Beam-specimen interactions

1) SCATTERING

- Interaction of electron with matter
- Elastic vs. inelastic scattering
- Electron trajectory
- Monte Carlo simulations

Beam – Specimen Interactions

Electron optical system controls:
- Beam voltage (1 – 50 keV)
- Beam current (pA – µA)
- Beam diameter (5 nm – 1 µm)
- Divergence angle

Small beam diameter is the first requirement for high spatial resolution.

Ideal: Diameter of area sampled = beam diameter
Real: Electron scattering increases diameter of area sampled = volume of interaction
**Types of scattering**

- **Elastic**
  - Inelastic

**Elastic scattering**

Direction component of electron velocity vector is changed, *but not magnitude.*

\[
\begin{align*}
\text{Target atom} & \quad \Phi_e \\
E_0 & \quad E_i \\
E_i & = E_0 \\
E_i & = \text{instantaneous energy after scattering} \\
\Rightarrow & \quad \text{Kinetic energy } \sim \text{ unchanged} \\
& \quad <1\text{eV energy transferred to specimen}
\end{align*}
\]

**Types of scattering**

- Elastic
  - Inelastic

**Inelastic scattering**

*Both direction and magnitude* components of electron velocity vector *change.*

\[
\begin{align*}
\text{Target atom} & \quad \Phi_i \\
E_0 & \quad E_i \\
E_i & < E_0 \\
E_i & = \text{instantaneous energy after scattering} \\
\Rightarrow & \quad \text{significant energy transferred to specimen} \\
\Phi_{\text{inelastic}} & < \Phi_{\text{elastic}}
\end{align*}
\]
**Elastic scattering**

Electron deviates from incident path by angle $\Phi_c$ (0 to 180°).

Results from interactions between electrons and coulomb field of nucleus of target atoms screened by electrons.

Cross section described by screened Rutherford model, and cross-section dependent on:

- atomic # of target atom
- inverse of beam energy

![Elastic Scattering Graphs](image)

**Inelastic scattering processes (1/2)**

1) **Plasmon excitation**

   Beam electron excites waves in the “free electron gas” between atomic cores in a solid (~ valence electron).

2) **Phonon Excitation**

   Excitation of lattice oscillations (phonons) by low energy loss events (<1eV)
   
   - Primarily results in heating

3) **Secondary electron emission**

   Semiconductors and insulators
   - Promote valence band electrons to conduction band
   - These electrons may have enough energy to scatter into the continuum
   - Low energy, mostly < 10eV

   In metals, conduction band electrons easily energized => can scatter out
Inelastic scattering processes (2/2)

4) Continuum X-ray generation (Bremsstrahlung)
   - Electrons decelerate in the coulomb field of target atoms
   - Energy loss converted to photon (X-ray) \( \Rightarrow \) Energy 0 to \( E_0 \)
   - Forms background spectrum
   - Depends on material density or average atomic number (Z-bar)

5) Ionization of inner shells
   - This is what interest us the most, as it produces X-ray characteristic of the analyzed material!

![Characteristic X-rays](image)

Electron with sufficiently high energy interacts with target atom

- Excitation: Ejects inner shell electron
- Decay (relaxation back to ground state):
  - Characteristic X-ray
  - Auger electron

Interaction volume

Scattering processes operate concurrently

- **Elastic scattering**
  - Beam electrons deviate from original path – diffuse through solid

- **Inelastic scattering**
  - Reduce energy of primary beam electrons until absorbed by solid
  - Limits total electron range

**Interaction volume = region over which beam electrons interact with the target solid**

- Deposits energy
- Produces radiation
- Three major variables
  - 1) Atomic #
  - 2) Beam energy
  - 3) Tilt angle

![Diagram](image)
Bethe equation:

\[ S = -\frac{dE}{dx} = 785 \frac{Z\rho}{AE} \ln \left( \frac{1.166E}{I} \right) \text{ (in eV/Å)} \]
Mean free path $\lambda$ and cross section $Q$ *inversely* correlated

Mean free path increases…

- With decreasing $Z$ and density
- With increasing beam energy *(except at very low voltage < 70 eV)*

Results in *volume of interaction*

$\Rightarrow$ Smaller interaction volume for…

- Higher $Z$ (∼ density)
- Lower beam energy

However…

**Interaction volume ≠ emission volume**

Interaction volume

Experimental evaluation at 20 keV of interaction volume using the etching method in polymethylmethacrylate (PMMA ∼ transparent thermoplastic)
Monte Carlo simulations

Length of step?
Mean free path of electrons between scattering events

Choice of event type and angle
• Random numbers
• Game of chance

- Can study interaction volumes in any target
- Detailed history of electron trajectory
- Calculated in step-wise manner

<table>
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<tr>
<th>Material</th>
<th>Density (g/cm³)</th>
<th>Z</th>
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<tbody>
<tr>
<td>Albite</td>
<td>2.62</td>
<td>11</td>
</tr>
<tr>
<td>Monazite</td>
<td>5.15</td>
<td>38</td>
</tr>
<tr>
<td>Gold</td>
<td>19.3</td>
<td>79</td>
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</table>
Mean Atomic Number $Z$ (or "Z-bar")

Mean atomic number reflects the average atomic number $Z$ of all atoms in a crystal. Function of atomic number AND the atomic weight of each atom:

$$
\bar{Z} = \frac{\sum W_i A_i Z_i}{\sum W_i A_i}
$$

- $W_i$: Atomic weight of $i$
- $A_i$: Site multiplicity
- $Z_i$: Atomic number

Example: FeTiO$_3$

$$
\bar{Z} = \frac{2889.24}{151.72} = 19.04
$$

<table>
<thead>
<tr>
<th>Atom</th>
<th>$W_i$</th>
<th>$A_i$</th>
<th>$Z_i$</th>
<th>$W_iA_iZ_i$</th>
<th>$W_iA_i$</th>
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<tbody>
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<td>26</td>
<td>1452.10</td>
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<tr>
<td>Ti</td>
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<td>1</td>
<td>22</td>
<td>1053.14</td>
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<tr>
<td>O</td>
<td>16.00</td>
<td>3</td>
<td>8</td>
<td>384.00</td>
<td>48.00</td>
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<tr>
<td>TOTAL</td>
<td></td>
<td></td>
<td></td>
<td>2889.24</td>
<td>151.72</td>
</tr>
</tbody>
</table>
Scattering

Key concept:
Cross section or probability of an event (likelihood of interaction between particles)

\[ Q = \frac{N}{n_t n_i} \text{ in cm}^2 \]

- \( N \) = # events / unit volume
- \( n_t \) = # target sites / unit volume
- \( n_i \) = # incident particles / unit area

Large cross section = high probability for an event

Mean Free Path

From knowledge of cross sections, can calculate mean free path \( \lambda \)

\[ \lambda = \frac{A}{N_0 \rho Q} \]

- \( A \) = atomic wt.
- \( N_0 \) = Avogadro’s number (6.02 x 10^{23} \text{ atoms/mol})
- \( \rho \) = density
- \( Q \) = cross section

Smaller cross section = greater mean free path
Mean Free Path in some solids

Mean free path in solids is in the order of 10-1000 Å, variable depending on the electron energy.

For ~15 keV electron energy, the mean free path in most solids is ~90 to 500 Å.

Inelastic scattering

Energy transferred to target atoms.
Kinetic energy of beam electrons decreases.

Note: Lower electron energy will now increase the probability of elastic scattering of that electron

Five principal inelastic scattering processes...

1) Plasmon excitation
2) Phonon Excitation
3) Secondary electron emission
4) Continuum X-ray generation (Bremsstrahlung)
5) Ionization of inner shells
Total scattering probabilities

Elastic events dominate over individual inelastic processes.

Max Born (~1926) Theory of atomic collisions
⇒ stopping power for a point charge travelling through a solid.

Hans Bethe 1930 Evaluates passage of charged particles through matter
⇒ probabilities of elastic and inelastic interactions.

From this, you can calculate the resulting range and energy of the charged particle, and with the ionization rate, the expected intensity of characteristic radiation.

Bethe’s ionization equation: the probability of ionization of a given shell (nl)

\[
\sigma_{nl} = \frac{6.51 \times 10^{-14}}{E_0 E_{nl}} Z_{nl} b_{nl} l n \left[ \frac{c_{nl} E_0}{E_{nl}} \right] \text{ cm}^2
\]

- \( E_0 \) = electron voltage
- \( E_{nl} \) = binding energy for the nl shell
- \( Z_{nl} \) = number of electrons in the nl shell

Bethe parameters

\[
b_{nl} = \text{“excitation factor”}
\]
\[
c_{nl} = 4E_{nl} / B_0 \quad (B \text{ is an energy ~ ionization potential})
\]

There are a number of important physical effects to consider for EPMA, but perhaps the most significant for determination of the analytical spatial resolution is electron deceleration in matter...

Rate of energy loss of an electron of energy \( E \) (in eV) with respect to path length, \( x \):

\[- \frac{dE}{dx}\]

⇒ Purpose of lab 4 (Monte Carlo simulations…)

9 – 22
Bethe's remarkable result: stopping power...

\[ S = -\frac{dE}{dx} = 2\pi e_0^4 N_0 Z\frac{\rho}{AE} \ln \left( \frac{\sqrt{e/2} E}{J} \right) \]

\( E \) = electron energy (eV)
\( x \) = path length
\( e \) = 2.718 (base of \( \ln \))
\( N_0 \) = Avogadro constant
\( Z \) = mean atomic number
\( \rho \) = density
\( A \) = atomic mass
\( J \) = mean excitation energy (eV)

Function of material density and “mean” atomic number

Or...

\[ S = -\frac{dE}{dx} = 785 \frac{Z\rho}{AE} \ln \left( \frac{1.166E}{J} \right) \text{ (in eV/Å)} \]

= rate of energy loss \( dE \) with distance travel \( dx \)

Joy and Luo (1989)

\[ S = -\frac{dE}{dx} = 785 \frac{Z\rho}{AE} \ln \left( \frac{1.166(E + k J_{exp})}{J_{exp}} \right) \text{ (in eV/Å)} \]

Modify with empirical factors \( k \) and \( J_{exp} \) to better predict low voltage behavior

Also: value of \( E \) must be greater than \( J / 1.166 \) or \( S \) becomes negative!
**Electron range**

What is the depth of penetration of the electron beam?

**Bethe Range**

\[
R = \int_{E_0}^{E=0} \frac{1}{dE/ds} \, dE
\]

Bethe equation:

\[
S = -\frac{dE}{dx} = 785 \frac{Z\rho}{AE} \ln \left( \frac{1.166E}{J} \right) \text{ (in eV/Å)}
\]

Approximation of \( R \) ... Henoc & Maurice (1976)

\[
R (cm) = \frac{f^2}{7.85 \times 10^4 \rho Z} \left[ EI \left( 2\log_e \frac{1.166E_0}{J} \right) - EI \left( 2\log_e \frac{1.166E_l}{J} \right) \right]
\]

**Kanaya – Okayama range:** approximates interaction volume dimensions

\[
R_{KO} = 0.0276 \ A \ E_0^{-0.67} / Z^{0.89} \rho
\]

- \( E_0 \) beam energy (keV)
- \( \rho \) density (g/cm³)
- \( A \) atomic wt. (g/mol)
- \( Z \) atomic #

**Monte Carlo electron path demonstrations**

- Backscatter electron
- Electron “dying” inside material
**Casino (2002)** McGill University
A. Real Couture, D. Drouin, R. Gauvin, P. Hovington, P. Homy, H. Demers

**Win X-Ray (2007)** Adds complete simulation of the X-ray spectrum and the charging effect for insulating specimens
McGill University group with E. Lifshin

**SS MT 95** (David Joy, modified by Kimio Kanda)

### Run and analyze effects of differing...
- Atomic Number
- Beam Energy
- Tilt angle

### Note changes in...
- Electron range
- Shape of volume
- BSE efficiency

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**Labradorite** \(-\text{Na}_{0.5}\text{Ca}_{0.5}\text{Al}_{1.5}\text{Si}_{2.5}\text{O}_{8}\). \(Z = 11\) at 15 kV
Labradorite [\( \sim \text{Na}_{3.5}\text{Ca}_{0.5}\text{Al}_{1.5}\text{Si}_{2.5}\text{O}_{8}, Z = 11 \)]
at 15 kV

Energy contours