Defect Sinks and Their Reactions

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Sink types

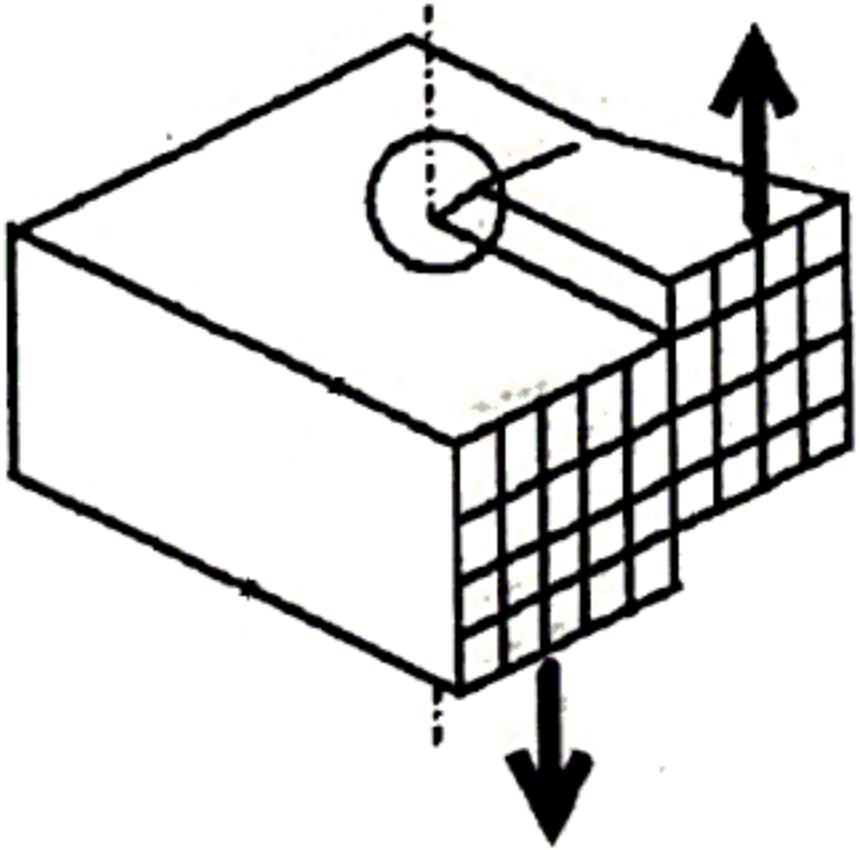
- Sinks can behave differently:
  - **Neutral sinks:** Neutral sinks show no preference for capturing one type of defect over another.
  - **Biased sinks:** Biased sinks show a preferential attraction for one defect over another.
  - **Variable sinks:** Variable sinks act as traps for defects which hold the defect but preserve its identity until annihilation or it is released.

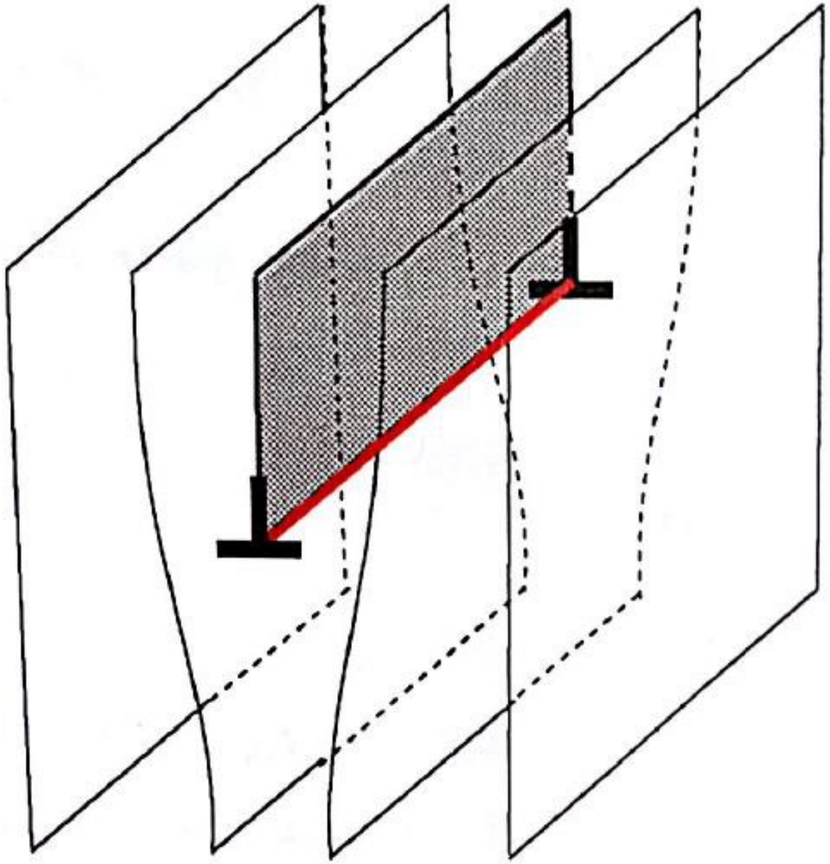
Coherent precipitates

Grain boundaries

Dislocations

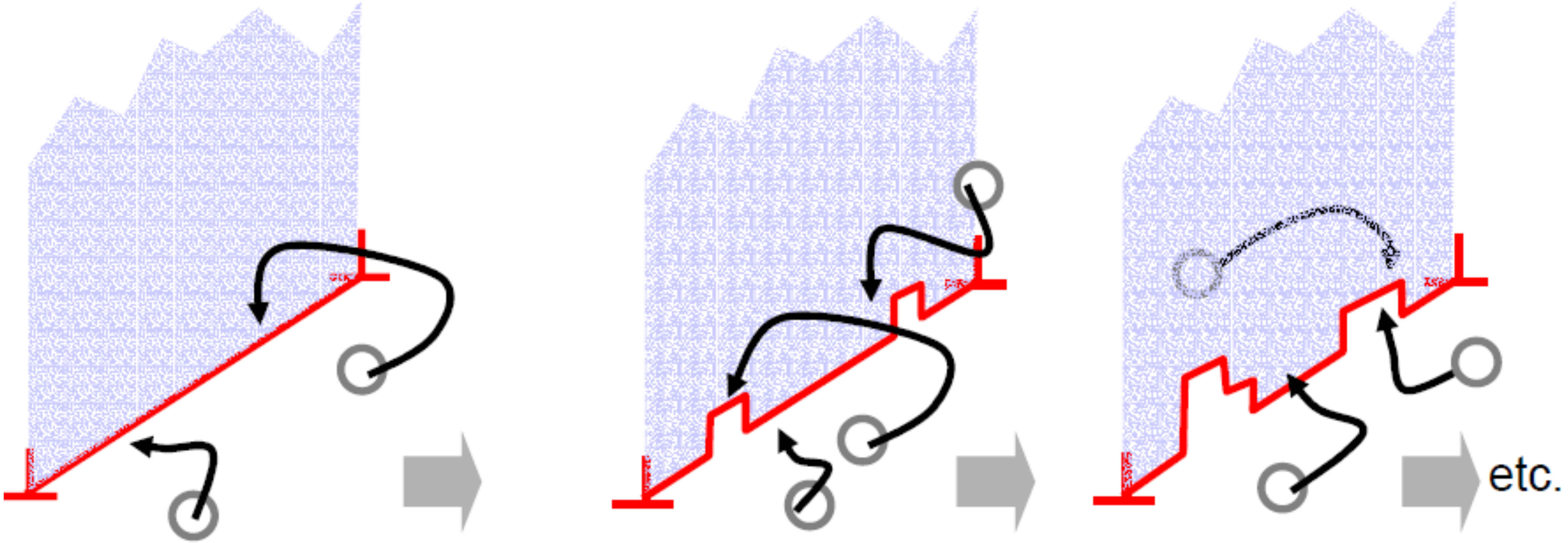
What are these?





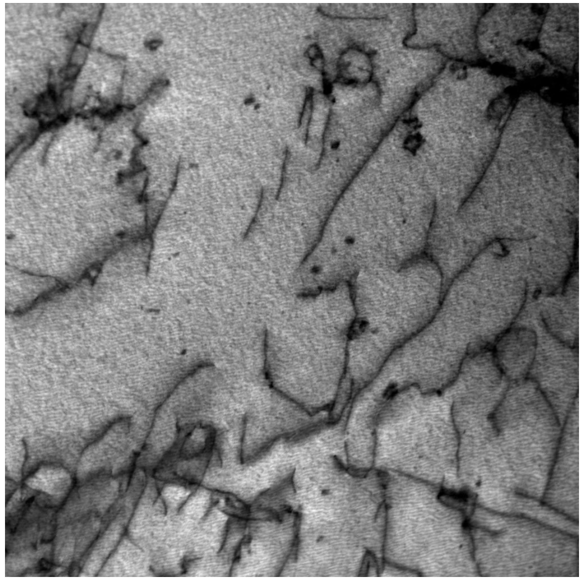
Sink Type I - Dislocations

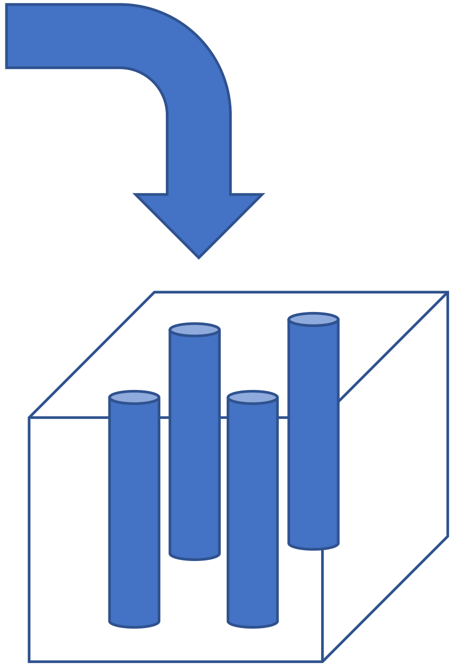
- Dislocation climb by vacancy absorption
- Leads to irradiation glide and creep



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 ($\mathbf{\rho_d}$ – 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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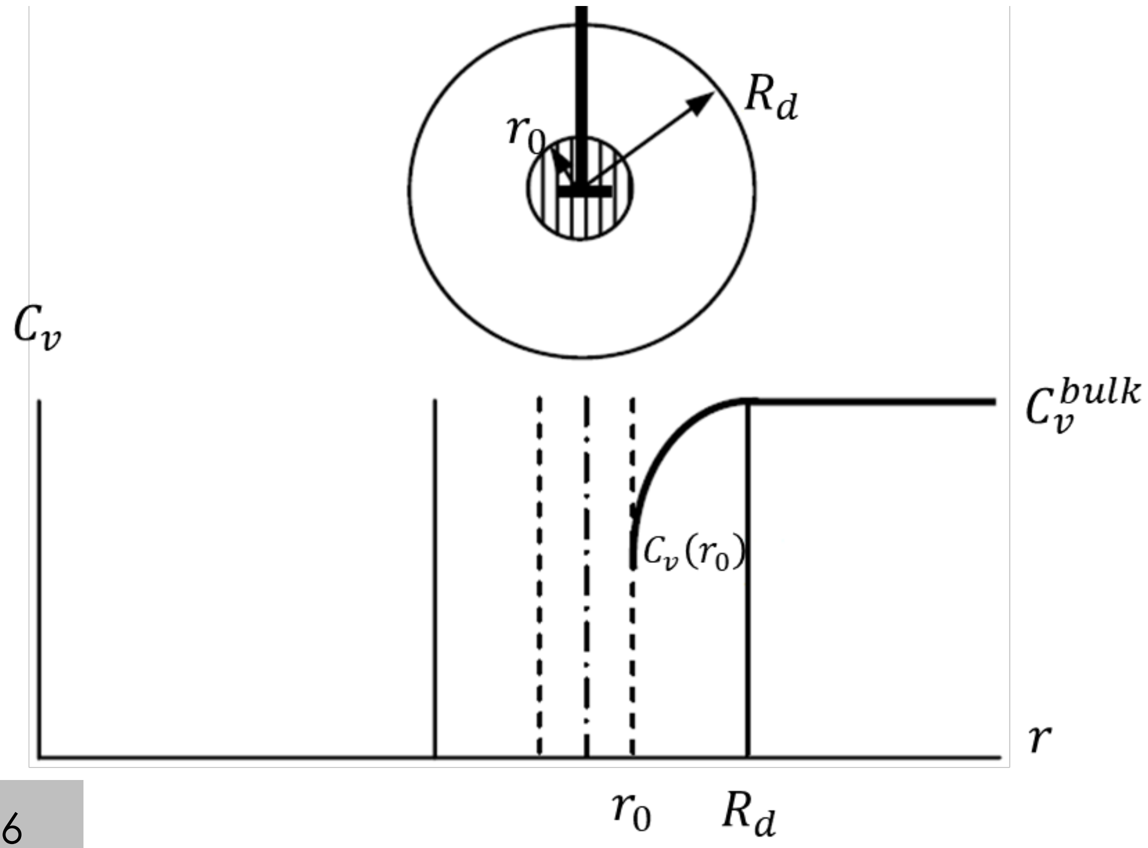

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Point Defect Absorption by Dislocations

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

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

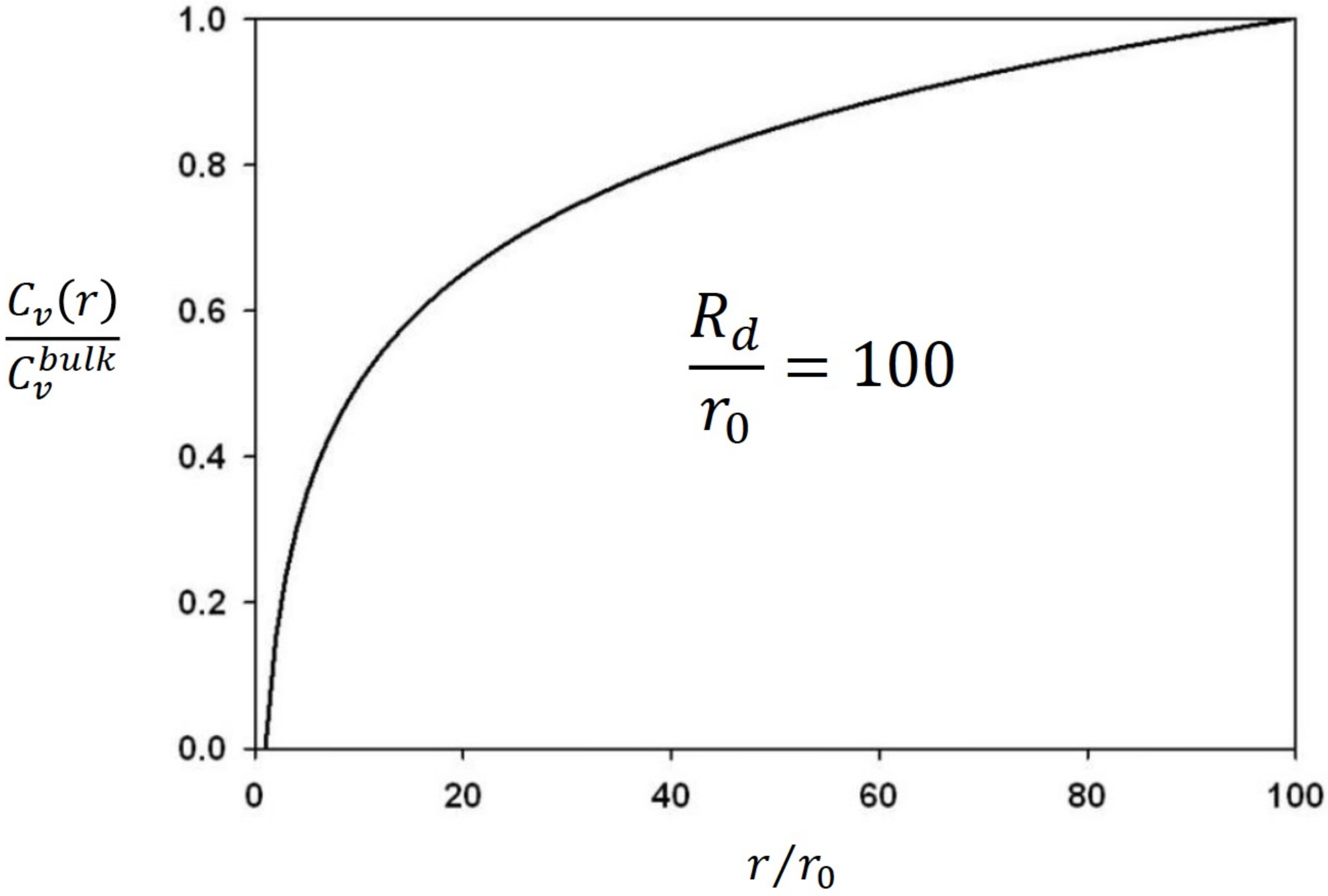
- The solution is then:

$$C_{i,v} = Aln(r) + B$$

- Using the boundary conditions established by our assumptions:

- Gives us:

Point Defect Absorption by Dislocations

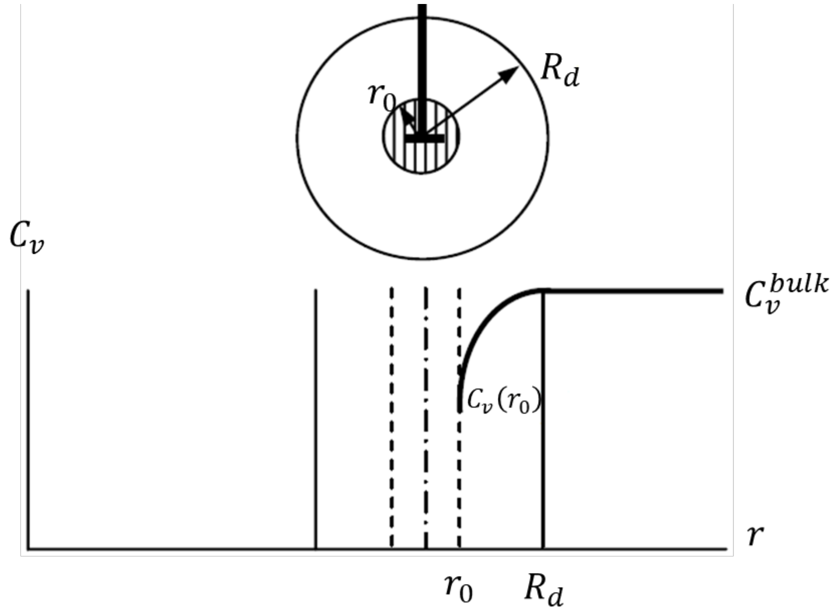


Point Defect Absorption by Dislocations

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

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

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



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:

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

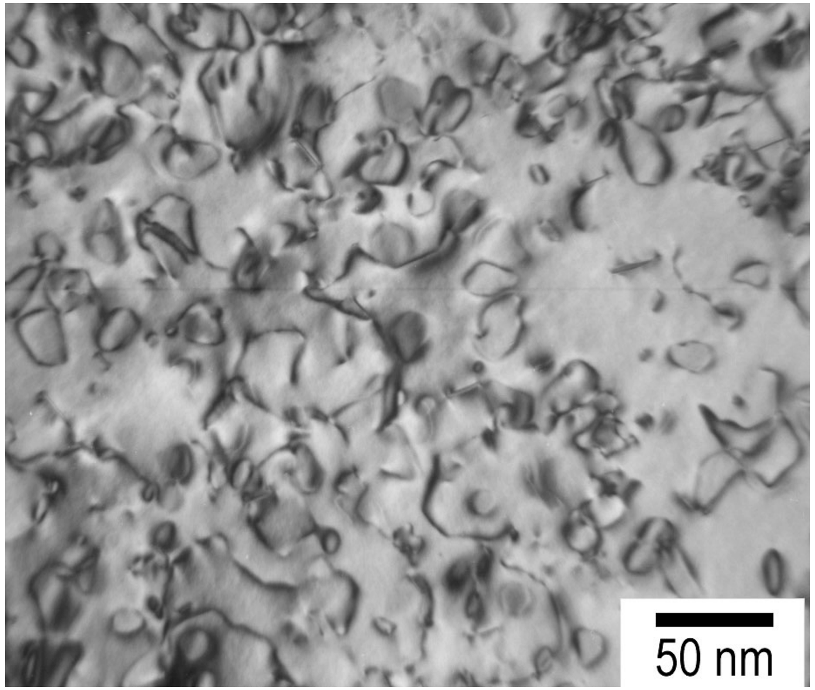
- Into the above giving:

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

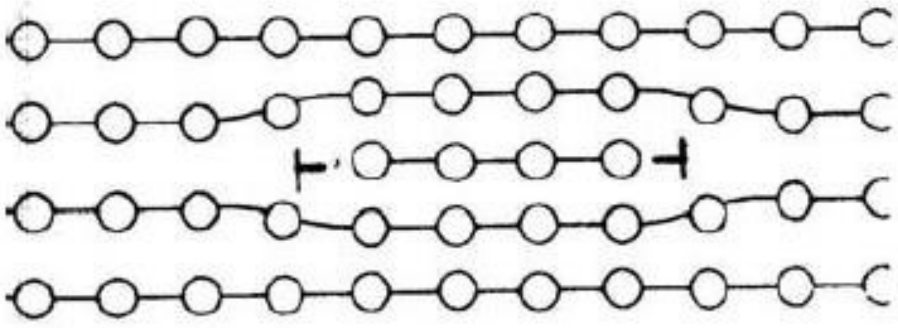
- Since there is $\mathbf{p_d}$ cm of dislocation line per cm^3:

Accounting for dislocation loops

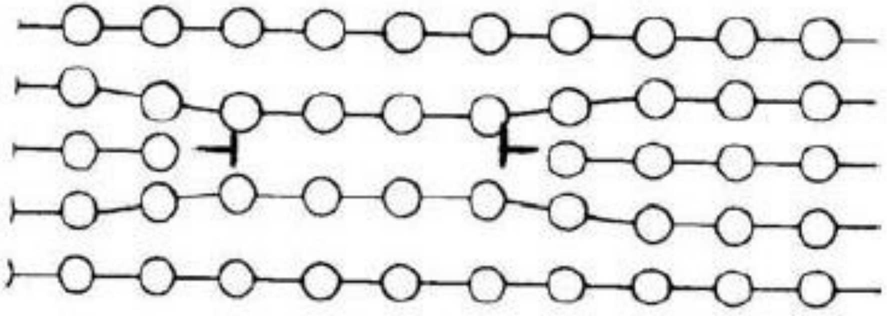
Dislocation Loops in Irradiated 316 SS (2 dpa)



Interstitial Loop

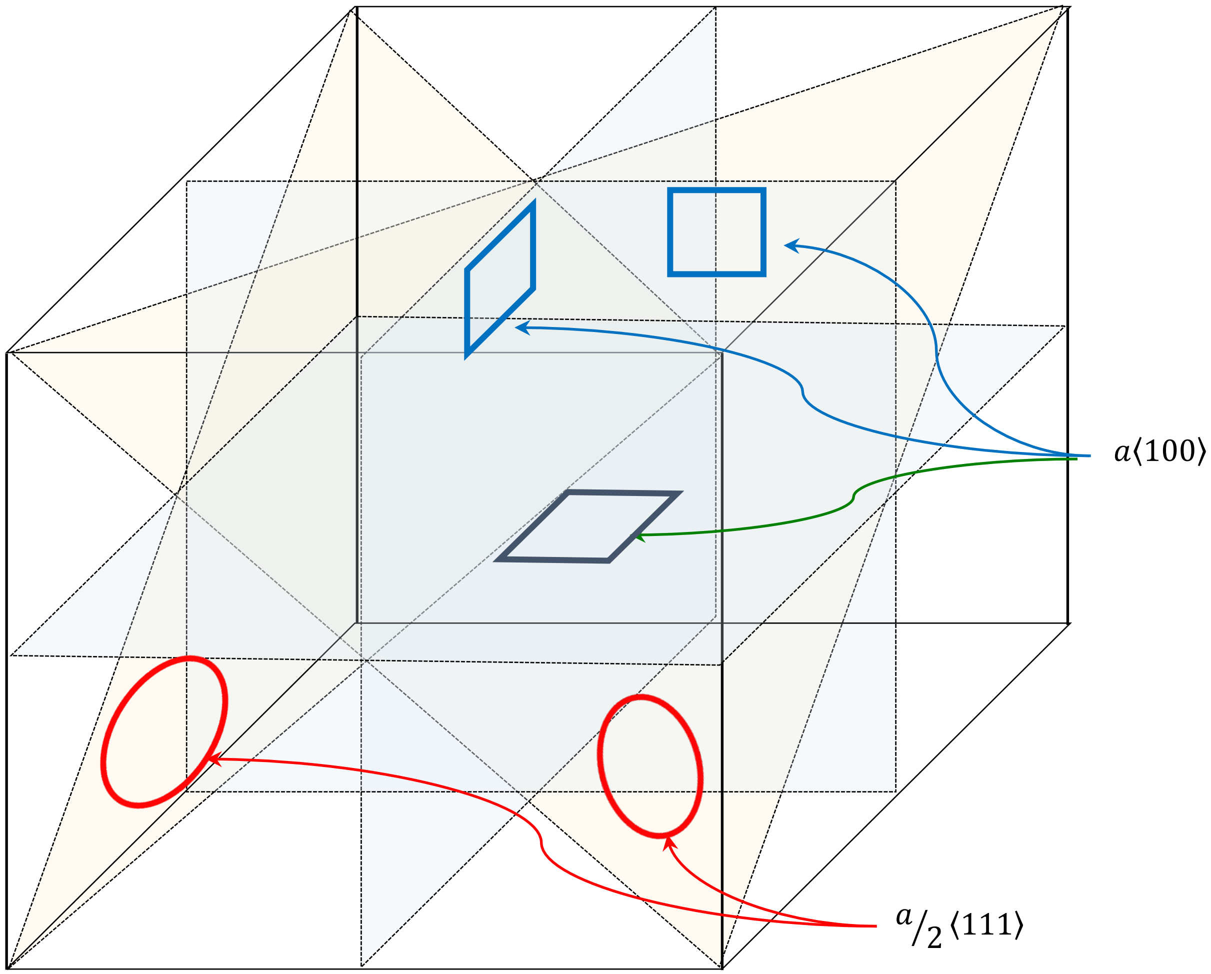


Vacancy Loop

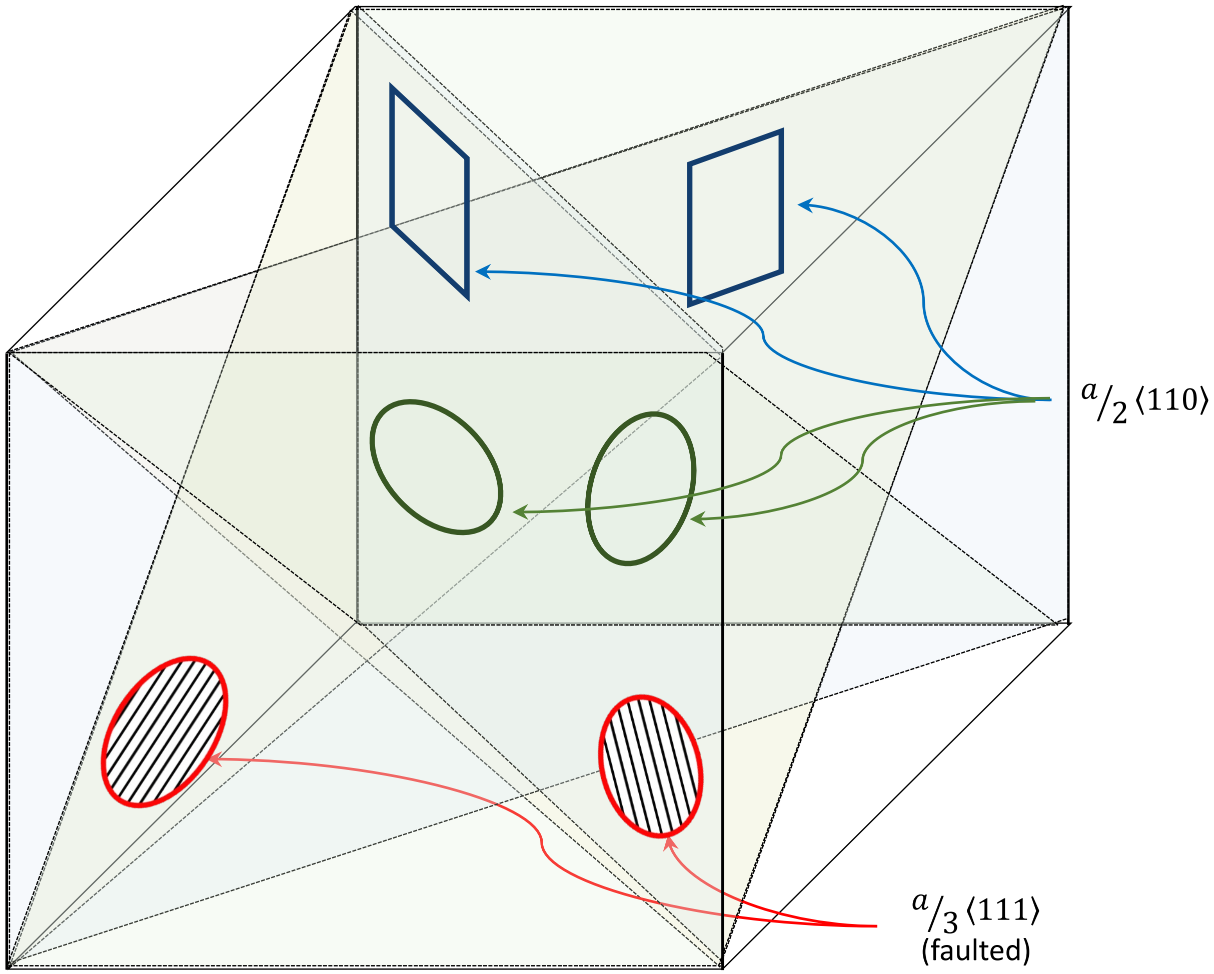


- Dislocation Loop: when a dislocation line forms a closed loop instead of extending until it reaches an interface
  - Character of the dislocation (edge, screw, mixed) changes continuously along the line
  - Loops typically grow

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



Body Centered Cubic
(BCC)



Face Centered Cubic
(FCC)

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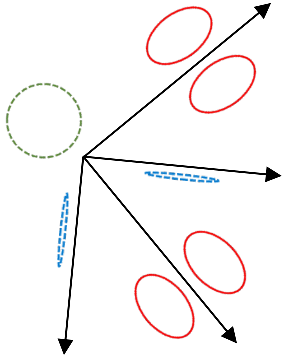
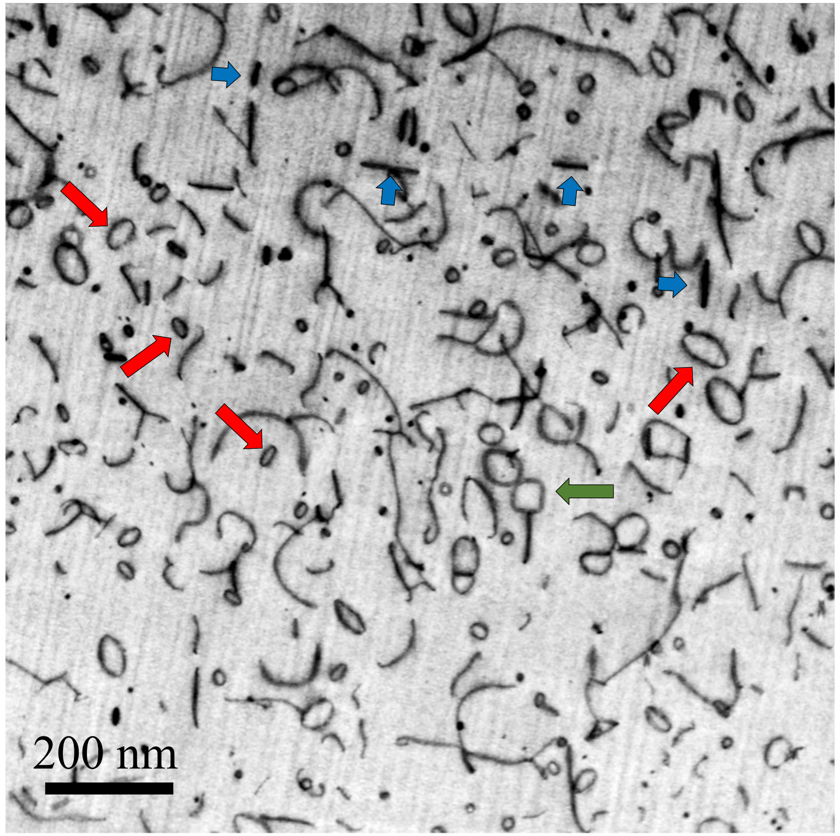
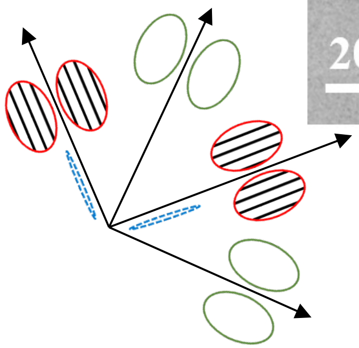
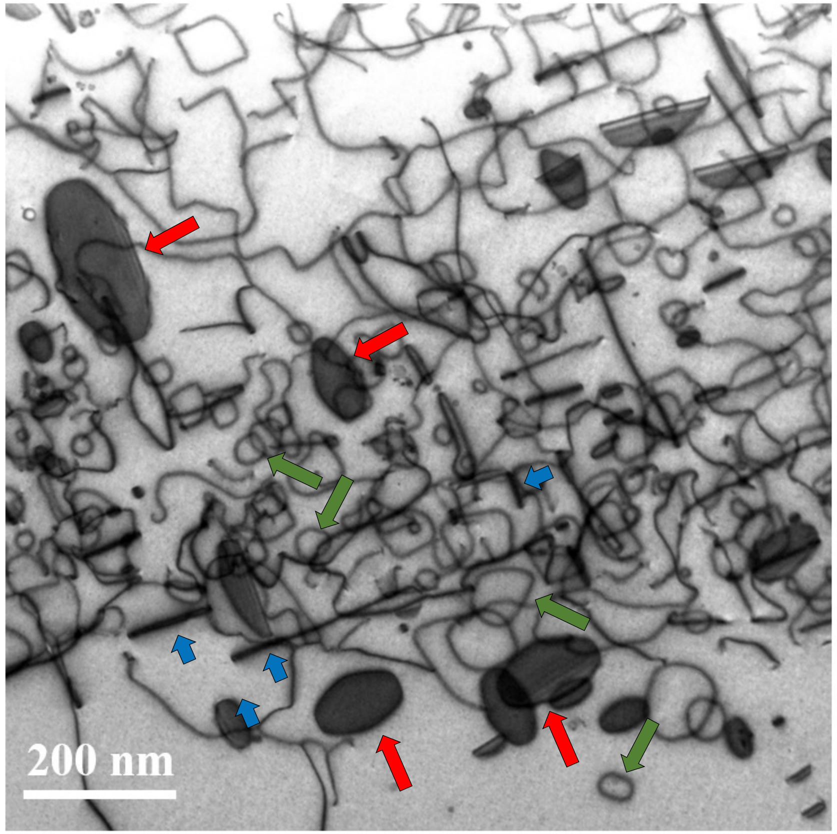




Body Centered Cubic
(BCC)

Imaging down
the [100] zone





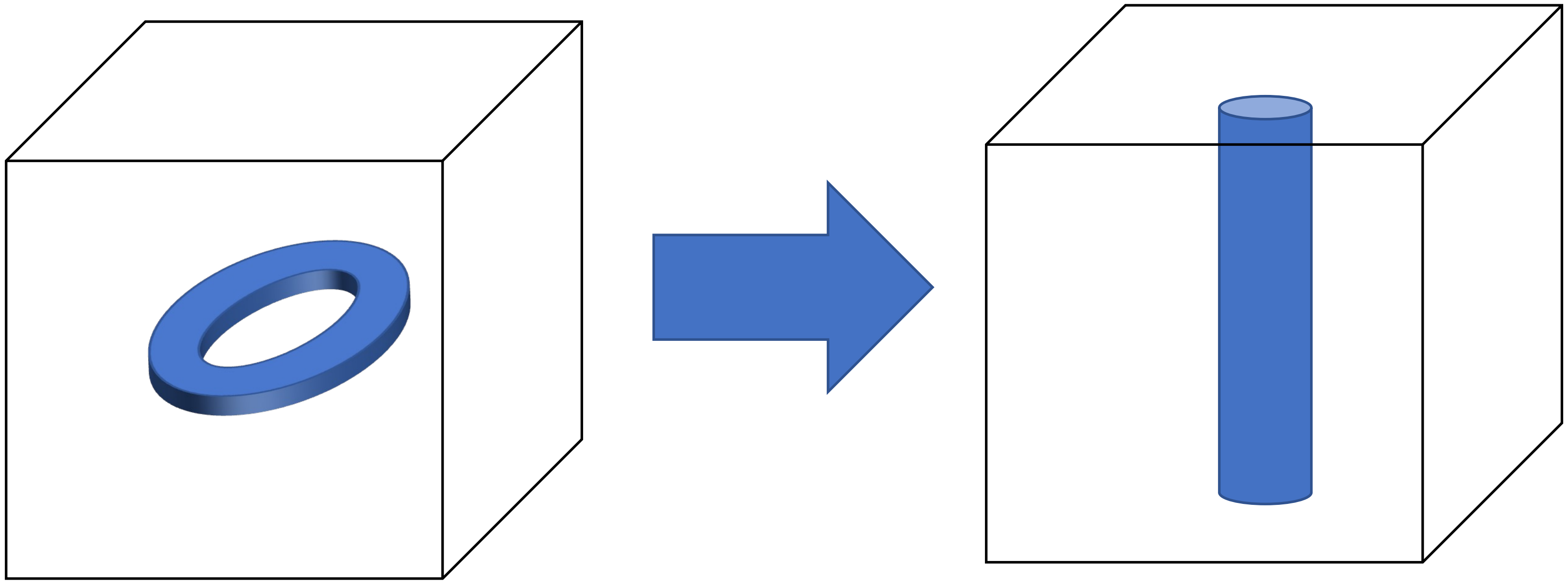
Face Centered Cubic
(FCC)

C. Parish, et al., *J. Mat. Res.*, **30**, 2020

P. Xiu, et al., *J. Nuc. Mat.*, **544**, 2021

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"



Last week F1 raced in the largest North American city by population. What city was it?

Sink types

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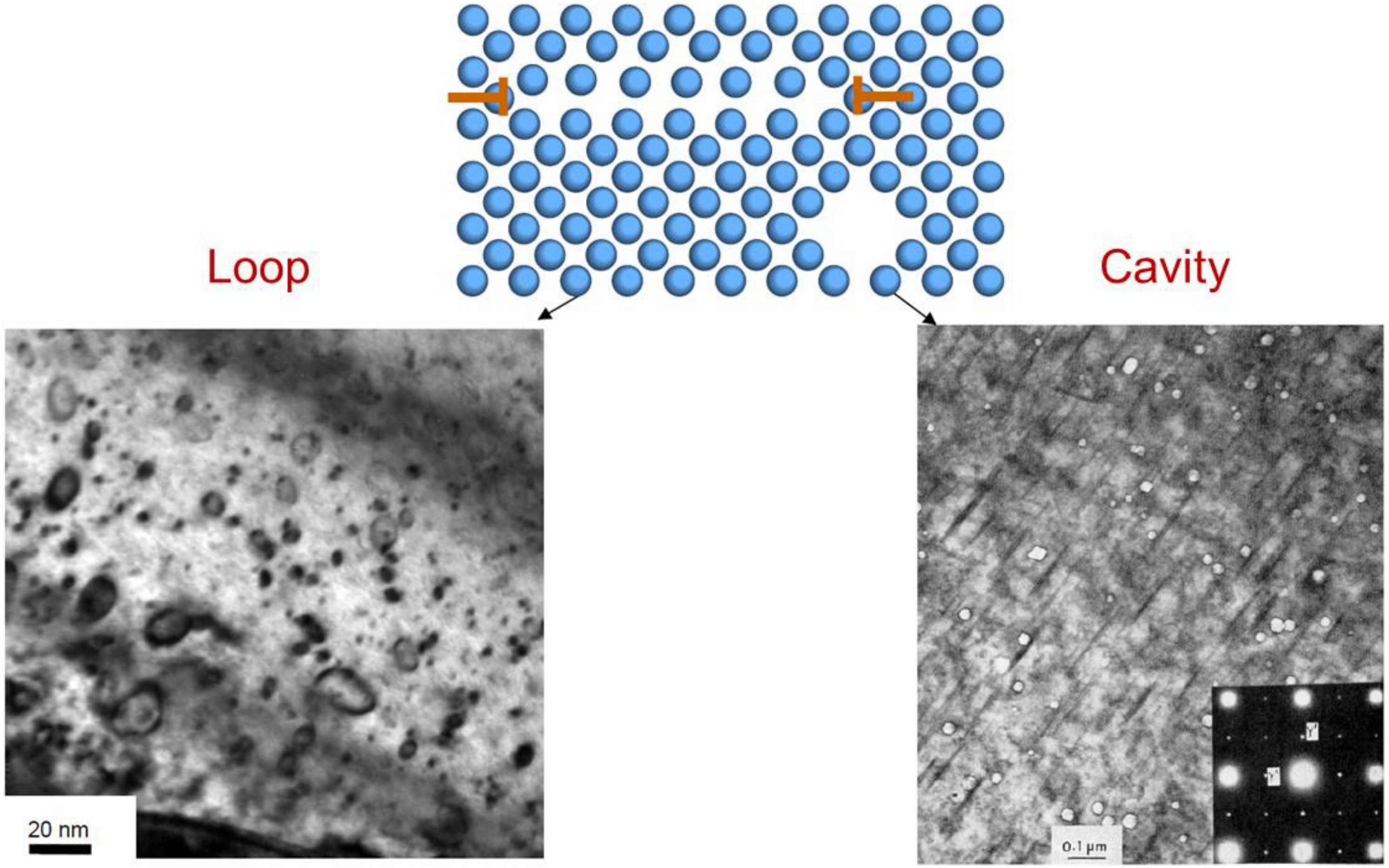
Coherent precipitates

Grain boundaries/Voids

Dislocations

Sink Type II - Cavities



- 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

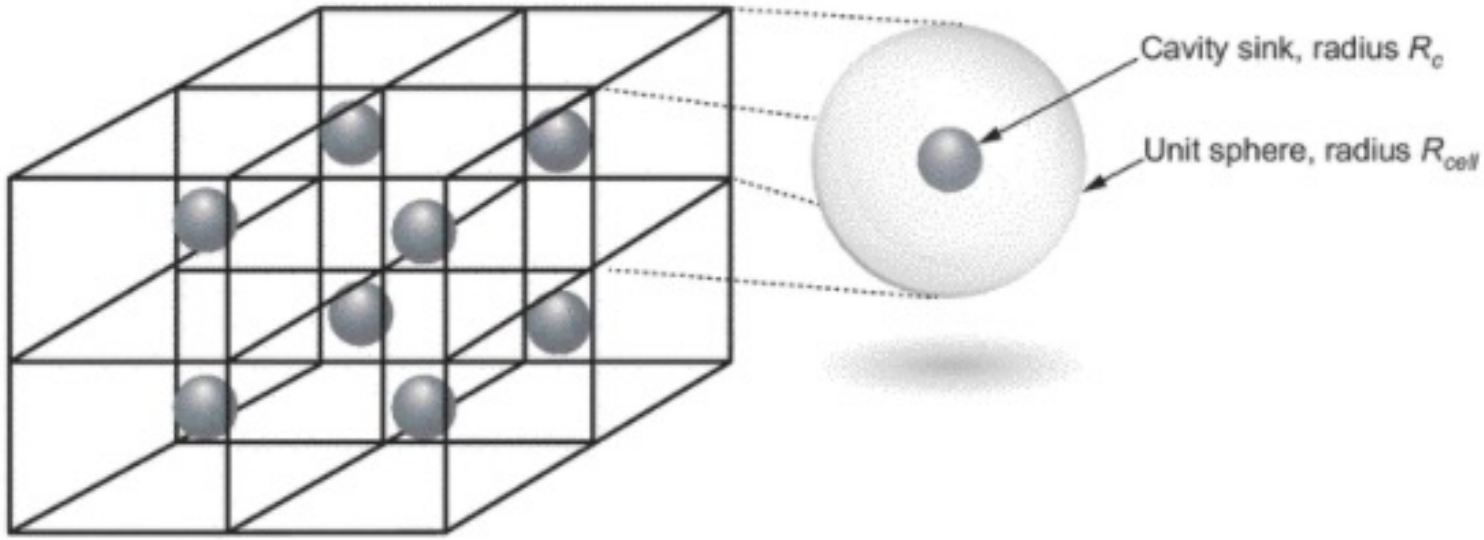
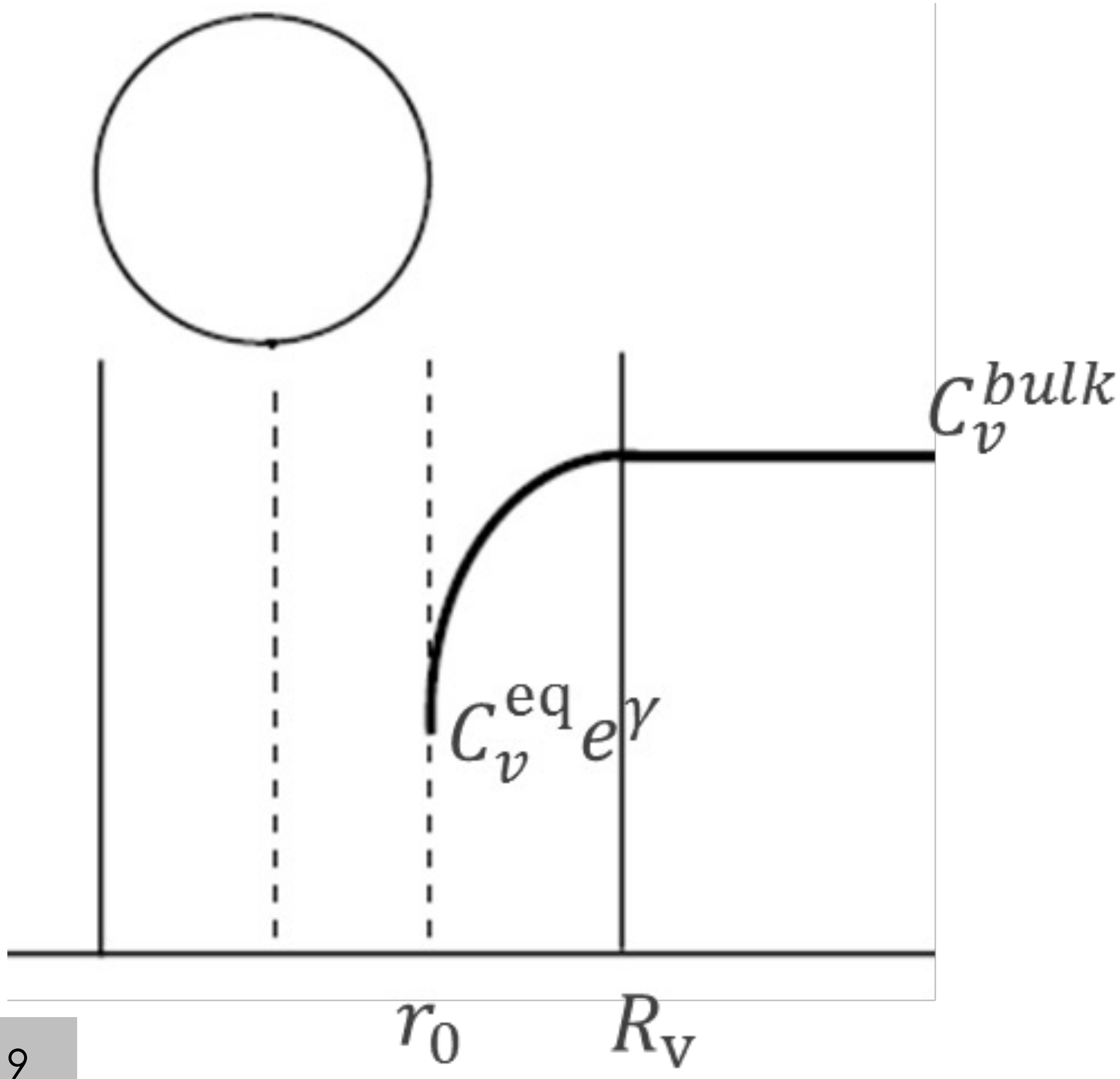


FIGURE 13.8: ***Spherical cavity sinks uniformly distributed in a solid. The cubes are unit cells for each sphere.***

- 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:

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

Sink Type II - Cavities

The rate of absorption per cavity is then given as:

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

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

$$J_v^C = 4\pi r_o N_c D_v C_v^{bulk}$$

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

Then:

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:

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

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

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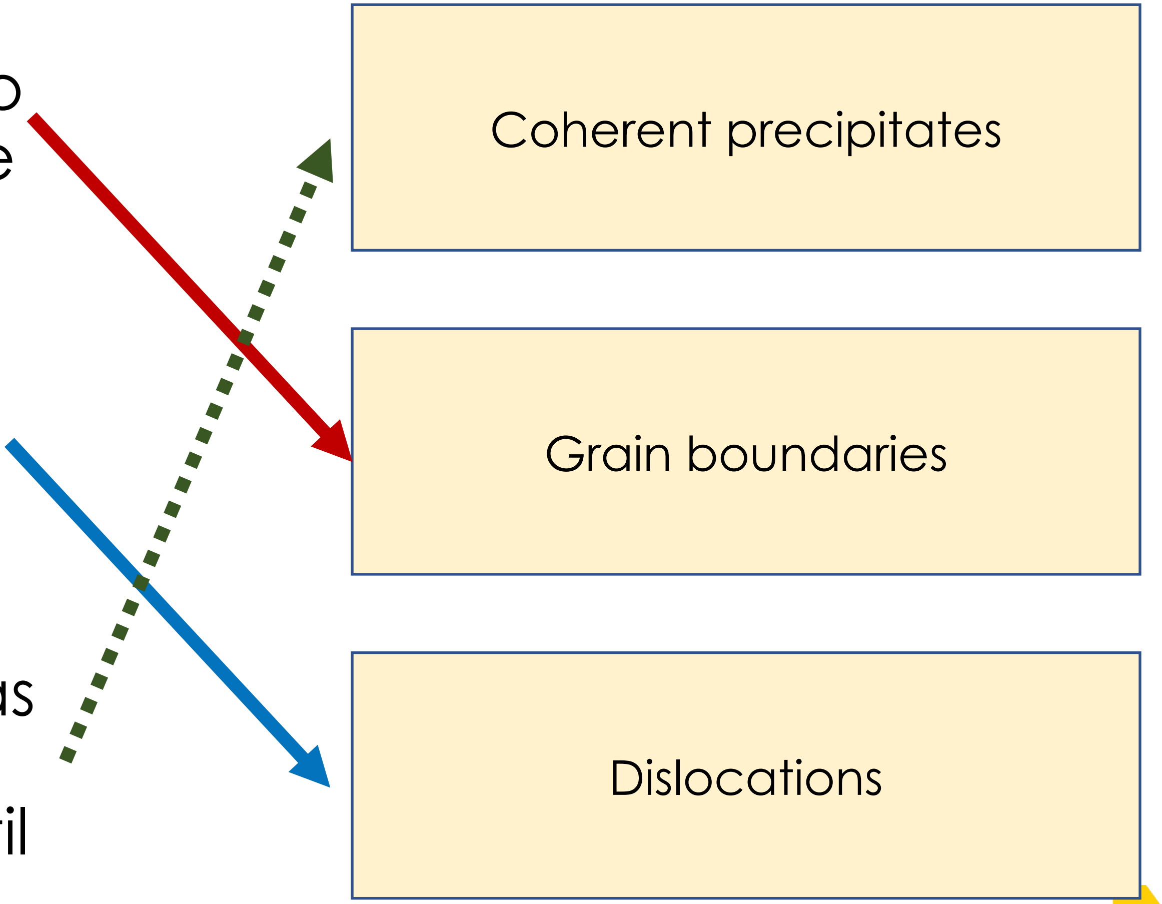
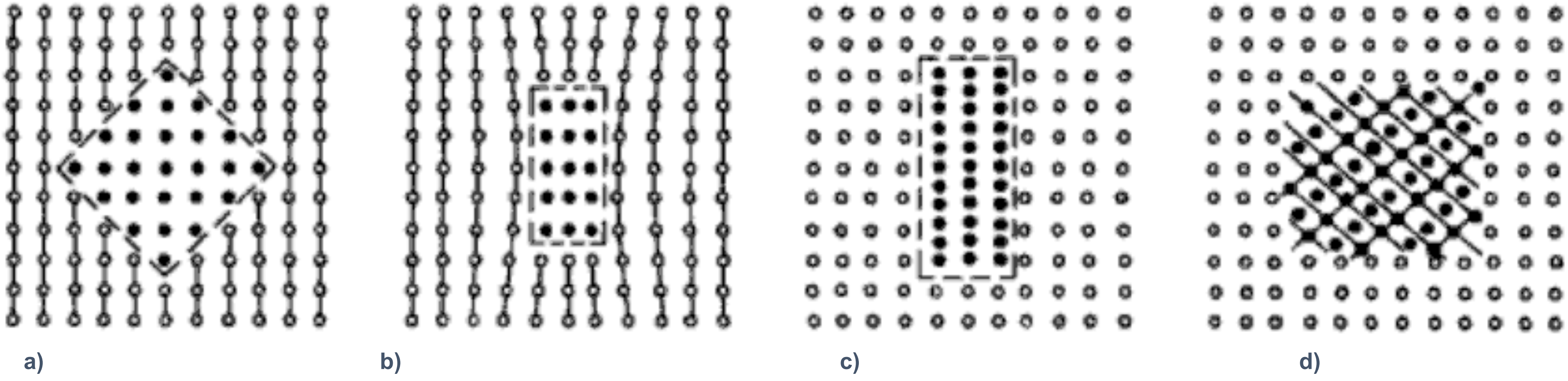


Sink Type III – Coherent Precipitates (PPTs)



- 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

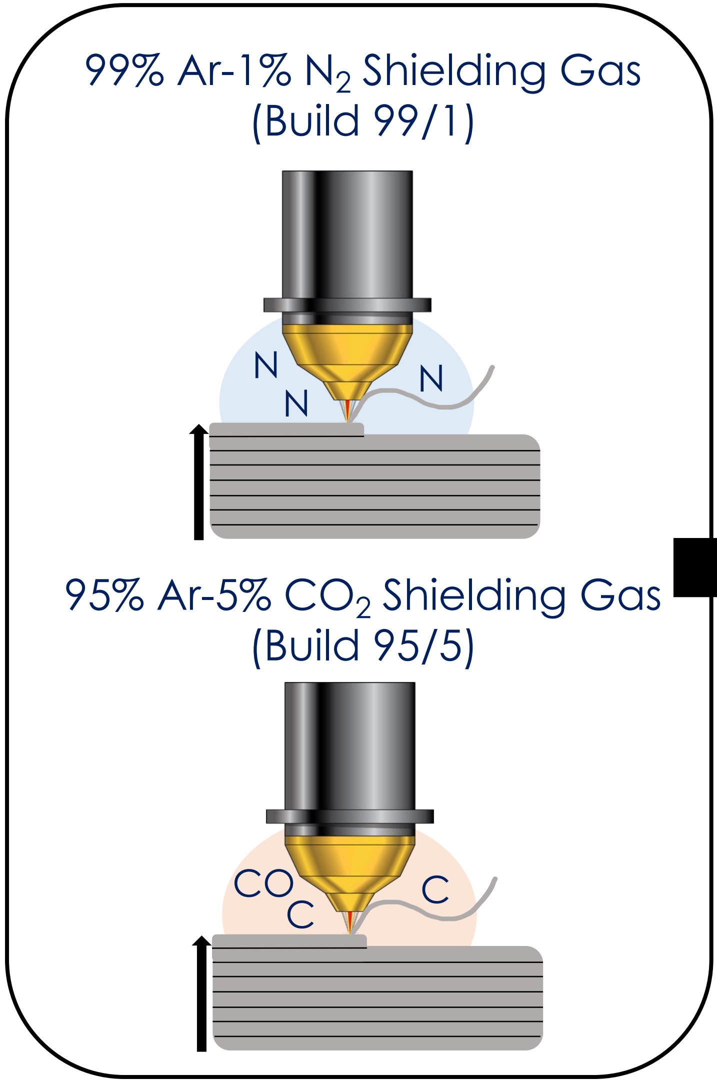
https://www.youtube.com/watch?v=zNZyAN9y3kY

Sink Type III – Coherent Precipitates (PPTs)

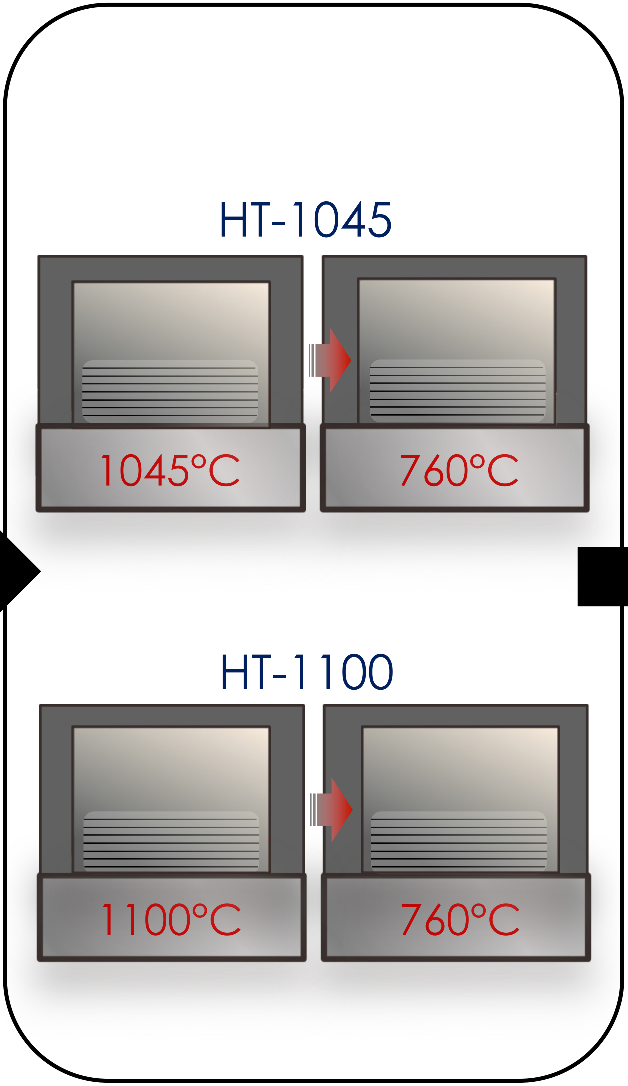
- Coherent precipitates act as traps
- Bias to interface depends on the other biased sinks present in the microstructure (such as dislocations!)
- Vacancies and interstitials reduce the strain field at the trap due to the lattice mismatch

WAAM Grade 91 Experimental Details

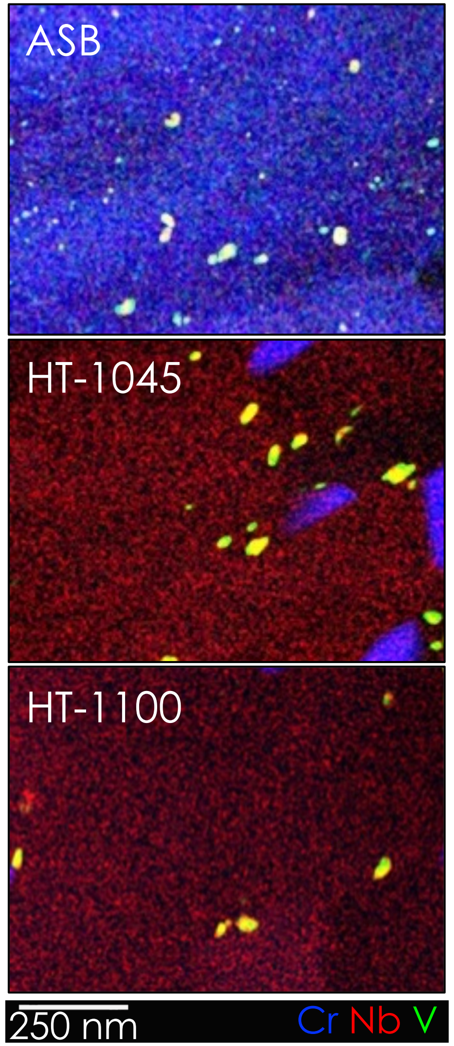
Control MX precipitate structure with C and N additions using different shielding gases



Build



Heat Treat



Characterize

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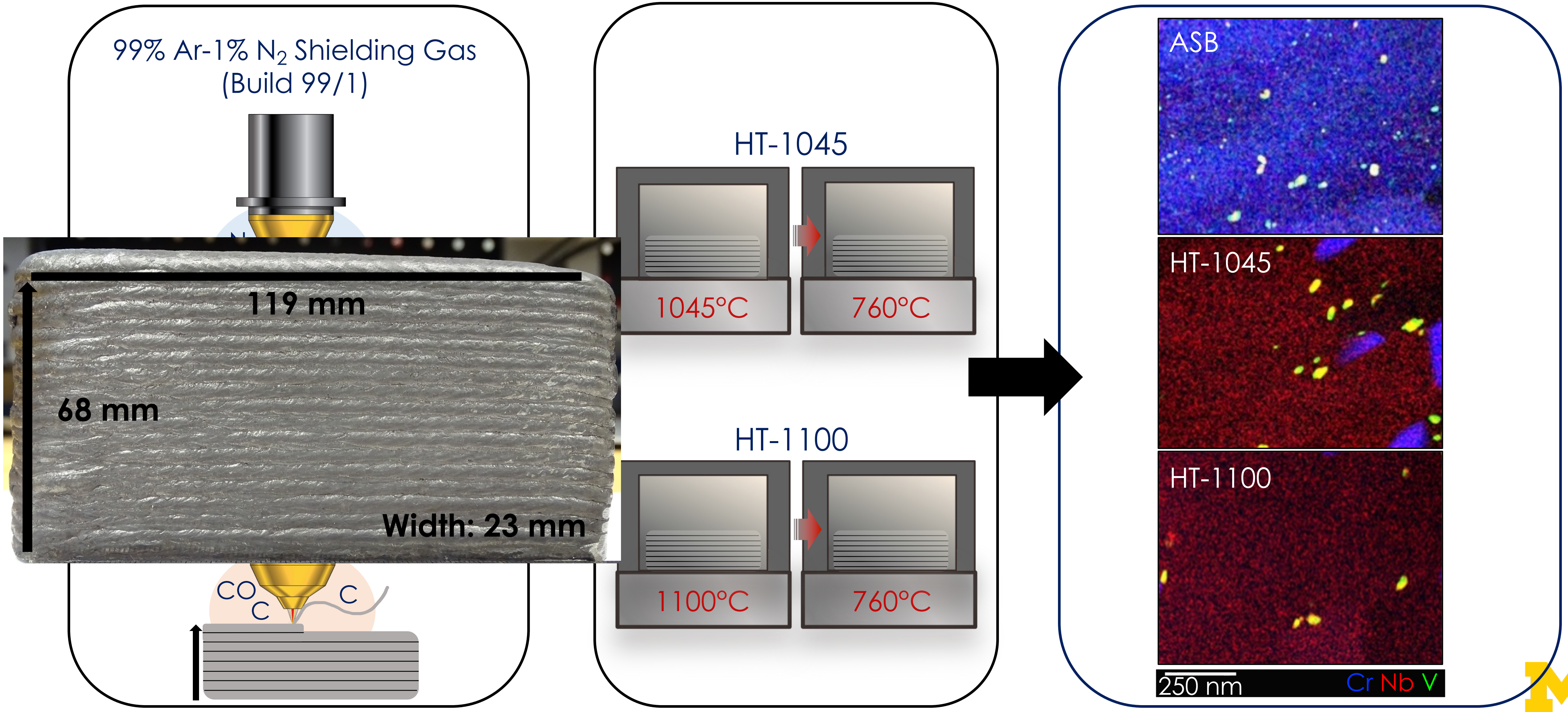
Wire Arc AM Experimental Details

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



Build

Heat Treat

Characterize

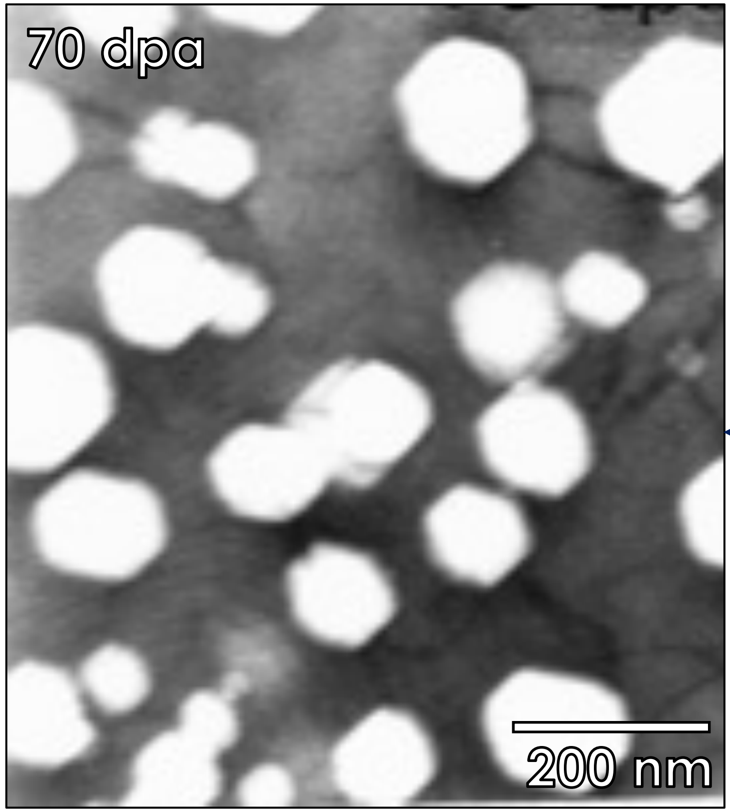
Shielding Gas Effect on Sink Strength

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

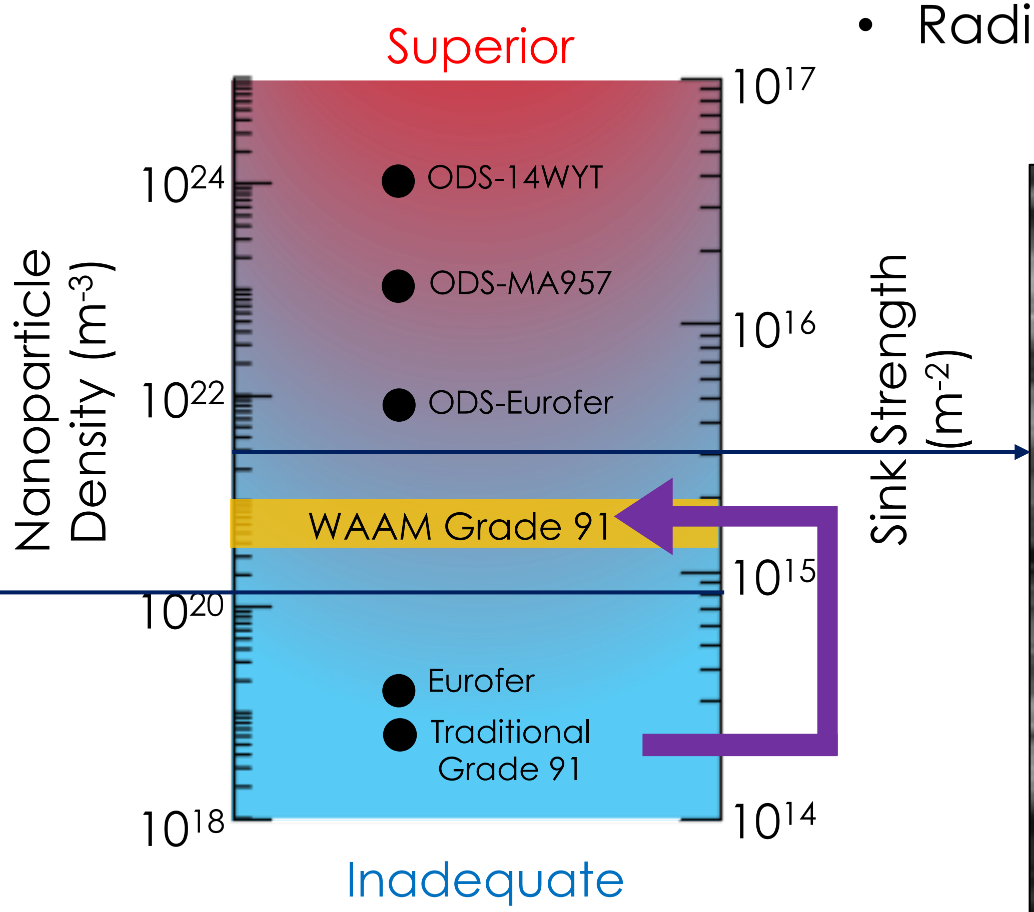
$S_{ppt} \sim 4\pi RN$

Critical sink strength value to prevent:

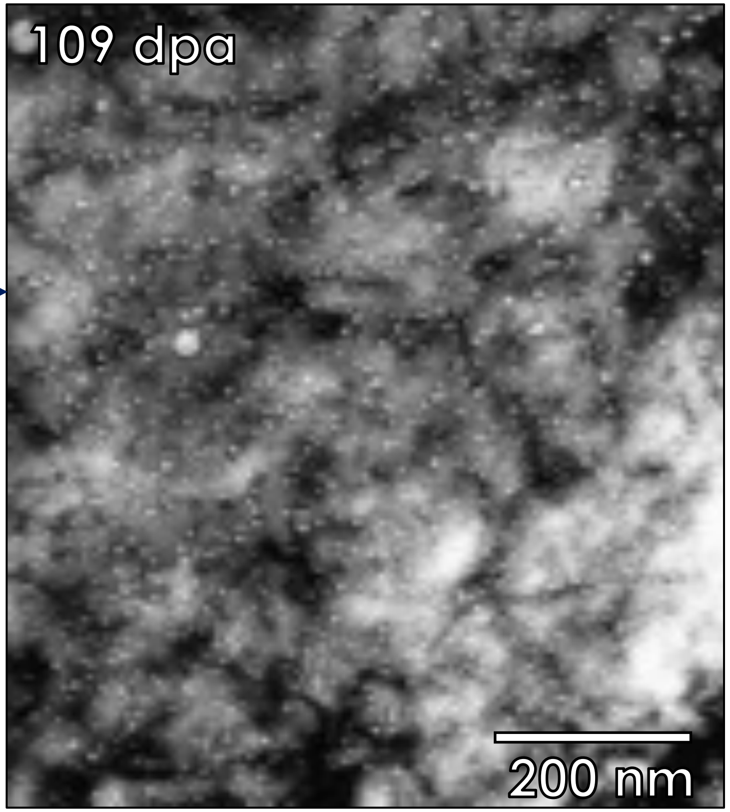
- Void swelling : 10^{15} m^{-2}
- Radiation hardening: 10^{16} m^{-2}



22% swelling



Increased gained from shielding gas use



0.5% swelling

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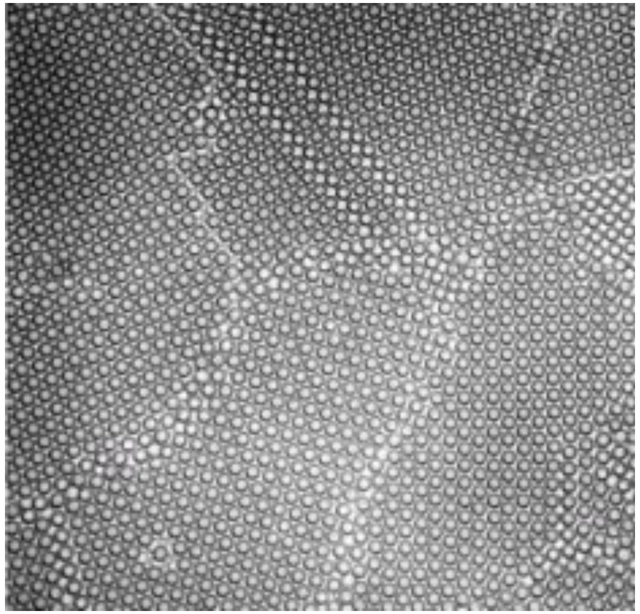
S.J. Zinkle and L.L. Snead, Ann Rev. Mat. Res., 44 (2014) 241

Putting it together:

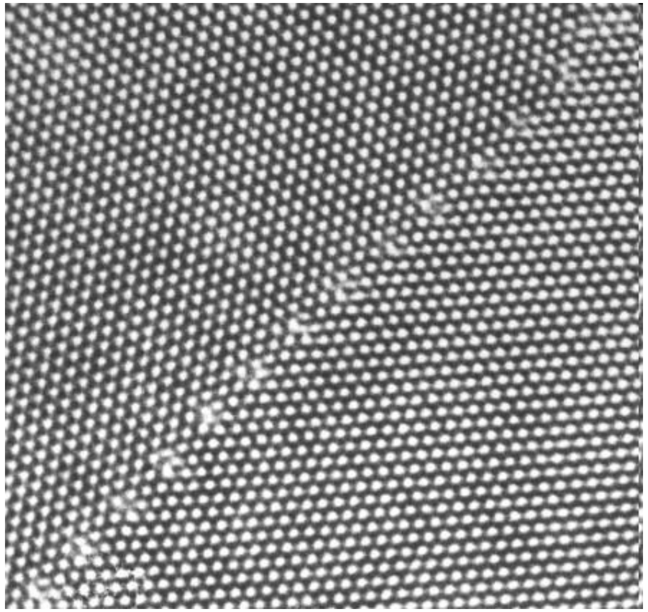
Table 5.2 Reaction rate constants for defect–sink reactions

Reaction	Rate constant	Sink strength	Eq. #
v + v	$K_{2v} = \frac{z_{2v}\Omega D_v}{a^2}$	–	Equation (5.58)
i + i	$K_{2i} = \frac{z_{2i}\Omega D_i}{a^2}$	–	Equation (5.58)
v + i	$K_{iv} = \frac{z_{iv}\Omega D_i}{a^2}$	–	Equation (5.61)
v, i + void			
Reaction rate control	$K_{vV} = \frac{4\pi R^2 D_v}{a}$ $K_{iV} = \frac{4\pi R^2 D_i}{a}$	$k_{vV}^2 = k_{iV}^2 = \frac{4\pi R^2 \rho_V}{a}$	Equation (5.65)
Diffusion control	$K_{vV} = 4\pi R D_v$ $K_{iV} = 4\pi R D_i$	$k_{vV}^2 = k_{iV}^2 = 4\pi R \rho_V$	Equation (5.84)
Mixed rate control	$K_{vV} = \frac{4\pi R D_v}{1+\frac{a}{R}}$ $K_{iV} = \frac{4\pi R D_i}{1+\frac{a}{R}}$	$k_{vV}^2 = k_{iV}^2 = \frac{4\pi R \rho_V}{1+\frac{a}{R}}$	Equation (5.102)
v, i + dislocation			
Diffusion control	$K_{vd} = \frac{2\pi D_v}{\ln(\mathscr{R}/R_{vd})}$ $K_{id} = \frac{2\pi D_i}{\ln(\mathscr{R}/R_{id})}$	$k_{vd}^2 = \frac{2\pi \rho_d}{\ln(\mathscr{R}/R_{vd})}$ $k_{id}^2 = \frac{2\pi \rho_d}{\ln(\mathscr{R}/R_{id})}$	Equations (5.99, 5.100)
Reaction rate control	$K_{vd} = z_{vd} D_v$ $K_{id} = z_{id} D_i$	$k_{vd}^2 = z_{vd}\rho_d$ $k_{id}^2 = z_{id}\rho_d$	Equation (5.67)
Mixed rate control	$K_{vd} = \frac{D_v}{\frac{1}{z_{vd}} + \frac{\ln(\mathscr{R}/R_{vd})}{2\pi}}$ $K_{id} = \frac{D_i}{\frac{1}{z_{id}} + \frac{\ln(\mathscr{R}/R_{id})}{2\pi}}$	$k_{vd}^2 = \frac{\rho_d}{\frac{1}{z_{vd}} + \frac{\ln(\mathscr{R}/R_{vd})}{2\pi}}$ $k_{id}^2 = \frac{\rho_d}{\frac{1}{z_{id}} + \frac{\ln(\mathscr{R}/R_{id})}{2\pi}}$	Equation (5.104)
v, i + grain boundary			
Diffusion control	$K_{vgb} = 4\pi D_v d$ $K_{igb} = 4\pi D_i d$ $K_{vgb} = \pi k D_v d^2$ $K_{igb} = \pi k D_i d^2$	$k_{gb}^2 = 24/d^2, \quad d < 10^{-3}$ cm $k_{gb}^2 = 6k/d, \quad d > 10^{-3}$ cm	Equation (5.115) Equation (5.116)
v, i + coherent ppt	$K_{vCP} = 4\pi R_{CP} D_v Y_v,$ $K_{iCP} = 4\pi R_{CP} D_i Y_i$	$k_{vCP}^2 = 4\pi R_{CP}\rho_{CP} Y_v,$ $k_{iCP}^2 = 4\pi R_{CP}\rho_{CP} Y_i$	Equation (5.120)

Sink Type IV – Grain Boundaries



Bubble Raft Model of Grain Boundaries

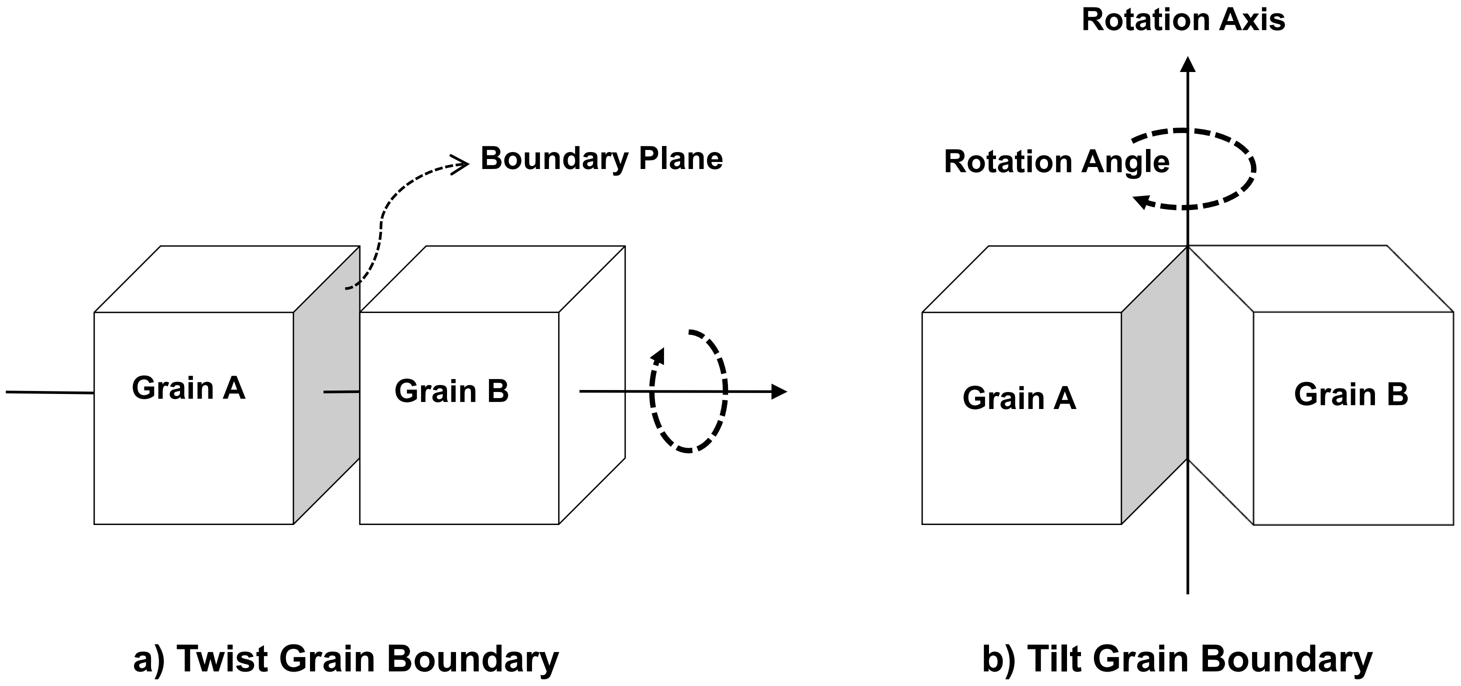


HRTEM image of a Σ19 GB in Al

- 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?