# Displacement Theory

K.G. Field[1,a],

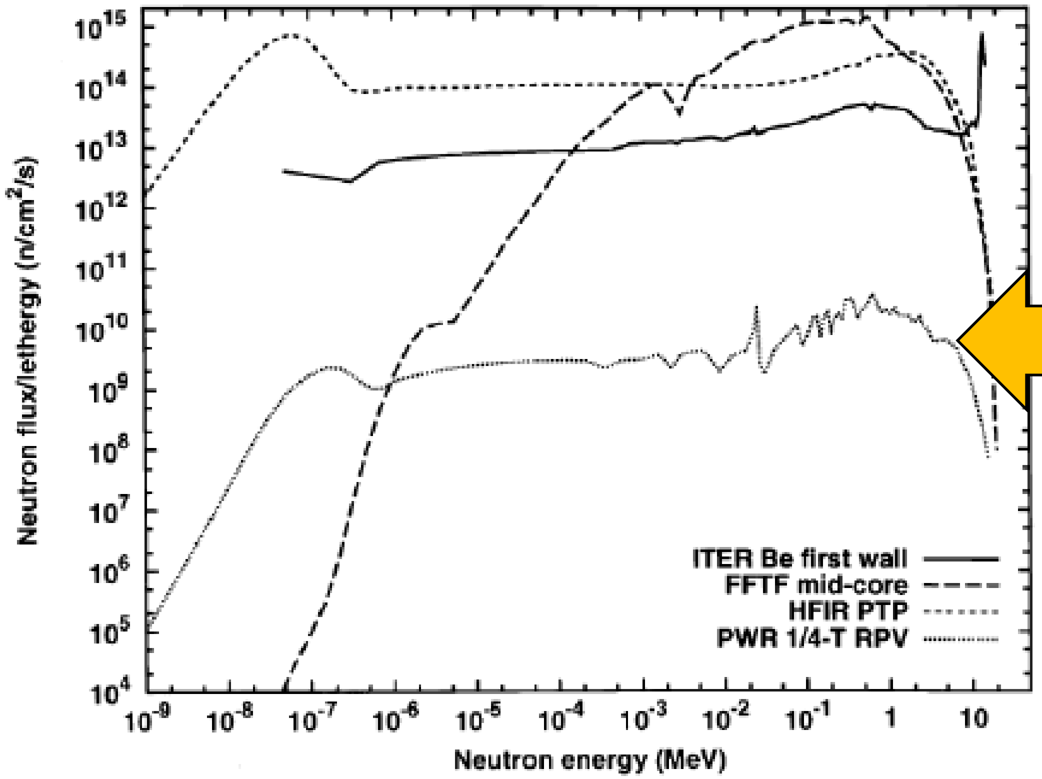
[a] kgfield@umich.edu

[1]University of Michigan

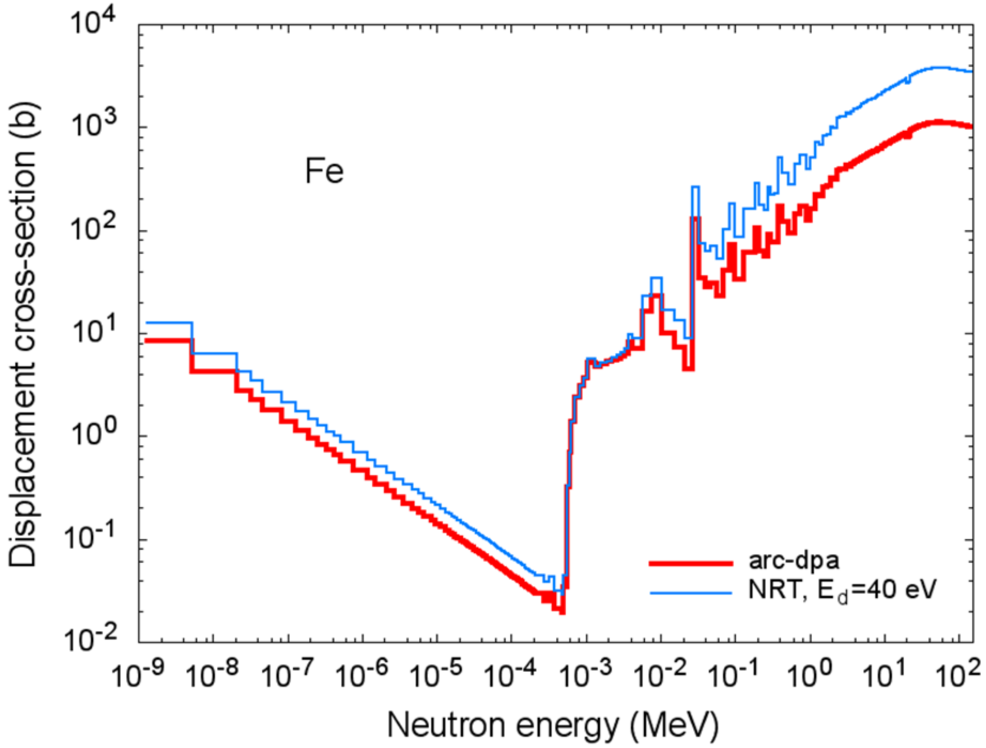
**HW due next Tuesday!**

NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# Cross sections then help us account for the energy spectrum of a given particle flux when converting to dpa




*Energy dependence of neutron flux in various irradiation environments: ITER (DT fusion), HFIR (light water moderated fission), FFTF (sodium moderated fission), and a commercial PWR (light water moderated fission) Source: R.E. Stollerand L.R. Greenwood, J. Nucl. Mater. 271-272 (1999)*




Displacement cross-section for iron calculated using data from ENDF/B-VIII.beta4 and using the arc-dpa model with parameters from Table II, and the NRT model. Source: A. Yu. Konobeyev (KIT)

NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# Summary of different analytical solutions for energy transfer cross sections

**Table 1.5** Energy transfer and energy transfer cross sections for various types of atom–atom collisions

| Type of collision | Energy transfer and energy transfer cross section | Equation in text |
|---|---|---|
| Hard sphere type (Born–Mayer potential) $\rho \sim r_e$ | $\sigma_s(E_i, T) = \frac{\pi B^2}{\gamma E_i}\left[\ln \frac{A}{\eta E_i}\right]^2$ | (1.87) |
| | $\overline{T} = \gamma E_i/2$ | (1.13) |
| Rutherford scattering (simple Coulomb potential) $\rho \ll a$ | $\sigma_s(E_i, T) = \frac{\pi b_0^2}{4}\frac{E_i \gamma}{T^2}$ | (1.102) |
| | $\overline{T} \approx E_d \ln\left(\frac{\gamma E_i}{E_d}\right)$ | (1.104) |
| Heavy ion (inverse square) $a/5 \leq \rho \leq 5a$ | $\sigma_s(E_i, T) = \frac{\pi^2 a^2 E_a \gamma^{1/2}}{8 E_i^{1/2} T^{3/2}}$ | (1.117) |
| | $\overline{T} = \left(\gamma E_i \check{T}\right)^{1/2}$ | (1.118) |
| Relativistic electrons | $\sigma_s(E_i, T) = \frac{4\pi a_0^2 Z^2 E_R^2}{m_0^2 c^4}\frac{1-\beta^2}{\beta^4} \times \left[1 - \beta^2 \frac{T}{\hat{T}} + \pi \frac{\alpha}{\beta}\left\{\left(\frac{T}{\hat{T}}\right)^{1/2} - \frac{T}{\hat{T}}\right\}\right]\frac{\hat{T}}{T^2}$ | (1.124) |

# Summary so far

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 **four** tasks to get towards a quantification of displacements for a given material system:

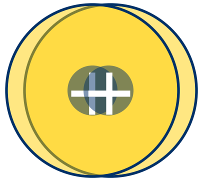
Task 1: Determine the ene

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

Task 2: Determine the sca

$$\phi = \pi - 2 \int_{\infty}^{r_0} \frac{b}{r^2}$$

Task 3: Described V(r) bas



= R<K-shell radi (Coulomb)

= <R<Lattice Constant (Born-Mayer)

Task 4: Combine Tasks 1-3 cross-sections

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

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

NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# Outline

Displacement theory:

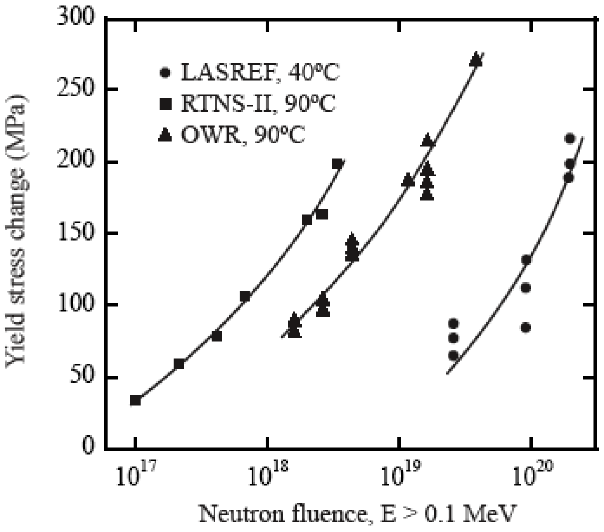
- Governing equations
- Determine $E_d$
- Kinchin-Pease Model
- Example!

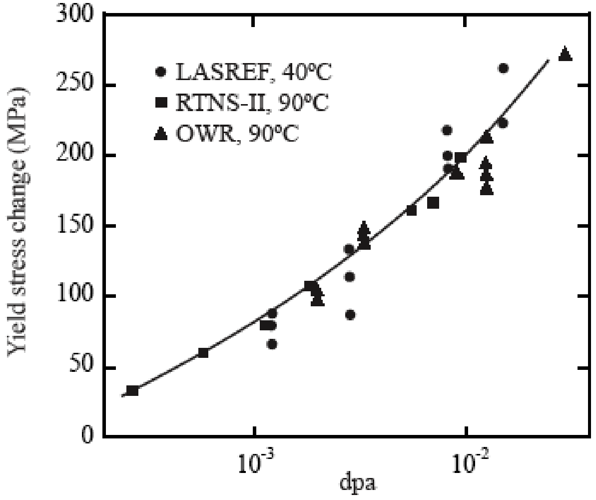
Quick Reminder Sheet Available

Goal: Find the displacements per atom for a given energy spectrum and material system

NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# We met our objective of finding σ($E_i$,T), now what?




- We're still interested in getting to the number of displacements per unit volume per unit time, e.g. dpa rate or dpa/s.

$$R_d = \frac{\#\, diplacements}{cm^3 s} = N \int_{\check{E}}^{\hat{E}} \phi(E_i) \underbrace{\int_{\check{T}}^{\hat{T}} \sigma_s(E_i, T)\, \upsilon(T)\, dT}\, dE_i$$

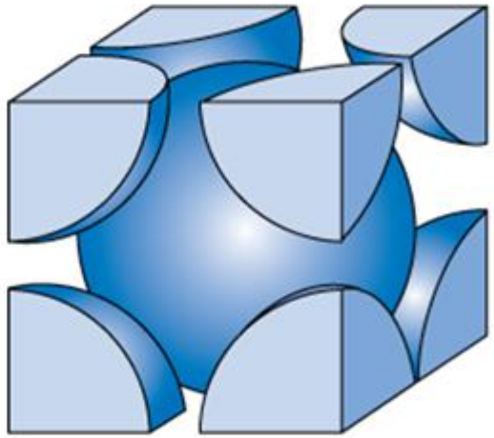
$\sigma_D(E_i)$ = energy dependent displacement cross section (cm$^2$)

$N$ = lattice atom density (#/cm$^3$)

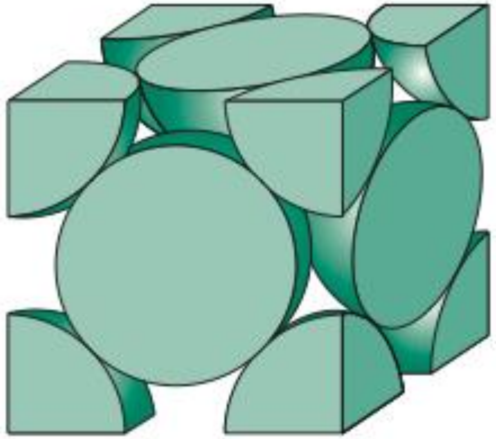
$\phi(E_i)$ = energy dependent particle flux (n/cm$^2$s)

Cover $K_o$

# Quick diversion on N…

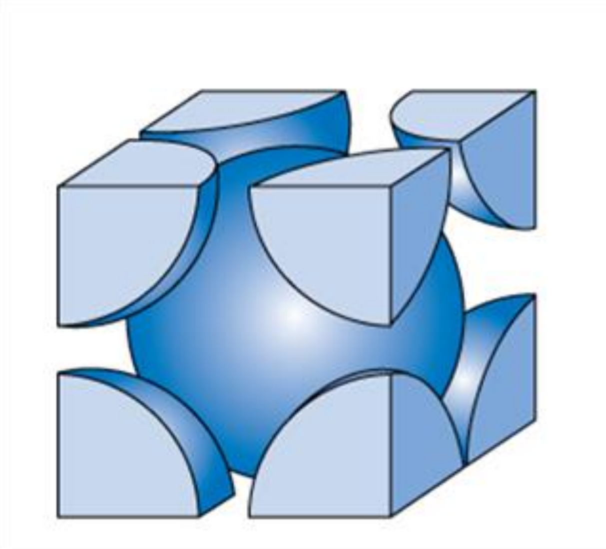


$$N = \frac{\#\, atoms\ in\ a\ unit\ cell}{a_o^3}$$

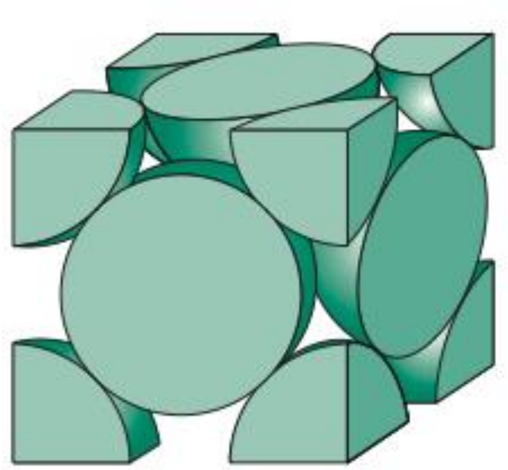


NUCLEAR ENGINEERING &
RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# Quick diversion on N…



$$N = \frac{\#\ atoms\ in\ a\ unit\ cell}{a_o^3}$$



NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# The displacement cross section

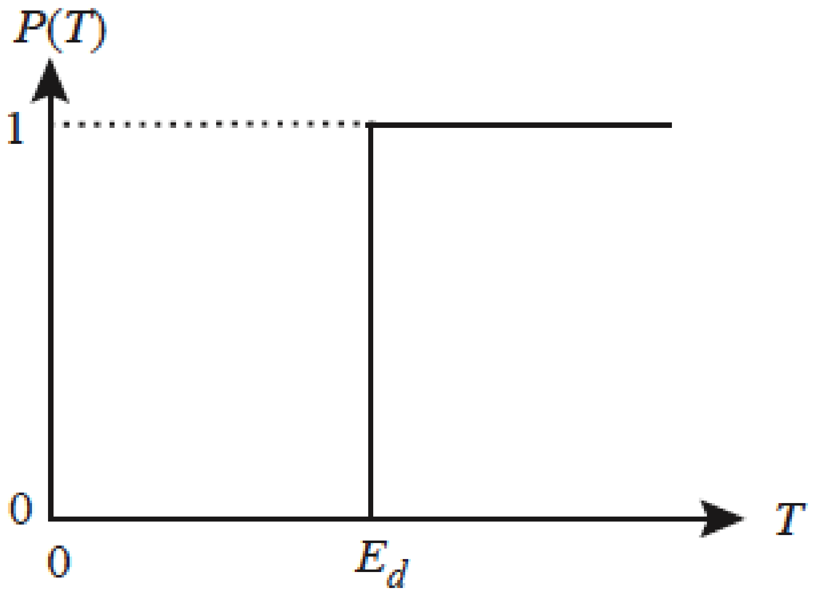
$$\sigma_D(E_i) = \int_{\check{T}}^{\hat{T}} \sigma_s(E_i, T)\, \upsilon(T)\, dT$$

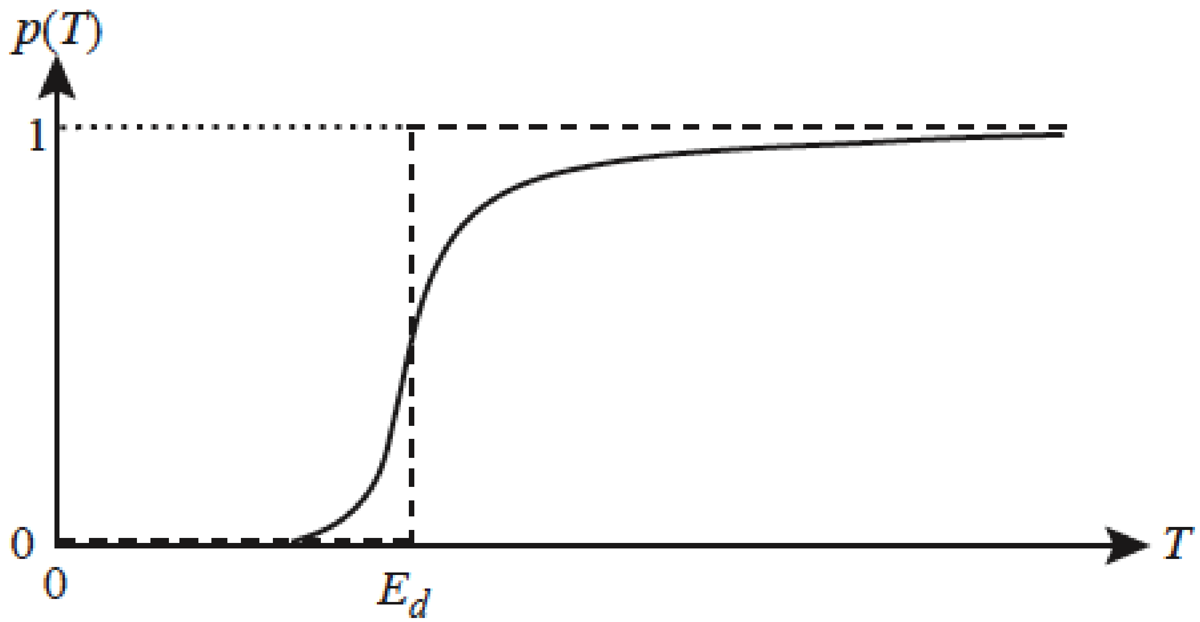
$\sigma_s(E_i, T)$ is the probability that a particle of energy $E_i$ will impart a recoil energy of $T$ to a struck lattice atom (last lecture!)

$\upsilon(T)$ is the number of displacements resulting from this type of collision

$\check{T} = E_d$ the minimum threshold displacement energy

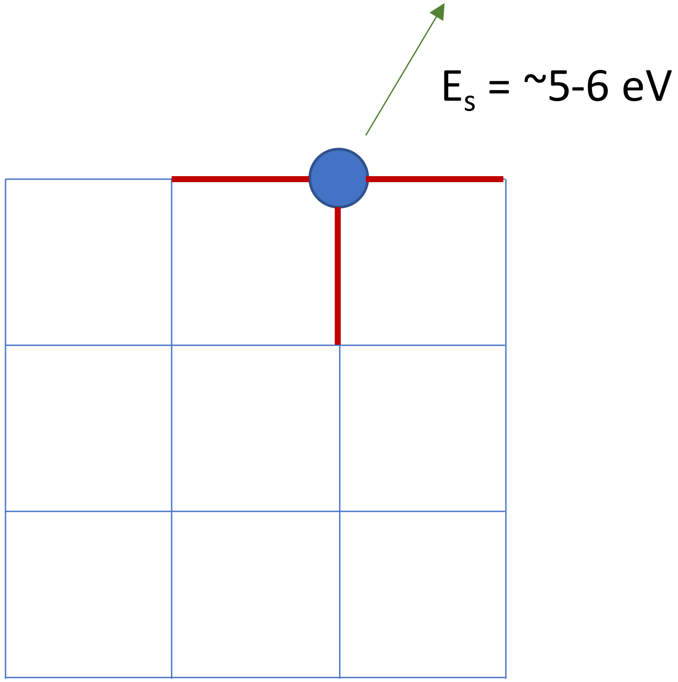
# Introducing the concept of displacement energy



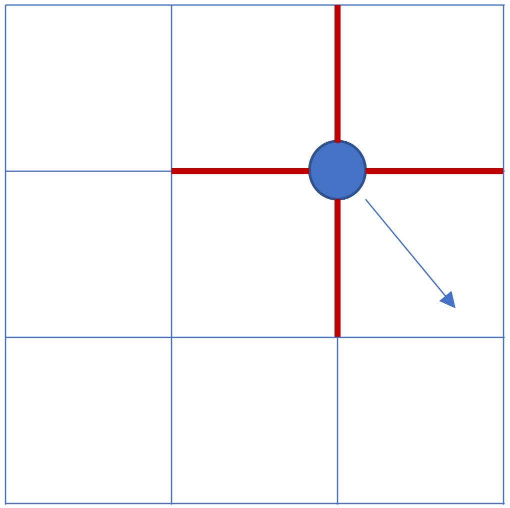




- Displacement energy, $E_d$:
  - If $T > E_d$ a displacement will occur
  - If $T < E_d$ energy transfer will cause an oscillation about the lattice site

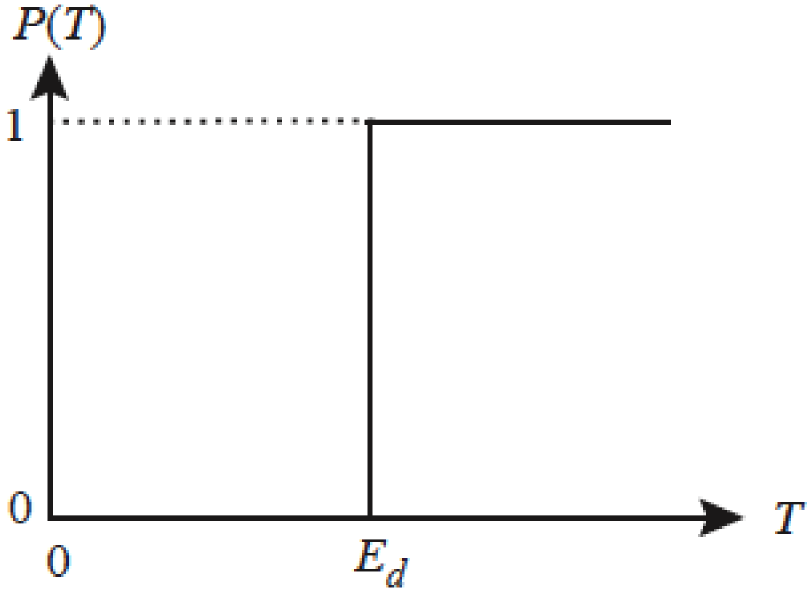
# Simple energy evaluation for $E_d$ (by Setiz)




Energy associated with sublimation

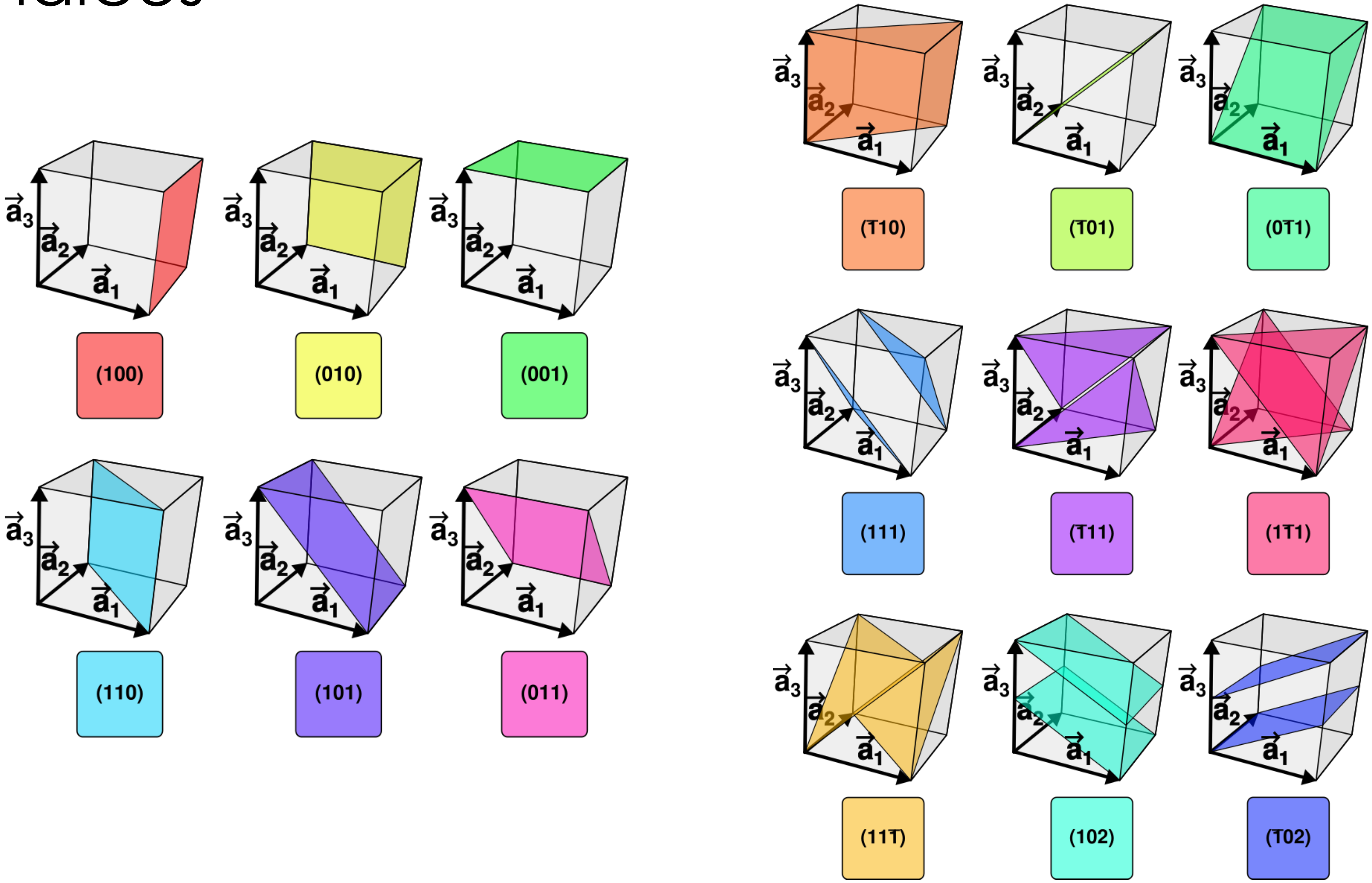


Energy associated with atom displacement



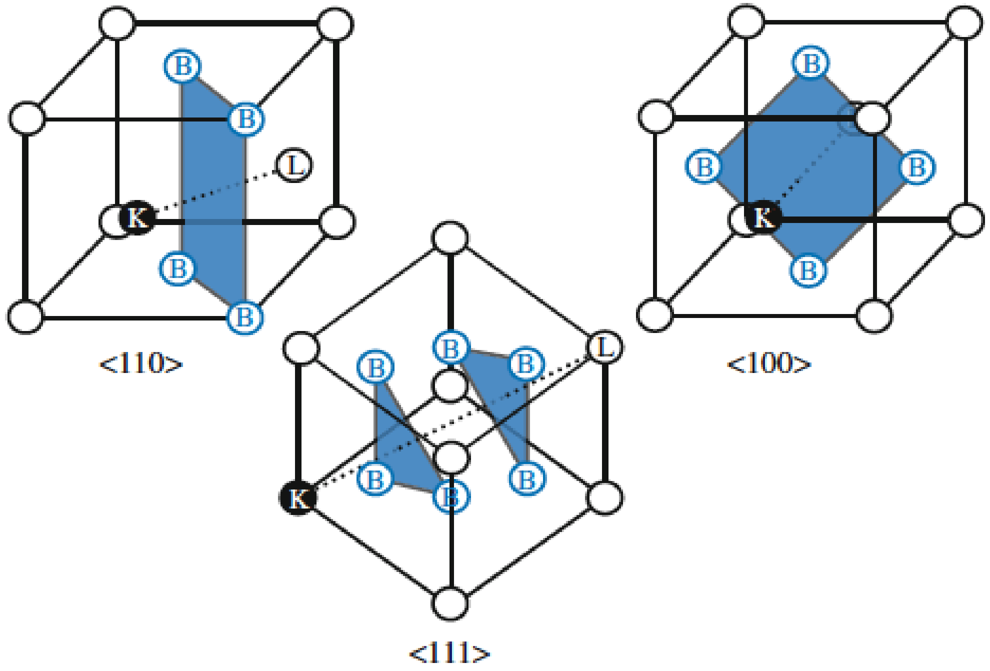

Bond Energy = ~1 eV

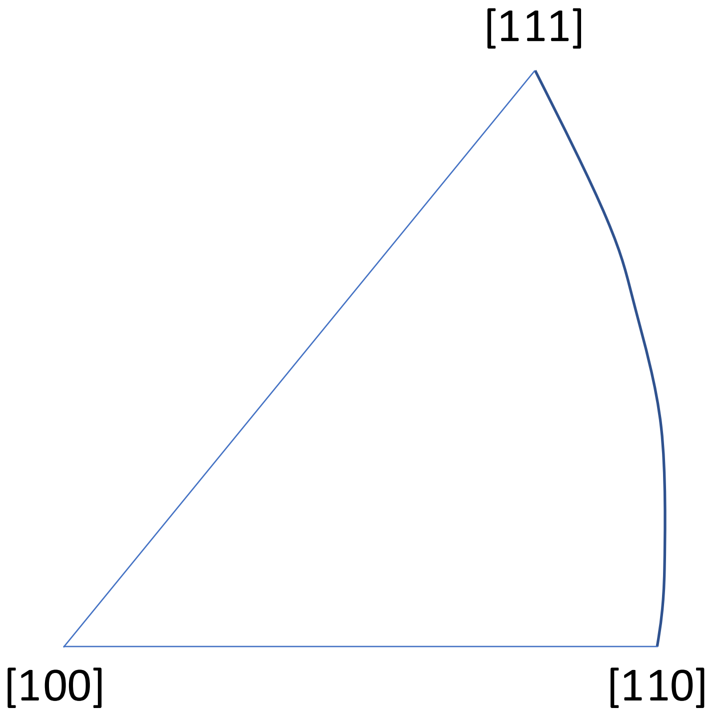
# Miller indices




NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

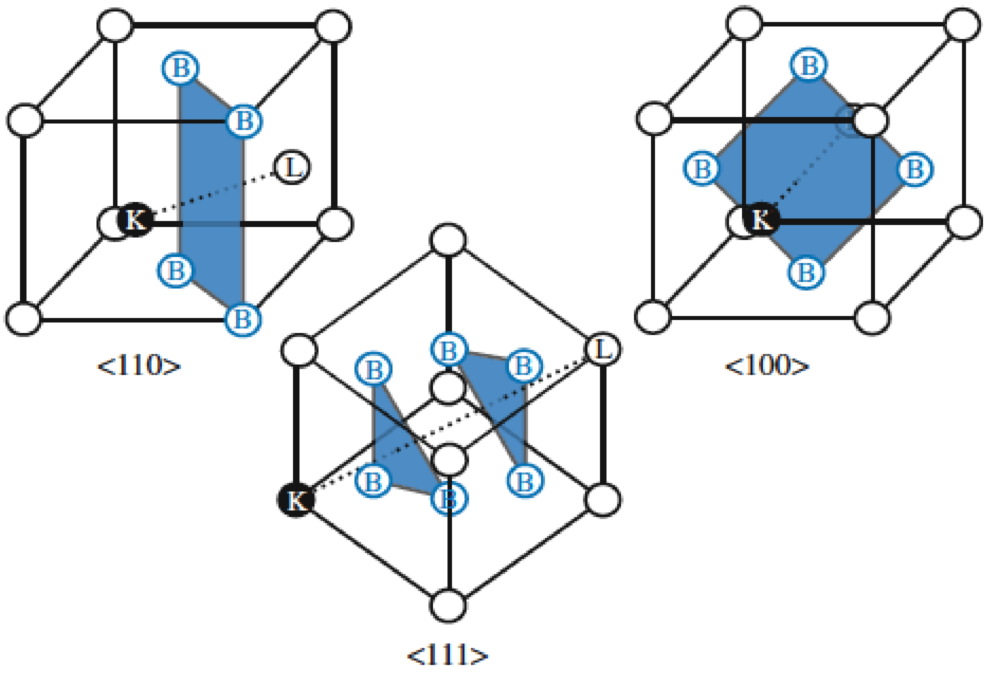
# Effect of crystallinity on $E_d$

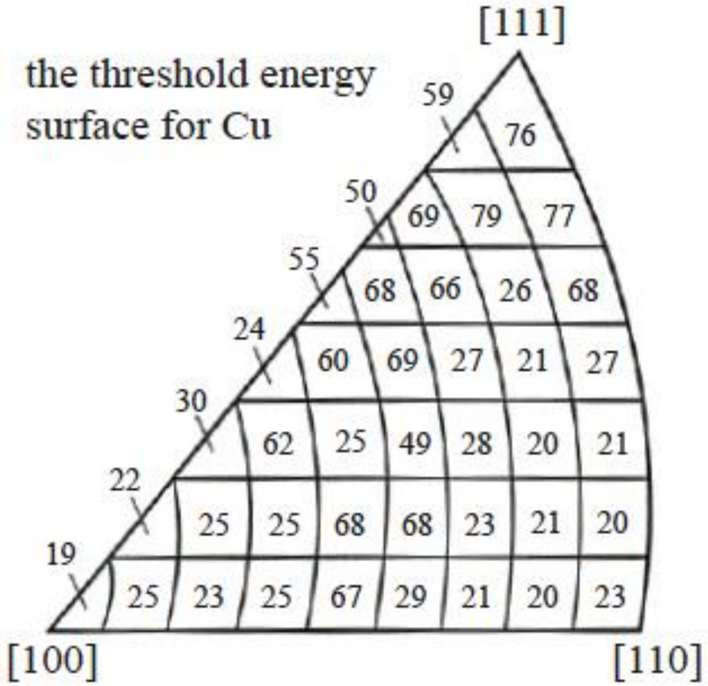



- $E_d$ is directionally dependent due to variances in the barrier based on the crystal structure and potential functions
- Import factors to consider:
  1. # of atoms seen by the moving atom (B in figure); greater # is harder
  2. Impact parameter (e.g. distance of closet approach); smaller is harder
  3. Distance to barrier; longer is harder

# Effect of crystallinity on $E_d$




- $E_d$ is directionally dependent due to variances in the barrier based on the crystal structure and potential functions
- Import factors to consider:
  1. # of atoms seen by the moving atom (B in figure); greater # is harder
  2. Impact parameter (e.g. distance of closet approach); smaller is harder
  3. Distance to barrier; longer is harder

# Practical applications for $E_d$

In practice, it is common to select an "effective" displacement energy or the orientation average value
→ *When using $E_d$ to determine displacements (for example using SRIM in ion irradiations) you must state what value was selected!*

| Metal | Lattice (*c/a*) | $E_{d,min}$ (eV) | $E_d$ (eV) |
|---|---|---|---|
| Al | fcc | 16 | 25 |
| Ti | hcp (1.59) | 19 | 30 |
| V | bcc | | 40 |
| Cr | bcc | 28 | 40 |
| Mn | bcc | -- | 40 |
| Fe | bcc | 20 | 40 |
| Co | fcc | 22 | 40 |
| Ni | fcc | 23 | 40 |
| Cu | fcc | 19 | 30 |
| Zr | hcp | 21 | 40 |
| Nb | bcc | 36 | 60 |
| Mo | bcc | 33 | 60 |
| Ta | bcc | 34 | 90 |
| W | bcc | 40 | 90 |
| Pb | fcc | 14 | 25 |
| Stainless Steel | fcc | | 40 |

NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# The Kinchin Pease (K-P) Approach:

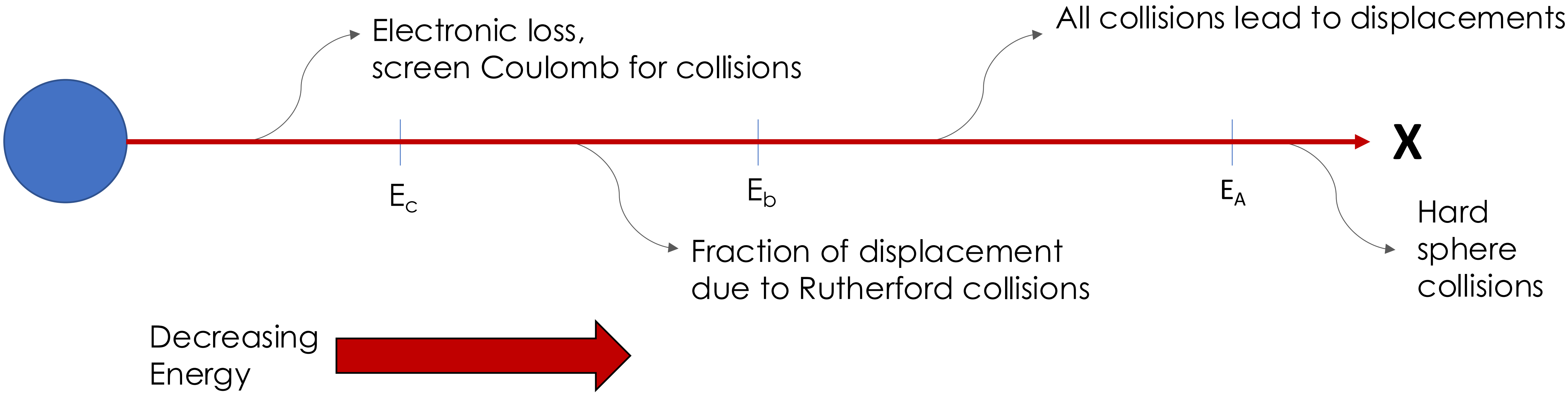
1. An atom is ejected from its lattice site if it receives kinetic energy greater than $E_d$
2. The moving atom will stay behind on the lattice site of the struck atom if the latter receives energy greater than $E_d$ while the former is left with energy less than $E_d$
3. Cascades are created by a sequence of 2-body elastic collisions between atoms
4. There exists a sharp 'ionization limit', $E_c$, where energy loss by electron stopping exists only, e.g.:

   $T > E_c$ no additional displacements

   $T < E_c$ electron stopping is ignored
5. Lattice sites are randomly located - no crystal structure effects
6. Energy transfer cross-section is given by the hard sphere model
7. Glancing collisions which can induce energy loss but not displacements are ignored

NUCLEAR ENGINEERING &
RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# Regimes of PKA energy



# Derivation for the Kinchin Pease (K-P) Approach:

- The total number of displacements produced by the PKA is equal to the total number produced by the two secondary recoils:

$$\upsilon(E_i) = \upsilon(E_i - T) + \upsilon(T)$$

- The probability that a PKA of energy $E_i$ transfers energy in the range $(T, T + dT)$

$$\frac{\sigma_s(E_i, T)dT}{\sigma_s(E_i)} = \frac{dT}{E_i}$$

- Weighing this partition of $T$ with this factor gives:

$$\upsilon(E_i) = \frac{1}{E_i}\int_0^{E_i}\big(\upsilon(E_i - T) + \upsilon(T)\big)dT = \frac{2}{E_i}\int_0^{E_i}\upsilon(T)dT$$

- Which yields:

$$\upsilon(E_i) = \frac{2E_d}{E_i} + \frac{2}{E_i}\int_{2E_d}^{E_i}\upsilon(T)dT$$

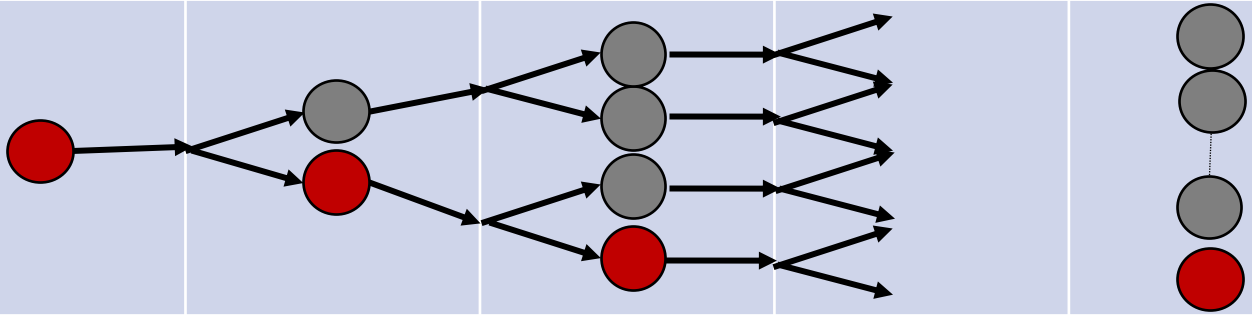
- Converting the integral equation to a differential equation with respect to $E_i$:

$$E_i\frac{d\upsilon}{dE_i} = \upsilon \Rightarrow \upsilon = \frac{E_i}{2E_d}, \text{for } 2E_d < E_i < E_c$$

NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

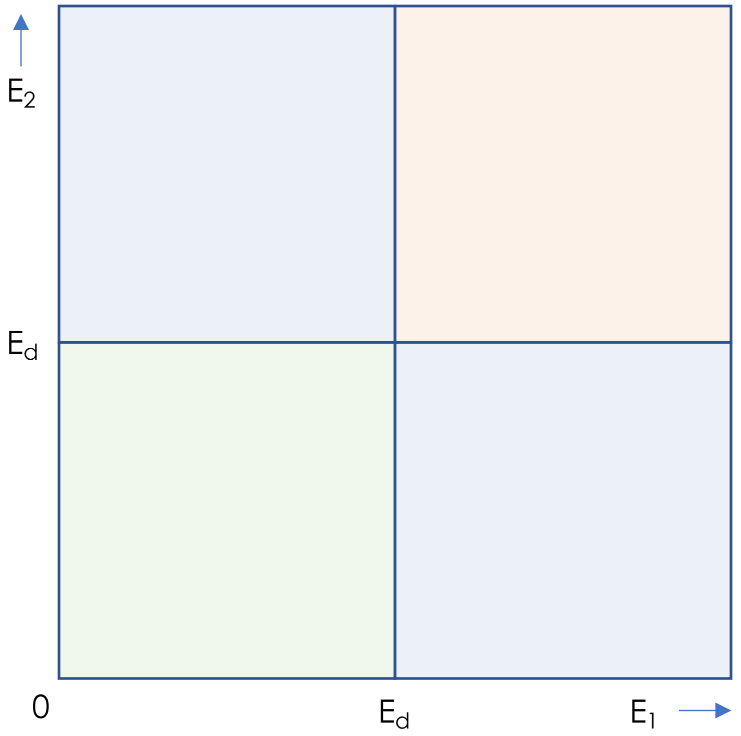
# Schematic for the Kinchin Pease (K-P) Approach:

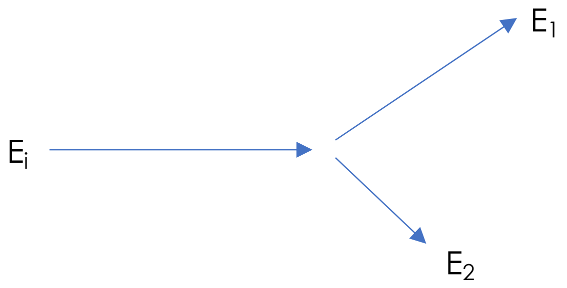
- Recall, for the hard-sphere model: $\bar{T} = {}^{\gamma E_i}/_2$ and $\gamma = 1 \Rightarrow \bar{T} = {}^{E_i}/_2$

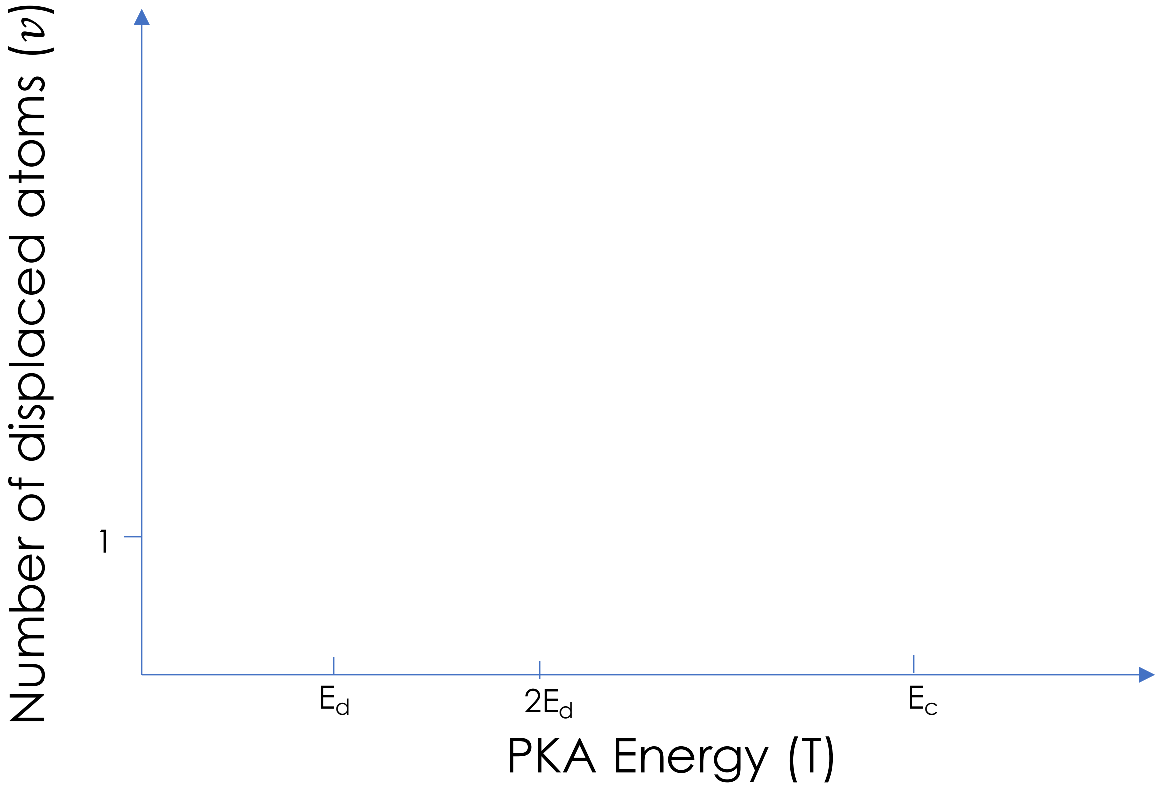
| **Collision #:** | 0 | 1 | 2 | | N | | $N_f$ |
|---|---|---|---|---|---|---|---|
| Schematic: |  | | | | | | |
| Average energy per knock-on | $E_i$ | $\frac{E_i}{2^1}$ | $\frac{E_i}{2^2}$ | | $\frac{E_i}{2^N}$ | | $2E_d$ |
| Number of displaced atoms | 1 | 2 | 4 | | $2^N$ | | $\frac{E_i}{2E_d}$ |

NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# The Kinchin Pease Approach:

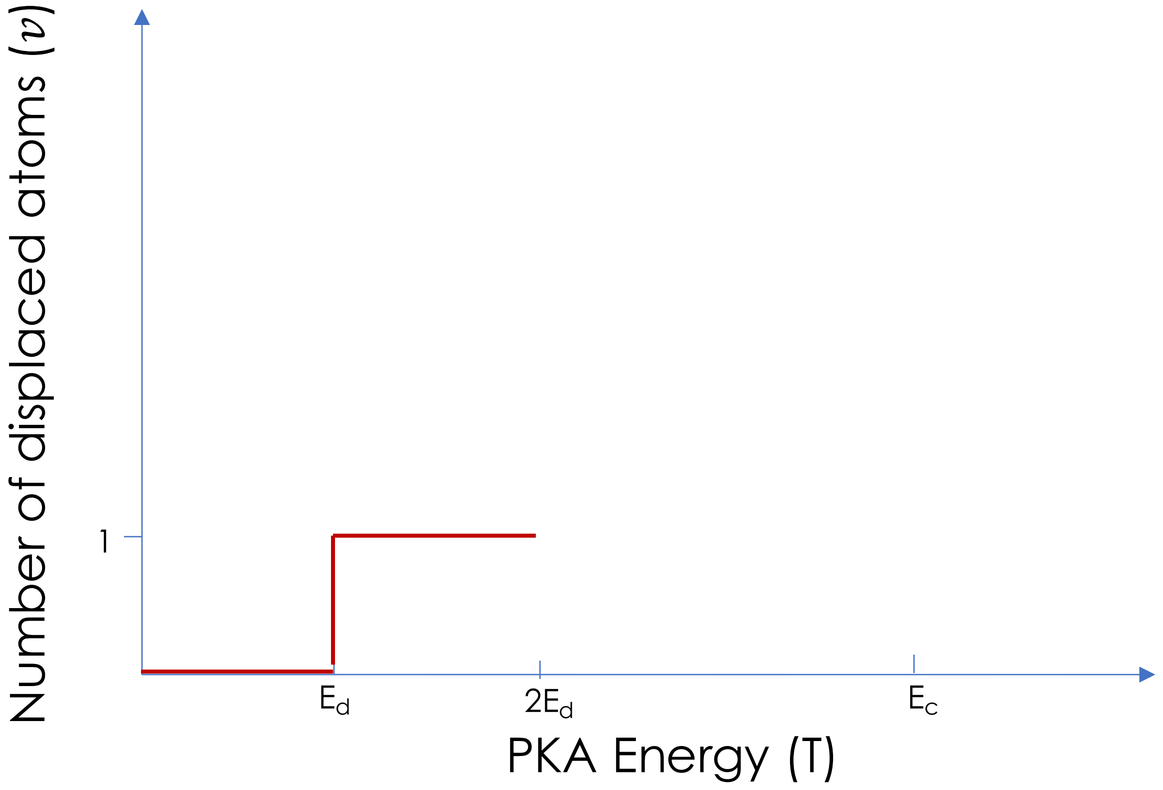



NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# The Kinchin Pease Approach:




NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# Example calculation…

Assume a pure piece of BCC iron is irradiated in a reactor with a monoenergetic flux of 5E13 $cm^3/s$ 1 MeV neutrons. Calculate the time it takes to reach 1 dpa in the iron sample.

NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# Example calculation…

# You might find this helpful:

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. 27 | 1 | Introduction | Notes / Recording | | |
| Thursday | Aug. 29 | 2 | Basic particle interactions | Notes / Recording | Midterm preference due by Friday | Alt. basic particle derivation |
| Tuesday | Sept. 3 | 3 | Collision Kinematics | Notes / Recording | | Collision Derivation |
| Thursday | Sept. 5 | 4 | Interatomic Potentials & Cross Sections | | | Flux/Fluence/Cross-sections/ener... ...ansfer quick review |
| Tuesday | Sept. 10 | 5 | Simple Disp. Theory | | Example | Displacement Integrals / C... |
| Thursday | Sept. 12 | 6 | Energy loss & K-P modifications | | | |
| Tuesday | Sept. 17 | 7 | Focus, Channel, Range - Guest Lecture (M. Lynch) | | PS1 due | |
| Thursday | Sept. 19 | 8 | Damage Cascades - Guest Lecture (M. Lynch) | | | Arc-dpa Paper |

NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

# Example calculation…

# Brain storming

- Why would the K-P model not be correct? (but reasonable)

# Summary so far

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

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

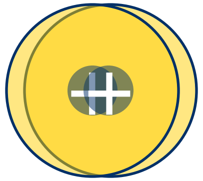
  Task 1: Determine the energy transferred to the PKA:

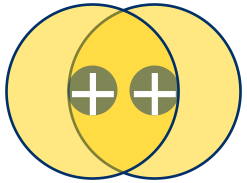
  $T = \frac{\gamma}{2} E_i (1 - \cos\phi)$ to get $\phi = f(T)$

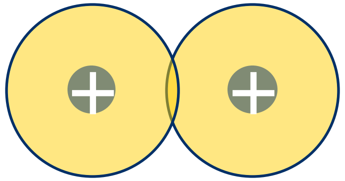
  Task 2: Determine the scattering angle based on the impact parameter:

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

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

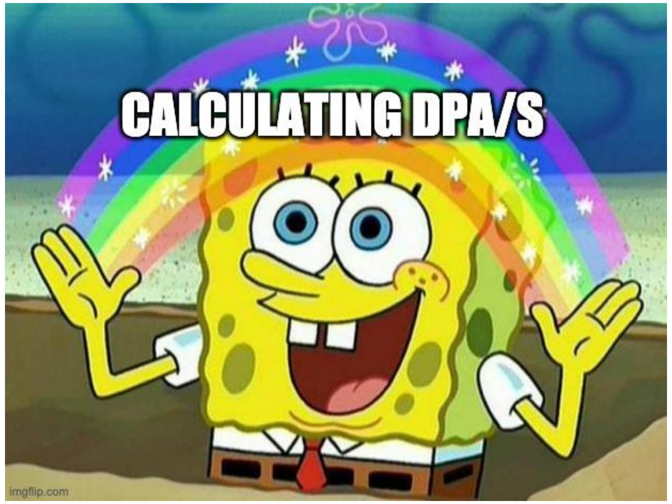

= R<K-shell radius (Coulomb)


= 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

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



# Questions?