Displacement Theory

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HW due next Tuesday!

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Reminder!

- 1 student has now done the Week 2 Knowledge Check (as of 8:42 am this morning)
- Problem Set 1 released, due next Tuesday
  - Look at it before next lecture so we can discuss any questions

NERS521 Radiation Materials Science: I

Fall 2025

Problem Set #1

Due Tuesday 9/16

Problem 1 (4 points)

A 2.0 MeV alpha particle (He ion) strikes a stationary Silicon (Si) atom in a head-on elastic collision. Given the following information:

Constant	Value
M_{alpha}	$4.00\ Da$
E_{alpha}	2.0 MeV
M_{Al}	$28.09\ Da$
$1\ Da$	$\frac{931.5\ MeV}{c^2}$
c	$3 \times 10^8\ m/s$

- The maximum energy transferred $\hat{T}$ to the Si atom
- The energy remaining in the alpha particle after the initial collision (E_f)
- The velocity of the Si atom (ν_{Si}) after the collision
- Redetermine the total energy transferred if the scattering angle was $\phi = 60^\circ$

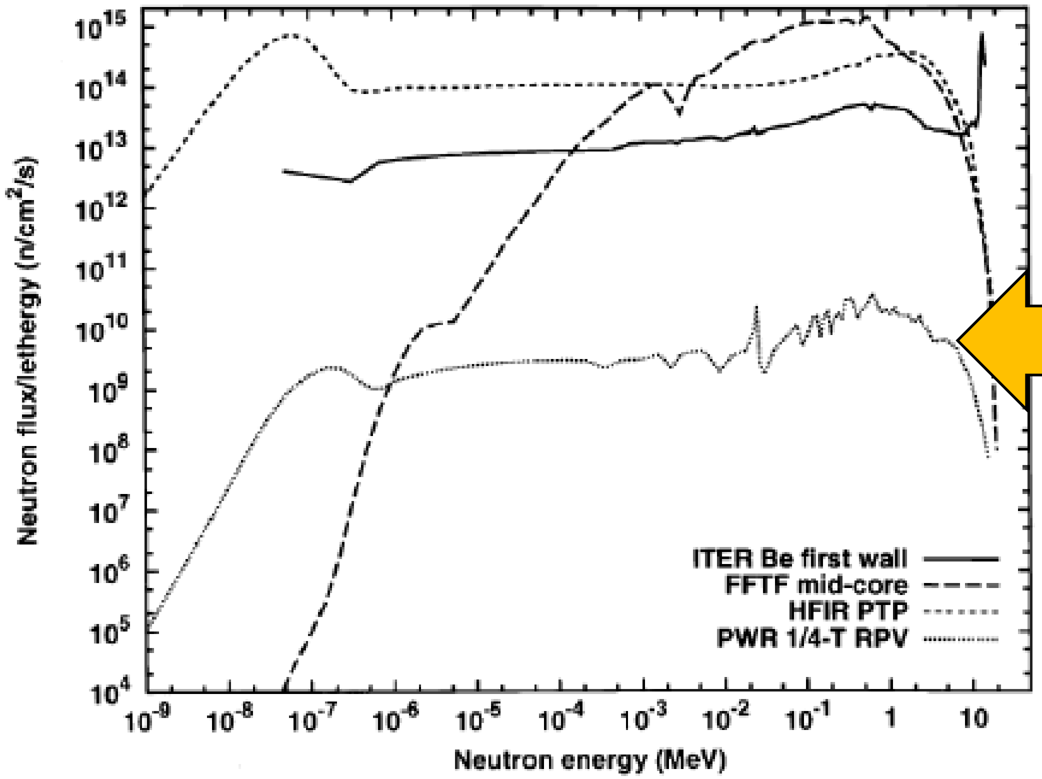
Problem 2 (2.5 points)

Assume a collision occurs between a light ion ($m_1 < 4$) that has an energy above 1 MeV where the Coulomb potential,

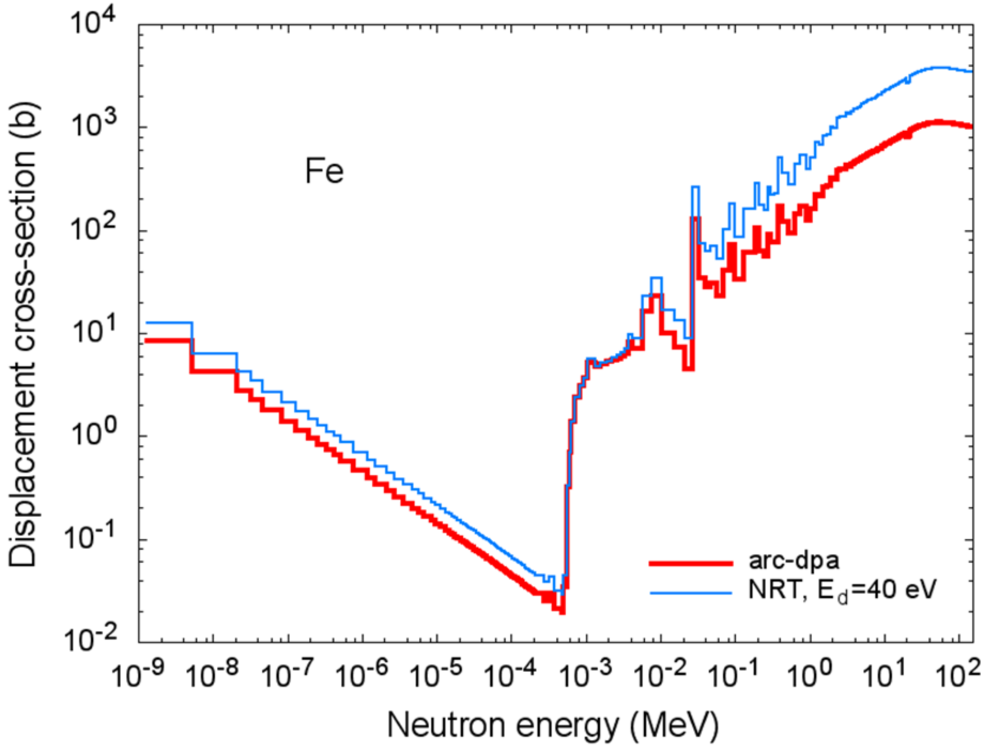
$$V(r) = \frac{Z_1 Z_2 \epsilon^2}{r}$$

is then a valid assumption. Using the relationship derived in class (or Eq. 1.77 in Was, 2nd edition) between impact parameter (b), and the interatomic potential ($V(r)$), derive the the equation governing the distance of closest approach during a head-on collision, $\rho(b = 0)$.

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)

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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) $a/5 \le \rho \le 5a$	$\sigma_s(E_i, T) = \frac{\pi^2 a^2 E_a \gamma^{1/2}}{8 E_i^{1/2} T^{3/2}}$	(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:

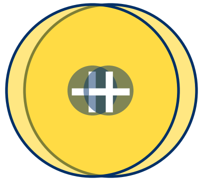
Task 1: Determine the ene

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

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 radiu
(Coulomb)

= <R<Lattice Constant
(Born-Mayer)

Task 4: Combine Tasks 1-3
cross-sections

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

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

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Outline

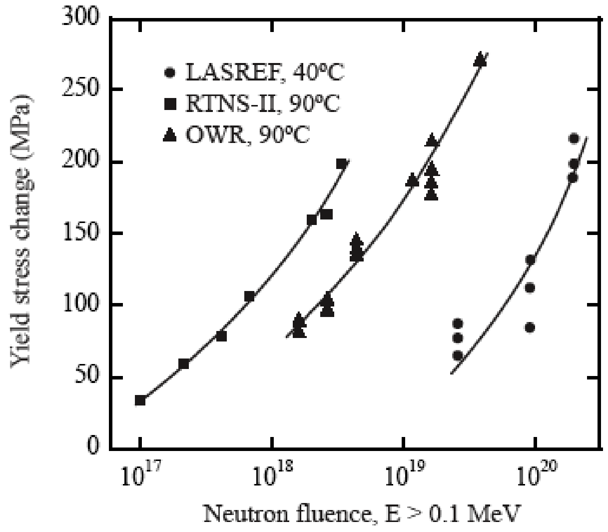
<u>Displacement theory:</u>

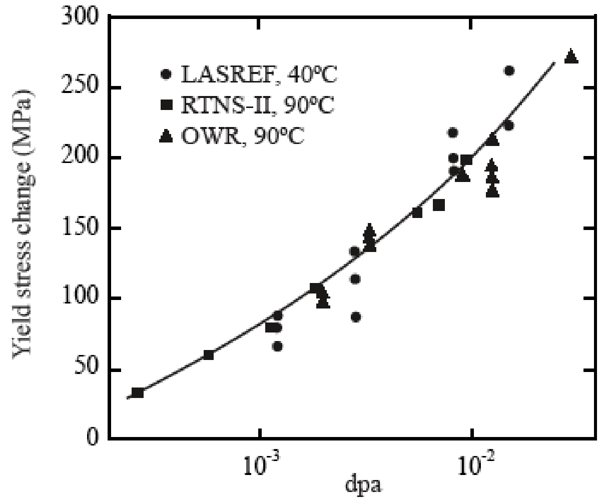
- Governing equations
- Determine E_d
- Kinchin-Pease Model
- Example!

Quick Reminder Sheet Available

<u>Goal:</u> Find the displacements per atom for a given energy spectrum and material system

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.

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

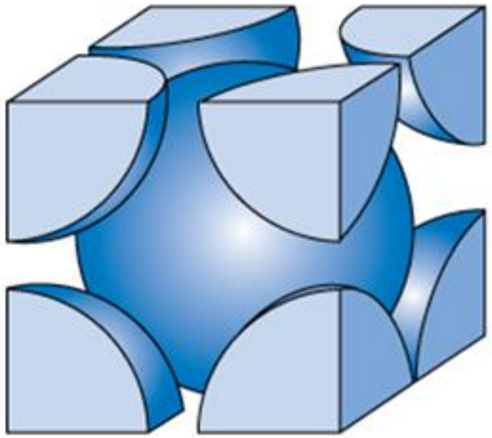
$\sigma_D(E_i)$ = energy dependent displacement cross section (cm^2)

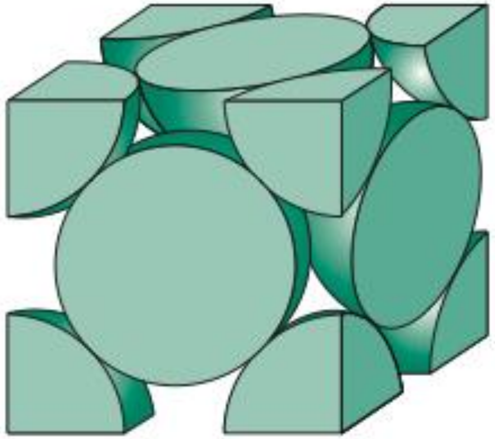
N = lattice atom density ($\#/cm^3$)

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

Cover K_o

Quick diversion on N…





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

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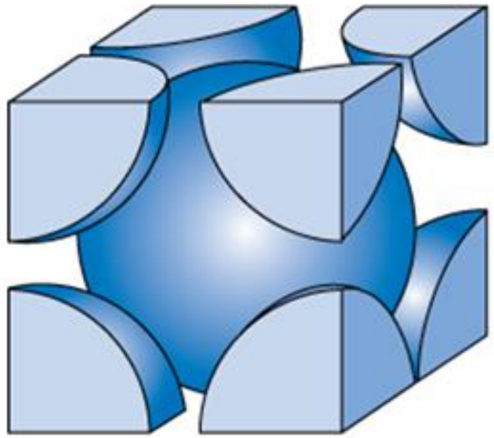
Quick diversion on N…



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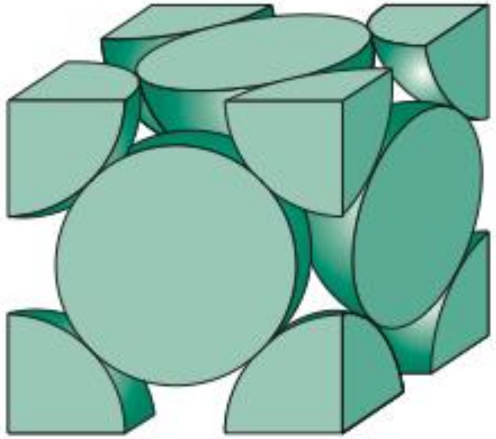


The displacement cross section

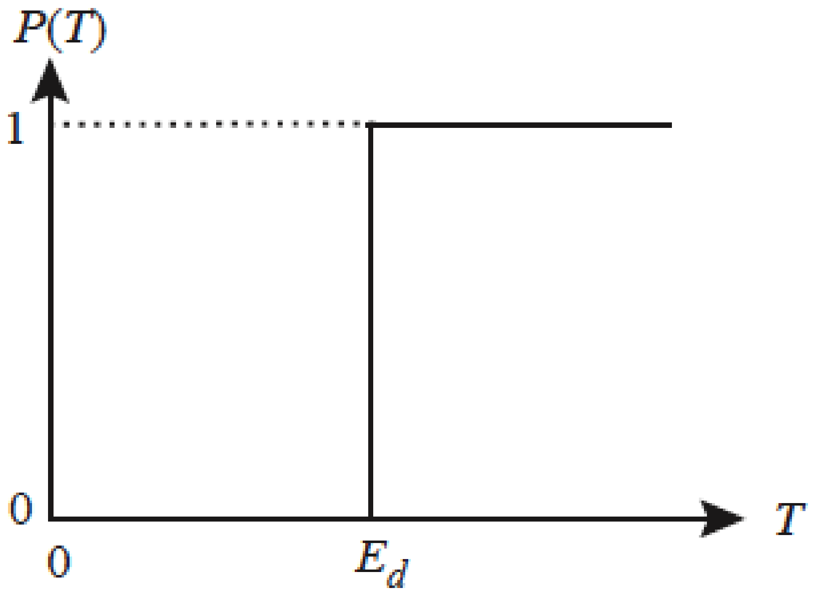
$$\sigma_D(E_i) = \int_{\check{T}}^{\hat{T}} \sigma_s(E_i, T)\, \upsilon(T)\, dT$$

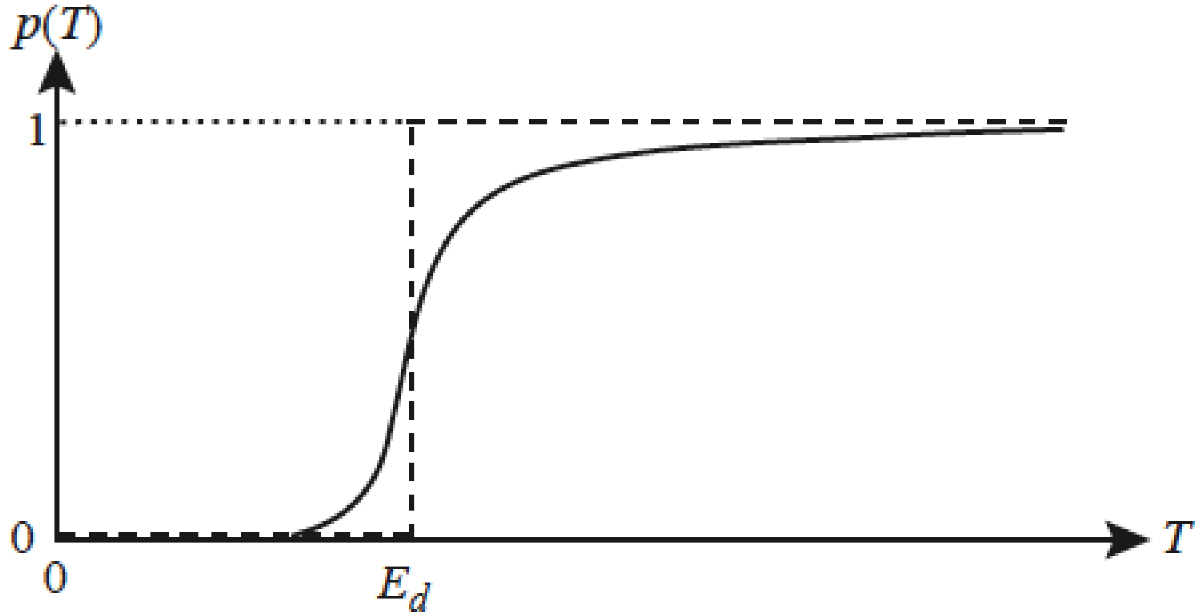
$\sigma_s(E_i, T)$ is the probability that a particle of energy E_i will impart a recoil energy of T to a struck lattice atom (last lecture!)

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

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

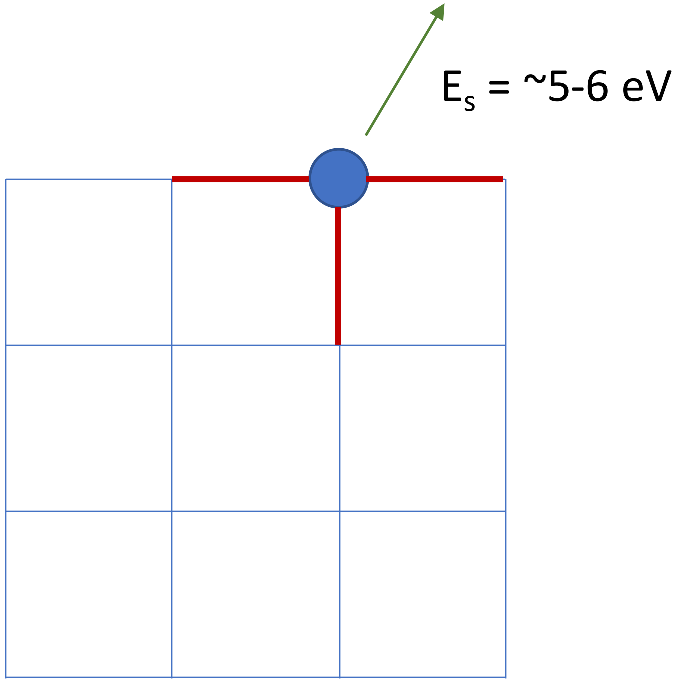
Introducing the concept of displacement energy



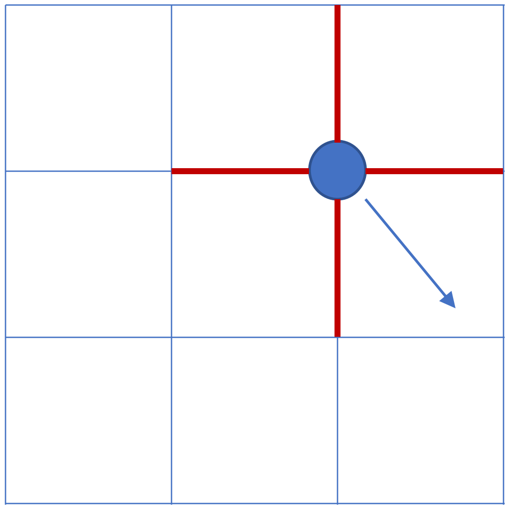


- Displacement energy, E_d:
  - If $T > E_d$ a displacement will occur
  - If $T < E_d$ energy transfer will cause an oscillation about the lattice site

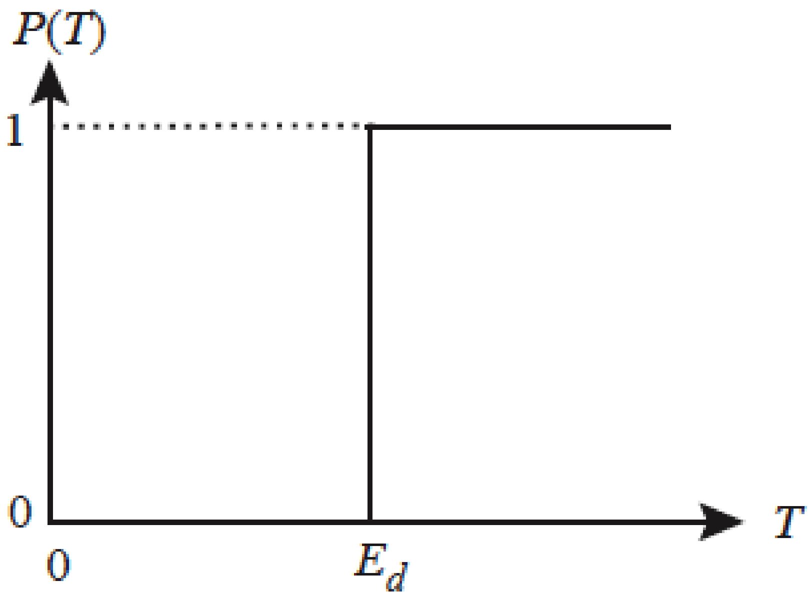
Simple energy evaluation for E_d (by Setiz)



Energy associated with sublimation

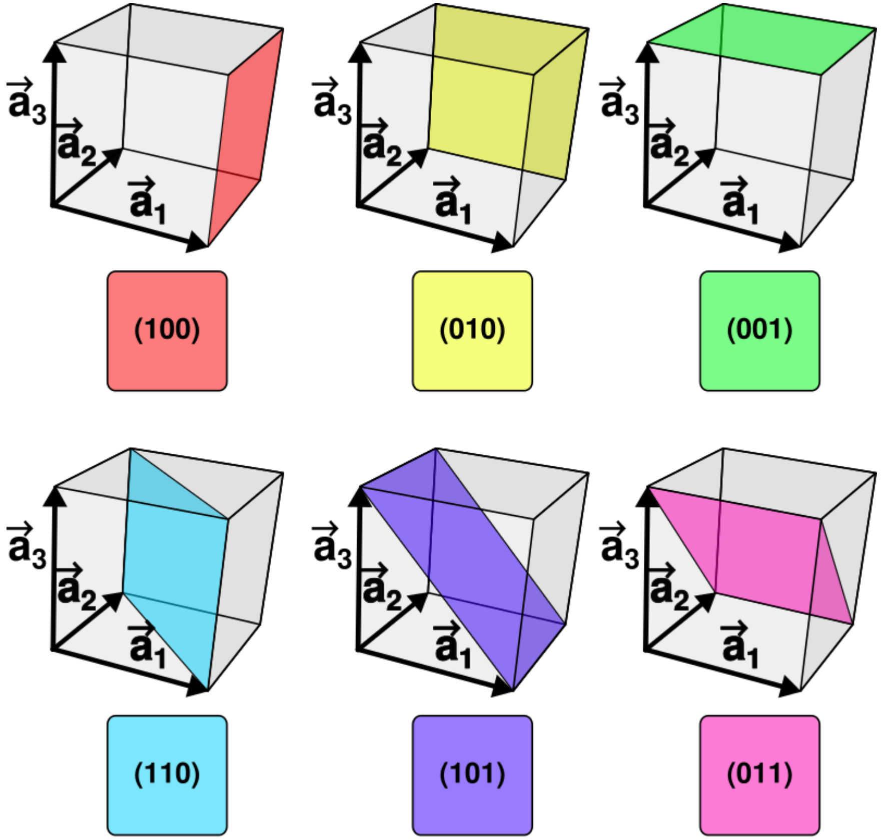


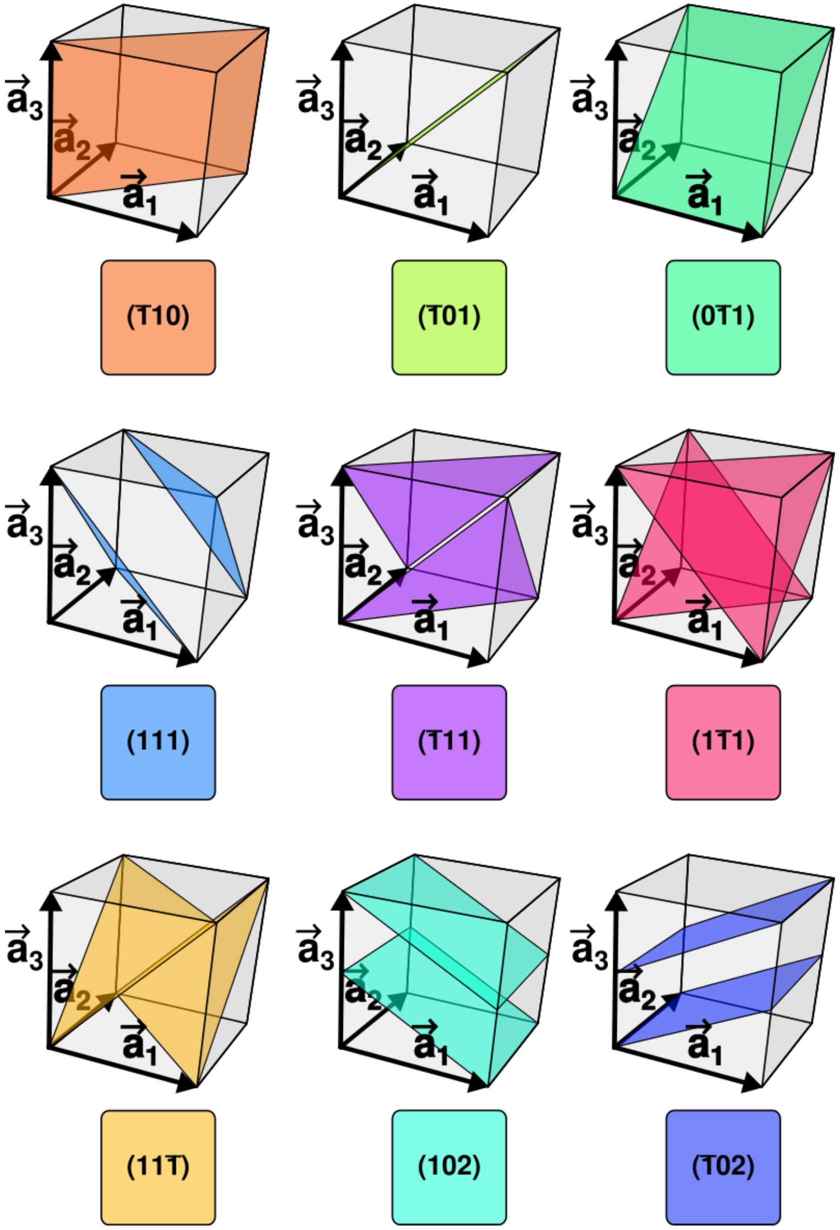
Energy associated with atom displacement



Bond Energy = ~1 eV

Miller indices





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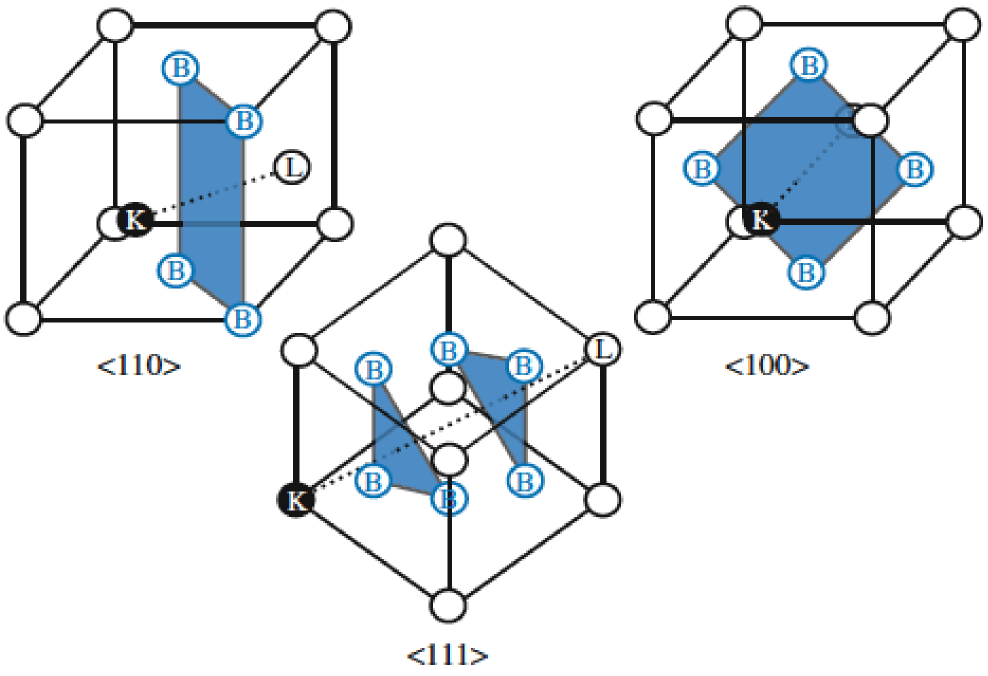
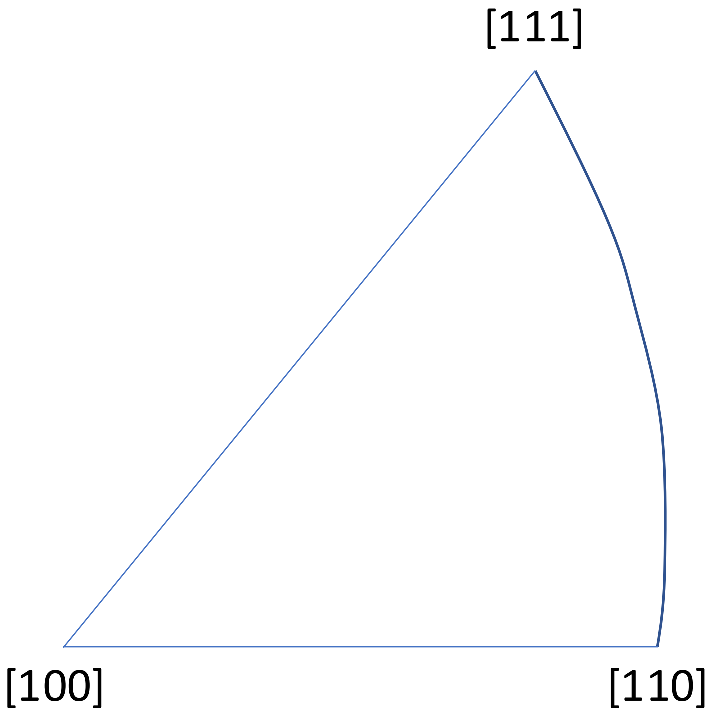
Effect of crystallinity on E_d





- 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

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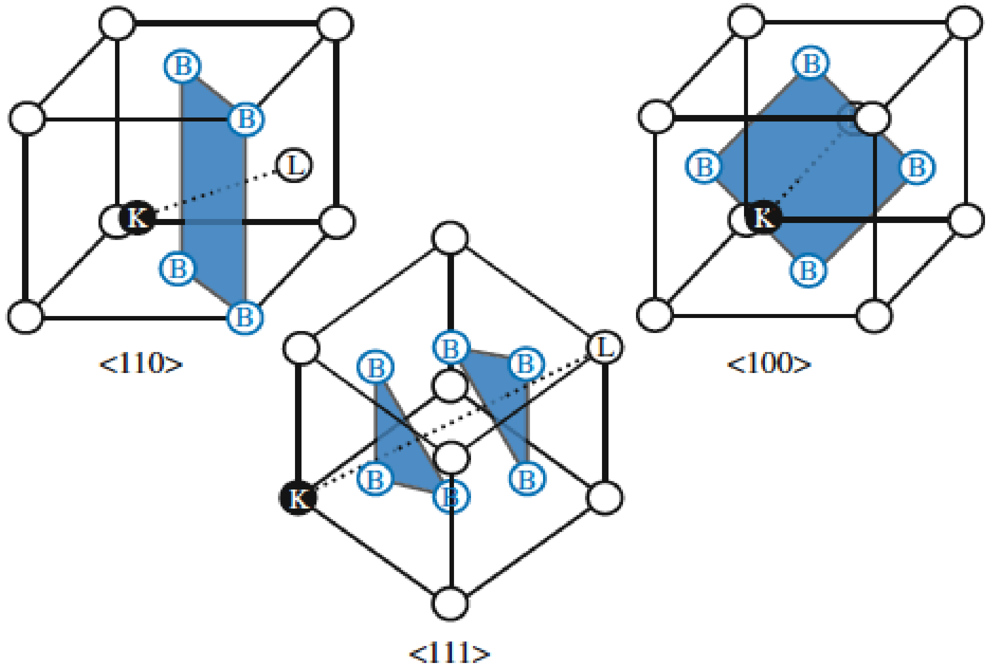
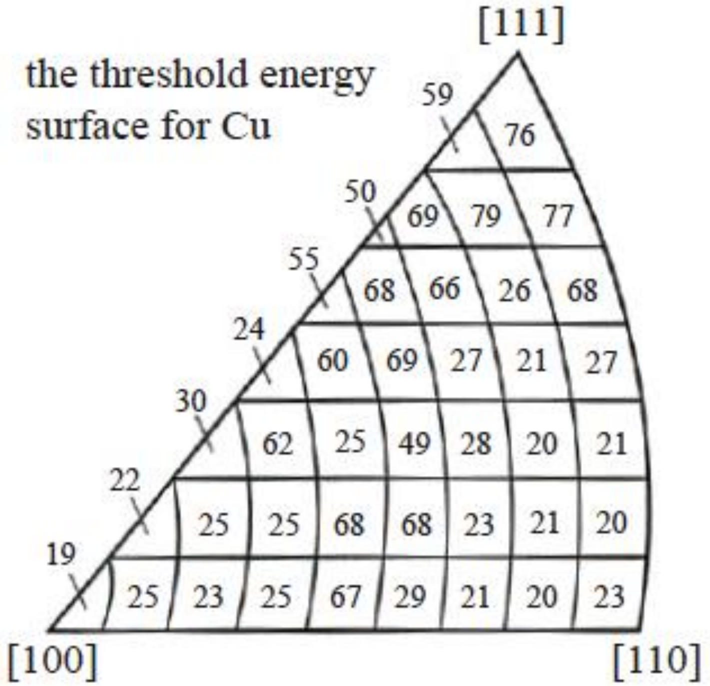
Effect of crystallinity on E_d





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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

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From 1982 to 1988, Formula 1 cars navigated a notoriously bumpy and demanding street circuit through downtown Detroit, weaving around the iconic Renaissance Center. The great Ayrton Senna famously won the final three events held on this layout. To the thousandth of a mile, what was the official length of this original Detroit Grand Prix track?

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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

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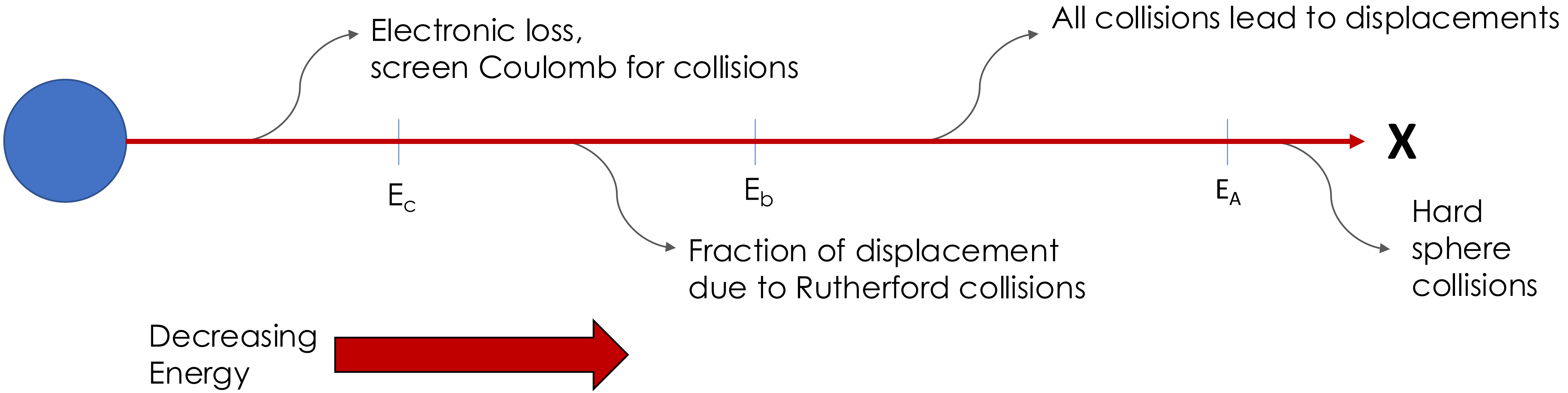
Regimes of PKA energy



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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:

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

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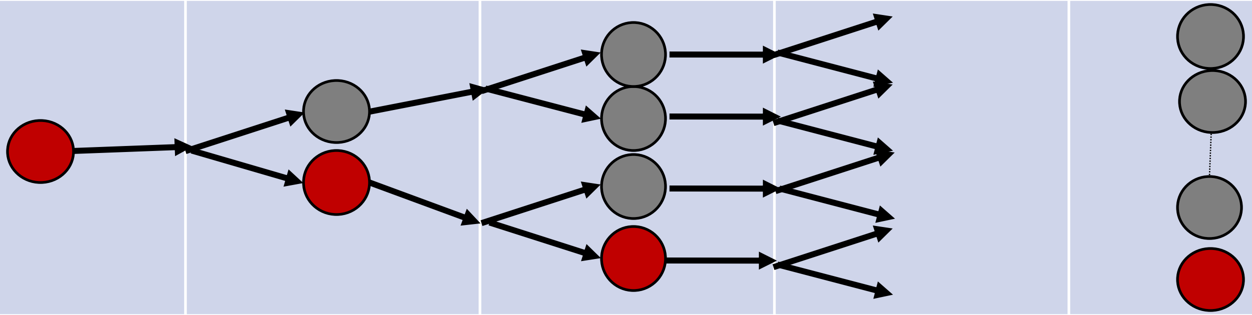
Schematic for the Kinchin Pease (K-P) Approach:

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

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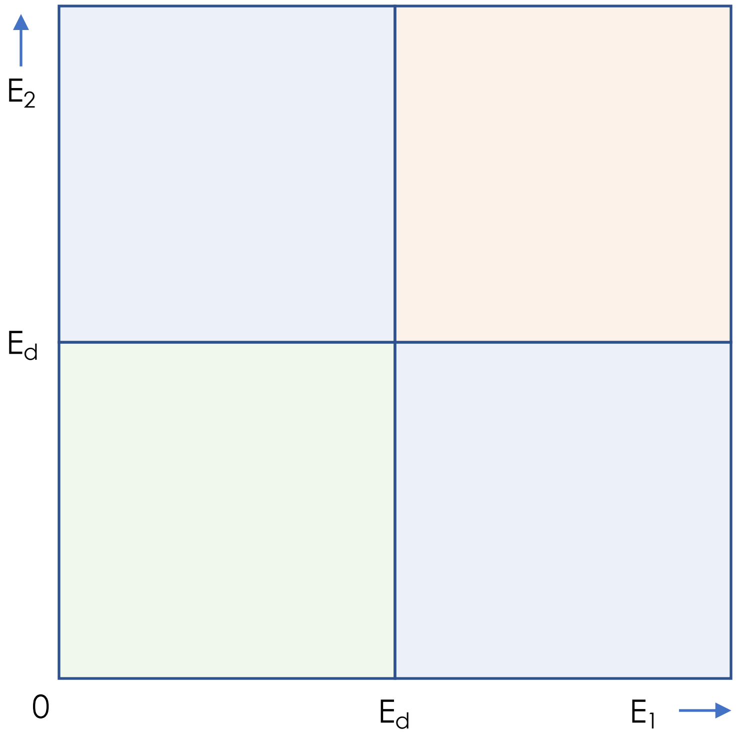
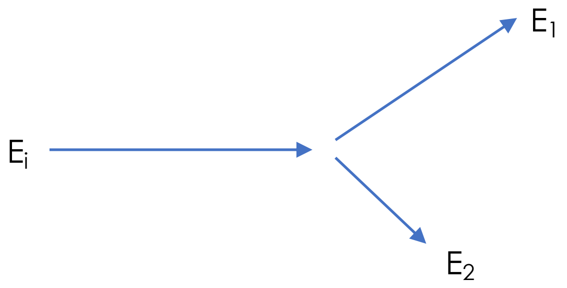
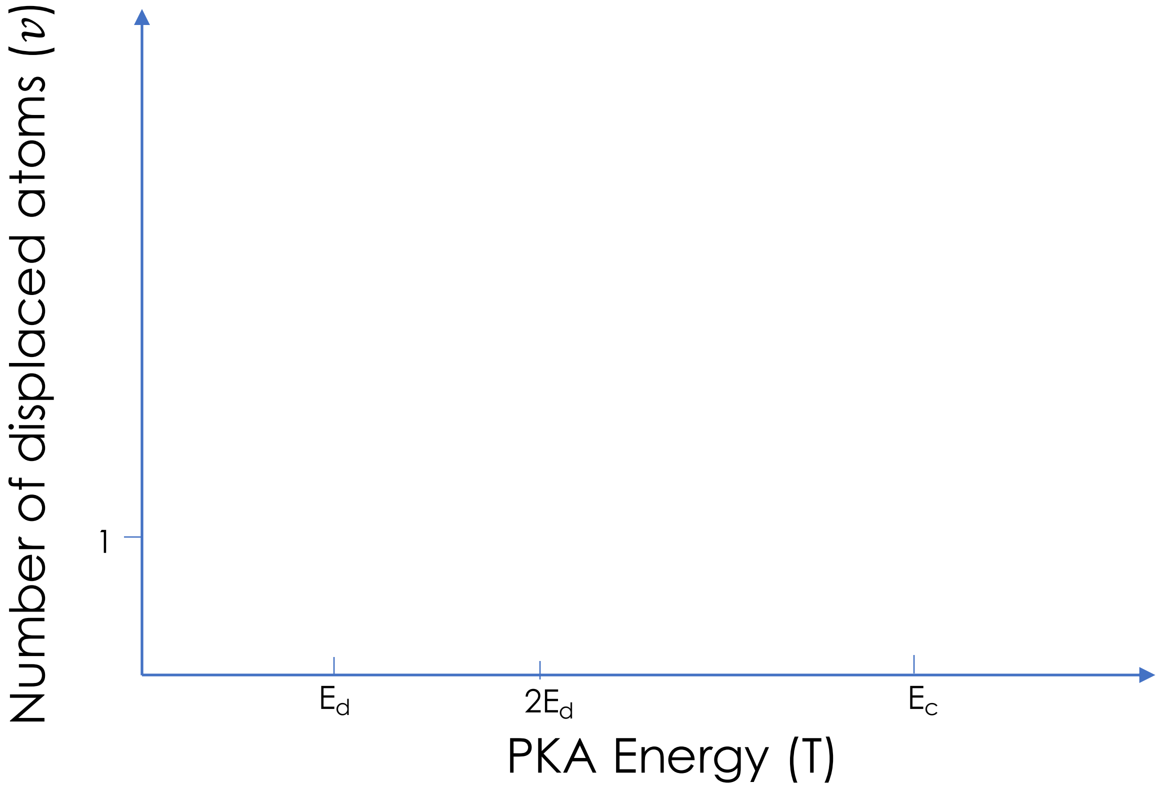
The Kinchin Pease Approach:







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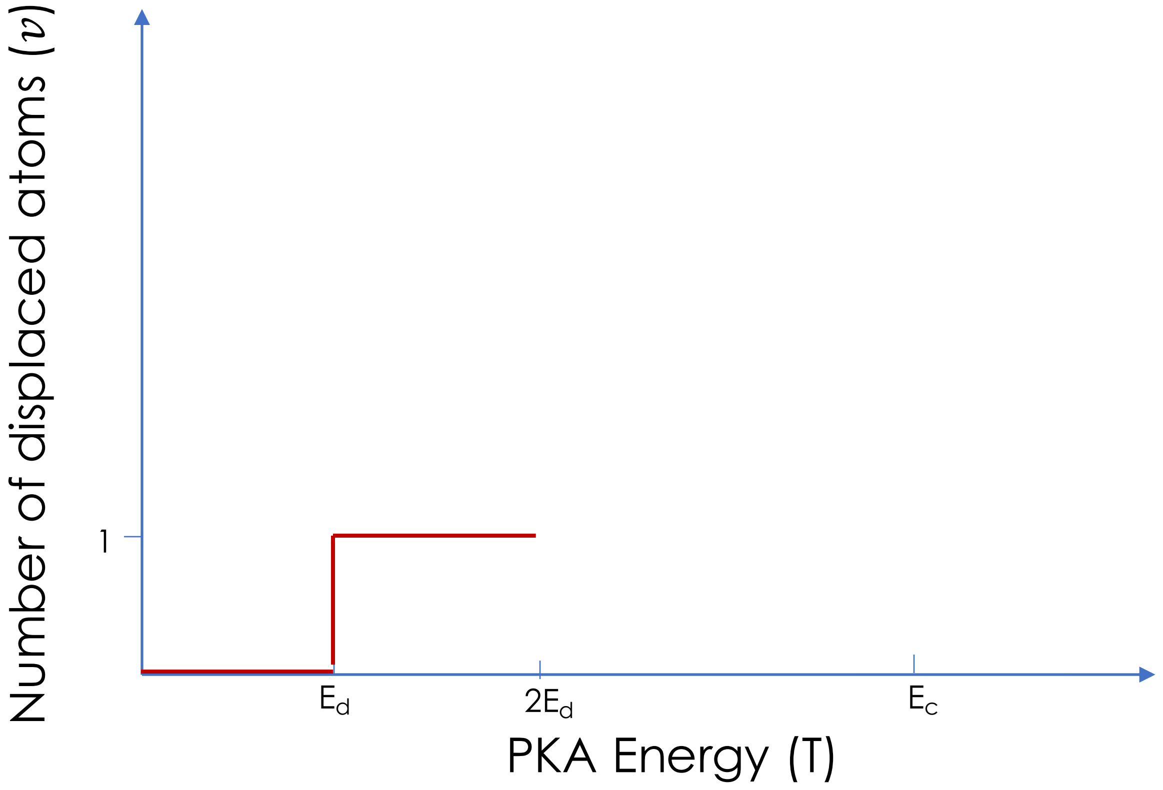
The Kinchin Pease Approach:



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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.

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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

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Example calculation…

Brain storming

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

Summary so far

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

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

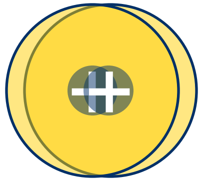
  Task 1: Determine the energy transferred to the PKA:

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

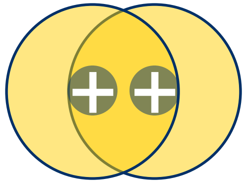
  Task 2: Determine the scattering angle based on the impact parameter:

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

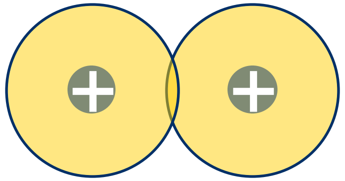
  Task 3: Described V(r) based on the distance of closest approach



= R<K-shell radius (Coulomb)



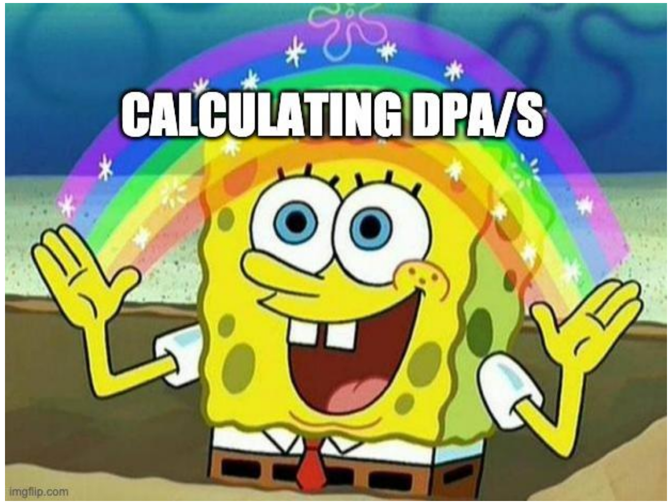
= K-shell<R<a_o (Screened Coulomb)



= <R<Lattice Constant (Born-Mayer)

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

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



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Questions?