

RIS + Defects

K.G. Field^{1,a},

^akgfield@umich.edu

¹University 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

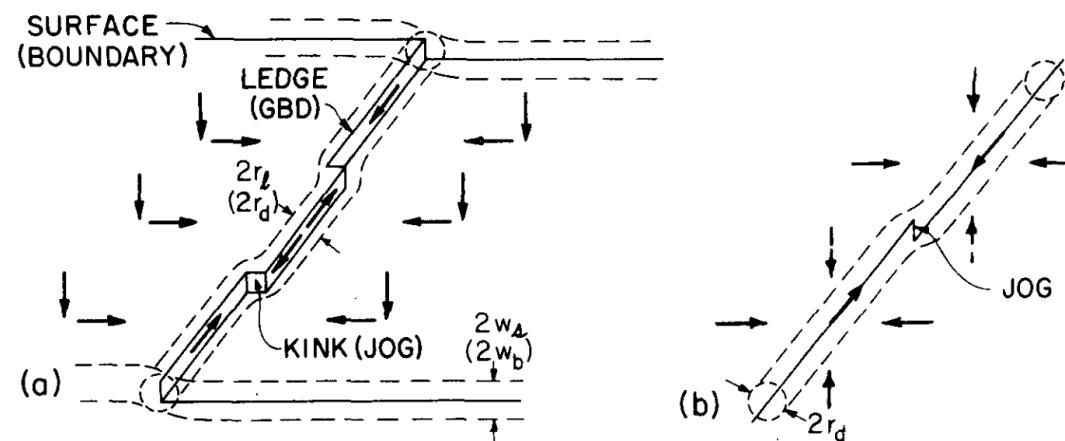


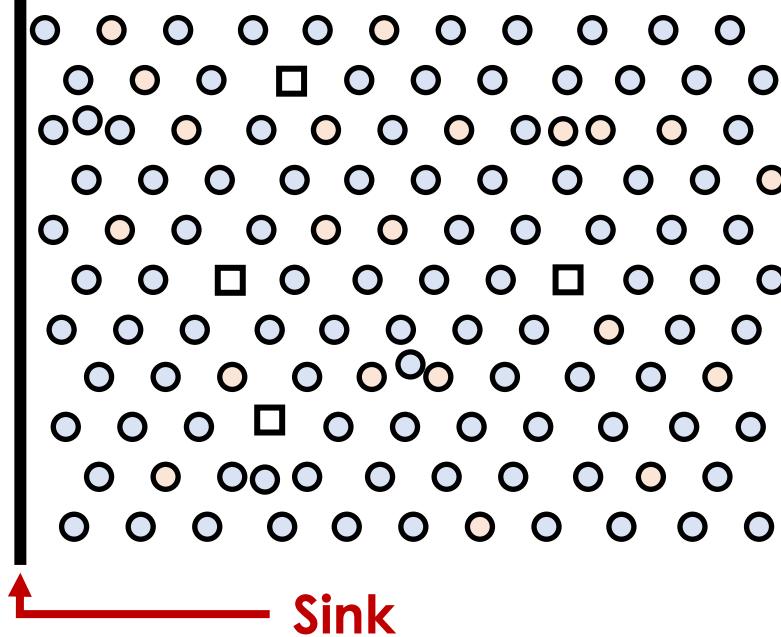
Fig. 4. Model for diffusion: (a) at void surface, or, alternatively, at grain boundary (parentheses); (b) at dislocation loop segment.

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



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:

$$J_i = J_A^i + J_B^i$$

mechanisms which it uses
↑ species of the flux

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

$$J_v = -(J_A^v + J_B^v)$$

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::

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

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_{0.75}A_{0.25}

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,

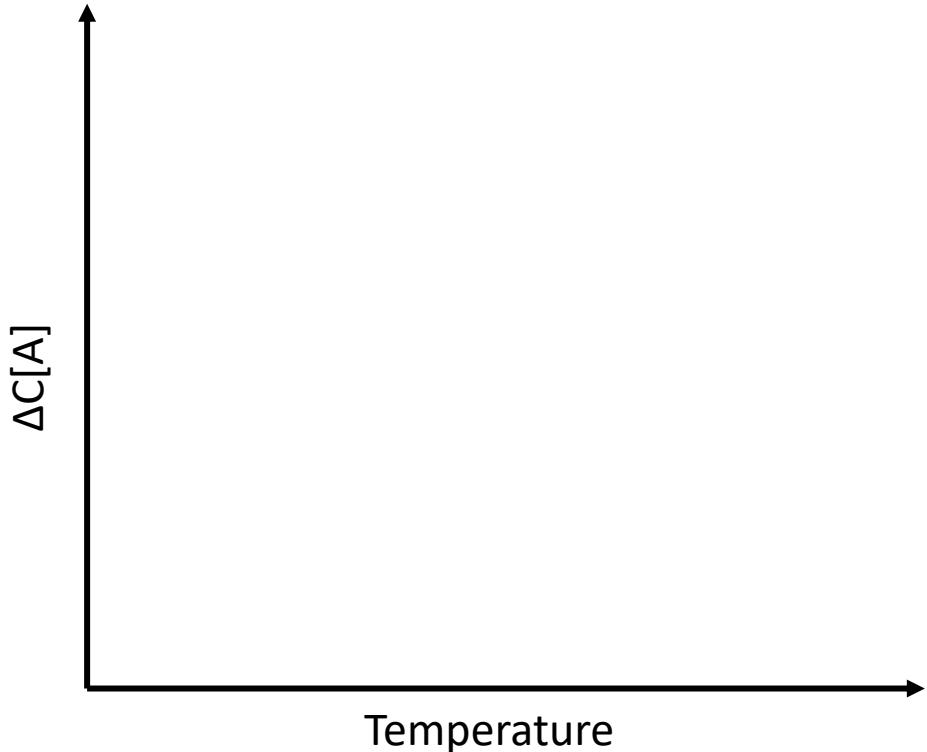
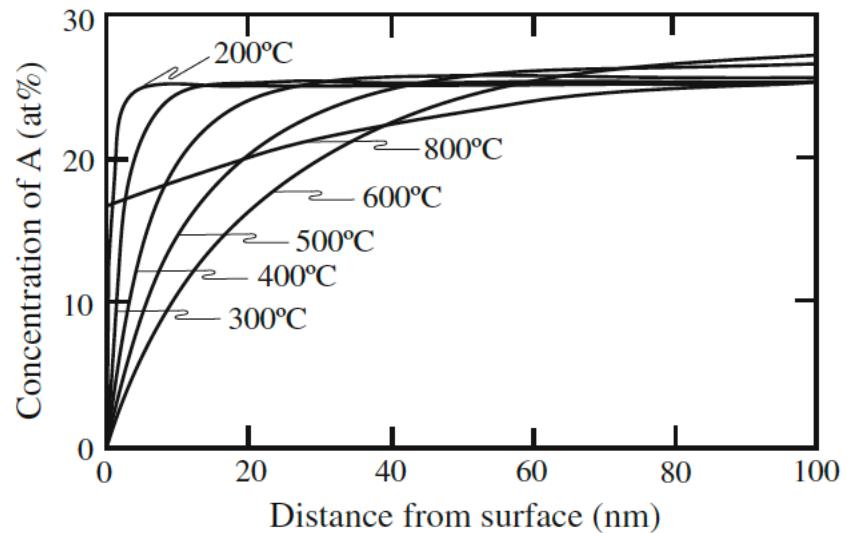
$$\frac{d_{Ai}}{d_{Bi}} \approx \exp\left(\frac{E_m^{Bi} - E_m^{Ai} + E_b^{Ai}}{k_B T}\right)$$

What is the current number of Bluey episodes?



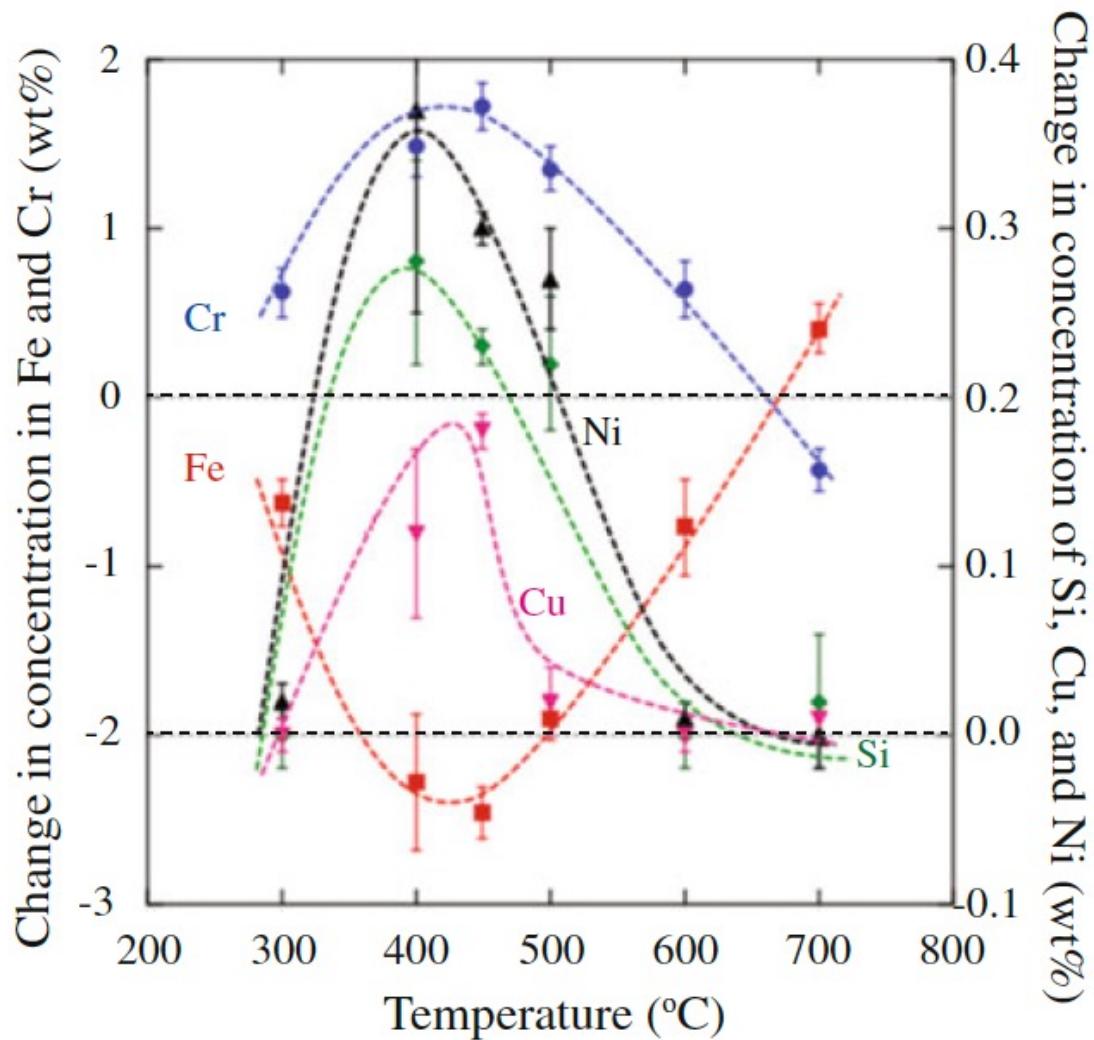
Temperature Dependence

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])



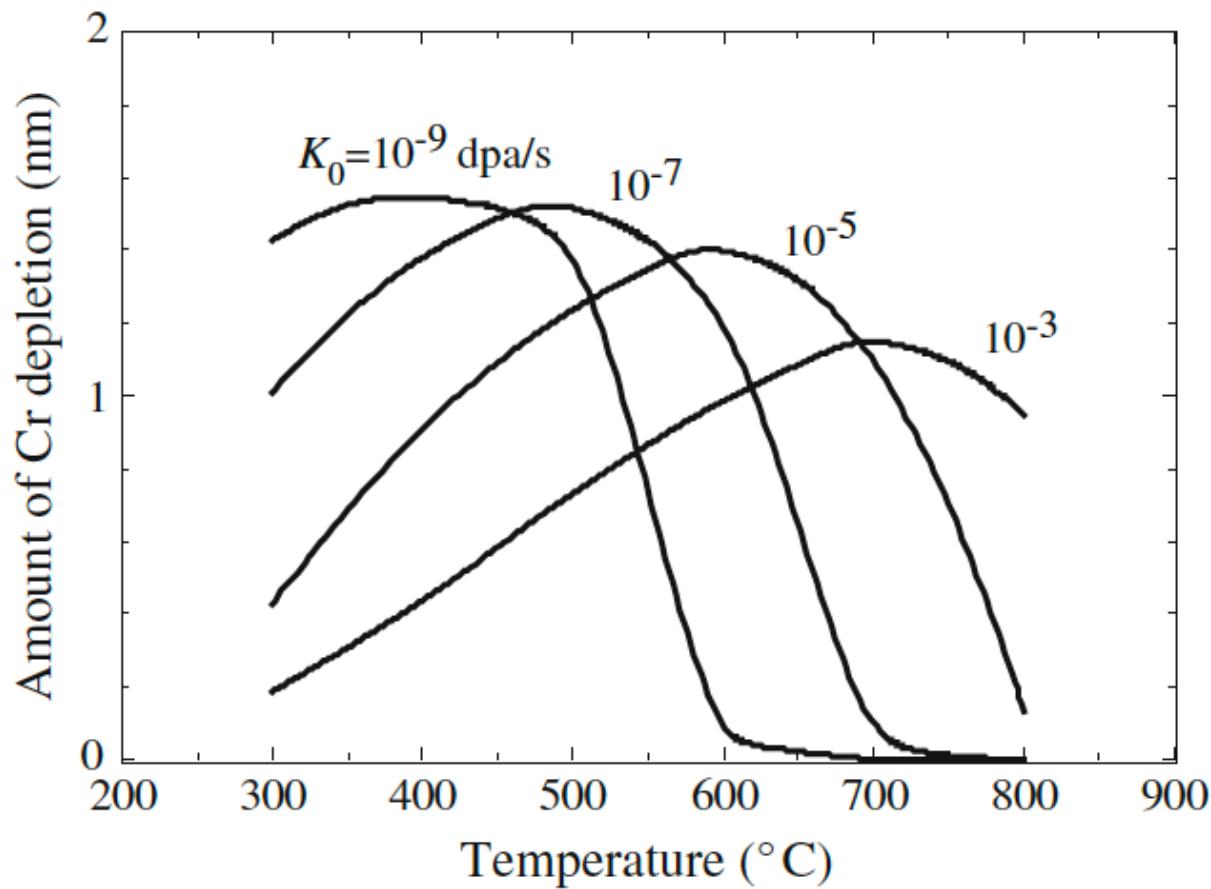
Temperature Dependence

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])

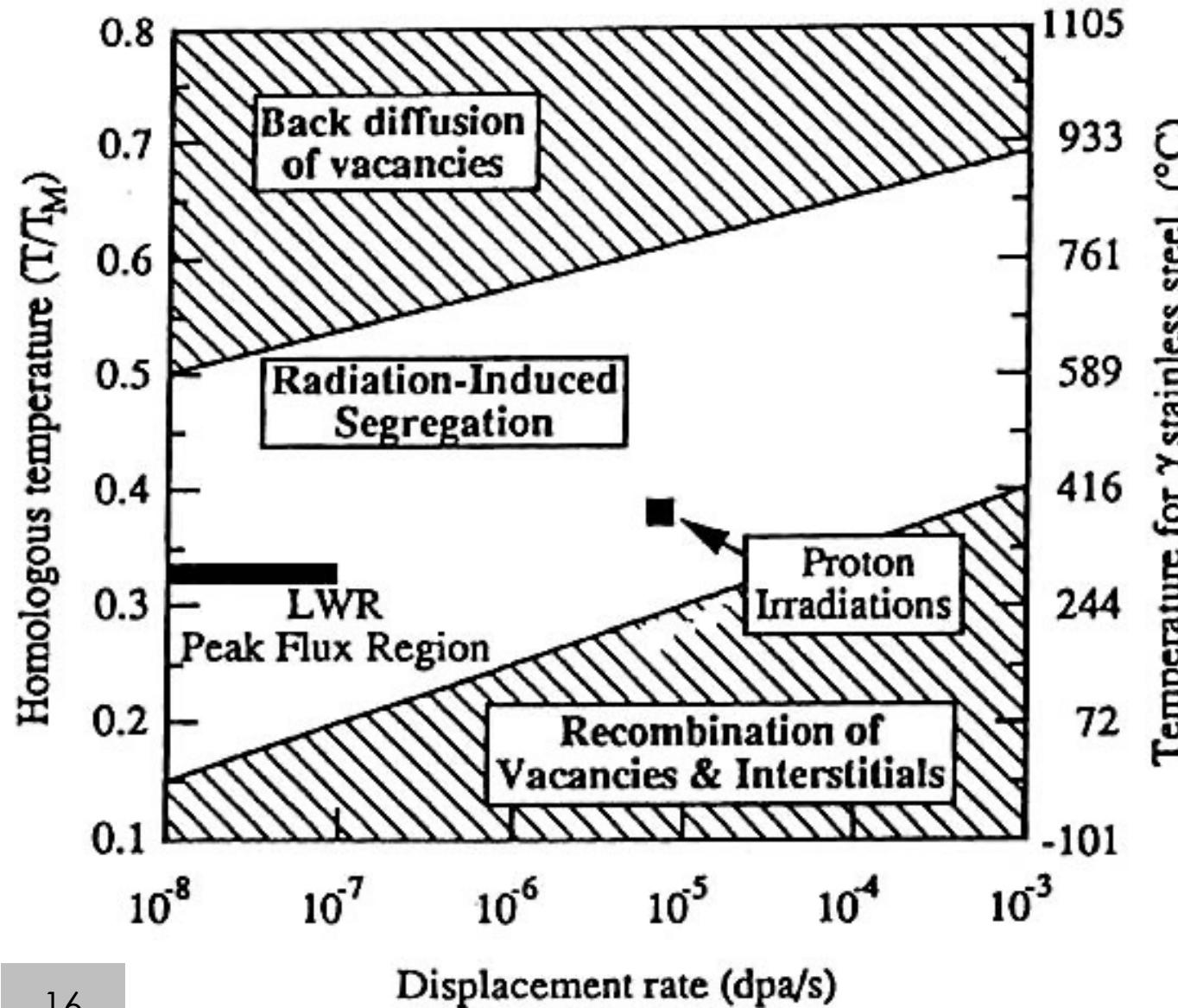


Dose Rate Dependence

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

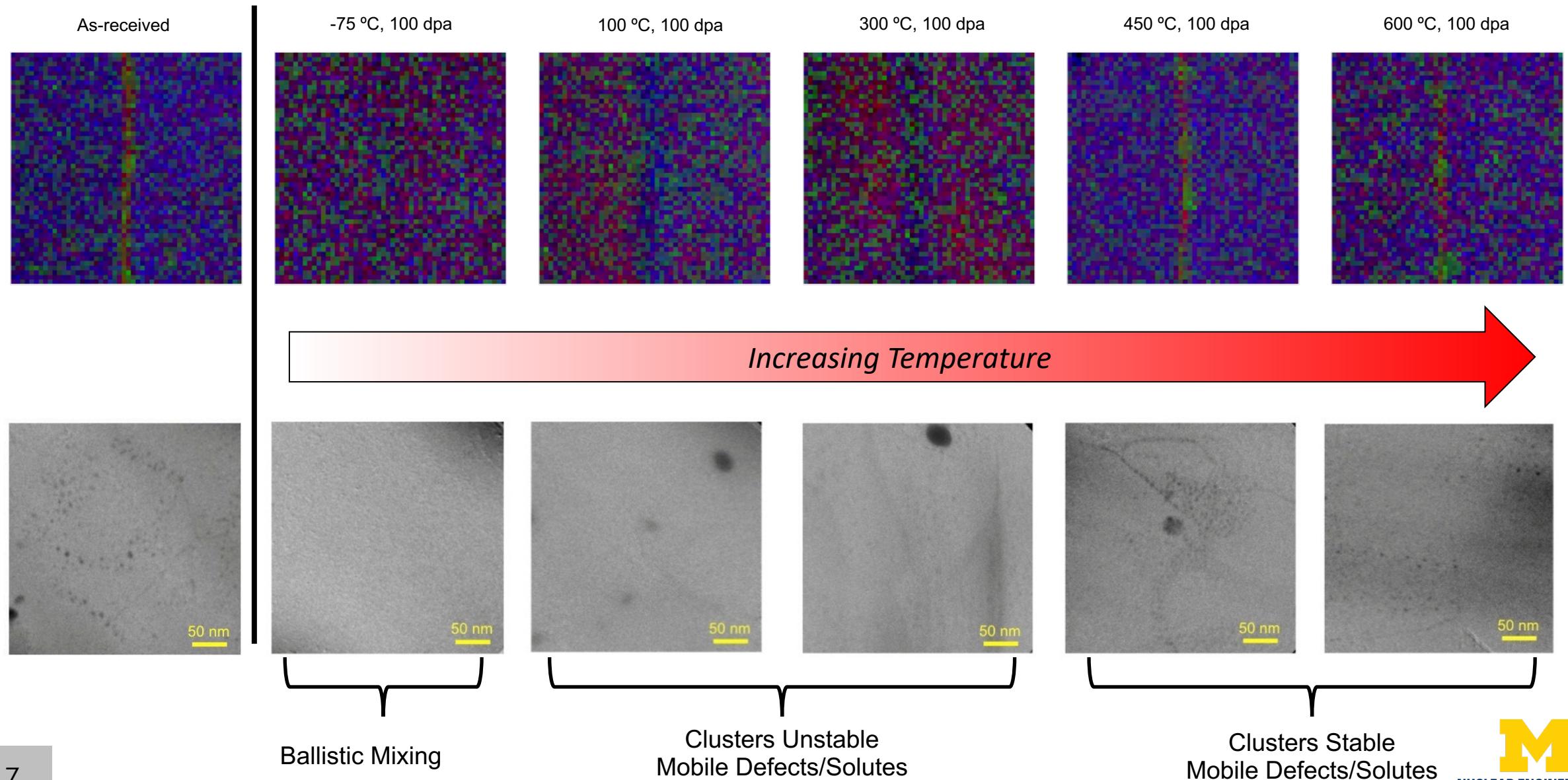


Temperature and Dose Rate Dependence

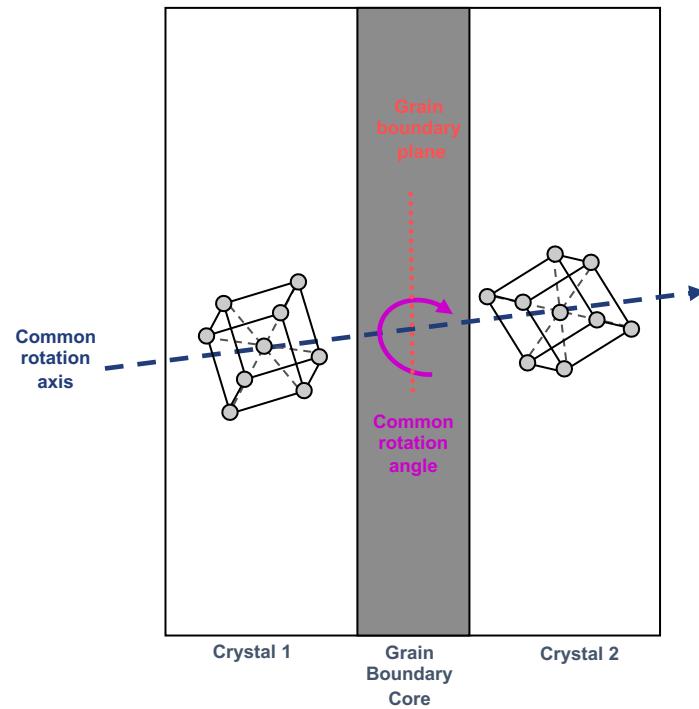


- The degree of segregation under irradiation will vary with temperature and dose rate.
- At low temperatures where defect mobility is limited, defect recombination dominates and RIS is minimal.
- At high temperatures where defect mobility and thermally induced defect populations are high, diffusion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

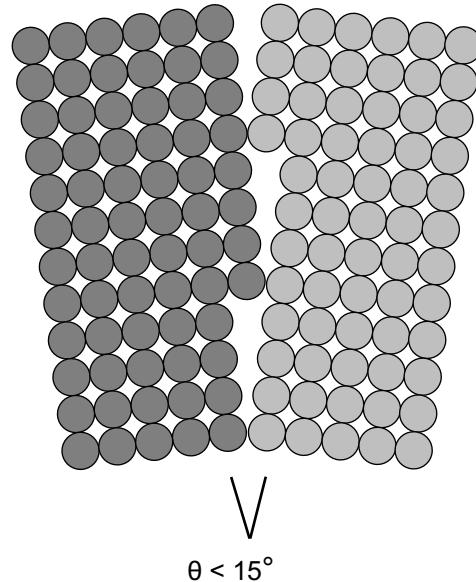
RIS is a “finger print” for defect mobility and loss



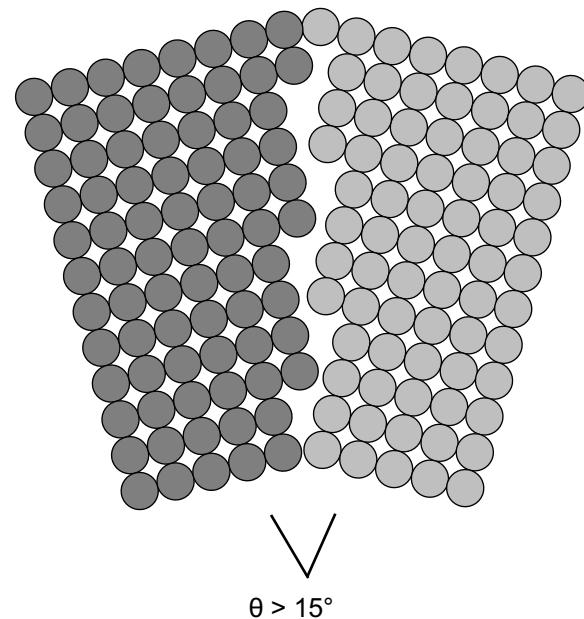
Grain Boundary Interfacial Structure Overview



Low Angle Grain Boundary

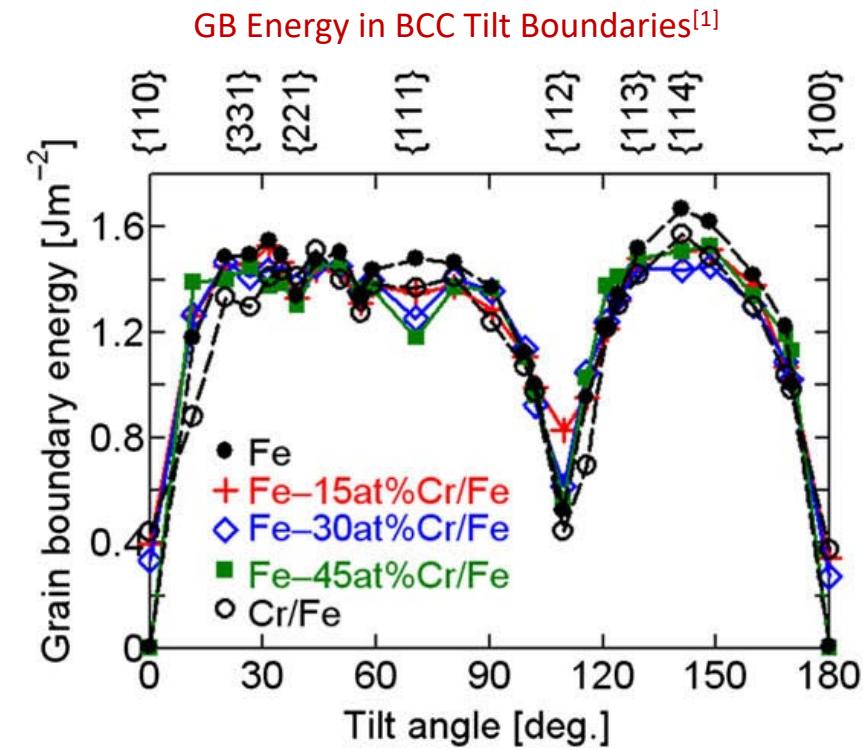
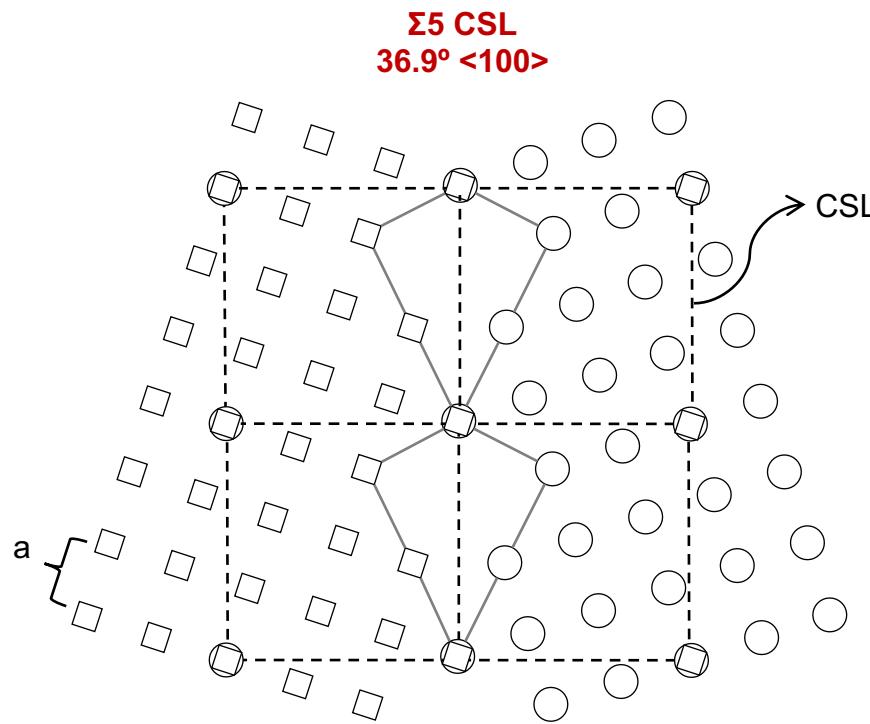


High Angle Grain Boundary



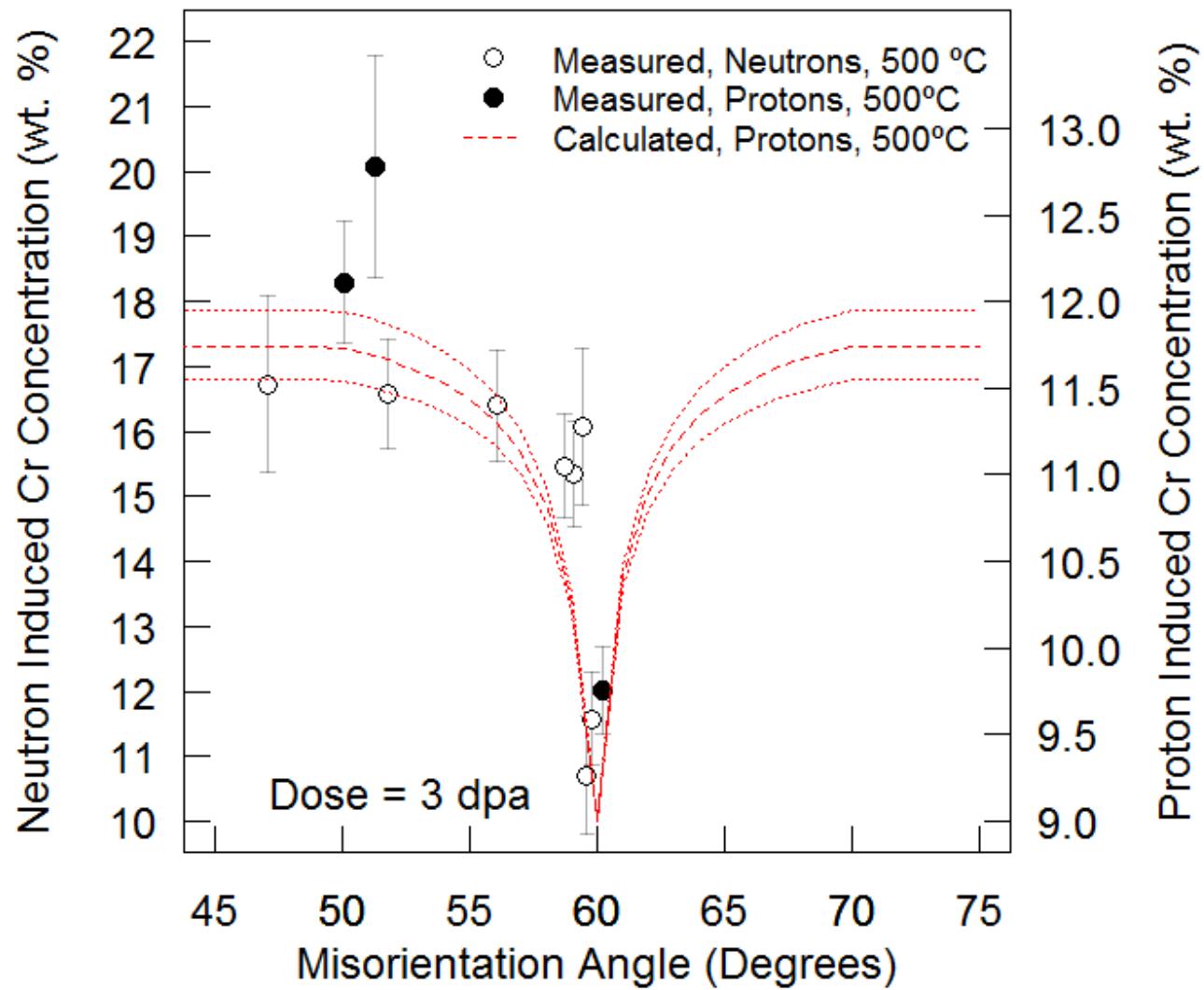
- Axis-angle representation for cubic materials helps describe GB structure:
 - **Axis:** The common crystallographic axis which comprises the boundary
 - **Angle (θ):** The degree of rotation between the two crystals along the axis
 - Axis-angle pairs describe GB: **low angle**, **high angle** or **special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

Coincident Site Lattice (CSL) Convention

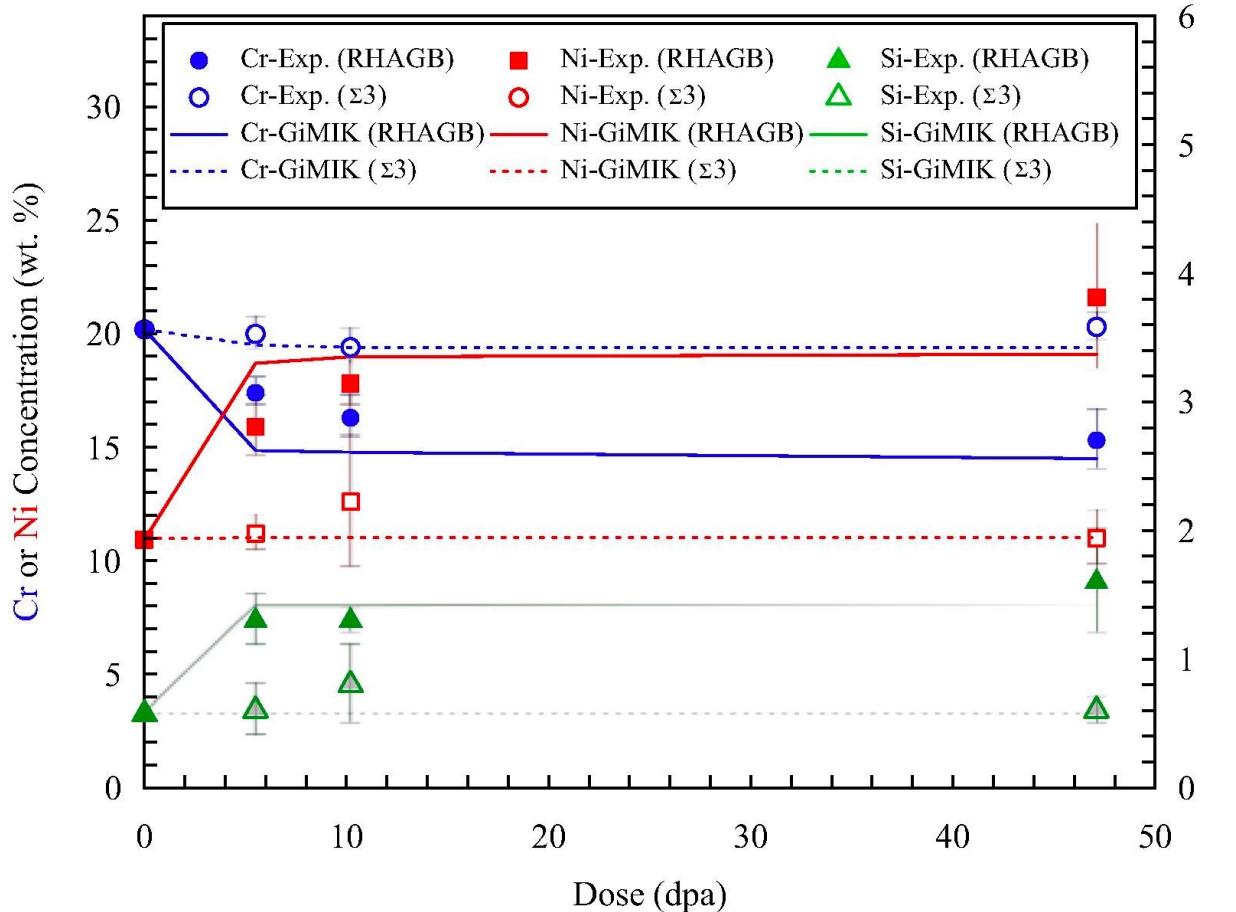
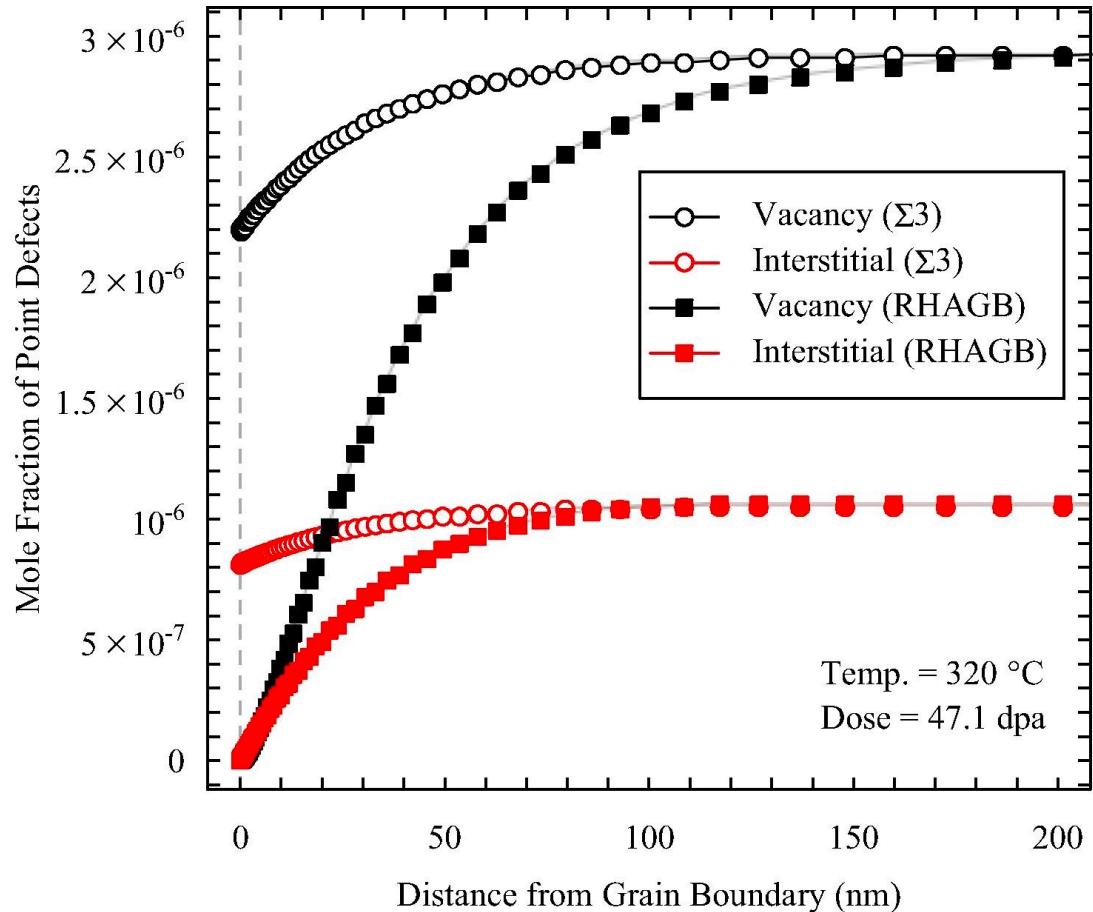


- CSL is a geometrical construction based on the geometry of the lattice
- Σ is the ratio between the area enclosed by a unit cell of coincidence sites and the standard unit cell
- Low Σ CSL boundaries have higher coherency compared to general HAGBs

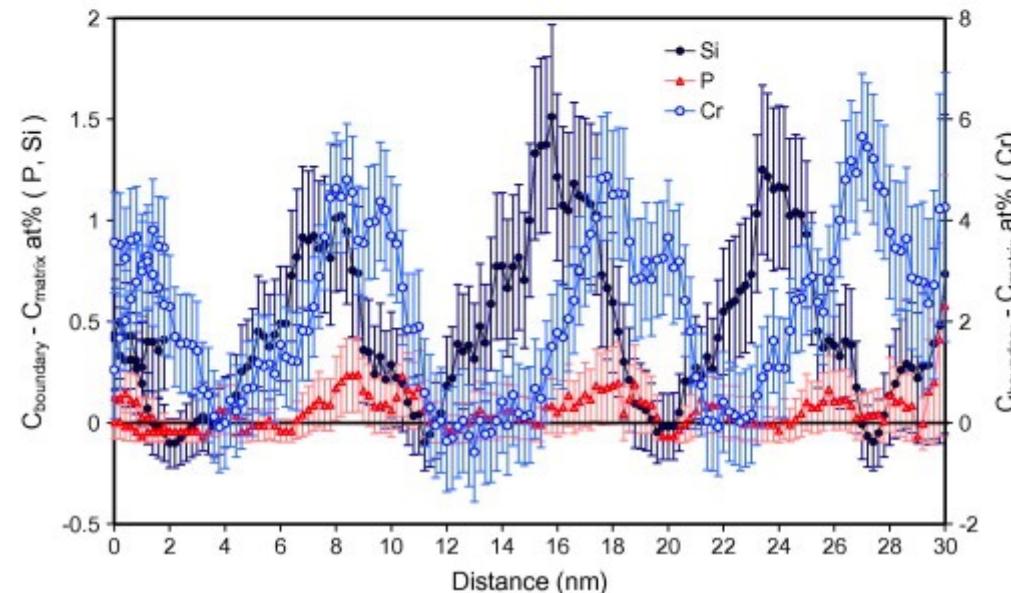
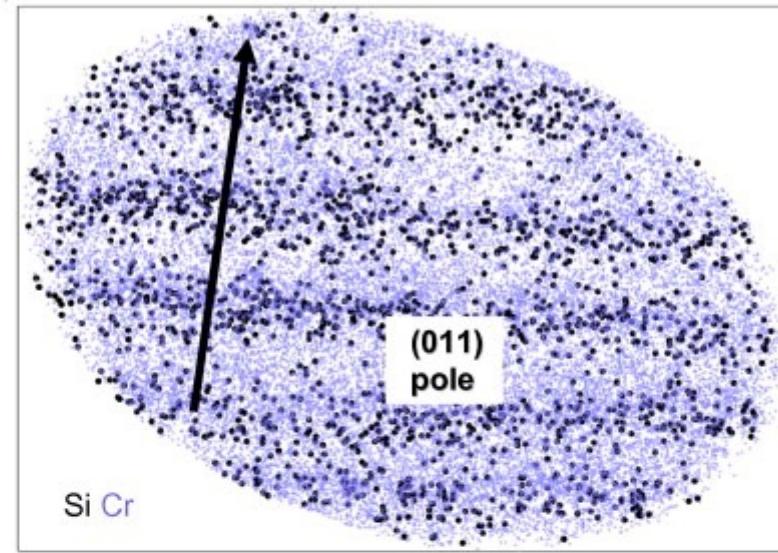
Example model and experimental data for BCC steels



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

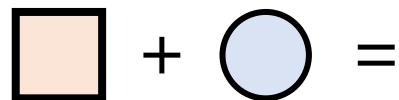
Goal:

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

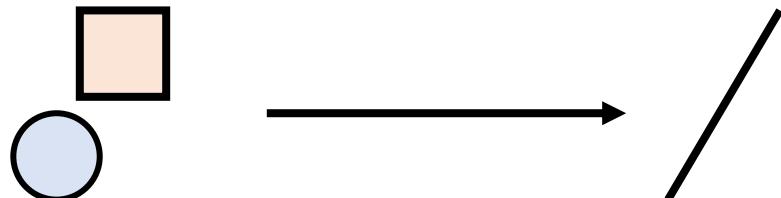


Options of vacancies and interstitials

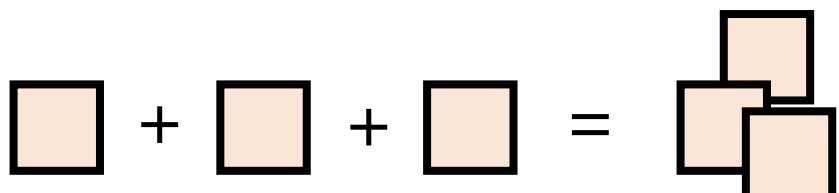
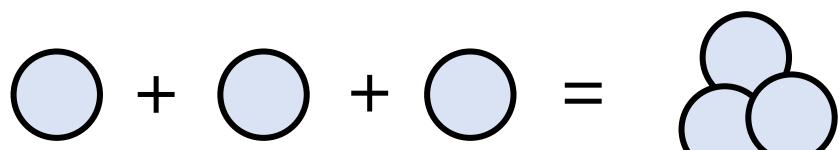
- Vacancies and interstitials can react with each other (recombination)



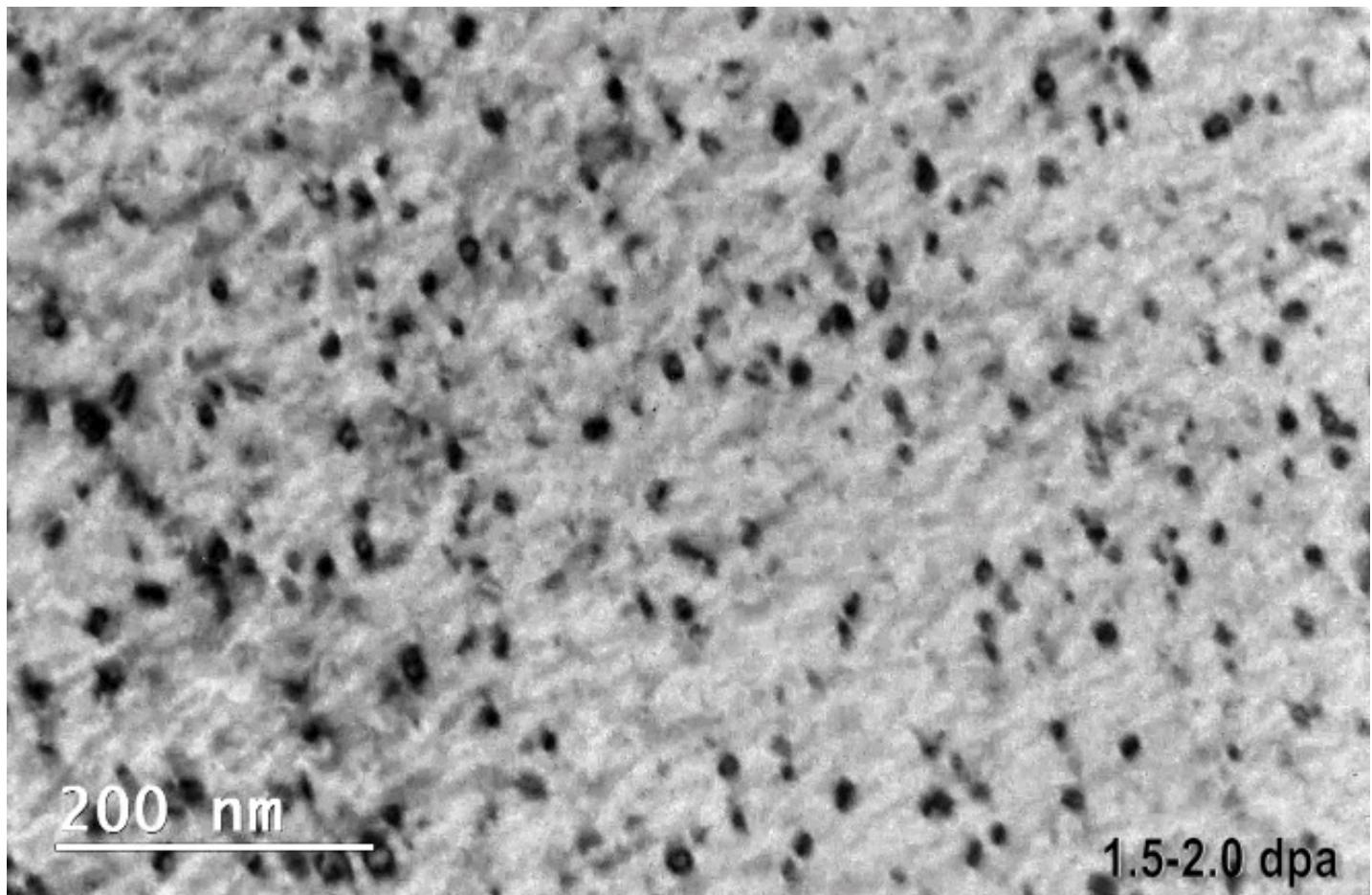
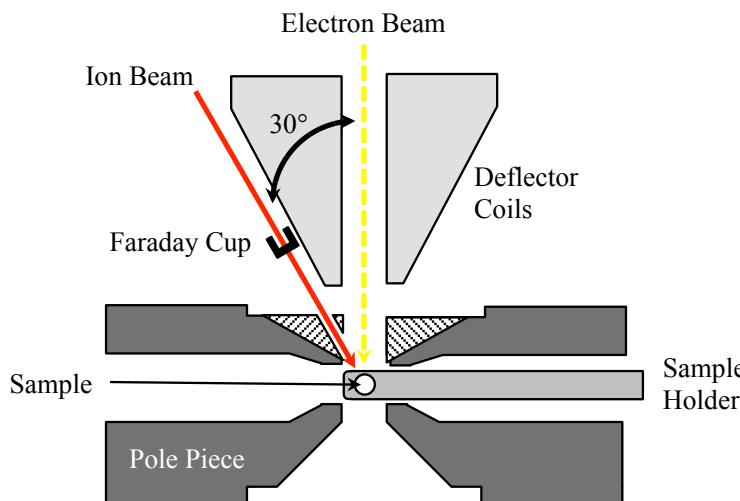
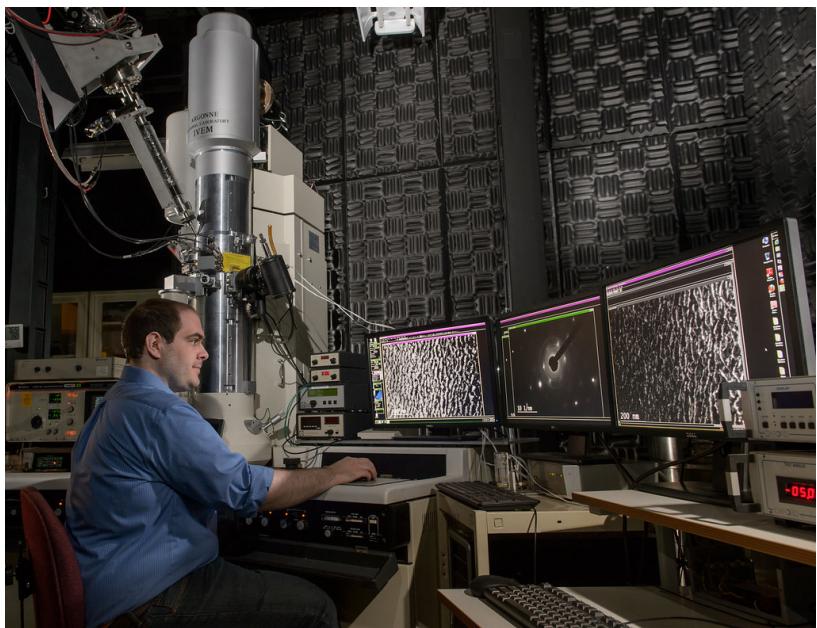
- They can react with defect sinks



- They can react with themselves



Dislocation Loop Formation

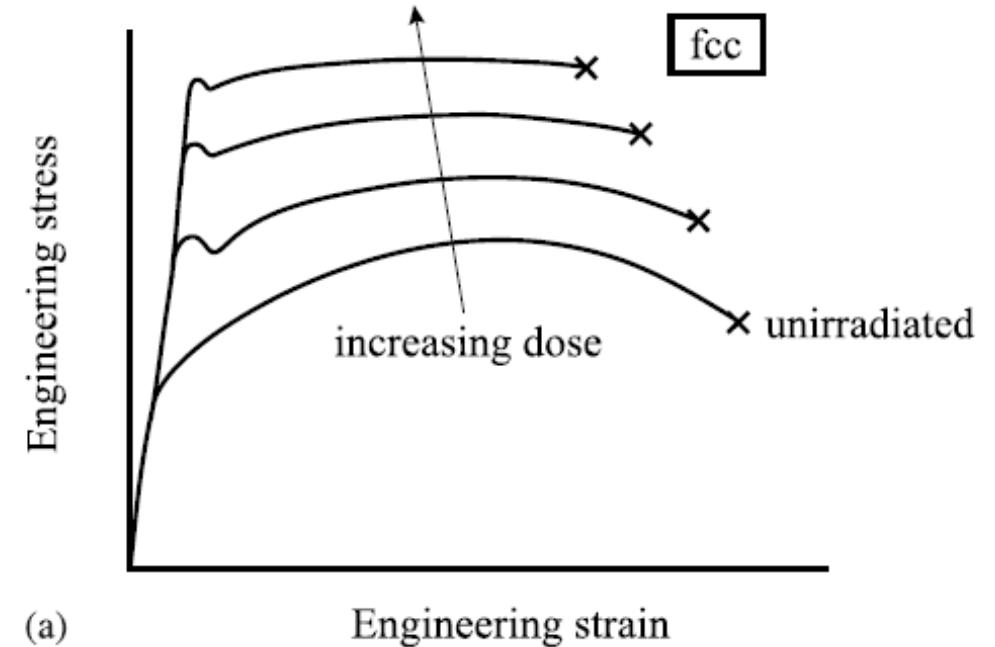
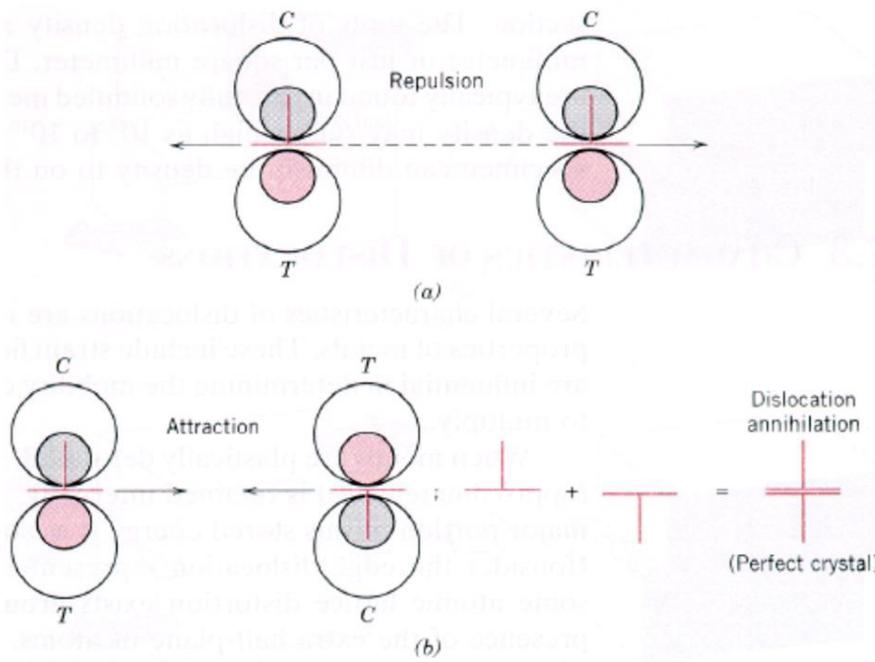


Video of in-situ ion irradiation of Fe-10Cr-4.8Al Gen I alloy irradiated at 320°C



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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

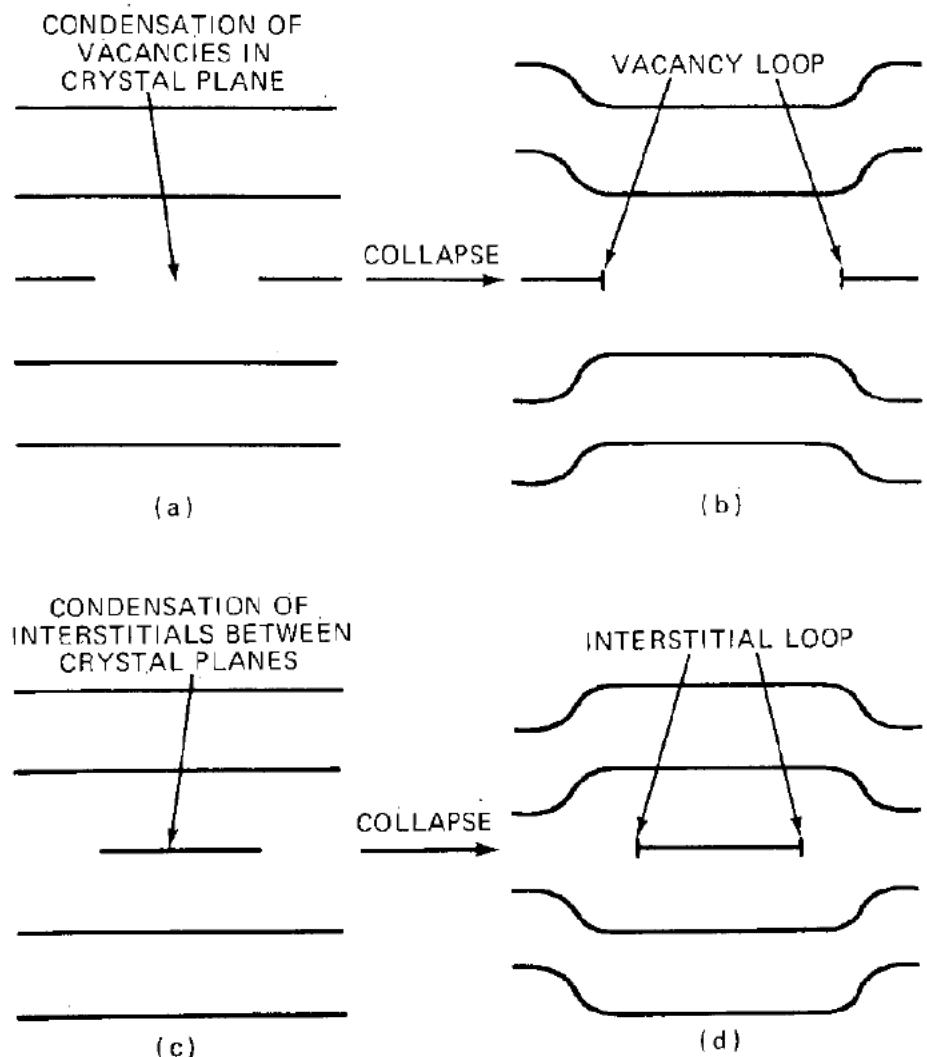
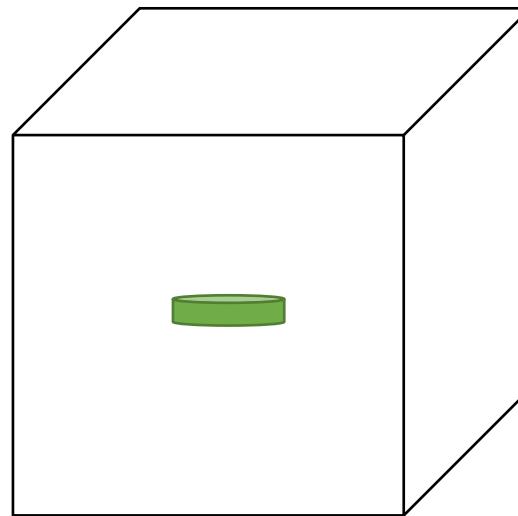
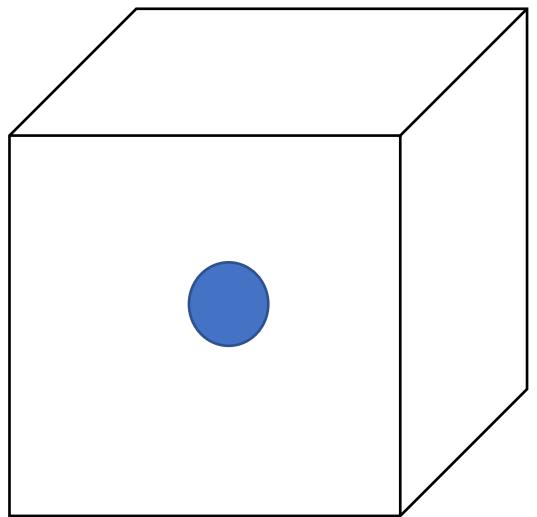


Fig. 18.4 Formation of vacancy loops and interstitial loops.

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?

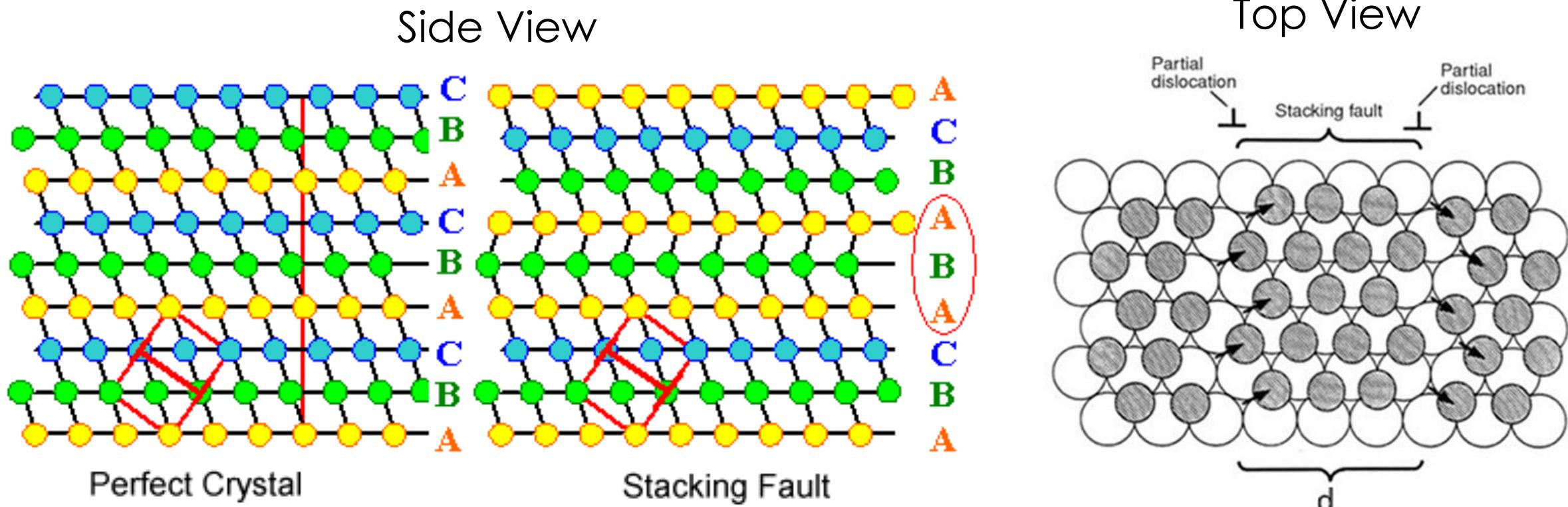


Dislocation Loop Formation

- 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)



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

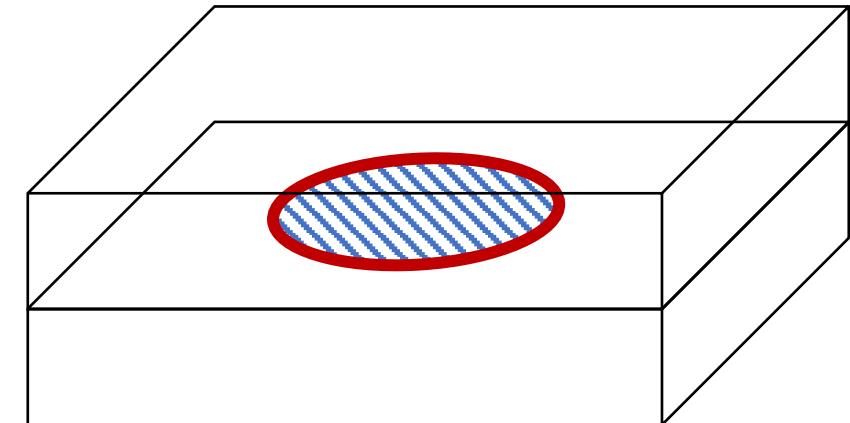
Interstitial Loops Formation

- 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



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?