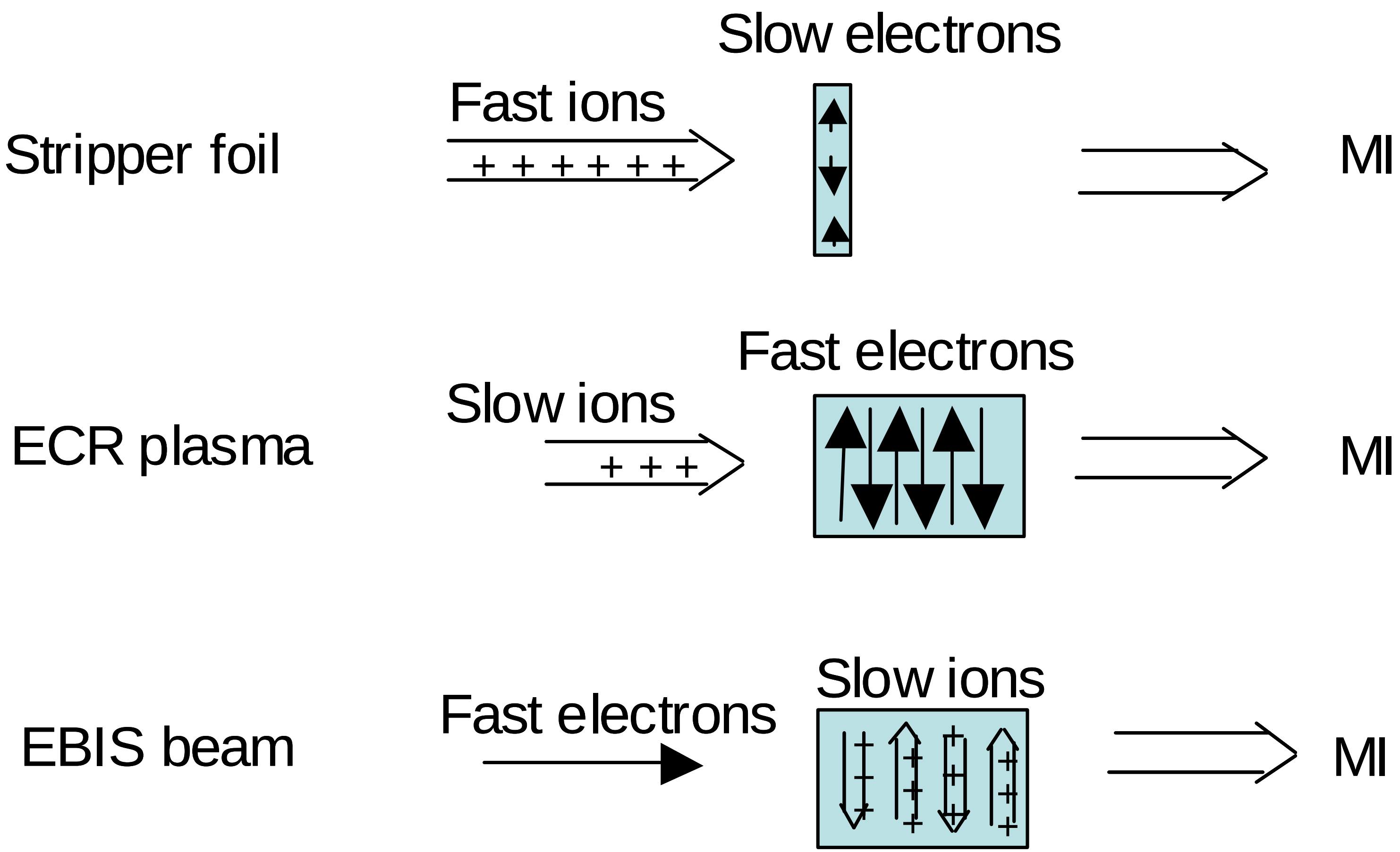
2) Ionisation: Electron impact ionisation and photo ionisation



The electron impact ionisation is the most fundamental ionisation process and most important for ion sources.

The cross section for the impact ionization is by orders of magnitudes higher than the cross section for the photo ionization.

The cross section depends on the mass of the colliding particle. Since the energy transfer of a heavy particle is lower, a proton needs for an identical ionization probability an ionization energy three orders of magnitudes higher than an electron.

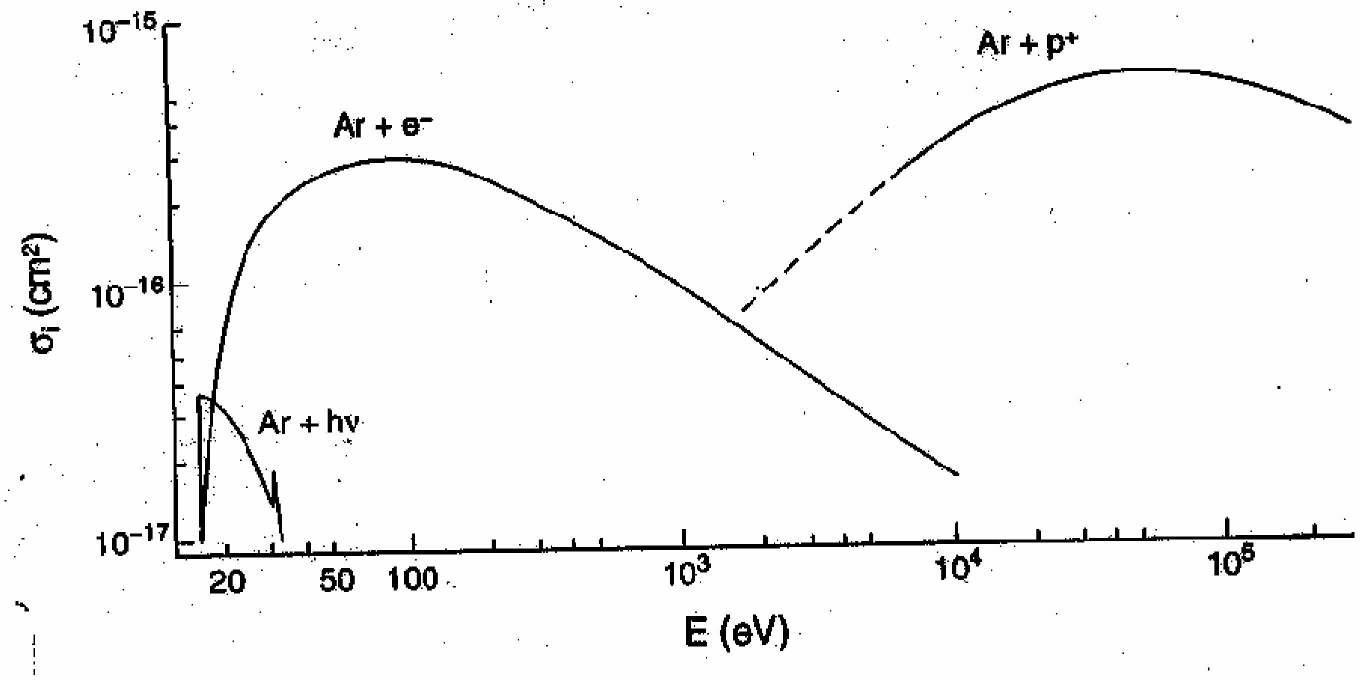
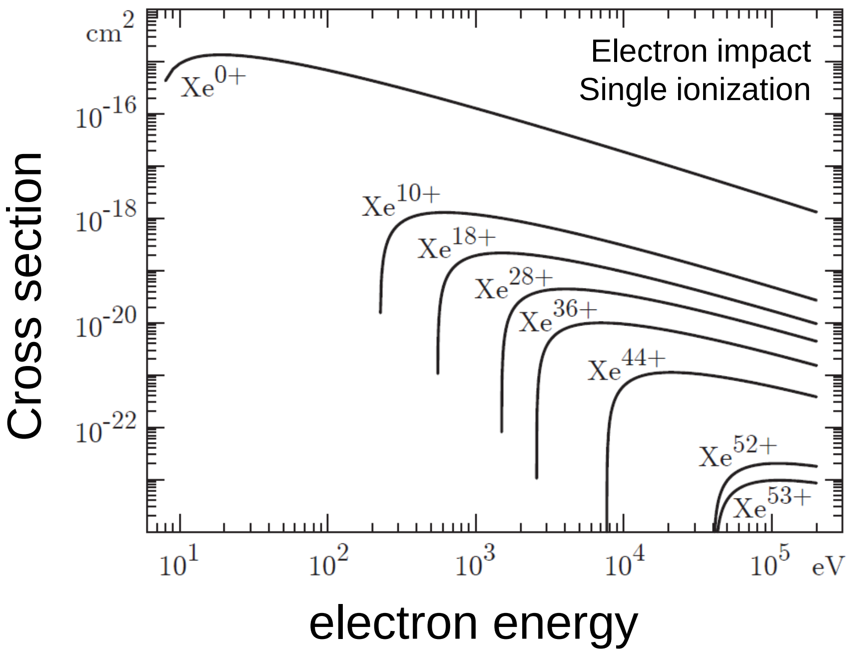
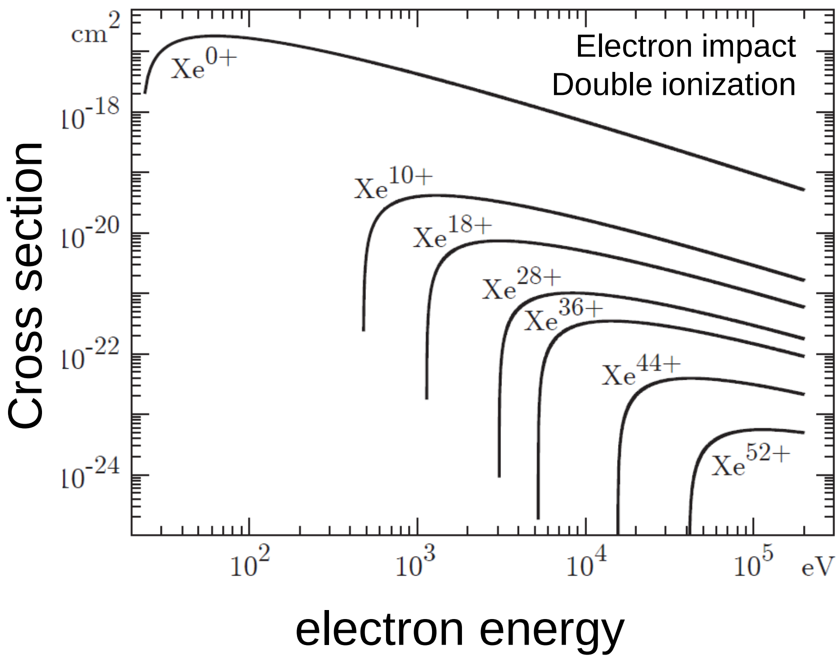


FIGURE 4
Ionization cross sections as functions of energy for ionizing collisions with fast electrons, protons, and photons. (From Winter, H., in *Experimental Methods in Heavy Ion Physics*, Springer-Verlag, Berlin, 1978. With permission.)

There are two different possibilities to produce multiple charged ions:

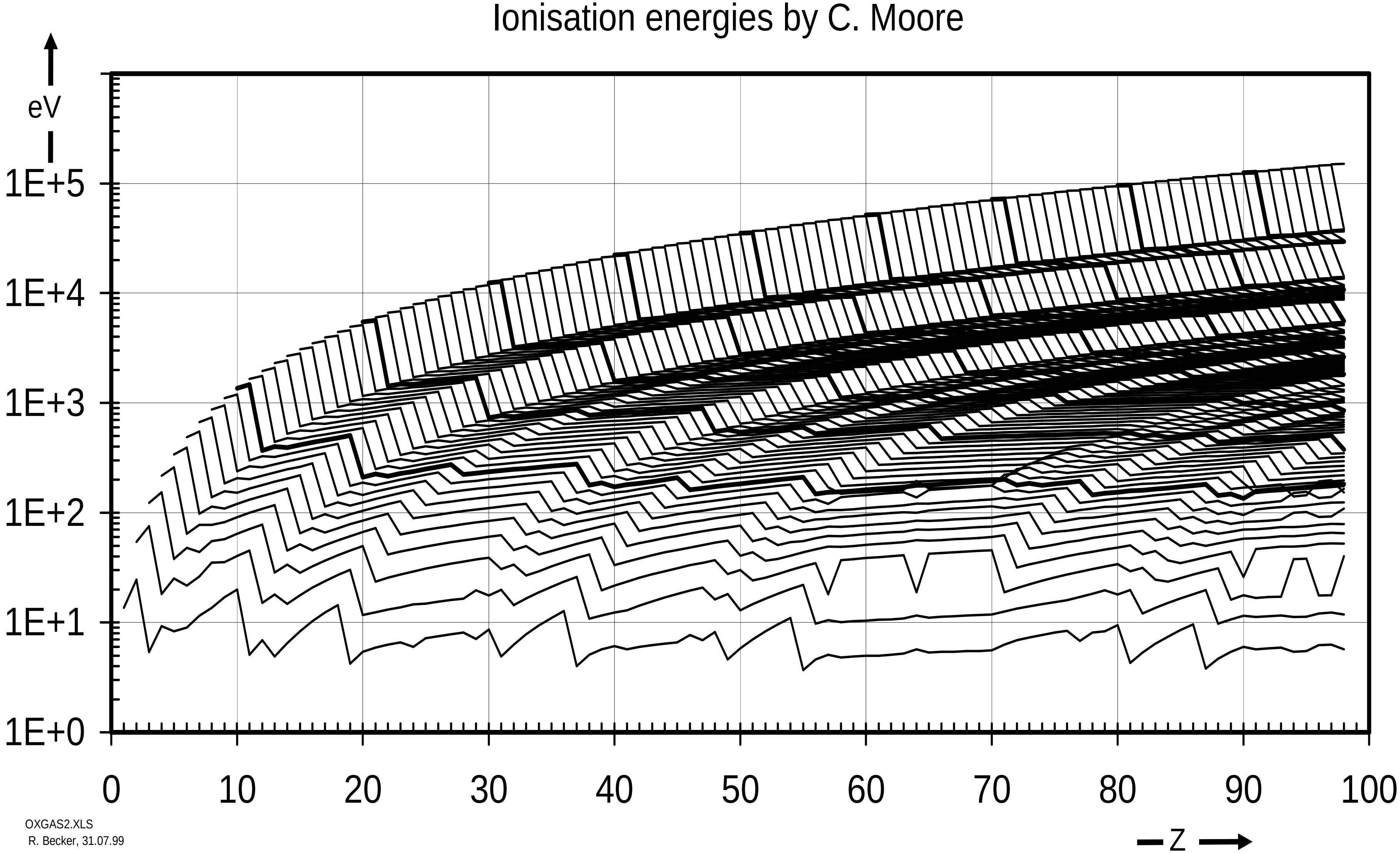
- in a single collision where many electrons are removed from the ion (double-ionization, triple-ionization, etc.
- multistep or successive ionization, where only one electron is removed per collision and high charge states are produced in different collisions





For energetic reasons the ionization releasing only one electron from the atomic shell is the most probable process. To produce highly charged ions the kinetic energy of the projectile electrons has to be at least equivalent to the n-th ionization potential.

- Ionisation energies up to 100 keV (U^{91+} --> U^{92+}) (see graphic below)
- shell structure of the atomic shells is clearly visible



Successive Ionisation: $A + e^- = A^+ + 2e^-$

The probability for removing one electron and changing the charge state of the ion from q→ q+1 is determined by the cross section $\sigma_{q \rightarrow q+1}$ [cm^2].

Are the cross sections for the successive ionization known, the average ionization time of the ions with charge state q can be approximated from the collision frequency:

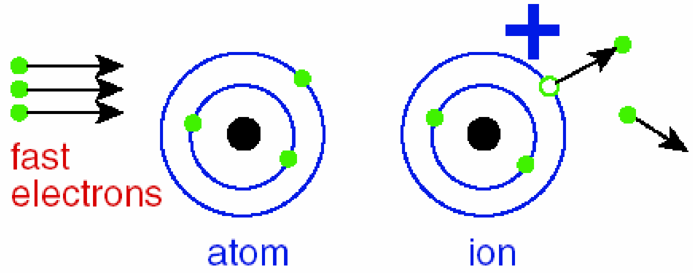
$$\nu_{q\rightarrow q+1} = n_e \cdot n_q v_e \sigma_{q\rightarrow q+1} \quad \left[\frac{1}{m^3 s}\right] \qquad (2.1)$$

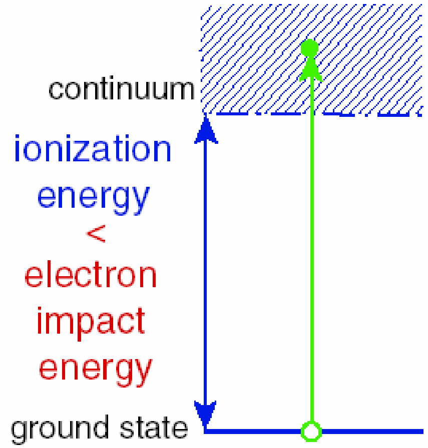
The time between to ionizing collisions is

$$\bar{\tau}_{q\rightarrow q+1} = \frac{n_q}{\nu_{q\rightarrow q+1}} = \frac{1}{n_e v_e \sigma_{q\rightarrow q+1}} = \frac{e}{j_e \sigma_{q\rightarrow q+1}} \qquad (2.2)$$

This applies to electrons with a well-defined kinetic energy.

$$j_e \cdot \bar{\tau}_{q\rightarrow q+1} = \frac{e}{\sigma_{q\rightarrow q+1}} \qquad (2.3)$$

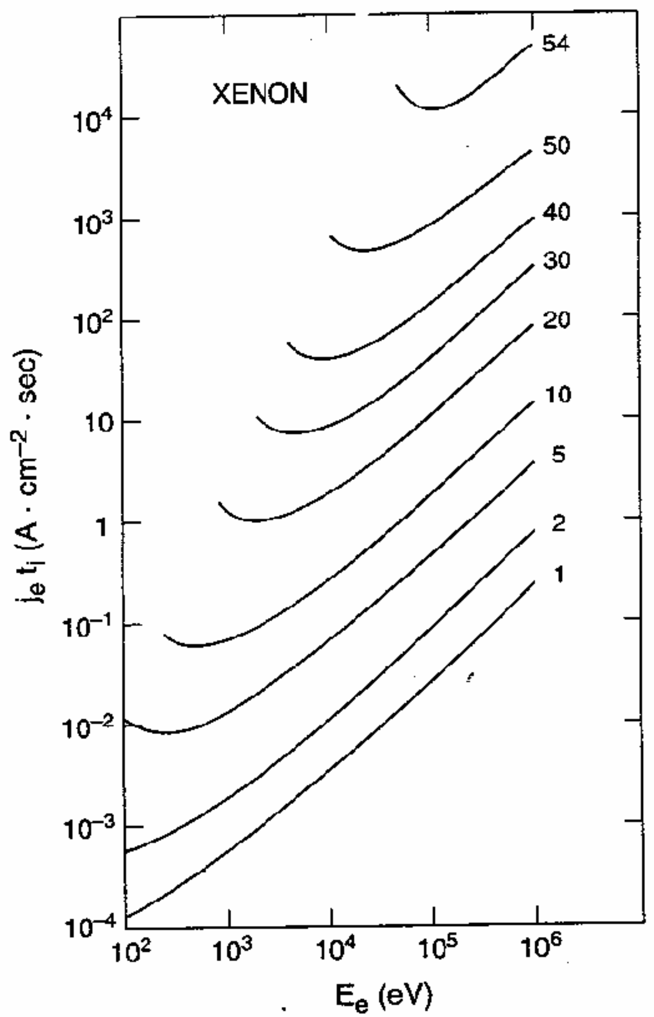




Principle of ionization by electron impact.

The average ionization time in the charge state q depends only on the cross section and the current density. This expression is called **IONISATION FACTOR**. (Sometimes it is defined as only the inverse cross section!) The average time necessary to reach the charge state q is therewith:

$$\bar{\tau}_q = \sum_{i=0}^{q-1} \bar{\tau}_{i\to i+1} = \frac{e}{j_e} \sum_{i=0}^{q-1} \frac{1}{\sigma_{i\to i+1}} \qquad (2.4)$$



Example on the right side:
The ionization factor j_e*t for different charge states of Xe, depending on the electron energy.

Approximation of the cross section and the ionization time for the production of bare ions from H-like ions using the Mosley's law for X-ray frequencies emitted in transitions from the continuum to the K-shell:

$$E_{i\to k}(Z) = 13.6 \cdot Z^2\,[eV] \quad \Rightarrow \quad \sigma_{z-1\to z} = 4.5 \cdot 10^{-14} \cdot \frac{\ln e}{e \cdot 13.6^2 Z^4} = \frac{9 \cdot 10^{-17}}{Z^4} \qquad (2.5)$$

Wherein $E = e \cdot E_{i\to k}(Z)$ ➔

$$j_e \tau_{z-1\to z} = \frac{e}{\sigma_{z-1\to z}} \approx \frac{eZ^4}{9 \cdot 10^{-17}} \approx \left(\frac{Z}{5}\right)^4 \qquad (2.6)$$

Argon can be ionized by 10 keV electrons,
ions of the heavy elements by up to 100 keV electrons and Uranium by 150 keV electrons. The resulting values for the ionization energy, cross section and ionization factor are summarized in the table on the left side.

Approximation of the cross section in quantum-mechanical calculations done by Bethe (1930) using the Born Approximation:

Scattering of a matter wave at a central potential V(r) for $E_{kin} >> E_{ion}$ (perturbation theory).
All electrons in an atom or ion contribute with their individual σ_{ei} to the total cross section σ, as long as the kinetic energy E_{kin} of the projectile is larger than the ionization energy P_i of these electrons.

Approximate Ionization Energies, Ionization Cross Sections, and Required jτ Values for Bare Ions

Ion	E_i(eV)	σ(cm²)	jτ(Cb/cm²)
C^{6+}	490	7.7×10^{-20}	2.1
N^{7+}	666	4.2×10^{-20}	3.8
O^{8+}	870	2.4×10^{-20}	6.5
Ne^{10+}	1360	1×10^{-20}	16
Ar^{18+}	4,400	9.5×10^{-22}	170
Kr^{36+}	17,600	6×10^{-23}	2,700
Xe^{54+}	39,700	1.2×10^{-23}	13,600
Pb^{82+}	91,400	2.2×10^{-24}	72,300
U^{92+}	115,000	1.4×10^{-24}	115,000

$$\sigma_{q\rightarrow q+1} = \sum_{i=1}^{N} \sigma_i = \sum_{i=1}^{N} q_i \sigma_{ei}$$

N = Number of subshells

All q_i electrons of the subshell contribute to the σ_i of the shell. The cross section for the ionization of the (n, l) - shell results from integration of the transition probabilities over all states n', l'→ k und the integration over the collision vector

$$\vec{q} = \frac{2\pi}{h} M(\vec{v} - \vec{v}')$$

with v before and v' after the collision. On receives

$$\sigma_i^{nl} = const \cdot Z_{nl} \frac{1}{E_{kin} E_{nl}} \ln\left(\frac{E_{kin}}{E_{nl}}\right)$$

Bethe et al., Ann. Physik 5 (1930) 325

For practical reasons the semi-empirical formula developed by Lotz 1967 for the energy dependence of the cross sections for the elements from H to Ca and for energies < 10 keV is commonly used. The error is given by maximal 10%.

The Lotz formula for the case of high ionization energies $E_{kin} >> P_i$ is:

$$\sigma_{q \to q+1} = 4.5 \cdot 10^{-14} \cdot \sum_{i=1}^{N} \frac{\ln\left(E_{kin} / P_i\right)}{E_{kin} \cdot P_i} \quad \left[\mathrm{cm}^2\right]$$

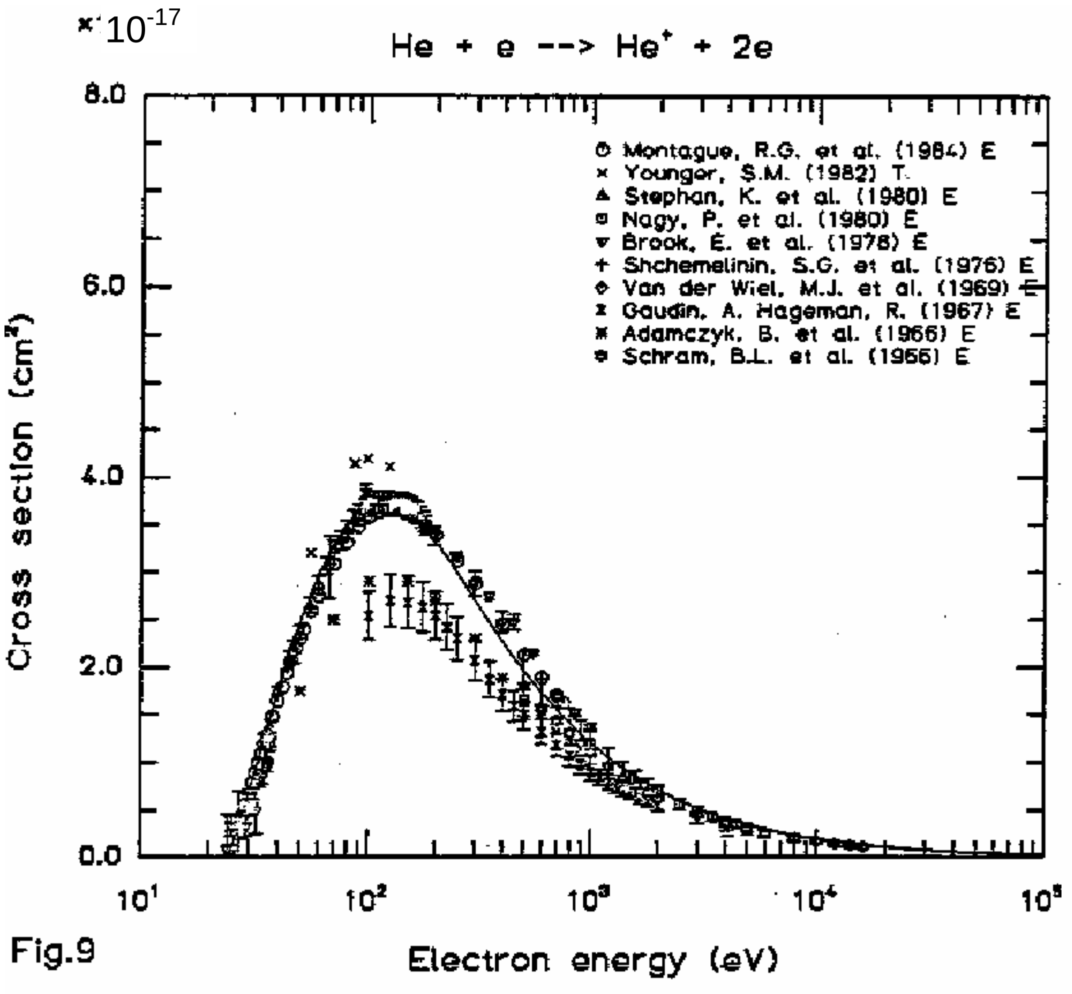
$P_i = E_{nl}$, N-subshells (2.7)

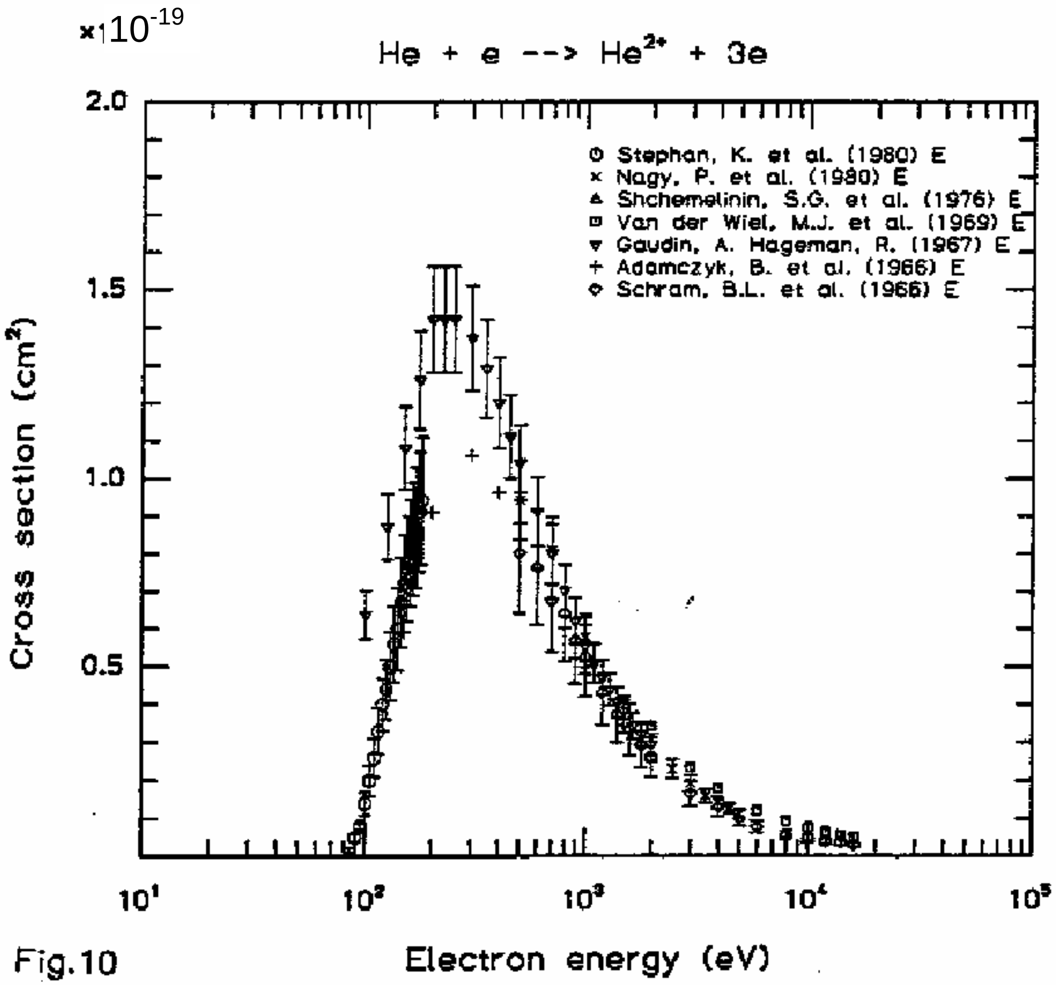
This expression is mostly used in calculations of the charge state distribution.

Examples for the dependence of the cross sections on the energy are shown for the case of He. The higher the initial charge state, the smaller is the cross section. Moreover the cross section is higher for atoms in an excited state.

Single ionisation

Multi-ionisation of He





Ionization of the excited state

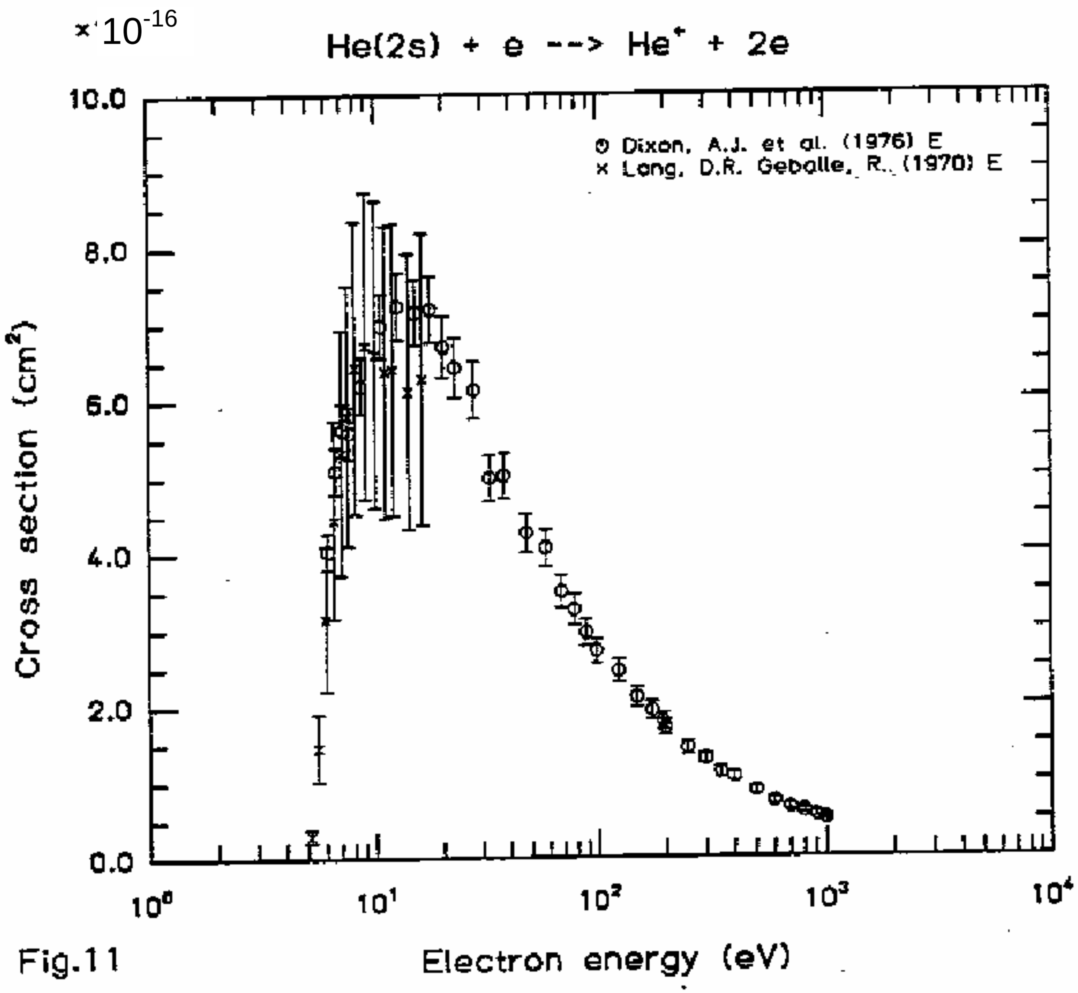


Fig.11

Ionisation of singly charged He

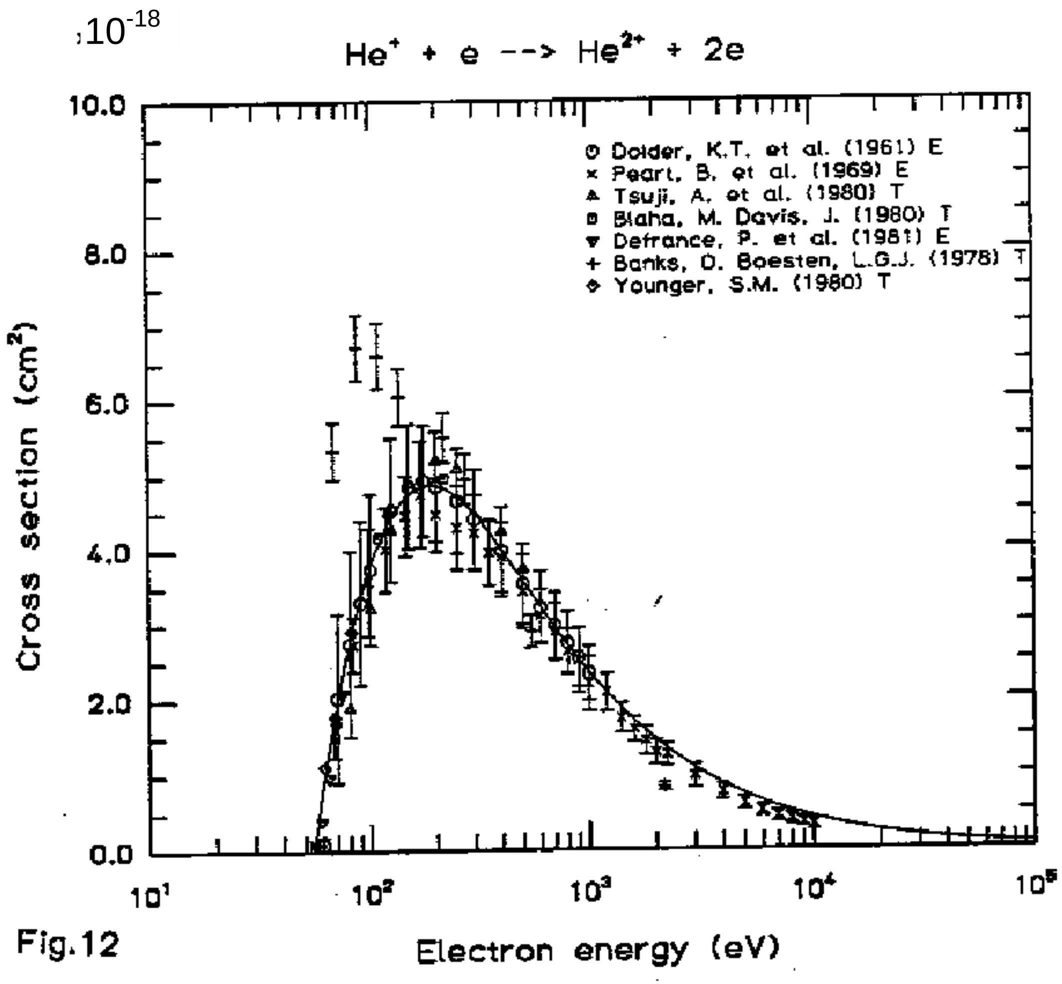


Fig.12

<u>Carlson-Correction for ionization energies:</u>

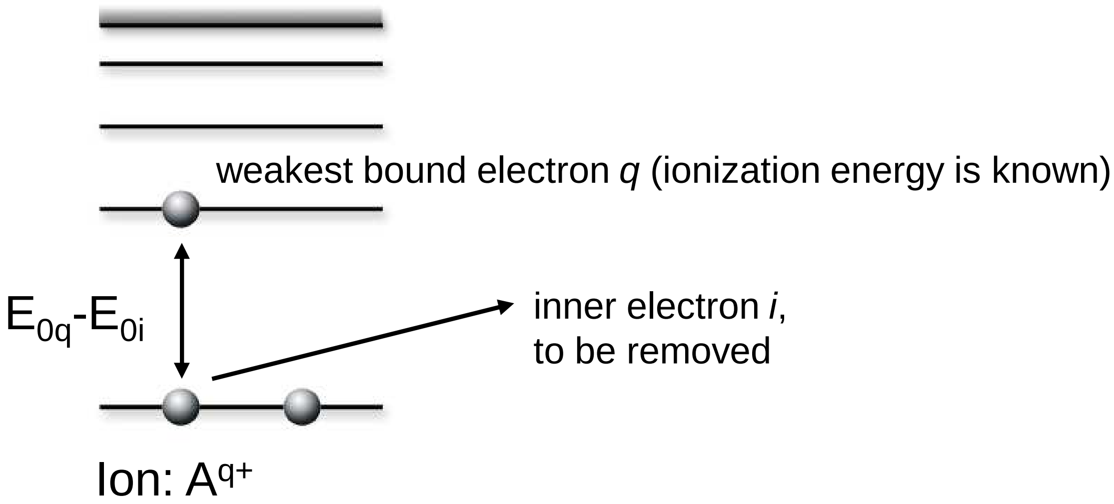
The ionization energies $P_{q,i}$ for ions with different charge states q, which does not describe the weakest bound electron are sometimes difficult to find in literature. They can be approximated with the Carlson-Correction (*T. A. Carlson et al., ORNL-4562 UC-34-Physics*).

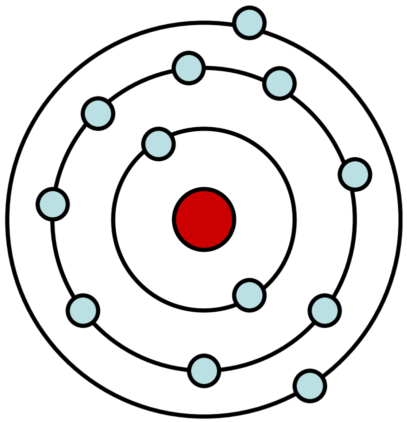
The ionization energy Pq,i is calculated from the ionization energy $W_i(q)$ of the ion with charge state q and the atomic binding energies of the electrons as follows:

$$P_i = E_{0i} + W_i(q) - E_{0q} \qquad (2.8)$$

E_{0i} = Binding energy of an electron in the i-th shell of the atom

E_{0q} = atomic binding energy of the electron, which is the weakest bound electron in the ion of the charge state q.





Because σ(E) has a maximum at a certain energy, the ionization factor j_e*τ has a minimum there. Basically the cross section for the last electron, which is removed, determines the ionisation time.

The optimal energy is given by

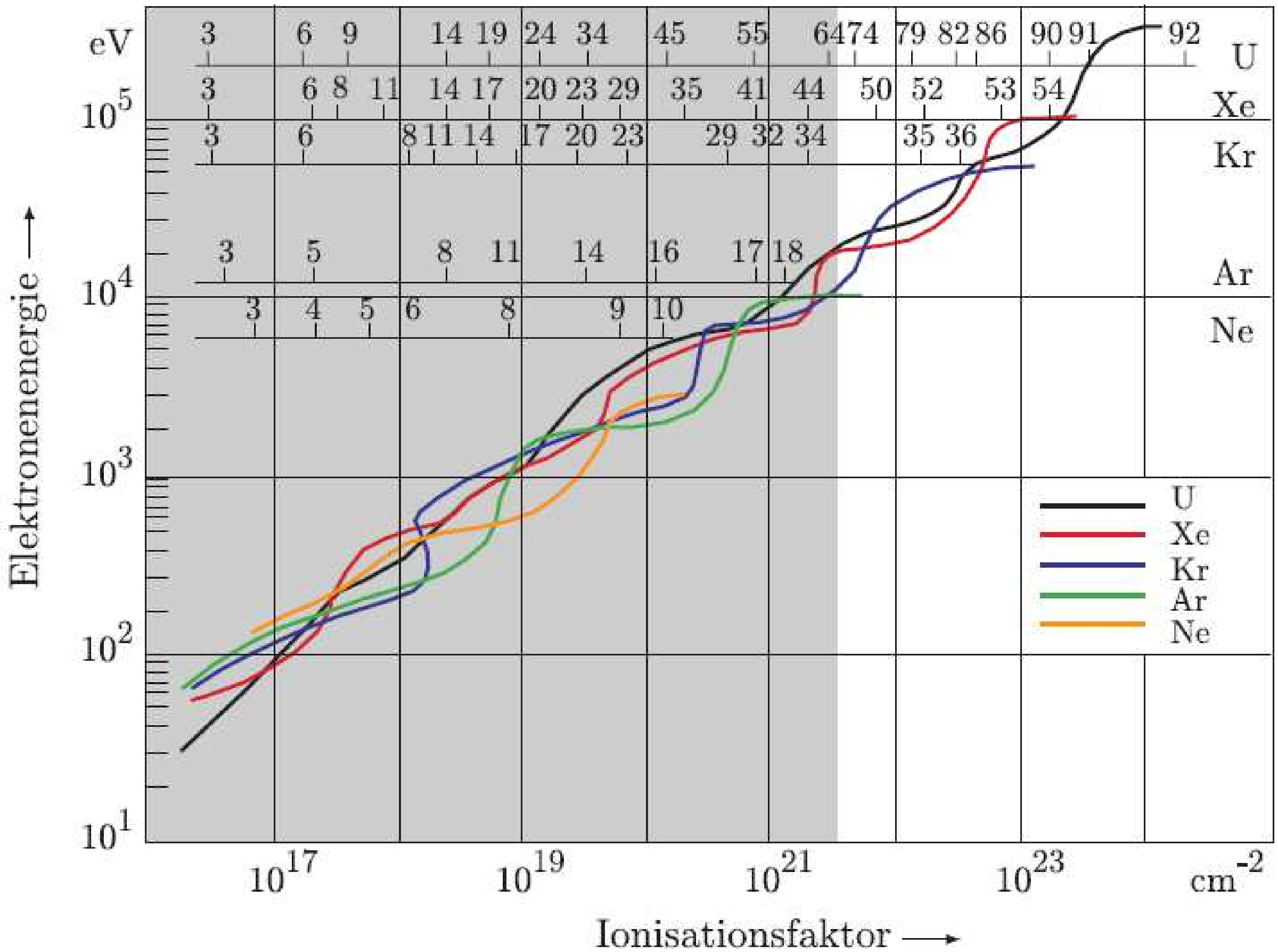
$$\frac{d\sigma_{z\to z+1}}{dE} = 4.5\cdot 10^{-14}\cdot\sum_{i=1}^{N}\frac{d}{dE}\left(\frac{\ln\left(E_{kin}/P_i\right)}{E_{kin}\cdot P_i}\right) = 0$$

$$\sum_{i=1}^{N}\frac{1}{P_i E^2}\left(1-\ln\left(\frac{E}{P_i}\right)\right) = 0 \quad\Rightarrow\quad E_{\max} = \exp\left(\frac{\sum_{i=1}^{N}\frac{1+\ln P_i}{P_i}}{\sum_{i=1}^{N} 1/P_i}\right) = e\cdot\exp\left(\frac{\sum_{i=1}^{N}\frac{\ln P_i}{P_i}}{\sum_{i=1}^{N} 1/P_i}\right)$$

For the optimal energy of the last electron, which is removed, follows: $E_{\max} \approx e\cdot\exp\left(\frac{\frac{\ln P_z}{P_z}}{1/P_z}\right) = e\cdot P_z$

Therewith the optimal energy is nearly e-times the ionization energy of the last electron that is removed from the ion with the charge state z.

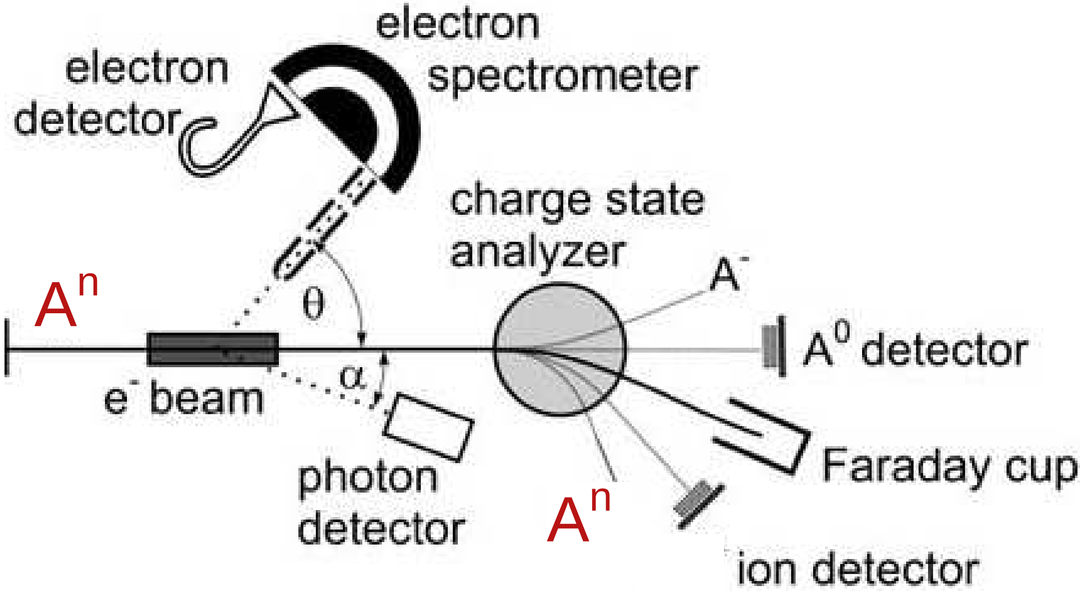
Ionization factor and optimal electron energy



Investigation of electron impact ionisation: ***Electron targets***

Investigation of electron-ion-collisions:

- Investigation of electron impact ionization
- Investigation of recombination processes
- Investigation of excitation processes

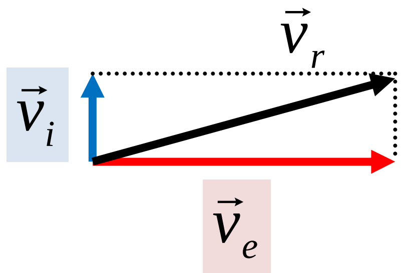


Measurement of rate coefficients R

$$R = \alpha \int n_e(\vec{r}) n_i(\vec{r}) d^3 r \qquad (2.9)$$

And there with the cross sections

$$\alpha = \langle \sigma \mathrm{v}_r \rangle = \int \sigma(\mathrm{v}_r) \mathrm{v}_r f(\mathrm{v}_r) d^3 \mathrm{v}_r \qquad (2.10)$$

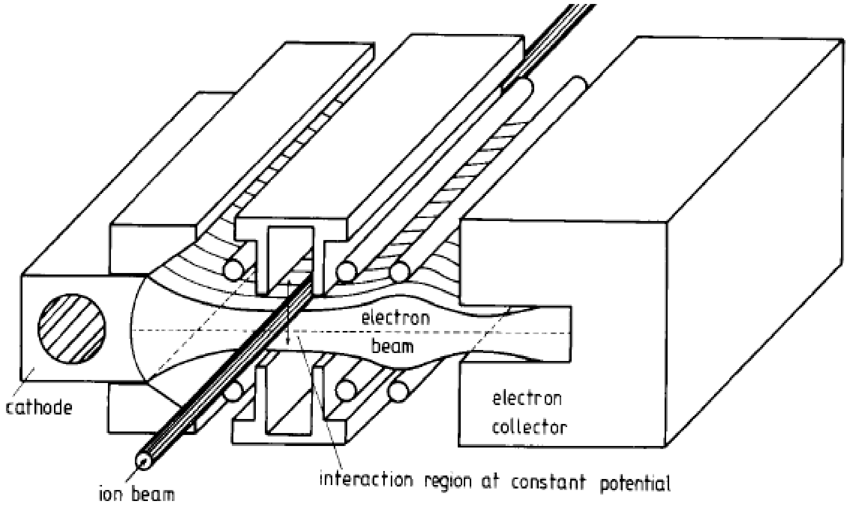


Important is the overlap of ion and electron beam

σ: cross section
n_e: electron density
n_i: ion density
v_r: collision velocity / relative velocity
$f(v_r)$: distribution function of the relative velocity

$$v_r = |\vec{v}_r| = |\vec{v}_e - \vec{v}_i| = \left(v_e^2 + v_i^2 - 2 v_e v_i \cos\theta\right)^{1/2}$$

Transversal electron target

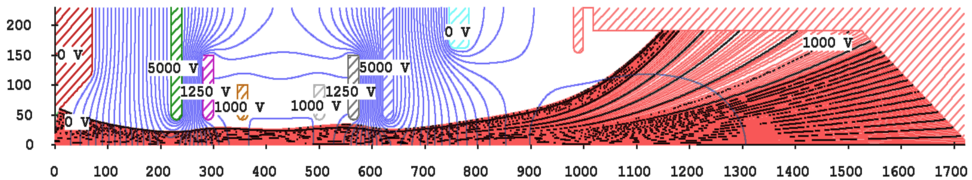


- “crossed beams technique”
- better energy resolution then gas target
- 10-15 cm long interaction region
- spectroscopic access is possible
- electrostatic focusing

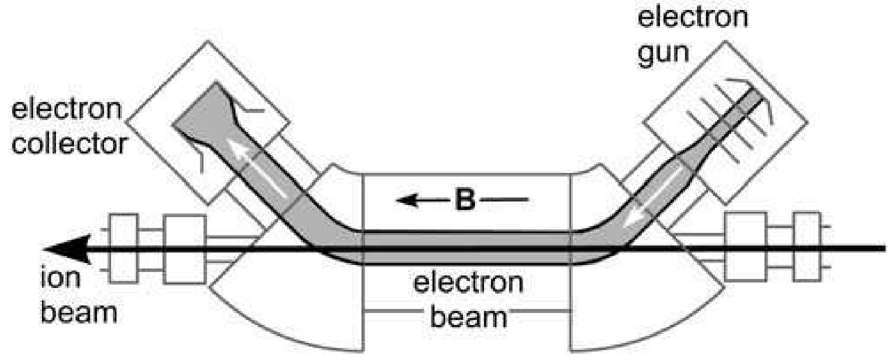
BUT:

- lower interaction rate as longitudinal electron target or gas target

0.061A/cm, R=8.19 mesh units, J=0.2 A/cm^2



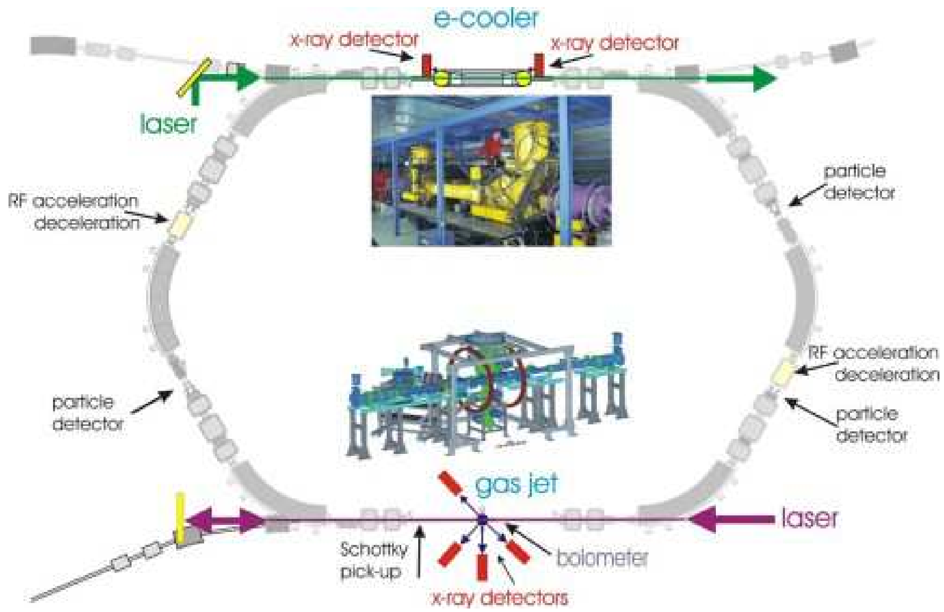
Longitudinal electron target



- „Merged beams“.
- also used as cooler for ion beams
- 2-2.5m long interaction region

BUT:

- limited access for spectroscopy



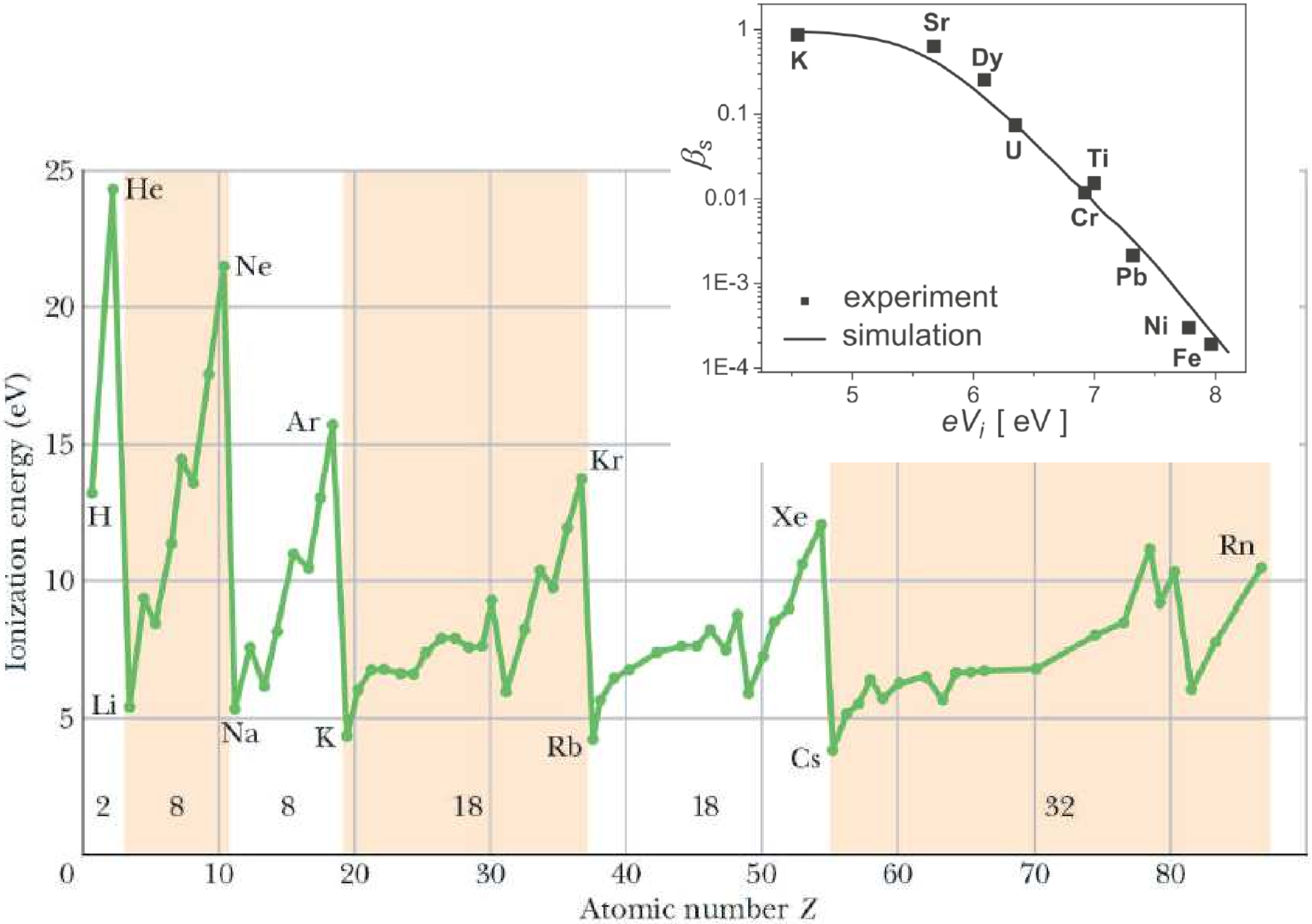
Photoionisation

The reaction is: $$A + h\nu = A^{+} + e^{-}$$

Atoms of a gas can be ionized by an intensive beam of photons with the adequate energy (photo ionization). Therefore the photon energy has to be $h \cdot \nu > e \cdot \varphi_i$. The energy of a photo electron is:

$$\frac{1}{2} m v_{\max}^{2} = h\nu - e\varphi_i$$

Ionisation energy
of atoms:



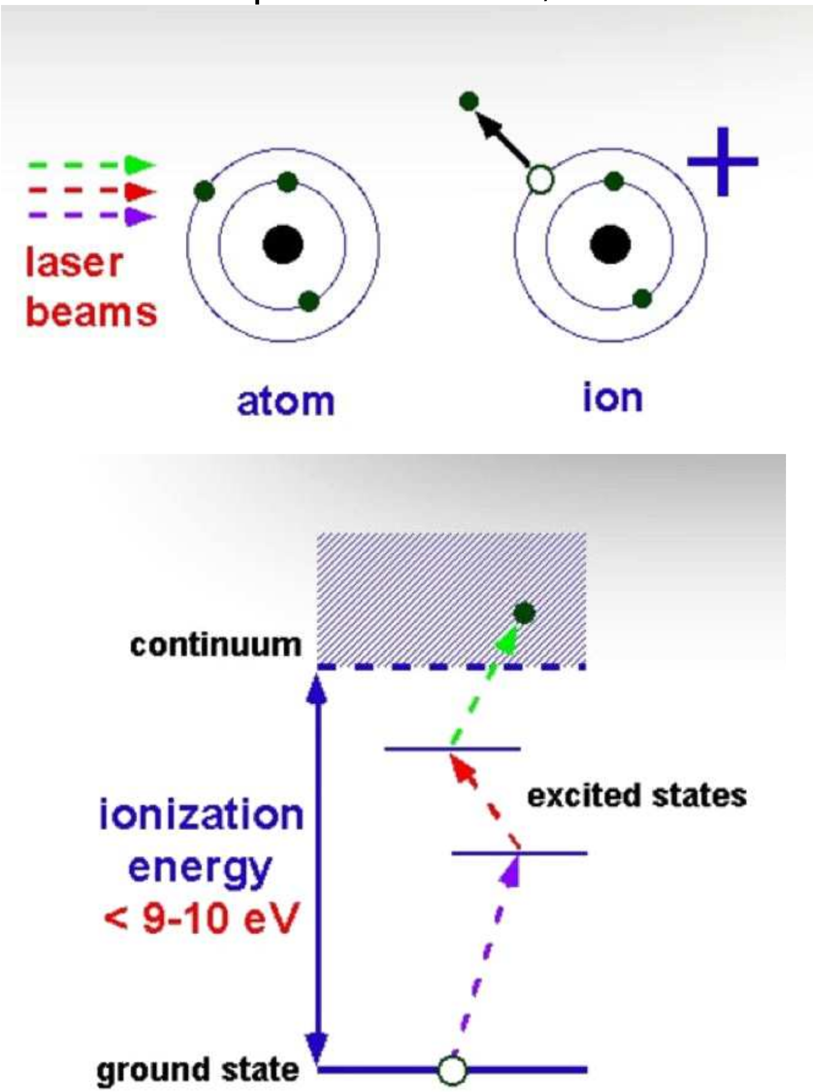
1 eV ➔ λ = 1.24 μm
(Indra red IR)

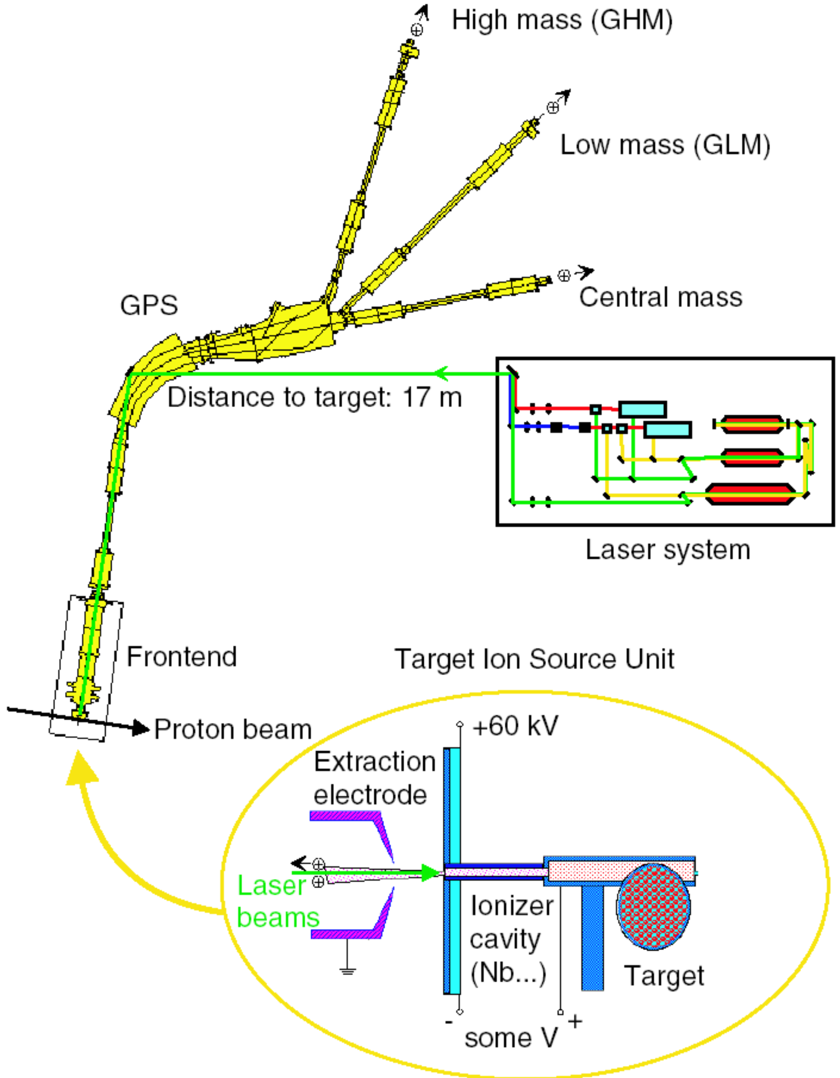
5 eV ➔ λ = 248 nm
(near UV)

In case of direct ionisation photons from the UV or X-ray region would be required.

Therefore the concept is

RILIS (Resonant ionisation laser ion source): Ionization via resonant excitation with three laser beams of frequencies f1 – f3, as shown in the following scheme





A prominent example for a RILIS is at ISOLDE/CERN (see picture).

Advantages of a RILIS: high selectivity, separation of surface-ionizing contaminations by adjusting the temperature of the cavity, high efficiency
In reality there a many more effects:

- Excitation into auto-ionizing state (AIS) with typical lifetimes of $10^{-15} - 10^{-10}$ s
- Excitation into Rydberg-states n = n*

Lifetime $\tau = \tau_0 \cdot (n^*)^3$

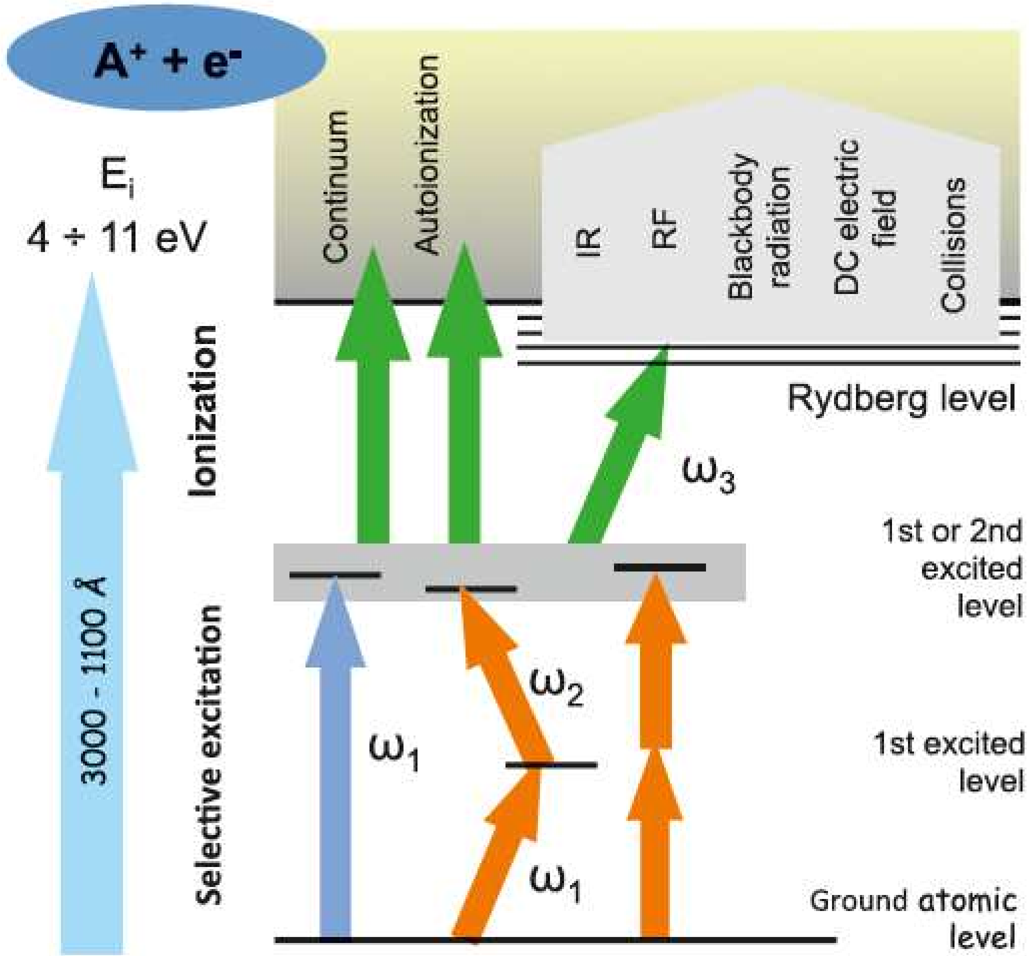
Binding energy $$E = R \cdot \frac{M}{M + m_e} \frac{Z^2}{(n^*)^2}$$

R = Rydberg constant

Radius of Rydberg atoms $\langle r \rangle = a_0 (n^*)^2$

Cross sections (orders of magnitude):

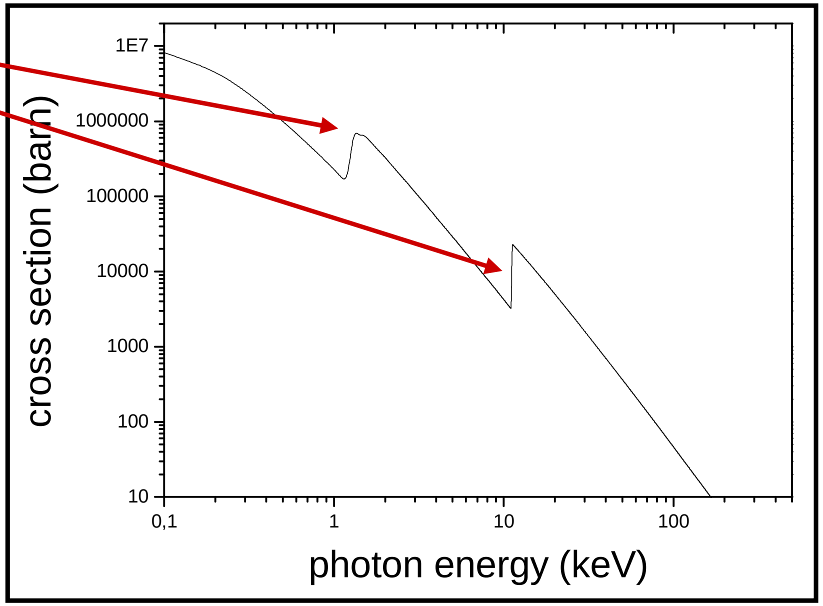
- Non-resonant (direct ionisation) → $\sigma = 10^{-19} - 10^{-17}$ cm^2
- AIS → $\sigma = 1.6 \cdot 10^{-14}$ cm^2
- Rydberg states → $\sigma \sim 10^{-14}$ cm^2



Cross section σ_p:

- σ_p has a strong dependence on the photon energy and the nuclear charge Z: $$\sigma_p \propto \frac{Z^{4-5}}{(\hbar\cdot\omega)^{7/2}}$$
- For a given atomic shell the cross section σ_p is the largest close to threshold, meaning where the photon energy reaches the ionization energy I (resonance/ threshold behavior):

$$\sigma_{max} : \hbar\cdot\omega \approx \mathrm{I_K}, \mathrm{I_L}, \mathrm{I_M}$$



- For high photon energies $\hbar\cdot\omega >> \mathrm{I_K}$ the ionization of the s-orbital is most probable and the K-shell ionization delivers the dominant contribution:

$$\sigma_{p_n} = \frac{1}{n^3}\cdot\sigma_K \quad \rightarrow \quad \sigma_p = \sigma_{p_K}\cdot\sum_{n=1}^{\infty}\frac{1}{n^3} = 1.2021\cdot\sigma_{p_K}$$

σ_{pn} : *cross section for RR into the K-shell*
n: *main quantum number*

- Description of σ_p as time-inverse effect to the radiative recombination by the Milne-formula:

$$g_{q+1}\cdot\sigma_{RR} = \frac{(\hbar\omega)^2}{2m_e c^2 E} g_q \cdot \sigma_P$$ with *g: statistical weights*