Defect Reactions + RIS Intro

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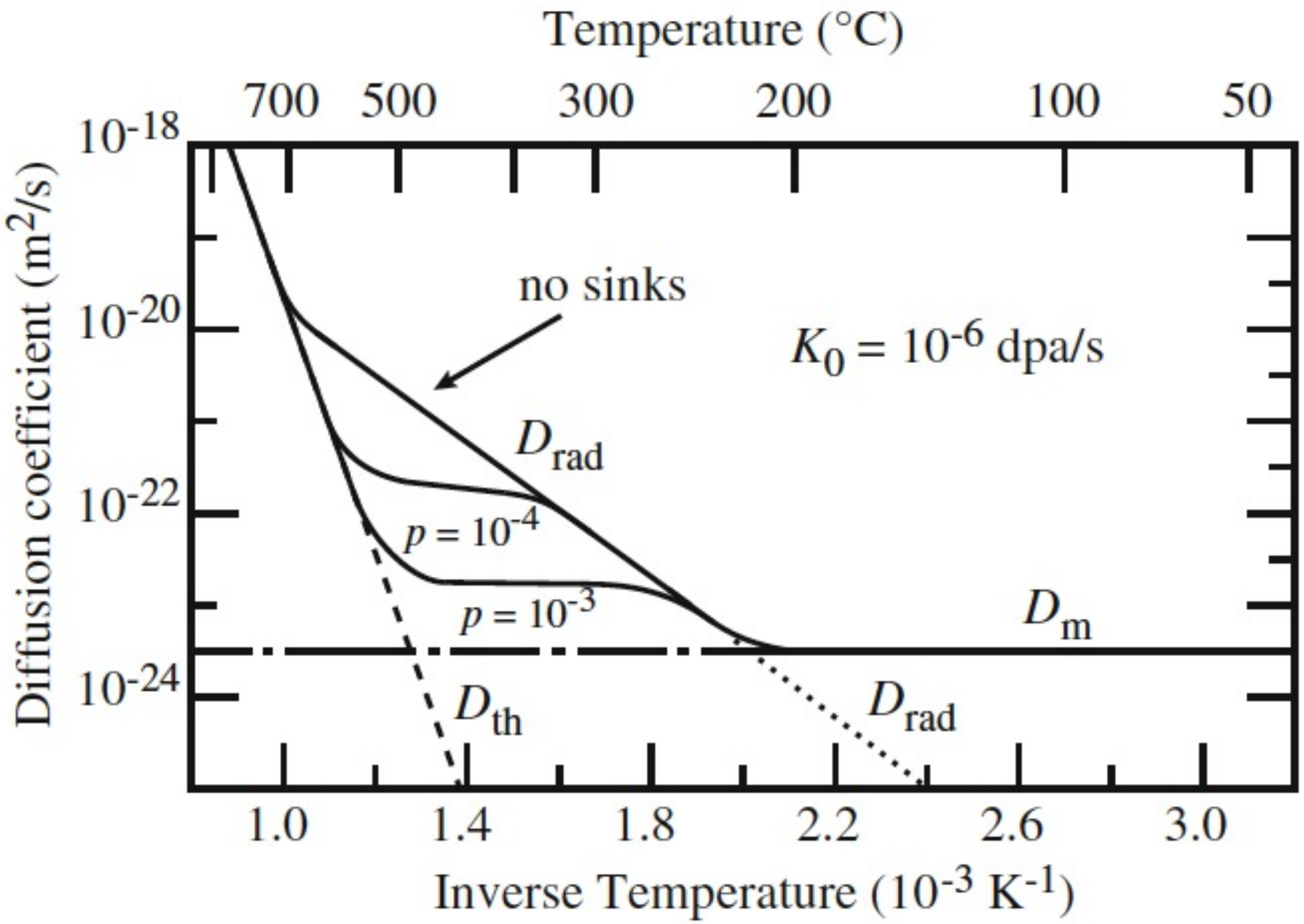
Pulling this now together:



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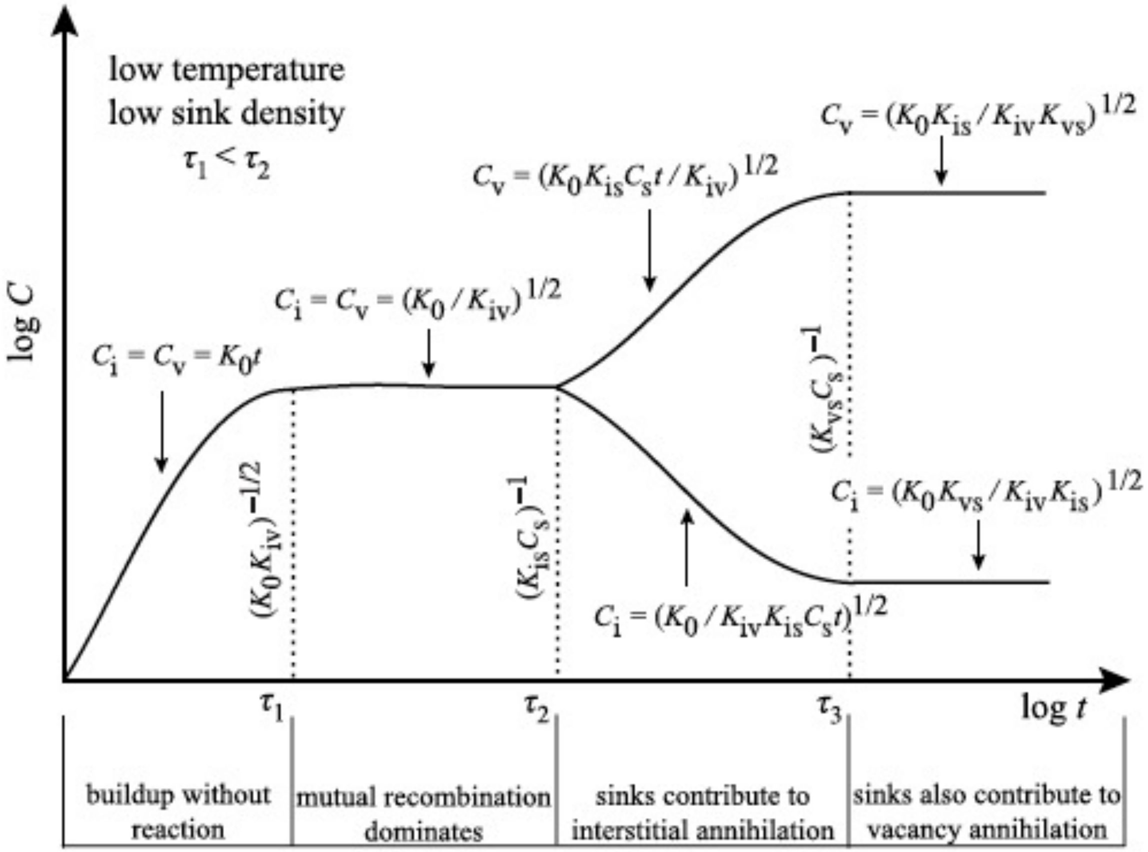

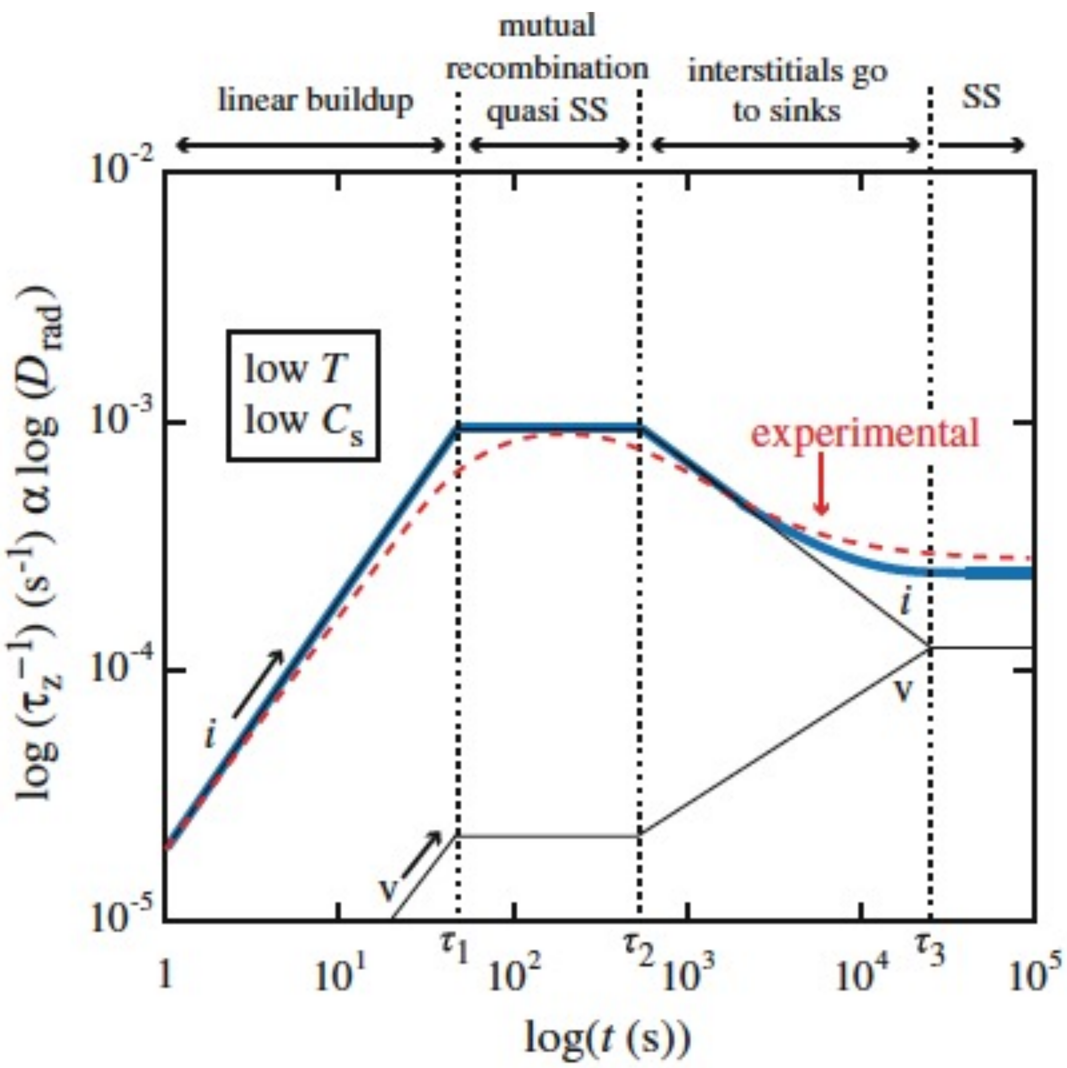

$\mathrm{Log}(D_{rad})$ vs. $\log(t)$

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Rate of Reaction

- We have now determined the relative change of C_i and C_v, but the ***rates are dependent on the reaction rate constant*** K_{AB} (s^{-1}), where the rate of reaction between A & B is:

$$K_{AB} C_A C_B \; reactions/cm^3 s$$

- Analogous to first order chemical reactions
- We will consider two types of reactions:
  - Defect-defect reactions
  - Defect-extended sinks reactions

Point-defect reactions with extended sinks

- To a *first approximation*, sinks at as “perfect” sinks
- In a perfect sink, all defects “stick” completely to the sink and never leak the sink -> think of these as black holes!
  - Result is the point-defect concentration at the surface of the sink is zero
- The rate of defect absorption at a sink is then:

- The sink strength describes the strength or affinity of a sink for defects and is measured in [length^{-2}]. Physically, k_j^{-1} is the mean distance a free defect of type j travels in the solid before becoming trapped.
- For discussion, we will assume unsaturable sinks

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Sink types

- Sinks can behave differently:

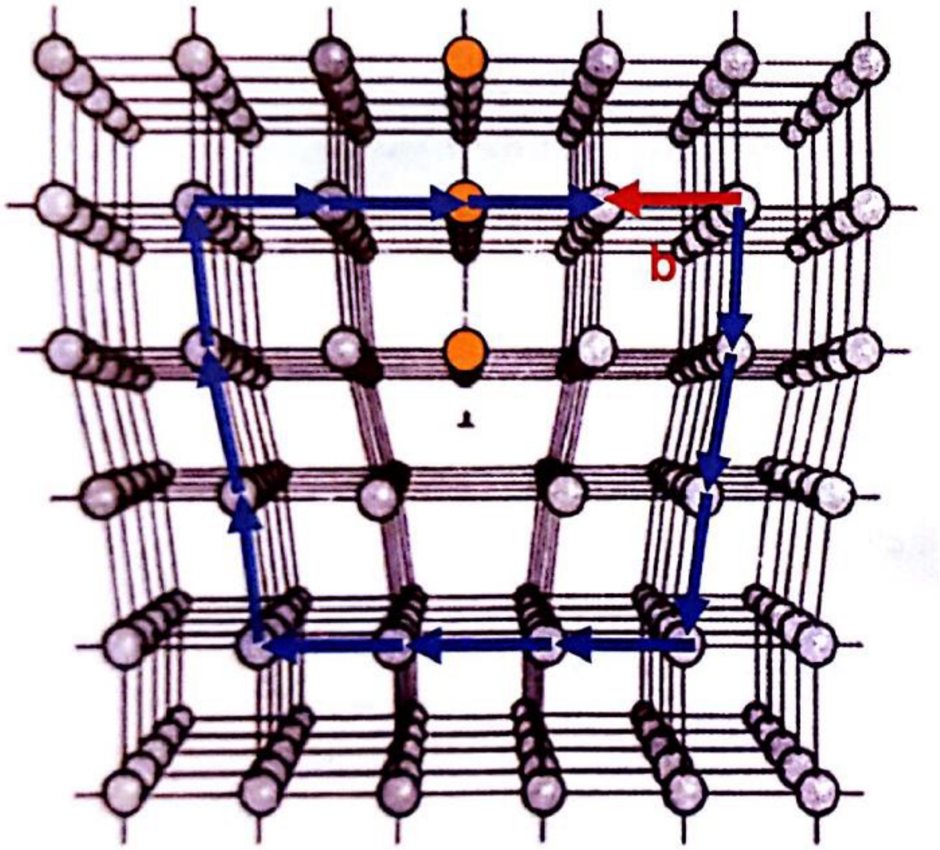
  - Neutral sinks:

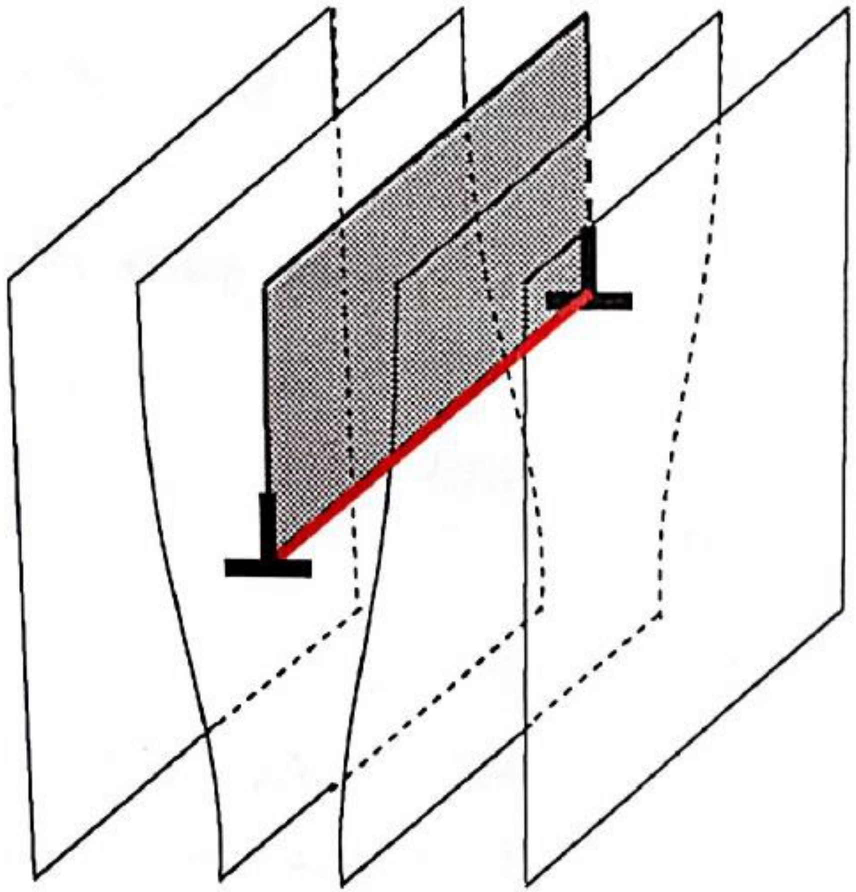
  - Biased sinks:

  - Variable sinks

Sink Type I - Dislocations

- Linear defect
- Edge dislocation is an additional half plane of atoms
- Burgers vector and slip plane defines dislocation





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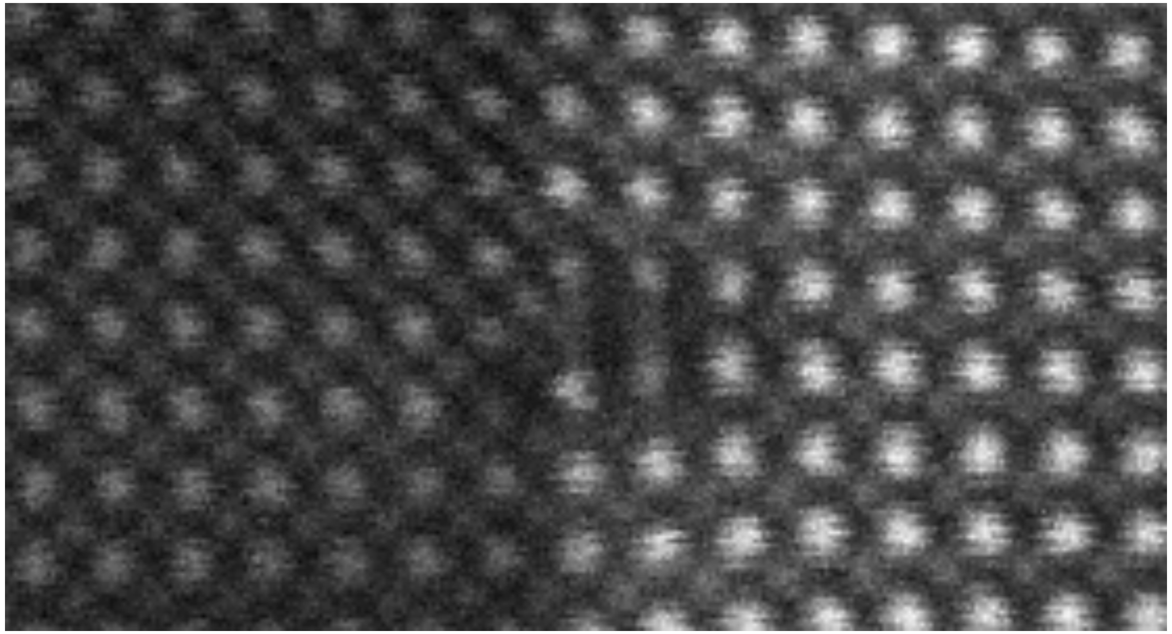
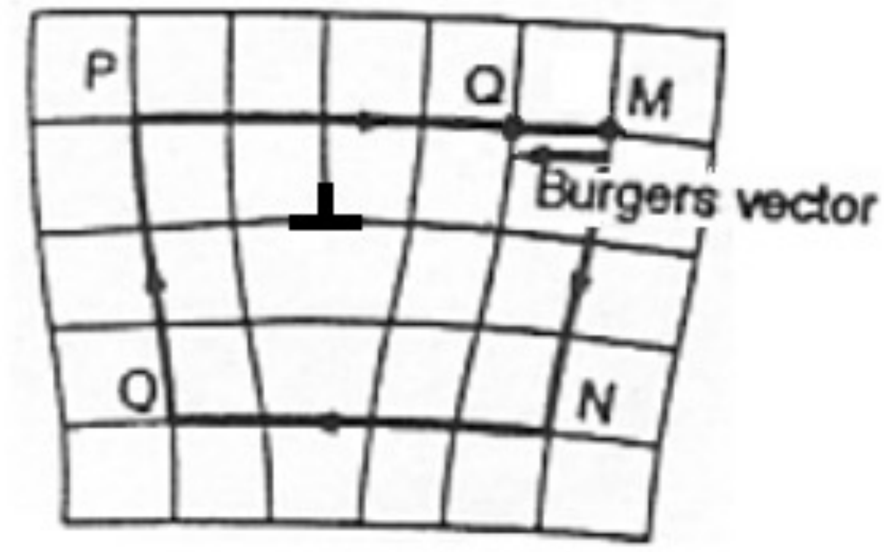
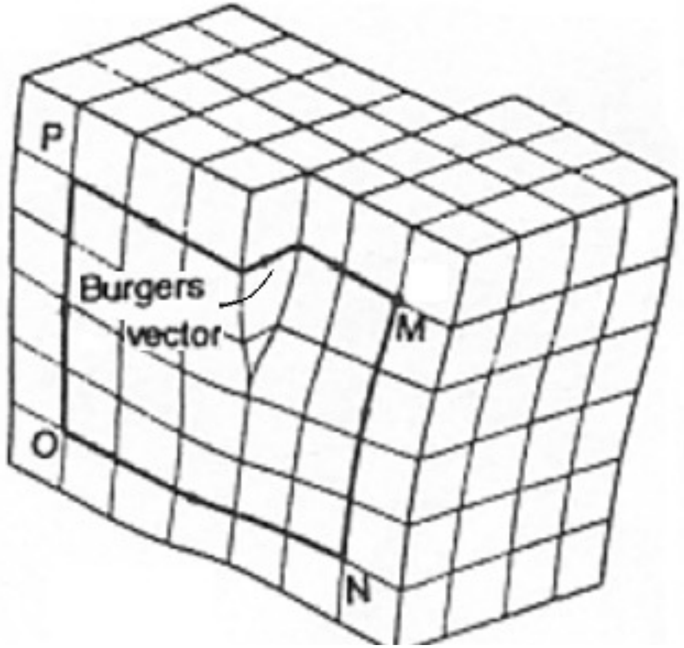


HAADF STEM Image of dislocation between $BaTiO_3$ and $SrTiO_3$

Sink Type I - Dislocations



Edge Dislocation

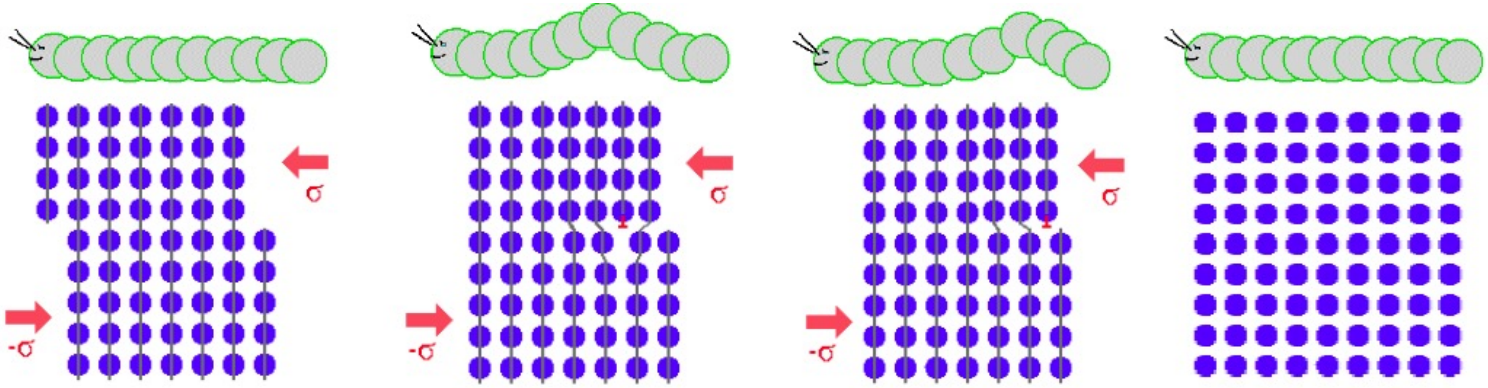


Screw Dislocation

- Three types: Edge, Screw, and Mixed
  - Edge dislocation: line is perpendicular to the Burgers vector
  - Screw dislocation: line is parallel to Burgers vector
  - Mixed dislocations: a combination of edge and screw characterisitics

Sink Type I - Dislocations

- Dislocation motion is the primary form of deformation in a material

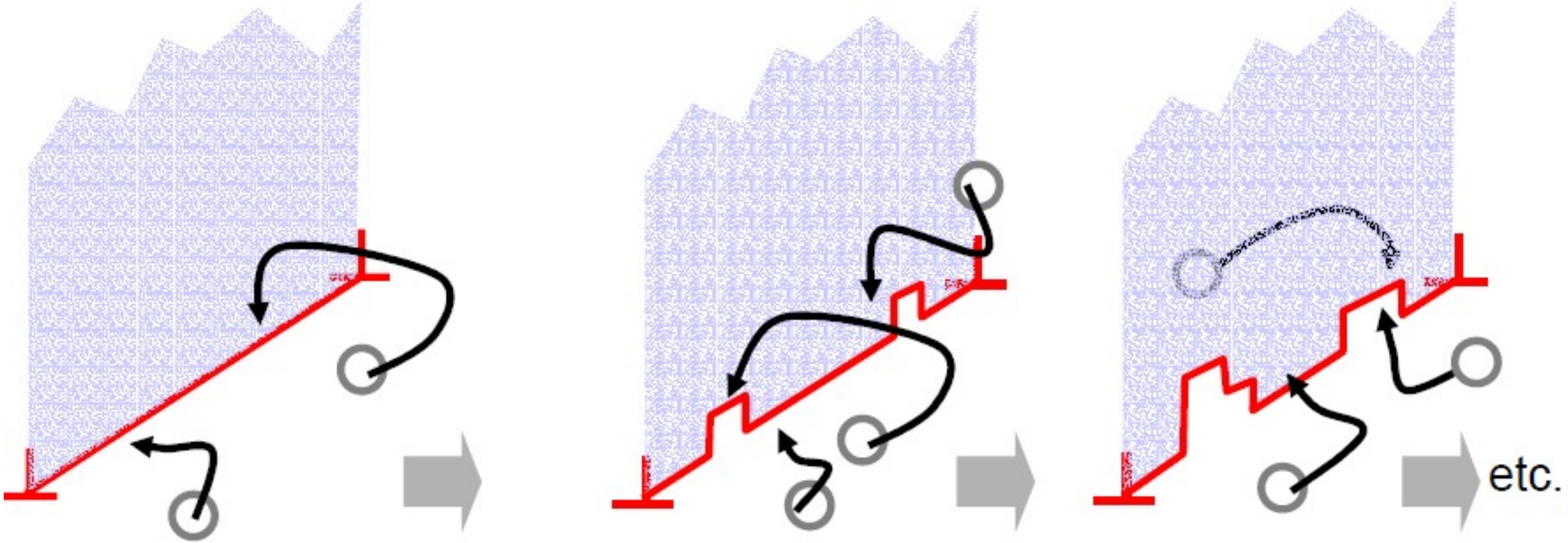


- Anything which impedes dislocation motion will strengthen the material, but may make it brittle
  - Defects which impede dislocation motion:
    - *Other dislocations*
    - *Interstitials*
    - *Impurities*
    - *Grain boundaries*
    - *Etc…*

www.people.virginia.edu/~lz2n/ mse201/mse201-defects.pdf

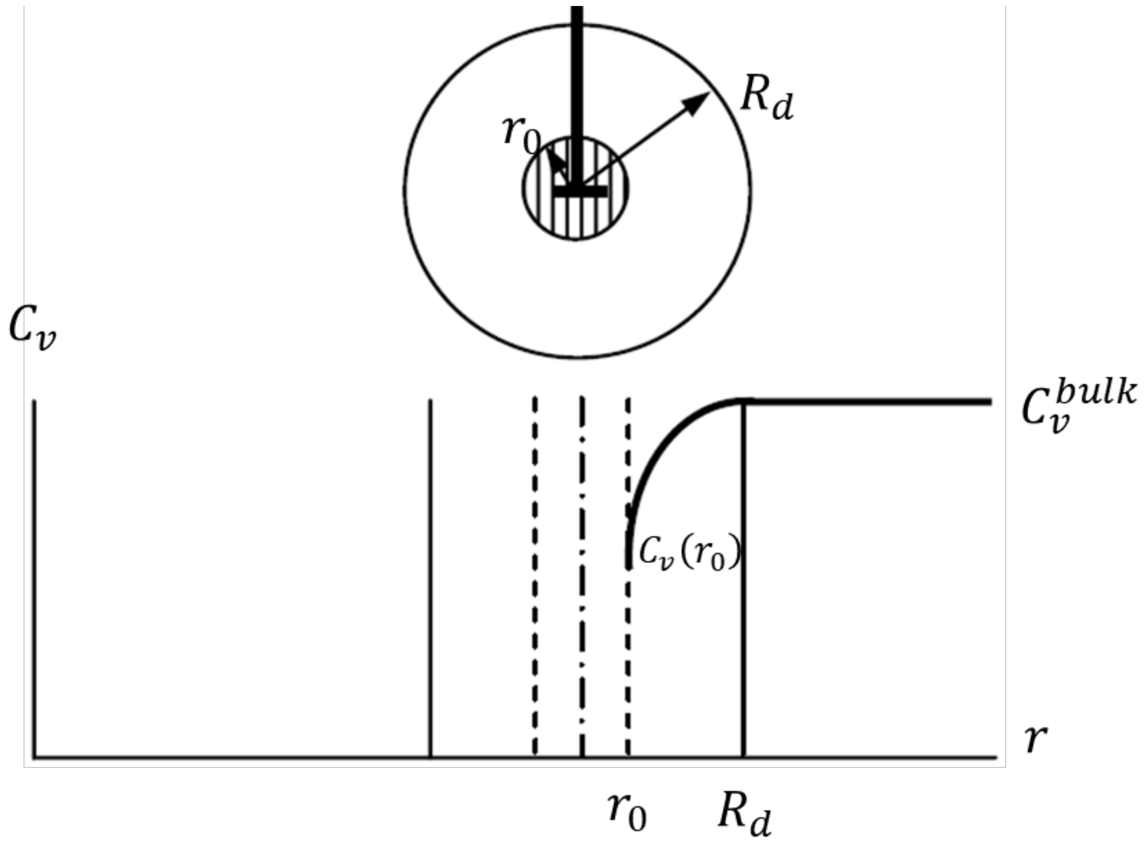
Sink Type I - Dislocations

- Dislocation climb by vacancy absorption
- Leads to irradiation glide and creep



Point Defect Absorption by Dislocations

- Net reduction of strain energy
- Absorption leads to jog formation and climb



- Assumptions to determine rate of absorption
  - Even distribution of dislocation line density ($\boldsymbol{\rho_d}$ – cm^{-2})
  - Only one type of dislocation defect
  - Defects enter but do not exit the dislocation core r_0
  - At a distance R_d the concentration of defects is equal to $C_{i,v}^{bulk}$
  - No influence of the dislocation strain field

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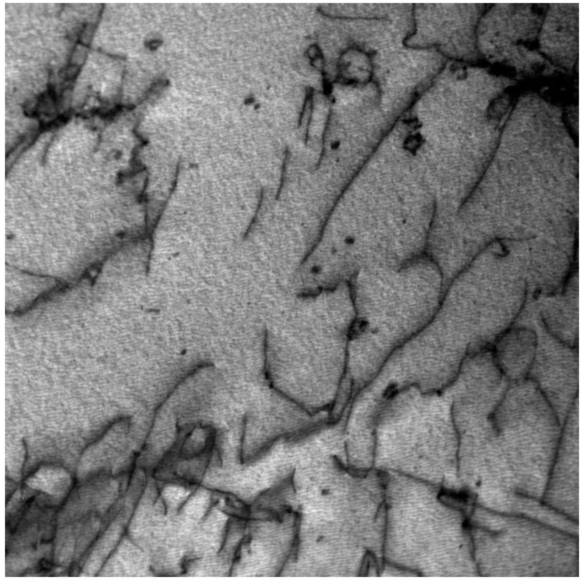

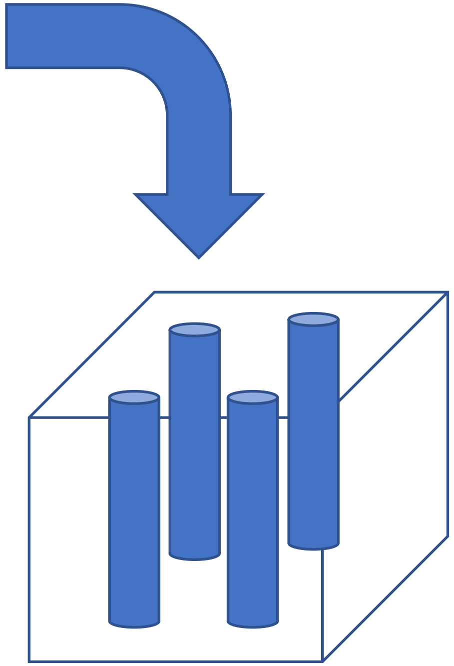

- Assumptions to determine rate of absorption
  - Even distribution of dislocation line density ($\mathbf{p_d}$ – cm^{-2})
  - Only one type of dislocation defect
  - Defects enter but do not exit the dislocation core r_0
  - At a distance R_d the concentration of defects is equal to $C_{i,v}^{bulk}$
  - No influence of the dislocation strain field

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Point Defect Absorption by Dislocations

- Our steady state assumption gives (in radial coordinates):

- The solution is then:

- Using the boundary conditions established by our assumptions:

- Gives us:

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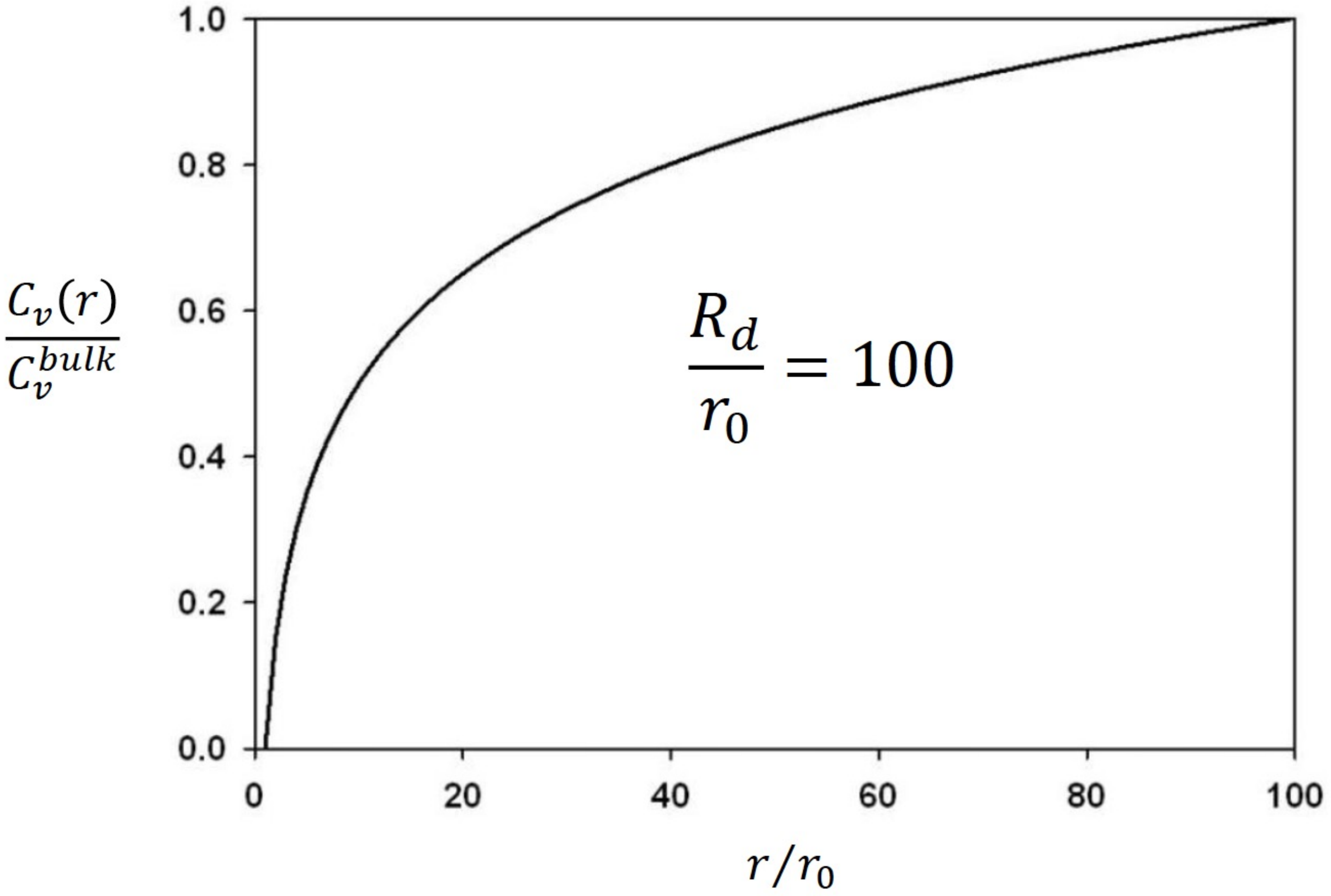
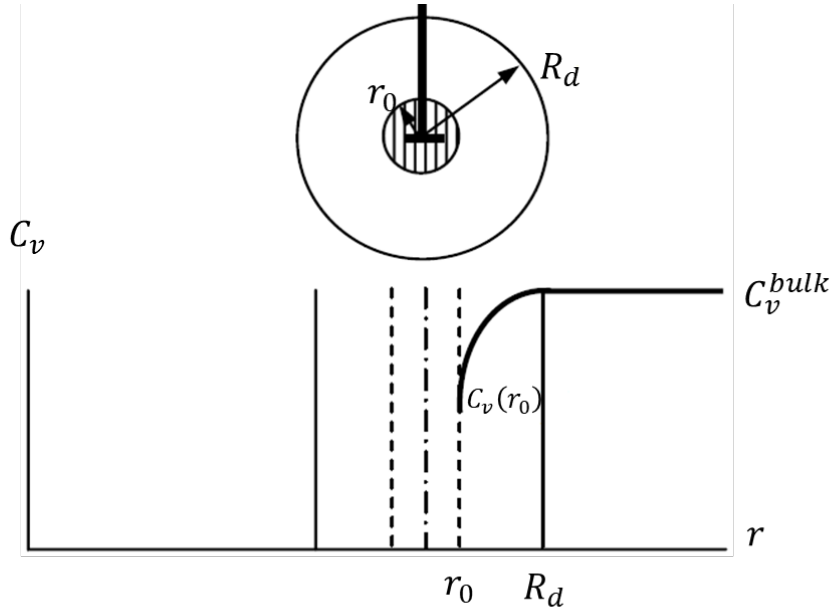
Point Defect Absorption by Dislocations



Point Defect Absorption by Dislocations



Point Defect Absorption by Dislocations

- We derived:

$$C_{i,v}(r) = C_{i,v}^{bulk} \frac{ln\frac{r}{r_0}}{ln\frac{R_d}{r_0}}$$

- and:

$$\frac{dC_{i,v}}{dr} = \frac{C_{i,v}^{bulk}}{ln\frac{R_d}{r_0}} \frac{1}{r}$$

- Rate of absorption per unit length of the dislocation:

- Since there is $\mathbf{p_d}$ cm of dislocation line per cm^3:

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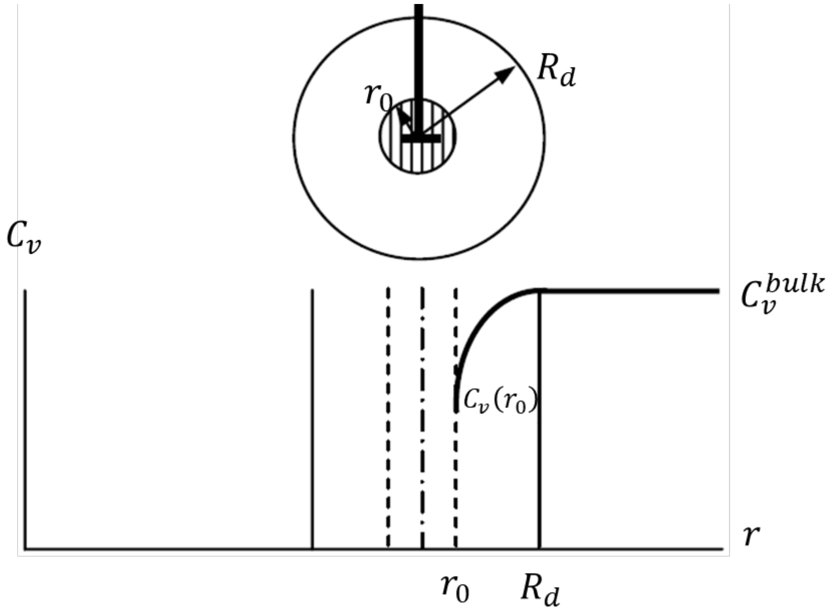
Point Defect Absorption by Dislocations

- For vacancies:

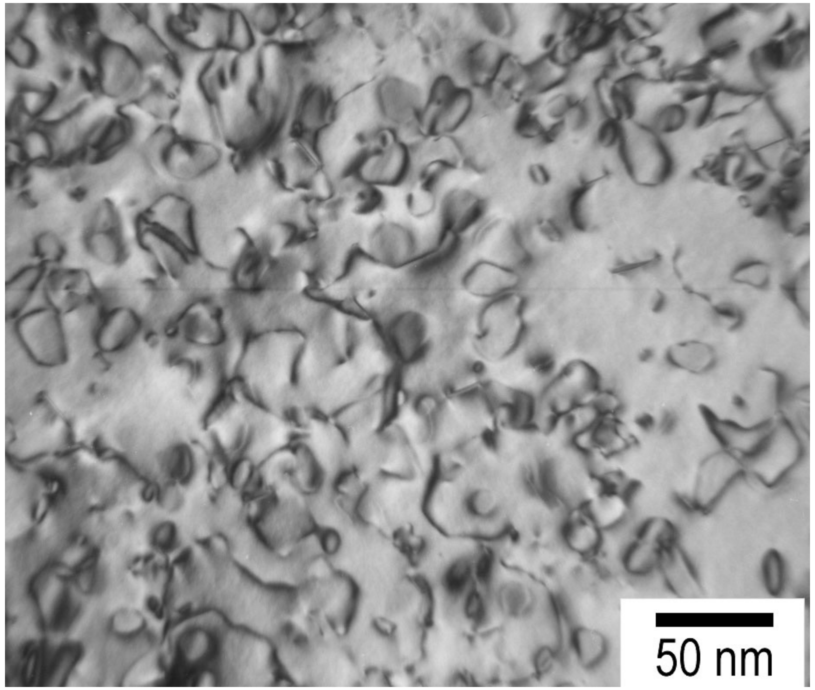
- For interstitials:



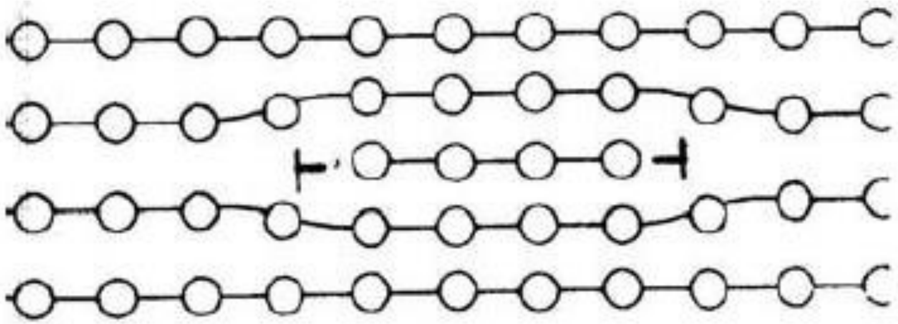
Influence of the dislocation strain field on interstitial is larger (no random walk)

Accounting for dislocation loops

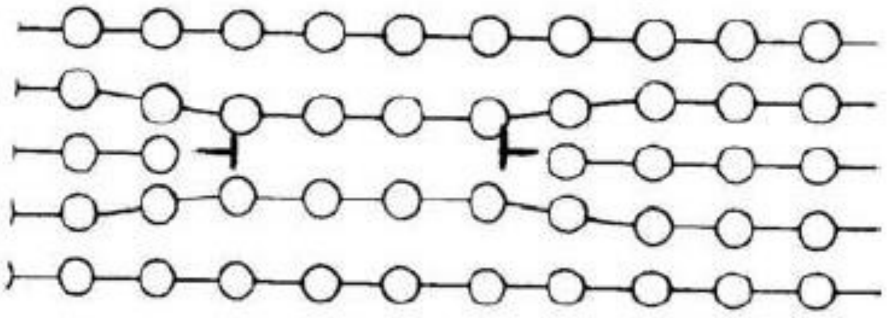
Dislocation Loops in Irradiated 316 SS (2 dpa)



Interstitial Loop



Vacancy Loop



- Dislocation Loop: when a dislocation line forms a closed loop instead of extending until it reaches an interface
  - Character of the dislocation (edge, screw, mixed) changes continuously along the line
  - Loops typically grow

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Accounting for dislocation loops

- We derived the reaction rate and sink strength for dislocation lines, but it is also used for dislocation loops. For loops ρ_d is used but with no consideration of geometry, e.g. the circular dislocation loops are effectively "straightened out"

Sink types

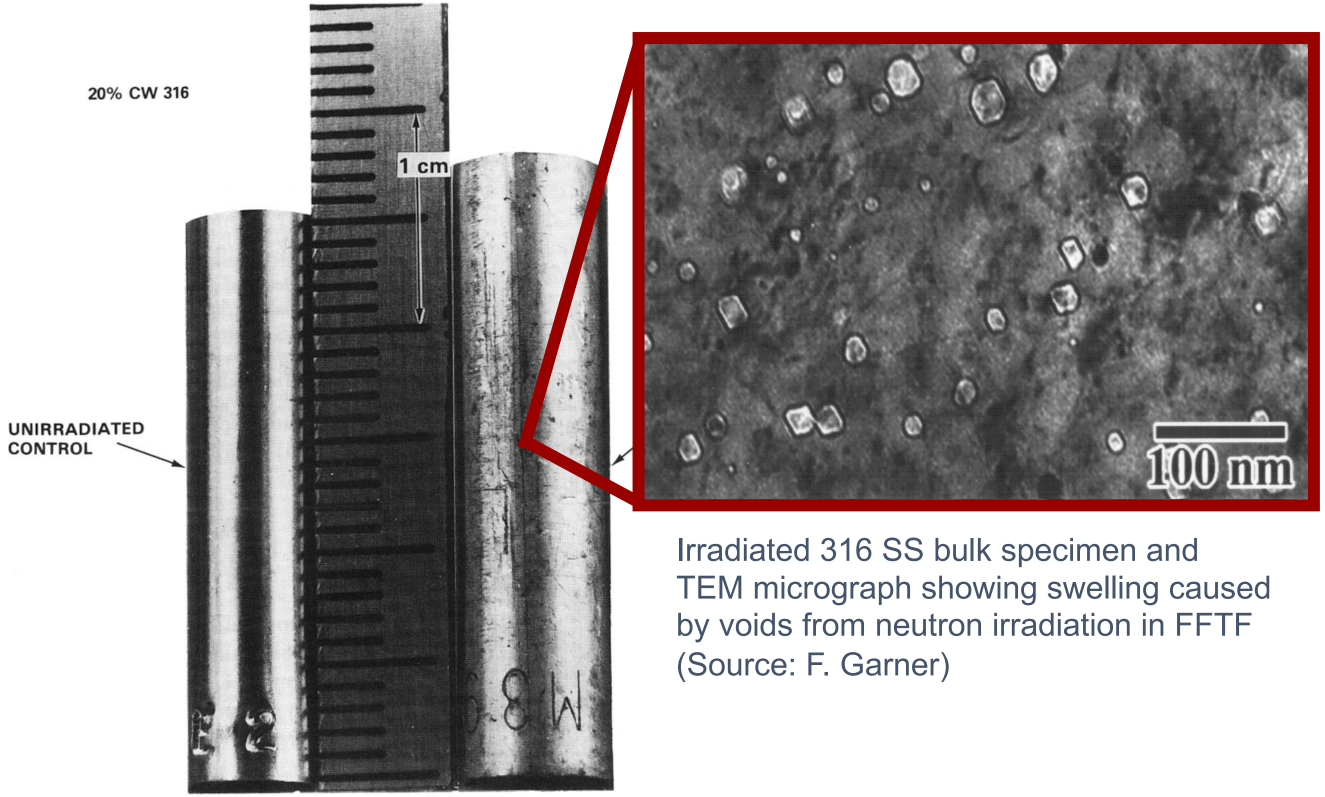
- Sinks can behave differently:

  - Neutral sinks: Neutral sinks show no preference for capturing one type of defect over another. Examples are voids and grain boundaries.

  - Biased sinks: Biased sinks show a preferential attraction for one defect over another. Examples are network dislocations.

  - Variable sinks: Variable sinks act as traps for defects which hold the defect but preserve its identity until annihilation or it is released. Examples are coherent precipitates.

Sink Type II - Cavities



Irradiated 316 SS bulk specimen and TEM micrograph showing swelling caused by voids from neutron irradiation in FFTF (Source: F. Garner)

- Cavities are due to vacancies (and possibly gas atoms) diffusing and coalescing together within the matrix
- Can lead to brittle fracture (bad!)

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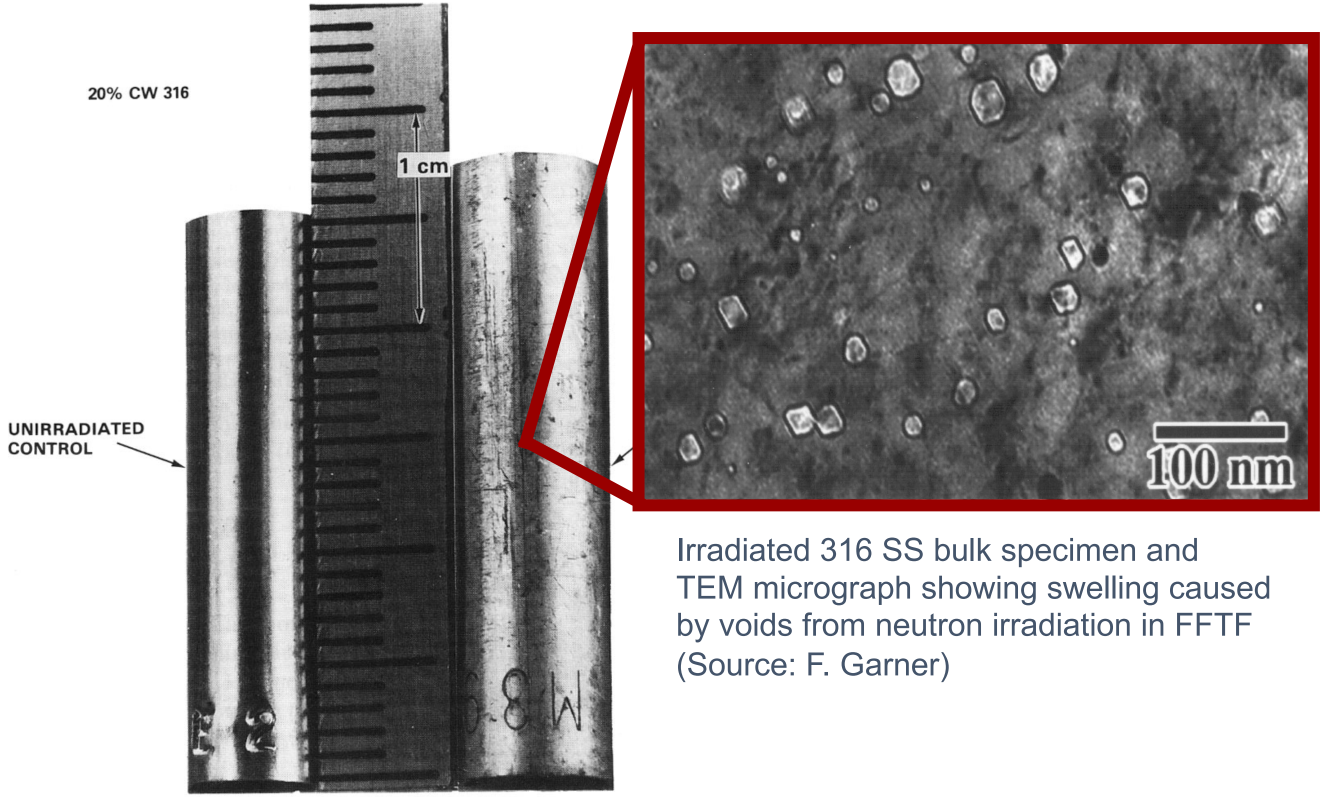
Sink Type II - Cavities



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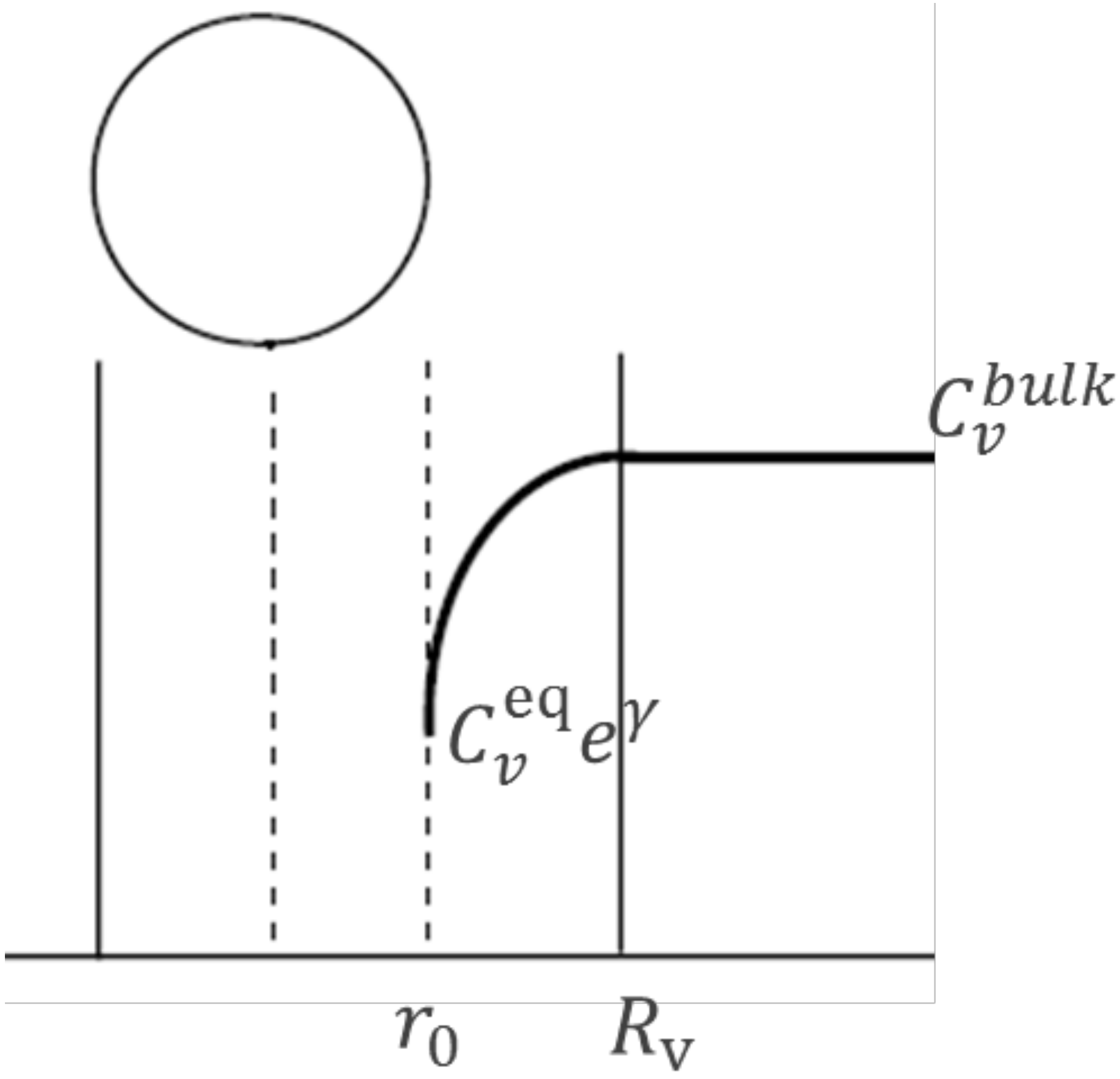
- Similar arguments for point defect absorption can be made in the case of voids:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dC_v}{dr}\right) = 0 \qquad \rightarrow C_v(r) = -\frac{A}{r} + B$$

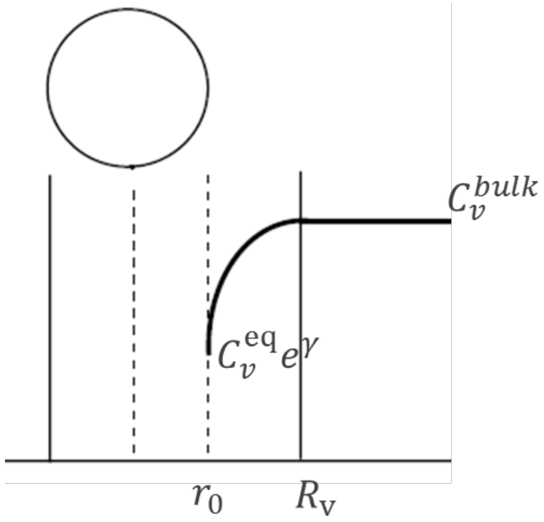
Sink Type II - Cavities



It is assumed that the boundary conditions are:

In these conditions:

Sink Type II - Cavities



Sink Type II - Cavities

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Point Defect Kinetic Equations

- If we neglect clustering:

$$\frac{\partial C_v}{\partial t} = K_0 - K_{iv}C_iC_v - \sum_s K_{vs}C_vC_s + D_v\nabla^2 C_v$$

$$\frac{\partial C_i}{\partial t} = K_0 - K_{iv}C_iC_v - \sum_s K_{is}C_vC_s + D_i\nabla^2 C_i$$

- Example of defect absorption to cavities:

$$\frac{\partial C_v}{\partial t} = K_0 - K_{iv}C_iC_v - z_v p_d D_v C_v + 4\pi R_c N_c D_v C_v$$

$$\frac{\partial C_i}{\partial t} = K_0 - K_{iv}C_iC_v - z_v p_d D_i C_i + 4\pi R_c N_c D_i C_i$$

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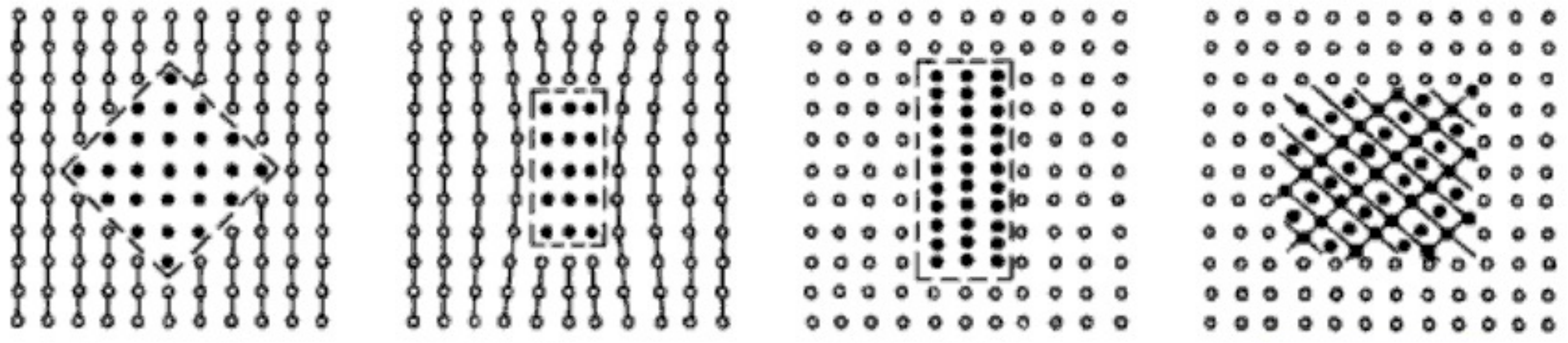
Sink Type III – Coherent Precipitates (PPTs)



a) b) c) d)

- Precipitates are the result of the local solubility limit being reached causing a new phase to form
- Precipitates can be either coherent, partially coherent or incoherent
  - Coherency: a perfect lattice match between the PPT and matrix
  - Coherency affects how dislocations interact with the PPT
  - Coherency can also affect diffusion in and around the PPT

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Sink Type III – Coherent Precipitates (PPTs)

- Precipitates impede dislocation motion
- Inclusion of precipitates can strengthen a material

https://www.youtube.com/watch?v=zNZyAN9y3kY

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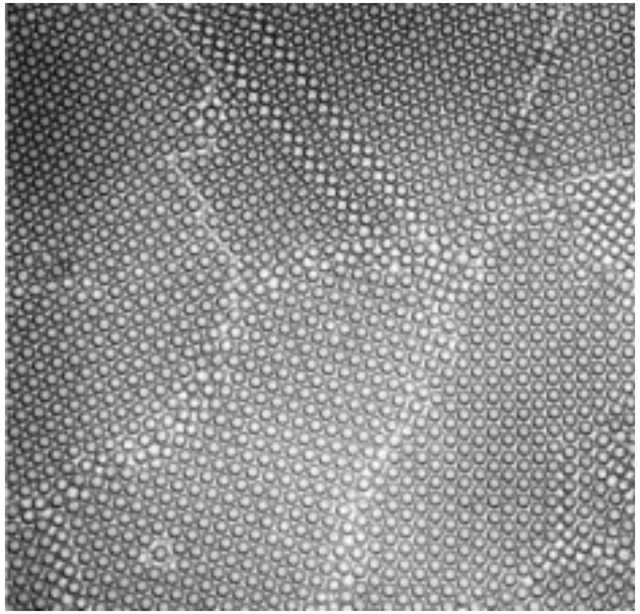
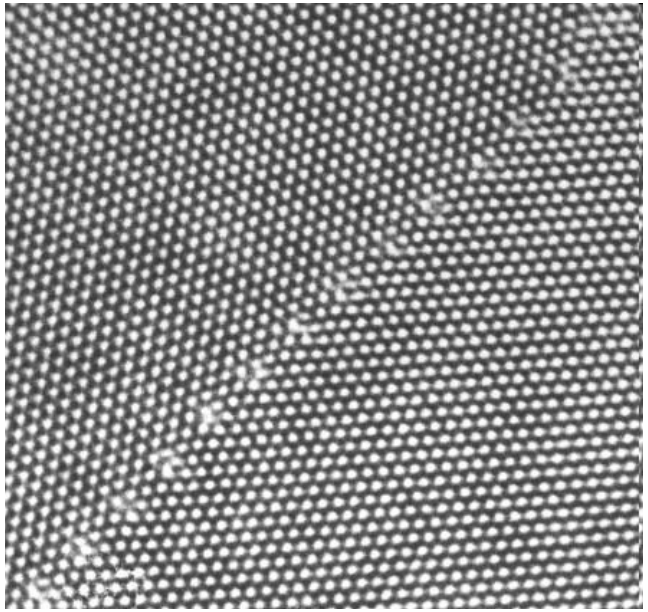
Sink Type III – Coherent Precipitates (PPTs)

Sink Type IV – Grain Boundaries



Bubble Raft Model of Grain Boundaries

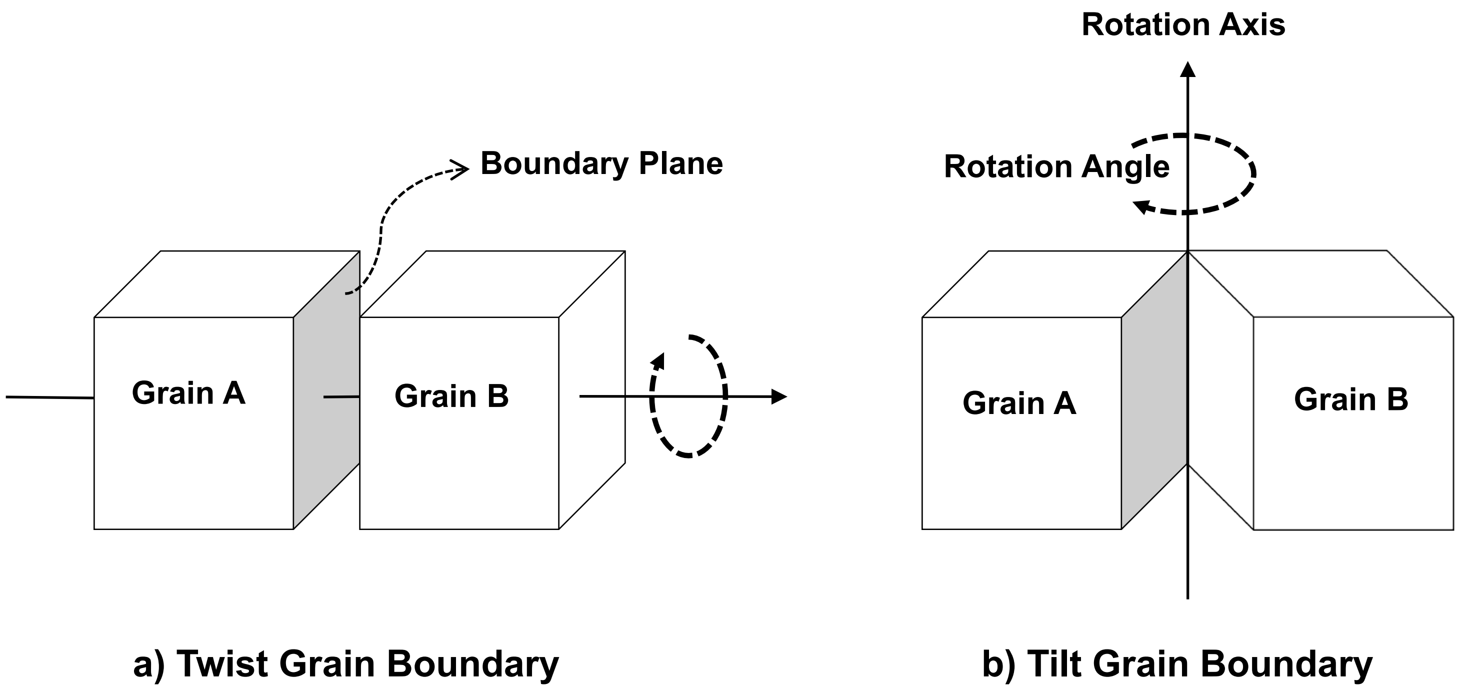


HRTEM image of a Σ19 GB in Al

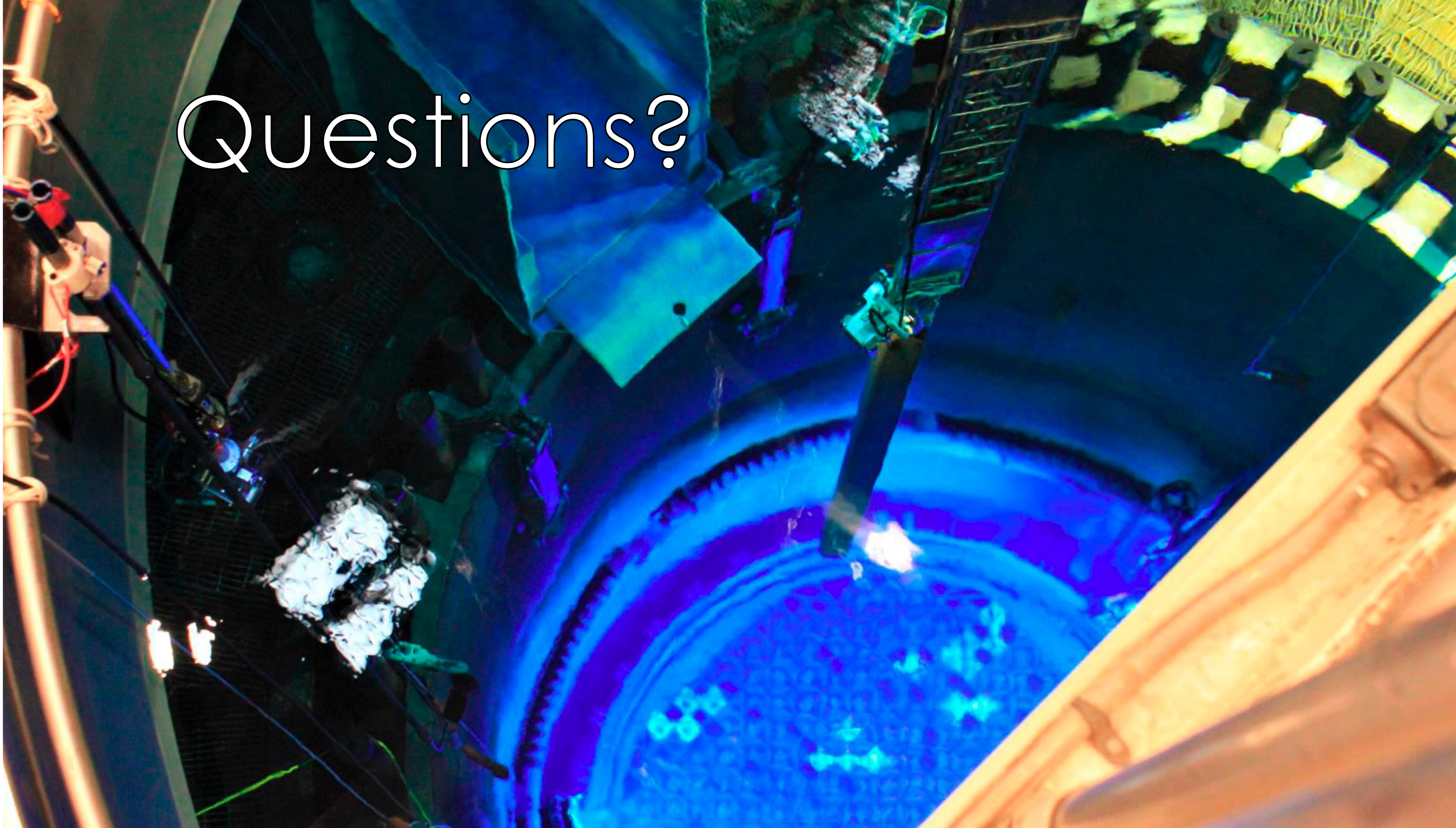
- A Grain Boundary is a general planar defect that separates regions of different crystalline orientation (i.e. *grains*) within a polycrystalline solid
- Grain boundaries can affect creep strength, yield strength, and diffusion

http://www.allenjhall.com/content/category/work/materials-science-and-engineering/

Sink Type IV – Grain Boundaries



- Grain boundaries can have twist, tilt, or mixed character
- Variations in the degree of misalignment between two adjacent grains are possible


Questions?