2. Overview of penetration mechanisms of energetic particles in matter
2.1. Penetration concepts

- For radiation penetrating matter (below the top atom layer) one can define:
  - **Mean depth ≈ Mean range** *(medeldjup, medelräckvidd, keskisyvyys, keskikantama)*
  - **Depth profile** *(djupprofil, syvyysjakauma)*: concentration distribution of implanted particles
  - **Straggling** *(spridning, leveys?)*: spread of depth profile, usually defined as the standard deviation of the mean
  - **Lateral straggling** *(lateral spridning, lateraalinen leveys)*: spread in lateral direction
Mathematical expressions

- These can be calculated using the usual mathematical expressions for probability distributions.

- A depth profile is in essence a probability distribution.

- Assume the depth profile is known as $c(z)$, and surface is at $z=0$. $c(z)$ obviously has to $> 0$ for all $z$.

- Then:
  - Total concentration of implanted material: $C = \int_{0}^{\infty} c(z)dz$
  - Mean range $\bar{R} = \frac{1}{C} \int_{0}^{\infty} zc(z)dz$
  - Straggling $\sigma = \frac{1}{C} \int_{0}^{\infty} (z - \bar{R})^2 c(z)dz$

- Also any other probability distribution concept can be used, e.g. median, skewness (*snedhet/vinous*), kurtosis (*kurtosis, huipukkuus*), full-width-half-maximum, etc.
Other terminology

- **Reflection** (*reflektion / sironia*): particle does not penetrate at all but is reflected
  - Or actually may penetrate to some depth but then is reflected back
- **Deposition** (*deposition / depositio*): particle stays in the substrate
  - This can be both deposition above the surface or deeper in
- **Sticking** (*stickande/klibbning / kiinnittyminen*): particle sticks on top of surface
- **Sputtering** (*sputring eller förstoftning / sputrautminen tai roiskuminen*): particles from inside material are kicked out due to the radiation process
Related measures

- **Reflection** (*reflektion / sironta*): measured with reflection coefficient, i.e. fraction of particles reflected (*reflektionskoefficient / sirontatekijä*)

- **Deposition** (*deposition / depositio*): measured with fraction of deposited particles

- **Sticking** (*stickande/klibbning / kiinnittyminen*): measured with sticking coefficient (*stickningskoefficient / kiinnittymistekijä*)

- **Sputtering** (*sputring eller förstoftning / sputrautminen tai roiskuminen*): measured with sputtering yield (*koefficient/utbyte / tuotto*) = number of outcoming atoms / number of incoming ions
Radiation exposure conditions

- Radiation impacting on a material can be monoenergetic or have an energy spread.
- It can come at a well-defined incoming angle (inkomstvinkel / sisääntulokulma) or with an angular distribution.
  - If it is a beam, it usually has a pretty precise incoming angle.
  - Beam spread: in reality even beams always have some spread, can be e.g. ± 0.5°. This is often ignored as insignificant.
- Accelerators typically have a well-defined energy, beam and angle θ. Simplified picture.
2.2 Overview of penetration

- A key aspect for the penetration of particles with matter is whether they are neutral or charged.
- Neutral particles do not interact with the electromagnetic force, and hence interact weakly with matter -> big ranges
  - MeV Neutrons: meters!
    - Scattering depends on mass difference, most efficient scattering by same mass particles = protons
    - Hence water good to slow down neutrons in nuclear reactors
  - Gammas: centimeters
    - E.g. 1 MeV gamma: 8 mm in lead, 44 mm in concrete

http://www.ndt-ed.org/EducationResources/HighSchool/Radiography/penetrationdepth.htm
Overview of penetration

- Charged particles interact strongly: likely lots of scattering, only small range
  - Electrons: E.g. 1 MeV electrons in Copper, adjacent equation by Potts gives 350 µm
  - Ions:
    - 1 MeV protons in Cu: 380 nm,
    - 1 MeV Au ions in Cu: 96 nm
    [Numbers from SRIM]

\[
x (\mu m) = \frac{0.1 \ E_0^{1.5}}{\rho}
\]

where \( E_0 \) = accelerating voltage (keV), and \( \rho \) = density (g/cm\(^3\))

http://www4.nau.edu/microanalysis/Microprobe/Interact-Volume.html
Overview of penetration

- Illustration [wikipedia]:
  - A sheet of paper is enough to stop alphas
  - An aluminum sheet enough to stop electrons
  - Gammas need more
  - Neutrons need meters of material
Illustration 2

Interaction of ionizing radiation with matter

α → bremsstrahlung
β → δ-electron
γ → n capture photon
n → recoil proton

charged particles interact strongly and ionize directly
neutral particles interact less, ionize indirectly and penetrate farther

[wikipedia: ionizing radiation]
2.2.1 Photons

- High-energy photons penetrating matter when slowing down can ionize electrons with the photoelectric effect and Compton scattering.
  - These in turn can excite atoms, and when these decay, they create additional photons.
    - These in turn can create additional ionized electrons.
    - These can create more photons…

- The end result is known as **electron-gamma cascades**
  (**elektron-gamma kaskader, elektroni-gamma-kaskadi/ryöppy**)

  - If the energy is higher than > 1022 keV, it can also produce electron-positron pairs, known as pair production.
    - Limit due to rest mass of electron, 511 keV.
Electron-gamma cascades

- From the explanation above, it is clear that both electrons and gammas can induce electron-gamma-cascades.
- Hence the penetration of both gammas and electrons can and are often treated with the same codes.
- Concept works down to energies ~ 100 eV – 1 keV.
  - Below that, e’s and γ’s do no longer behave particle-like but quantum wave functions => very difficult to model and understand.
2.2.1 Electrons

1. See above! High-energy single electron penetration is similar to gammas.
2. But a beam of monoenergetic electrons at energies around 100 keV are the basis of transmission electron microscopy (TEM) operation, and in that case can be treated in a wave mechanics way.

- TEM operation can be well understood and modelled with waves, which scatter from the electrons of atoms as scattering centers.
- There is no paradox here, the issue just reflects the basic quantum mechanical particle-wave duality, i.e. that depending on aim, matter can be either treated as particles or waves.
Electron – nucleus knock-ons

- Electrons can also with a small but not insignificant probability hit nuclei.
- This (usually) is an elastic binary collision governed by classical kinematics.
- Often (e.g. in TEM’s) main source of radiation damage.
- Basic classical binary collision equations give the maximum energy transfer to an atom of mass $m_{atom}$ as

$$E_{\text{max,atom}} = \frac{4 m_{\text{electron}} m_{\text{atom}}}{(m_{\text{electron}} + m_{\text{atom}})^2} E_{\text{electron}}$$

where $E_{\text{electron}}$ is the kinetic energy of the electron and $E_{\text{max,atom}}$ the maximum energy an atom can receive.
Electron – nucleus knock-ons

However, for high electron energies one needs to use the relativistic kinematics version of this equation, which is

\[ E_{\text{max, atom}} = \frac{2ME (E+2mc^2)}{(m+M)^2c^2+2ME} \]

where the notation has been shortened with

\[ m_{\text{electron}} = m, \ m_{\text{atom}} = M, E_{\text{electron}} = E \]

Of course the probability of a direct knock-on leading to the maximum energy transfer is very small, but this is still an important equation since it allows calculating the threshold displacement energy.
McKinley-Feshbach equation

- Calculation of the full displacement probability is complicated, but the McKinley-Feshbach equations provide a good approximation [Phys. Rev. 74 (1948) 1759]
  - Useful reference on implementation: [Lucasson, Phys. Rev. 127 (1962) 485]
- Cross section is slightly complicated:

\[
\sigma = \frac{4 Z^2 E_R^2}{m^2 c^4} \left( \frac{T_{\text{max}}}{T_{\text{thr}}} \right) \pi a_0^2 \left( \frac{1 - \beta^2}{\beta^4} \right) \left\{ 1 + 2 \pi \alpha \beta \left( \frac{T_{\text{thr}}}{T_{\text{max}}} \right)^{1/2} \right\} 

- \frac{T_{\text{thr}}}{T_{\text{max}}} \left[ 1 + 2 \pi \alpha \beta + (\beta^2 + \pi \alpha \beta) \ln \left( \frac{T_{\text{max}}}{T_{\text{thr}}} \right) \right] \right\}
\]

(5)

where \( Z \) is the atomic number of the displaced atom, \( E_R \) the Rydberg energy (13.6 eV), \( a_0 \) the Bohr radius of the hydrogen atom \( (5.3 \times 10^{-11} \text{ m}) \), \( \beta = v/c \), and \( \alpha = Z/137 \). It can be seen that \( \sigma \) increases with increasing \( Z \), therefore heavier atoms should be displaced more easily; however, due to momentum conservation (equation (3)), the energy transfer is lower. At very high projectile energies \( (E \gg E_d) \) a higher displacement rate can be expected for heavier atoms.

McKinley-Feshbach equation

- This is widely used still as sort of a standard, but it is good to remember it is approximate.
- Right top is a comparison to experiments from the original paper.
- Right bottom: decrease of cross section with energy.

Figure 5. Comparison of theory and experiment at electron energy of 2 Mev. The solid line is given by the theory. The triangles give the experimental points as obtained by Van de Graaff, Buechner et al.

Figure 3. Differential cross section $d\sigma/d\Omega$ of the displacement of a carbon nucleus by an electron as a function of the energy $T$ transferred to the nucleus ($E = 1$ MeV, $T_0 = 10$ eV).

Comparison of electron interaction cross sections

- For carbon atoms:

Table 1. Cross sections $\sigma$ for the interaction of electrons (100 keV) with an agglomerate of carbon atoms (Coslett 1978).

<table>
<thead>
<tr>
<th>Process</th>
<th>$\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ionization</td>
<td>$2.0 \times 10^6$ barn</td>
</tr>
<tr>
<td>Plasmon excitation</td>
<td>$1.5 \times 10^6$</td>
</tr>
<tr>
<td>X-ray emission (K-shell)</td>
<td>$2.5 \times 10^4$</td>
</tr>
<tr>
<td>Displacement of an atom</td>
<td>$1.8 \times 10^2$</td>
</tr>
<tr>
<td>Elastic collision (diffraction)</td>
<td>$10^6$</td>
</tr>
</tbody>
</table>

[Coslett, 1978 J. Microsc. 113 113–29]

- Hence the atom displacement cross section is indeed small, but it can be dominating for damage production, since in many materials ionization does not produce any damage...
2.2.3 Neutrons

- Neutrons do not interact significantly with electrons, but mainly with atomic nuclei via the nuclear forces.
- Since the radius of nuclei and the range of the nuclear forces is of the order of fm (femtometers), the collision probability is very small => hence the long ranges of neutrons in matter.
- Neutrons can interact with several different processes with the atoms, the most important of which are:
  1. Elastic scattering
  2. Inelastic scattering
  3. \((n,2n)\) reactions
  4. \((n,\gamma)\) reactions
Elastic neutron scattering

- The elastic neutron scattering can be calculated with classical kinematics, similar to electrons.
- But since the nature of the interaction is different, it is not exactly the same equations.
Elastic neutron cross sections

The calculation gives

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

with

$$\gamma = \frac{4mM}{(M + m)^2}$$

where $E_i$ is the initial energy of the neutron of mass $m$, $T$ is the energy transferred to the atom of mass $M$, and $\phi$ is the scattering angle in center-of-mass coordinates (see picture on previous page)
Elastic neutron cross sections

- The angular dependence is as follows
- The maximum corresponds to a knock-on collision for backward scattering of the neutron, and is the same equation as given for maximum energy transfer for electrons
- A further calculation (see Was sect. 1.1.1) gives as an example the following values for the average energy transfer in a collision:

\[ T \approx \frac{\gamma E_i}{2} \]

- 1 MeV n on C: \( \gamma = 0.28 \quad \tilde{T} = 0.14 \text{MeV} \)
- 1 MeV n on Fe: \( \gamma = 0.069 \quad \tilde{T} = 0.035 \text{MeV} \)
- 1 MeV n on U: \( \gamma = 0.017 \quad \tilde{T} = 0.009 \text{MeV} \)
Inelastic neutron scattering

- Inelastic neutron scattering becomes important for neutron energies above 1 MeV
- It means scattering of a neutron such that the kinetic energy is not preserved, but goes into a excitation of the (potential) energy of the nucleus
- Written as a nuclear reaction equation: $^A\text{X}(n,n')^A\text{X}^*$ where $^A\text{X}$ is the isotope (e.g. $^{14}\text{N}$ or $^{11}\text{B}$) and the asterisk $^*$ denotes that the nucleus has become excited
(n,2n) reactions

- This class of nuclear reactions becomes significant above 8 MeV [Was]
- It means nuclear reactions of the type $^A_X (n,2n) ^{A-1}X$
(n,γ) reactions

- The (n,γ) reactions are important at thermal neutron energies, e.g. in nuclear reactors for $^{235}\text{U}$.
- They mean reactions where a nucleus absorbs a neutron, but the process releases a γ photon, $^A\text{X}(n, \gamma)^{A+1}\text{X}$.
- This is significant for damage production because the nucleus gets a recoil energy from the emitted gamma particle (since also photons have a momentum $p = E/c$).
- The recoil energy the atom receives is of the order of a few 100 eV’s, which is enough for damage production!
Total neutron effects

- The calculation of neutron effects of materials is complicated by the fact that neutron spectra in nuclear reactors are very complicated in shape.
- Different energies have different reactions, so the total damage estimation requires integration over the neutron spectra, all reactions and damage production.

[M.R. Gilbert et al 2012 Nucl. Fusion 52 083019]
2.2.4 Ions

- Energetic ions interact with matter with 3 different mechanisms:
  1. Collisions with nuclei/atom cores
  2. Collisions with electrons, via several different mechanisms
  3. At high energies via nuclear reactions

- The ion-nucleus collisions are at high energies classical binary collisions under a Coulomb repulsive potential

- Since the ion mass is much higher than that of the electrons, the interaction with electrons slows down the ion, but does not change its path

- The nuclear reactions can (as for neutrons) be very complicated
The slowing down process of an ion impacting on a surface can be roughly illustrated as follows:

- Collisions with electrons
- Collisions with nuclei

Ion penetration depth

[Picture: Kai Nordlund]
Animation of slowing down

- Computer simulation for 30 keV Xe impacting on Au
  - Each sphere an atom, cross section picture
  - More on these simulations later
The concept of stopping power

Since the electronic collisions only slow down the ion, and the number of collisions is at high energies large, the effect of the electrons can be considered to be an average frictional force slowing down the ion

This is known as the **electronic stopping power** (elektronisk uppbromsning / elektroninen jarruuntuminen)

The collisions with ions can also be averaged and then considered a nuclear stopping power (nukleär uppbromsning / ydinten välinen jarruuntuminen?)

The nuclear reactions can also be averaged and considered a nuclear reaction stopping power (kärnreaktionsuppbromsning / ydinreaktiojarruuntuminen)
Stopping power

- The total stopping power can be then written as

\[ S = S_n + S_e + S_{\text{reactions}} \]

- The typical energy dependence of these is qualitatively typically as follows:
  - The estimates for the energies are very rough!

![Graph showing log stopping power vs. log energy with different contributions labeled: Sn, Se, and Sreactions.]

- Bragg peak (not to be confused with x-ray Bragg peaks!)
Energy dependence

- The shape of these curves explains why the earlier plot showed straight path atom motion initially, when electronic stopping dominates, and then more curved and dense collisional region when nuclear collisions become significant.
- More on this later
Charge states, ion vs. atom vs. recoil

- An interesting question is, what is the charge state of an ion after it enters a material!? 

- At energies corresponding to low electronic stopping powers, below the Bragg peak, the ion loses its initial charge state after penetrating a couple of atom layers, and after that is essentially neutral
  
  - A more scientific way of putting the same thing: when its velocity is below the Fermi velocity of the material, it moves within the Born-Oppenheimer approximation, and its charge state is the same as if it would be at rest

  [this is known experimentally from so called hollow atom studies]
This implies that for velocities below the Bragg peak, the ‘history’ of the ion/atom does not matter.

Hence damage production by implanted ion, or atomic recoils produced by neutrons, electrons or gammas are only a function of the initial kinetic energy of the moving ion/atom, i.e.

\[
\text{Damage} = \text{Damage(Initial Energy)}
\]

Moreover, it means that wrt. damage production below the Bragg peak, “ion=atom=recoil”

This is a major simplification for predicting damage production!
What produces the actual damage? Good news-2

- In metals, excited electrons do not (with very few exceptions) produce damage.
- In ionic and organic materials they may, in semiconductors occasionally.
- Hence in metals and usually in semiconductors, all damage is produced by the atomic recoils – regardless of whether they come from $\alpha$, $\beta$, $\gamma$ particles or neutrons.
  - And also in ionic materials, the atomic recoils often dominate.
- Because of this, a separate chapter is dedicated to the issue of damage production by atoms in materials.
What happens around and above the Bragg peak?

- Around and above the Bragg peak in stopping power?
- Around the Bragg peak, the ion has some memory of its previous charge state, and above it strong memory
  - The ion is in some highly charged state
- In non-metallic materials, the high level of electronic excitations can produce damage directly in the material
  - Nuclear stopping insignificant = no atomic collisions
- Since the ion at the same time moves in an essentially straight path, this implies that one produces straight tracks of damage in the material
Swift heavy ions

- This regime is known as the **swift heavy ion** (*rask tunga jon / ripeä raskas-ioni*) one
  - Damage known as ion tracks (*jonspår / ioniraita*)
- Occurs in nature due to natural radioactive decay
- Are produced by high-energy accelerators, now a hot topic for research
  - Fundamental mechanism by which swift ion electron excitations translate into the track damage not known!
  - Intense current research

http://www.detectingdesign.com/radiometricdating.html
Ion track production threshold

- The tracks are only observed to be produced above some materials-specific threshold in the stopping power.
- Hence a limited energy range around the Bragg peak in stopping.

[Review on swift heavy ions: D. Kanjijal, Current Science, 80(12):1560, 2001]
Computer simulation codes

- There is a range of computer software for simulating the ion penetration
- Many kept up by a software database at the OECD Nuclear Energy Agency (NEA) in Paris
- Neutronics:
  - SPECTR for neutron recoil spectra, NJOY, etc.
- Photons and electron-gamma cascades:
  - EGS4 – a modular tool that can be implemented in various geometries, PENELOE
- Wide-purpose radiation transport on the meso- and macroscopic scale:
  - FLUKA, GEANT4 (especially for radiation detectors in particle accelerators in space)
What should you have learned from this section?

- You know the basic concepts for radiation penetration, reflection, surface interactions, etc.
- You know how to characterize a particle penetration depth profiles
- You know the basics of how deep different kinds of particles penetrate in materials, and roughly what the physical mechanisms are behind this
- You understand that many different kinds of irradiation eventually produce the final damage by knock-on atoms