

# NERS 521 Study Guide

(Solutions **Bolded**)

# 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	Topic	Lecture Notes	Assignments	Other resources/details
Monday	Aug. 30	<a href="#">Introduction</a>	<a href="#">Recording</a> / No notes	-	-
Wednesday	Sept. 1	<a href="#">Basic particle interactions</a>	<a href="#">Recording</a> / <a href="#">Notes</a>	-	<a href="#">Alt. basic particle derivation</a>
Monday	Sept. 6	<span style="color:green">No lecture - Labor Day<span>	-	-	-
Wednesday	Sept. 8	<a href="#">Collision Kinematics</a>	<a href="#">Recording</a> / <a href="#">Notes</a>	<a href="#">PS#1</a>	<a href="#">Flux/Fluence/Cross-sections/energy transfer quick review</a>
Monday	Sept. 13	<a href="#">Interatomic Potentials &amp; Cross Sections</a>	<a href="#">Recording</a> / <a href="#">Notes</a>	-	<a href="#">Displacement Integrals</a>
Wednesday	Sept. 15	<a href="#">Simple Disp. Theory</a>	<a href="#">Recording</a> / <a href="#">Notes</a>	-	<a href="#">Cross section conversions</a>
Monday	Sept. 20	<a href="#">Energy loss &amp; K-P modifications</a>	<a href="#">Recording</a> / <a href="#">Notes</a>	<span style="color:red">PS1 due<span>	
Wednesday	Sept. 22	<a href="#">Focus, Channel, Range</a>	<a href="#">Recording</a> / <a href="#">Notes</a>	<a href="#">PS1 Sol.</a>	
Monday	Sept. 27	<a href="#">Damage Cascades</a>	<a href="#">Recording</a> / <a href="#">Notes</a>	<a href="#">PS#2</a>	<a href="#">Arc-dpa Paper</a>

# Summary of topics covered

## 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	Topic	Lecture Slides	Assignments	Other resources
Wednesday	Sept. 29	<a href="#">Point Defects</a>	<a href="#">Recording</a> / <a href="#">Notes</a>		
Monday	Oct. 4	<a href="#">Defect Motion</a>	<a href="#">Recording</a> / <a href="#">Notes</a>	<span style="color:red">PS 2 due<span>	
Wednesday	Oct. 6	<a href="#">Point Defect Kinetics</a>	<a href="#">Recording</a> / <a href="#">Notes</a>	<a href="#">PS2 Sol.</a>	
Monday	Oct. 11	<a href="#">Kinetics + RED</a>	<a href="#">Recording</a> / <a href="#">Notes</a>	<a href="#">PS3</a>	
Wednesday	Oct. 13	<a href="#">Defect Reactions</a>	<a href="#">Recording</a> / <a href="#">Notes</a>	PS3 updated	

# 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:

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

# 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:

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

# 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?

**$p$  is the distance of closest approach and  $V(r)$  is the interatomic potential, where  $p$  helps define the correct potential to use while the potential describes the repulsive force between the two colliding particles. Both are needed to determine the energy transfer in a collision event.**

# 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. **Coloumb**
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



# 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

# $N$ 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 (**2**)

-FCC (**4**)

# 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 its previous position
- **The struck atom is assumed to resume to its 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:

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

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

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

$$\check{T} = T_{\min} = E_d$$

# 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.

**No, the equation is not correct since  $T_{max}$  is less than  $E_c$  where  $E_c$  can be approximated assuming the atomic weight of iron is roughly the value in keV, e.g.  $E_c^{Fe} = 0.056 MeV$**

# 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 its energy.

-**True**

-False

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

-True

-**False** (large scale cascades)

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

-**True**

-False

# 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** (it shortens the time of quasi steady, e.g.  $t_2$  approaches  $t_1$ )

# 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.

# Diffusion during irradiation

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** ( $D_i \gg D_v$ )

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 to you have in your answer?

- Low** (*platelet precipitates will have a surface area calculation like a cylinder, meaning you would expect  $2\pi$  somewhere in the solution*)

- Moderate

- High