

Potentials and Cross Sections

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Simple Recap from Last Lecture:



*Size of visual indicates amount of charge/interaction potential NOT size of atom/ion

Importance of Interatomic Potentials:

- Required to estimate the number of displaced atoms produced by a primary knock-on atom
- Needed to capture the physics of energy loss for a charged particle
- Used to determine the mean free paths for the displacement of atoms
- Used in the determination of focusing and channeling

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

There exists no single function that describes all interactions between atoms

The first part of this lecture will focus on some of the simpler functional forms for potential functions

Interactions between ions and atoms requires use of interatomic potentials

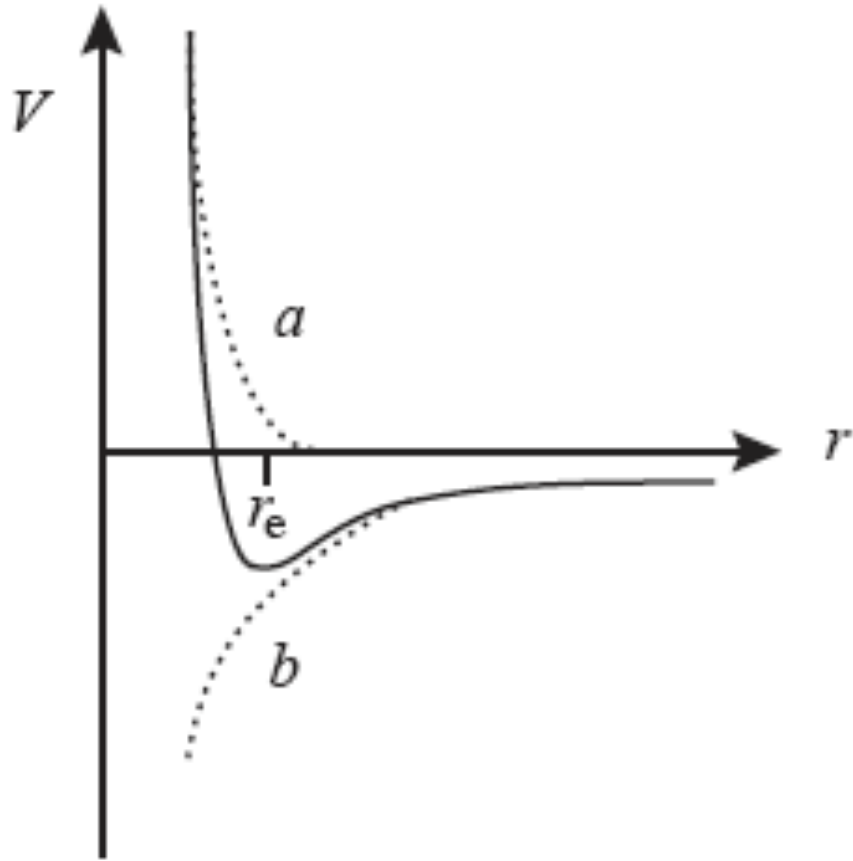


Figure 1.8 in Was, pg. 20

Interactions between ions and atoms requires use of interatomic potentials

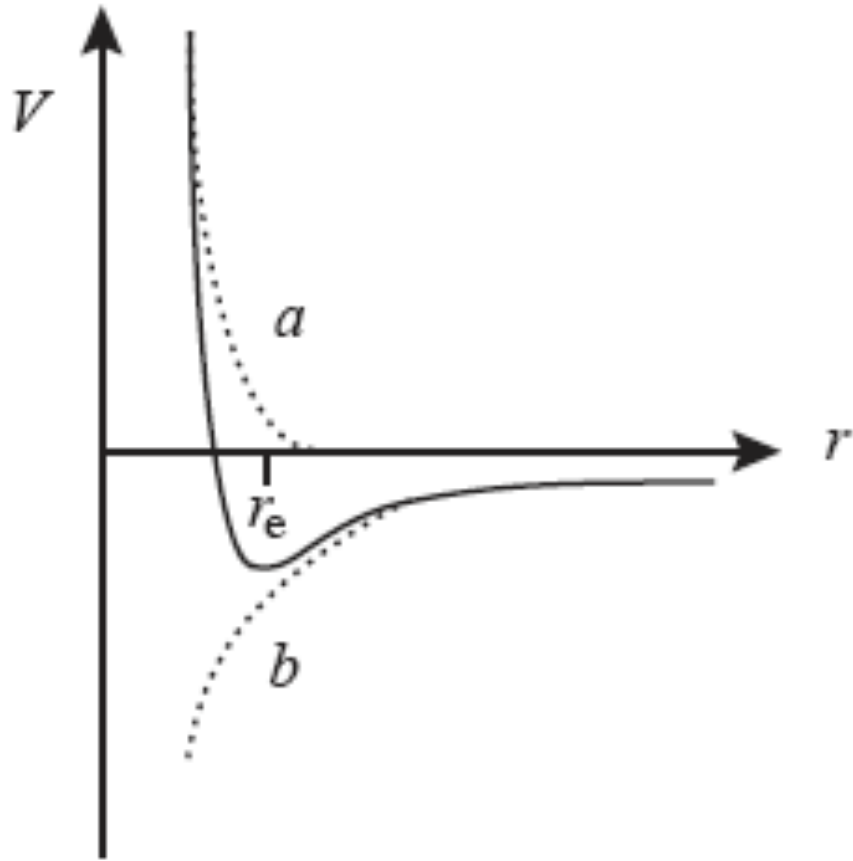


Figure 1.8 in Was, pg. 20

Interactions between ions and atoms requires use of interatomic potentials

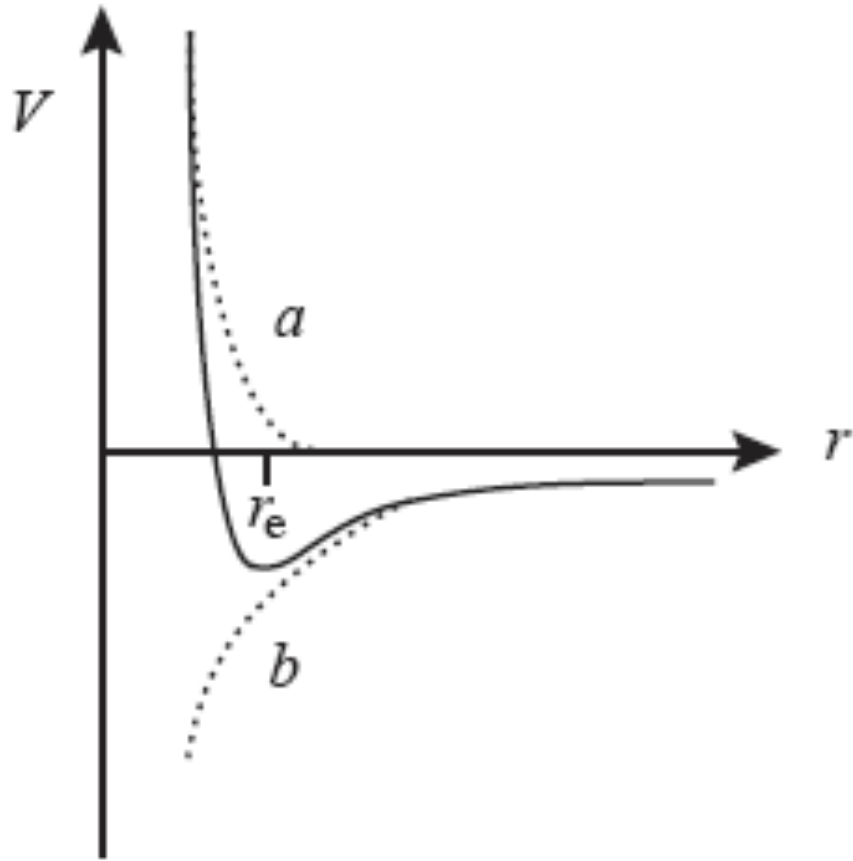
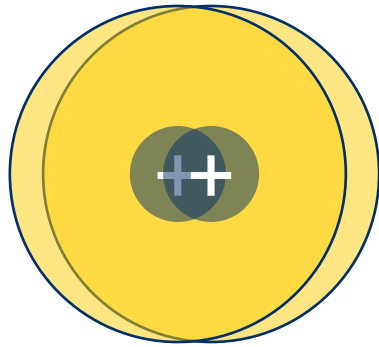
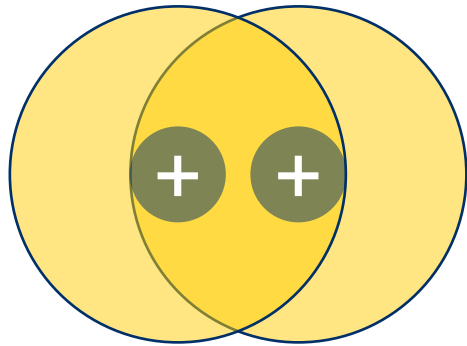


Figure 1.8 in Was, pg. 20

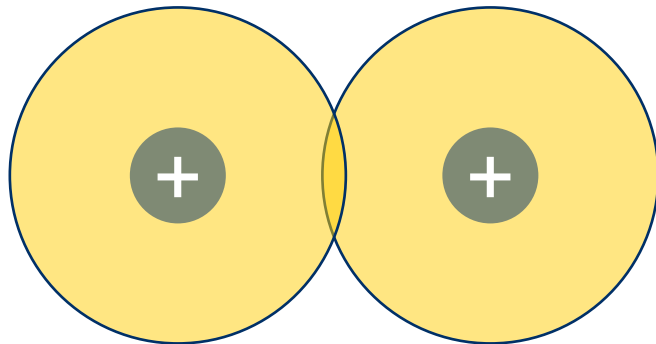
A visual of what this looks like...



$R < \text{K-shell radius}$
(Coulomb)



$\text{K-shell radius} < R < \text{Lattice Constant}$
(Screened Coulomb)



$R < \text{Lattice Constant}$
(Born-Mayer)

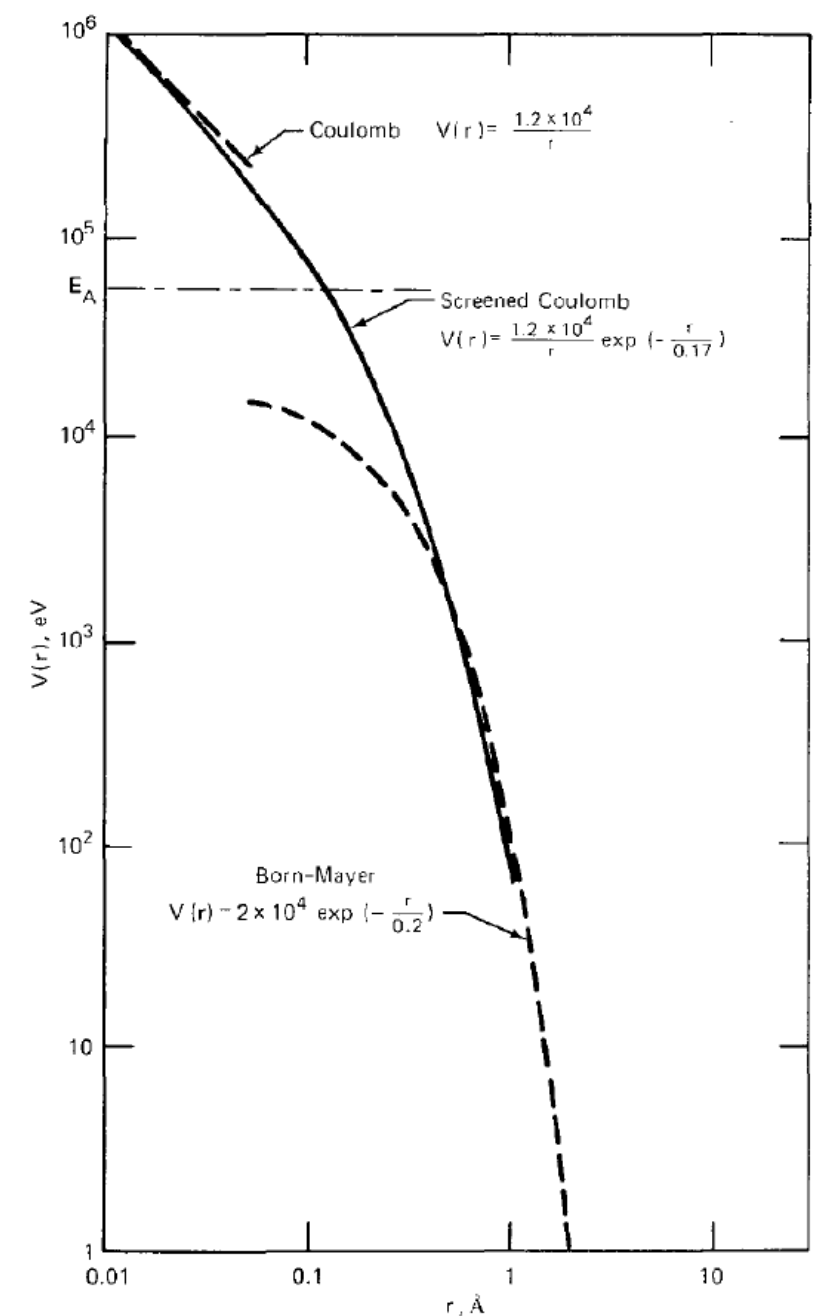
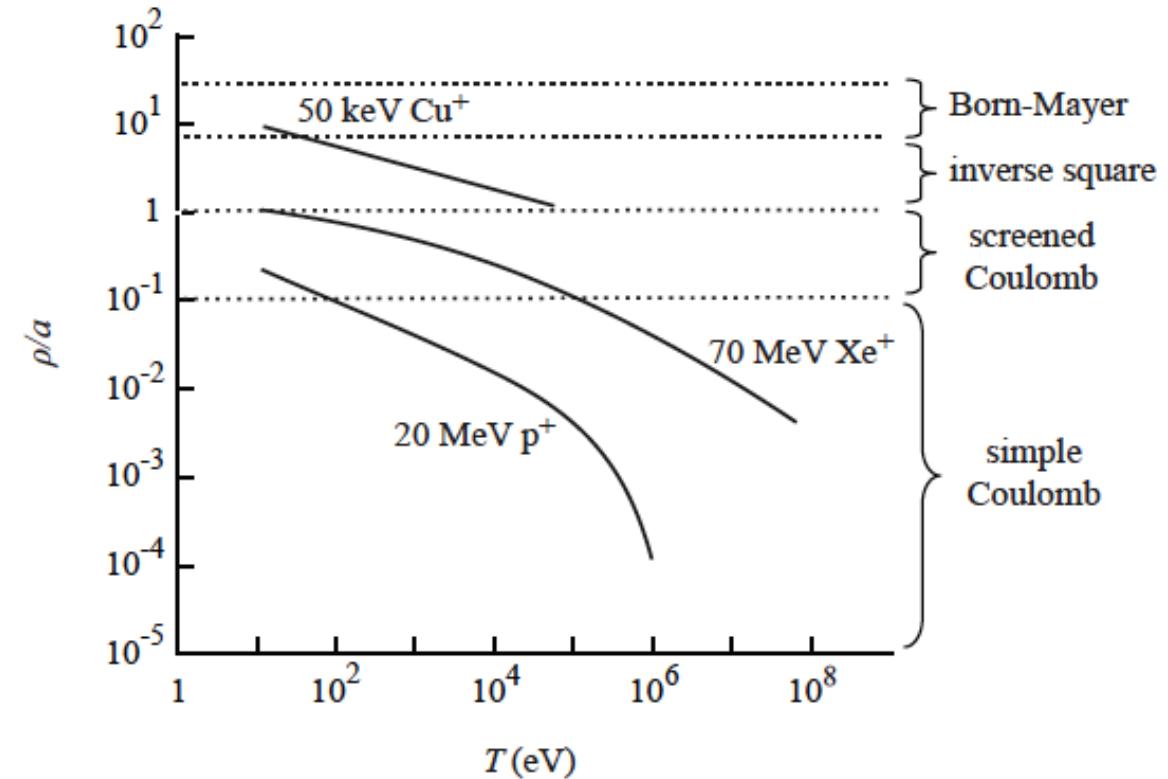


Fig. 17.5 Composite potential function for interaction between copper atoms.

Potential	Equation	Range of Applicability	Definitions	Eqn in text
Hard sphere	$0 \text{ for } r > r_0$ $\infty \text{ for } r < r_0$	$10^{-1} < T < 10^3 \text{ eV}$	r_0 = size of atom	(1.46)
Born-Mayer	$V(r) = A \exp(-r/B)$	$10^{-1} < T < 10^3 \text{ eV}$ $a_0 < r \leq r_e$	A, B determined from elastic moduli	(1.47)
Simple Coulomb	$\frac{Z_1 Z_2 \epsilon^2}{r}$	light ions of high energy $r \ll a_0$		(1.48)
Screened Coulomb	$\left(\frac{Z_1 Z_2 \epsilon^2}{r} \right) \exp(-r/a)$	Light ions $r < a_0$	a_o = Bohr radius a = screening radius	(1.49)
Brinkman I	$\frac{Z^2 \epsilon^2}{r} e^{(-r/a)} \left(1 - \frac{r}{2a} \right)$	$r < a$	$a \cong a_0 / Z^{1/3}$	(1.51)
Brinkman II	$\frac{A Z_1 Z_2 \epsilon^2 \exp(-Br)}{1 - \exp(-Ar)}$	$Z > 25$ $r < 0.7 r_e$	$A = \frac{0.95 \times 10^{-6}}{a_o} Z_{eff}^{7/2}$ $B = Z_{eff}^{1/3} / C a_o$ $C \cong 1.5$	(1.52)
Firsov	$\frac{Z_1 Z_2 \epsilon^2}{r} \chi \left[(Z_1^{1/2} + Z_2^{1/2})^{2/3} \frac{r}{a} \right]$	$r \leq a_0$	χ is screening function	(1.56)
TFD Two Center	$\frac{Z^2 \epsilon^2}{r} \chi \left(Z^{1/3} \frac{r}{a} \right) - \alpha Z + \bar{\Lambda}$	$r < r_b (3a_0)$	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)

Classification of Ions

- Type 1: Light energetic ions with $E_i > 1$ MeV
 - $\rho \ll a$ and Coulomb collision are dominant
- Type 2: Energetic heavy ions, $E_i > 10^2$ MeV, $M \sim 10^2$
 - $\rho \ll a$ for head-on collisions \rightarrow Coulomb potential
 - $\rho \sim a$ for glancing collisions \rightarrow Screened Coulomb
- Type 3: Low energy heavy ions, $E_i < 1$ MeV (e.g. from an ion accelerator or recoils from an earlier collision)
 - $a < \rho < 5a \rightarrow$ Inverse power potential or Brinkman potential (need to include screened Coulomb and B-M terms)



Summary

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

Task 1: Determine the energy transferred to the PKA:

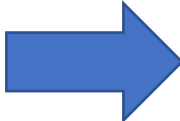
$$T = \frac{\gamma}{2} E_i (1 - \cos \phi) \text{ to get } \phi = f(T)$$

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 $V(r)$ to enable the calculation of cross sections

Rest of Lecture

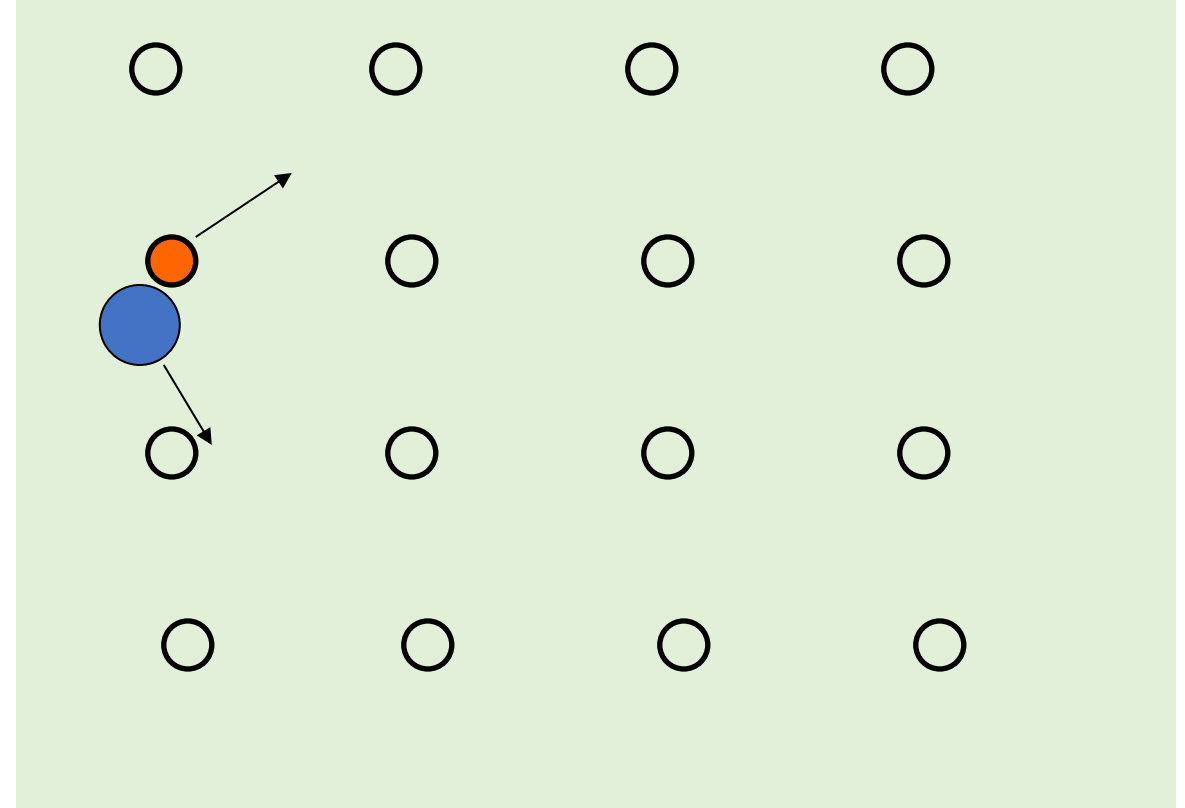
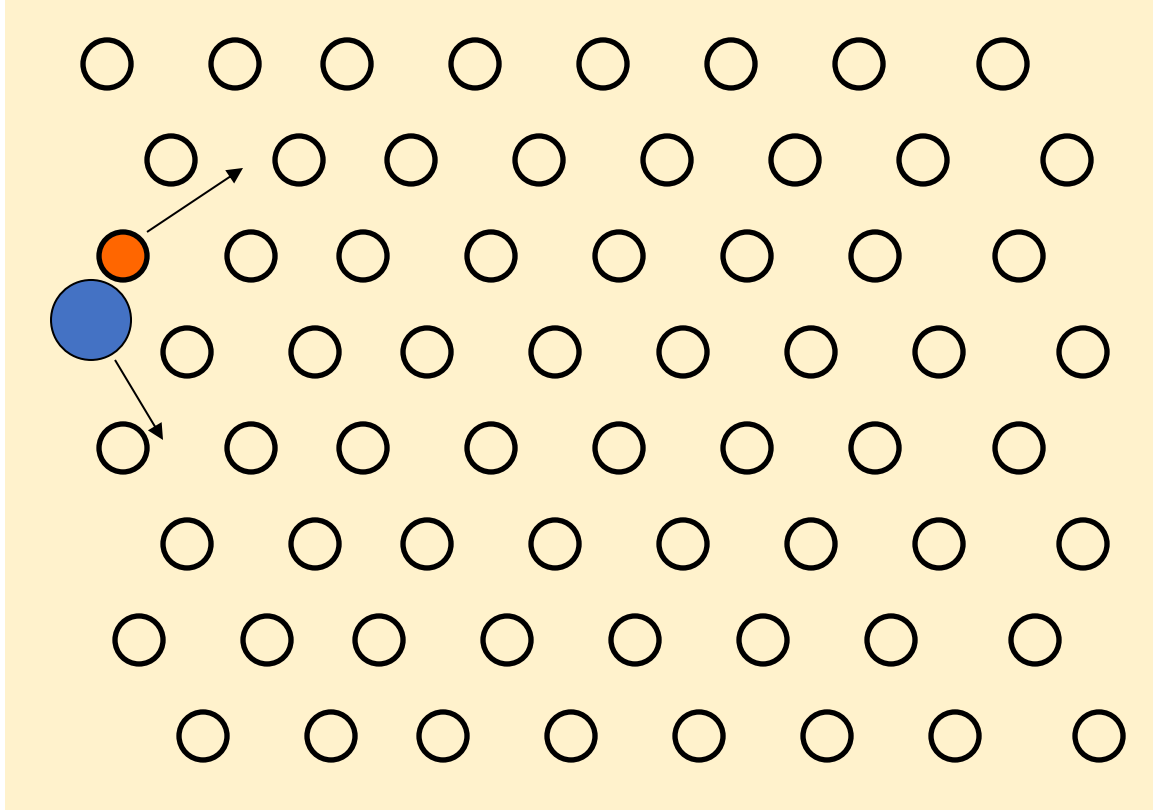


$\sigma_s(E_i, T) = 2\pi b \frac{db}{d\phi} \frac{d\phi}{dT}$



According to <https://ehlenbachscheese.com/> Wisconsin has the most licensed cheesemakers than any other state. How many licensed cheesemakers are in the state of Wisconsin

Simple thought experiment:



What material (yellow or green) has a higher probability of scattering the PKA?

Outline

Cross-Section:

- Definition
- Methods of determining σ_s
- Examples
- Mean kinetic energy

Goal: Find the energy transfer probability between two particles



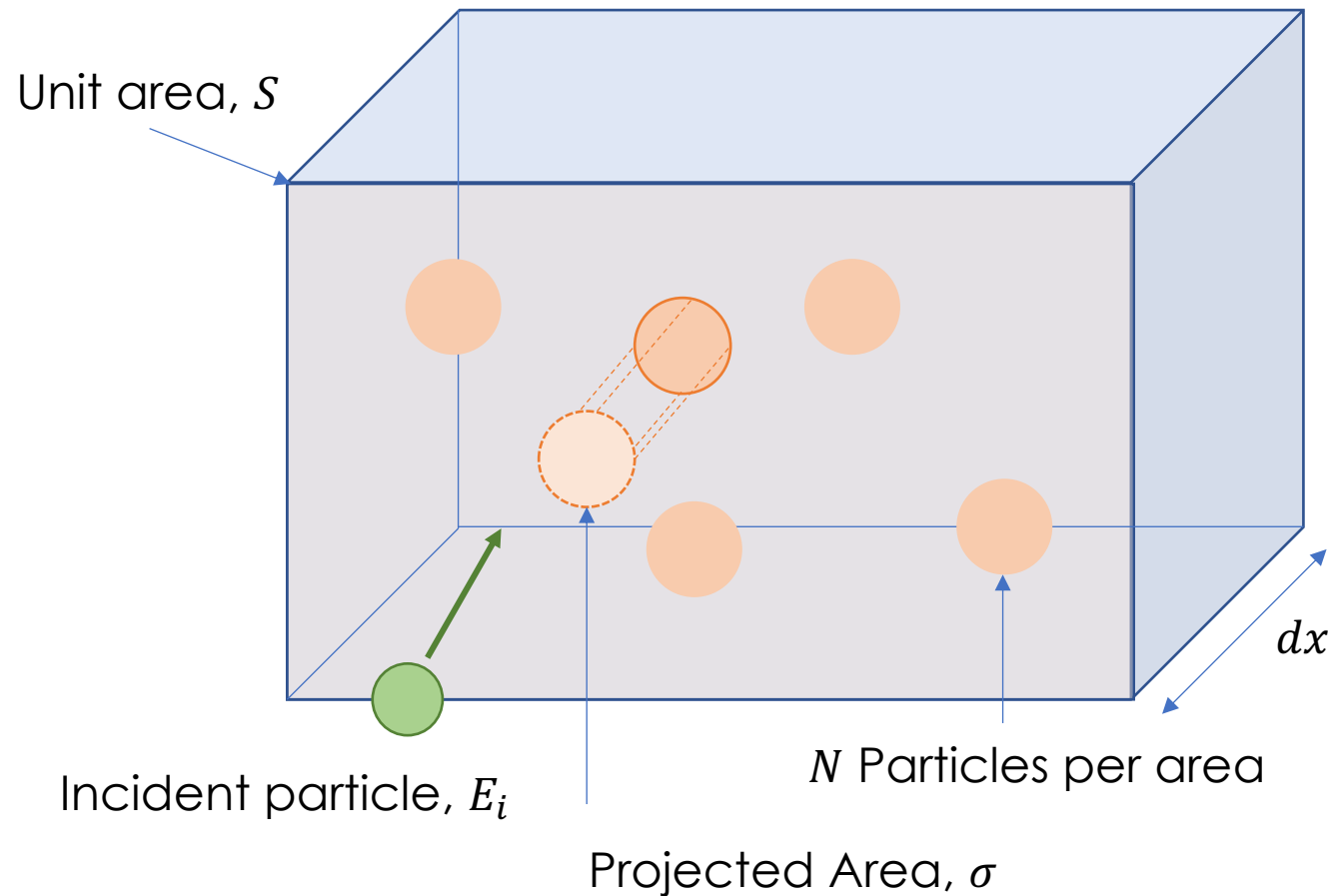
Quick Reminder Sheet:

<https://umich.instructure.com/courses/470114/pages/cross-section-conversions>



Definition, simple schematic, and maths

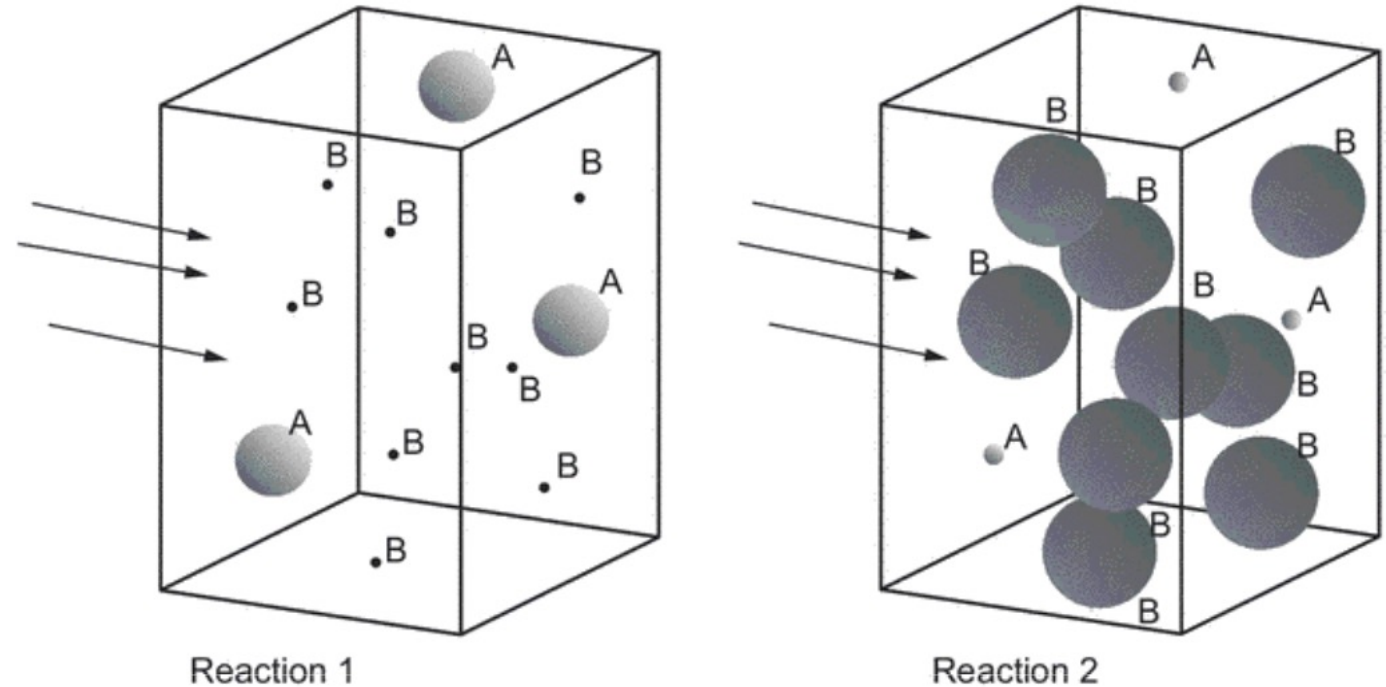
The probability of occurrence of a particular reaction between the atoms in the solid and the incident particle flux is represented by a **cross section**



Probability of a collision with a target atom is proportional to dx and N :

Cross section will depend on the reaction

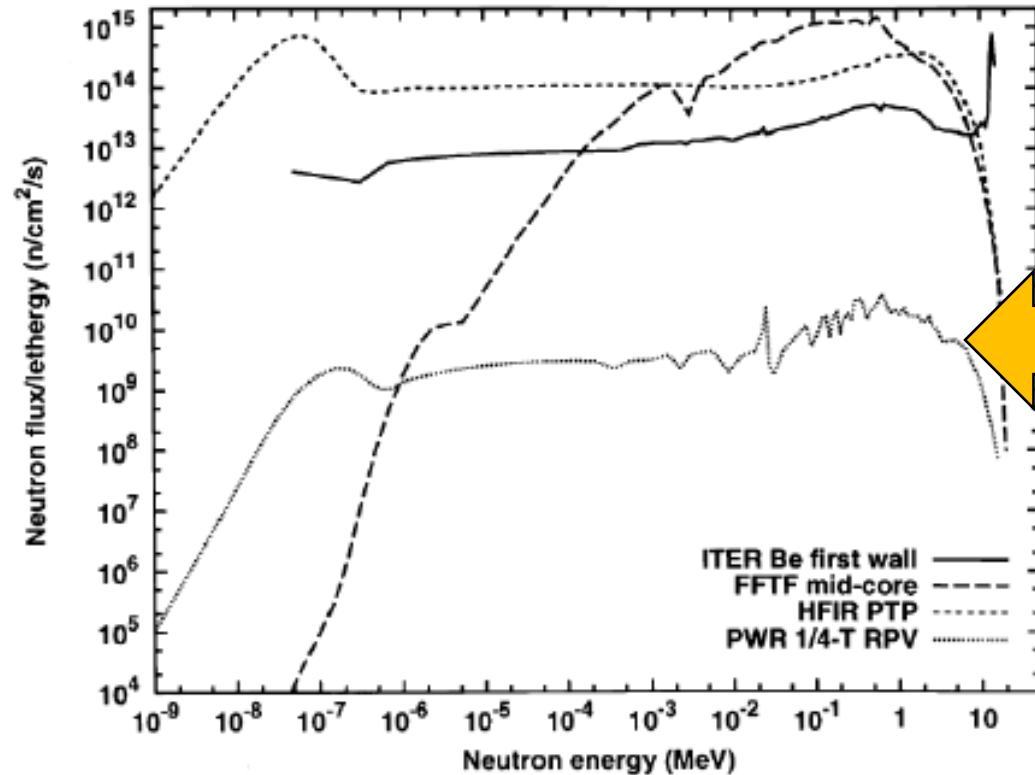
The cross section effectively assigns an apparent size to the atoms based on the probability of a given reaction based on the given particle flux (energy) spectrum



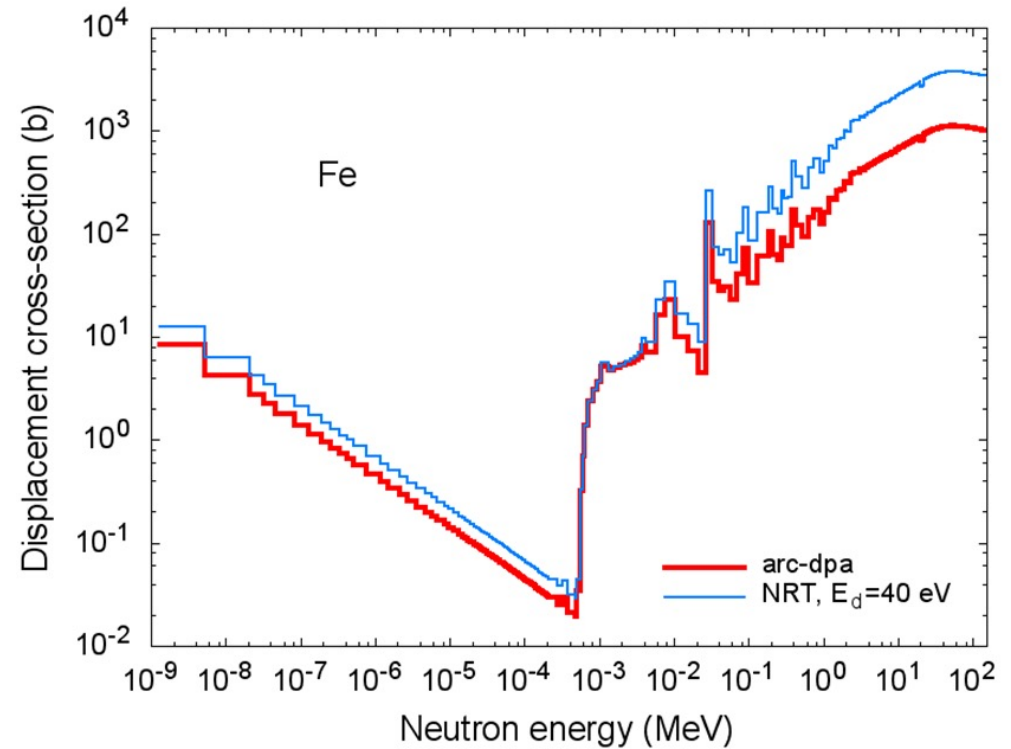
2.2: Schematic representation of the microscopic cross section concept. If A atoms are U-235 and B atoms are B-10, then Reaction 1 would be nuclear fission, for which the U-235 atoms have a large cross section and the B atoms do not, while Reaction 2 could be the (n, α) reaction, for which the cross section of U-235 is much smaller than that of B-10.



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)

σ_s definitions

Total scattering cross sections $\sigma_s(E_i)$:

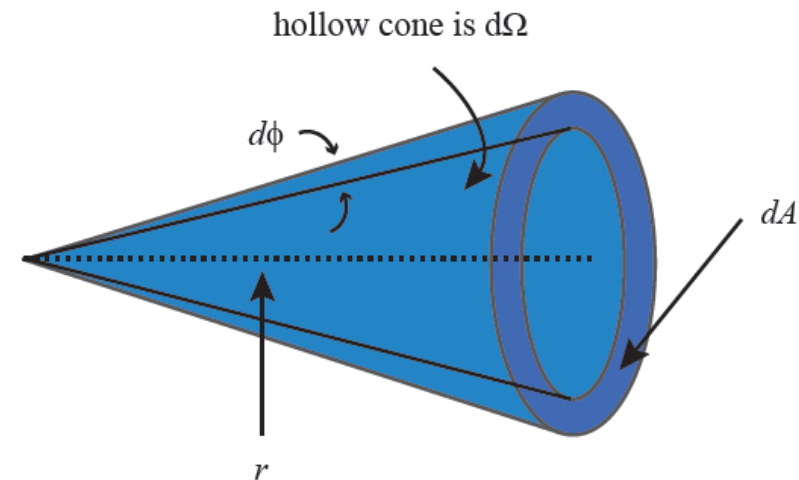
- $N\sigma_s(E_i)dx$: The probability of the collision of an incident particle with a target in dx

Differential energy transfer cross-sections $\sigma_s(E_i, T)$:

- $N\sigma_s(E_i, T)dTdx$: The probability of the collision in dx transferring energy in the range of $T + dT$ to the target particle

Differential angular cross-sections $\sigma_s(E_i, \phi)$:

- $N\sigma_s(E_i, \phi)d\Omega dx$: The probability of the collision in dx scattering the incident particle into a COM angle in the range of $(\phi, d\Omega)$



σ_s definitions

Total scattering cross sections $\sigma_s(E_i)$:

- $N\sigma_s(E_i)dx$: The probability of the collision of an incident particle with a target in dx

Differential energy transfer cross-sections $\sigma_s(E_i, T)$:

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Differential angular cross-sections

$\sigma_s(E_i, \phi)$:

- $N\sigma_s(E_i, \phi)d\Omega dx$: The probability of the collision in dx scattering the incident particle into a COM angle in the range of $(\phi, d\Omega)$

σ_s relationships

$$\sigma_s(E_i, T)dT = \sigma_s(E_i, \phi)d\Omega$$

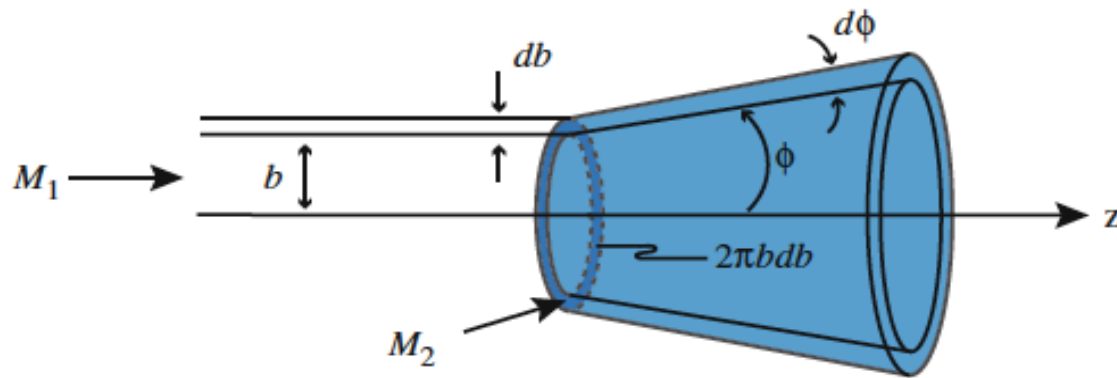
$$\sigma_s(E_i) = \int_{T_{min}}^{T_{max}} \sigma_s(E_i, T)dT$$

$$\begin{aligned}\sigma_s(E_i) &= \int_0^\Omega \sigma_s(E_i, \phi)d\Omega \\ &= 2\pi \int_0^\phi \sigma_s(E_i, \phi) \sin \phi d\phi\end{aligned}$$



Back to impact parameter – Differential Energy Transfer Cross Section

- Particles which enter b and $b + db$ will be scattered into ϕ about $d\phi$ with energies T to $T + dT$



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

- The **total cross section** for collisions with T anywhere in the range of T_{\min} and T_{\max} is:

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

Known:

$V(r)$ = interaction potential

The method then:

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

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

$\sigma_s(E_i)$

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

Finish



Known:

$V(r)$ = interaction potential

Classic scattering integral:

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

Energy transfer:

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

Differentiate to get $2bdb$
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Differential Cross Section:

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

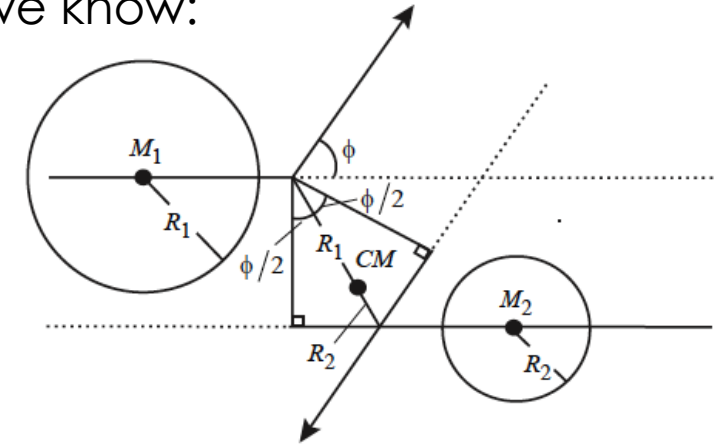
$$\sigma_s(E_i) = \int_{T_{min}}^{T_{max}} \sigma_s(E_i, T) dT$$

Hard sphere example – find $\sigma_s(E_i, T)$ and $\sigma_s(E_i)$:

From our collision kinematics lecture, we know:

$$V(\rho) = \frac{M_2}{M_1 + M_2} E_i \quad \text{For head-on}$$

If we back-off a bit we get →



Known:

$V(r)$ = interaction potential

Classic scattering integral:

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

Energy transfer:

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

Differentiate to get $2bdb$
as a function of T and dT

Differential Cross Section:

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

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

Hard sphere example – find $\sigma_s(E_i, T)$ and $\sigma_s(E_i)$:

Then:

$$\sigma_s(E_i, T) = 2\pi\rho \cos \phi/2 \frac{\rho}{2} \sin \phi/2 \frac{2}{\gamma E_i \sin \phi}$$



An alternate solution method! – Page 9-11 Was, 2nd Edition

- Use our relationships and knowledge of solid angles

$$\sigma_s(E_i, T) dT = \sigma_s(E_i, \phi) d\Omega$$

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

$$\begin{aligned} \sigma_s(E_i) &= \int_0^\Omega \sigma_s(E_i, \phi) d\Omega \\ &= 2\pi \int_0^\phi \sigma_s(E_i, \phi) \sin \phi d\phi \end{aligned}$$

We are still interested in obtaining the probability that a given T will be imparted to the recoil atom. This depends on the differential cross section. We define $\sigma_s(E_i, \phi) d\Omega$ as the probability of a collision that scatters the incident particle into a center-of-mass angle in the range $(\phi, d\Omega)$ where $d\Omega$ is an element of solid angle about the scattering direction ϕ . Since differential probabilities written in transformed variables are equivalent, $\sigma_s(E_i, \phi)$ can be written in terms of CM variables:

$$\sigma_s(E_i, \phi) d\Omega = \sigma_s(E_i, T) dT. \quad (1.15)$$

Using Fig. 1.3 to relate $d\Omega$ to $d\phi$, we have by definition:

$$d\Omega = dA/r^2, \quad (1.16)$$

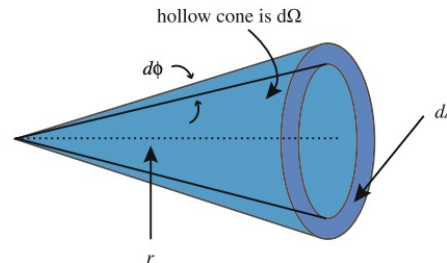
and from Fig. 1.4, we have:

$$d\Omega = \frac{rd\phi(2\pi r \sin \phi)}{r^2} = 2\pi \sin \phi d\phi. \quad (1.17)$$

Substituting Eq. (1.17) into Eq. (1.15) yields:

$$\sigma_s(E_i, T) dT = \sigma_s(E_i, \phi) d\Omega = 2\pi \sigma_s(E_i, \phi) \sin \phi d\phi. \quad (1.18)$$

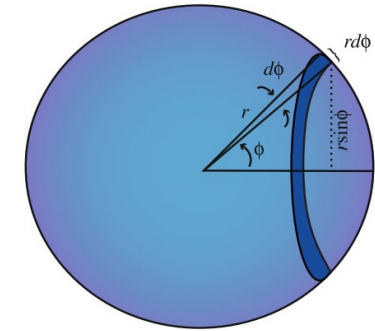
Fig. 1.3 Scattering into the solid angular element $d\Omega$ defined by dA/r^2



10

1 The Radiation Damage Event

Fig. 1.4 The solid angle $d\Omega$ subtended at the scattering angle ϕ by the incremental angle $d\phi$



Since $T = \frac{\gamma}{2} E_i (1 - \cos \phi)$ then $dT = \frac{\gamma}{2} E_i \sin \phi d\phi$, and we have:

$$\sigma_s(E_i, T) = \frac{4\pi}{\gamma E_i} \sigma_s(E_i, \phi). \quad (1.19)$$

Figure 1.5 shows the difference in the differential scattering cross section in units of area per unit solid angle versus area per unit angle as in Eq. (1.18). Although the number of atoms scattered through an angle increment $d\phi$ about $\phi = \pi/2$ is greater than that through an angular increment $d\phi$ about $\phi = 0$ or π (Fig. 1.5(a)), the number intercepting the spherical surface per unit of solid angle is constant over all angles, ϕ (Fig. 1.5(b)). Hence, $dT/d\phi$ varies in a sinusoidal manner with ϕ , but $dT/d\Omega$ is independent of ϕ .

Using Eqs. (1.2) and (1.18), the total elastic scattering cross section is as follows:

$$\sigma_s(E_i) = \int \sigma_s(E_i, \phi) d\Omega = 2\pi \int \sigma_s(E_i, \phi) \sin \phi d\phi.$$

If we assume that elastic scattering in the CM system is independent of scattering angle (i.e., scattering is isotropic), Fig. 1.6, then:

$$\sigma_s(E_i) = \int \sigma_s(E_i, \phi) d\Omega = 2\pi \sigma_s(E_i, \phi) \int \sin \phi d\phi = 4\pi \sigma_s(E_i, \phi), \quad (1.20)$$

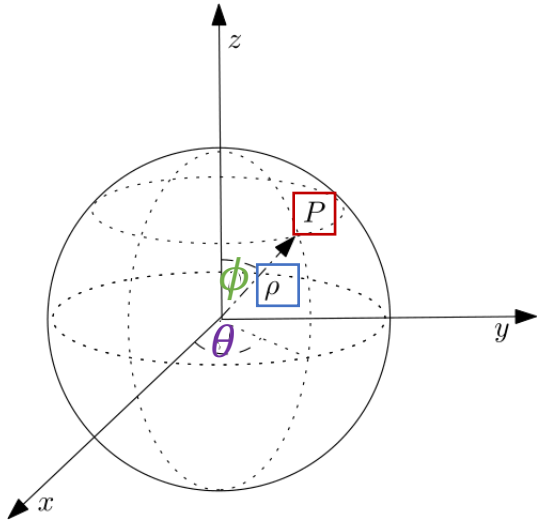
and

$$\sigma_s(E_i, T) = \frac{\sigma_s(E_i)}{\gamma E_i}, \quad (1.21)$$



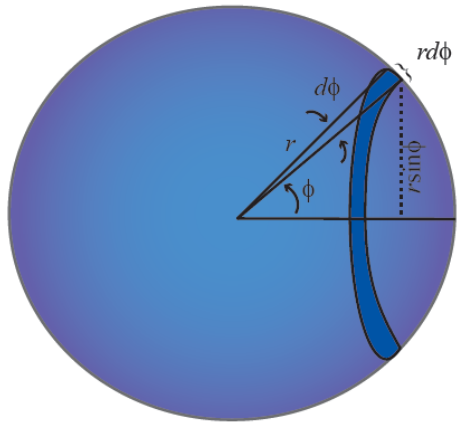
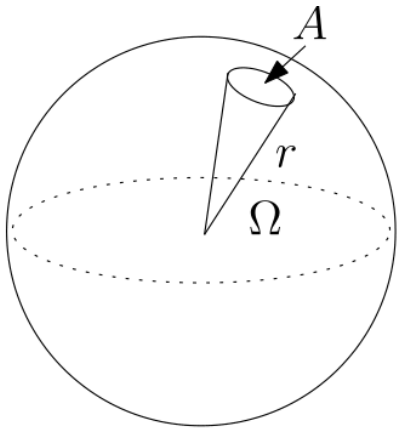
Solid angle definitions and relationships

- Solid angle vector in cartesian coordinates



$$\vec{P} = \vec{x} + \vec{y} + \vec{z} = \rho \sin \phi \cos \theta + \rho \sin \phi \sin \theta + \rho \cos \phi$$

- Solid angle vector in spherical coordinates:
 - 1 steradian (sr) = 1 rad², where $4\pi^2$ sr = sphere



$$d\Omega = \frac{A}{r^2}$$

$$d\Omega = \frac{\rho^2 \sin \phi d\theta d\phi}{\rho^2} = \sin \phi d\theta d\phi$$

$$d\Omega = \sin \phi d\phi \int_0^{2\pi} d\theta = 2\pi \sin \phi d\phi$$

...Then for simple, elastic neutron-nucleus interactions

- The mean energy transfer is then:

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

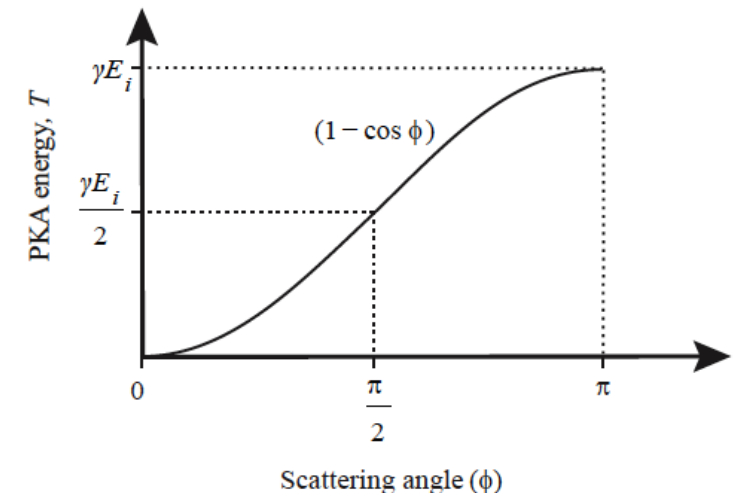
Where usually: $\hat{T} =$ and $\check{T} = E_d$

- Elastic isotropic neutron-nuclear collisions:

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

∴ Average energy:

$$\bar{T} \approx \frac{\gamma E_i}{2}$$



Summary of different analytical solutions

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) $\rho \ll a$	$\sigma_s(E_i, T) = \frac{\pi b_0^2 E_i \gamma}{4 T^2}$	(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)

Tips, help, and other examples

- I highly recommend Section 12.3.5 starting on page 534 of Olander and Motta

12.3.5 Ion-atom scattering; general binary collision dynamics

A collision between two particles that have an interaction potential $V(r)$ and which collide with an *impact parameter* p is shown in Figure 12.6. It is desired to find the orbit of two particles in an elastic collision and to relate the interaction potential to the differential cross section $\sigma(E, \theta)$.

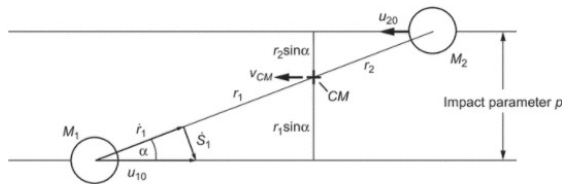


FIGURE 12.6: Geometry for derivation of elastic collision between an energetic ion and a stationary atom, interacting by a potential $V(r)$.

In the system considered, a particle mass M_1 is moving initially with kinetic energy E toward an initially stationary particle mass M_2 . The center of mass (CM) is located on the line joining the two masses at a distance

$$r_1 = \frac{M_2}{M_1 + M_2} r \quad \text{and} \quad r = r_1 + r_2 \quad (12.28)$$

from the mass M_1 . The initial velocity of particle 1 in the center-of-mass system, u_{10} , is decomposed into two perpendicular components \dot{r}_1 and \dot{S}_1 , such that $\vec{u}_{10} = \dot{r}_1 + \dot{S}_1$. The line between the particles makes an angle α with the initial direction of the particles in the CM system. Only the initial kinetic energy in the CM system is convertible to potential energy, and this is written

$$E_{CM} = \frac{1}{2} (M_1 + M_2) v_{CM}^2, \quad (12.29)$$

and using Equation (12.3):

$$E_{CM} = \frac{M_1}{M_1 + M_2} E = \frac{M_1}{M_1 + M_2} \left[\frac{M_1 v_{10}^2}{2} \right] \quad (12.30)$$

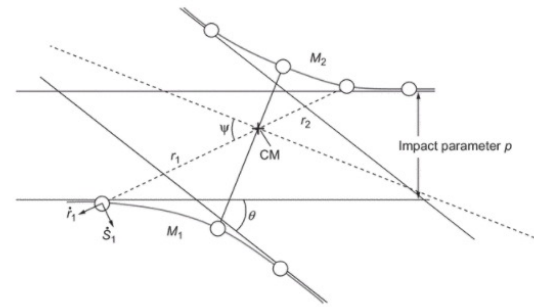


FIGURE 12.7: Geometry during the collision in center-of-mass coordinates.

where E is the initial kinetic energy of particle 1 in the laboratory frame. Now using conservation of energy and angular momentum during the collision, it is possible to derive a relationship between the scattering angle in the center of mass θ and the impact parameter p . The trajectory of the particles as they interact and are deflected by angle θ are shown in Figure 12.7.

Conservation of energy

As the two energetic particles approach each other, they convert kinetic energy into potential energy, $V(r)$, so that at the distance of closest approach, the kinetic energy is minimized. Conservation of energy for the system is

$$E_{CM} = V(r) + \frac{1}{2} M_1 u_{10}^2 + \frac{1}{2} M_2 u_{20}^2 = V(r) + \frac{1}{2} M_1 (\dot{r}_1^2 + \dot{S}_1^2) + \frac{1}{2} M_2 (\dot{r}_2^2 + \dot{S}_2^2). \quad (12.31)$$

The tangential speed \dot{S} is equal to $r\dot{\psi}$, so Equation (12.31) is

$$E_{CM} = V(r) + \frac{1}{2} M_1 (\dot{r}_1^2 + r_1^2 \dot{\psi}^2) + \frac{1}{2} M_2 (\dot{r}_2^2 + r_2^2 \dot{\psi}^2), \quad (12.32)$$



Summary

Where we are going:

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

- 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:

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

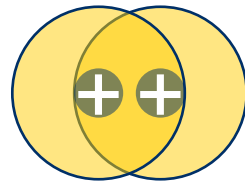
Task 2: Determine the scattering angle based on the impact parameter:

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

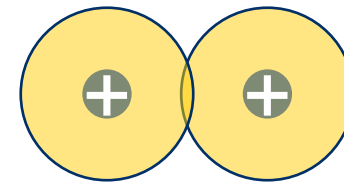
Task 3: Described $V(r)$ based on the distance of closest approach



= 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?

