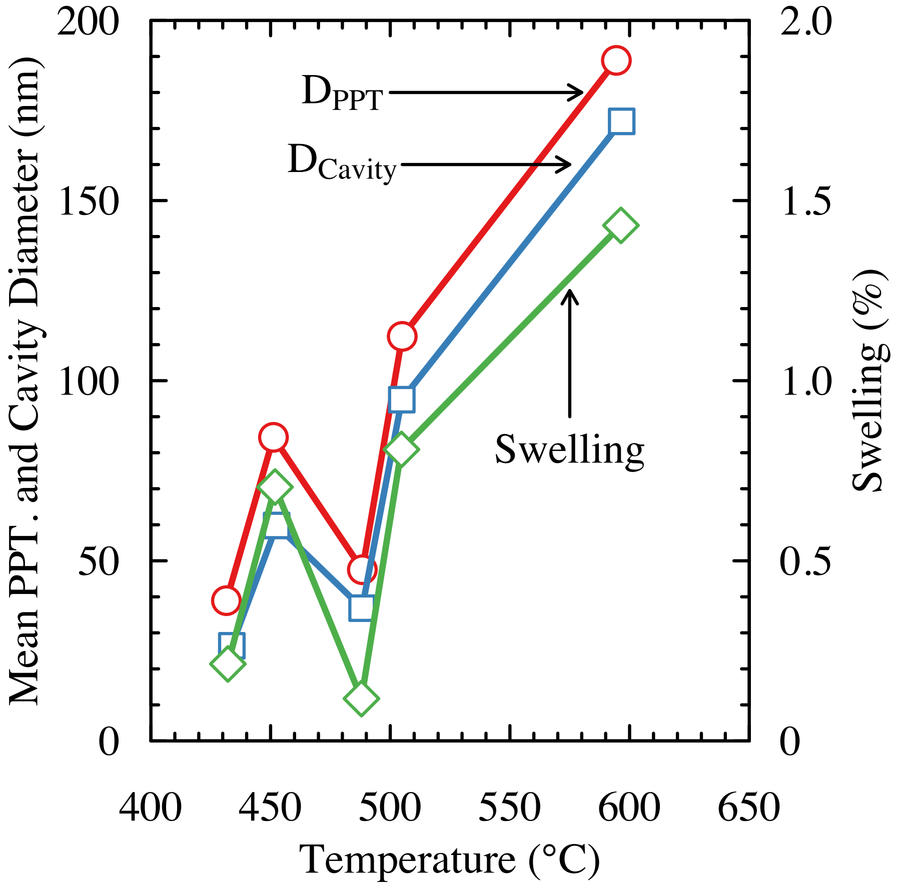
$$\frac{dr}{dt} = \frac{\Omega}{r}\left[\begin{pmatrix}\text{Radiation-induced}\\ \text{plus thermal}\\ \text{vacancy influxes}\end{pmatrix} - \begin{pmatrix}\text{Radiation-induced}\\ \text{interstitial influx}\end{pmatrix} - \begin{pmatrix}\text{Thermal}\\ \text{vacancy outflux}\end{pmatrix}\right]$$

And the last term, which is the thermal emission term (E) is proportional to the cavity surface eg. $E \propto C_v^e(r)$ where $C_v^e(r)$ is dependent on the cavity size, the temperature, and the internal pressure by,

$$C_v^e(r) = C_v^0 \, exp\left[\left(\frac{2\gamma}{r} - P\right)\frac{\Omega}{kT}\right]$$

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

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



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Influence of phase stability and cavity growth

- Remember, our cavity growth rate equation in simple terms:

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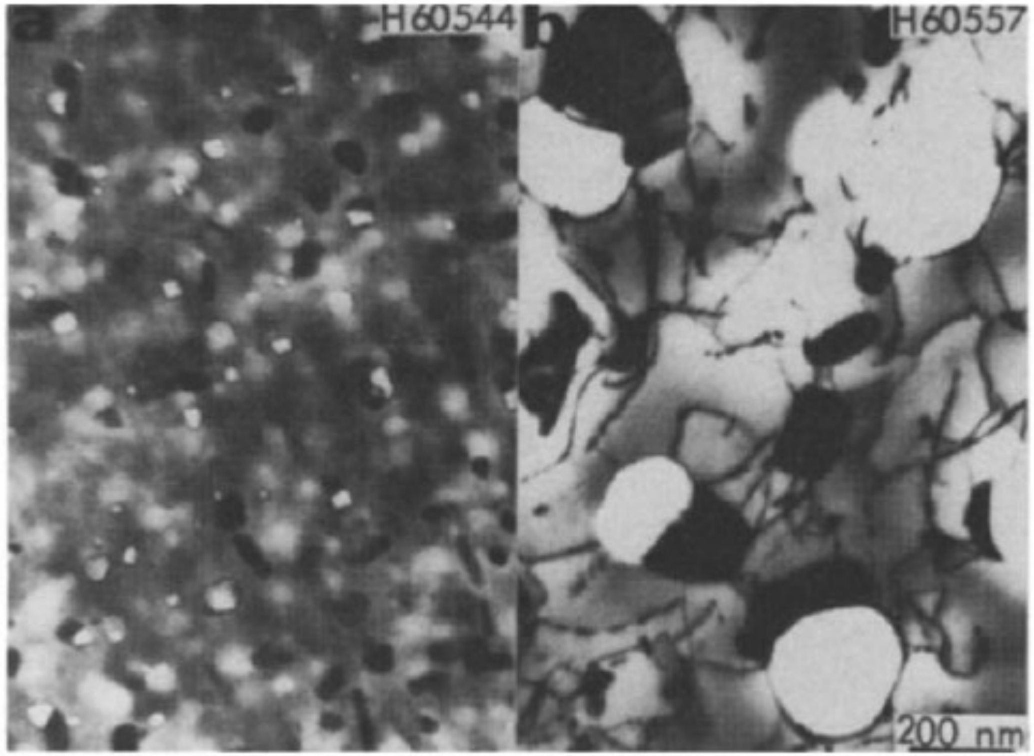
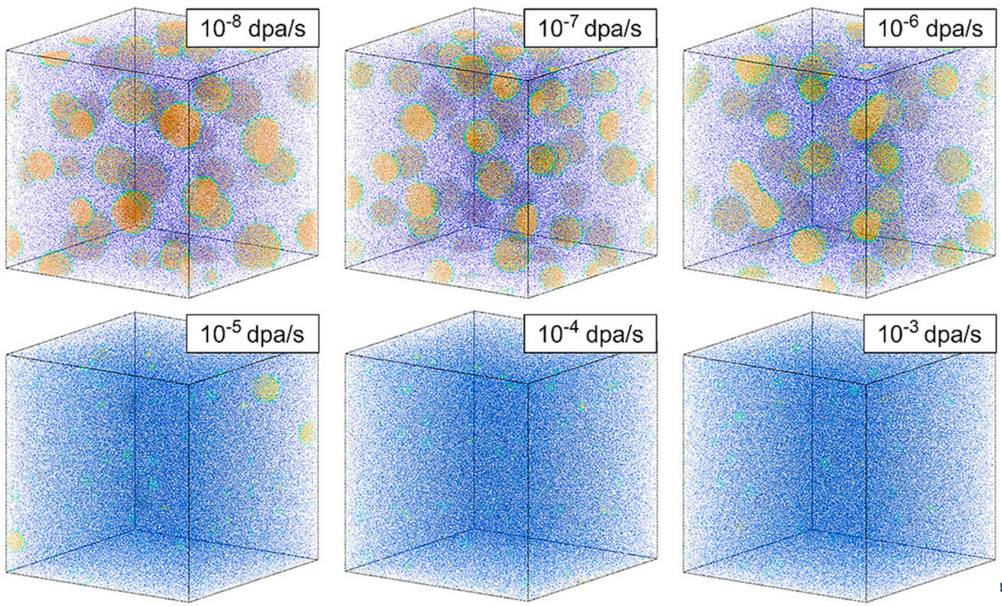


Fig. 2. Cavity-particle association in LS1C irradiated to ~35 dpa in EBR-II at (a) 425°C, (b) 600°C.

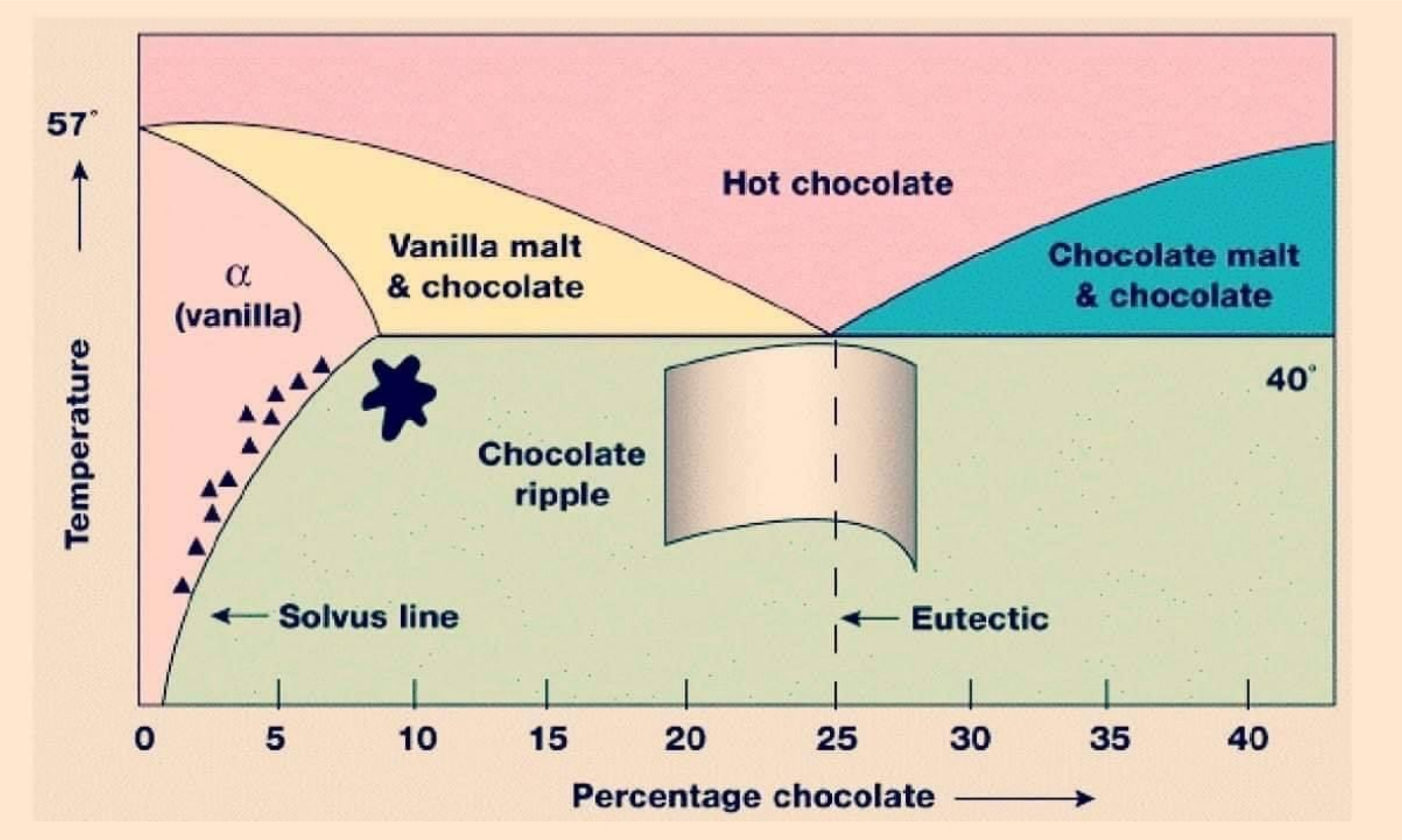
Two primary irradiation induced phase transformation types:

1. 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
2. Requires compositional changes
   1. Induced precipitation from solid solution
   2. Dissolution of precipitates

Irradiation flux effect on α' precipitation in Fe-Cr



Food for thought



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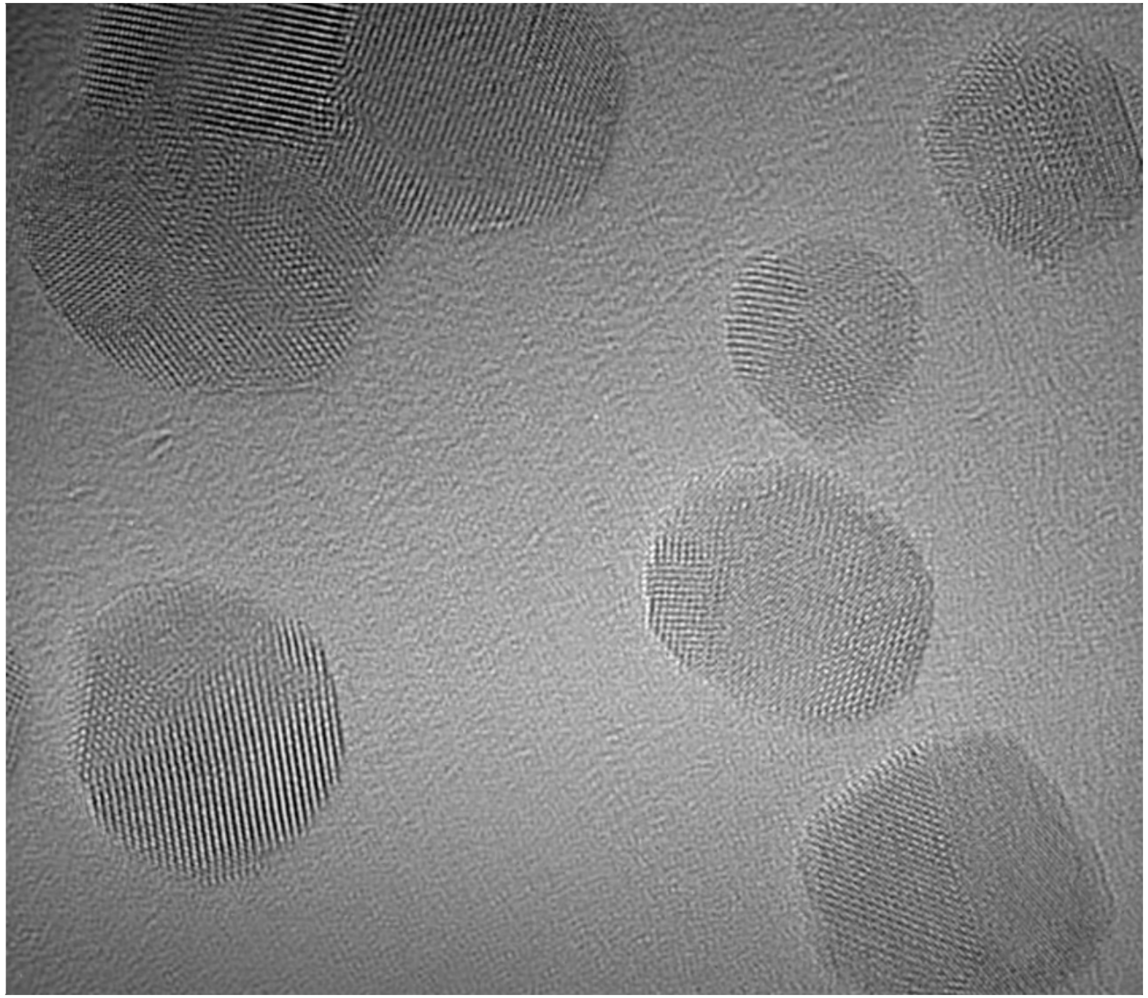
Ostwald Ripening

- 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 then



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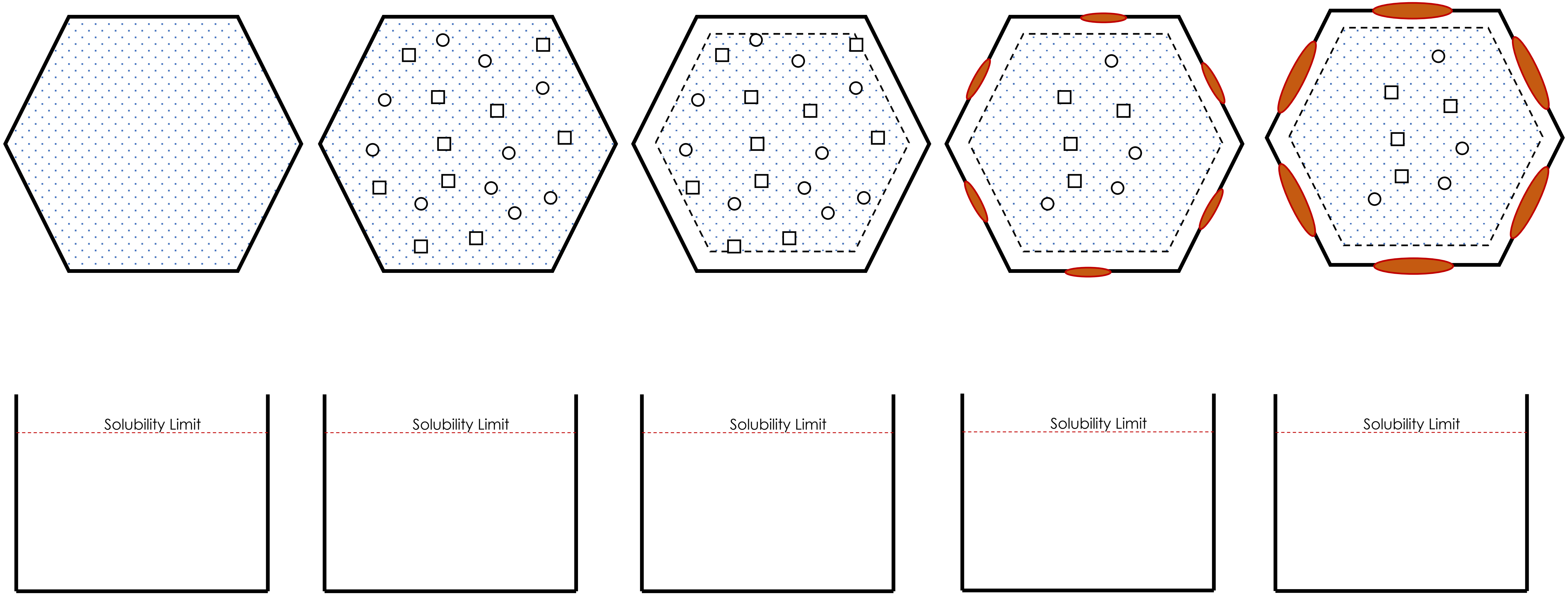
Phase transformations with changes in composition

RIS and Radiation-induced precipitation



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RIS and Radiation-induced precipitation

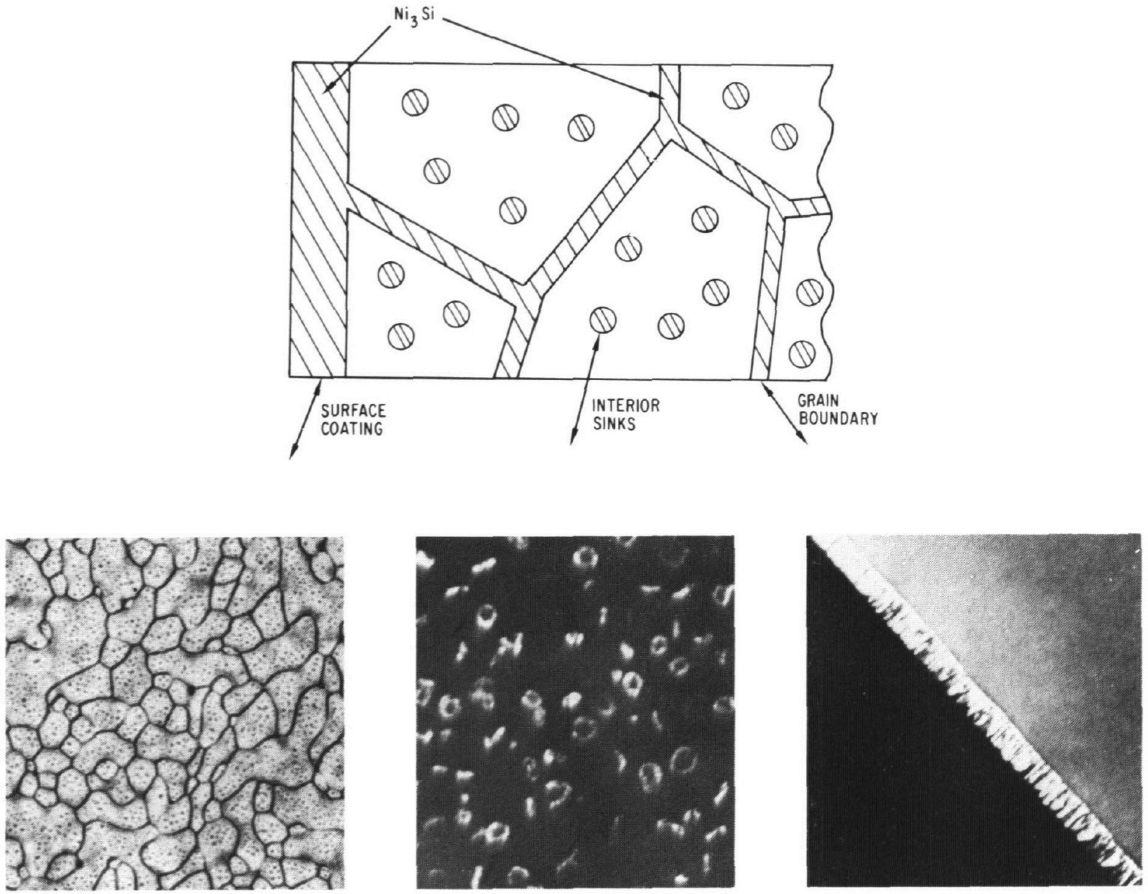

Fig. 1. Formation of γ'-Ni_3Si on defect sinks in a solid solution Ni-Si alloy because of RIS. The dark-field micrographs from the work of K.-H. Robrock and P. R. Okamoto show: (a) the anti-phase domain structure in a contiguous surface coating; (b) toroidal γ'-precipitates on interstitial loops; and (c) a grain boundary coated with γ'.

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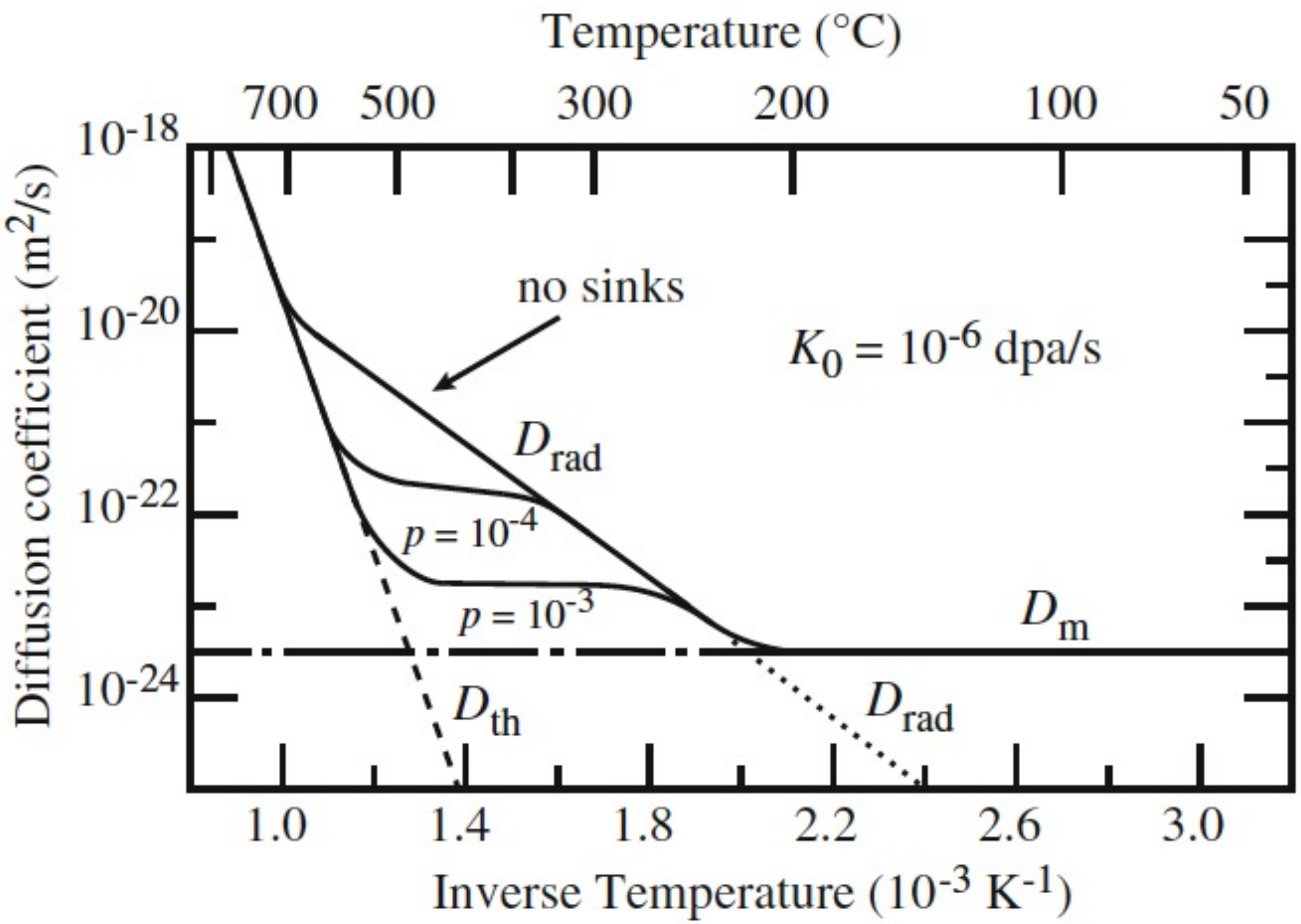
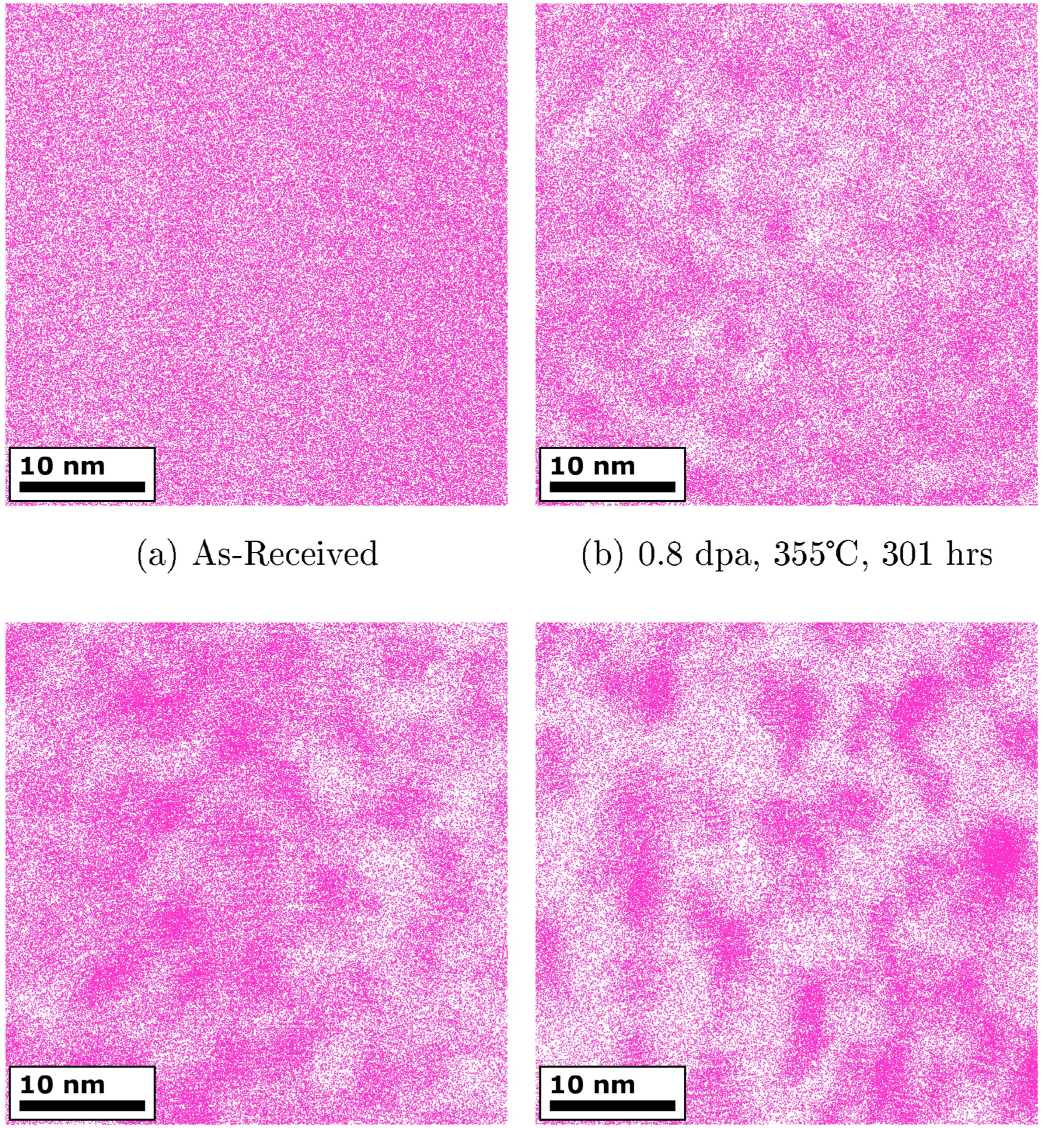
Radiation-enhanced effects on kinetics





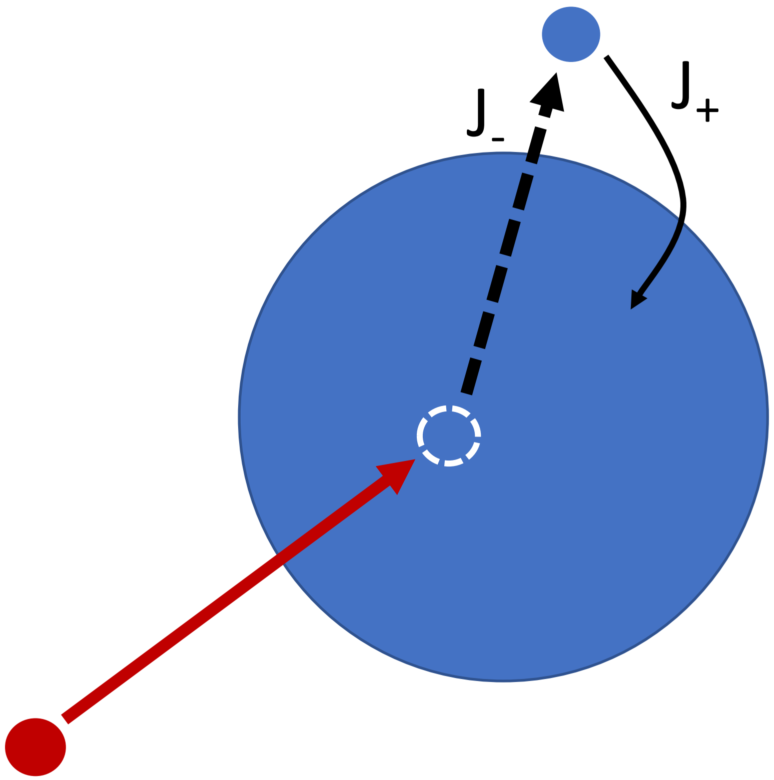
(a) As-Received

(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

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

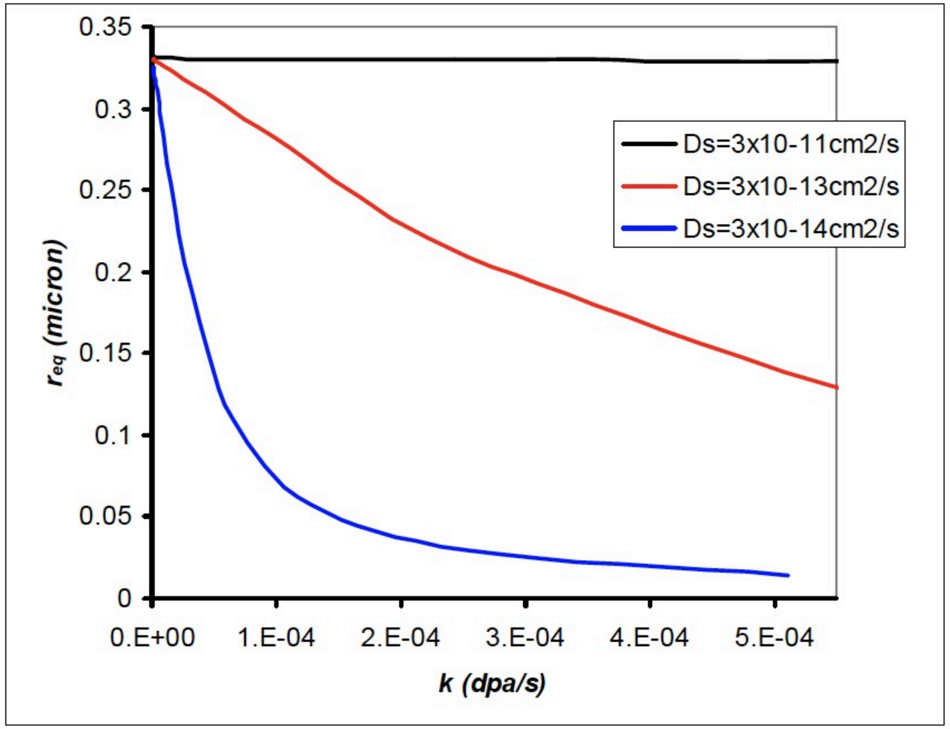


Figure 24.13: Equilibrium radius for a precipitate subjected to recoil dissolution as a function of displacement rate for three values of the solute diffusion coefficient. x_S=1% and C_p=66%.

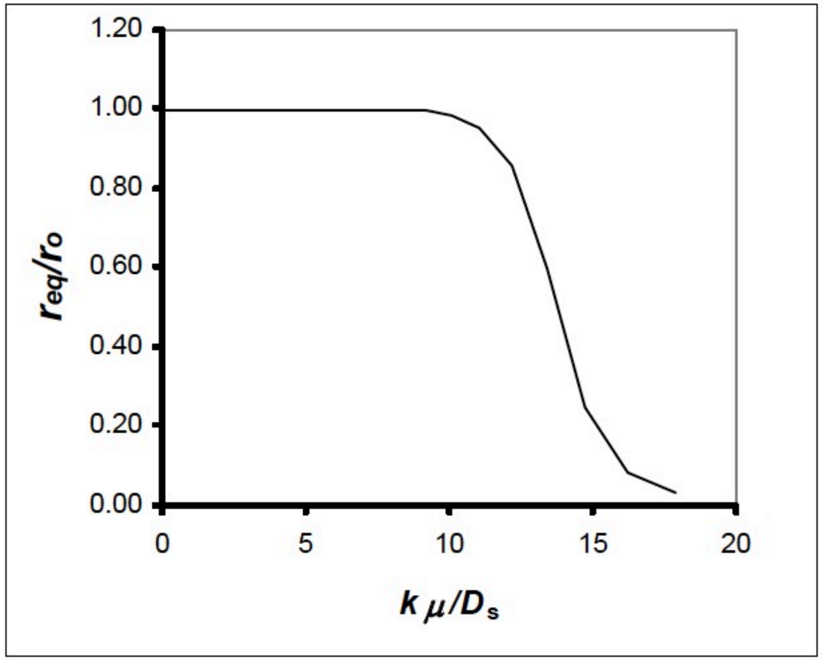
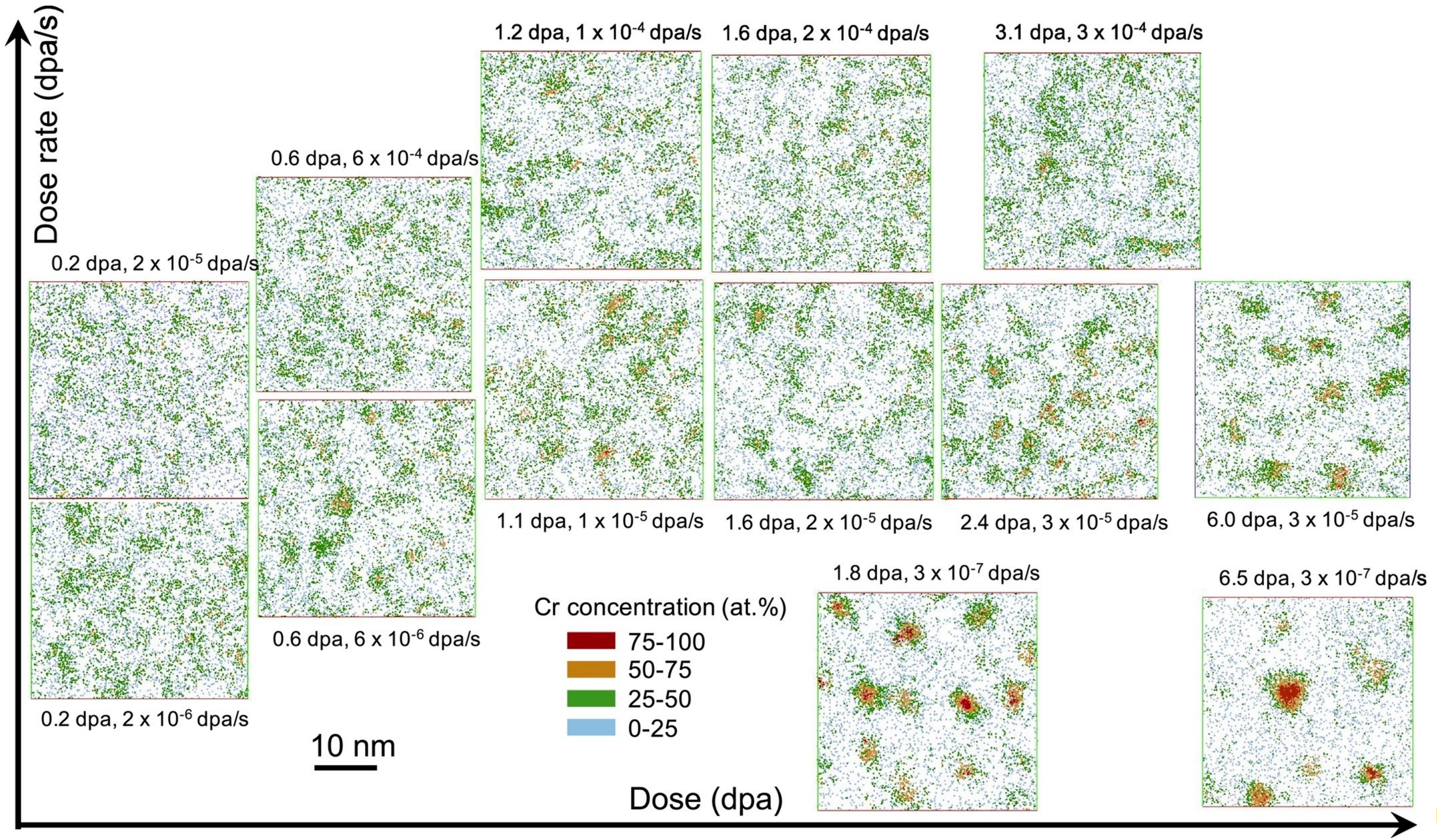


Figure 24.14: Ratio of equilibrium precipitate radius to radius in the absence of recoil dissolution, versus parameter $\frac{k\mu}{D_s}$.



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Radiation-induced precipitate dissolution

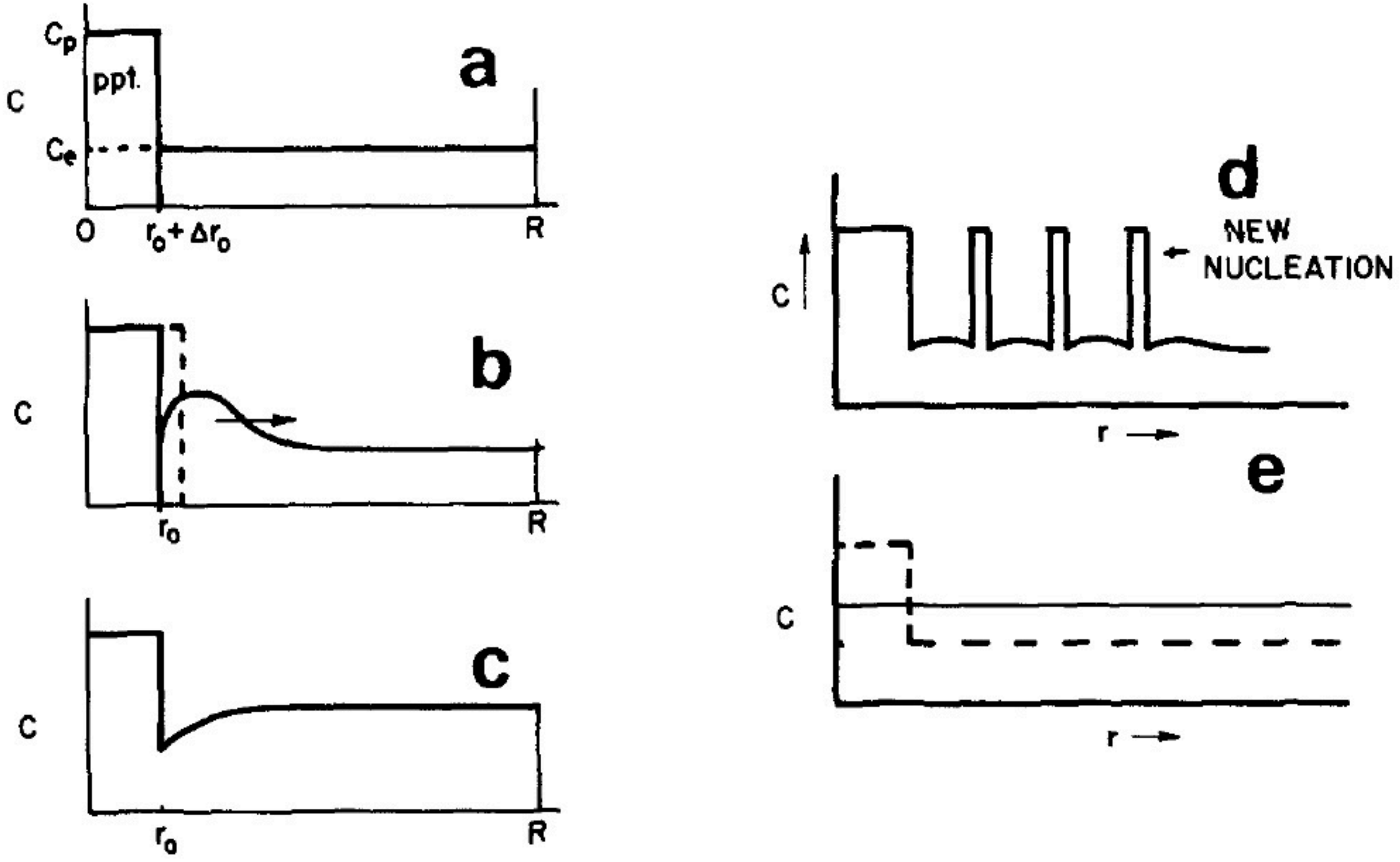
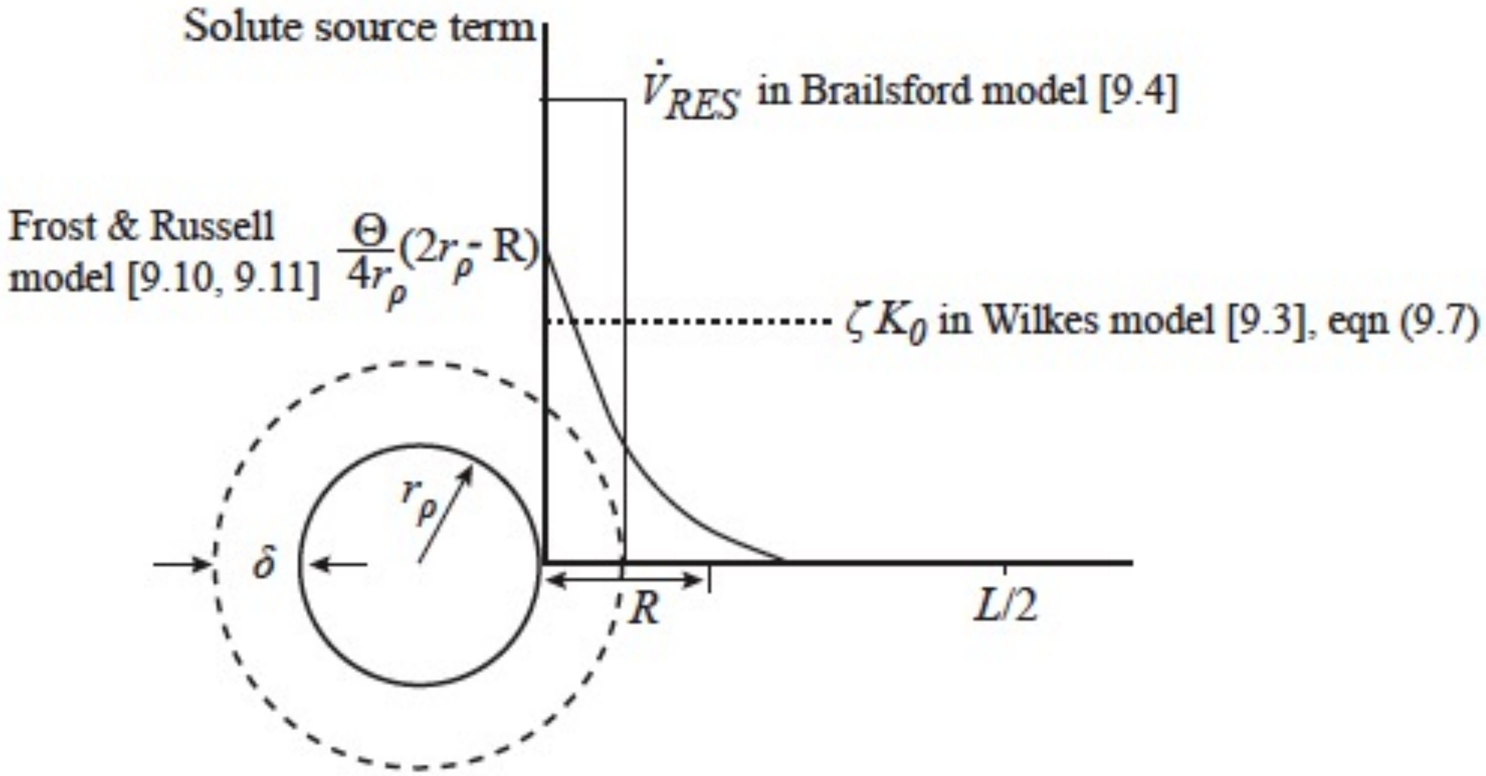


Fig. 3. A schematic diagram of concentration variations in a precipitate cell: (a) before irradiation with a precipitate of radius $r_0 + \Delta r$ in equilibrium with a uniform matrix concentration c_e; (b) when irradiation begins surface disssolution causes a local solute supersaturation some of which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



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: Simplest. Similar to that derived in class and uses rate theory. Proposed inverse Ostwald ripening:

$$\frac{dr_p}{dt} = -\delta K_0 \Omega + \frac{3DC}{4\pi r_p C_p} - r_p^2 D_p$$

- Wilkes model – pg. 489-492 in Was: Uses a cell model and add in a source term that is uniform in cell:

$$r_o^3 - r_p^3 = [. \qquad](\qquad)$$

- Frost and Russell – pg. 492-493 in Was: Provides for a source term for redeposited solute as a function of radius.

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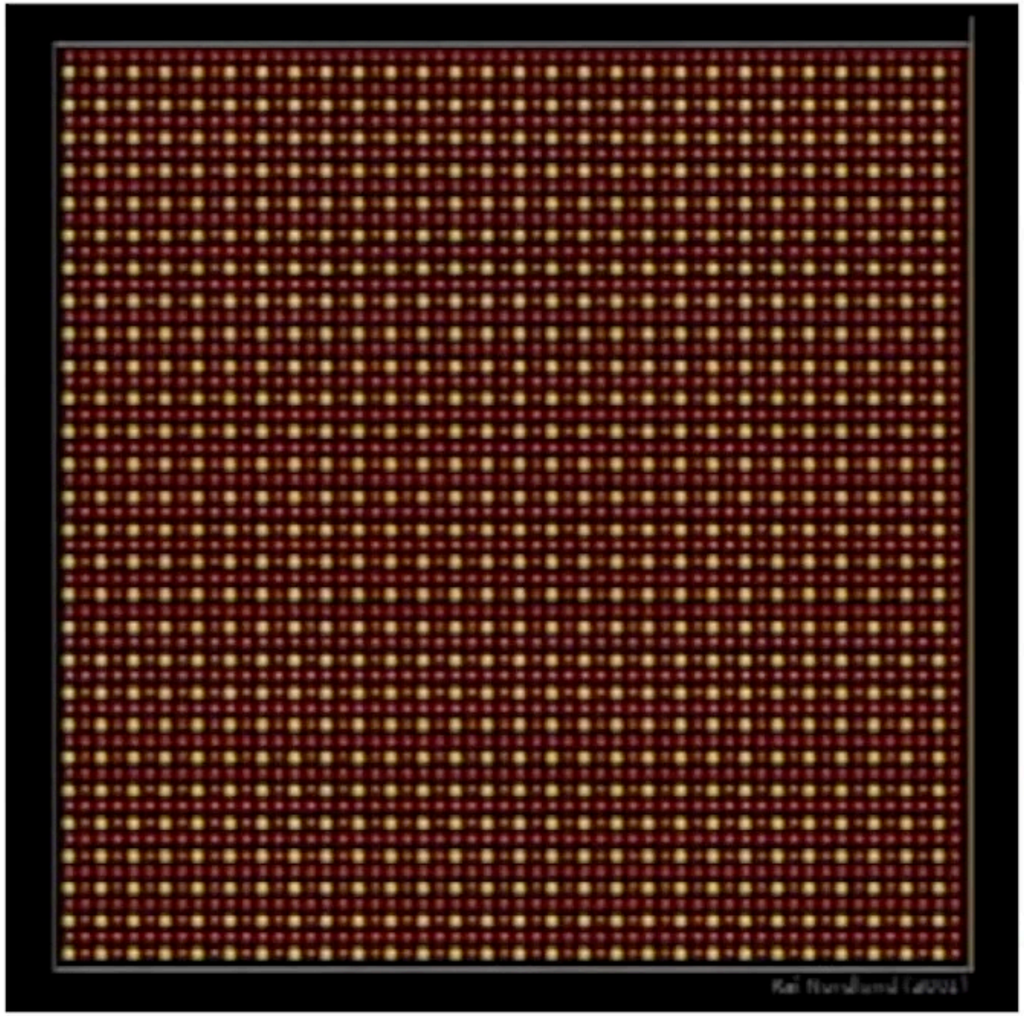
Phase transformations without changes in composition

Radiation Disordering

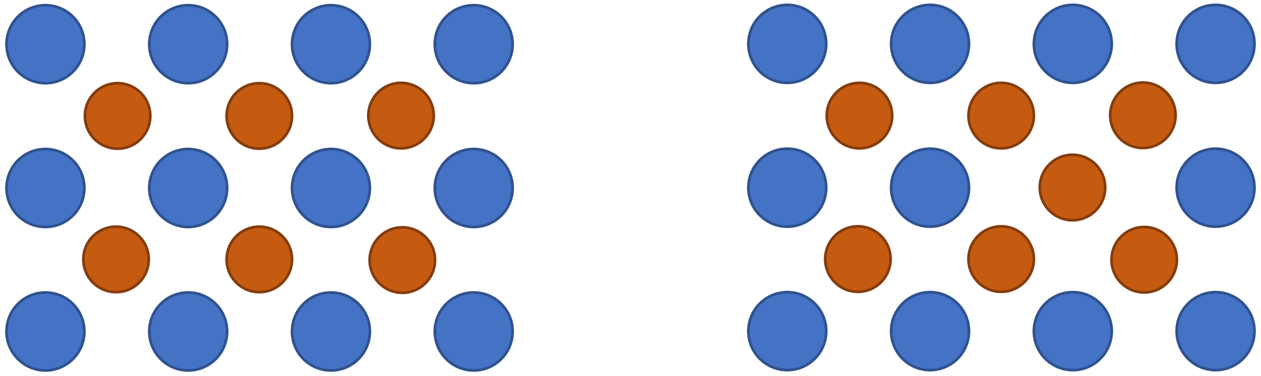
9.1 Irradiation-induced disordering.
Disordering of Cu_3Au (L12 structure)
by bombardment with 10 keV Au ions.
(courtesy K. Nordlund, University of Helsinki)



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:

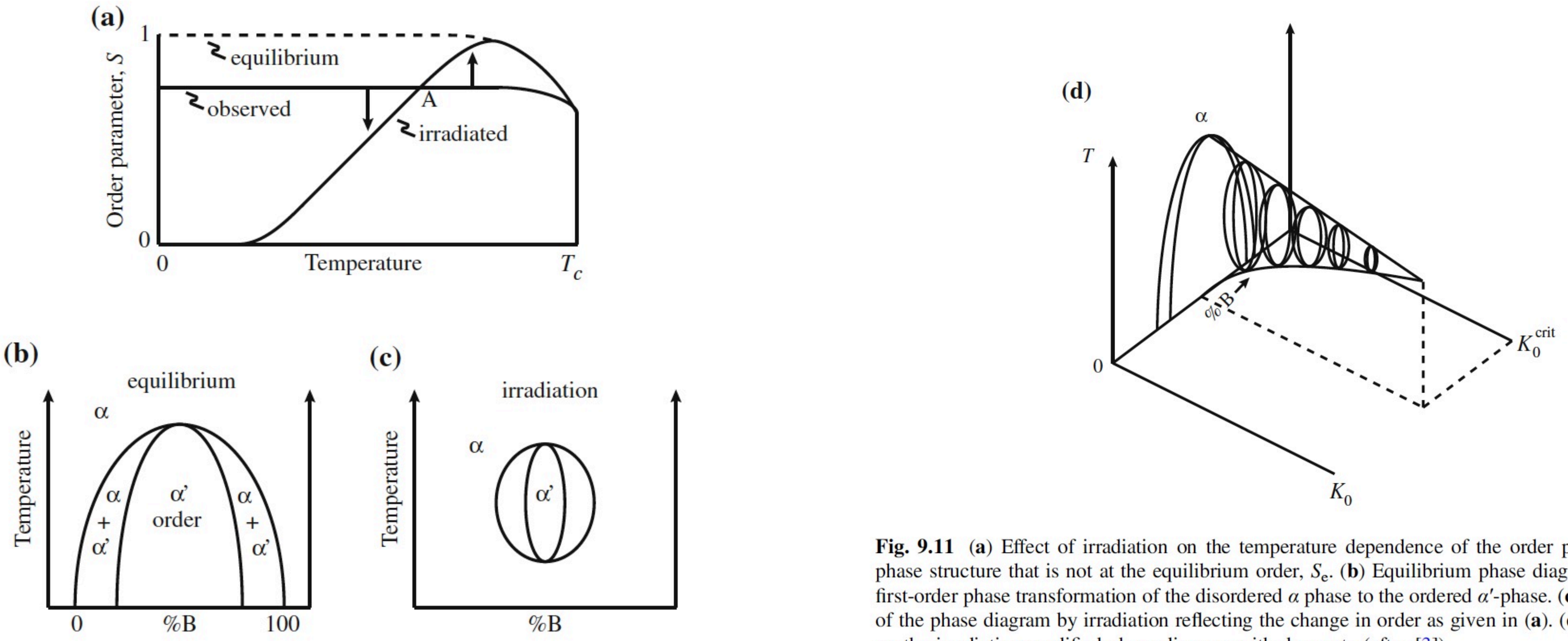
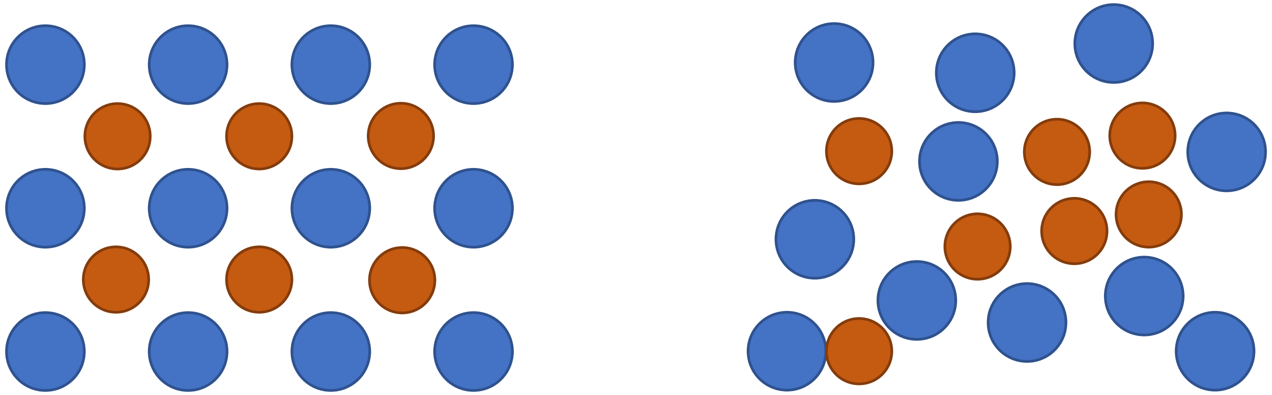


Fig. 9.11 (**a**) Effect of irradiation on the temperature dependence of the order parameter for a phase structure that is not at the equilibrium order, S_e. (**b**) Equilibrium phase diagram showing a first-order phase transformation of the disordered α phase to the ordered α'-phase. (**c**) Modification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

- 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

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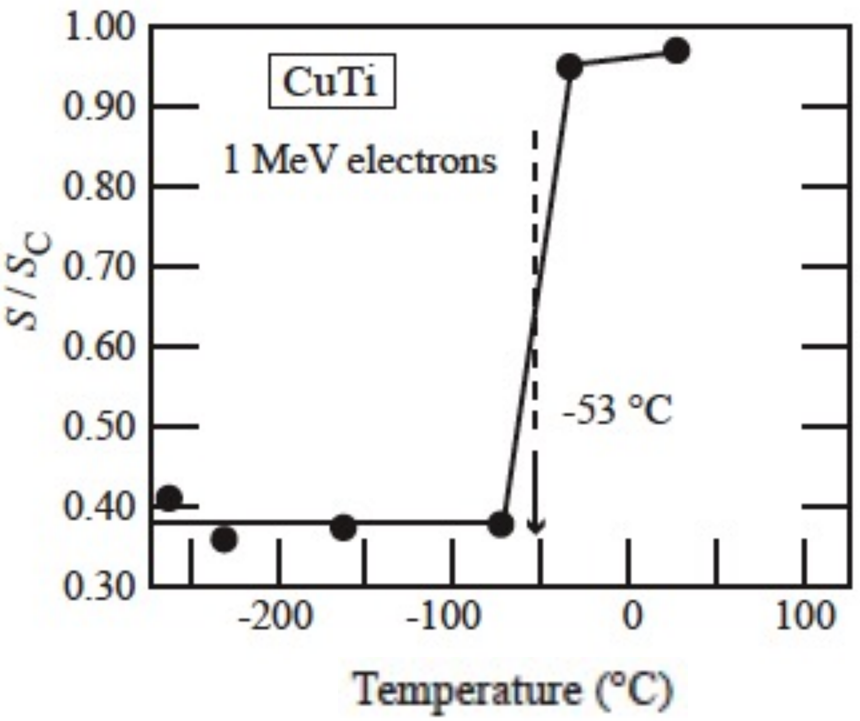
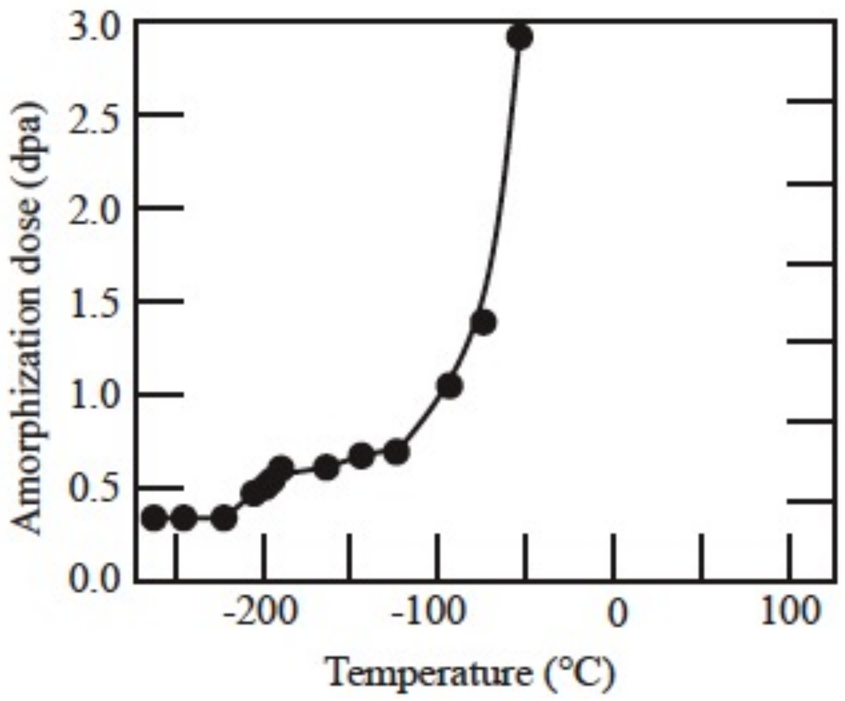
Temperature dependence of amorphization



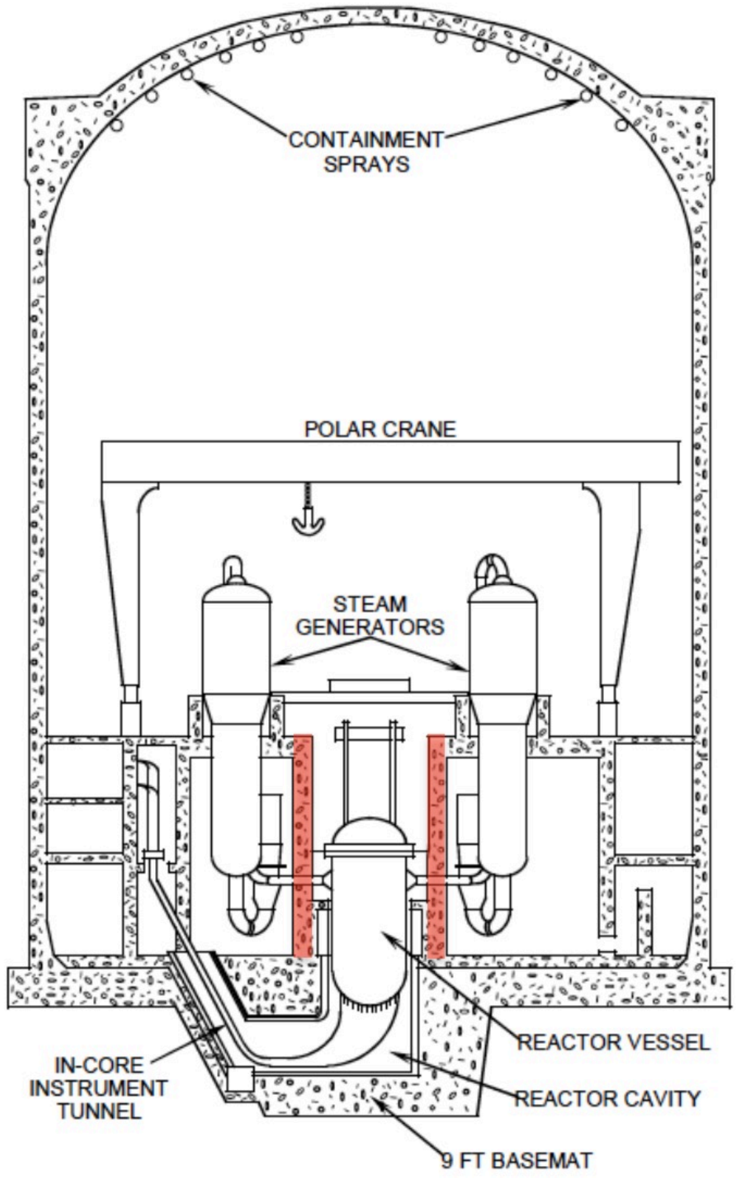
a

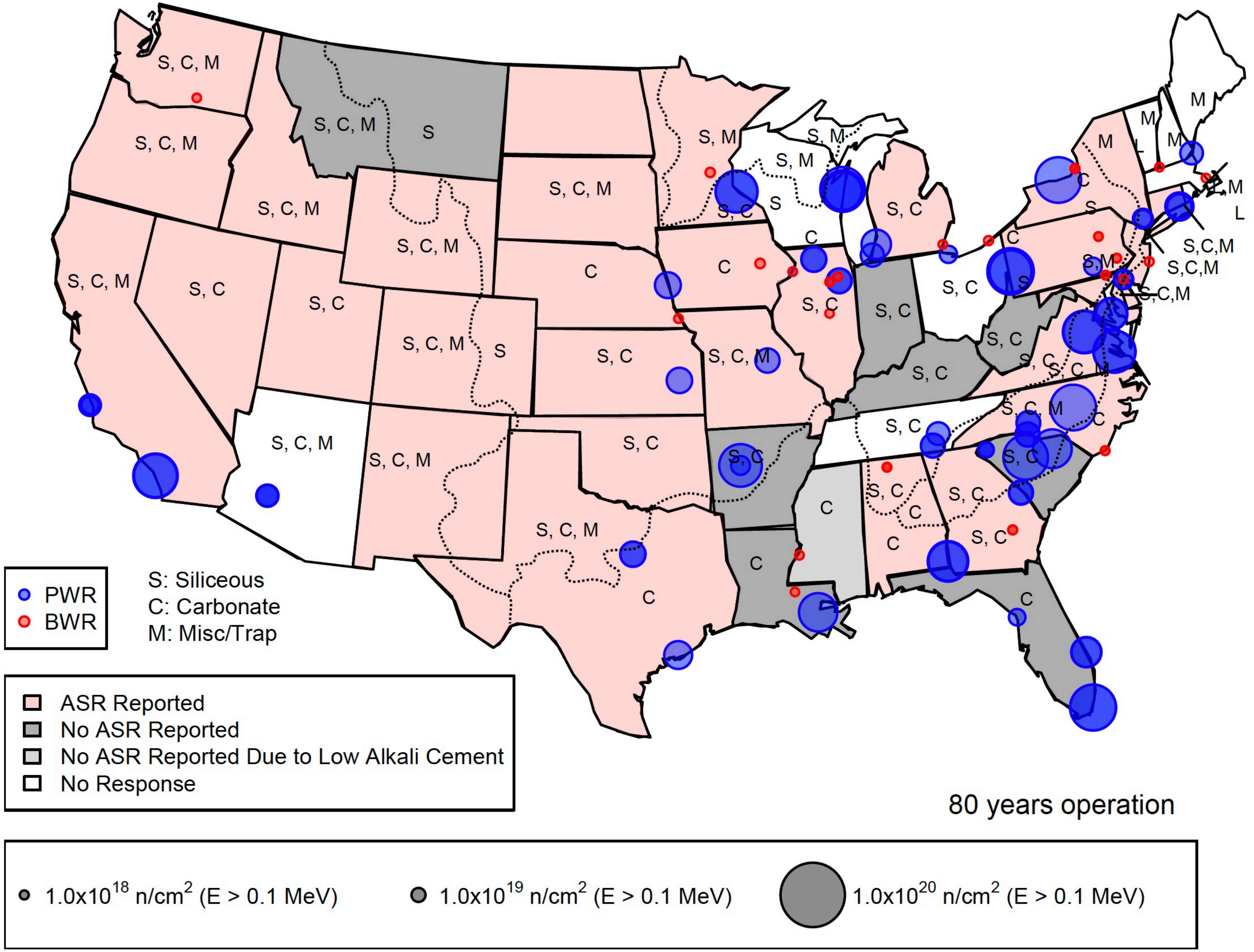


b

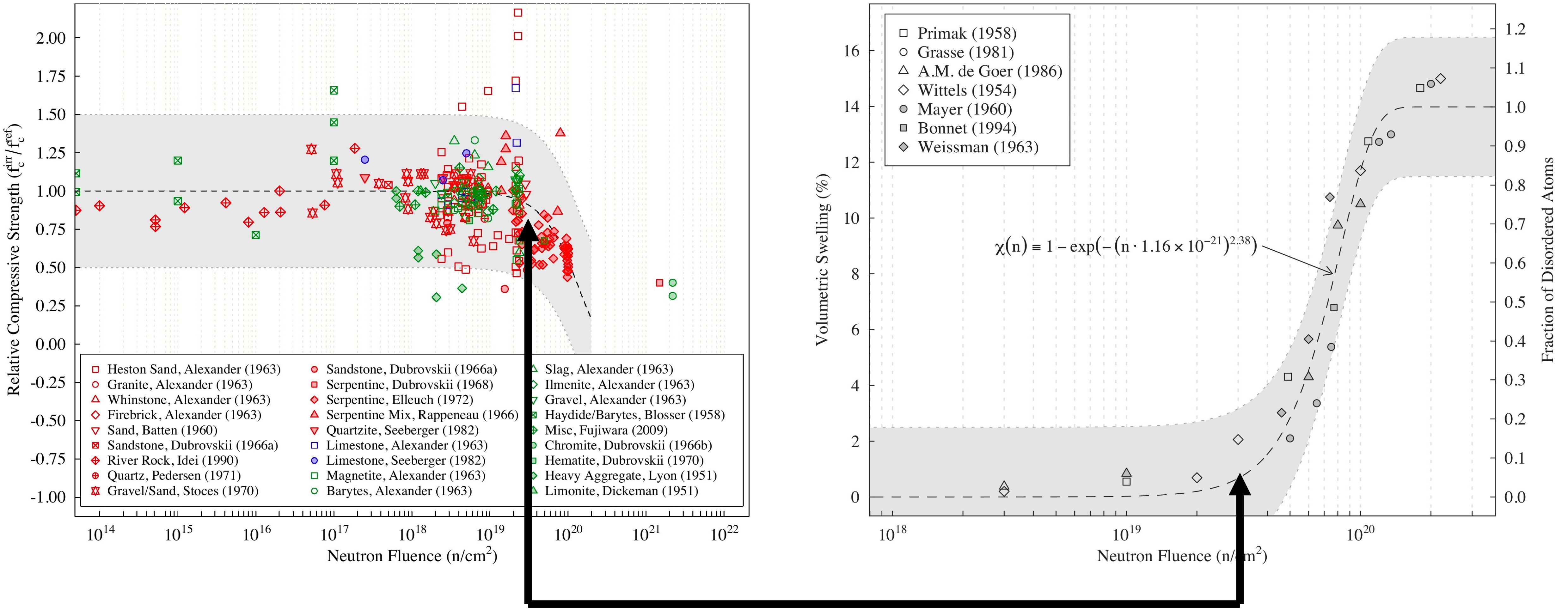
Temperature dependence of a) the long-range order parameter S/S_C, and b) the critical amorphization dose for CuTi, irradiated with 1 MeV electrons

Irradiation-induced amorphization





Irradiation-induced amorphization



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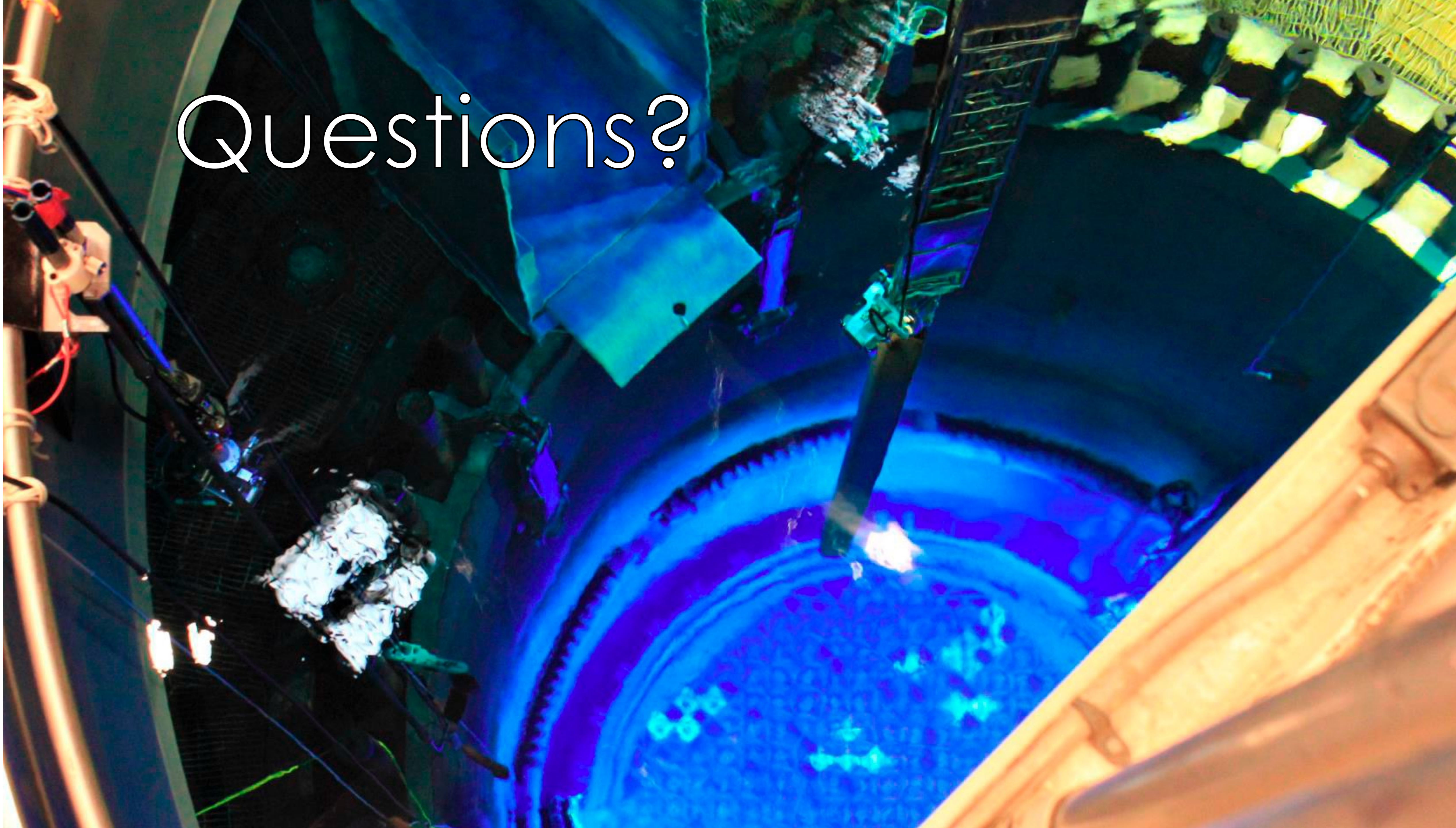
Questions?