B. Reiserf

EXAM, Atomic and Molecular Interactions 2014 Ia (Schlathölter), 6/11/2014, 10:00-12:00

1. **Rutherford scattering**

   1.5 MeV α-particles impinge on a very thin gold foil (Z_{Au}=79) with carbon contaminations.

10 a) What is the distance of closest approach between α-particle and a gold/carbon atom? How does this compare to nuclear size and typical radial distributions of atomic electrons? Why is this comparison relevant for Rutherford scattering?

10 b) What is the impact parameter of α-particles scattered through 90°?

10 c) Draw a sketch of the backscattering spectrum with energetic positions and relative heights of the peaks. Discuss the spectrum. How would the spectrum change, if the contaminated gold foil was much thicker? How would it change, if the carbon had the form of a thin film on top of the thick gold foil?

2. **Stopping power**

   Over a wide range of kinetic energies, ions moving through matter lose their energy predominantly by interactions with electrons.

10 a) Sketch the electronic stopping power curve as a function of ion kinetic energy. Explain, why the curve has a maximum. Explain why different mechanisms dominate at high and low kinetic energy, respectively. Does the curve look qualitatively similar for electrons, antiprotons and neutrons?

9 b) In a Rutherford backscattering experiment, 10 MeV H ions interact with an Aluminum target covered by a 100 nm thick layer of water (H_2O, density: 1 g/cm^3). Use the Bethe-Bloch formula, to estimate the kinetic energy of those α-particles, which were backscattered from Aluminium atoms directly behind the water layer.

9 c) Radiotherapy with energetic photons or MeV ions can be used to treat tumors, because the deposited energy can e.g. induce DNA damage via various mechanisms. It is currently under investigation, if metal nanoparticles (e.g. Gold (Z=79), Platinum (Z=78)) in the tissue can improve the cancer-cell killing effect of the radiation for energetic photons and MeV ions. What could the mechanism be?

3. **Charge exchange**

7 a) Consider the charge exchange reaction $O^{8+}+H \rightarrow O^{7+}+H^+$ and determine the cross section using the classical overbarrier model. Into which O^{7+} n-level is the electron predominantly captured?

8 b) Sketch the electron capture cross section in ion-atom collisions as a function of collision energy. Discuss the three different capture mechanism that play a role in the different energy regimes.

8 c) Assume the charge exchange reaction $O^{8+}+N \rightarrow O^{5+} + N^{3+}$. The 3 electrons are captured into higher lying O n-levels. Discuss, how such a highly excited "hollow" system de-excites into the ground state. Why can the de-excitation be a problem for the experimental determination of the cross section?

4. **Molecular physics**

   What is the Born-Oppenheimer approximation and why is it important?

6

87/100

Exam A&M I 2014; Bernd Rietberg; 5190597.

Exercise (1)

(1) a) Closest Approach:

$$d_{min} = \frac{z_1 z_2}{E} =$$

$z_1 = 2$

$z_2 = 79; 6$

$E = \frac{1,5 \cdot 10^6}{27,2}$

$$d_{min,C} = \frac{2 \cdot 6}{1,5 \cdot 10^6 / 27,2}$$

$= 2,2 \cdot 10^{-4}$ a.u.

$= 2,2 \cdot 10^{-4} \cdot 5,29 \cdot 10^{-11}$ m

$= 1,2 \cdot 10^{-14}$ m

$= \underline{1,2 \cdot 10^{-5}}$ nm, For Carbon

Gold $\rightarrow d_{min} = \frac{2 \cdot 79}{1,5 \cdot 10^6 / 27,2} = 2,9 \cdot 10^{-3}$ a.u.

$\rightarrow 2,9 \cdot 5,29 \cdot 10^{-3} \cdot 10^{-11} = 1,5 \cdot 10^{-13}$ m

$= \underline{1,5 \cdot 10^{-4}}$ nm For Gold

An atoms radius is in the order of Angstrom (Å), or 10^{-10} m, therefore this is much smaller than the radius of the atom; ie. the electron distribution radius. On the other hand, it is larger than the radius of the nuclei.

This is important, because For Rutherford Scattering to occur, the distance of closest approach must be ~~[illegible]~~ smaller than the radial distribution of the electrons ~~[illegible]~~, and larger than the radius of the nuclei, so that no nuclear reactions will occur, and we have a Roughly coulomb- or partly shielded coulomb-interaction between the nuclei → Rutherford Scattering.

(1) b) impact Parameter ($\Theta = 90°$)

$$b = \frac{z_1 z_2}{2E}$$

$z_1 = 2$; $Z_2 = 79$; $E = \frac{1,5 \cdot 10^6}{27,2}$

$Z_2 = 79$ $b = 1,4 \cdot 10^{-3}$ a.u. For Gold.

$Z_2 = 6$ $b = 1,1 \cdot 10^{-4}$ a.u. For Carbon.

(1) c) Backscatter energies:

$$\frac{E_1}{E_0} = K = \frac{(M_2 - M_1)^2}{(M_2 + M_1)^2} \rightarrow E_{1,gold} \approx \left(\frac{197-4}{197+4}\right)^2 E_0$$

$$= 0,92\ E_0 = 1,4\ MeV$$

✓

$$E_{1,carbon} = \frac{(12-4)^2}{(12+4)^2} E_0$$

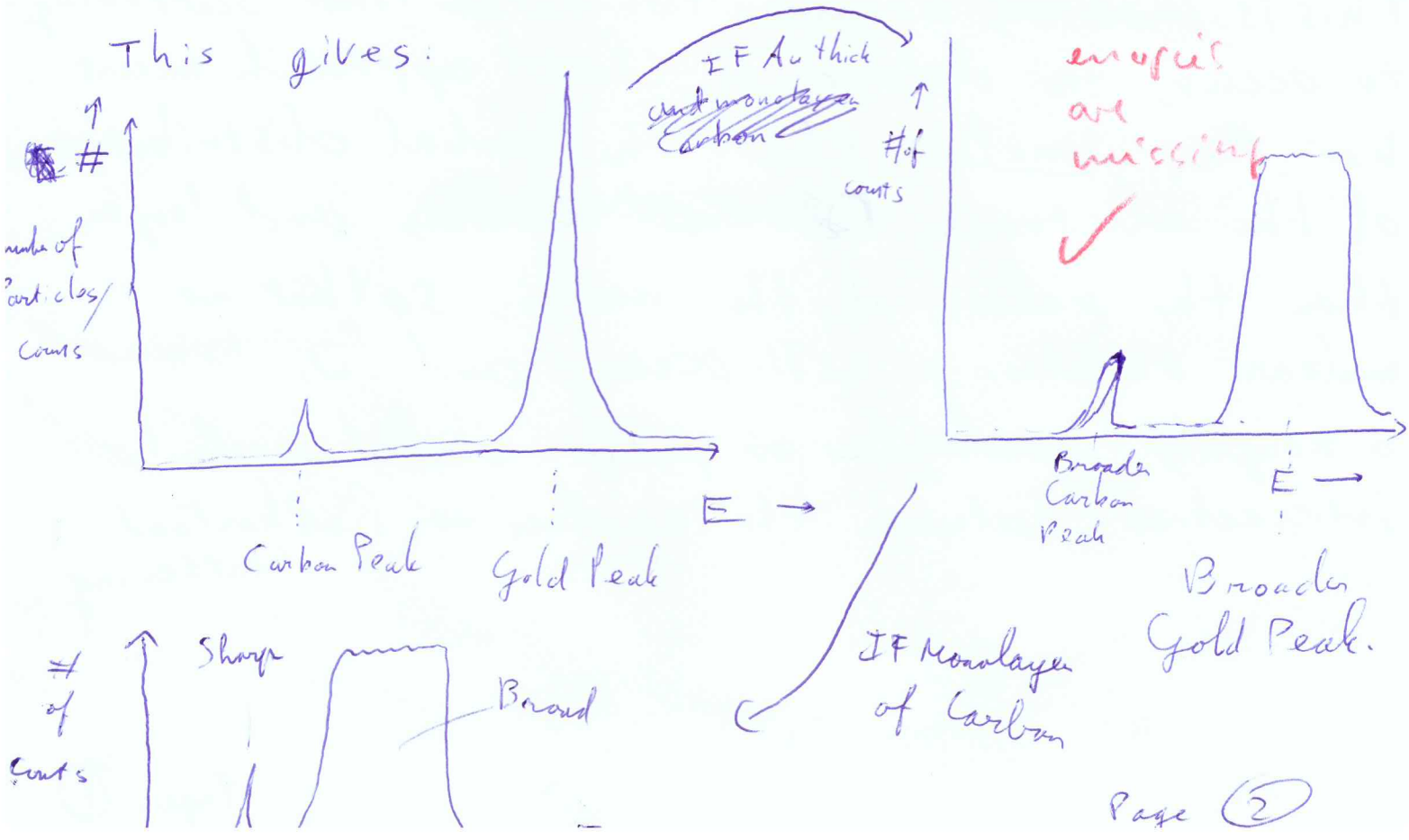
$$= \frac{1}{4} E_0 = 0,38 MeV.$$

Relative Heights:

$$\frac{\delta_A}{\delta_B} = \frac{Z_A^2}{Z_B^2} = \frac{6^2}{79^2} \rightarrow \delta_A = \frac{6^2}{79^2}\delta_B = 0,0058\ \delta_B$$

✓

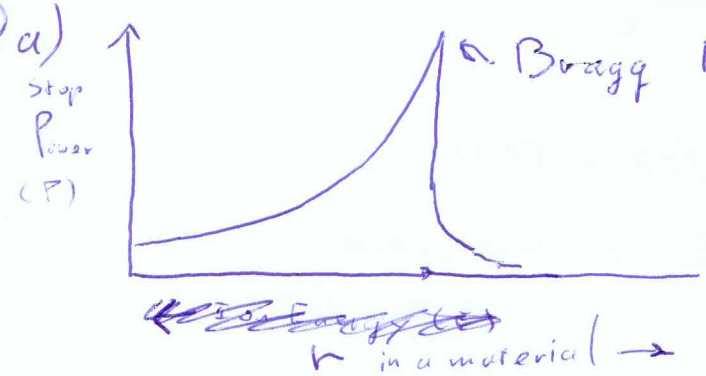
This gives:

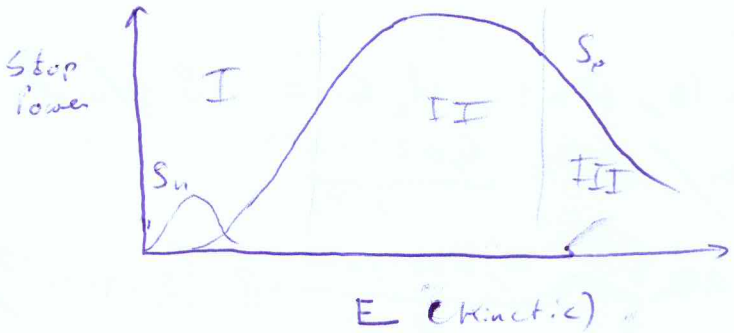


Exam A&MI 2014, Bernd Rietberg
S1905597

Exercise (2)

2a)





As one can see in the top picture, ions interact much more with matter as their energy decreases.
The second Picture shows the Stopping Power vs Energy
In the low energy Regime, There is more interaction with the environment with increasing E_x. (I)
But, at High energies, the Interaction Cross Section becomes smaller with increasing E (Due to very short interaction times), thus resulting in a downwards Curve. (III)
In the intermediate regime, (II), one goes from the High to the Low interaction, thus resulting in a maximum

For e^- and p^-; this would be similar because these are charged particles, and thus interact with electrons.
For Neutrons, it would not Because these are not Charged Particles and thus interact differently with

2b) Bethe Bloch:

$$\frac{-dE}{dx} = \frac{4\pi Z_1^2}{m_e v^2} n \ln \frac{2 m_e v^2}{I}$$

{ $Z_1 = 1$ and θ

{ $I = 10 \cdot Z_1\ eV = 10 Z_1 / 27,2$ a.u.

{ $v^2 = \frac{2E}{M} = \frac{2 \cdot 10^7 / 27,2}{1836} = 400,0$ a.u.

Determination of n_O and n_H.

n_O: # el per unit Volume:

- Atomic Weight of Water: $O = 16$; $H = 1$: $H_2O = 18$ g/mol.
- number of Water Particles / cm³: $\frac{6,022 \cdot 10^{23}}{18}$.

→ number of Oxygen electrons per a.u.³: $\frac{6,022 \cdot 10^{23}}{18} \cdot 8 \cdot (5,29 \cdot 10^{-9})^3$

$$n_O = 0,040 \text{ O.el/a.u.}^3$$

n_H: $\frac{6,022 \cdot 10^{23}}{18} \cdot 2 \cdot (5,29 \cdot 10^{-9})^3 = 0,010$ H.el/a.u.³

$$\frac{-dE}{dx} = \frac{4\pi}{400} 0,040 \ln \frac{400 \cdot 2}{(10/27,2)} + \frac{4\pi 8^2}{400} \cdot 0,04 \ln \frac{400 \cdot 2}{(80/27,2)}$$

$$= 0,453 \text{ a.u.}$$

$$\rightarrow -\frac{dE}{dx} = \frac{0,453 \cdot 100 \cdot 10^{-9}}{27,2} = 3,9 \cdot 10^{-12} \text{ eV}?$$

→ Energy of the incoming H (10 MeV) stays roughly the same.

$$K = \frac{E_1}{E_0} = \frac{(M_2 - M_1)^2}{(M_2 + M_1)^2} \rightarrow E_1 = \frac{(27-1)^2}{(27+1)^2} \cdot \frac{10 \cdot 10^6}{27,2}$$

$$= 3,17 \cdot 10^5 \text{ eV}$$

a.u.

Exam A&MI 2014; Bernd Richberg S1905599

Exercise 2c & 3.

(2c) One can see from the Bethe-Bloch formula that Heavy nanoparticles absorb more ion energies. element
Thus, Gold and Platinum nanoparticles would simply heat up alot, destroying the surrounding tissue.

Nanoparticles could be tuned so that they absorb very strongly in the ~~UV~~ regime of the ~~X-ray~~ photon-Radiotherapy-beam. Thus, the Photons would be much more absorbed, again heating and destroying the surrounding tissue. For ~~Radio~~ Photon-therapy, this might increase the focus of the deposited energy, thus leaving other tissue intact. For ion therapy, this would also be the case, but that's a far less problem than with Photon therapy

(3a) $\delta = \pi \cdot R_c^2 = \pi \cdot \left(\frac{1+2\sqrt{q}}{IP_H} \right)^2$

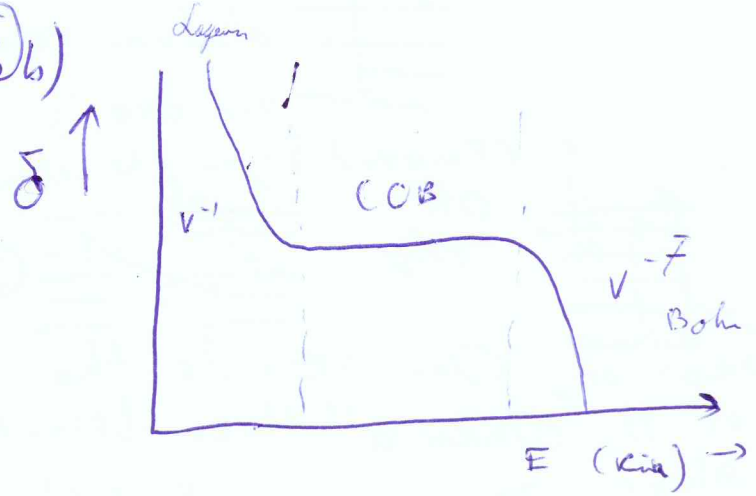
$IP_H = 13,6\ eV = \frac{13,6}{27,2}\ a.u. = 0,5\ a.u.$

$\delta = \pi \cdot \left(\frac{1+\sqrt{8}}{0,5} \right)^2 = 184\ a.u.^2$

Which n-level?:

$E = \frac{q^2}{2n^2} \Rightarrow n = \sqrt{\frac{q^2}{2E}} = \sqrt{\frac{8^2}{1,0}} = 8.$

(3b)

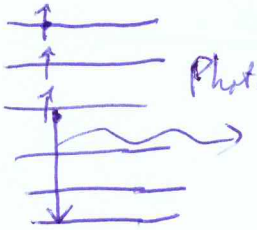


As one can see, for low energies, the probability of electron capture goes with $1/v$ of the ion. This is the Lagevin-region, and is the 'Chemistry' region. It has to do with the polarizability of the ions.

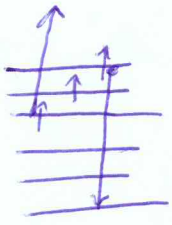
In the Over Barrier Regime, there is much less interaction time, thus polarizability does not play a role. Here, the probability is constant with V.

In the Bohr or High energy regime, the electrons get 'stripped' from the ion, and there is very little chance for electron capture by the ion. This is because the interaction time is Very low/small ✓

(3)c) This can be by a variety of de-excitations. For instance, a 'normal' de-excitation can occur;



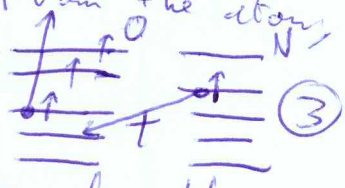
Or an Auger desexitation;



Where one electron relaxes and one is removed from the atom;

Or other Auger's like:

OR



To determine the Cross Section, One needs the IP's of The first 3 electrons of N. When all these different Relaxation-Mechanisms take place, one can not find the right value of the IP's of N; For instance $N^{2+} \rightarrow N^{3+}$. ✓

Also, Mechanisms as described in Figure (3) can happen, which

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Exercise (4)

(4) The Born-Oppenheimer approximations states that the WaveFunction describing states of energy in atoms, can be rewriten in terms of an electronic, Vibrational, Rotational and nuclear part.

$$\Psi = \Psi_{el.} \cdot \Psi_{vib.} \cdot \Psi_{Rot} \cdot \Psi_{nucl.}$$ (✓)

Usually, the Wave Functions are determined with Fixed nuclei that are at an optimized distance.

It is important because it drastically reduces the number of variables needed to calculate certain excitations. Also, it gives us a nice view of how electronic transitions take place, e.g. vibrational vs electronic excitations

With this model, one can define transitions, guess their relative energies and oscillator strengths (Vibrational is low energy relative to el. for instance), etc.