

# Midterm Review

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# Midterm Logistics

- **IN CLASS**
- Written to take the full 80 minutes
- Use of “cheat sheet” permitted. One sheet of paper, letter size, front and back is OK
  - To be stapled and provided with midterm
  - **...if you need to use the sheet to answer every question, you will run out of time**
- Likely:
  - 3-6 multiple choice/answer
  - 2-4 true/false
  - 2-3 multiple-part (2-4 parts) questions w/ limited calculations (but, you can do the calculations if you find that helpful)

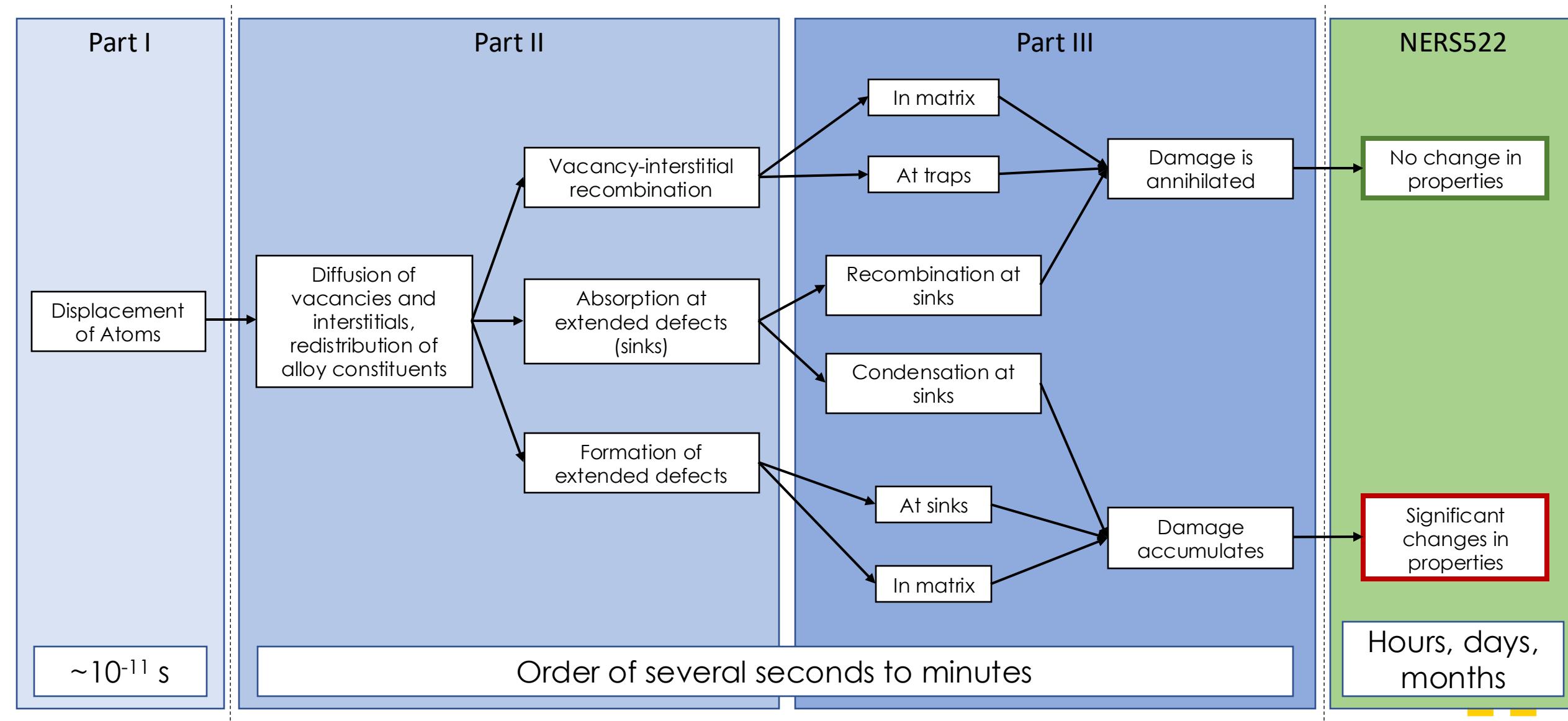


# Midterm Hints and Tricks

- **Easy grading means happy grading**
  - That means to clearly write and box answers (this goes for homework as well, PLEASE!)
  - Write out all steps, errors in one part will not be counted against future parts ***IF*** I can track down the error
- If you had to make an assumption, write what it was! I am looking for mastery in reasoning based on the fundamentals, sometimes you will assume something that I hadn't consider – listing it/describing it helps me determine your mastery of the topic
- Do the multi-part questions first, these take the most time



# Flow chart for radiation damage



# Summary of Topics Covered

Day	Date	Lec. #	Topic	Lecture Notes	Assignments	Other resources/details	Pre-Readings
Tuesday	Aug. 26	1	<a href="#">Introduction</a>	<a href="#">Notes</a> / <a href="#">Recording</a>			
Thursday	Aug. 28	2	<a href="#">Basic particle interactions</a>	<a href="#">Notes</a> / <a href="#">Recording</a>		<a href="#">Alt. basic particle derivation</a>	<a href="#">Was C.1</a> , Pg. 4-8 / <a href="#">Basics of collisions review</a> 
Tuesday	Sept. 2	3	<a href="#">Collision Kinematics</a>	<a href="#">Notes (from 2024)</a> / <a href="#">Recording</a>		<a href="#">Collision Derivation</a>	Derivation: <a href="#">O&amp;M 12.3.5</a>
Thursday	Sept. 4	4	<a href="#">Interatomic Potentials &amp; Cross Sections</a>	<a href="#">Notes</a> / <a href="#">Recording</a>	<a href="#">PS#1 assigned</a> / <a href="#">Week 2 KC</a>	<a href="#">Flux/Fluence/Cross-sections/energy transfer quick review</a>	
Tuesday	Sept. 9	5	<a href="#">Simple Disp. Theory</a>	<a href="#">Notes</a> / <a href="#">Recording</a>	<a href="#">Example</a> / <a href="#">Wk1 - KC Due</a>	<a href="#">Displacement Integrals</a> / <a href="#">Cross section conversions</a>	
Thursday	Sept. 11	6	<a href="#">Energy loss &amp; K-P modifications</a>	<a href="#">Notes</a> / <a href="#">Recording</a>	<a href="#">Week 3 KC</a>		
Tuesday	Sept. 16	7	<a href="#">Focus, Channel, Range</a>	<a href="#">Notes</a> / <a href="#">Recording</a>	<a href="#">PS1 due - Solutions</a>		
Thursday	Sept. 18	8	<a href="#">Damage Cascades</a>	<a href="#">Notes</a> / <a href="#">Recording</a>	<a href="#">PS#2 assigned</a> / <a href="#">Week 4 KC</a>	<a href="#">Arc-dpa Paper</a>	

Part II: Point Defect Generation, Recombination, and Mobility

Objective: Apply knowledge from the radiation damage event to determine the point defect generation in material systems

Day	Date	Lec. #	Topic	Lecture Notes	Assignments	Other resources/details	Pre-Readings
Tuesday	Sept. 23	9	<a href="#">Point Defects</a>	<a href="#">Notes</a> / <a href="#">Recording</a>			
Thursday	Sept. 25	10	<a href="#">Defect Motion</a>	<a href="#">Notes</a> / <a href="#">Recording</a>	<a href="#">Week 4 KC</a>		
Tuesday	Sept. 30	11	<a href="#">Point Defect Kinetics</a> - Guest lecture	<a href="#">Recording</a>	<a href="#">PS2 due - Solutions</a>		
Thursday	Oct. 2	12	<a href="#">Kinetics + RED</a> - Guest lecture	<a href="#">Recording</a>		<a href="#">Derivation for <math>C_s + i</math> regime</a> / <a href="#">Example Problem</a>	
Tuesday	Oct. 7	13	<a href="#">Defect Reactions</a>		<a href="#">PS#3 assigned</a> / <a href="#">Week 5 &amp; 6 KC</a>		

# Point Defect Kinetic Equations

- If we neglect clustering:

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

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

- Example of defect absorption to cavities:

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

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



# Energy Transfer to the PKA ( $T$ )

The energy transfer due to a hard sphere collision can be calculated using:

$$T = \frac{\gamma}{2} E_i (1 - \cos \theta)$$

The maximum energy transfer,  $\hat{T}$  is then:

- $E_i$
- $\gamma E_i$
- $\frac{\gamma E_i}{2}$

# Energy Transfer to the PKA ( $T$ )

The energy transfer due to a hard sphere collision can be calculated using:

$$T = \frac{\gamma}{2} E_i (1 - \cos \theta)$$

The average energy transferred is then:

- $E_i$
- $\gamma E_i$
- $\frac{\gamma E_i}{2}$

# Units of Radiation Damage ( $T$ )

DPA stands for:

- Displacements per atom
- Damage per atom
- Displacement potential of an atom
- Down plane acceleration

# Classic scattering integral equation

The classic scattering angle equation enables the evaluation of the scattering angle based on the interaction between two particles and is given as:

$$\phi = \pi - 2 \int_{\infty}^p \frac{b}{r^2} \frac{dr}{\sqrt{1 - \frac{V(r)}{\Sigma} - \frac{b^2}{r^2}}}$$

What is  $p$  and  $V(r)$  in this equation? What is the importance of these parameters in determining the radiation damage event?

# Summary

- We've accomplished **four** tasks to get towards a quantification of displacements for a given material system:

Task 1: Determine the energy transferred to the PKA:

$$T = \frac{\gamma}{2} E_i (1 - \cos \phi) \text{ to get } \phi = f(T)$$

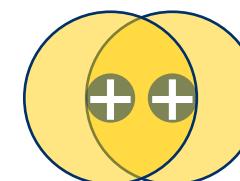
Task 2: Determine the scattering angle based on the impact parameter:

$$\phi = \pi - 2 \int_{\infty}^{r_0} \frac{b}{r^2} \frac{dr}{\sqrt{1 - \frac{V(r)}{\Sigma} - \frac{b^2}{r^2}}}$$

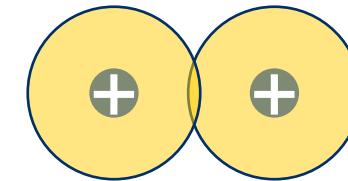
Task 3: Described  $V(r)$  based on the distance of closest approach



= R<K-shell radius  
(Coulomb)



= K-shell<R< $a_o$   
(Screened Coulomb)



= <R<Lattice Constant  
(Born-Mayer)

Task 4: Combine Tasks 1-3 to get total and differential energy transfer cross-sections

$$\sigma_s(E_i, T) dT = 2\pi b db$$

$$\sigma_s(E_i) = \int_{T_{min}}^{T_{max}} \sigma_s(E_i, T) dT$$

Where we are going:

$$dpa/s = N \int_{\check{E}}^{\hat{E}} \Phi(E_i) \int_{\check{T}}^{\hat{T}} \sigma(E_i, T) \nu(T) dT dE_i$$



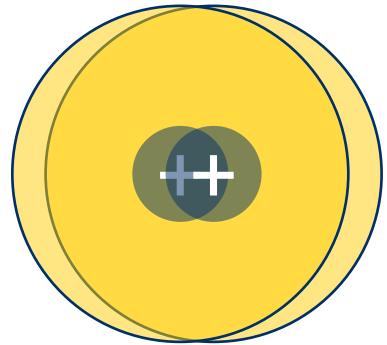
# Interatomic Potentials

1. When  $p$  (or  $r$  in slide notes) is less than radius of a typical lattice atom ( $a_0$ ) the electrons are in the internuclear space which screen the total nuclear charge. What is the appropriate interatomic potential to use in this case?
2. Coloumbic
3. Screened Coloumb
4. Hard sphere
5. Born-Mayer
6. The interatomic potential will change depending on the type of ion and the incident ion energy for an ion irradiation experiment.

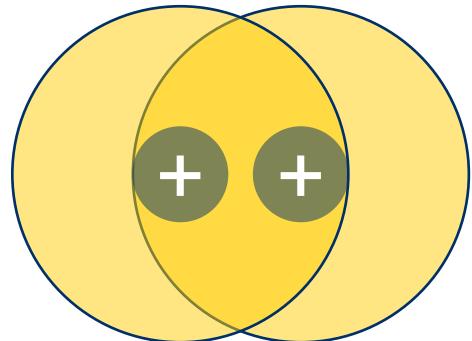
-True

-False

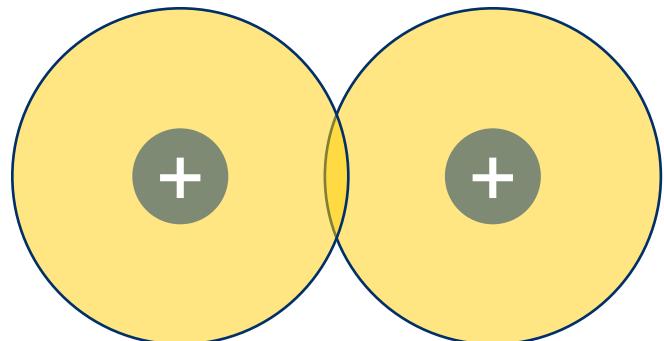
# Importance of Interatomic Potentials



$R <$ K-shell radius  
(Coulomb)



K-shell radius < R < Lattice Constant  
(Screened Coulomb)



$< R <$ Lattice Constant  
(Born-Mayer)

Potential	Equation	Range of Applicability	Definitions	Eqn in text
Hard sphere	$0 \text{ for } r > r_0$ $\infty \text{ for } r < r_0$	$10^{-1} < T < 10^3 \text{ eV}$	$r_0 = \text{size of atom}$	(1.46)
Born-Mayer	$V(r) = A \exp(-r/B)$	$10^{-1} < T < 10^3 \text{ eV}$ $a_0 < r \leq r_e$	$A, B$ determined from elastic moduli	(1.47)
Simple Coulomb	$\frac{Z_1 Z_2 \epsilon^2}{r}$	light ions of high energy $r \ll a_0$		(1.48)
Screened Coulomb	$\left( \frac{Z_1 Z_2 \epsilon^2}{r} \right) \exp(-r/a)$	Light ions $r < a_0$	$a_o = \text{Bohr radius}$ $a = \text{screening radius}$	(1.49)
Brinkman I	$\frac{Z^2 \epsilon^2}{r} e^{(-r/a)} \left( 1 - \frac{r}{2a} \right)$	$r < a$	$a \equiv a_0/Z^{1/3}$	(1.51)
Brinkman II	$\frac{AZ_1 Z_2 \epsilon^2 \exp(-Br)}{1 - \exp(-Ar)}$	$Z > 25$ $r < 0.7r_e$	$A = \frac{0.95 \times 10^{-6}}{a_o} Z_{\text{eff}}^{7/3}$ $B = Z_{\text{eff}}^{1/3} / Ca_o$ $C \approx 1.5$	(1.52)
Firsov	$\frac{Z_1 Z_2 \epsilon^2}{r} \chi \left[ (Z_1^{1/2} + Z_2^{1/2})^{2/3} \frac{r}{a} \right]$	$r \leq a_0$	$\chi$ is screening function	(1.56)
TFD Two Center	$\frac{Z^2 \epsilon^2}{r} \chi \left( Z^{1/3} \frac{r}{a} \right) - \alpha Z + \bar{\Lambda}$	$r < r_b (3a_0)$	$r_b = \text{radius at which the electron cloud density vanishes}$	(1.57)
Inverse square	$\frac{2E_r}{e} (Z_1 Z_2)^{5/6} \left( \frac{a_o}{r} \right)^2$	$a/2 < r < 5a$	$E_R = \text{Rydberg energy} = 13.6 \text{ eV}$	(1.59)



# Total Cross Section

The interatomic potential, scattering integral, energy transfer and relationships between differential cross sections are all used to determine the total cross section for a particle-particle interaction.

- True
- False

Known:

$$V(r) = \text{interaction potential}$$

The method then:

Start

Provides  $b^2$  in terms of  $\phi$  thru:

Classic scattering integral:

$$\phi = \pi - 2 \int_{\infty}^p \frac{b}{r^2} \frac{dr}{\sqrt{1 - \frac{V(r)}{\Sigma} - \frac{b^2}{r^2}}}$$

Cast in terms of  $T$  using:

Energy transfer:

$$T = \frac{\gamma E_i}{2} (1 - \cos \phi)$$

Differentiate to get  $2bdb$  as a function of  $T$  and  $dT$

Plug into:

Differential Cross Section:

$$\sigma_s(E_i, T) dT = 2\pi b db$$

$$\sigma_s(E_i, T) = 2\pi b \frac{db}{d\phi} \frac{d\phi}{dT}$$

Finish

...and use

$$\sigma_s(E_i) = \int_{T_{min}}^{T_{max}} \sigma_s(E_i, T) dT$$

$$\sigma_s(E_i)$$



# $N$ for common crystal structures

$N$  is the atomic volume of the cell and can be determined by:

$$N = \frac{\text{num. atoms in a unit cell}}{a_0^3}$$

What then are the number atoms in the unit cell for:

-BCC

-FCC

# Displacement Energy $E_d$

Based on the Kinchin-Pease model, if an energetic particle has an energy less than  $E_d$ , then what happens to the struck atom?

- The struck atom is displaced from the lattice site and is presumed to come to rest at a location in the lattice different from it's previous position
- The struck atom is assumed to resume to it's lattice site after interaction

Displacement energy,  $E_d$ , is crystal directionally dependent.

- True
- False

# Kinchin Pease Approach I

You are asked to calculate the dpa/s based on a monoenergetic flux of neutrons into BCC iron. You determine you need to calculate the damage cross section,  $\sigma_D(E_i)$ , using your notes you determine the equation to do this calculation is:

$$\sigma_D(E_i) = \int_{\check{T}}^{\hat{T}} \sigma_s(E_i, T) v(T) dT = \frac{\sigma_s(E_i)}{\gamma E_i} \int_{\check{T}}^{\hat{T}} v(T) dT <\!p\!>$$

What equations should you use for  $\check{T}$  and  $\hat{T}$ ?

## Kinchin Pease Approach II

You have correctly identified in the previous slide that  $\hat{T}$  is the maximum energy transfer. You calculate this using  $T_{max} = \hat{T} = \gamma E_i$  and get a value of  $0.025 MeV$ . Based on this value is using the following equation the correct approach?

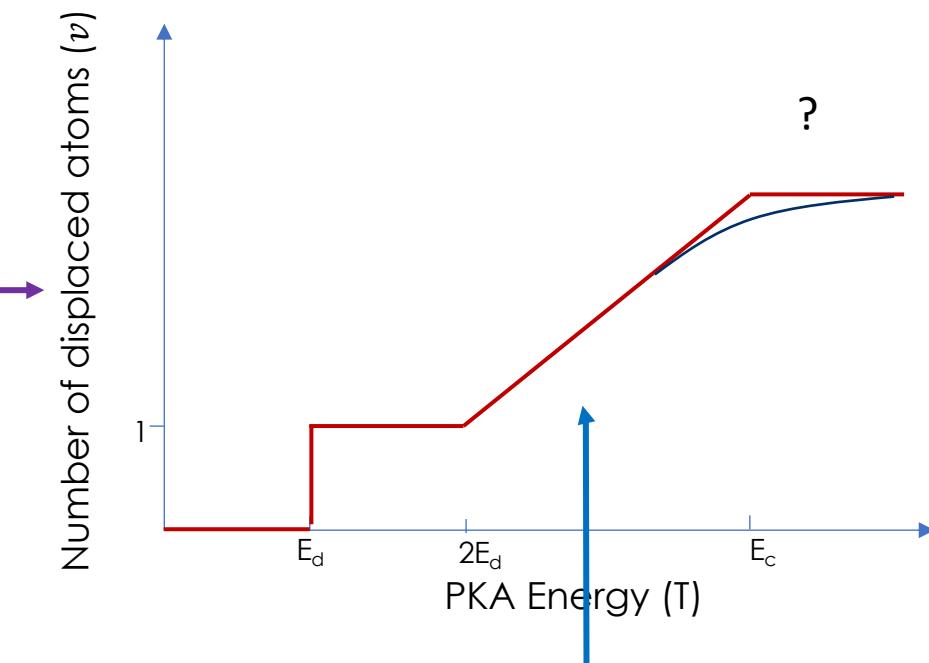
$$\sigma_D(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i} \left( \int_0^{E_d} 0dT + \int_{E_d}^{2E_d} 1dT + \int_{2E_d}^{E_c} \frac{T}{2E_d} dT + \int_{E_c}^{\gamma E_i} \frac{E_c}{2E_d} dT \right)$$

Hint: The atomic weight of Fe is 55.85.

# Point Defect Kinetic Equations

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

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



$$T = \frac{1}{2} \frac{4mM}{(m+M)^2} (1 - \cos \varphi) E_i$$

$$\gamma = \frac{4mM}{(m+M)^2}$$

$$T = \frac{1}{2} \gamma (1 - \cos \varphi) E_i$$

$$T_{max} = \gamma E_i$$



# Stopping Powers

A high energy ( $>1$  MeV) heavy ion is injected into a bulk material. The ions will undergo energy loss as it passes through the material and come to rest at some position away from the implantation surface. The primary energy loss at high energy (e.g. early in range) is \_\_\_\_\_ and at low energy is \_\_\_\_\_.

- Nuclear, electronic
- Electronic, nuclear

# Focusing and channelling

Most crystalline materials will experience focusing and/or channeling events when irradiated with energetic particles. This is due to preferential directions and planes in the atomic structure. Focusing and channeling act then to increase the number of displacements under irradiation.

- True
- False

# Range

At high energy, ions will typically undergo \_\_\_\_\_ that lead to \_\_\_\_\_. At the energy is decreased of the ions they will undergo \_\_\_\_\_ that leads to \_\_\_\_\_. Once the the energy reaches below \_\_\_\_\_ the ions no longer cause displacements and come to rest a short distance further into the material.

- High angle collisions; high energy loss; low angle collisions; low energy loss;  $E_d$
- Low angle collisions; high energy loss; high angle collisions; low energy loss;  $E_d$
- Low angle collisions; low energy loss; high angle collisions; high energy loss;  $E_c$
- Low angle collisions; low energy loss; high angle collisions; high energy loss;  $E_d$

# Cascades and Damage

The cascade morphology is strongly dependent on the mass of the incident ion and it's energy.

- True
- False

Heavy ions will commonly cause small scale cascades with vacancy rich cores.

- True
- False

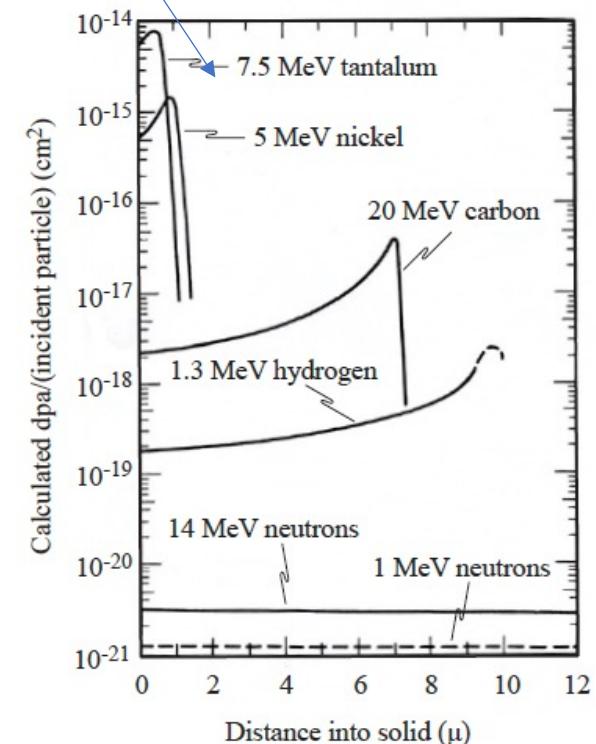
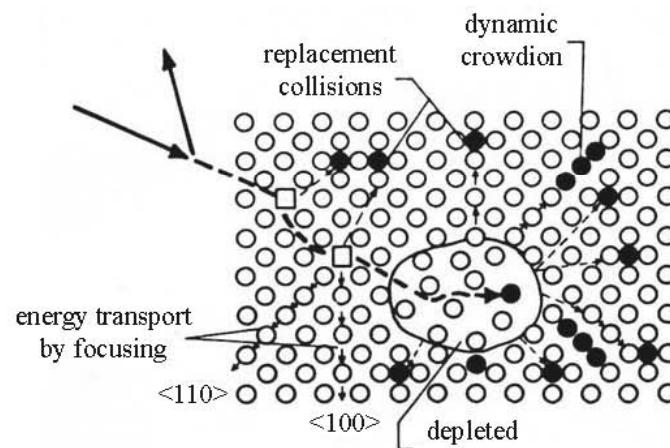
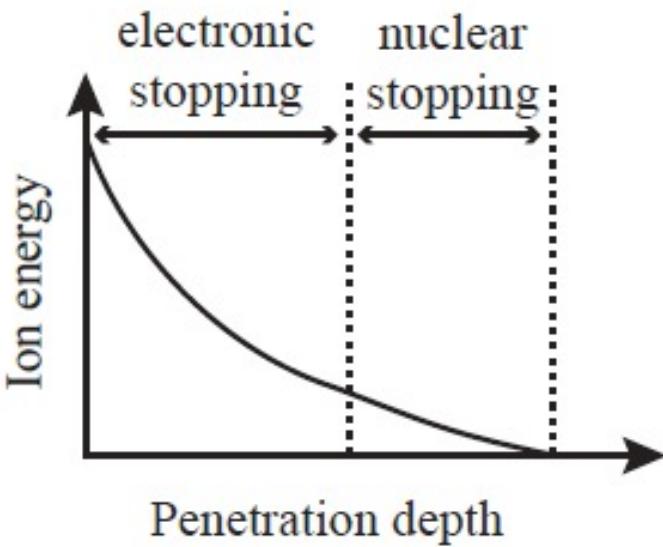
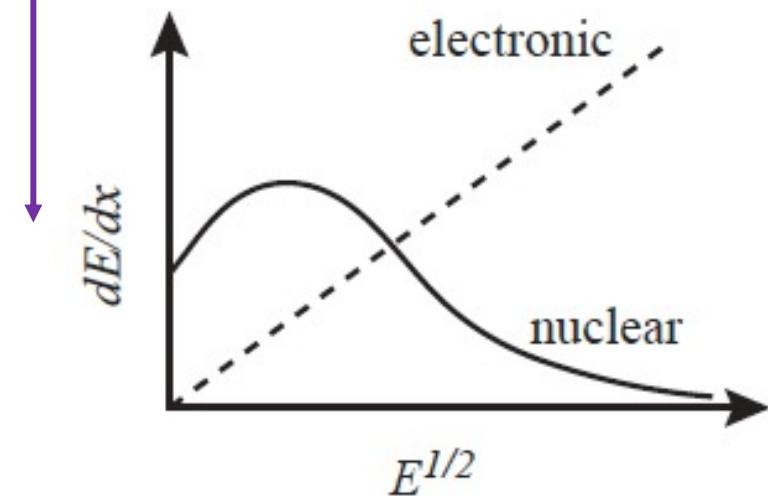
The Kinchin Pease and NRT approach don't account for enhanced recombination in metals in a cascade

- True
- False

# Point Defect Kinetic Equations

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

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



# Point Defects

You are asked to calculate the concentration of vacancies and interstitials at  $\frac{1}{3}$  the melting point of a metal. You find that  $C_i^{eq} > C_v^{eq}$ , should you check your work?

- Yes
- No

The primary point defect diffusion mechanisms are (select all that apply):

- Exchange
- Ring
- Vacancy
- Interstitial
- Interstitialcy
- Dumbell
- Crowdion

# Defect Reactions I

For a low temperature, low sink density regime the order of different regimes for  $C_v$  and  $C_i$  as a function of irradiation time are:

- Mutual recombination; build up without reaction; sinks contribute to interstitial annihilation; sinks annihilate both vacancies and interstitials
- Build up without reaction; mutual recombination; sinks contribute to interstitial annihilation; sinks annihilate both vacancies and interstitials
- Build up without reaction; sinks contribute to interstitial annihilation; sinks annihilate both vacancies and interstitials; mutual recombination

The effect of increasing the sink strength in the system would be to move  $t_3$  closer to  $t_2$ .

-True

-False

## Defect Reactions II

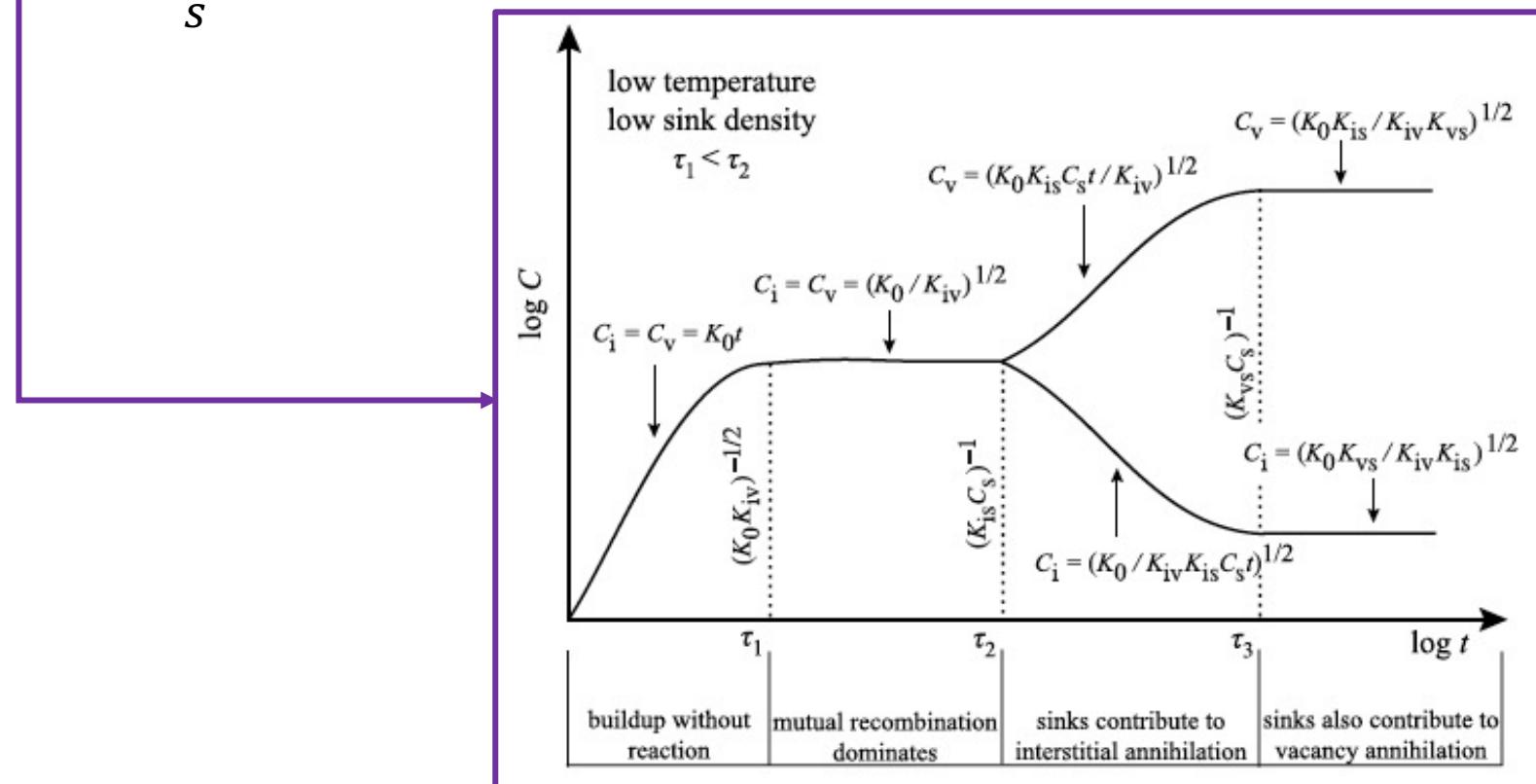
You are asked to calculate the time when vacancies arrive at sinks to determine the time to reach steady state conditions in a material using the point defect rate theory equations. Your answer comes out to be only a few seconds and a fractional dose. Should you go back and check your work?

- Yes
- No
- There is no time to check my work either way because I didn't study for the exam. I am just happy to have numbers on the page.

# Point Defect Kinetic Equations

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

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



# Diffusion during irradiation

Irradiation in metals under irradiation will tend to accelerate diffusion at intermediate temperatures due to increases in the point defect concentrations due to displacements.

- True
- False

Diffusion-based processes tend to be controlled by vacancy-based diffusion.

- True
- False

At low irradiation temperatures radiation effects tend to be \_\_\_\_\_ because of \_\_\_\_\_ diffusion and at high temperatures radiations effects tend to be \_\_\_\_\_ because of \_\_\_\_\_ resulting in bell-curve shaped graphs of radiation effect magnitude as a function of irradiation temperature.

- Recombination dominated; sluggish; thermal diffusion limited; high concentration of vacancies
- Thermal diffusion limited; sluggish; recombination dominated; high defect sink concentration
- Damage limited; high; moderate; high concentration of interstitials

# Sinks and defect reactions

Grain boundaries and voids act as \_\_\_\_\_.

- Neutral sinks
- Biased sinks
- Variable sinks

You are asked to derive the reaction rate for a platelet precipitate and get a pre-factor of  $4\pi$  to account for the geometry. How much confidence do you have in your answer?

- Low
- Moderate
- High

# Point Defect Kinetic Equations

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

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

- 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.

