Rutherford Backscattering Spectrometry

EMSE-515
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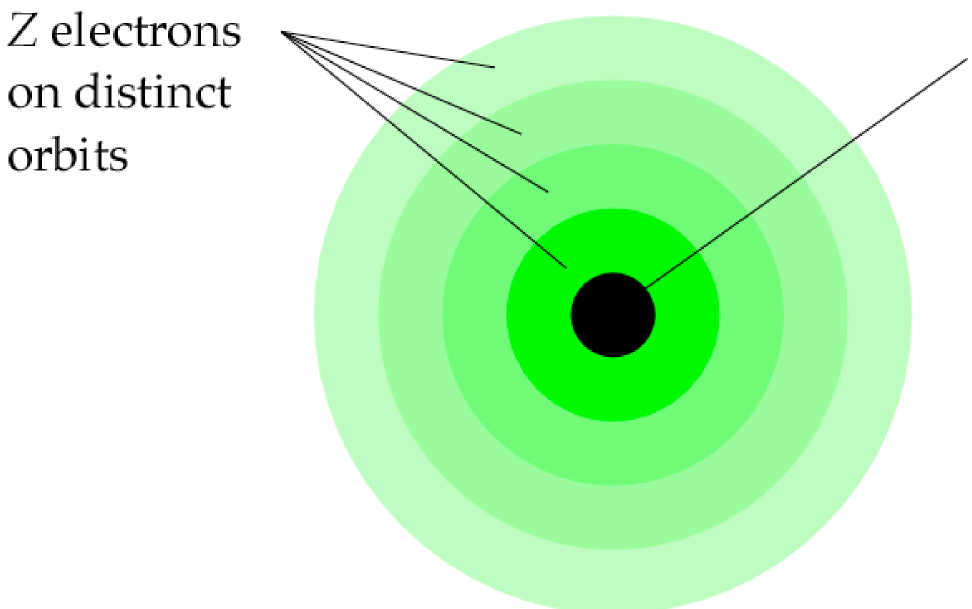
F. Ernst

Bohr's Model of an Atom



$$E_n = -13.58\ \text{eV} \cdot \frac{Z^2}{n^2}$$

$$a_0 = \frac{\hbar^2}{m e^2} = 0.053\ \text{nm}$$

$$r_n = \frac{n^2}{Z} \cdot a_0$$

- existence of central *core* established by single collision, large-angle scattering of alpha particles ($^4He^{2+}$)

→ basis of Rutherford back-scattering spectrometry (RBS)

Principle of RBS

- exposed specimen surface to beam of (light) MeV particles
- *elastic* collisions with (heavy) atoms of target

→ Coulomb scattering in a central-force field

- can be described by classical mechanics
- but: specimen will eventually stop beam particles

→ sufficient penetration of the target requires beam particles with kinetic energy in the MeV range

→ accelerator!

NEC 5SDH Accelerator

NEC 5SDH Accelerator

- 1.7 MV tandem pelletron
- 3.4 MeV protons
- 5.1 MeV alpha particles
- N ions with energies in excess of 7.0 MeV
- detectors
  - Si surface barrier detector
  - NaI(Ti) scintillator
  - liquid nitrogen-cooled Si(Li) detector

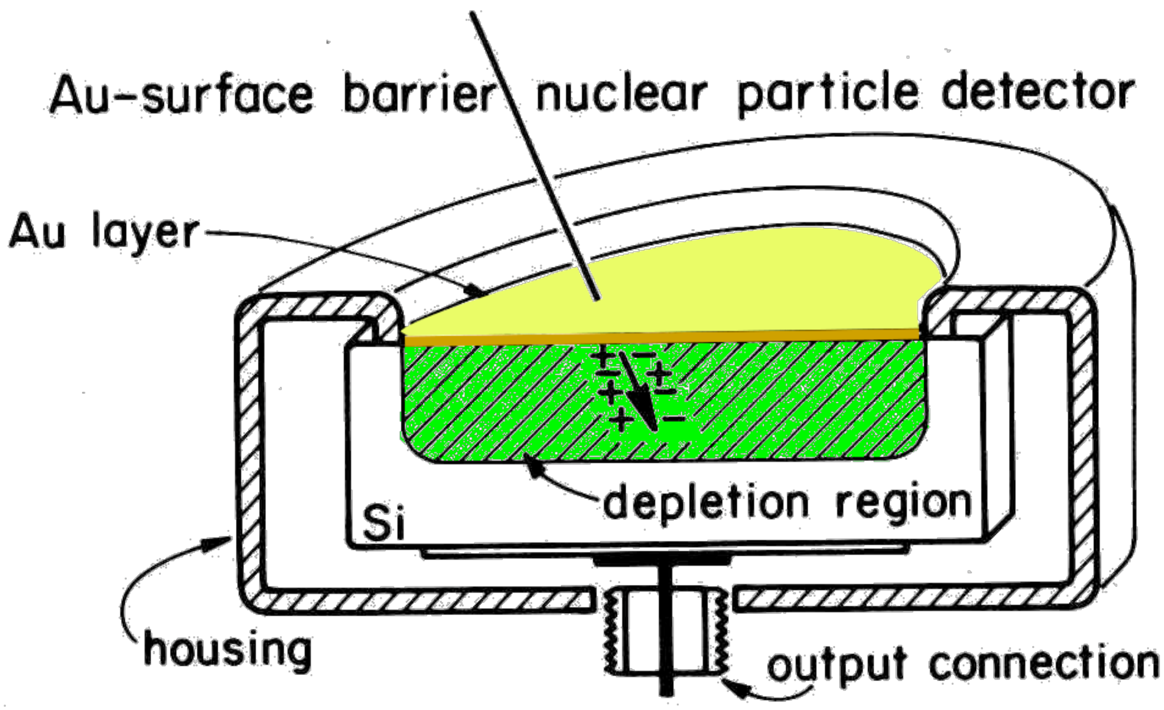
NEC 5SDH Accelerator

- detectors enable detection of
  - scattered ions
  - characteristic gamma rays
  - characteristic x-rays
- can be used for the following experimental techniques:
  - RBS
  - PIXE (particle induced X-ray emission)
  - NRA (nuclear reaction analysis)
  - sample temperatures from 77 to 1000 K

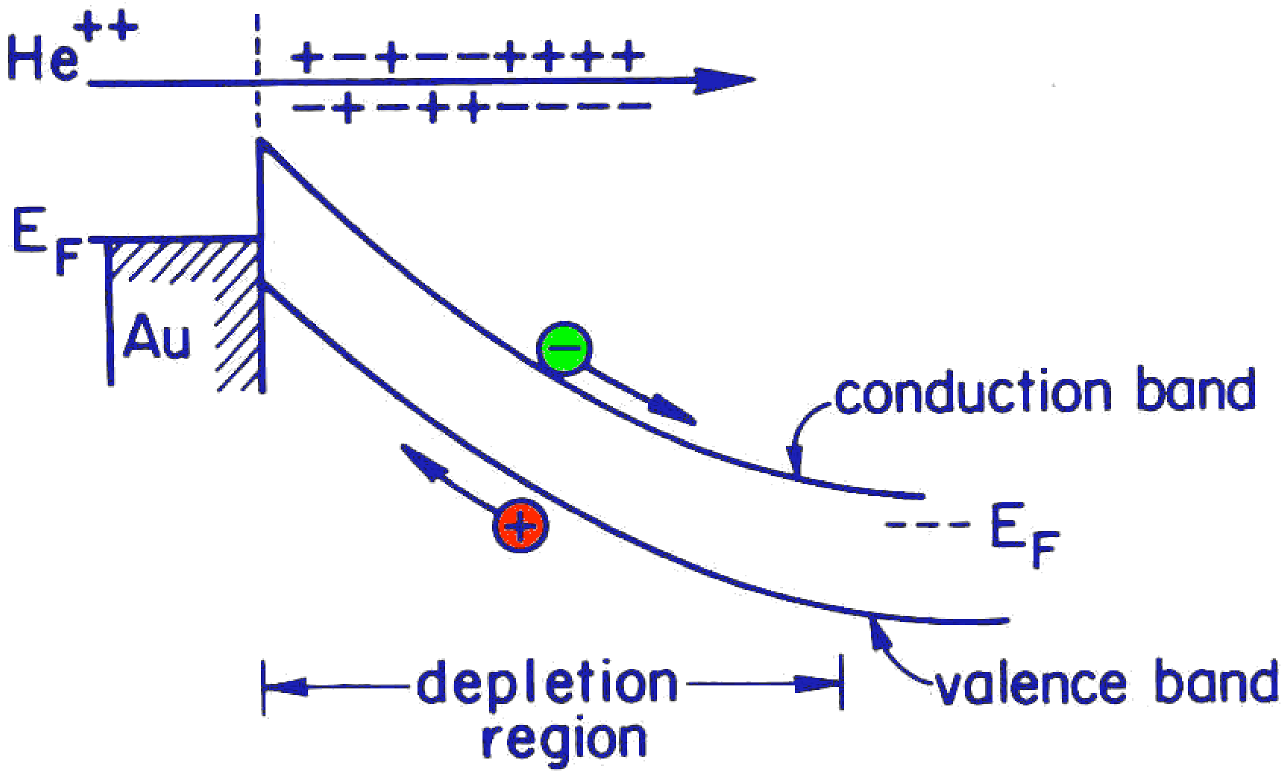
Detection of Scattered Particles

- semiconductor nuclear particle detector
- resolve rate and kinetic energy of scattered particles
- most systems use a *surface-barrier*, solid state detector
    - Schottky-barrier diode
    - reverse-biased
    - incident particle generates electron–hole pairs
    - collected to electrodes
    - voltage pulse, proportional to particle energy
    - collect counts in voltage bins of multichannel analyzer

Surface Barrier, Solid State Detector



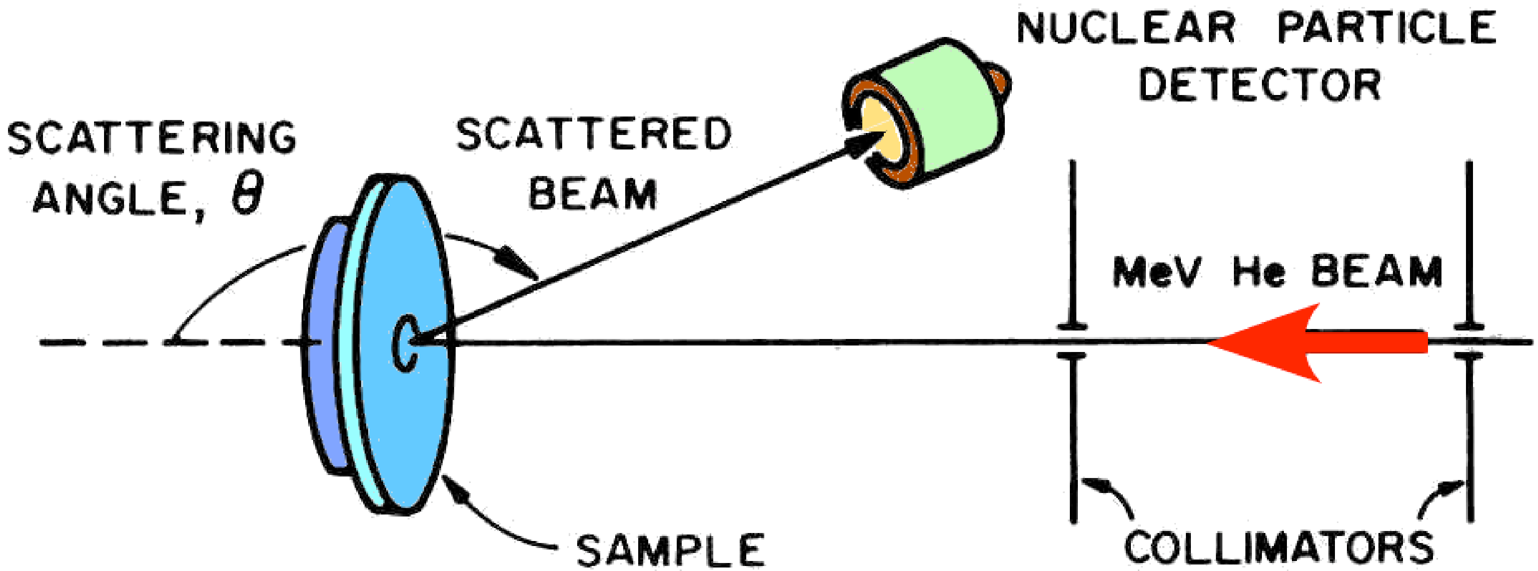
Surface Barrier, Solid State Detector



Resulting Spectrum Properties

- statistics of electron-hole pair generation
- noise in output signal
- limited energy resolution
- typical energy resolution: $10 \ldots 20$ keV
- backscattering analysis with 2.0 MeV ^{4}He particles can resolve isotopes up to about mass 40 (clorine isotopes, for example)
- mass resolution decreases with increasing atomic mass of the target
- example: ^{181}Ta and ^{201}Hg cannot be distinguished

Experimental Setup for RBS



Experimental Setup for RBS

- beam of mono-energetic particles (^{4}He)
- in vacuum
- backscattering

  → energy transfer to (stationary) target atoms

  → primary particle looses kinetic energy

- amount depends on masses of incident particle and target atom
- energy loss provides “signature” of target atoms

Characteristics of RBS

- multi-element depth concentration profiles
- fast, non-destructive analysis (no sample preparation or sputtering required)
- matrix independent (unaffected by chemical bonding states)
- quantitative without standards
- high precision (typically $\pm 3\,\%$
- high sensitivity
  - e. g. 10^{11} Au/cm^2 on Si
  - depends on Z and sample composition

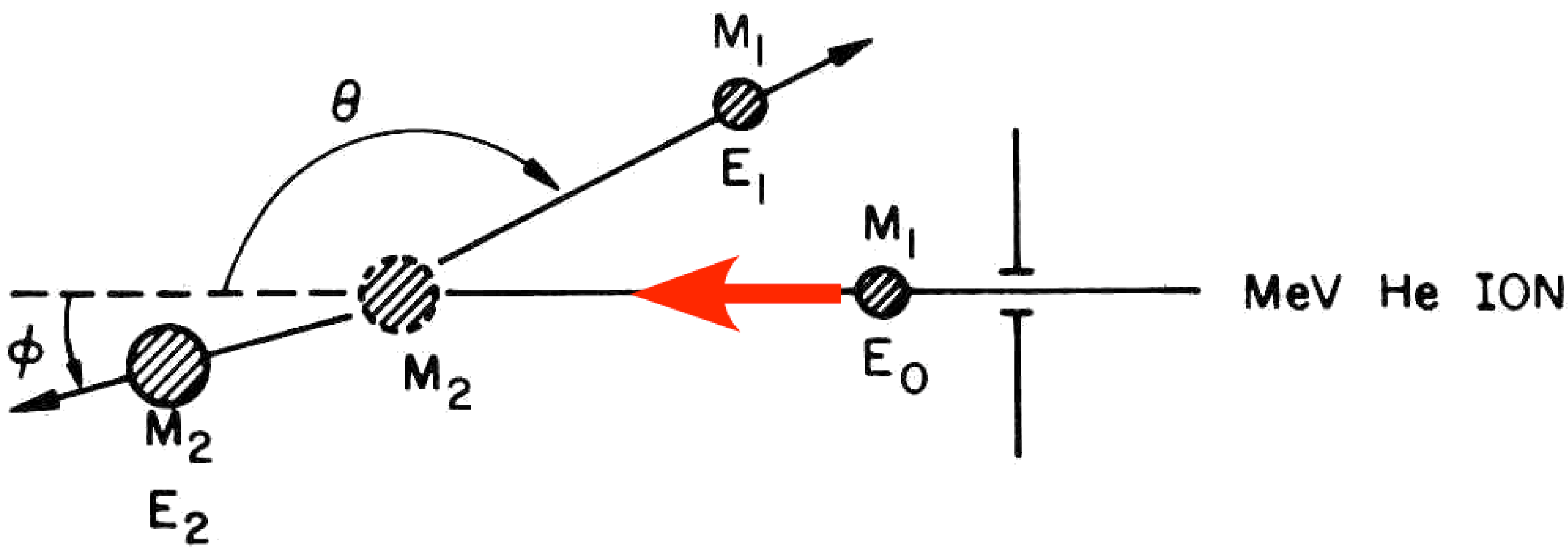
Characteristics of RBS

- depth range: between 0 and 1 mm
- depth resolution ≈ 2 nm near the surface
- spatial definition:
  - beam spot size $0.5 \ldots 2.0$ mm
  - map or raster option to 7 cm $\times$ 7 cm

Typical Applications of RBS

- absolute thickness of films, coatings, and surface layers (in atoms/cm^2)
- surface/interface contaminant detection (oxide layers, adsorbates, etc.)
- interdiffusion kinetics of thin films (metals, silicides, etc.)
- elemental composition of complex materials (phase identification, alloy films, oxides, ceramics, etc.)
- quantitative dopant profiles in semiconductors
- process control monitoring
  - composition
  - contaminant control

Kinematics of Elastic Collisions



Kinematics of Elastic Collisions

- RBS: elastic Coulomb scattering

→ calculate energy transfer in the framework of classical mechanics

- applying the conservation principle of energy and momentum
- energy:

$$\frac{M_1}{2}v^2 = \frac{M_1}{2}v_1^2 + \frac{M_2}{2}v_2^2$$

v: velocity of beam particle before collision;
v_1: velocity of beam particle after collision;
v_2: velocity of target particle after collision;
M_1: mass of beam particle;
M_2: mass of target particle.

Kinematics of Elastic Collisions

- momentum:

$$
\begin{aligned}
p &= p_1 + p_2 \\
\Longrightarrow \quad M_1 v &= M_1 v_1 + M_2 v_2
\end{aligned}
$$

p: momentum of beam particle before collision;
p_1: momentum of beam particle after collision;
p_2: momentum of target particle after collision.

- components parallel and normal to the axis (direction of the incident beam):

$$
\begin{aligned}
M_1 v &= M_1 v_1 \,\mathrm{Cos}[\theta] + M_2 v_2 \,\mathrm{Cos}[\theta] \\
\wedge \quad 0 &= M_1 v_1 \,\mathrm{Sin}[\theta] + M_2 v_2 \,\mathrm{Sin}[\theta]
\end{aligned}
$$

Kinematics of Elastic Collisions

- for the ratio of particle velocities, these expressions yield

$$\frac{v_1}{v} = \frac{\pm\sqrt{M_2^2 - M_1^2 \operatorname{Sin}[\theta]^2} + M_1 \operatorname{Cos}[\theta]}{M_1 + M_2},$$

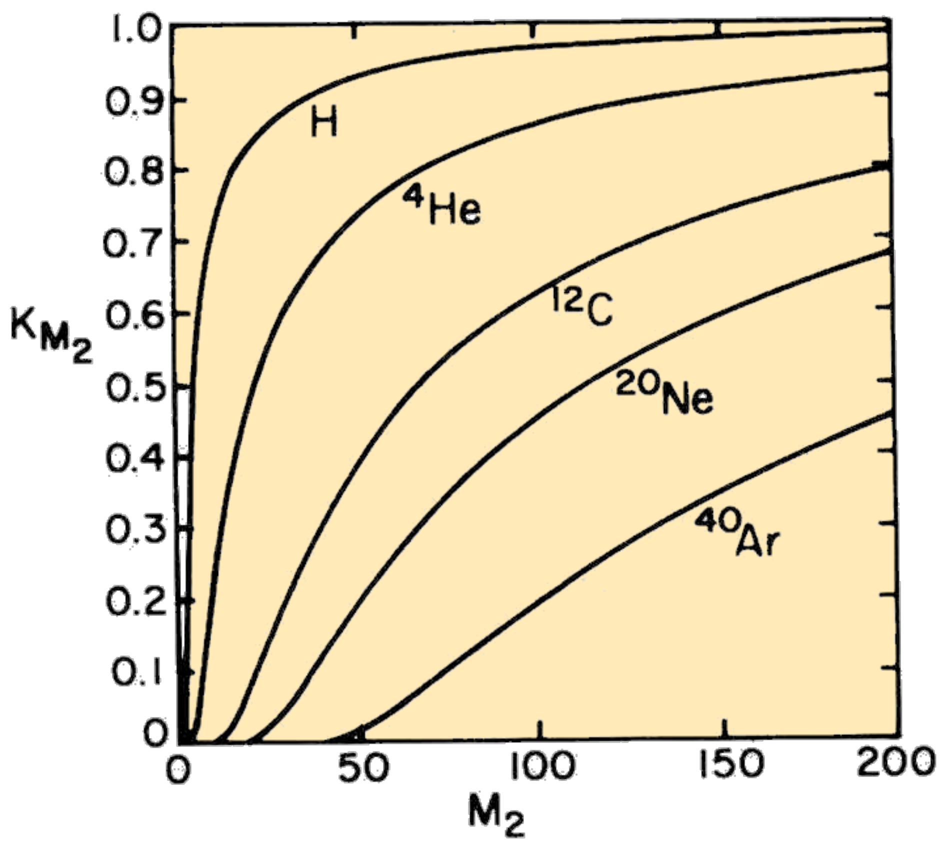
where the plus sign holds for

$$M_1 < M_2$$

- ratio of the projectile energies for $M_1 < M_2$ is known as "kinematic factor" K_{M_2}

Kinematic Factor

- K_M for a scattering angle $\theta = 170^\circ$ as a function of the target mass M_2 for different beam particles:



Kinematic Factor

- the sensitivity for small differences ΔM_2 becomes a maximum for $\theta = 180^\circ$

$\Rightarrow$ $\theta = 180^\circ$ is the preferred position for the detector

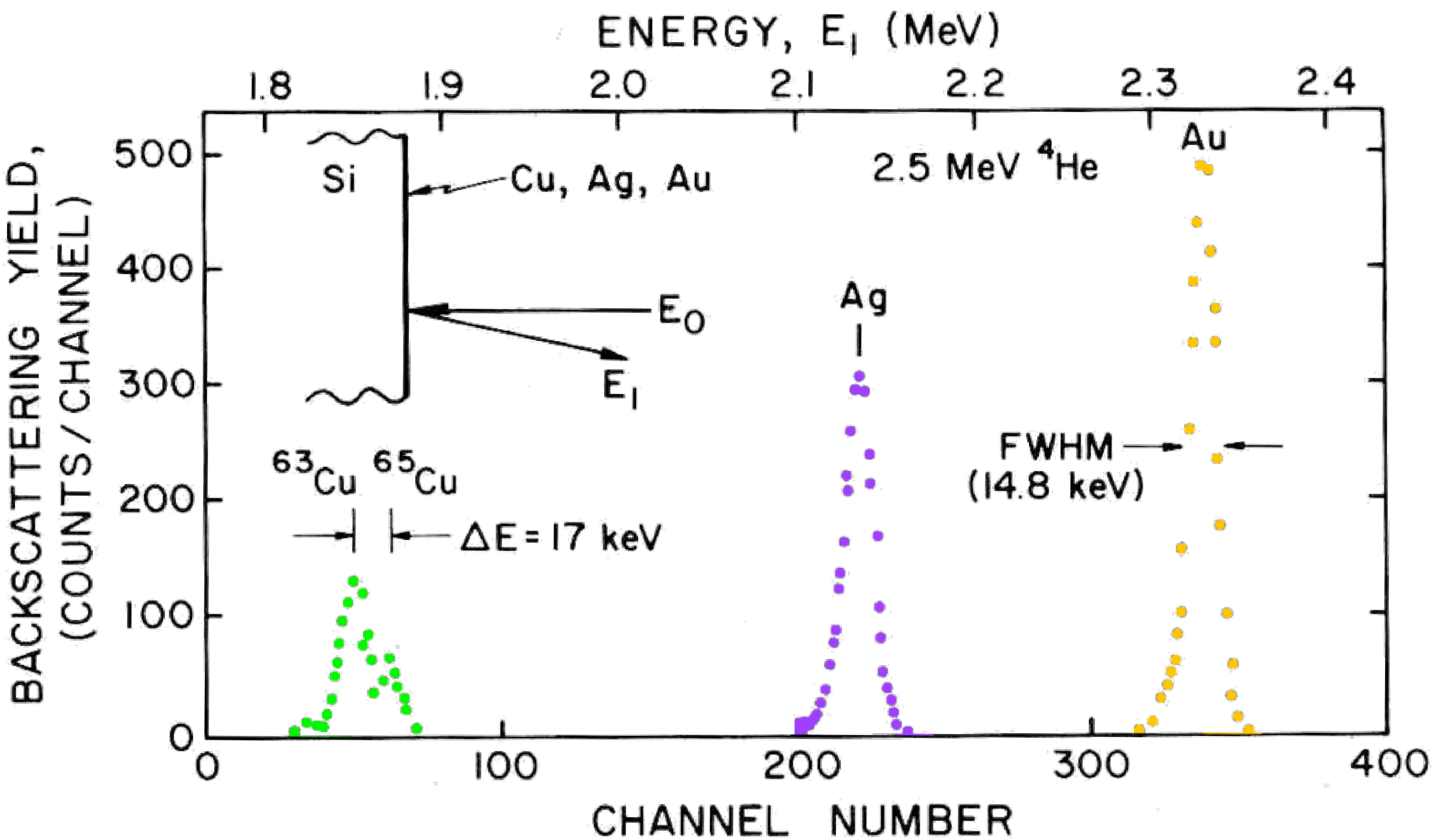
$\rightarrow$ "back-scattering"

- in practice (to accommodate the detector size):
detector at $\theta \approx 180^\circ$

Example of RBS Spectra

- ≈ 1 ML of different noble metals:
  - $^{63,\,65}$Cu
  - $^{107,\,109}$Ag
  - ^{197}Au
  - $\theta = 170°$
- 2.5 MeV ^{4}He ions

Example of RBS Spectra



Discussion

- RBS can detect less than one monolayer of heavy elements!
- peaks representing the elements
  - well separated
  - easy to identify
- determination of *absolute* coverage?

→ requires knowledge on absolute cross-section (see below)

- limits of mass resolution ↔ separation of isotope peaks

Discussion

- Cu:
  - ^{63}Cu ($K = 0.777$) and ^{65}Cu ($K = 0.783$)
  - energy difference $\Delta E_1 = 17\,\text{keV}$ for $2.5\,\text{MeV}$ [4]
  - → somewhat larger than detector resolution ($\approx 15\,\text{keV}$)
  - ⇒ Cu isotopes are resolved
- Ag:
  - ^{107}Ag and ^{109}Ag
  - $\Delta E_1 = 6\,\text{keV}$
  - → *smaller* than energy resolution of detector
  - Ag isotopes *not* resolved

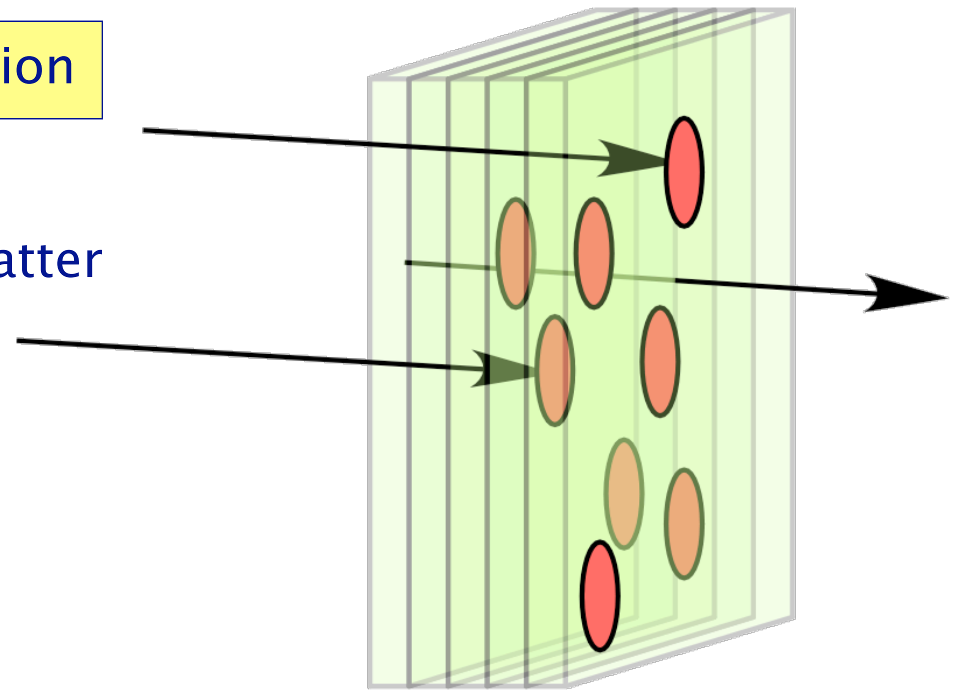
Scattering Cross Section

- probability of scattering is equal to fraction of sample area "blocked" by scatters

- important concept for scattering problems:

scattering cross section

→ effective " target area" presented by each scatter (atom)



Scattering Cross Section

- scattering cross section can be considered for specific kinds of scattering events, for example:
  - elastic scattering → σ_{el}
  - inelastic scattering → σ_{inel}
- *thin* samples:
  - target areas of individual scatters do not overlap

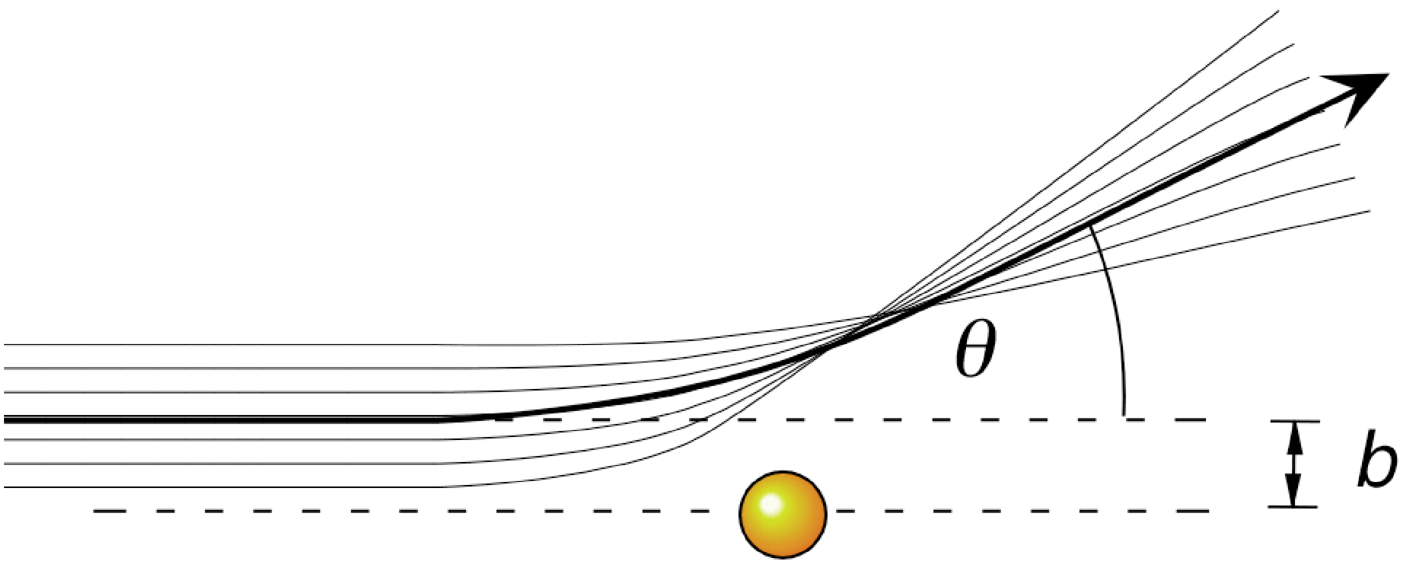
  → N scatterers block area $N \cdot \sigma$
  - fraction of "rays" removed from incident beam:

$$\frac{N\sigma}{A} = \frac{N\sigma x}{Ax} = \rho\sigma x$$

x: sample thickness; $\rho \equiv N/Ax$: number density of scatterers.

Impact Parameter

- scattering is generally anisotropic
- depends on impact parameter b



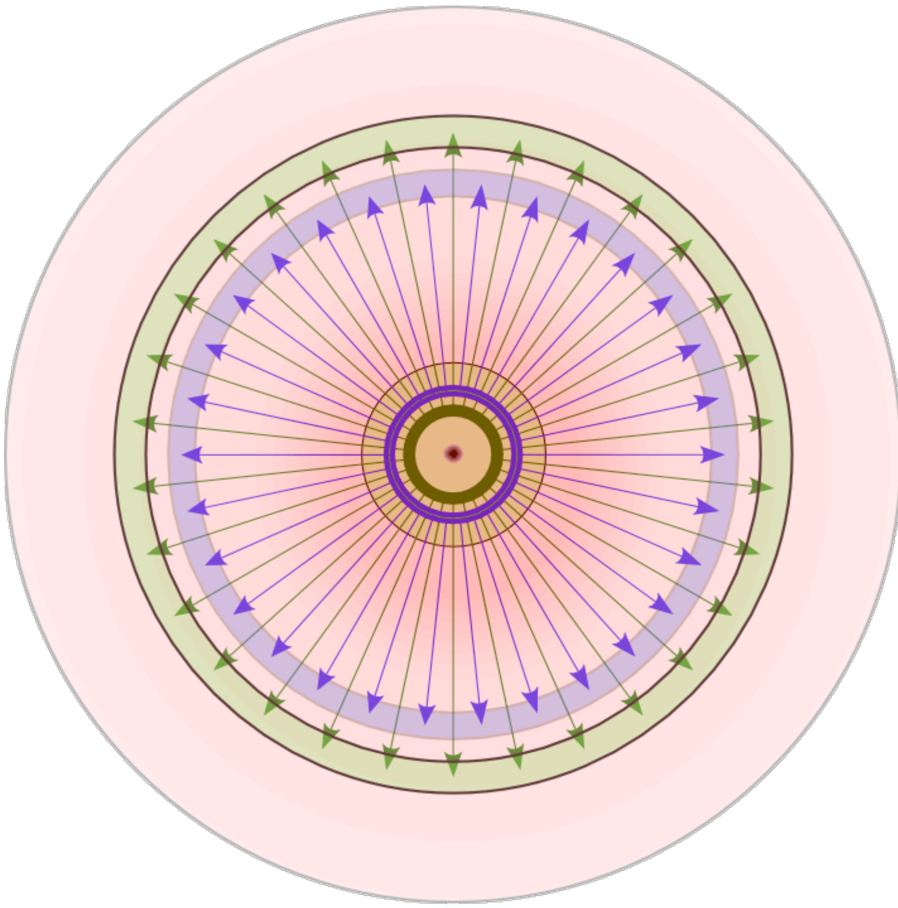
Differential Scattering Cross-Section

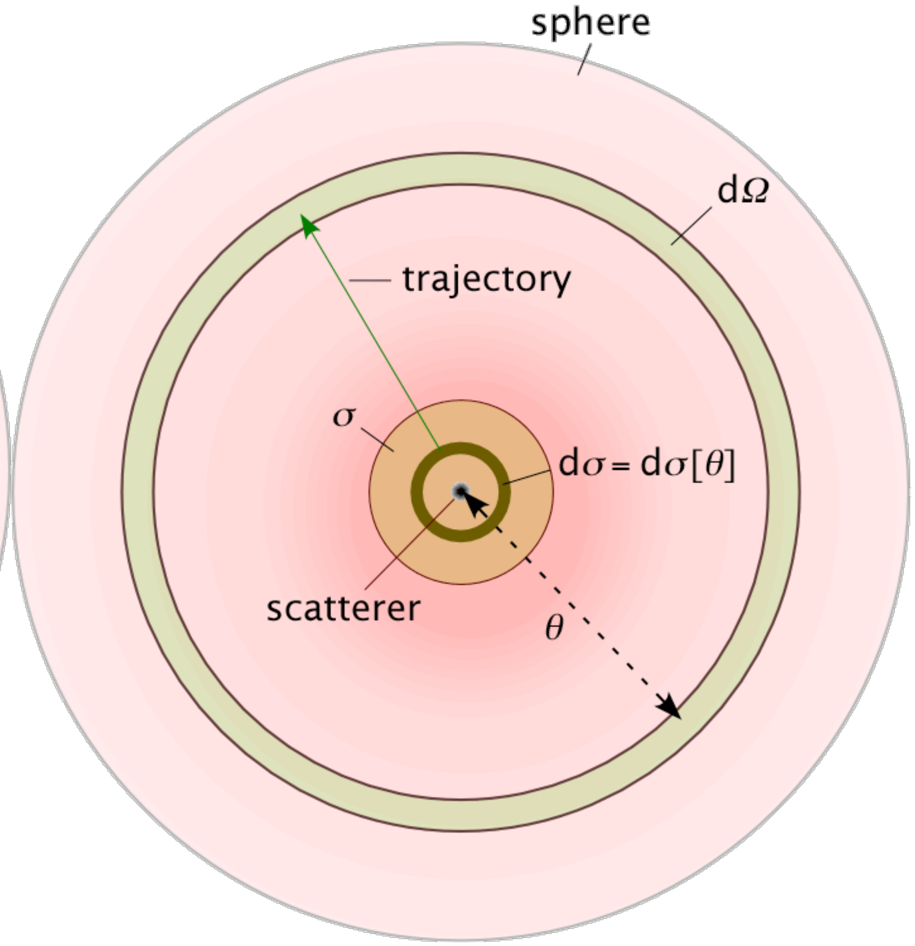
- scattering angle θ *decreases* with increasing b
- for increasing b, $\theta \to 0$ (forward scattering)
- angular distribution of scattered particles?
- important concept:

differential scattering cross section:

$$\frac{d\sigma}{d\Omega}$$

View Along Incident Beam Direction





Differential Scattering Cross Section

- interpretation of differential scattering cross section:
  - piece of area $\mathrm{d}\sigma$ offered by the scatterer for scattering into a particular increment $\mathrm{d}\Omega$ in solid angle
  - $\mathrm{d}\sigma$ varies with the location of $\mathrm{d}\Omega$, characterized by the scattering angle θ:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}[\theta]$$

- relation between increment in scattering angle θ and increment in solid angle:

$$\mathrm{d}\Omega = 2\pi \,\mathrm{Sin}[\theta]\mathrm{d}\theta$$

Differential Scattering Cross-Section

- relation between increment in scattering angle θ and increment in solid angle:

$$d\Omega = 2\pi \, \mathrm{Sin}[\theta] d\theta$$

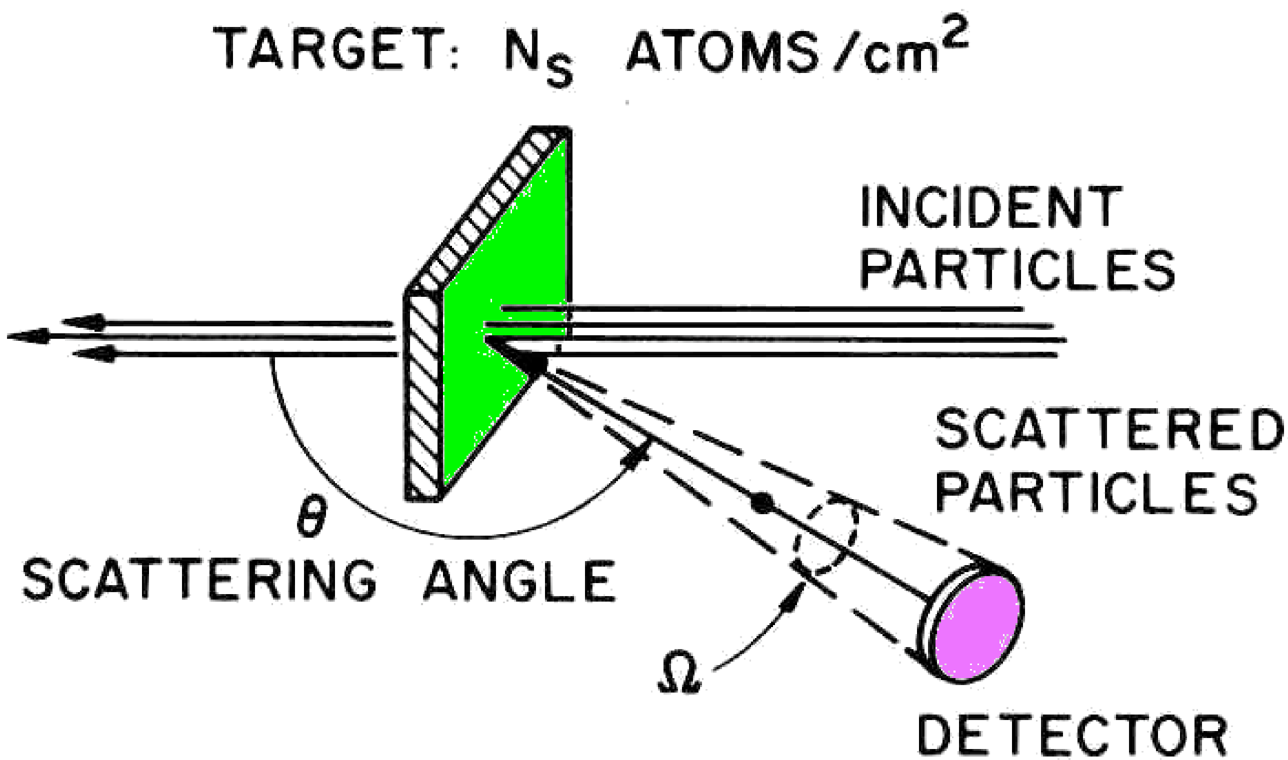
- in backscattering spectrometry, the detector solid angle ΩD is *small* – typically $< 10^{-2}$ sterad

- therefore, one often uses an *average* differential cross-section:

$$\sigma[\theta] = \frac{1}{\Omega_D} \int_{\Omega_D} \frac{d\sigma}{d\Omega} d\Omega,$$

where σ is usually called “scattering cross-section”

Differential Scattering Cross-Section



Quantification

- consider thin target of thickness t with N atoms/cm^3, thus

$$N_{\mathrm{S}} = Nt$$

  target atoms per unit area

- total number of incident particles: Q

- number of particles detected by the detector positioned at scattering angle θ: $Q_{\mathrm{D}}[\theta]$

→ to infer N_{S} from Q_{D}, one needs to know $\sigma[\theta]$, the “scattering cross-section:”

$$Q_{\mathrm{D}}[\theta] = \sigma[\theta] \cdot \Omega_{\mathrm{D}} \cdot Q \cdot N_{\mathrm{S}}$$

Quantification

- $\sigma[\theta]$ can be calculated from the force that acts during the collision

- since high-energy particles penetrate up to the core of the target atom, this force mainly corresponds to an un-screened Coulomb repulsion between the two positively charged nuclei

- one-body formulation of this problem:

  - scattering by a central force

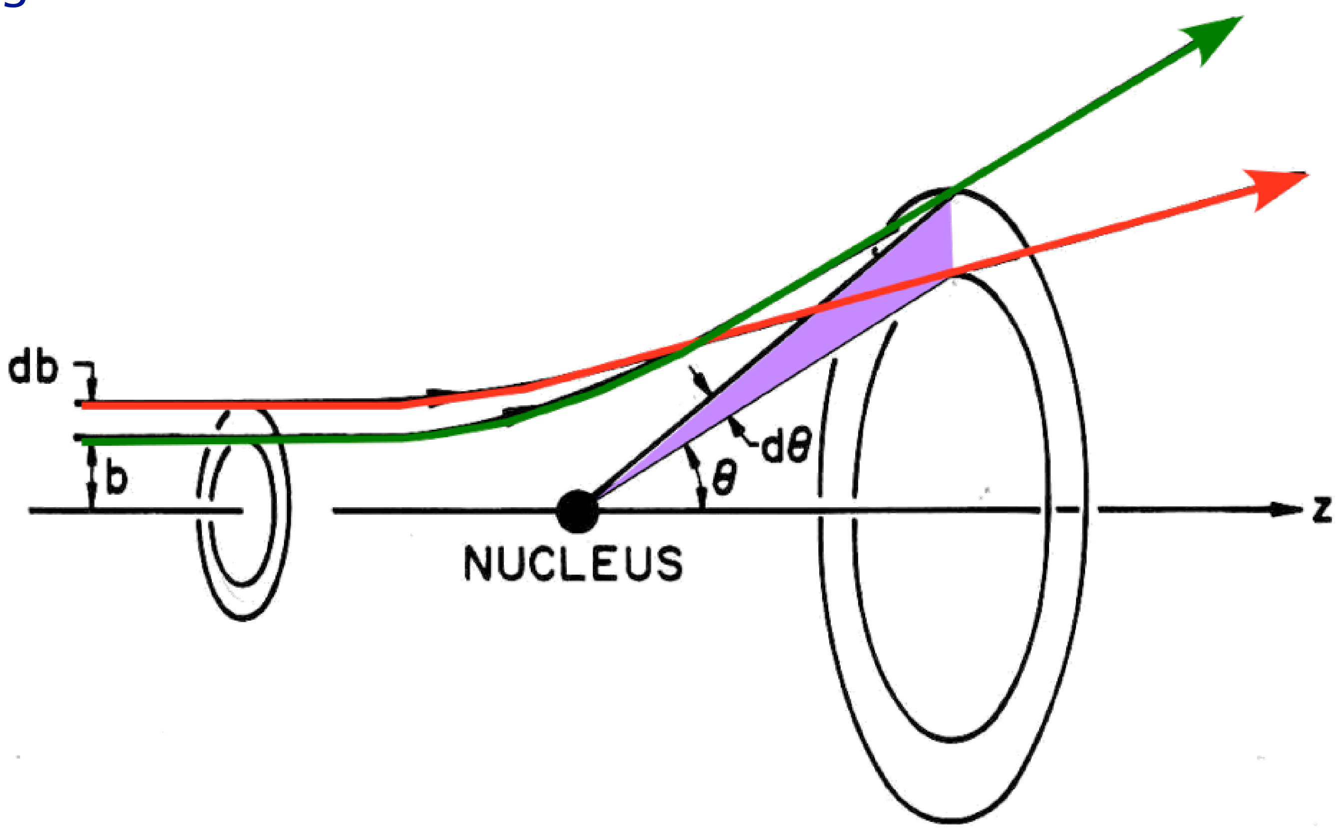
  - conservation of kinetic energy

  - impact parameter b

  - rotational symmetry

Quantification

- particles with impact parameters between b and $b + \mathrm{d}b$ are deflected into an annular region spanned by scattering angles between θ and $\theta + \mathrm{d}\theta$



Quantification

- the area of this region is

$$\mathrm{d}\Omega = 2\pi\,\mathrm{Sin}[\theta]\mathrm{d}\theta$$

- recall definition of the scattering cross-section:

$$\mathrm{d}\sigma = \sigma[\theta]\mathrm{d}\Omega$$

→ annular area enclosing scattering angles $[\theta,\ \theta + \mathrm{d}\theta]$ is related to annular area

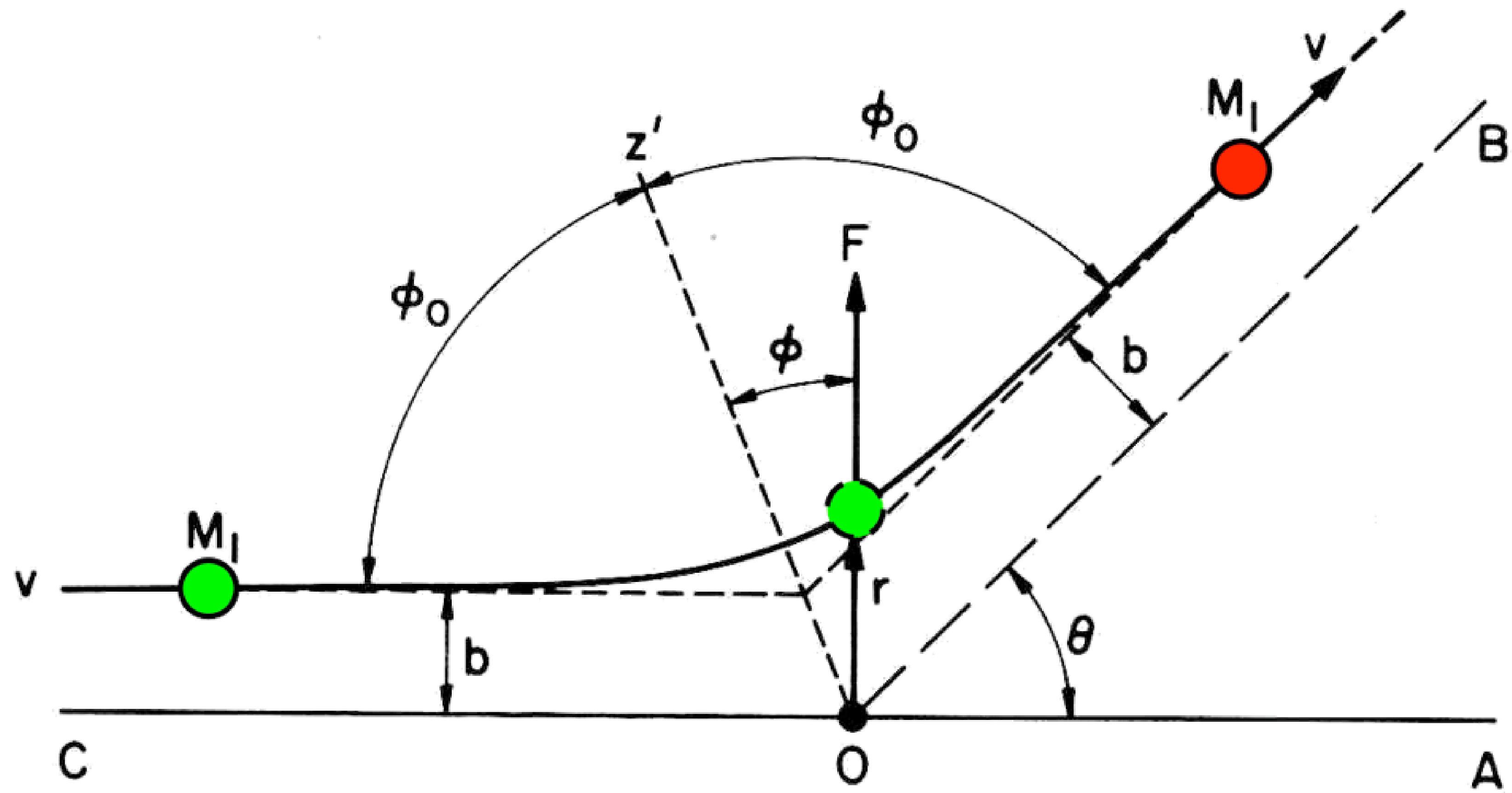
$$\mathrm{d}\sigma = 2\pi b\mathrm{d}b$$

by

$$2\pi b\mathrm{d}b = -\sigma[\theta]\cdot 2\pi\,\mathrm{Sin}[\theta]\mathrm{d}\theta$$

Central Force Scattering

- geometry of RBS:



Central Force Scattering

- central force!

$\Rightarrow$ scattered particle travels on a *hyperbolic* trajectory

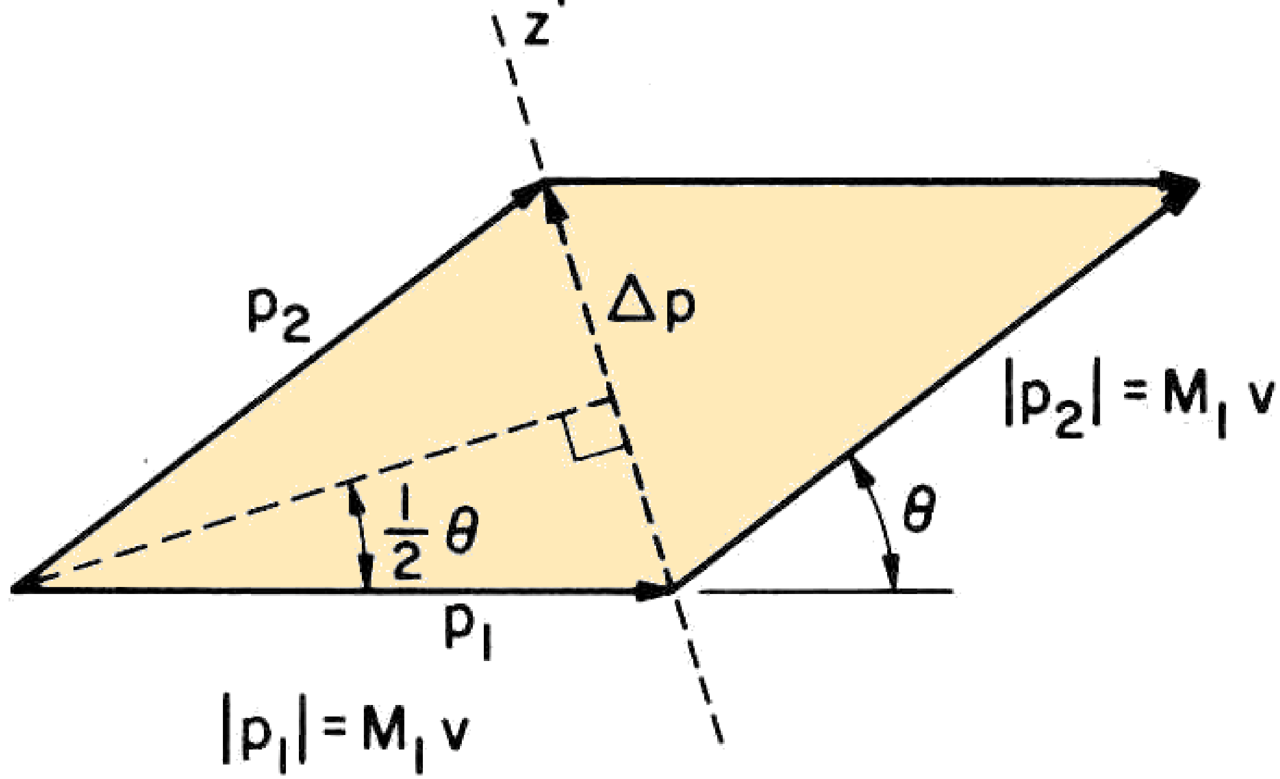
- elastic scattering by a central force $\Rightarrow$ conservation of
  - kinetic energy
  - magnitude of the momentum (direction generally changes)

$\rightarrow$ total change in momentum,

$$\Delta \boldsymbol{p} \equiv \boldsymbol{p}_1 - \boldsymbol{p},$$

is along the z' axis

Conservation of Momentum



Central Force Scattering

- for this geometry,

$$\frac{\Delta p/2}{M_1 v} = \text{Sin}\left[\frac{\theta}{2}\right] \quad \Longleftrightarrow \quad \Delta p = 2M_1 v\,\text{Sin}\left[\frac{\theta}{2}\right]$$

- Newton's second law:

$$\boldsymbol{F} = \dot{\boldsymbol{p}} \Rightarrow \mathrm{d}\boldsymbol{p} = \boldsymbol{F}\mathrm{d}t$$

- the force $\boldsymbol{F}$ is the Coulomb repulsion between the scattered particle and the target particle:

$$F = \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{r^2}$$

ε_0: electric constant; $Z_{1,2}$: atomic numbers; e: electron charge; r: distance.

Central Force Scattering

- since the angular momentum is conserved under a central force,

$$
\begin{aligned}
M_1 v b &= M_1 r^2 \frac{\mathrm{d}\phi}{\mathrm{d}t} \\
\Rightarrow \quad \frac{\mathrm{d}t}{\mathrm{d}\phi} &= \frac{r^2}{v b}
\end{aligned}
$$

- inserting this result and the expression for the Coulomb force into the above equation for Δp yields

$$
\begin{aligned}
\Delta p &= \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{r^2}\int \mathrm{Cos}[\phi]\frac{r^2}{v b}\mathrm{d}\phi \\
&= \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{v b}\int \mathrm{Cos}[\phi]\mathrm{d}\phi
\end{aligned}
$$

Central Force Scattering

- this implies

$$\Delta p = \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{v\, b}\left(\mathrm{Sin}[\phi_2] - \mathrm{Sin}[\phi_1]\right)$$

- according to the geometry of the scattering process,

$$\phi_1 = -\phi_0, \quad \phi_2 = +\phi_0, \quad 2\phi_0 + \theta = \pi$$

- it follows that

$$\mathrm{Sin}[\phi_2] - \mathrm{Sin}[\phi_1] = 2\,\mathrm{Sin}\left[\frac{\pi}{2} - \frac{\theta}{2}\right]$$

- combining this with the above equation for Δp yields

$$\Delta p = \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{v\, b}\left(2\,\mathrm{Sin}\left[\frac{\pi}{2} - \frac{\theta}{2}\right]\right) = \frac{2}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{v\, b}\mathrm{Cos}\left[\frac{\theta}{2}\right]$$

Central Force Scattering

- this yields a relationship between the impact parameter b and the scattering angle θ:

$$b = \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{M_1 v^2}\,\mathrm{Cot}\left[\frac{\theta}{2}\right] = \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{2E}\,\mathrm{Cot}\left[\frac{\theta}{2}\right]$$

- using the previous equation

$$2\pi b\,\mathrm{d}b = -\sigma[\theta]\cdot 2\pi\,\mathrm{Sin}[\theta]\mathrm{d}\theta,$$

the scattering cross-section can be expressed as

$$\sigma[\theta] = -\frac{b}{\mathrm{Sin}[\theta]}\frac{\mathrm{d}b}{\mathrm{d}\theta}$$

Central Force Scattering

- inserting the geometrical relationships

$$\mathrm{Sin}[\theta] = 2\,\mathrm{Sin}\left[\frac{\theta}{2}\right]\mathrm{Cos}\left[\frac{\theta}{2}\right]$$

$$\mathrm{d}\,\mathrm{Cot}\left[\frac{\theta}{2}\right] = -\frac{\mathrm{d}\theta}{2\,\mathrm{Sin}[\theta/2]^2}$$

yields the cross-section originally derived by Rutherford:

$$\sigma[\theta] = \left(\frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{4E}\right)^2 \frac{1}{\mathrm{Sin}[\theta/2]^4}$$

Central Force Scattering

- the closest approach d of the scattered particle to the target particle is given by equating its kinetic energy to its potential energy at a distance d away from the core of the target particle:

$$d = \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{E}$$

- inserting this into the Rutherford expression for the scattering cross-section yields

$$\sigma[\theta] = \frac{(d/4)^2}{\mathrm{Sin}[\theta/2]^4}$$

- for $\theta = \pi$ this yields

$$\sigma[\pi] = (d/4)^2$$

Central Force Scattering

- for 2 MeV He ions ($Z_1 = 2$ incident on Ag ($Z_2 = 47$) this yields a closest particle–scatterer distance of

$$d = 6.8 \cdot 10^{-5}\,\mathrm{nm}$$

⇒ much (!) smaller than the Bohr radius
(radius of a hydrogen atom, $5 \cdot 10^{-2}$ nm)

- the cross-section for scattering to $\theta = \pi$ is

$$\sigma[\theta] = 2.98 \cdot 10^{-10}\,\mathrm{nm}^2 = 2.89 \cdot 10{-}28\,\mathrm{m}^2 \equiv 2.89\,\mathrm{barn}$$

$1\,\mathrm{barn} := 10^{-28}\,\mathrm{m}^2$

Conclusion

- conclusions for materials scientists:

The use of an unscreened cross-section is justified.

RBS is a powerful, quantitative method.

- conclusion for physicists and philosophers:

THE WORLD IS "EMPTY!"