

# RIS + Defects

K.G. Field<sup>1,a</sup>,

<sup>a</sup>kgfield@umich.edu

<sup>1</sup>University of Michigan



NUCLEAR ENGINEERING &  
RADIOLOGICAL SCIENCES  
UNIVERSITY OF MICHIGAN

# Radiation Induced Segregation (RIS)

- RIS at grain boundaries
- Some “classic” examples
- Modeling RIS in binary alloys

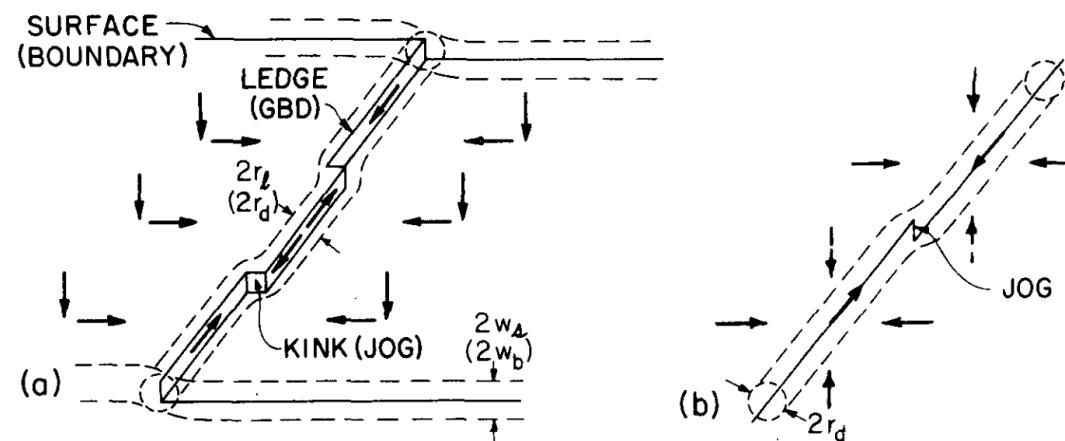
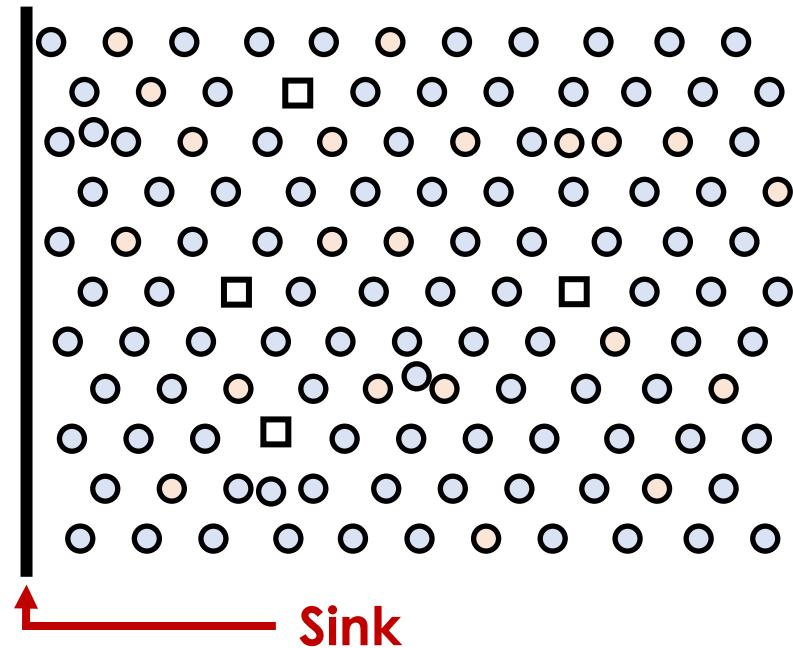


Fig. 4. Model for diffusion: (a) at void surface, or, alternatively, at grain boundary (parentheses); (b) at dislocation loop segment.

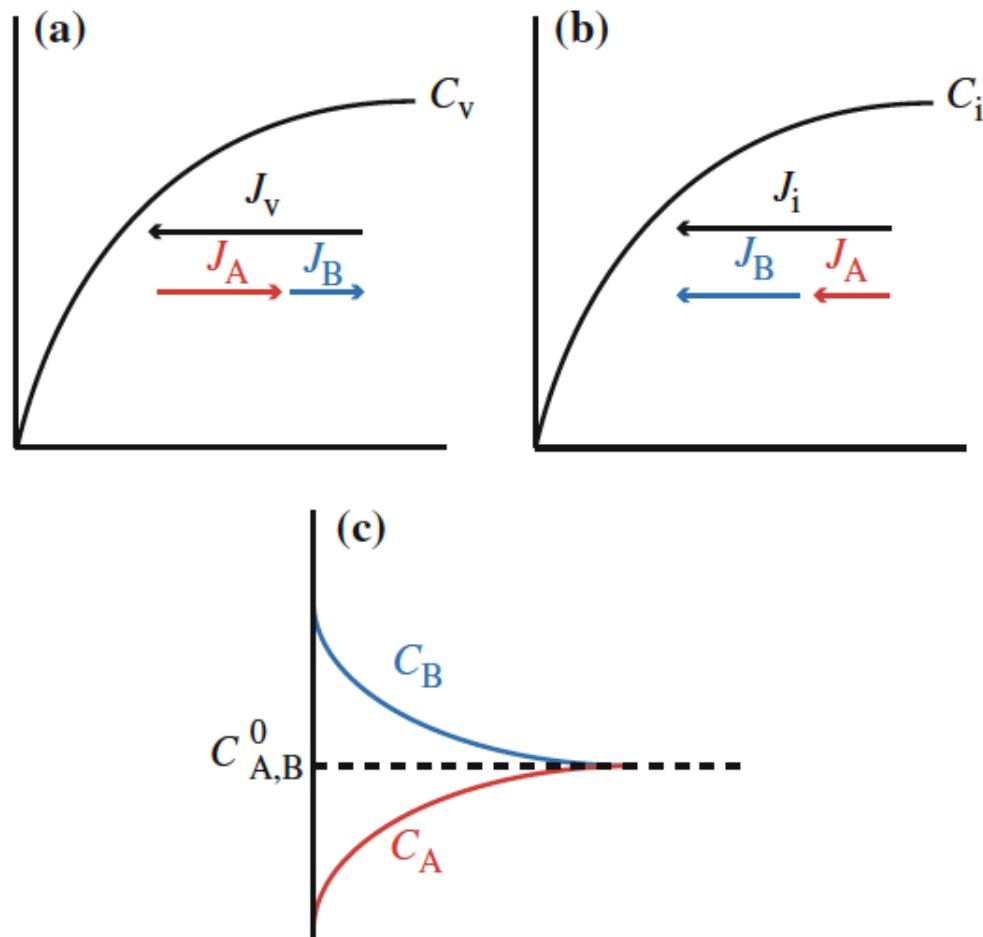
- **Goal:** Understand the role of diffusion imbalances on the occurrence of RIS in multi-component alloys



# RIS visual

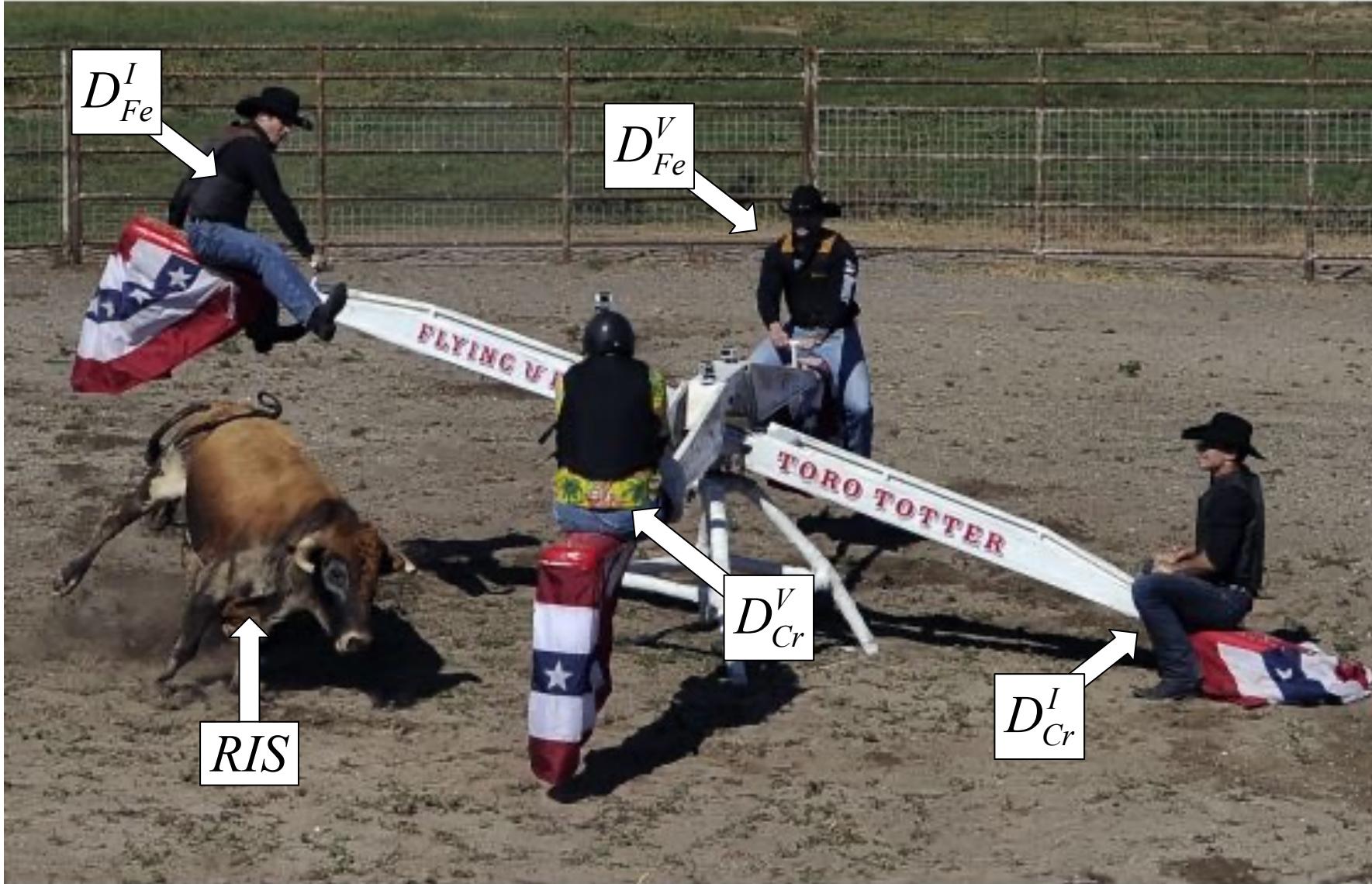


- Motion of defects means motion of atoms



**Fig. 6.2** Schematic of radiation-induced segregation in a binary, 50 % A–50 % B system showing (a) the development of the vacancy concentration profile by the flow of vacancies to the grain boundary balanced by an equal and opposite flow of A and B atoms, but not necessarily in equal numbers, (b) the development of the interstitial concentration profile by the flow of interstitials to the grain boundary balanced by an equal flow of A and B atoms migrating as interstitials, but not necessarily in equal numbers, (c) the resulting concentration profiles for A and B

# RIS becomes a balancing act



Let's model a concentrated alloy of A & B atoms, e.g.  $A_xB_{x-1}$

Assumptions:

- A & B atoms are distributed uniformly throughout (e.g. no long or short range ordering)
- Sink is acting in the perfect sink condition (black hole)

First, let's define the general kinetics equations

Since we now have A & B atoms:

$$\frac{\partial C_\nu}{\partial t} = -\nabla J_\nu + K_0 - K_{i\nu} C_i C_\nu$$

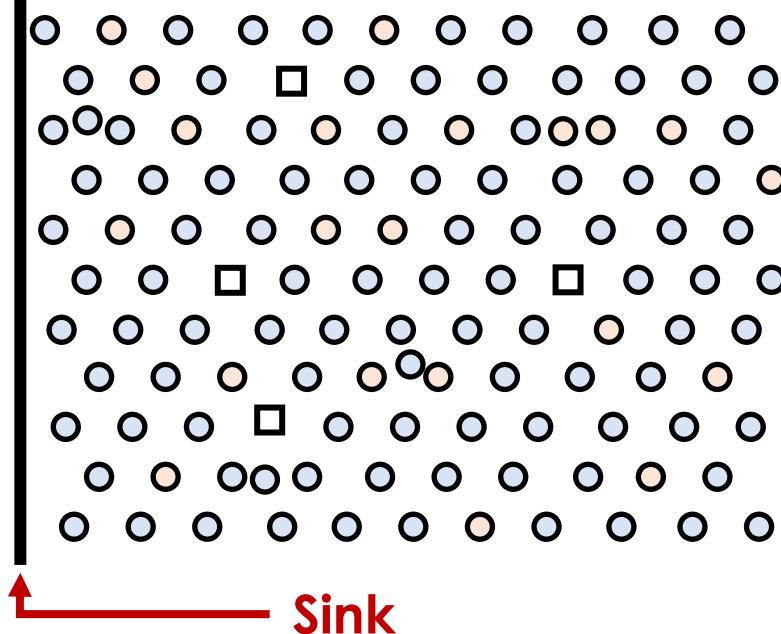
$$\frac{\partial C_A}{\partial t} = -\nabla J_A$$

$$\frac{\partial C_i}{\partial t} = -\nabla J_i + K_0 - K_{i\nu} C_i C_\nu$$

$$\frac{\partial C_B}{\partial t} = -\nabla J_B$$

Let's model a concentrated alloy of A & B atoms, e.g.  $A_xB_{x-1}$

Now, let's write the flux in terms of  $i$ ,  $v$ ,  $A$  &  $B$



The flux of interstitials will be the combined flux of A and B atoms via interstitial hopping:

The flux of vacancies will be the combined flux of A and B atoms via vacancy hopping:

Let's model a concentrated alloy of A & B atoms, e.g.  $A_xB_{x-1}$

We now need to define the partial diffusion coefficients, since the flux (e.g.,  $J_x$ ) is proportional to the partial diffusion coefficients:

Let's model a concentrated alloy of **A** & **B** atoms, e.g.  $A_xB_{x-1}$

Writing out all the diffusion coefficients in terms of partial diffusion coefficients:

$$D_A^v = d_{Av} N_v \quad D_v^A = d_{Av} N_A \quad \left. \begin{array}{l} \\ \end{array} \right\} \text{Vacancies}$$

$$D_B^v = d_{Bv} N_v \quad D_v^B = d_{Bv} N_B \quad \left. \begin{array}{l} \\ \end{array} \right\} \text{Vacancies}$$

$$D_A^i = d_{Ai} N_i \quad D_i^A = d_{Ai} N_A \quad \left. \begin{array}{l} \\ \end{array} \right\} \text{Interstitials}$$

$$D_B^i = d_{Bi} N_i \quad D_i^B = d_{Bi} N_B \quad \left. \begin{array}{l} \\ \end{array} \right\} \text{Interstitials}$$



Let's model a concentrated alloy of **A** & **B** atoms, e.g.  $A_xB_{x-1}$

The total diffusion coefficients are::

$$D_v = D_v^A + D_v^B = d_{Av} N_A + d_{Bv} N_B \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} \text{Defects}$$
$$D_i = D_i^A + D_i^B = d_{Ai} N_A + d_{Bi} N_B \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} \text{Atoms}$$
$$D_A = D_A^v + D_A^i = d_{Av} N_v + d_{Ai} N_i \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} \text{Atoms}$$
$$D_B = D_B^v + D_B^i = d_{Bv} N_v + d_{Bi} N_i \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} \text{Atoms}$$

Let's model a concentrated alloy of A & B atoms, e.g.  $A_xB_{x-1}$

$$J_A = -D_A \alpha \nabla C_A + d_{Av} N_A \nabla C_v - d_{Ai} N_A \nabla C_i$$

$$J_B = -D_B \alpha \nabla C_B + d_{Bv} N_B \nabla C_v - d_{Bi} N_B \nabla C_i$$

$$J_v = d_{Av} N_v \alpha \nabla C_A + d_{Bv} N_v \alpha \nabla C_B - D_v \nabla C_v = (d_{Av} - d_{Bv}) N_v \alpha \nabla C_A - D_v \nabla C_v$$

$$J_i = -d_{Ai} N_i \alpha \nabla C_A - d_{Bi} N_i \alpha \nabla C_B - D_i \nabla C_i = -(d_{Ai} - d_{Bi}) N_i \alpha \nabla C_A - D_i \nabla C_i$$

Let's model a concentrated alloy of A & B atoms, e.g.  $A_xB_{x-1}$

$$\frac{\partial C_v}{\partial t} = \nabla [ - (d_{Av} - d_{Bv}) \alpha \Omega C_v \nabla C_A + D_v \nabla C_v ] + K_o - K_{iv} C_i C_v$$

$$\frac{\partial C_i}{\partial t} = \nabla [ (d_{Ai} - d_{Bi}) \alpha \Omega C_i \nabla C_A + D_i \nabla C_i ] + K_o - K_{iv} C_i C_v$$

$$\frac{\partial C_A}{\partial t} = \nabla [ D_A \alpha \nabla C_A + \Omega C_A (d_{Ai} \nabla C_i - d_{Av} \nabla C_v) ]$$

Let's model a concentrated alloy of A & B atoms, e.g.  $A_xB_{x-1}$

$$\nabla C_A = \frac{N_A N_B d_{Bi} d_{Ai}}{\alpha(d_{Bi} N_B D_A + d_{Ai} N_A D_B)} \times \left( \frac{d_{Av}}{d_{Bv}} - \frac{d_{Ai}}{d_{Bi}} \right) \nabla C_v$$

If  $\frac{d_{Ai}}{d_{Bi}} > \frac{d_{Av}}{d_{Bv}}$  →

# Example Alloy B<sub>0.75</sub>A<sub>0.25</sub>

Given:  $E_m^{Av} \sim 0.8 \text{ eV}$        $E_m^{Ai} \sim 0.10 \text{ eV}$

$E_m^{Bv} \sim 1.28 \text{ eV}$        $E_m^{Bi} \sim 0.15 \text{ eV}$

Will A or B atoms enrich at the sinks?

# Interstitial Binding

Solutes can tightly bind to interstitials forming interstitial solute complexes, this can be accounted for by,

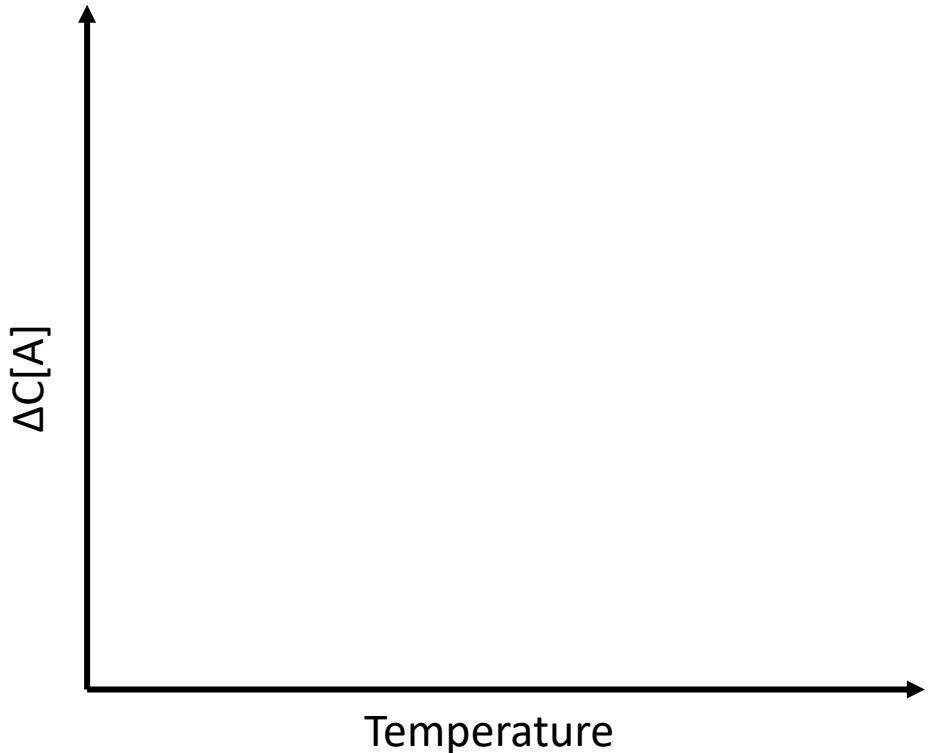
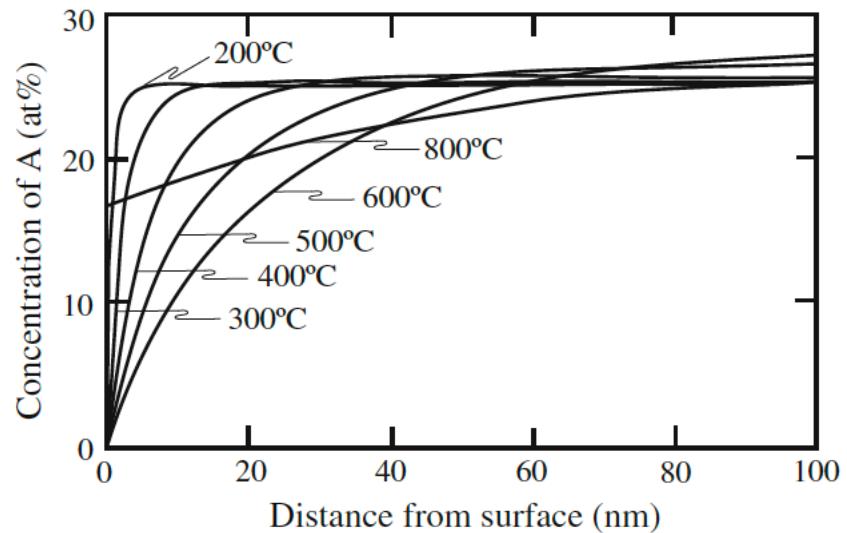
$$C_{Ai} = C_i \frac{C_A \exp\left(\frac{E_b^{Ai}}{k_B T}\right)}{C_A \exp\left(\frac{E_b^{Ai}}{k_B T}\right) + C_B}$$

Or simply,

$$\frac{d_{Ai}}{d_{Bi}} \approx \exp\left(\frac{E_m^{Bi} - E_m^{Ai} + E_b^{Ai}}{k_B T}\right)$$

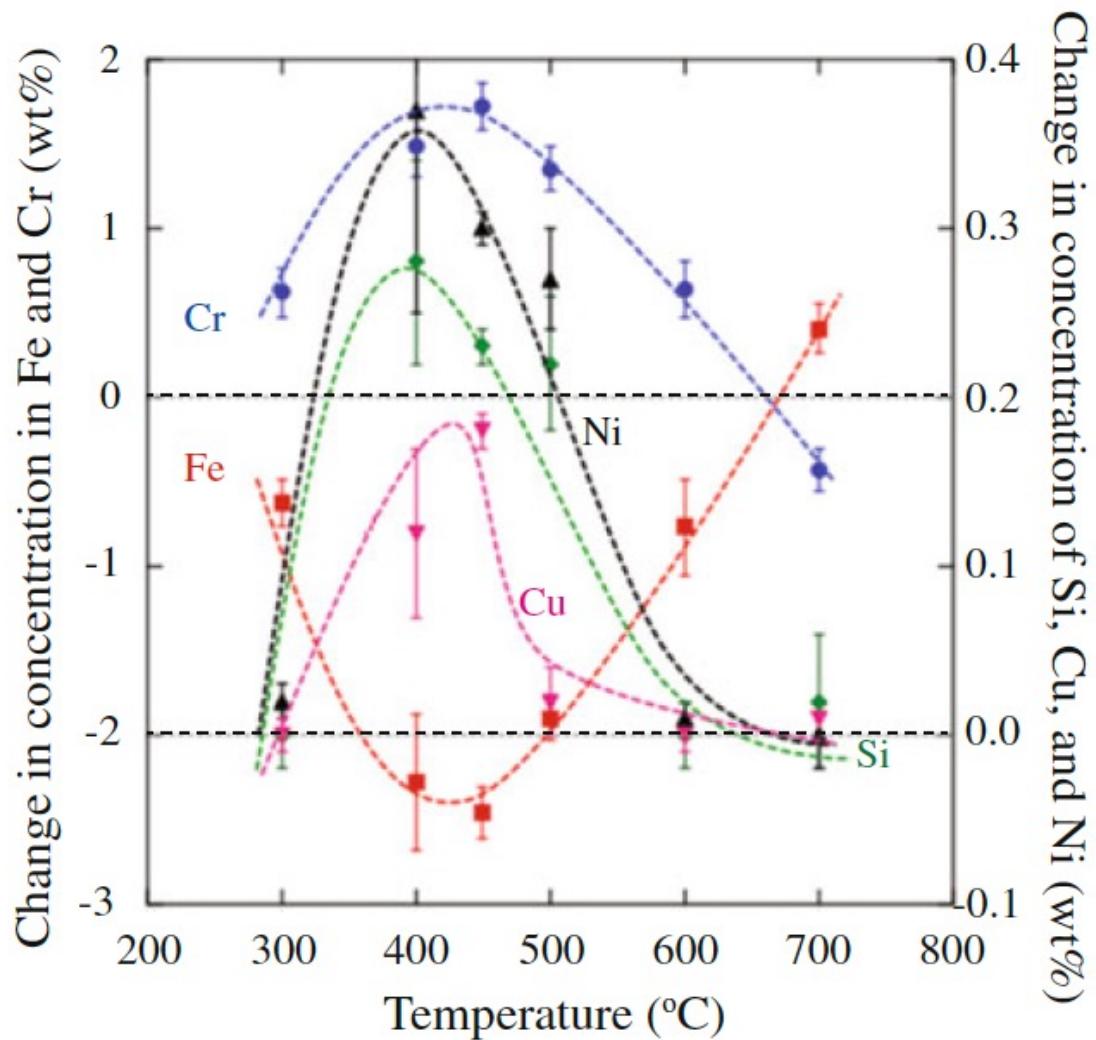
# Temperature Dependence

**Fig. 6.7** Steady-state concentration profiles of element A as a function of temperature for the same alloy and irradiation conditions as shown in Fig. 6.3 (after [4])



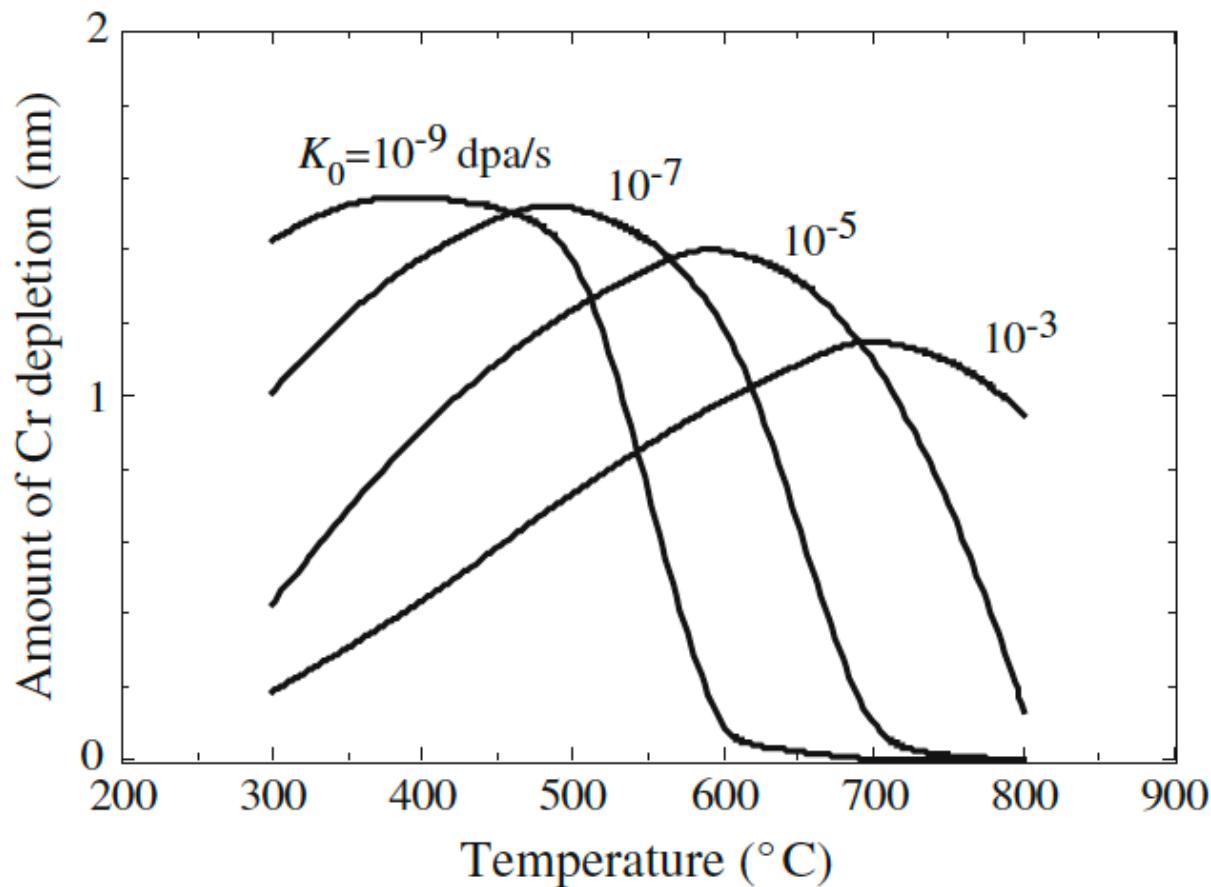
# Temperature Dependence

**Fig. 6.23** Grain boundary composition as a function of temperature in alloy T91 irradiated to 3 dpa with 2.0 MeV protons (after [26])

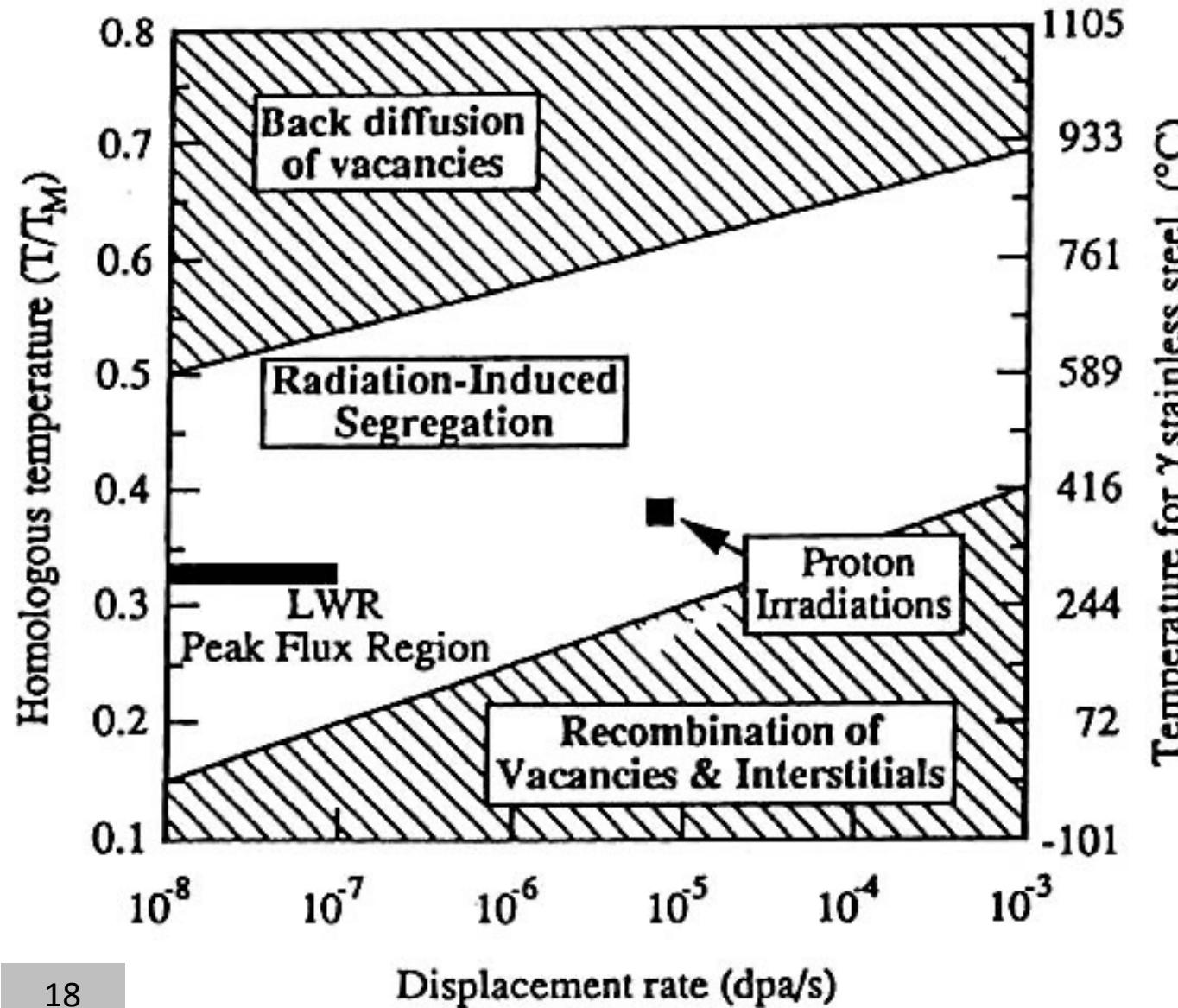


# Dose Rate Dependence

**Fig. 6.9** Dose rate dependence of grain boundary chromium depletion calculated using the MIK model for RIS (after [13, 14])

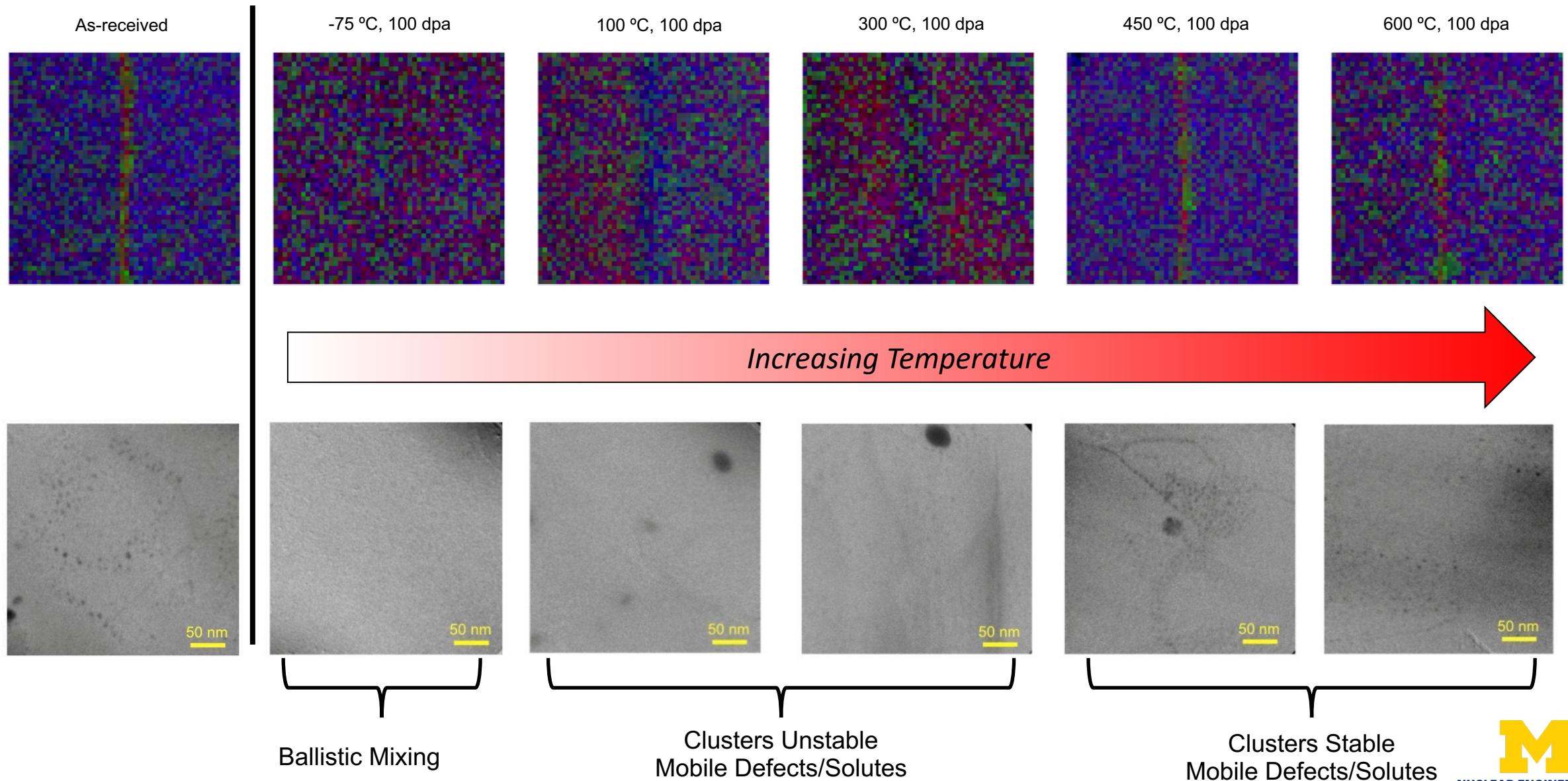


# Temperature and Dose Rate Dependence

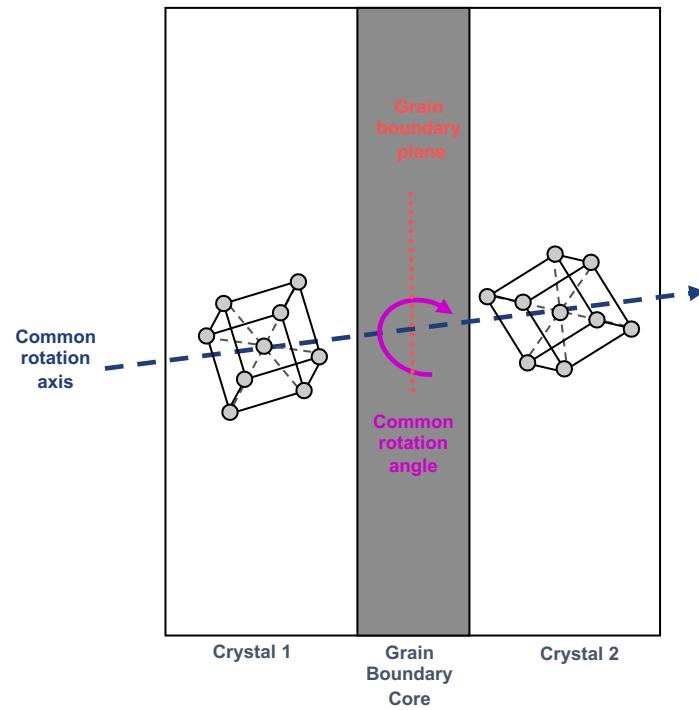


- The degree of segregation under irradiation will vary with temperature and dose rate.
- At low temperatures where defect mobility is limited, defect recombination dominates and RIS is minimal.
- At high temperatures where defect mobility and thermally induced defect populations are high, diffusion works to prevent or remove any composition gradients.
- At intermediate temperatures, however, RIS will occur.

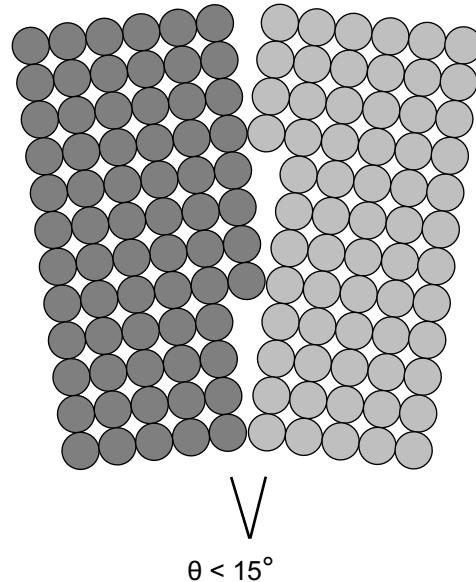
# RIS is a “finger print” for defect mobility and loss



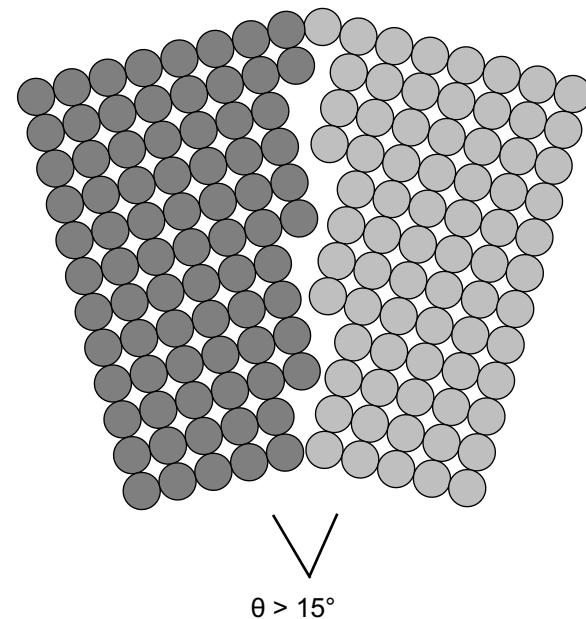
# Grain Boundary Interfacial Structure Overview



Low Angle Grain Boundary

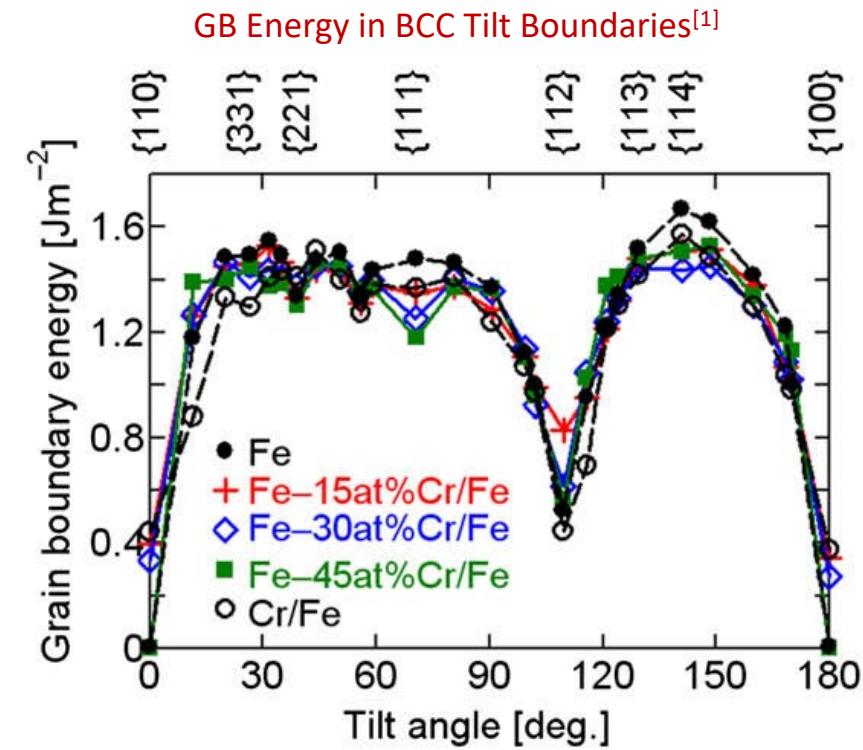
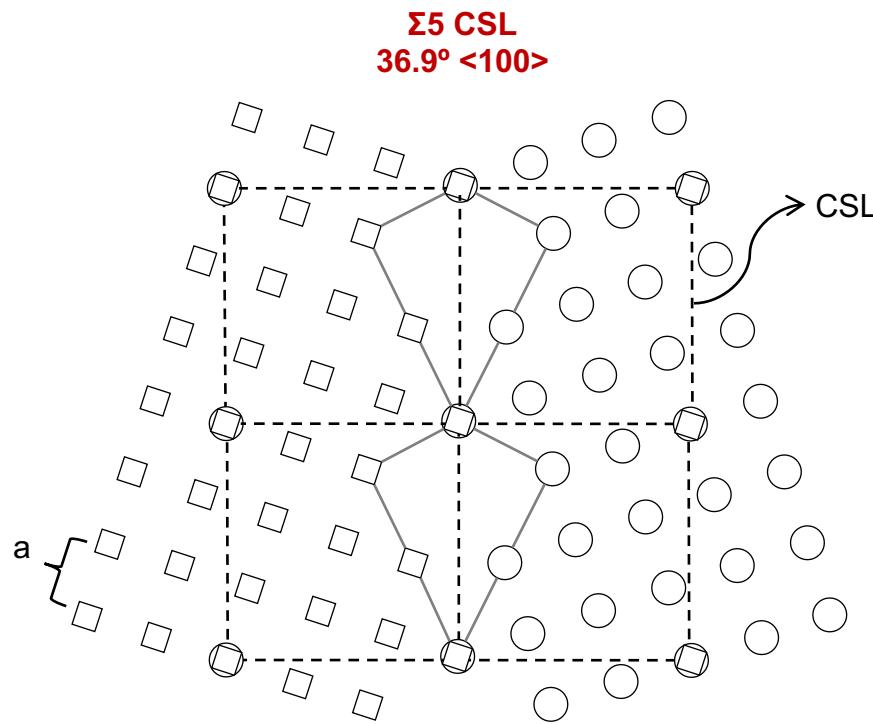


High Angle Grain Boundary



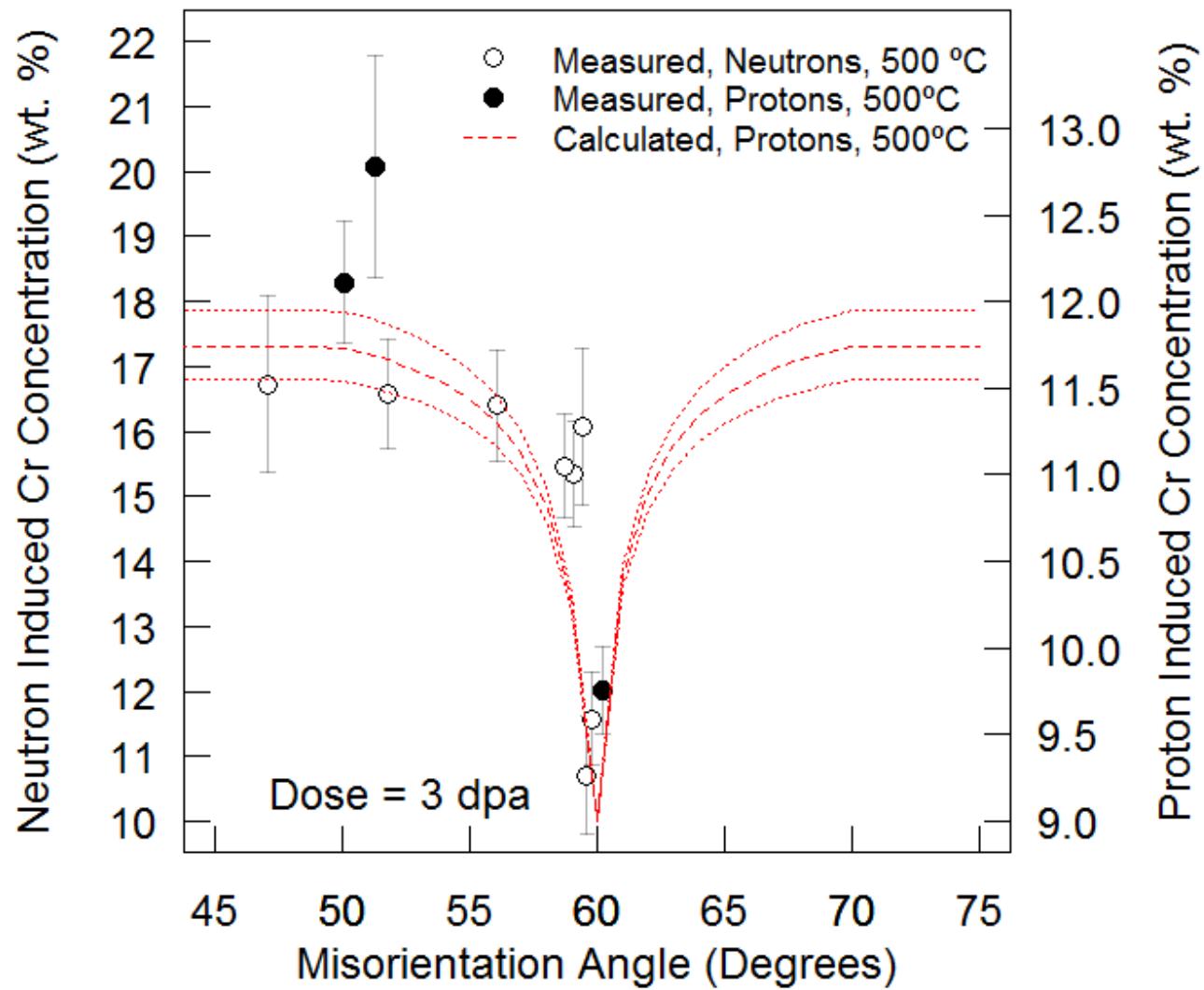
- Axis-angle representation for cubic materials helps describe GB structure:
  - **Axis:** The common crystallographic axis which comprises the boundary
  - **Angle ( $\theta$ ):** The degree of rotation between the two crystals along the axis
  - Axis-angle pairs describe GB: **low angle**, **high angle** or **special (low- $\Sigma$ ) GB**

# Coincident Site Lattice (CSL) Convention

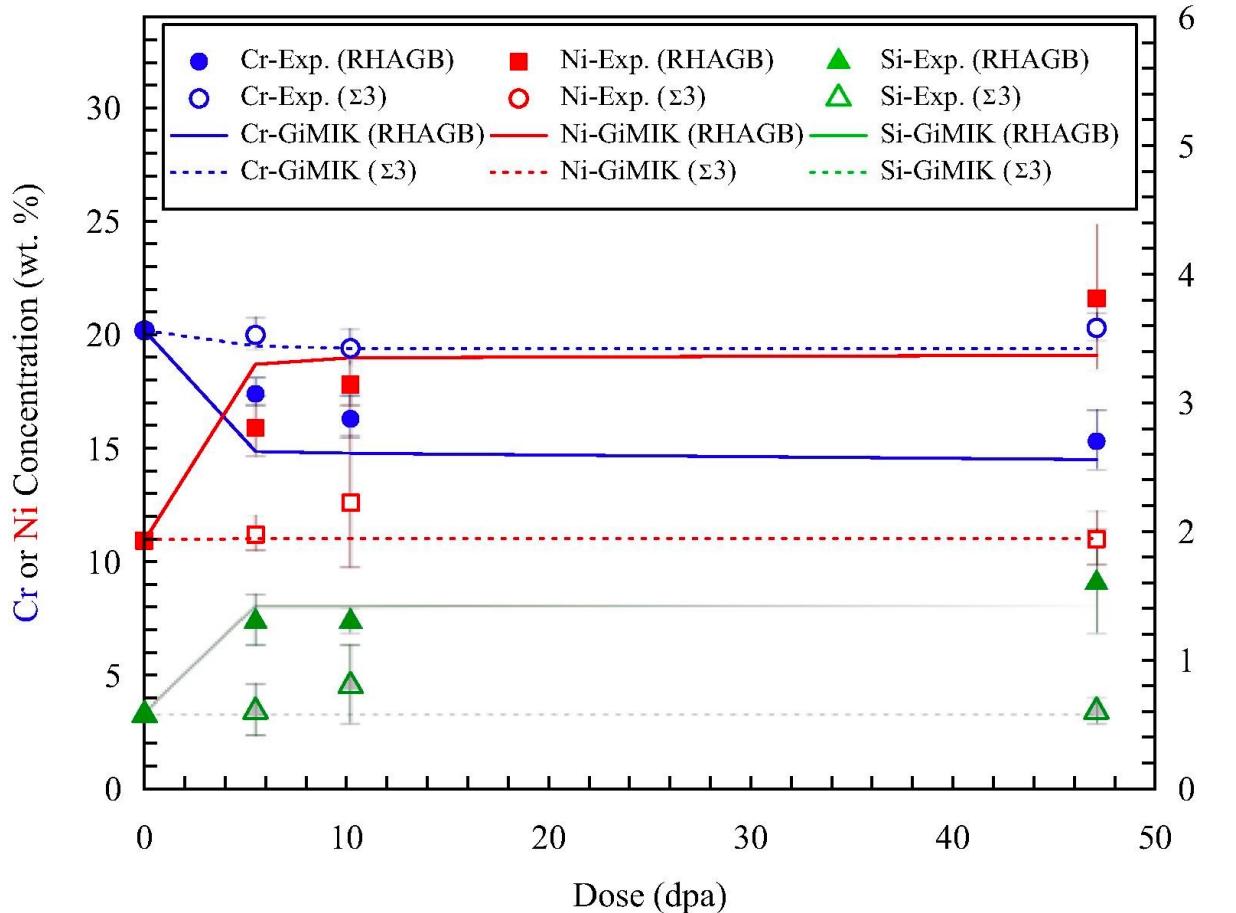
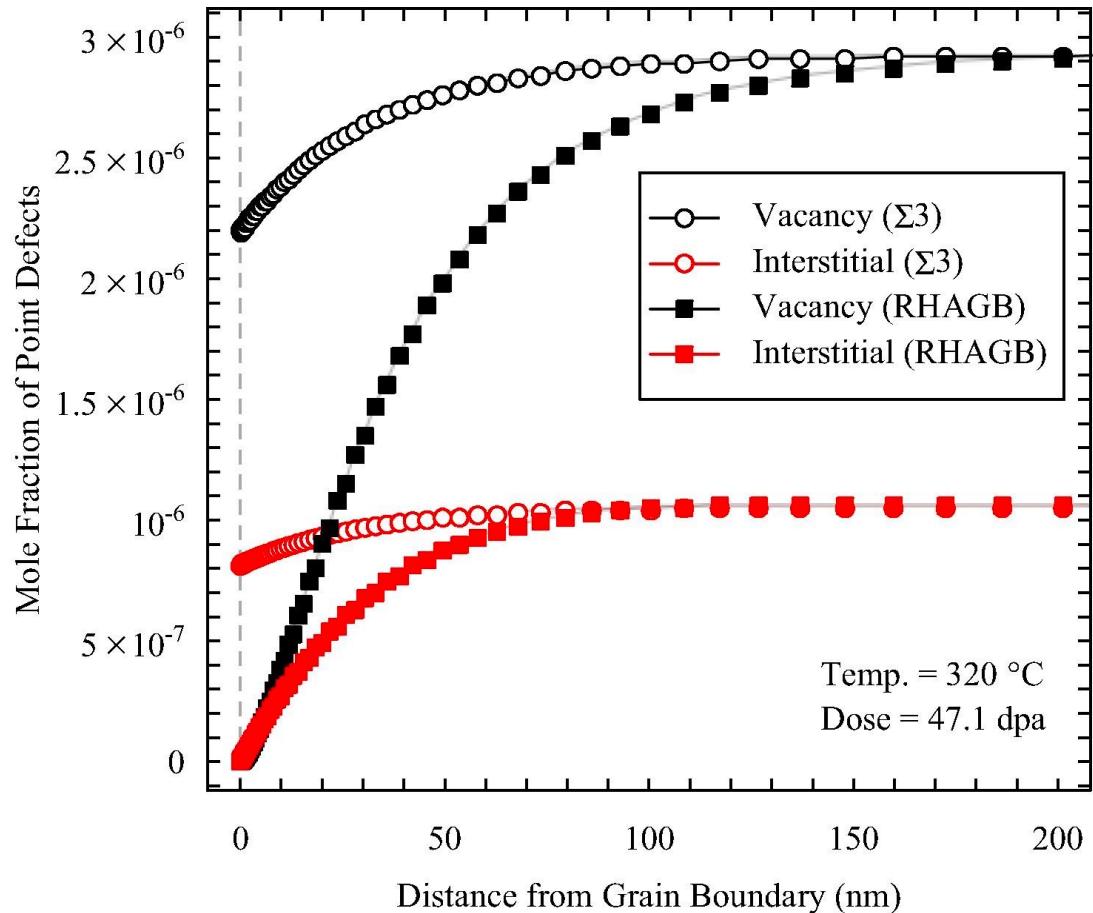


- CSL is a geometrical construction based on the geometry of the lattice
- $\Sigma$  is the ratio between the area enclosed by a unit cell of coincidence sites and the standard unit cell
- Low  $\Sigma$  CSL boundaries have higher coherency compared to general HAGBs

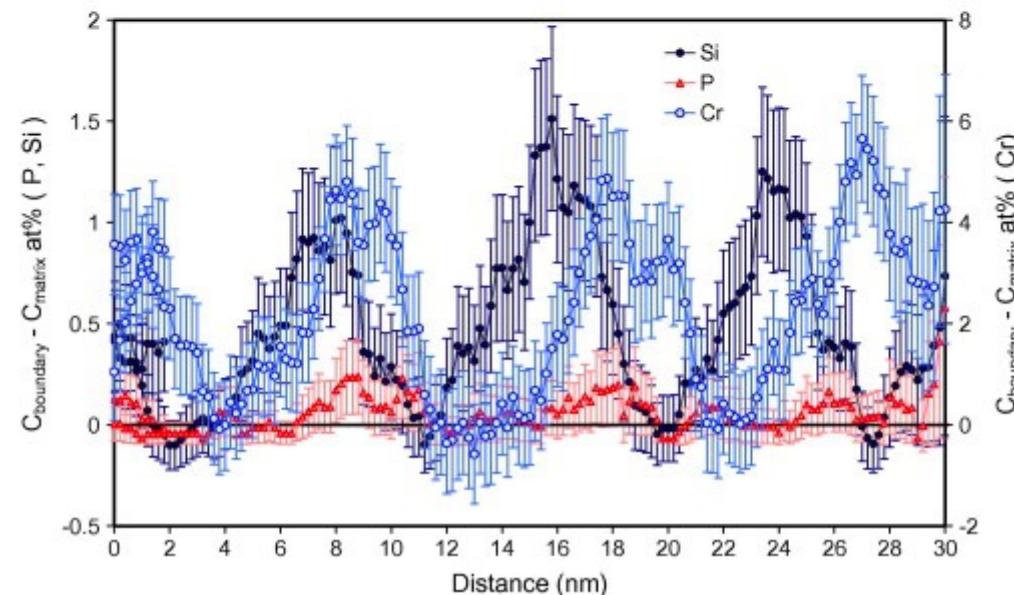
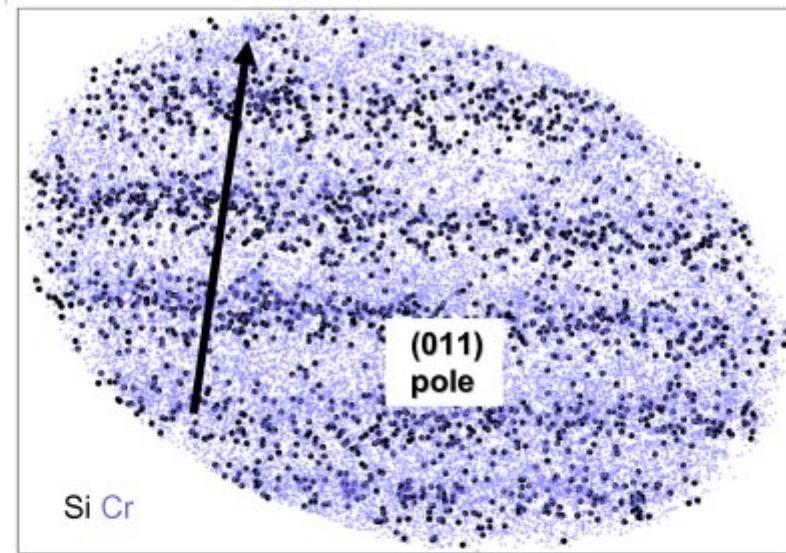
# Example model and experimental data for BCC steels



# Example model and experimental data for FCC steels



# Segregation to grain boundary dislocations



# Outline

## **Defect Energetics:**

- Role of loops on material response
- Interstitial loop formation and energetics
- Vacancy loop vs. void formation

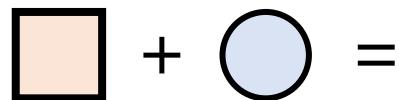
## **Goal:**

1. Understand the energetics associated with the formation of extended defects and the corresponding responses as a function of temperature and dose/dose rate.

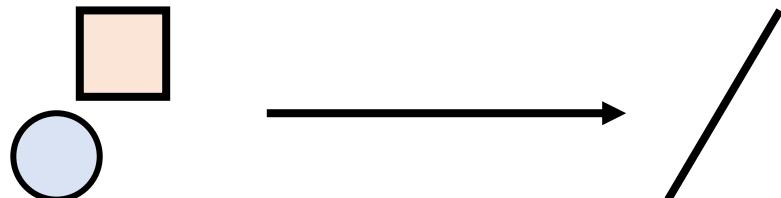


# Options of vacancies and interstitials

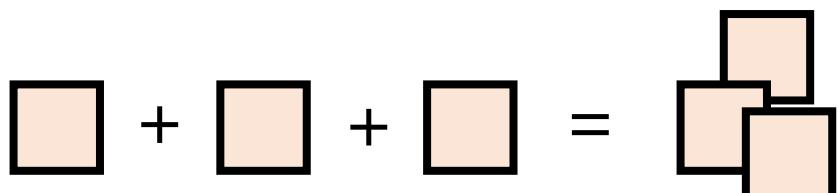
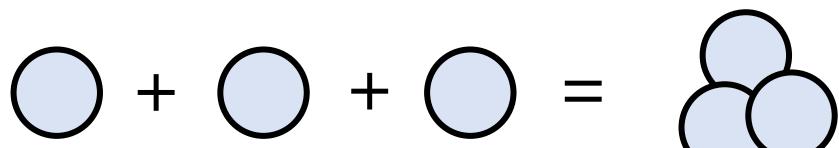
- Vacancies and interstitials can react with each other (recombination)



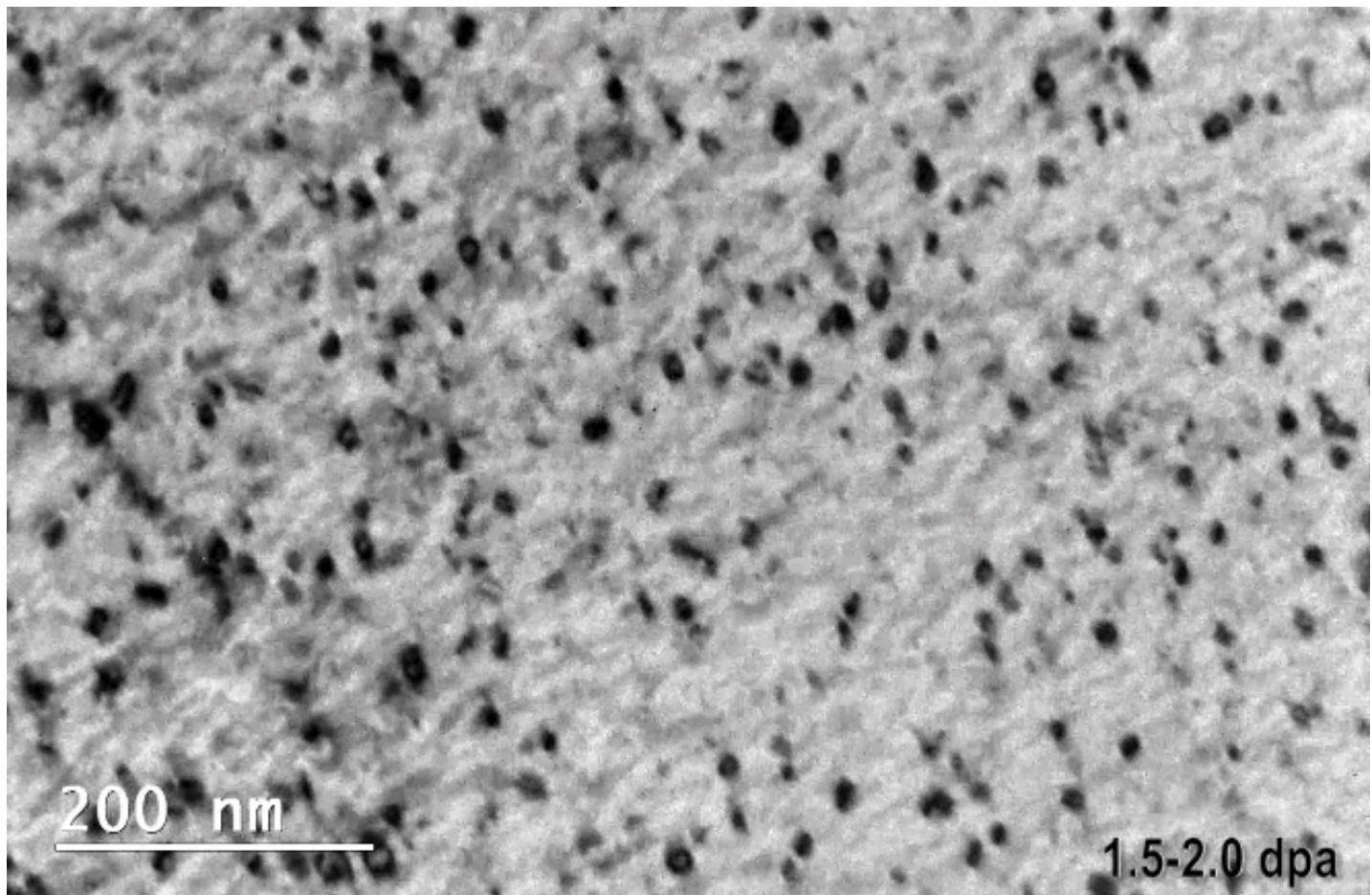
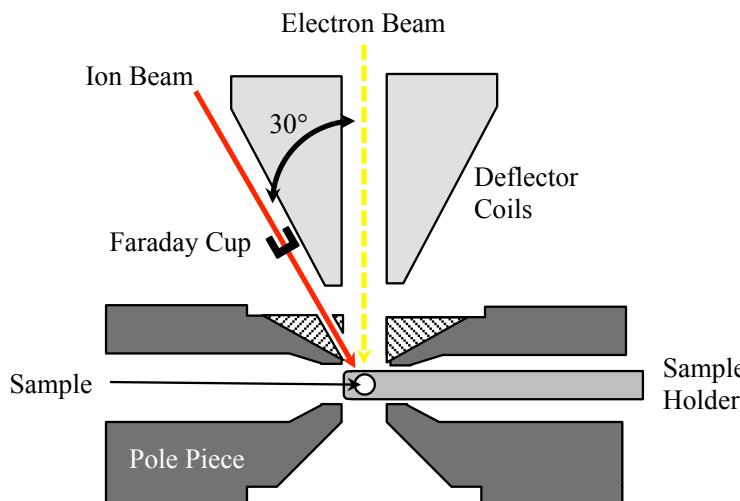
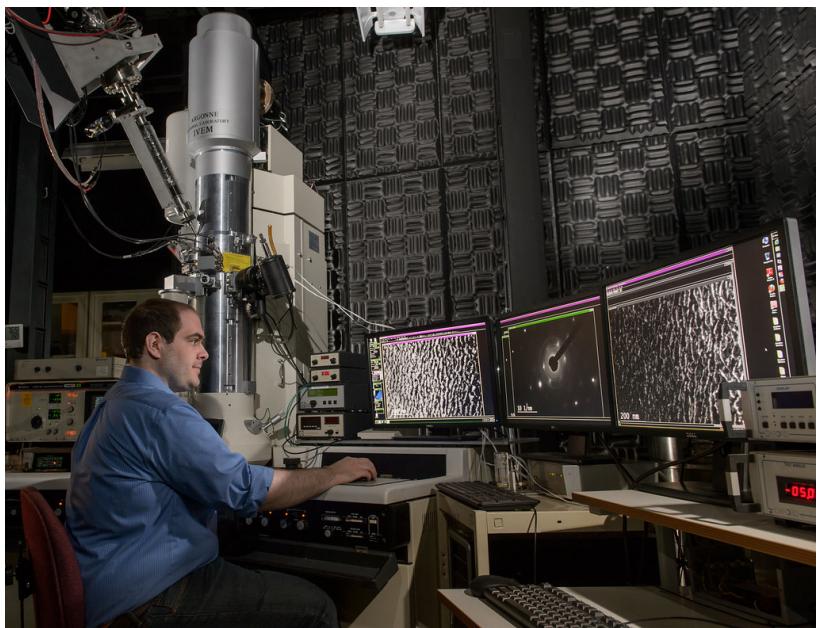
- They can react with defect sinks



- They can react with themselves



# Dislocation Loop Formation

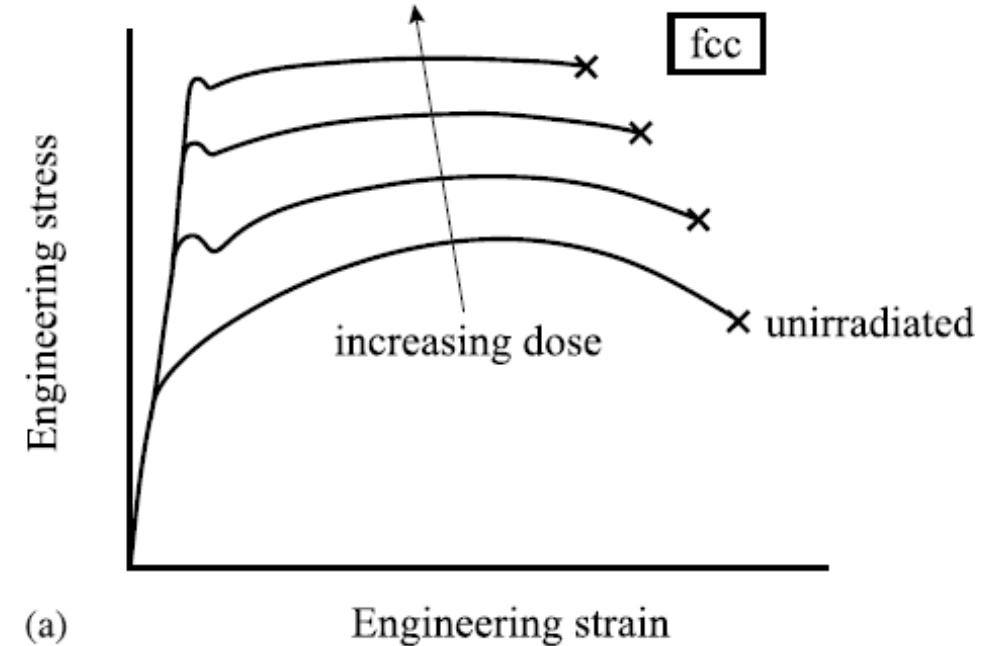
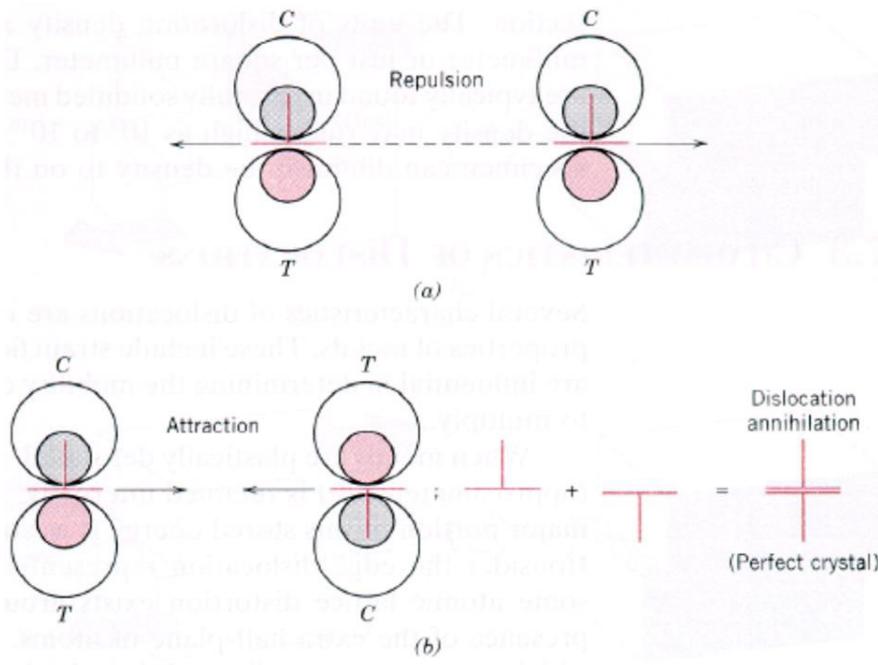


Video of in-situ ion irradiation of Fe-10Cr-4.8Al Gen I alloy irradiated at 320°C



NUCLEAR ENGINEERING &  
RADIOLOGICAL SCIENCES  
UNIVERSITY OF MICHIGAN

# Effects of dislocation loops on mechanical properties



- Slowing down or impeding dislocation motion in metals results in **hardening** but can also lead to **embrittlement**
- Dislocation loop formation by irradiation will cause this hardening and embrittlement response



# Dislocation Loop Formation

- In any crystal lattice there are close packed planes (e.g. most densely packed)
  - Normal to the closed pack plane is lattice planes that are widely separated
- Loops can be considered as a condensation of radiation-produced vacancies or interstitials

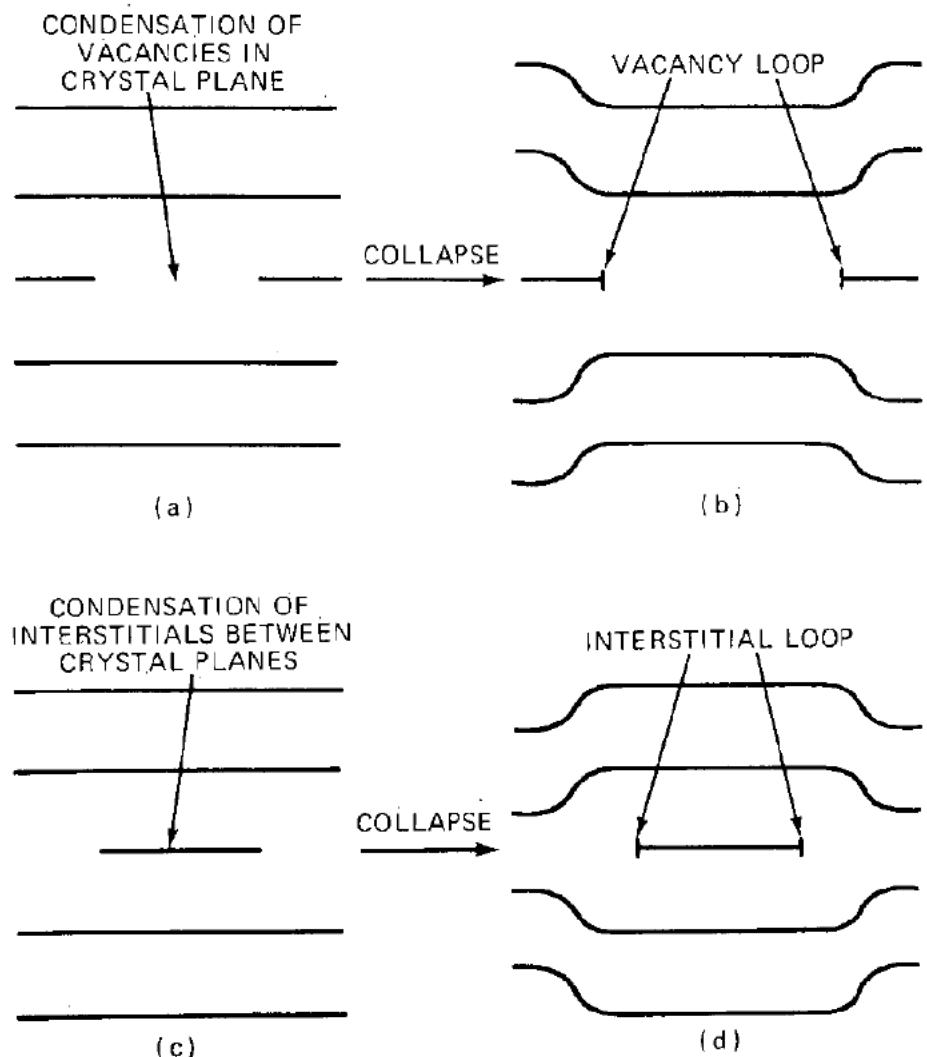
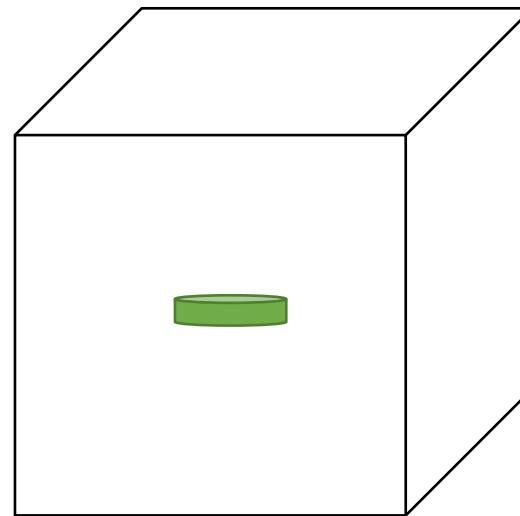
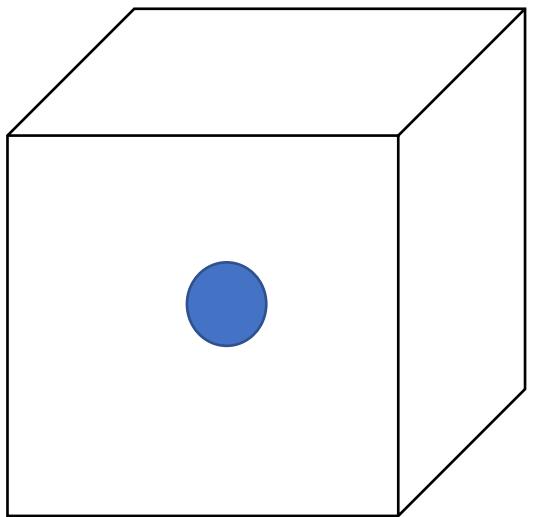


Fig. 18.4 Formation of vacancy loops and interstitial loops.

# A simple though experiment



If we placed a sphere and a disc into a finite volume of material, what aspects of those features would help define the change in energy for the total system?



# Dislocation Loop Formation

- Loops formed from interstitial atoms or vacancies can be distinguished in three ways:
  1. The **Burgers vector** (magnitude and direction)
  2. The **stacking fault** (if any) contained by the loop
  3. The **nature** (e.g. vacancy or interstitial loops)

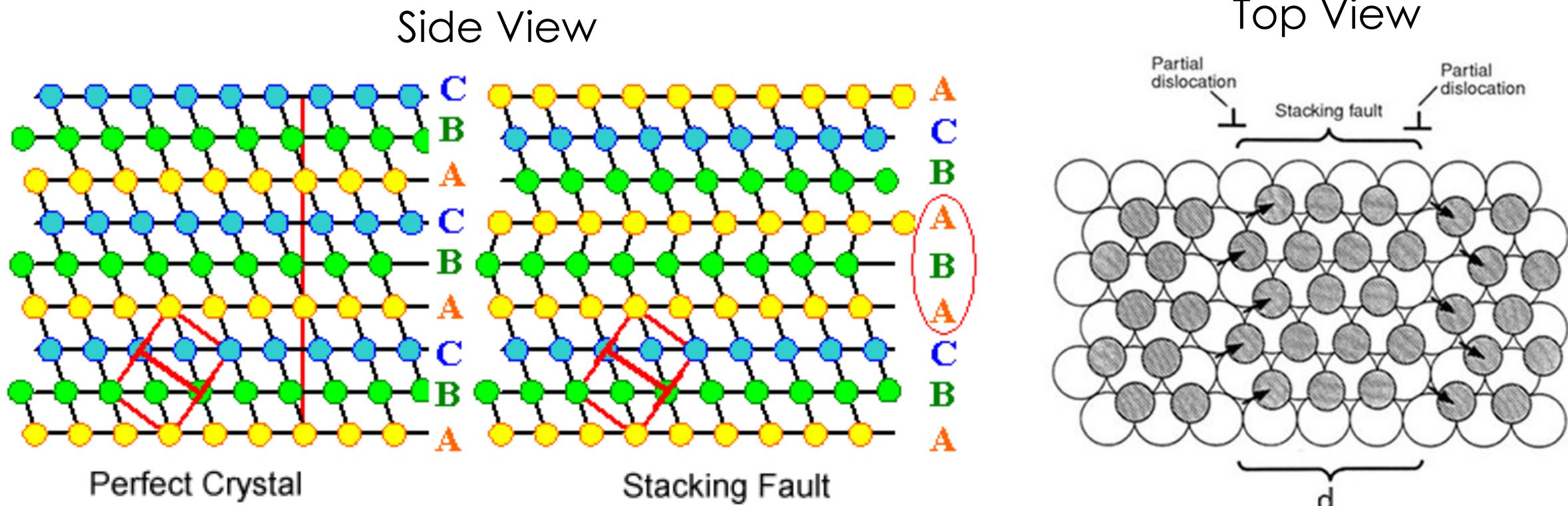


# Interstitial Loops Formation

- Let's first consider interstitial loop formation:
- Formation of extended defects occurs between closed packed planes
- In FCC materials, this can cause a break in the stacking sequence leading to stacking faults (also known as Frank loops)
- Disc/platelet of defects it the minimum energy configuration for defect clusters when the number of defects is small



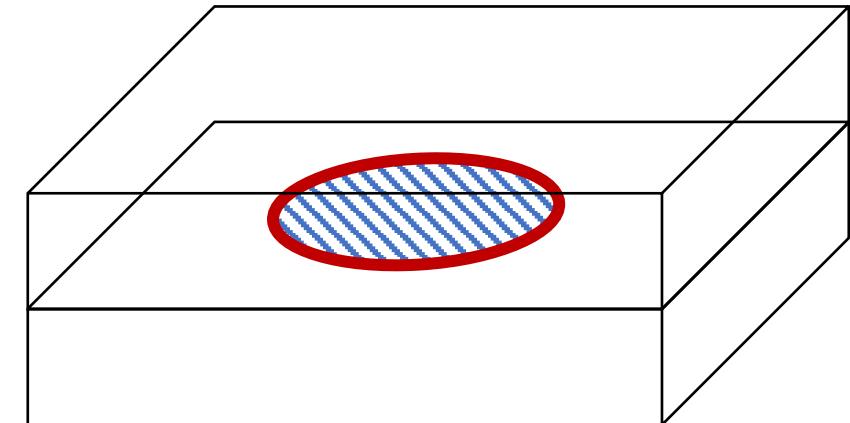
# What is a stacking fault?



- The shifted portion of the partial dislocation location is a “stacking fault”
  - more simply it is a “mistake” in the layering of atoms
- Found in closed-packed face centered cubic and hcp crystals because only the second-nearest neighbors are different at the fault

# Dislocation loop energy in FCC alloys

- For FCC, we must consider both the energy created because of the loop and of the possible stacking fault:





# Questions?