

# Defect Sinks and Their Reactions II

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# Welcome back!

- Class logistics

- Today:

- 1. Primary lecture on defect reactions at sinks (~55 minutes)
    2. Lecture break (~5 minutes)
    3. Midterm feedback with CRLT

- Wednesday (10/27)

- 1. Review and Q&A to last weeks guest lecture
      - *Watch it if you haven't!*
    2. Midterm review and discussion

- Next Monday (11/1)

- **Midterm**

- In-class
    - 80 minutes
    - 1 page – 1 sided "helper sheet" allowed (Equations/constants provided anyways)
    - Course text allowed (open book)
    - Simple function/graphing calculator allowed



# Point Defect Kinetic Equations

- If we neglect clustering:

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

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



# Sink types

- Sinks can behave differently:

- **Neutral sinks:** Neutral sinks show no preference for capturing one type of defect over another.

Coherent precipitates

- **Biased sinks:** Biased sinks show a preferential attraction for one defect over another.

Grain boundaries

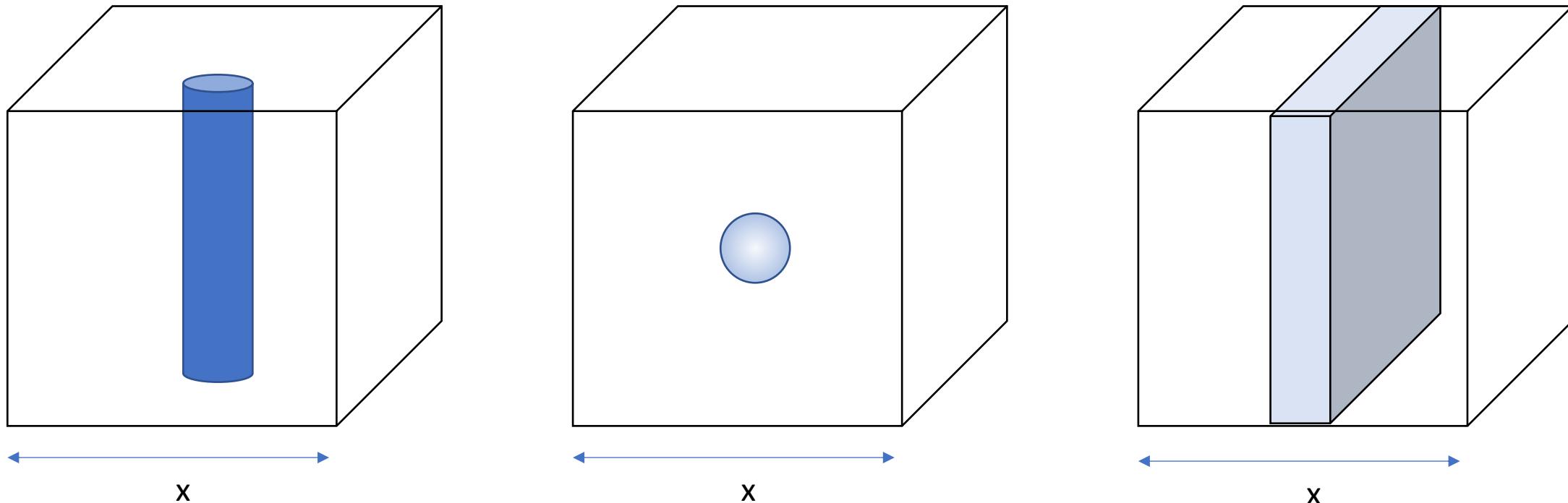
- **Variable sinks:** Variable sinks act as traps for defects which hold the defect but preserve its identity until annihilation or it is released.

Dislocations



# A simple thought experiment for $K_{vs}/K_{is}$

- Assume unbiased defect sink, radius/length of interaction is  $10a_0$

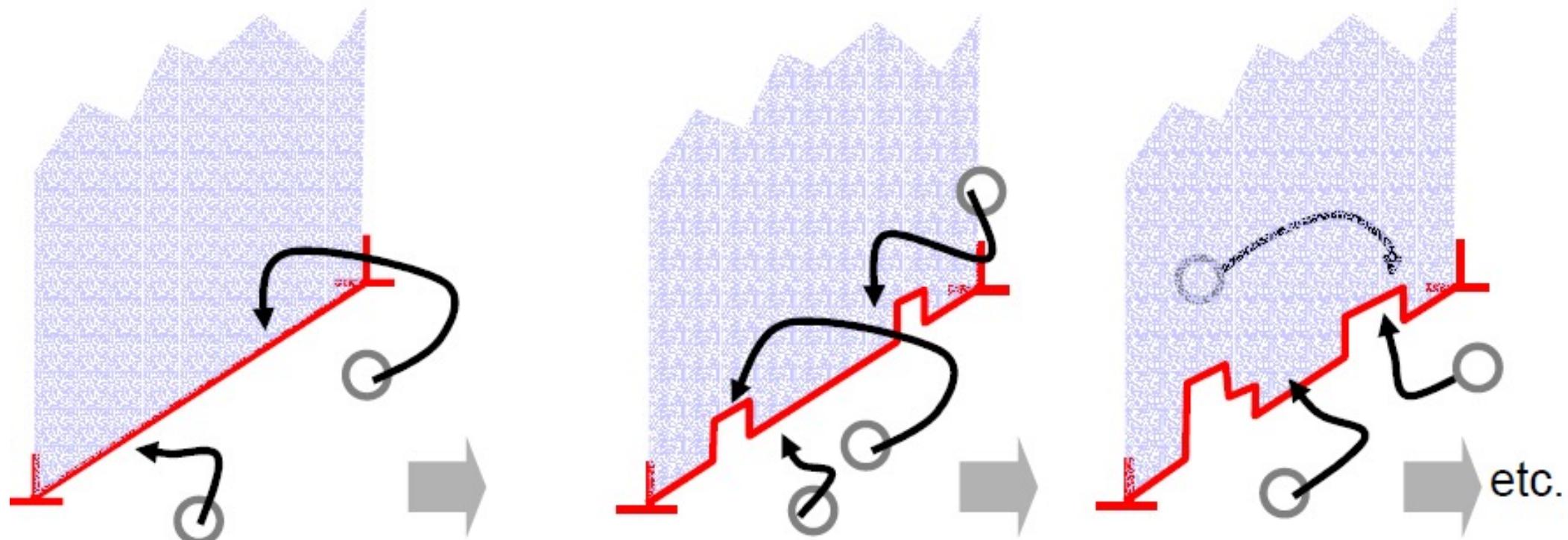


What sink will have the highest reaction rate (e.g. sink strength)?



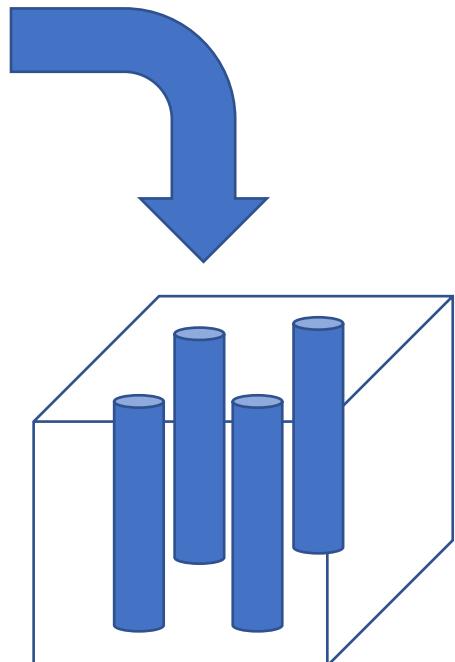
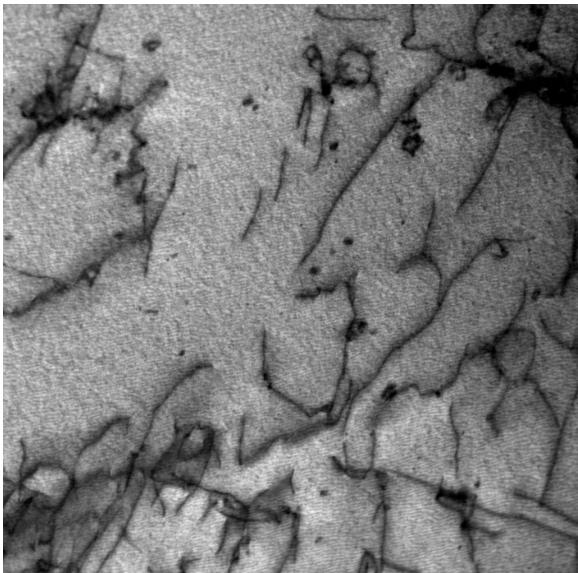
# Sink Type I - Dislocations

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



# Point Defect Absorption by Dislocations

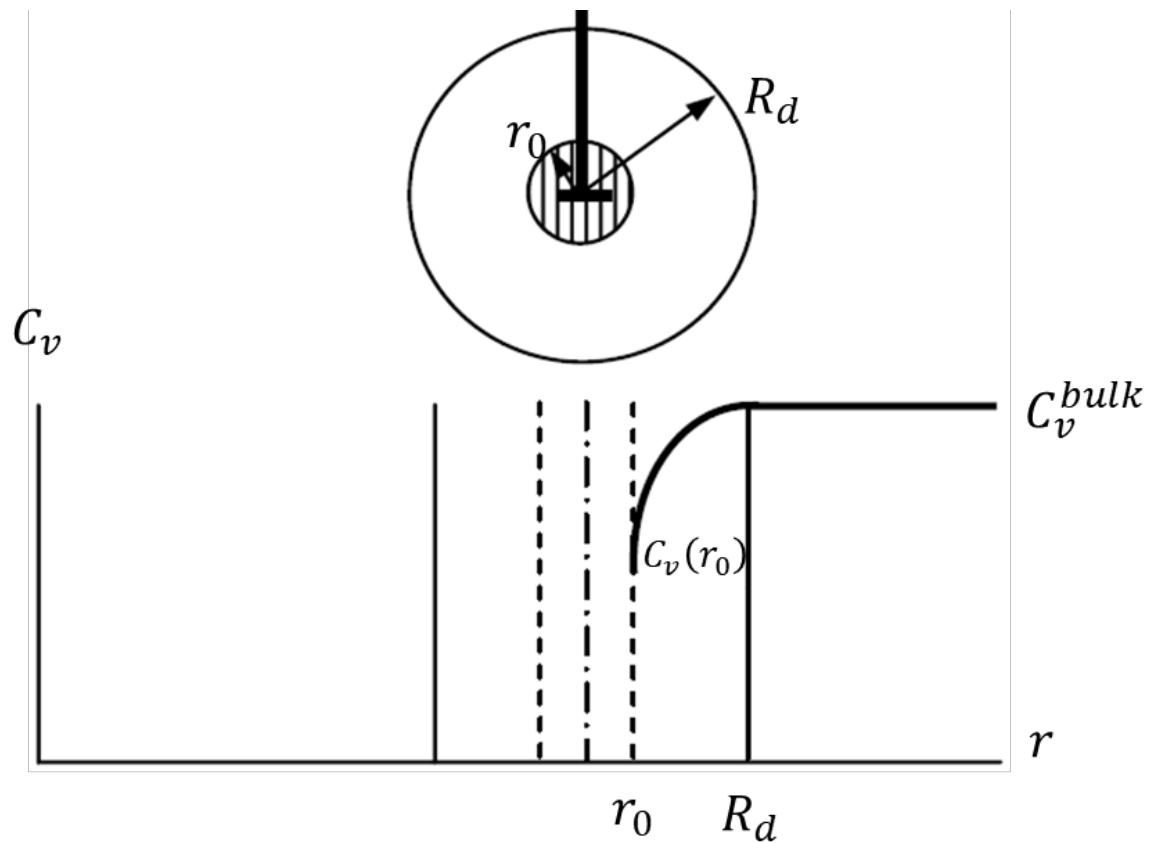
- Net reduction of strain energy
- Absorption leads to jog formation and climb



- Assumptions to determine rate of absorption
  - Even distribution of dislocation line density ( $p_d$  – cm<sup>-2</sup>)
  - 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):

$$\frac{1}{r} \frac{d}{dr} \left( r \frac{dC_{i,v}}{dr} \right) = 0$$

- The solution is then:

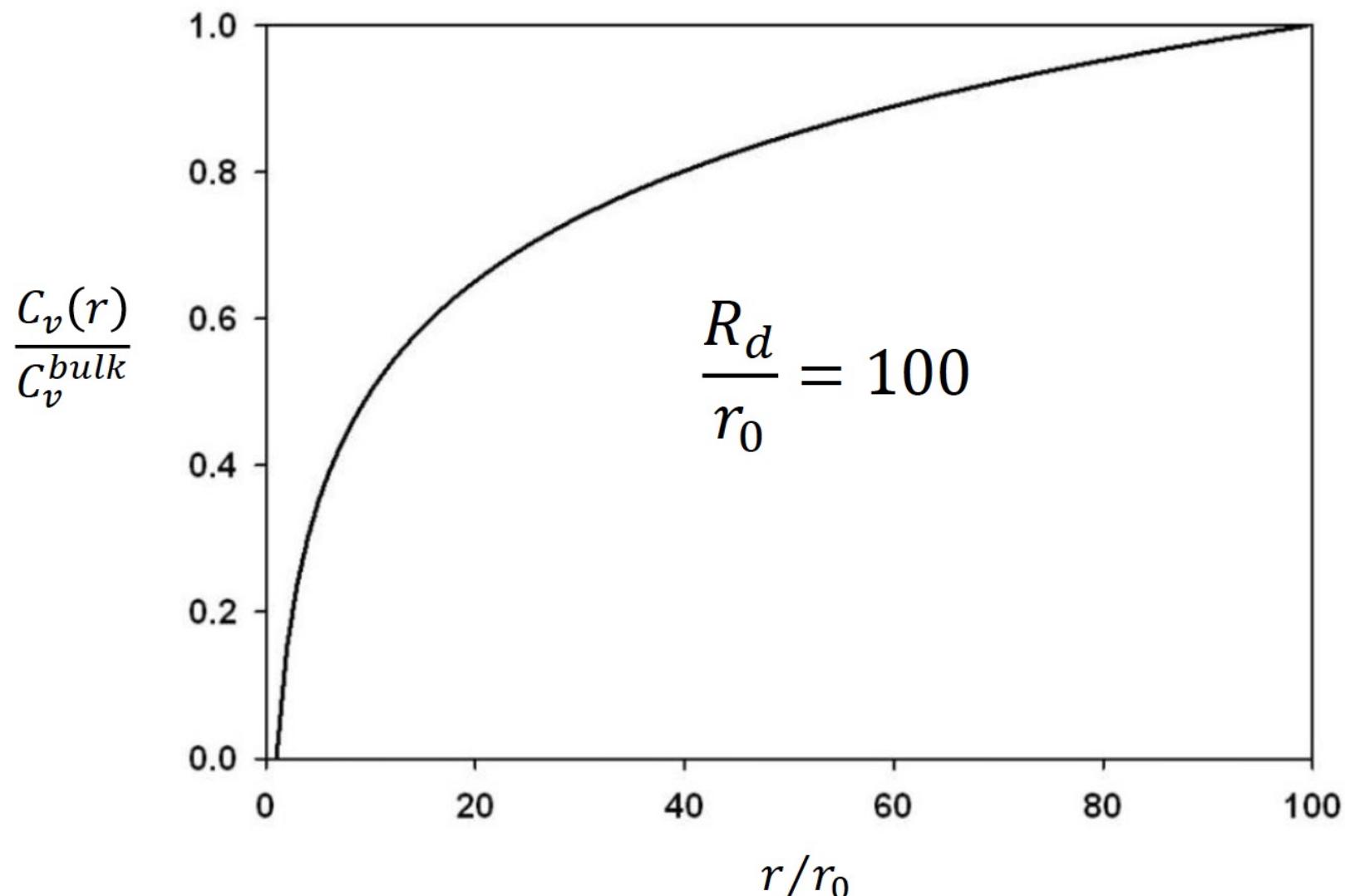
$$C_{i,v} = A \ln(r) + B$$

- Using the boundary conditions established by our assumptions:

- Gives us:



# Point Defect Absorption by Dislocations

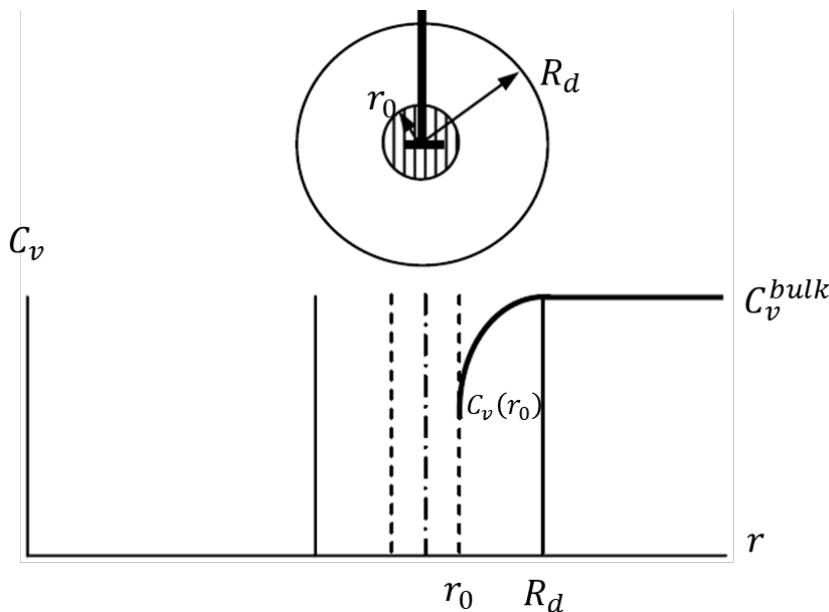


# Point Defect Absorption by Dislocations

We now need the rate of absorption per unit length of the dislocation, e.g. the flux to the line dislocation:

$$j^{disl} = \frac{\text{disl. surface area} \times \text{defect flux}}{\text{dislocation length}}$$

$$j^{disl} = \frac{2\pi r_o L \times \text{defect flux}}{L} = 2\pi r_o \times \text{defect flux}$$



The defect flux is dependent on the diffusion of the defects and their concentration, giving:

$$j^{disl} = 2\pi r_o D_{i,v} \left( \frac{dC_{i,v}}{dr} \right)_{r_o}$$



# Point Defect Absorption by Dislocations

- Now that we have:

$$j^{disl} = 2\pi r_o D_{i,v} \left( \frac{dC_{i,v}}{dr} \right)_{r_o}$$

- We can substitute our previous equation:

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

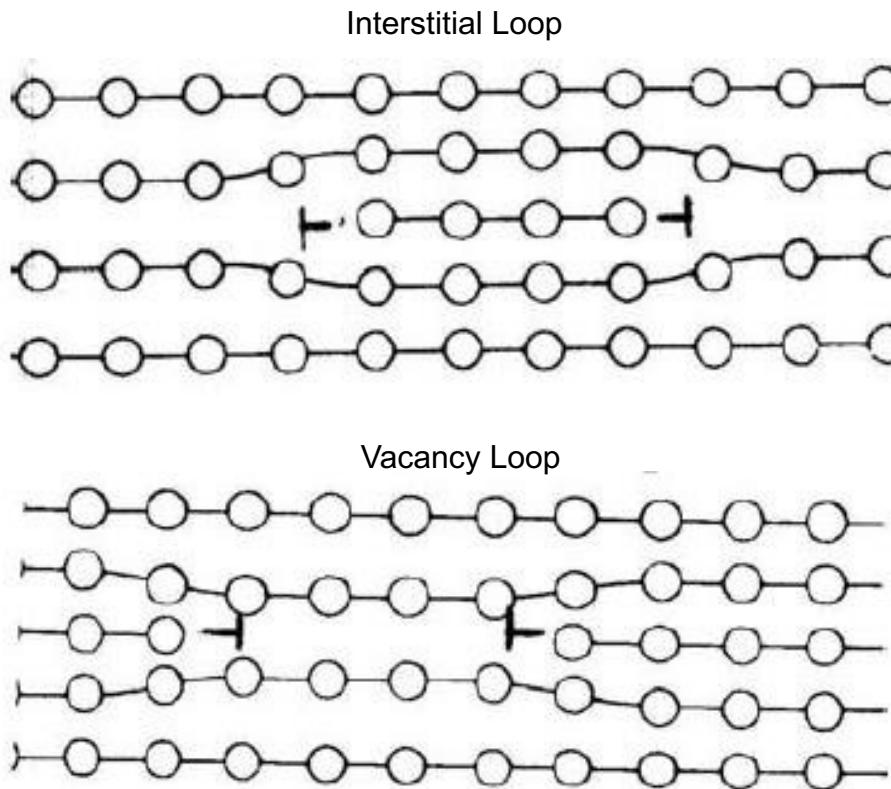
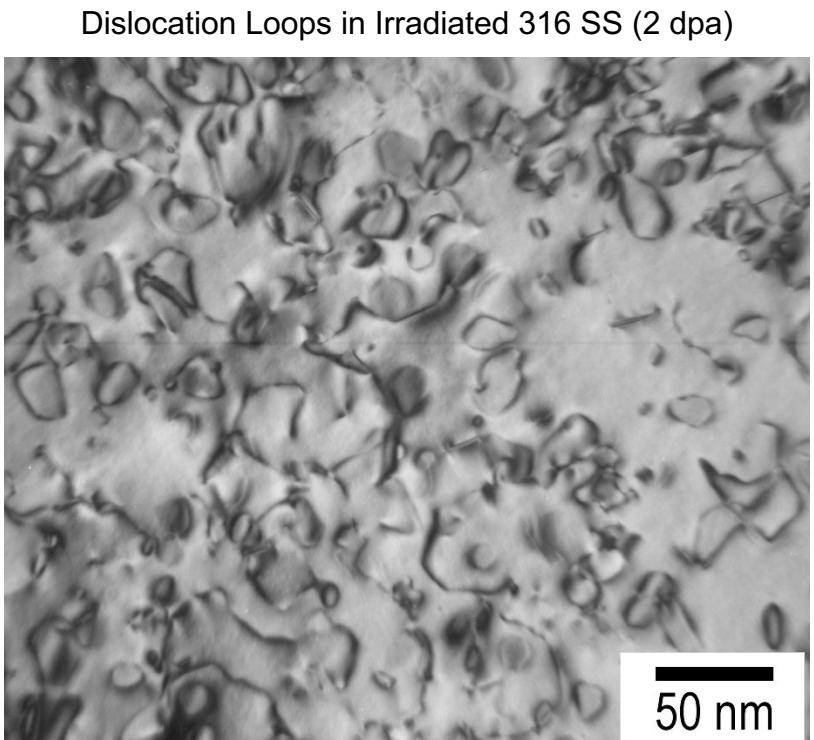
- Into the above giving:

$$j^{disl} = 2\pi r_o D_{i,v} \frac{C_{i,v}^{bulk}}{\ln \frac{R_d}{r_0}}$$

- Since there is **p<sub>d</sub>** cm of dislocation line per cm<sup>3</sup>:

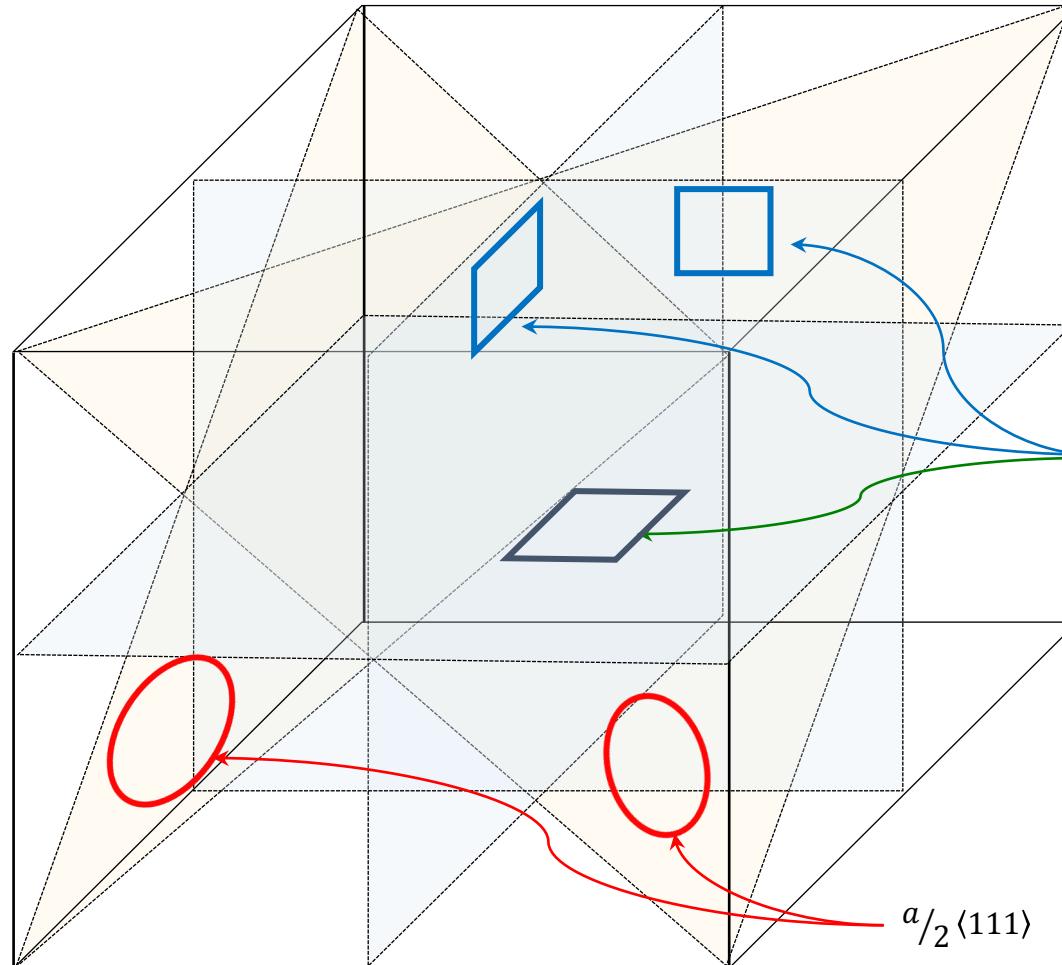


# Accounting for dislocation loops

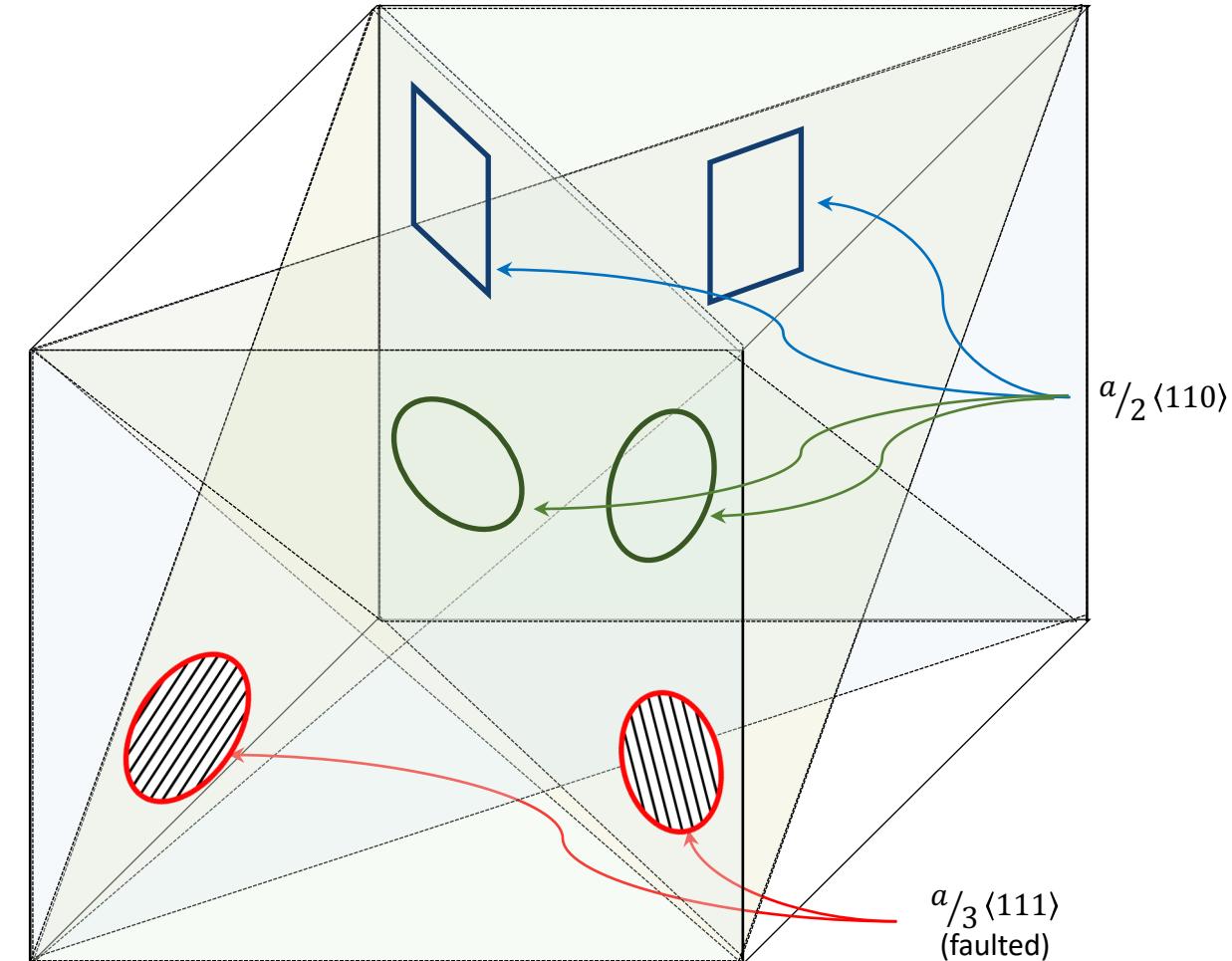


- Dislocation Loop: when a dislocation line forms a closed loop instead of extending until it reaches an interface
  - Character of the dislocation (edge, screw, mixed) changes continuously along the line
  - Loops typically grow

For most BCC and FCC materials the Burgers vector and habit plane are well known



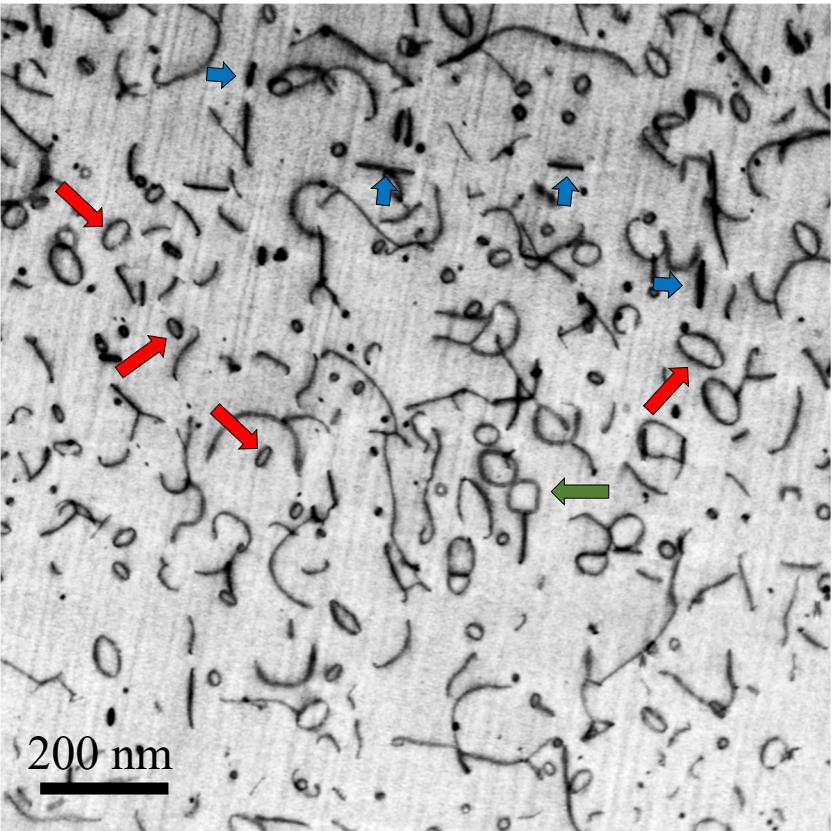
Body Centered Cubic  
(BCC)



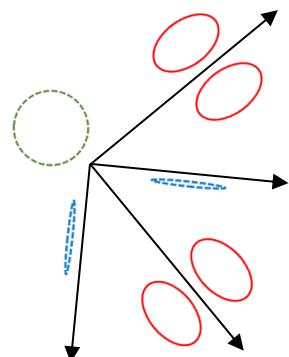
Face Centered Cubic  
(FCC)



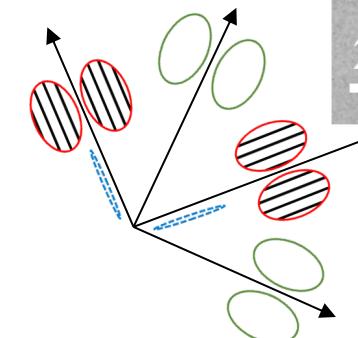
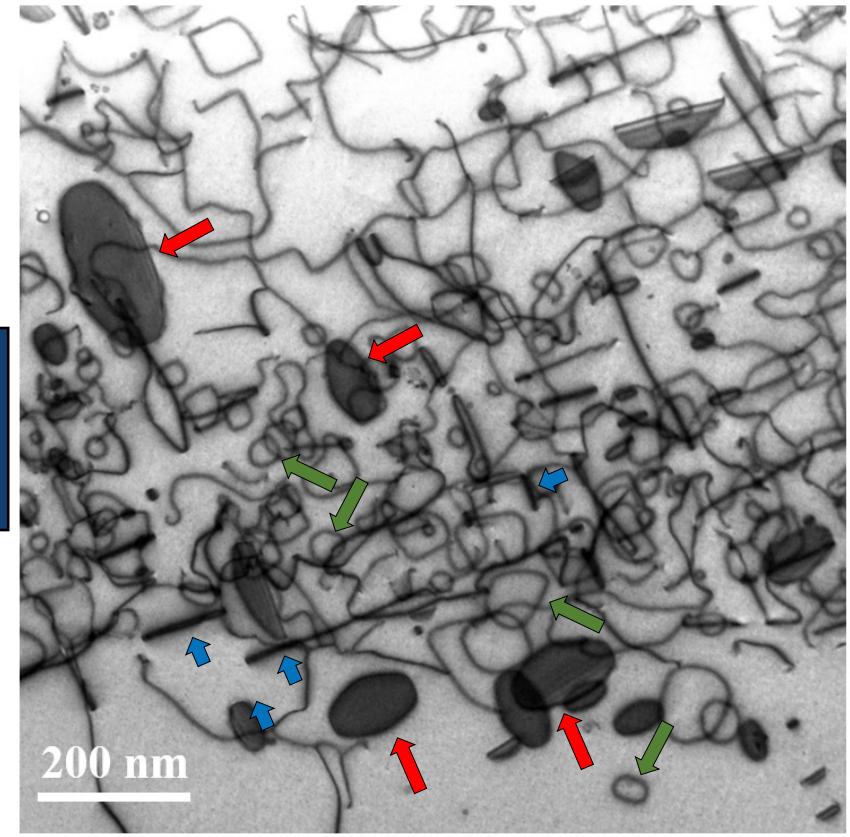
For most BCC and FCC materials the Burgers vector and habit plane are well known



Body Centered Cubic  
(BCC)



Imaging down  
the [100] zone



Face Centered Cubic  
(FCC)

# 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  $p_d$  is used but with no consideration of geometry, e.g. the circular dislocation loops are effectively “straightened out”



# Sink types

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Coherent precipitates

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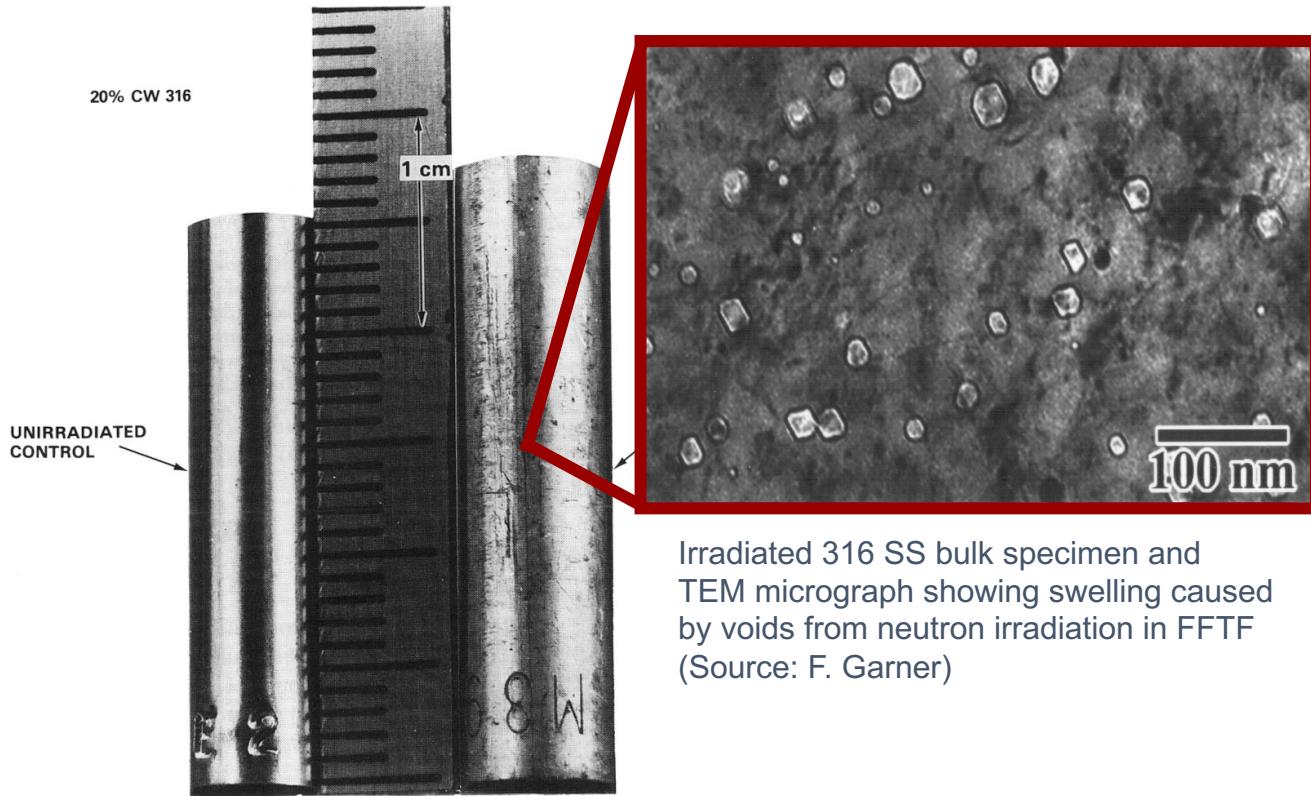
Grain boundaries

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

Dislocations



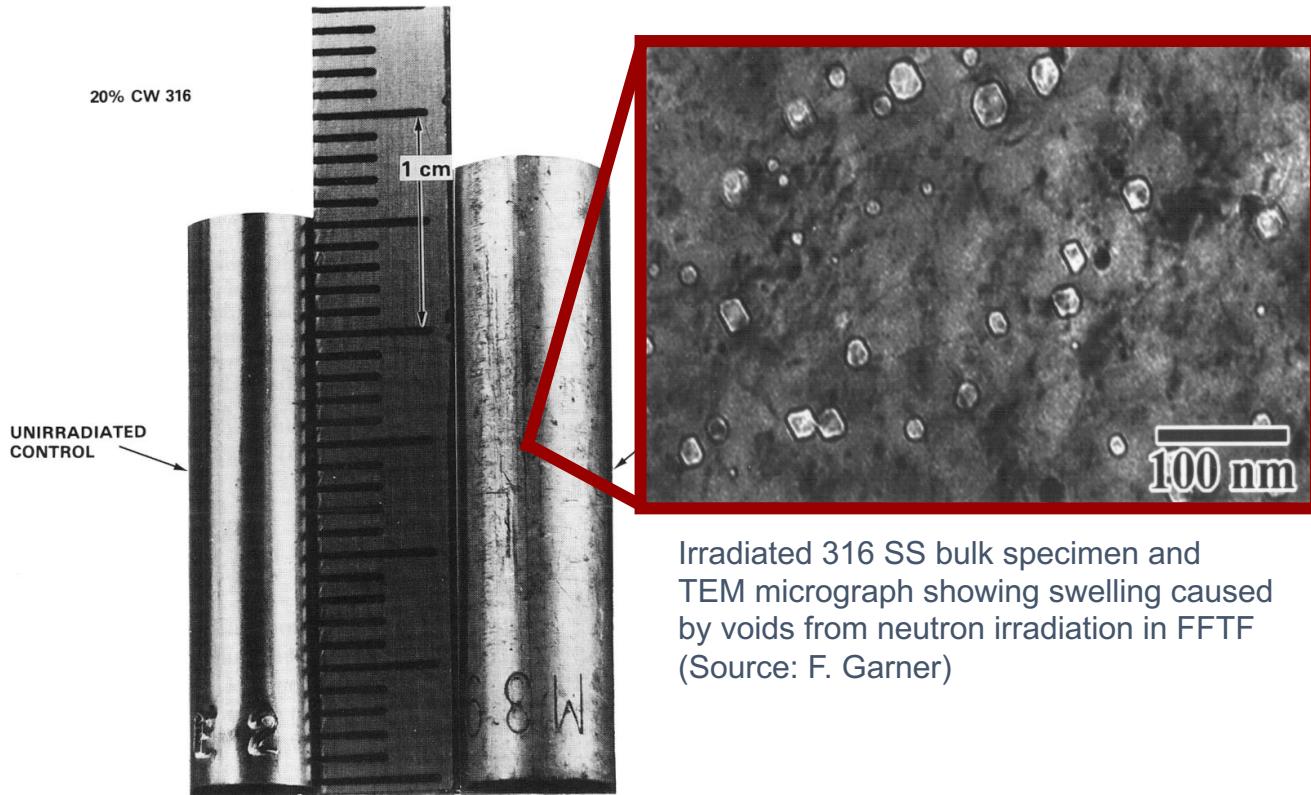
# Sink Type II - Cavities



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!)

# Sink Type II - Cavities



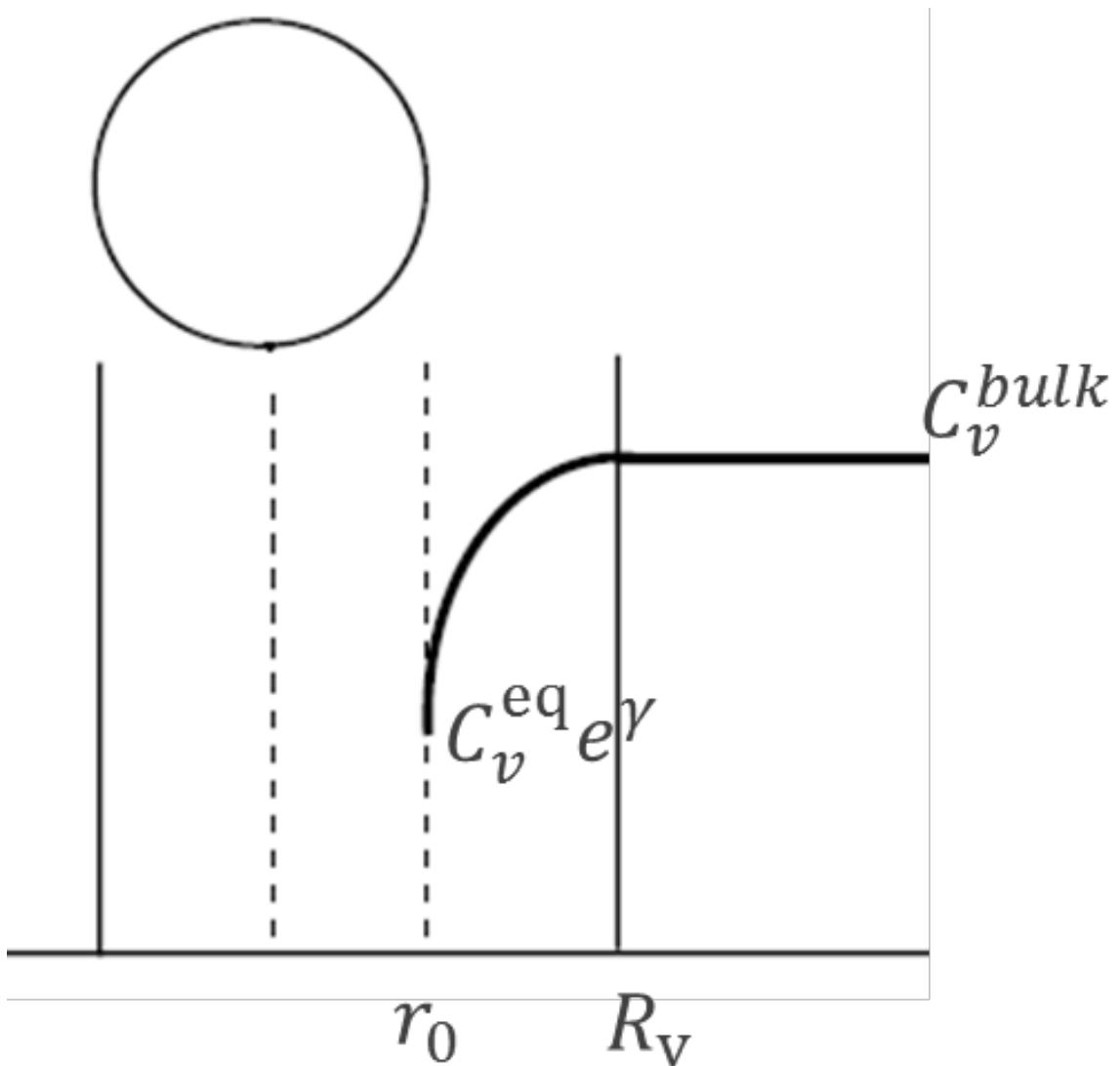
Irradiated 316 SS bulk specimen and  
TEM micrograph showing swelling caused  
by voids from neutron irradiation in FFTF  
(Source: F. Garner)

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

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



# Sink Type II - Cavities



It is assumed that the boundary conditions are:

In these conditions:

$$\frac{C_v(r) - C_v(r_o)}{C_v^{bulk} - C_v(r_o)} = 1 - \frac{r_o}{r}$$

# Sink Type II - Cavities

The rate of absorption per cavity is then given as:

$$j_{i,\nu}^{Cavity} = 4\pi r_o D_{i,\nu} C_{i,\nu}^{bulk}$$

Considering all cavities using  $N_c$  (cavities per unit volume), we get:

$$J_\nu^C = 4\pi r_o N_c D_\nu C_\nu^{bulk}$$

$$J_i^C = 4\pi r_o N_c D_i C_i^{bulk}$$

Then:



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

- Example of defect absorption to cavities:

$$\frac{\partial C_v}{\partial t} = K_0 - K_{iv}C_iC_v - z_vp_dD_vC_v + 4\pi R_cN_cD_vC_v$$

$$\frac{\partial C_i}{\partial t} = K_0 - K_{iv}C_iC_v - z_vp_dD_iC_i + 4\pi R_cN_cD_iC_i$$



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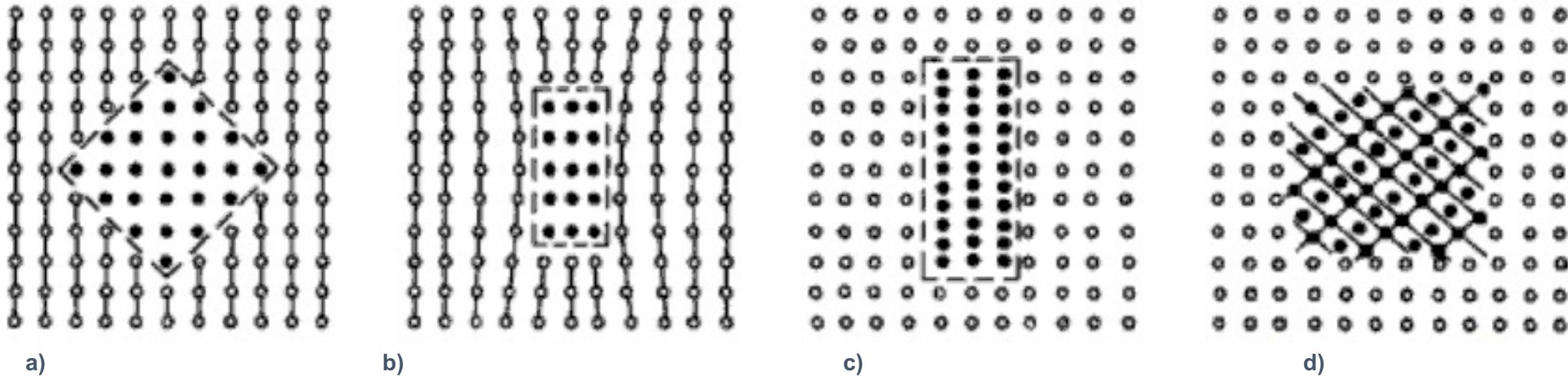
Grain boundaries

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

Dislocations



# Sink Type III – Coherent Precipitates (PPTs)



- 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



# Sink Type III – Coherent Precipitates (PPTs)



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

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



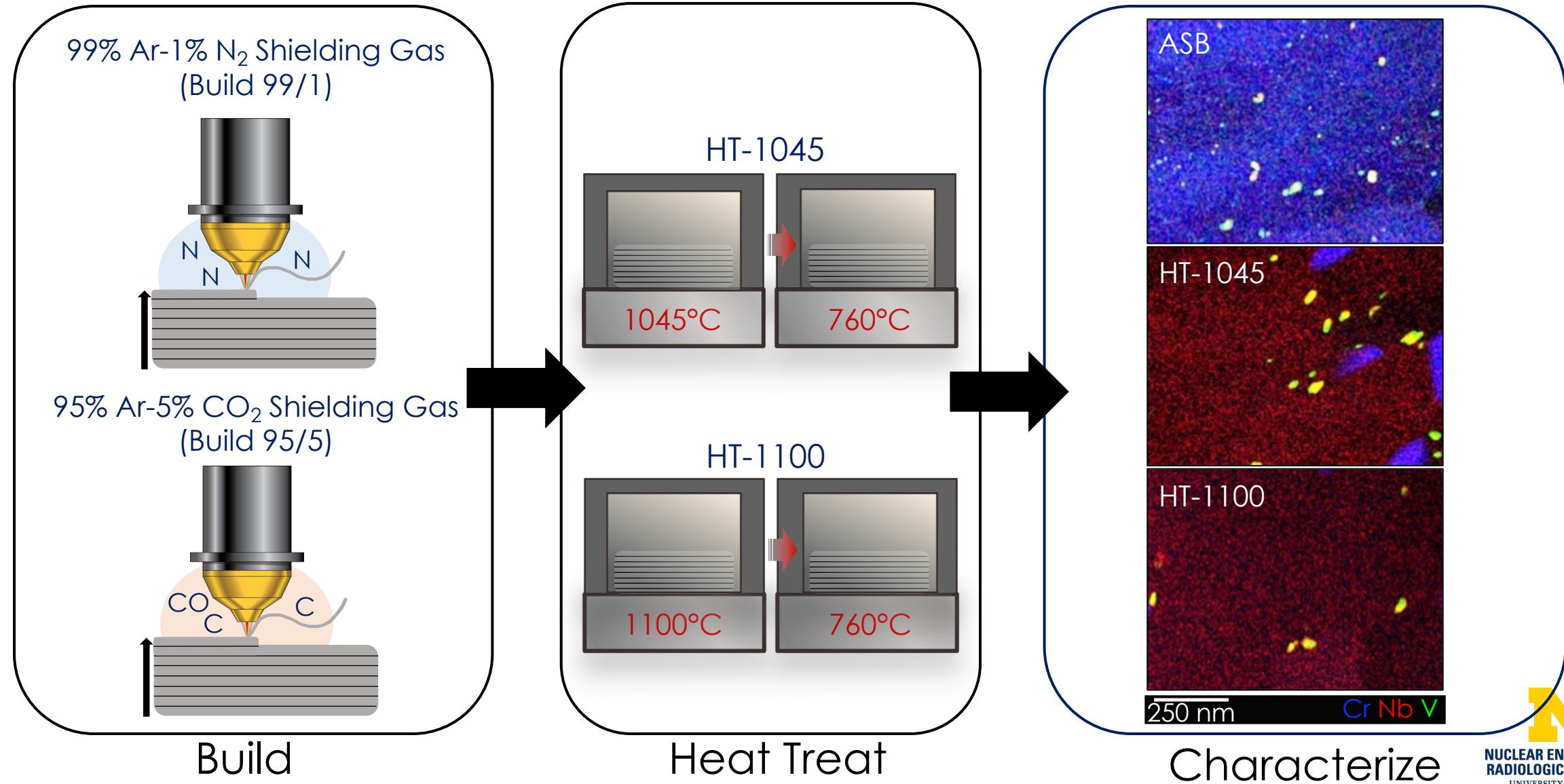
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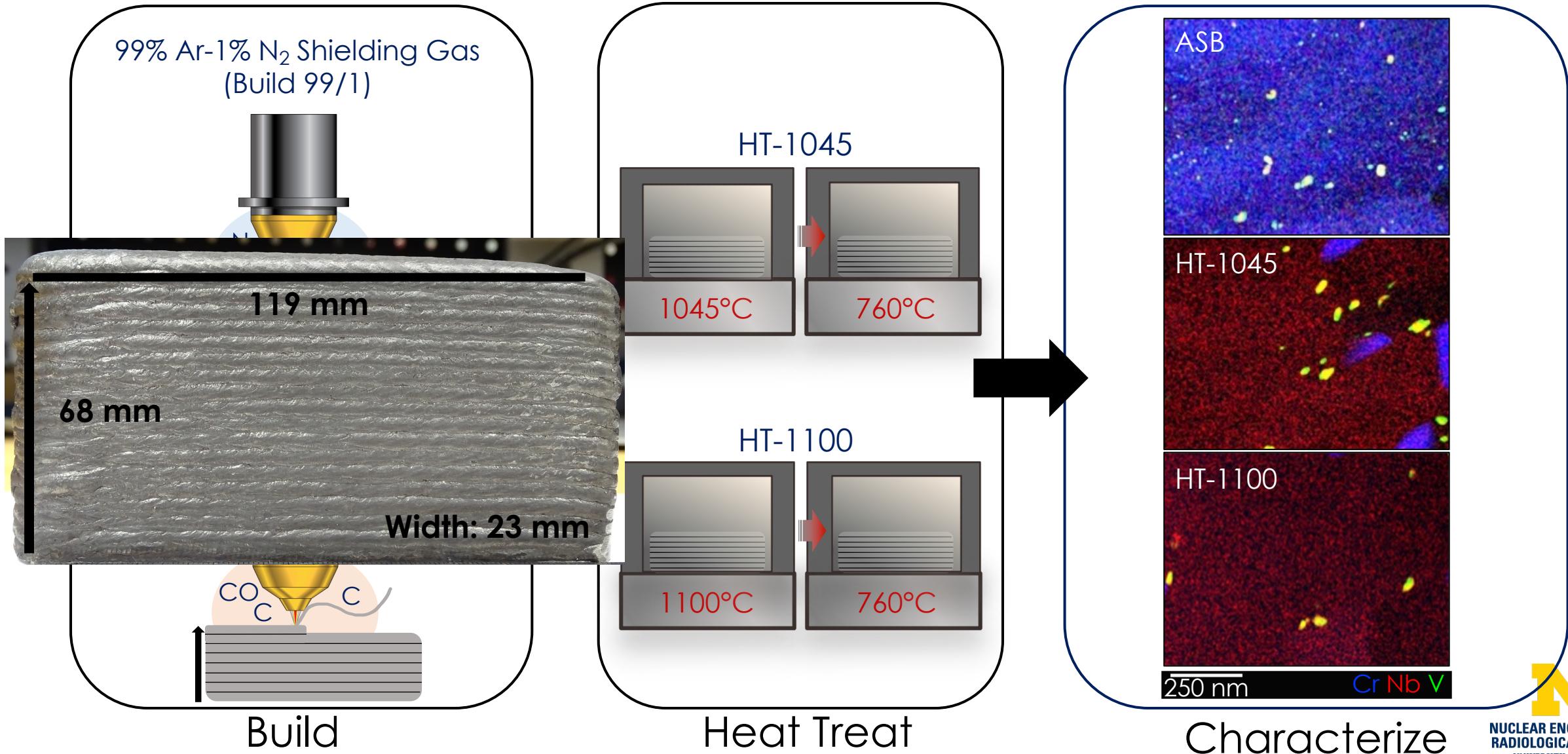
# WAAM Grade 91 Experimental Details

Control MX precipitate structure with C and N additions using different shielding gases



# Wire Arc AM Experimental Details

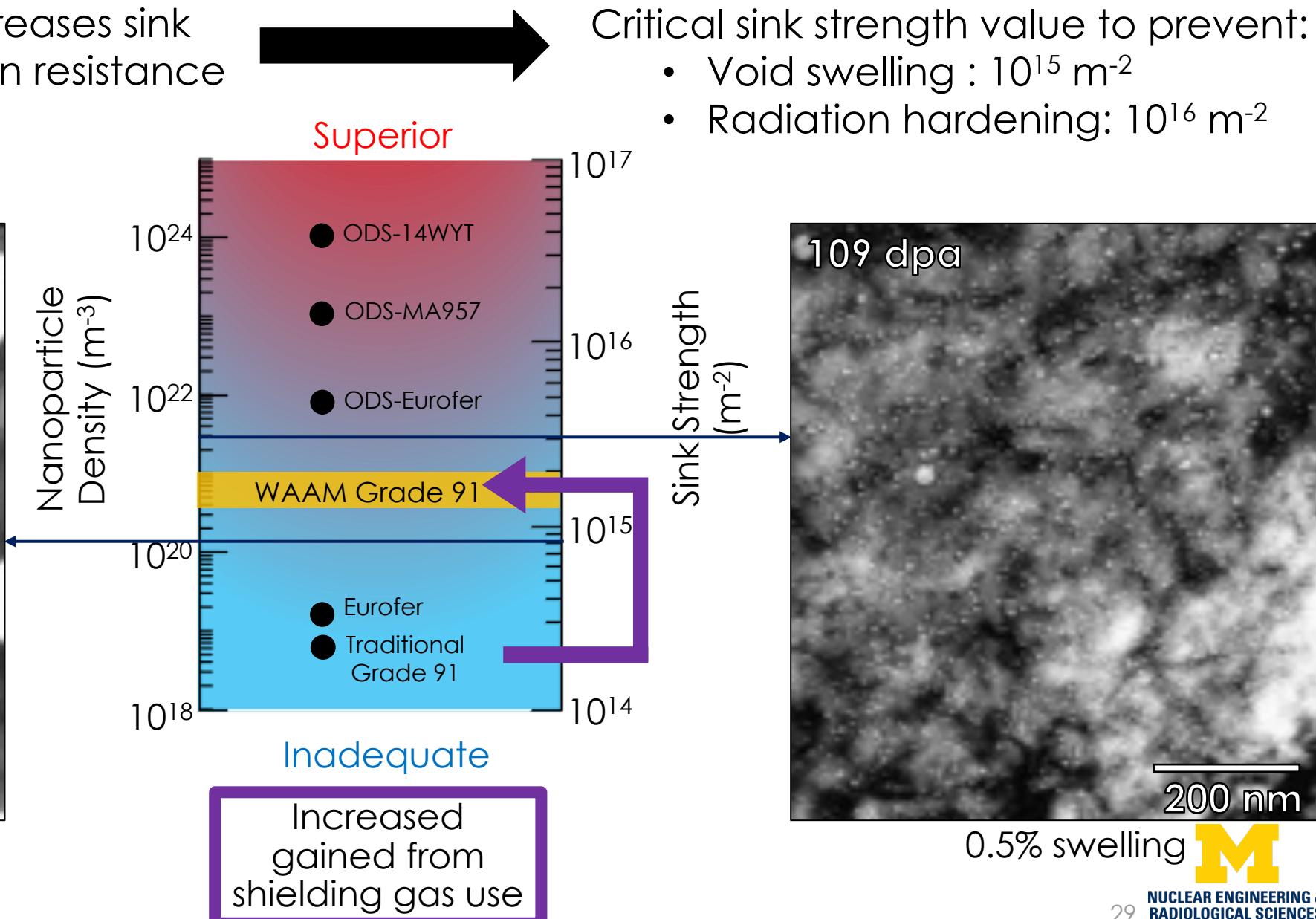
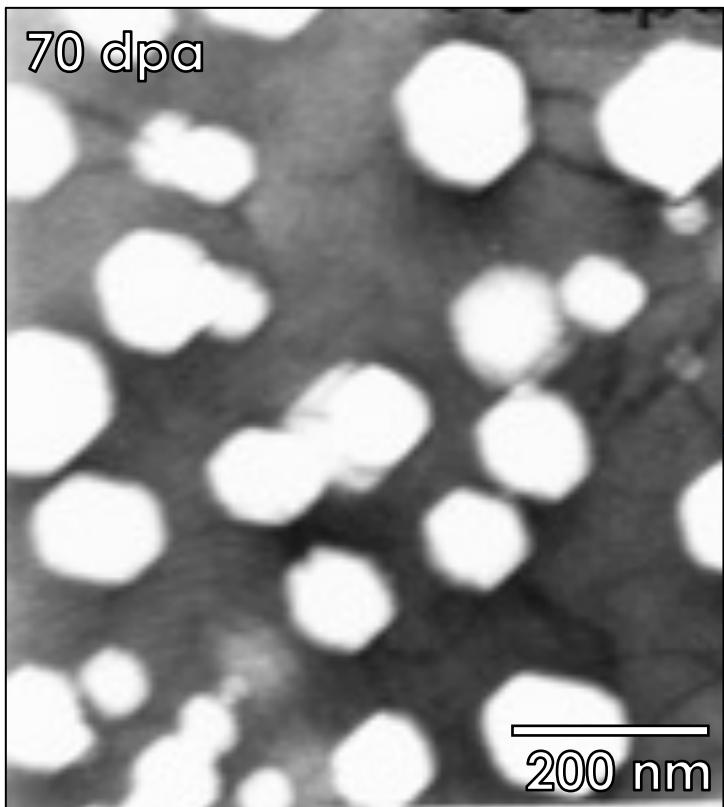
Control MX precipitate structure with C and N additions using different shielding gases



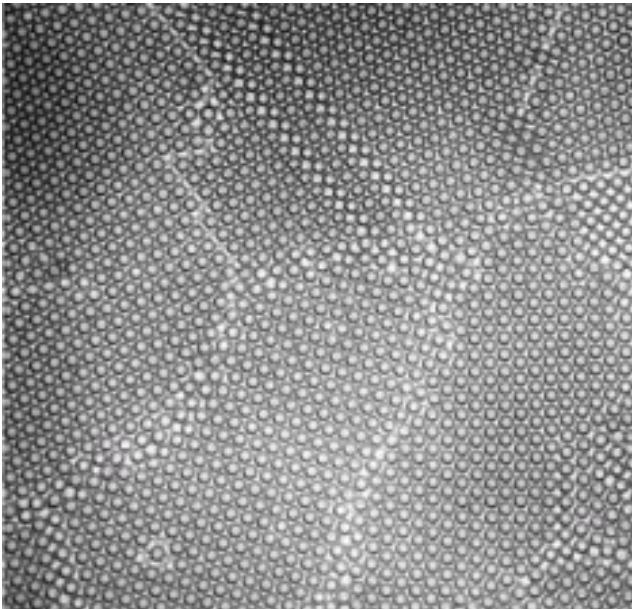
# Shielding Gas Effect on Sink Strength

Nanoscale precipitation increases sink strength and hence radiation resistance of a material

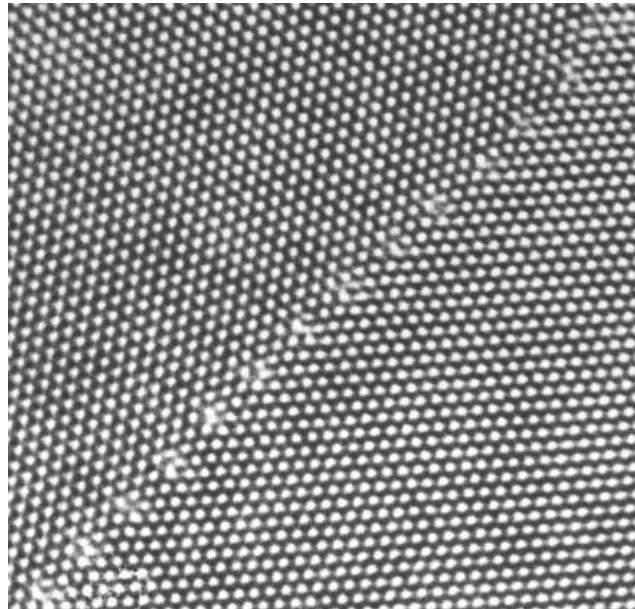
$$S_{\text{ppt}} \sim 4\pi RN$$



# Sink Type IV – Grain Boundaries



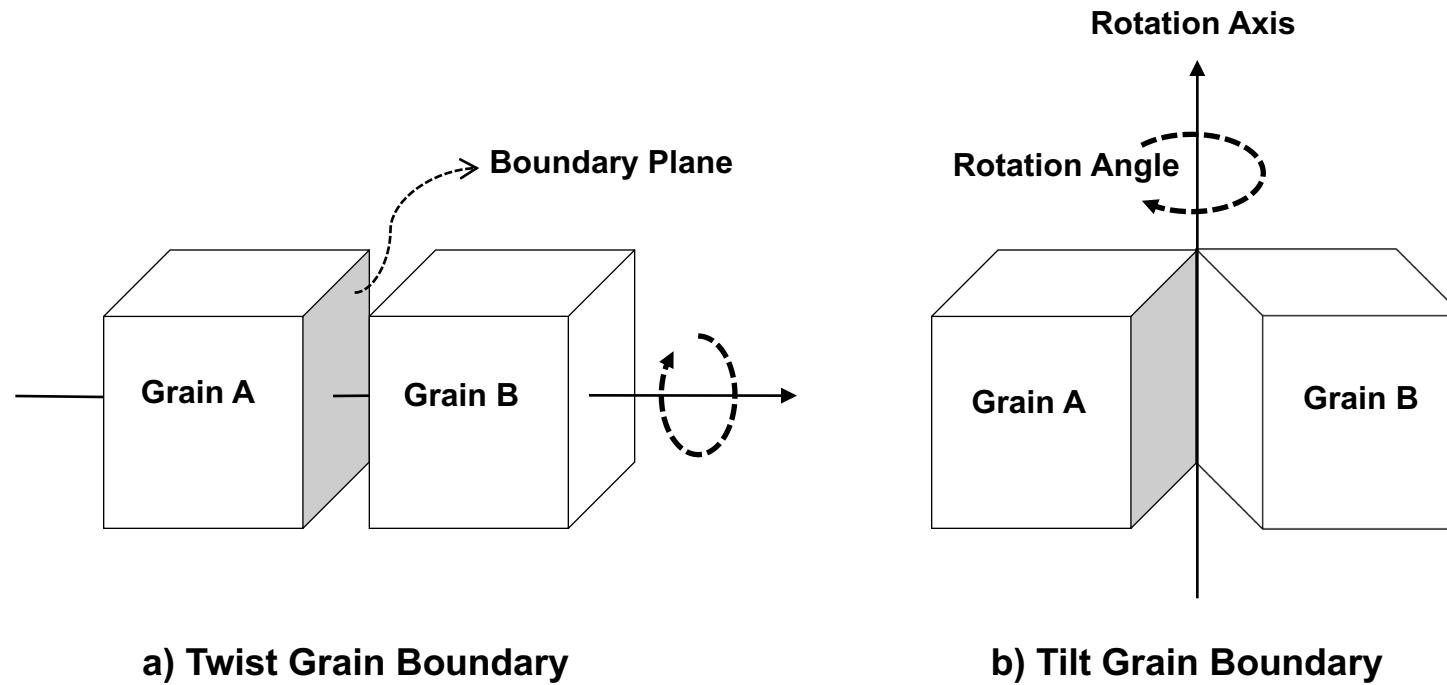
Bubble Raft Model of Grain Boundaries



HRTEM image of a  $\Sigma 19$  GB in Al

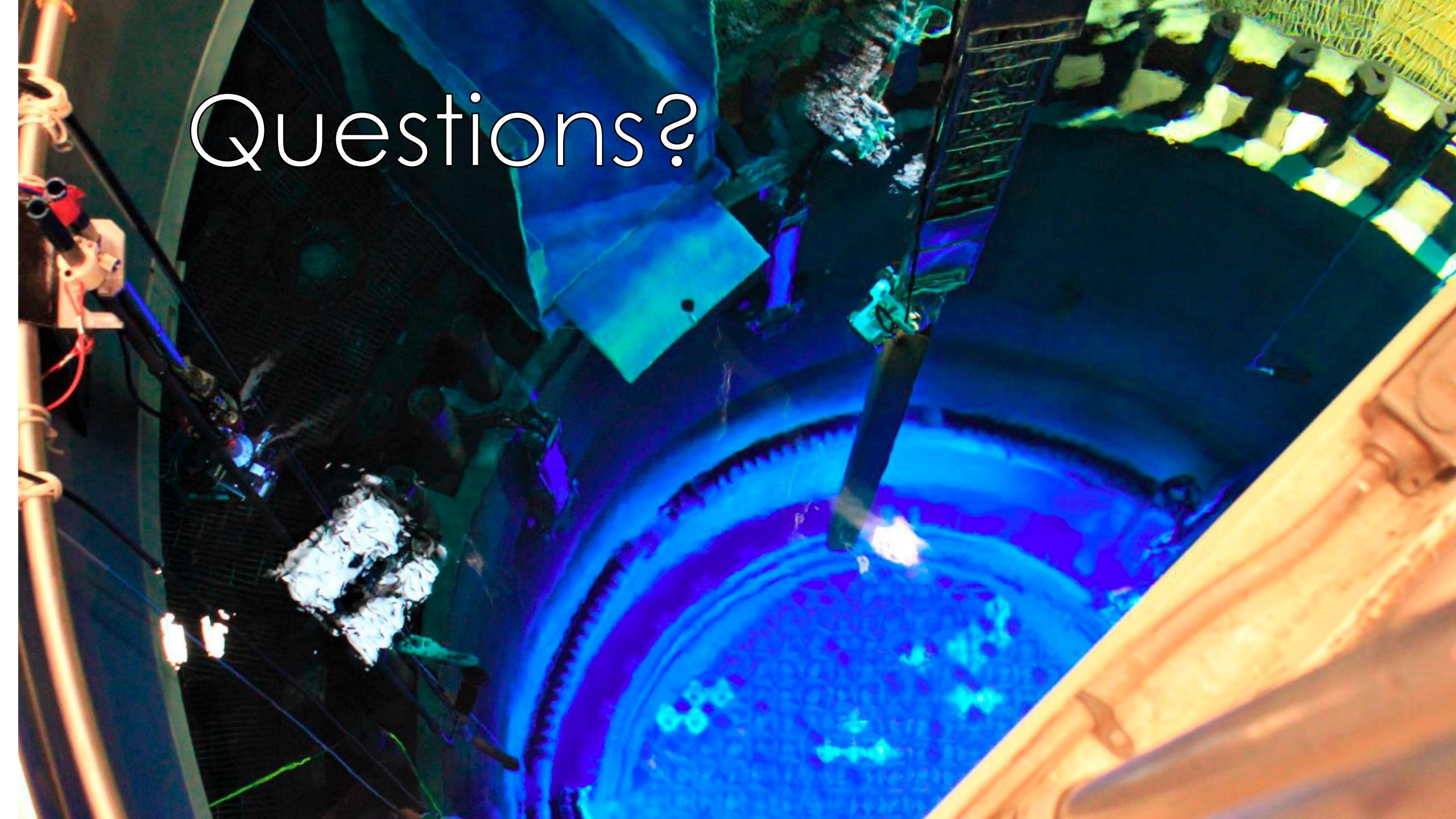
- A Grain Boundary is a general planar defect that separates regions of different crystalline orientation (i.e. grains) within a polycrystalline solid
- Grain boundaries can affect creep strength, yield strength, and diffusion

# 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?