Midterm Review

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Midterm Logistics

My preference would be:

A take-home midterm with 6-10 questions with some questions being multipart worked problems (e.g., need to do math/calculations). The exam would be done over Canvas with a 3 hr time limit (plus accommodations if requested) but designed to be completed in ~90 minutes. The exam would be released on 10/26 and be open for completion until 10/31. Questions can be e-mailed, but rapid response would only be possible on 10/30 - questions asked would be posted to Canvas.	6 respondents	43 %	✓
A midterm project assignment. This would be a multistep project that would require students to calculate factors like dpa, ion range, diffusion all to determine the concentration of steady state point defects at discrete points along the ion(s) range. It would require light coding/excel work and would be expected to take 2-5 hrs to complete. The project would be posted on 10/25 and due 11/1. The submission would a short lab-style write up where prompts/sections to complete would be provided.	4 respondents	29 %	
A normal "midterm" that would be administered in class on 10/26. Students would be tested on general concepts with 6-8 questions with limited worked problems (e.g. won't need a calculator). Some questions would be multi-part while others might be simple selection/multiple choice. A make up exam time would be provided, ideally the following week on 11/30 for students with academic leave or undue stress exemptions. This would likely occur the morning of 11/30 but the time and location would be determined only if this option is selected. The exam is designed to take a full 90 minutes.	4 respondents	29 %	

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Midterm Logistics

- ON CANVAS (auto graded'ish)
- Released on 10/26 – 8 am
- Due on 10/31 – 11:59 pm
- Designed for 90 minutes but timed for 3 hrs (180 mins)
- Open book/open resources
  (but if you need to flip through the book to find answers you will run out of time)
- Currently:
  - 5 multiple choice
  - 1 multiple answer
  - 2 true/false
  - 2-3 multiple part (2-4 parts) questions – limited calculations (but you can do the calculations if you find that helpful)

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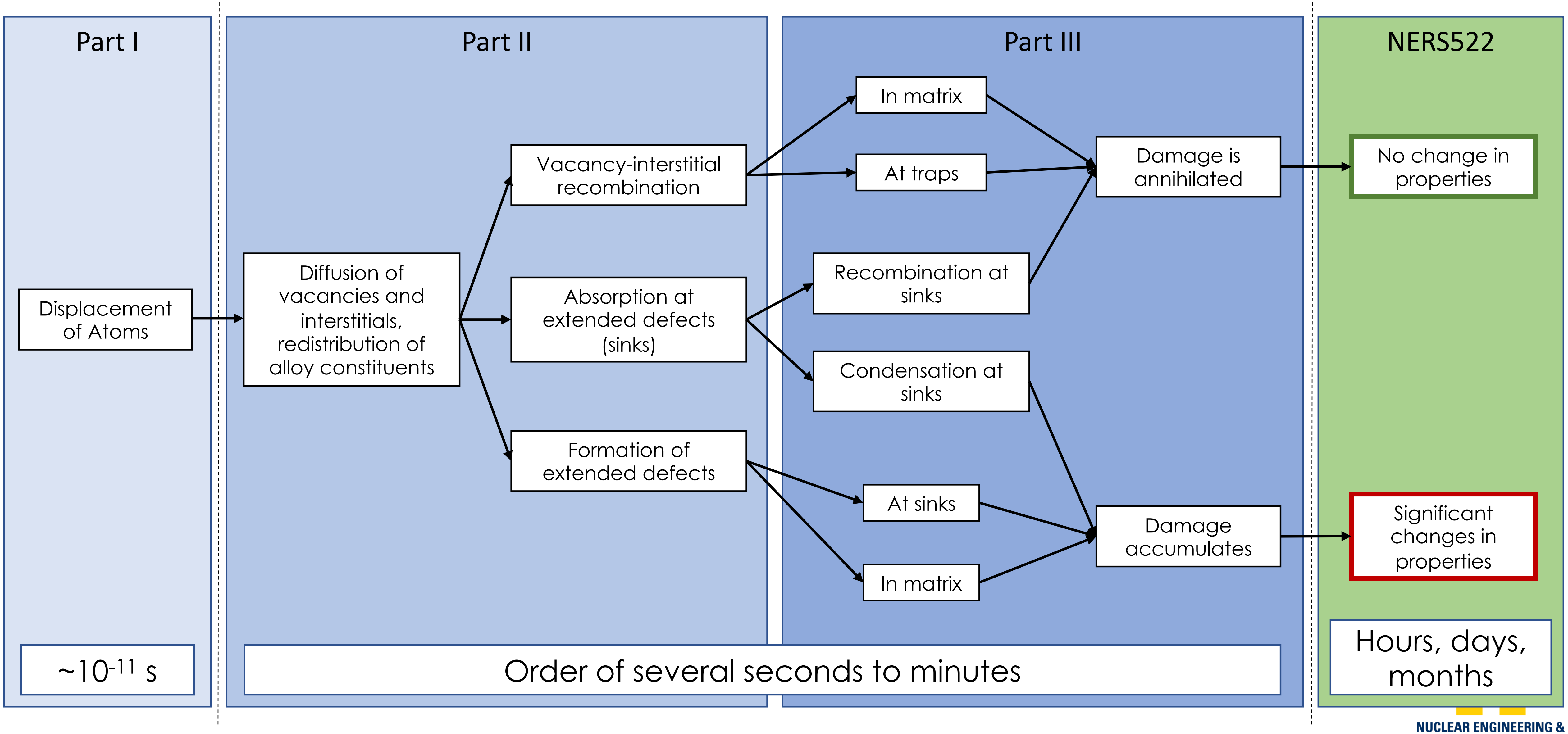
Flow chart for radiation damage



Louis Mansur, "Mechanisms & Kinetics of Radiation Effects in Metals and Alloys", in: Kinetics of Nonhomogeneous Processes, 1987

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Summary of Topics Covered

Part I: The Radiation Damage Event

Objective: Develop a fundamental understanding of the physics of the radiation damage event

Day	Date	Lec. #	Topic	Lecture Notes	Assignments	Other resources/details
Tuesday	Aug. 29	1	Introduction	Notes / Recording		
Thursday	Aug. 31	2	Basic particle interactions	Notes / Recording		Alt. basic particle derivation
Tuesday	Sept. 5	3	Collision Kinematics	Notes / Recording		Collision Derivation
Thursday	Sept. 7	4	Interatomic Potentials & Cross Sections	Notes / Recording	PS#1	Flux/Fluence/Cross-sections/energy transfer quick review
Tuesday	Sept. 12	5	Guest Lecture Simple Disp. Theory - Charles Hirst	Notes / Recording	Example	Displacement Integrals / Cross section conversions
Thursday	Sept. 14	6	Guest Lecture Energy loss & K-P modifications - Charlies Hirst	Notes / Recording		
Tuesday	Sept. 19	7	Range	Notes / Recording	PS1 due	
Thursday	Sept. 21	8	Damage Cascades	Notes / Recording		Arc-dpa Paper

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
Tuesday	Sept. 26	9	Point Defects	Notes / Recording	PS#2	
Thursday	Sept. 28	10	Defect Motion	Notes / Recording	PS#1 soln.	
Tuesday	Oct. 3	11	Guest Lecture - Computational Modelling (Fei Gao)	Notes / Recording		Prof. Field out of town
Thursday	Oct. 5	12	Point Defect Kinetics	Notes / Recording	PS2 due / PS#3	
Tuesday	Oct. 10	13	Kinetics + RED	Notes / Recording		Derivation for $C_s + i$ regime / Example Problem
Thursday	Oct. 12	14	Defect Reactions	Notes / Recording		

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:

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

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

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Energy Transfer to the PKA (T)

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

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

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

- E_i
- γE_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:

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

The average energy transferred is then:
- E_i
- γE_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 intergral 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

Where we are going:

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

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

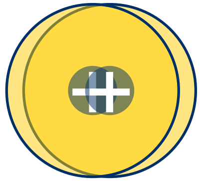
  Task 1: Determine the energy transferred to the PKA:

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

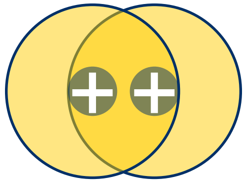
  Task 2: Determine the scattering angle based on the impact parameter:

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

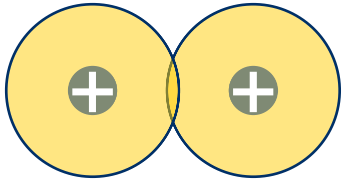
  Task 3: Described V(r) based on the distance of closest approach



= 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

  $$\sigma_s(E_i, T)dT = 2\pi b db \qquad \sigma_s(E_i) = \int_{T_{min}}^{T_{max}} \sigma_s(E_i, T)dT$$

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

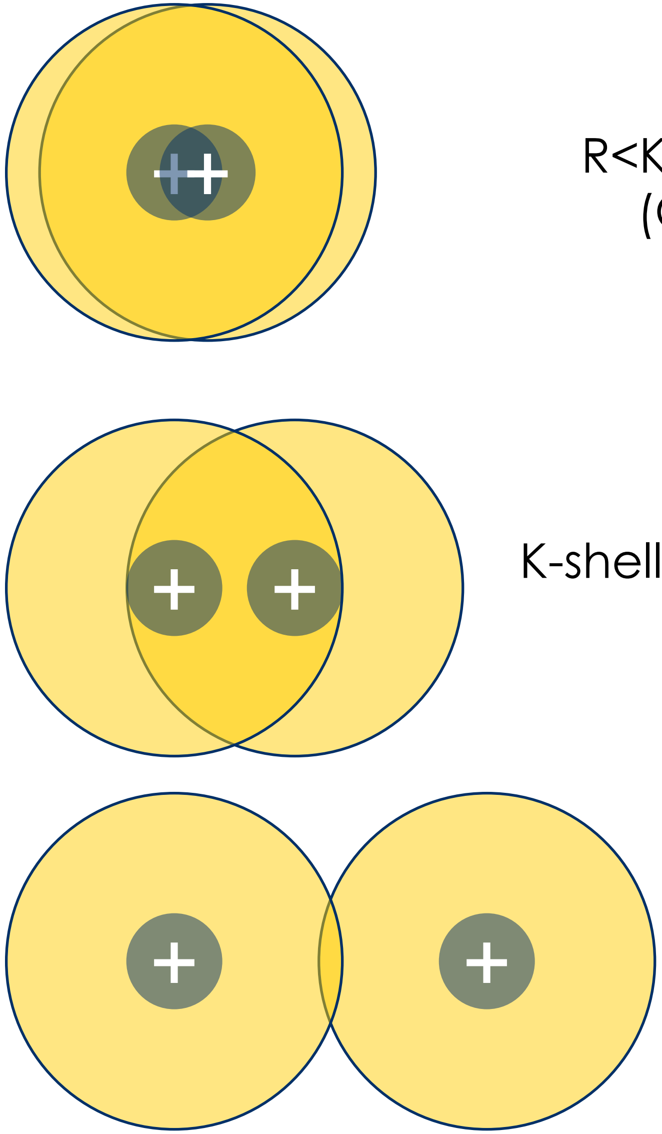
3. Screened Coloumb

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	$0 \quad for \; r > r_0$ $\infty \quad for \; r < r_0$	$10^{-1} < T < 10^3$ eV	r_0 = size of atom	(1.46)
Born-Mayer	$V(r) = A\exp(-r/B)$	$10^{-1} < T < 10^3$ eV $a_0 < r \le r_e$	A,B determined from elastic moduli	(1.47)
Simple Coulomb	$\frac{Z_1 Z_2 \varepsilon^2}{r}$	light ions of high energy $r << a_0$		(1.48)
Screened Coulomb	$\left(\frac{Z_1 Z_2 \varepsilon^2}{r}\right)\exp(-r/a)$	Light ions $r < a_0$	a_o = Bohr radius a = screening radius	(1.49)
Brinkman I	$\frac{Z^2\varepsilon^2}{r} e^{(-r/a)}\left(1-\frac{r}{2a}\right)$	$r < a$	$a \cong a_0/Z^{1/3}$	(1.51)
Brinkman II	$\frac{A Z_1 Z_2 \varepsilon^2 \exp(-Br)}{1-\exp(-Ar)}$	$Z > 25$ $r < 0.7 r_e$	$A = \frac{0.95\times10^{-6}}{a_o} Z_{eff}^{7/}$ $B = Z_{eff}^{1/3}/Ca_o$ $C \cong 1.5$	(1.52)
Firsov	$\frac{Z_1 Z_2 \varepsilon^2}{r}\chi\left[\left(Z_1^{1/2}+Z_2^{1/2}\right)^{2/3}\frac{r}{a}\right]$	$r \le a_0$	χ is screening function	(1.56)
TFD Two Center	$\frac{Z^2\varepsilon^2}{r}\chi\left(Z^{1/3}\frac{r}{a}\right) - \alpha Z + \overline{\Lambda}$	$r < r_b\ (3a_0)$	r_b = 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 = Rydberg energy = 13.6 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

The method then:

Known:

$V(r)$ = interaction potential

Provides b^2 in terms of ϕ 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:

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

…and use

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

$$\boldsymbol{\sigma_s(E_i)}$$

Start

Finish

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

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N for common crystal structures

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

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

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, $\sigma_D\left(E_i\right)$, using your notes you determine the equation to do this calculation is:

$$\sigma_D(E_i) = \int_{\check{T}}^{\hat{T}} \sigma_s(E_i, T)\upsilon(T)dT = \frac{\sigma_s(E_i)}{\gamma E_i} \int_{\check{T}}^{\hat{T}} \upsilon(T)dT$$ <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?

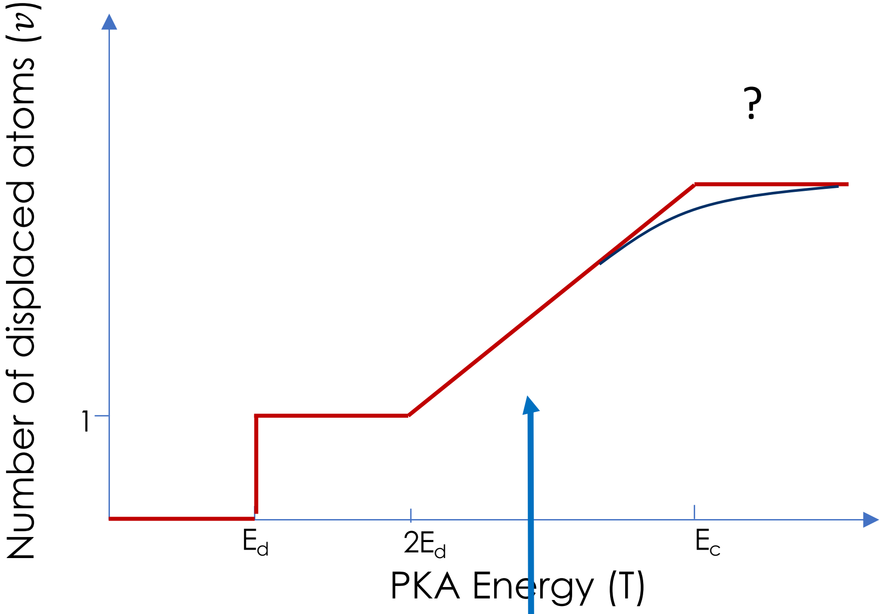
$$\sigma_D(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i}\left(\int_0^{E_d} 0 dT + \int_{E_d}^{2E_d} 1 dT + \int_{2E_d}^{E_c} \frac{T}{2E_d} dT + \int_{E_c}^{\gamma E_i} \frac{E_c}{2E_d} dT\right)$$

Hint: The atomic weight of Fe is 55.85.

Point Defect Kinetic Equations

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

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



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

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

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

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

?

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

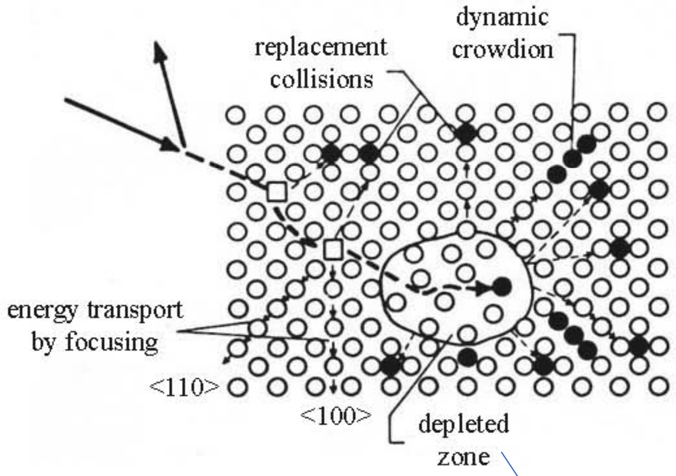
Heavy ions will commonly cause small scale cascades with vacancy rich cores.
-True
-False

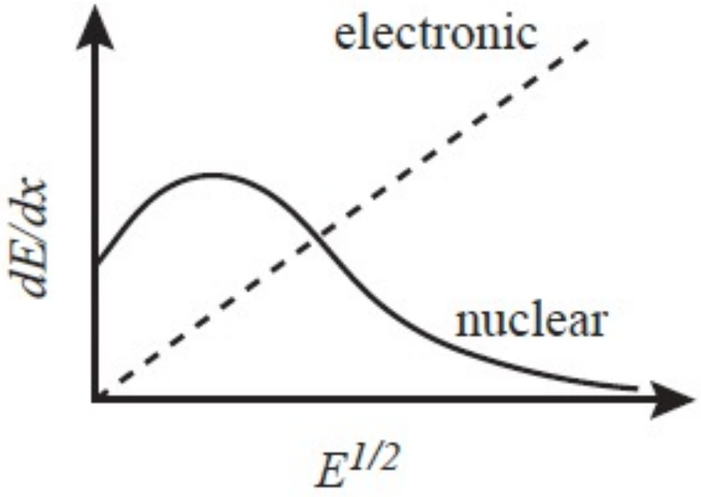
The Kinchin Pease and NRT approach don't account for enhanced recombination in metals in a cascade
-True
-False

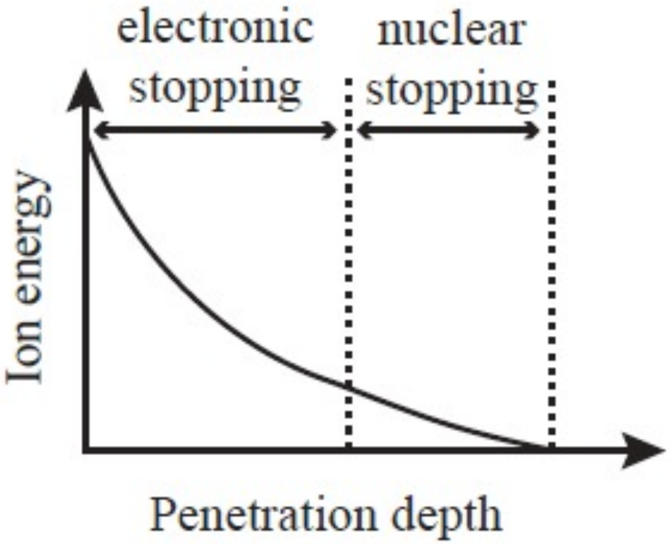
Point Defect Kinetic Equations

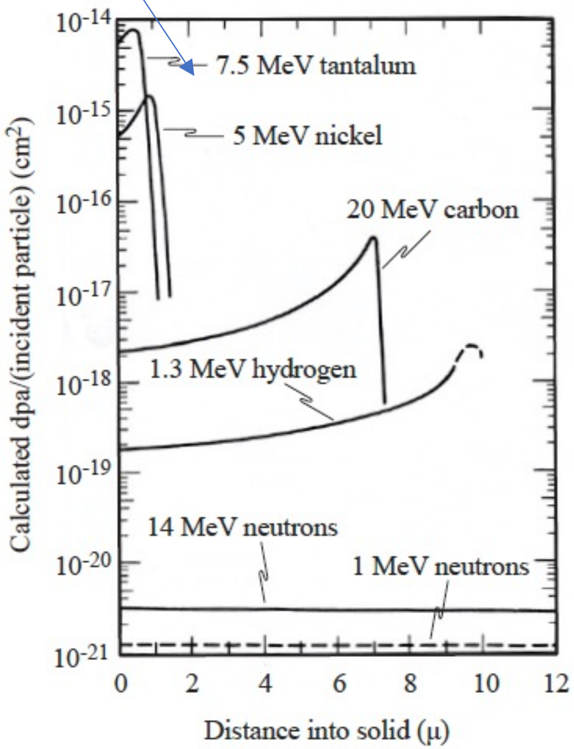
$$\frac{\partial C_v}{\partial t} = \boxed{K_0} - K_{iv}C_iC_v - \sum_s K_{vs}C_vC_s + D_v\nabla^2 C_v$$

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









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

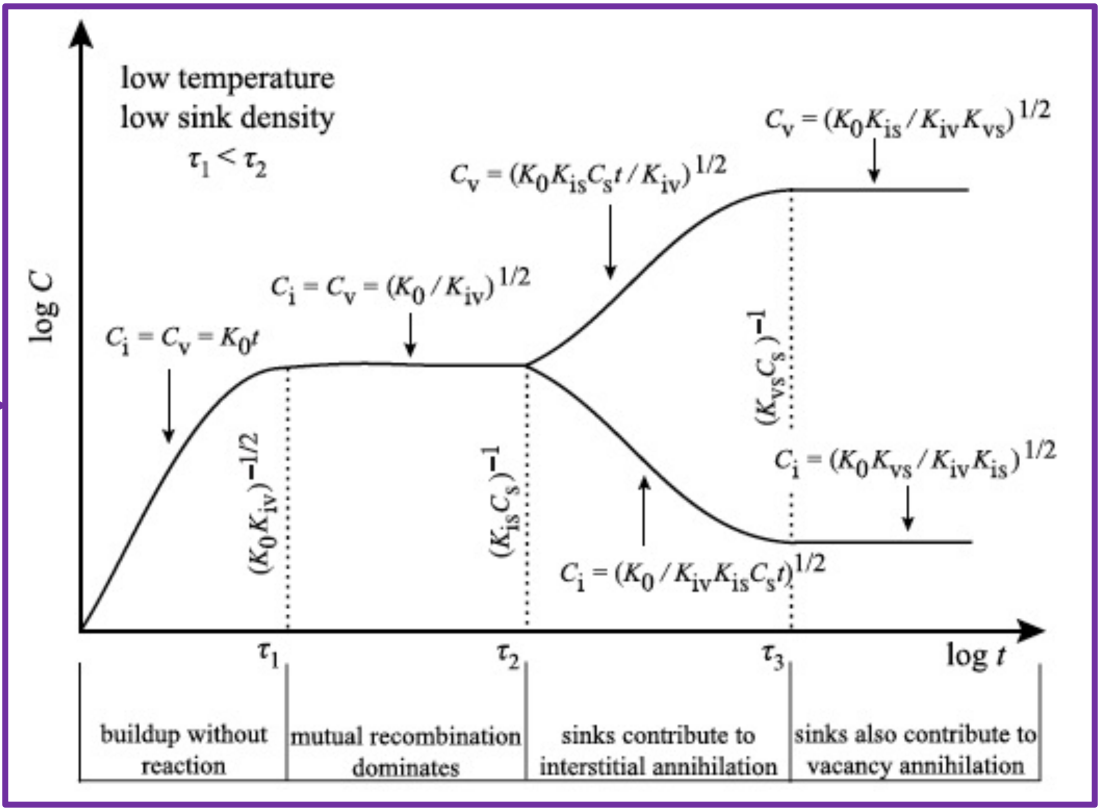
-No

-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 4π to account for the geometry. How much confidence to you have in your answer?

-Low

-Moderate

-HIgh

Point Defect Kinetic Equations

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

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

- 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.