

# Displacement Theory

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**NUCLEAR ENGINEERING &  
RADIOLOGICAL SCIENCES**  
UNIVERSITY OF MICHIGAN

# Summary so far

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

Where we are going:

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

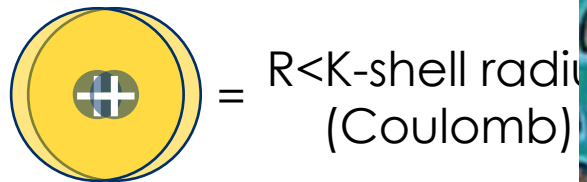
Task 1: Determine the energy

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

Task 2: Determine the scattering

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

Task 3: Described  $V(r)$  based on



Task 4: Combine Tasks 1-3 to calculate cross-sections

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

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



=  $\langle R \rangle$  Lattice Constant (Born-Mayer)

# Outline

## Displacement theory:

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

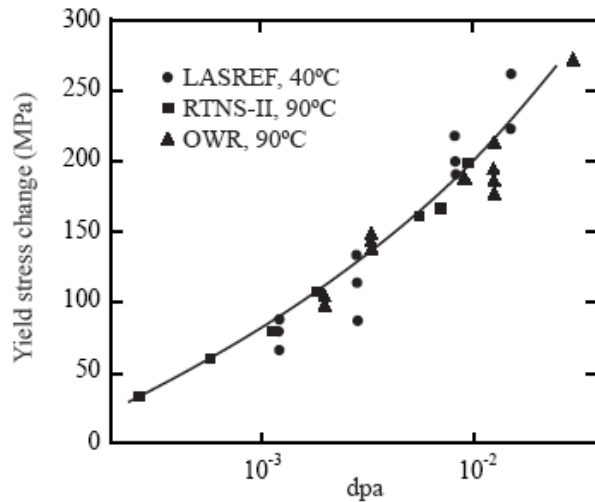
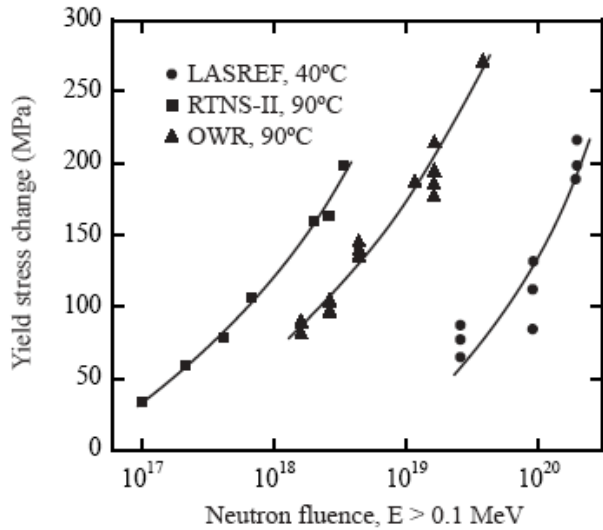


Quick Reminder Sheet Available

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



# We met our objective of finding $\sigma(E_i, T)$ , 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.

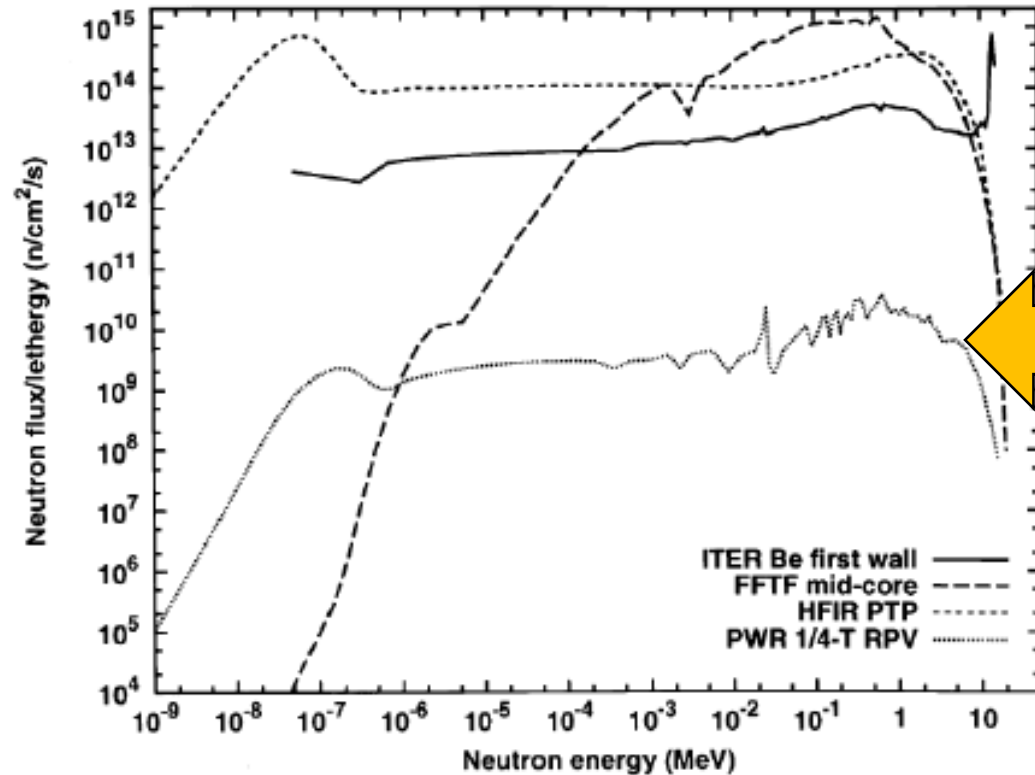
$$R_d = \frac{\# \text{ displacements}}{\text{cm}^3 \text{ s}} = N \int_{\check{E}}^{\hat{E}} \underbrace{\phi(E_i) \int_{\check{T}}^{\hat{T}} \sigma_s(E_i, T) v(T) dT}_{\sigma_D(E_i)} dE_i$$

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

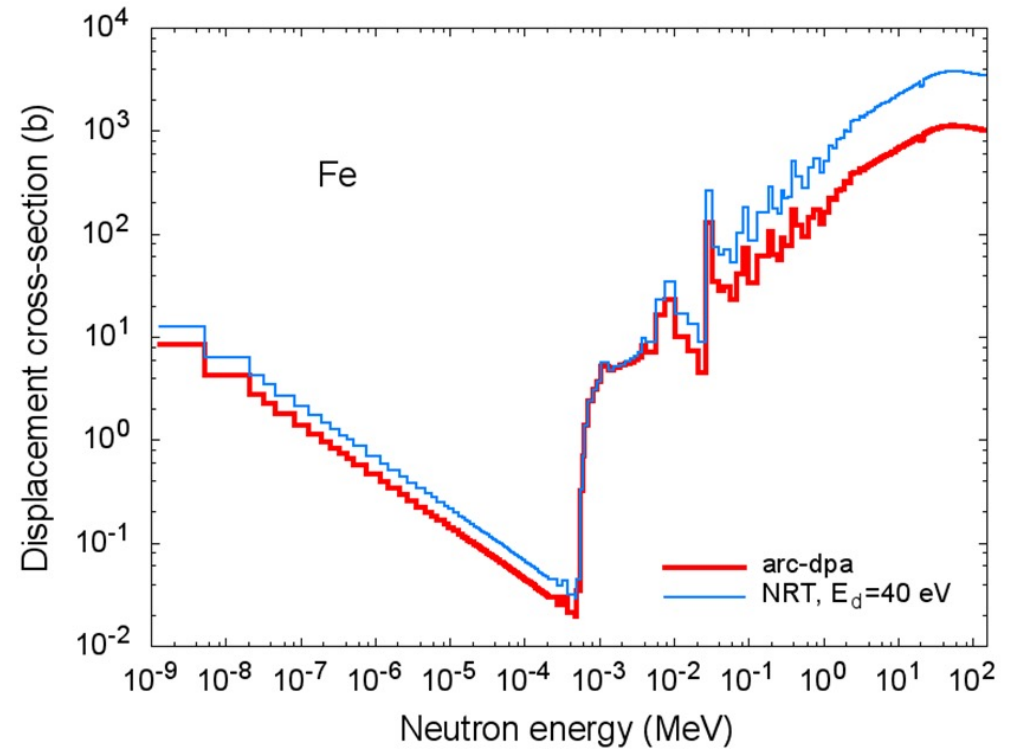
$N$  = lattice atom density ( $\#/\text{cm}^3$ )

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

# 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. Stoller and 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)



# The displacement cross section

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

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

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

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



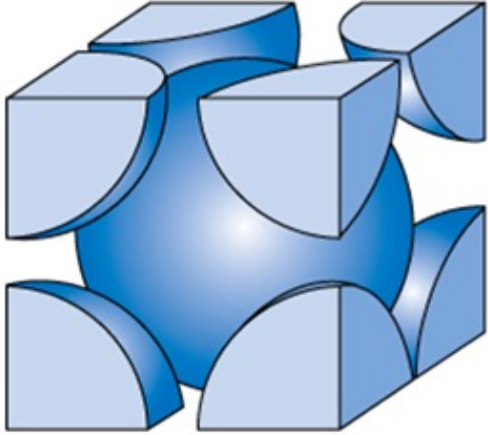
# Summary of different analytical solutions for energy transfer cross sections

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

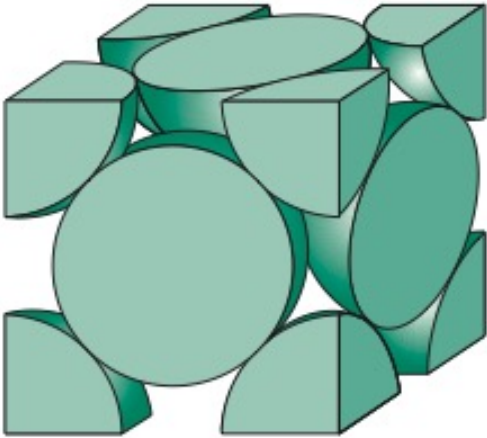
Type of collision	Energy transfer and energy transfer cross section	Equation in text
Hard sphere type (Born–Mayer potential) $\rho \sim r_e$	$\sigma_s(E_i, T) = \frac{\pi B^2}{\gamma E_i} \left[ \ln \frac{A}{\eta E_i} \right]^2$	(1.87)
	$\bar{T} = \gamma E_i / 2$	(1.13)
Rutherford scattering (simple Coulomb potential) $\rho \ll a$	$\sigma_s(E_i, T) = \frac{\pi b_0^2}{4} \frac{E_i \gamma}{T^2}$	(1.102)
	$\bar{T} \approx E_d \ln \left( \frac{\gamma E_i}{E_d} \right)$	(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)
	$\bar{T} = (\gamma E_i \tilde{T})^{1/2}$	(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)



# Quick diversion on N...

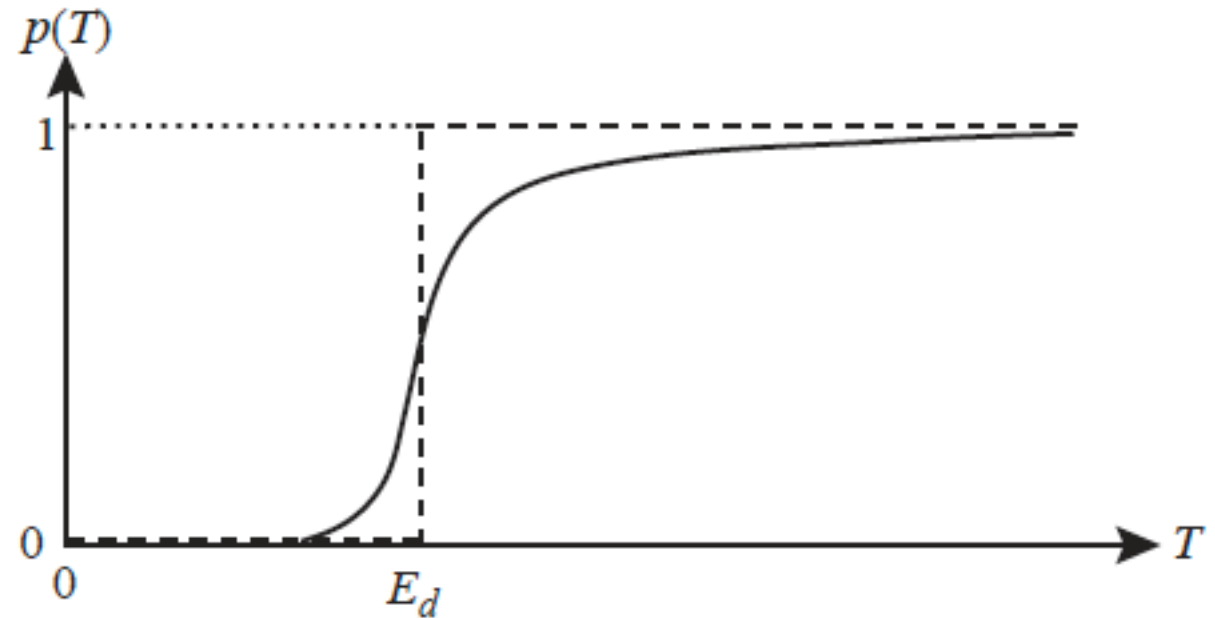
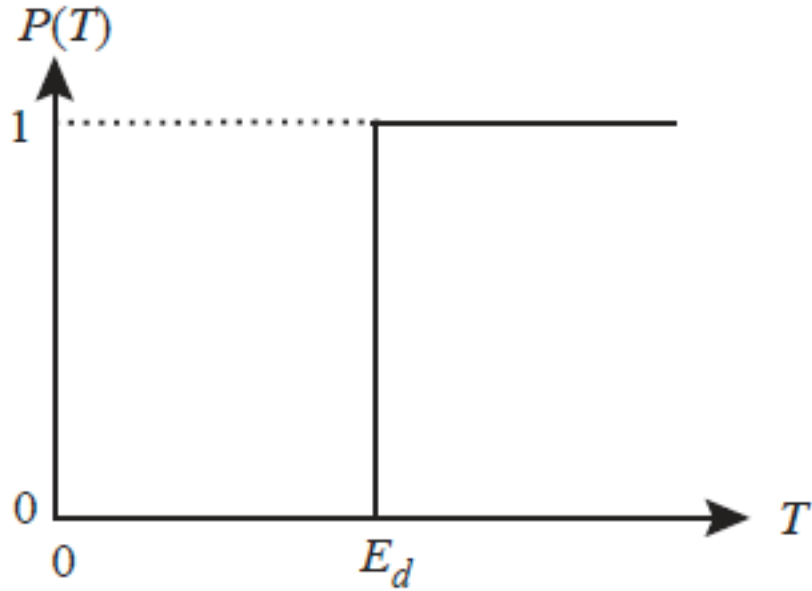


$$N = \frac{\text{\# atoms in a unit cell}}{a_o^3}$$



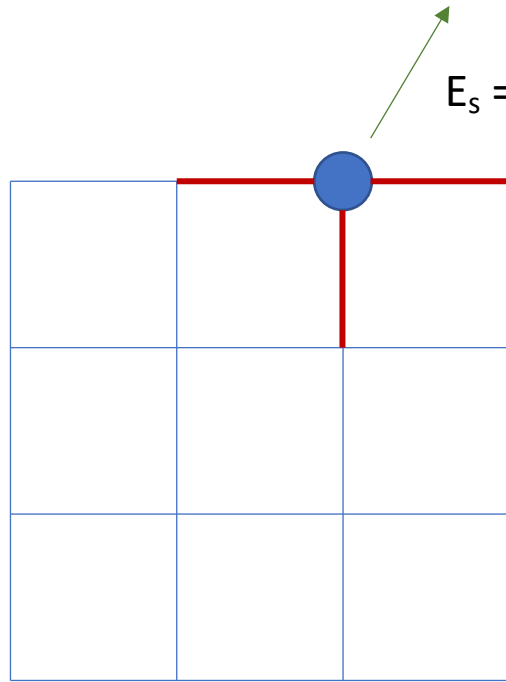


# Introducing the concept of displacement energy



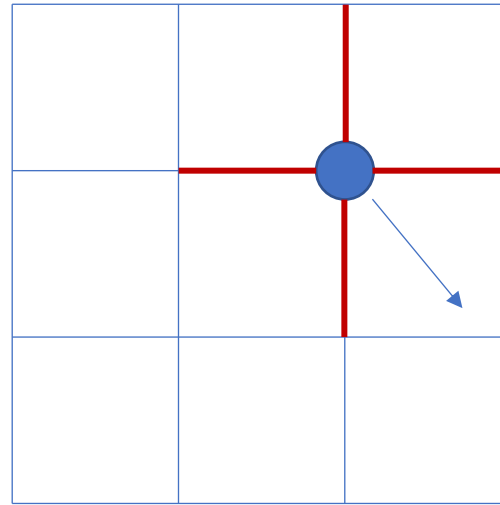
- Displacement energy,  $E_d$ :
  - If  $T > E_d$  a displacement will occur
  - If  $T < E_d$  energy transfer will cause an oscillation about the lattice site

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

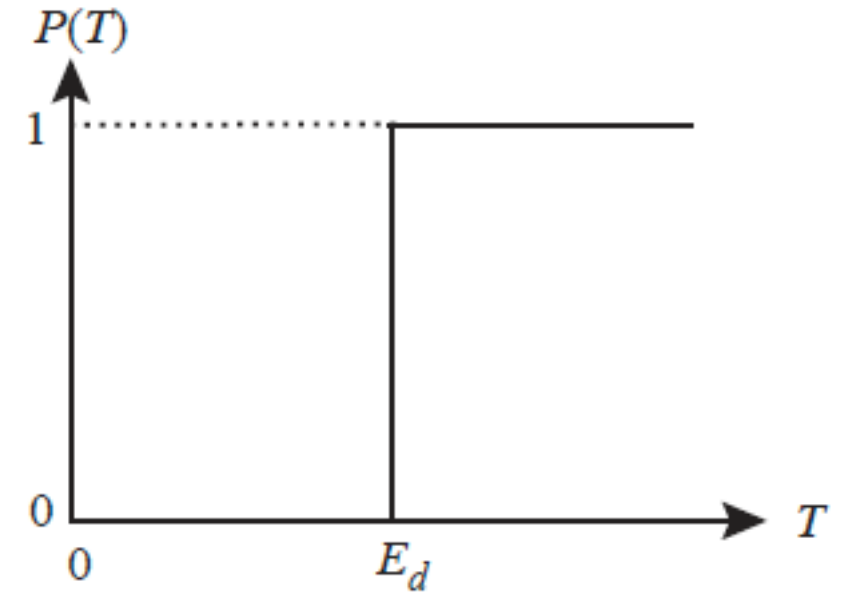


Energy associated with sublimation

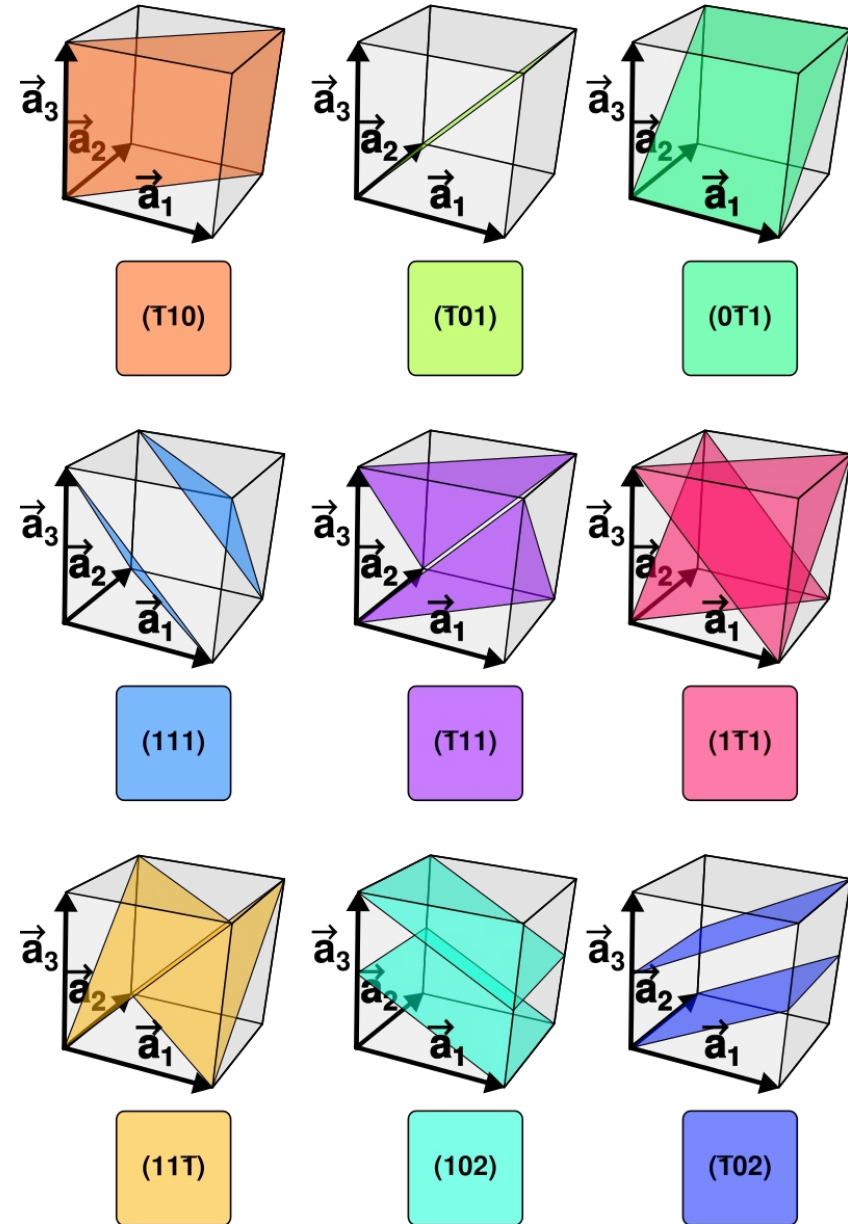
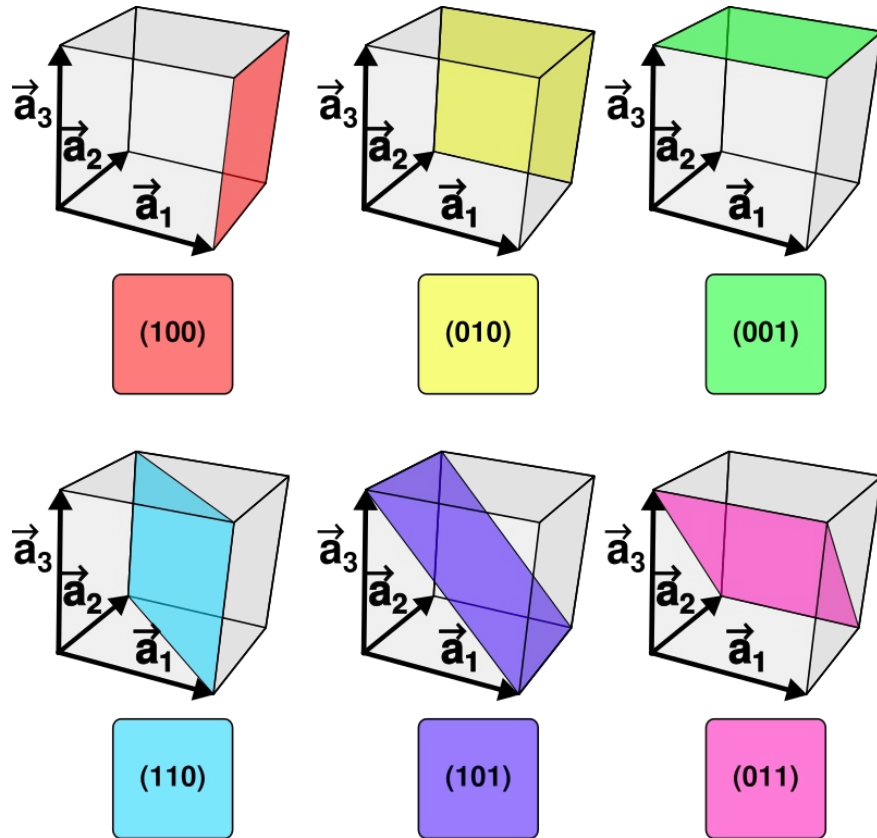
Bond Energy =  $\sim 1 \text{ eV}$



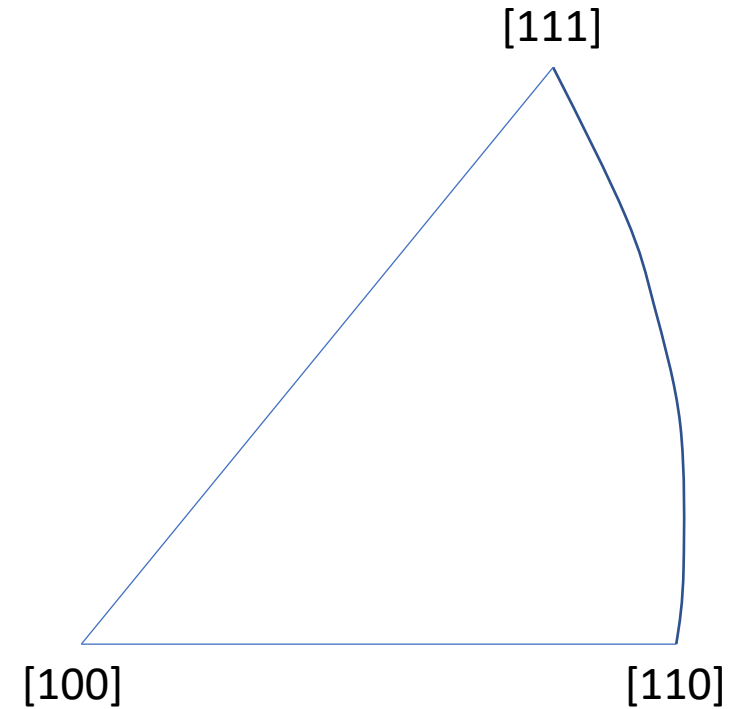
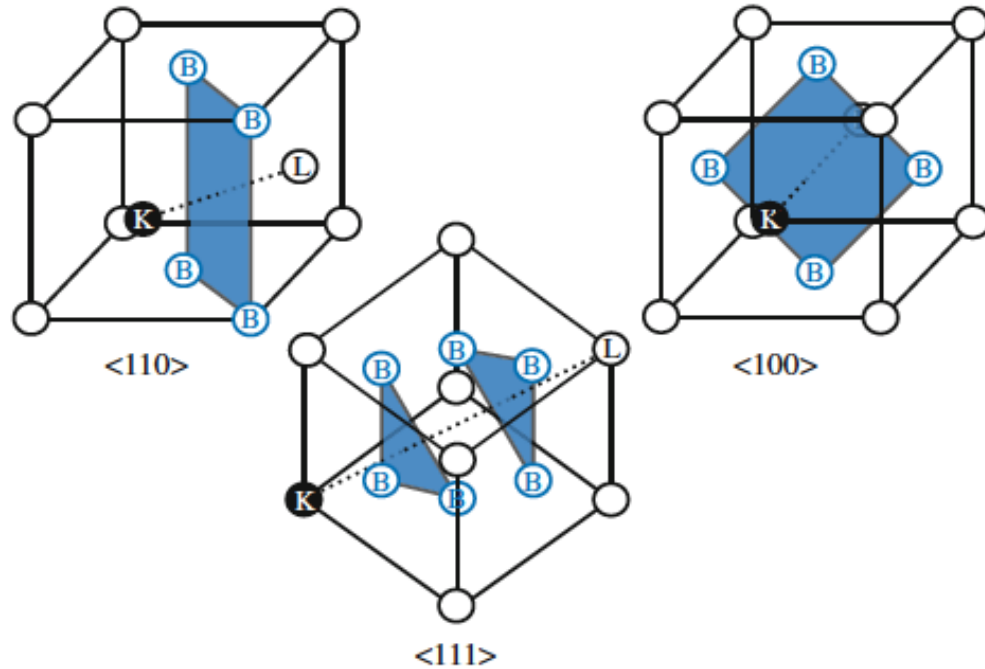
Energy associated with atom displacement



# Miller indices

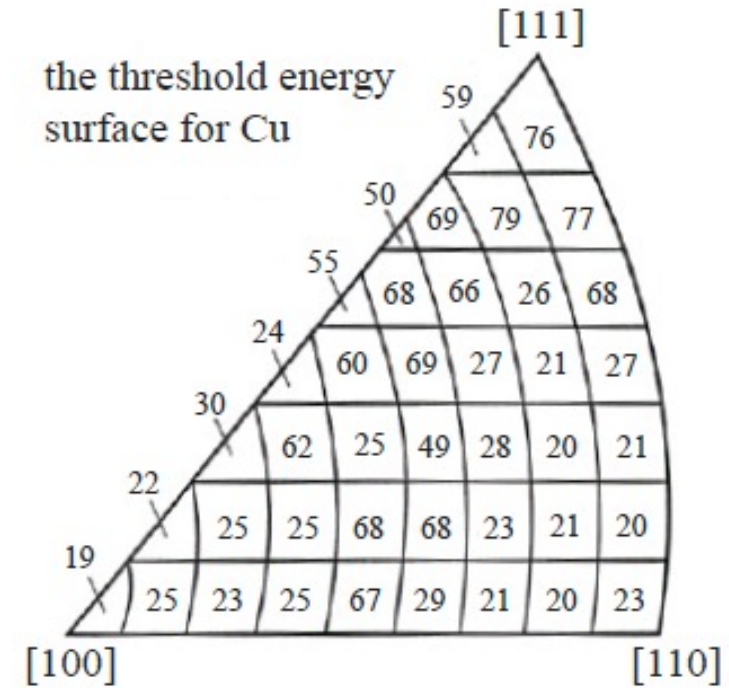
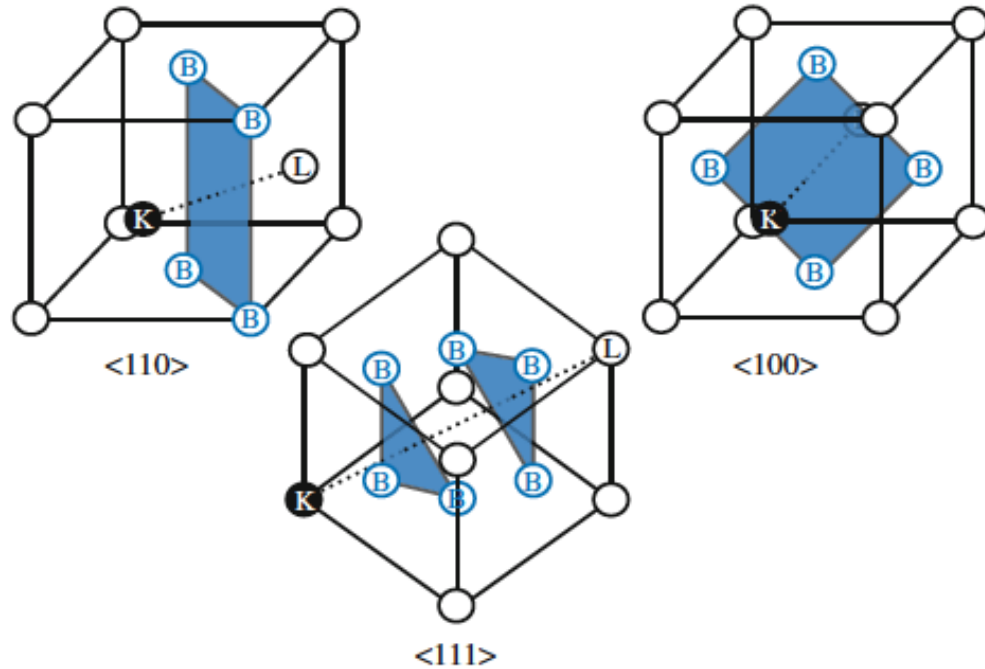


# Effect of crystallinity on $E_d$



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

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# 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!*

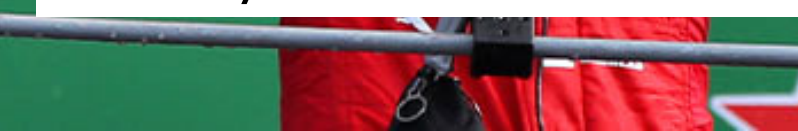
Metal	Lattice (c/a)	$E_{d,min}$ (eV)	$E_d$ (eV)
Al	fcc	16	25
Ti	hcp (1.59)	19	30
V	bcc		40
Cr	bcc	28	40
Mn	bcc	--	40
Fe	bcc	20	40
Co	fcc	22	40
Ni	fcc	23	40
Cu	fcc	19	30
Zr	hcp	21	40
Nb	bcc	36	60
Mo	bcc	33	60
Ta	bcc	34	90
W	bcc	40	90
Pb	fcc	14	25
Stainless Steel	fcc		40







The “Monza Curse” is an ongoing curse that dictates that the P1 finisher of the Italian Grand Prix will end the race the following year in a did not finish or DNF. According to this curse, who will DNF at next years race?



# The Kinchin Pease (K-P) Approach:

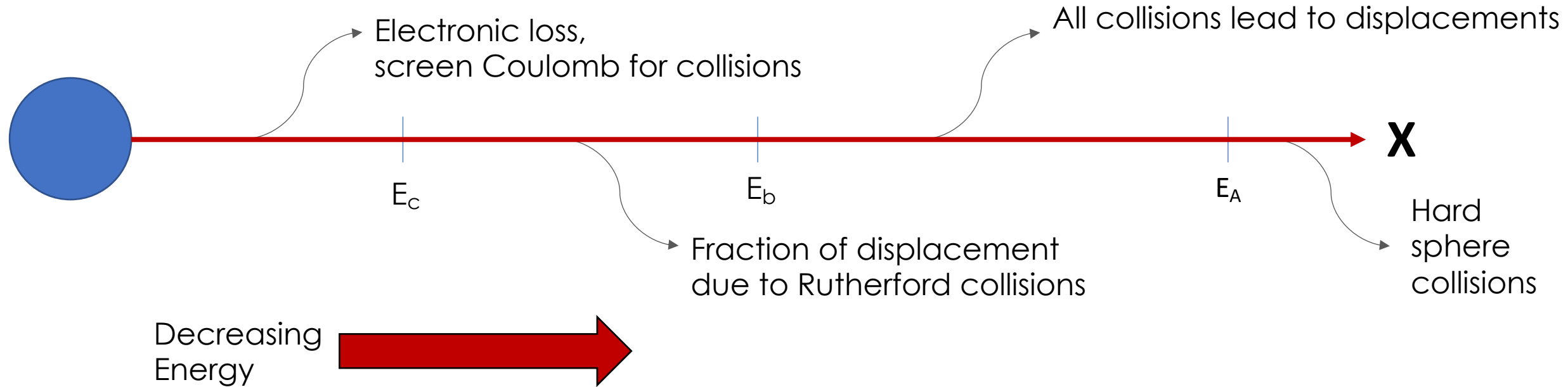
1. An atom is ejected from its lattice site if it receives kinetic energy greater than  $E_d$
2. The moving atom will stay behind on the lattice site of the struck atom if the latter receives energy greater than  $E_d$  while the former is left with energy less than  $E_d$
3. Cascades are created by 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

# 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:

$$v(E_i) = v(E_i - T) + v(T)$$

- 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:

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

- Which yields:

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

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



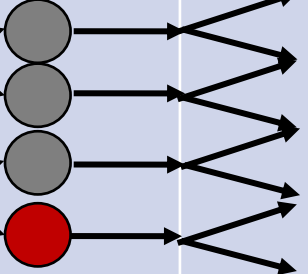
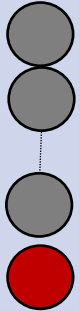
$$E_i \frac{dv}{dE_i} = v \Rightarrow v = \frac{E_i}{2E_d}, \text{ for } 2E_d < E_i < E_c$$





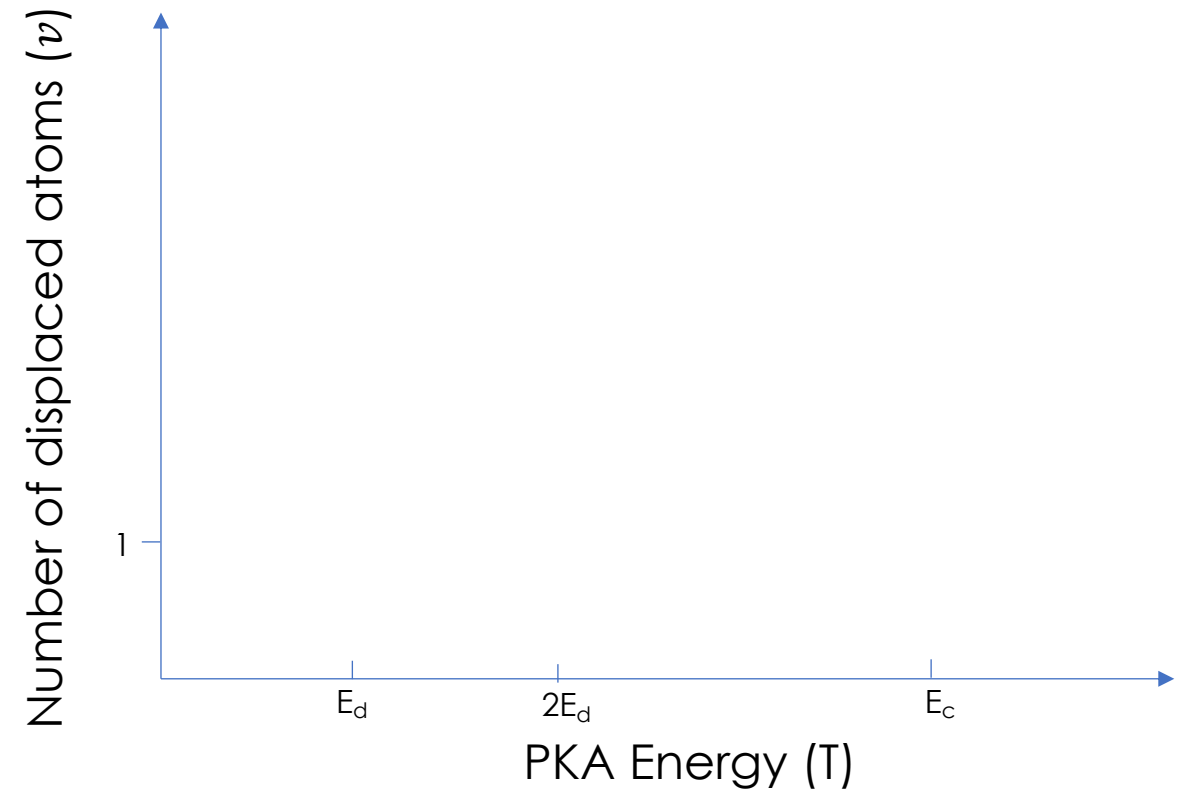
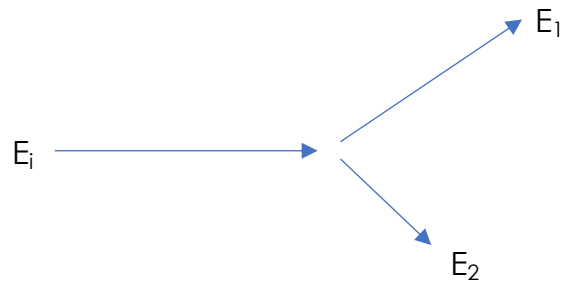
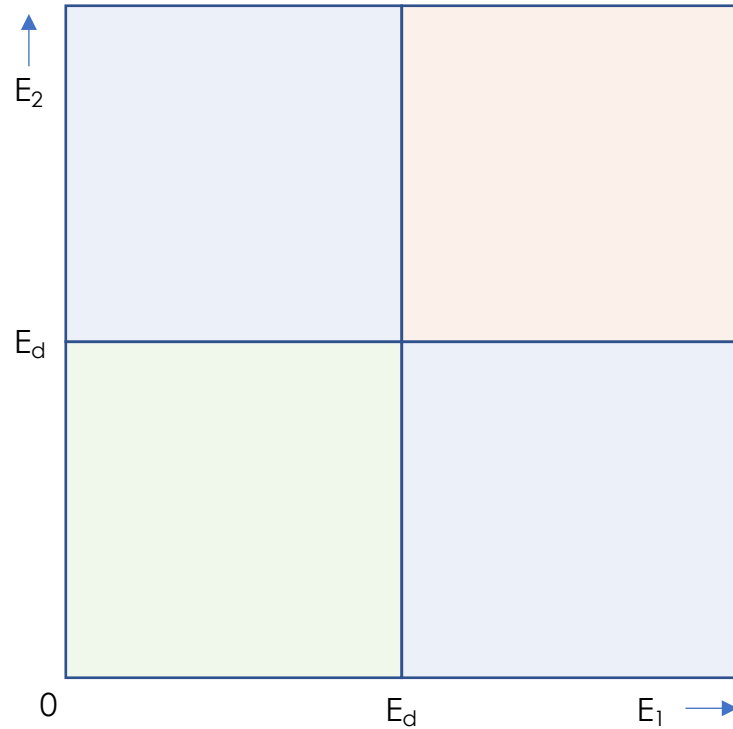
# Schematic for the Kinchin Pease (K-P) Approach:

- 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	$E_i$	$\frac{E_i}{2^N}$	$\frac{E_i}{2^N}$		$\frac{E_i}{2^N}$		$2E_d$
Number of displaced atoms	1	2	4		$2^N$		$\frac{E_i}{2E_d}$

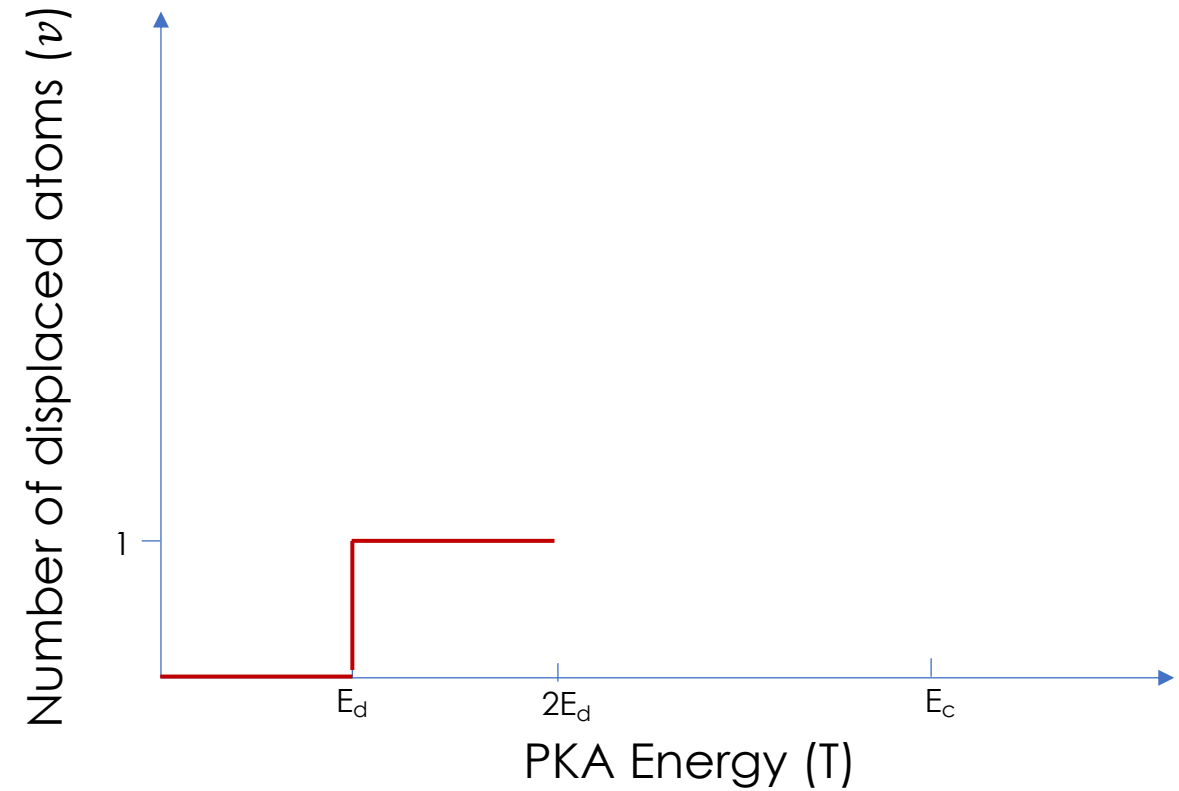


# The Kinchin Pease Approach:





# The Kinchin Pease Approach:



# Example calculation...

Assume a pure piece of BCC iron is irradiated in a reactor with a monoenergetic flux of  $5 \times 10^{13} \text{ cm}^{-2}/\text{s}$  1 MeV neutrons. Calculate the time it takes to reach 1 dpa in the iron sample.

# Example calculation...

# 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. 30	1	<a href="#">Introduction</a>	<a href="#">Notes</a> / <a href="#">Recording</a>	-	-
Thursday	Sept. 1	2	<a href="#">Basic particle interactions</a>	<a href="#">Notes</a> / <a href="#">Recording</a>	-	<a href="#">Alt. basic particle derivation</a>
Tuesday	Sept. 6	3	<a href="#">Collision Kinematics</a>	<a href="#">Notes</a> / <a href="#">Recording</a>		<a href="#">Collision Derivation</a>
Thursday	Sept. 8	4	<a href="#">Interatomic Potentials &amp; Cross Sections</a>	<a href="#">Notes</a> / <a href="#">Recording</a>	<a href="#">PS#1</a>	<a href="#">Flux/Fluence/Cross-sections/Energy transfer quick review</a>
Tuesday	Sept. 13	5	<a href="#">Simple Disp. Theory</a>		-	<a href="#">Displacement Integrals / Versions</a>
Thursday	Sept. 15	6	<a href="#">Energy loss &amp; K-P modifications</a>		-	
Tuesday	Sept. 20	-	<a href="#">Focus, Channel, Range</a>	-	PS1 due	-
Thursday	Sept. 22	7	<i>No lecture - Prof. Field out of town</i>			
Tuesday	Sept. 27	8	<a href="#">Damage Cascades</a>		PS#2	<a href="#">Arc-dpa Paper</a>



# Brain storming

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



# Summary so far

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

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

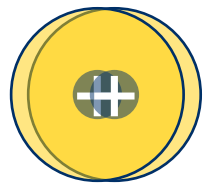
Task 1: Determine the energy transferred to the PKA:

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

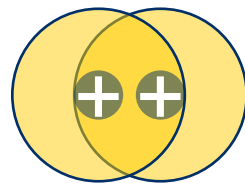
Task 2: Determine the scattering angle based on the impact parameter:

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

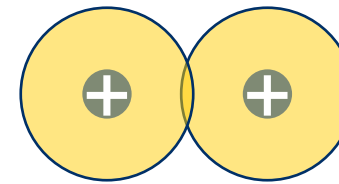
Task 3: Described  $V(r)$  based on the distance of closest approach



= R < K-shell radius  
(Coulomb)



= K-shell < R <  $a_0$   
(Screened Coulomb)

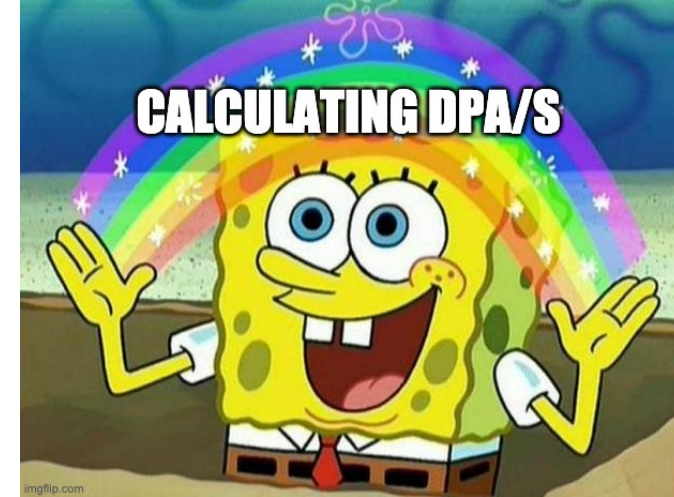


= < R < Lattice Constant  
(Born-Mayer)

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

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

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





Questions?

