



The Abdus Salam
International Centre for Theoretical Physics



SMR.1744 - 27

SCHOOL ON ION BEAM ANALYSIS AND ACCELERATOR APPLICATIONS

13 - 24 March 2006

Low energy scattering

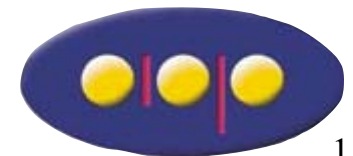
Peter BAUER
Johannes Kepler Universität Linz, Austria

Low Energy Ion Scattering

Peter Bauer

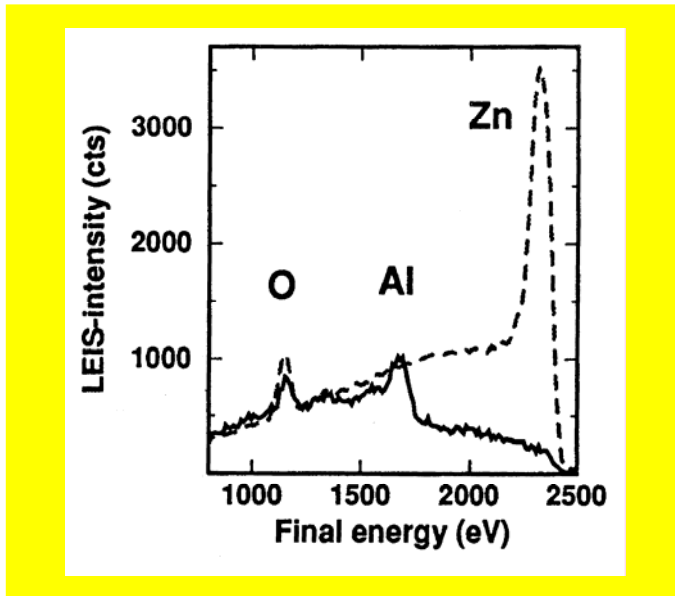
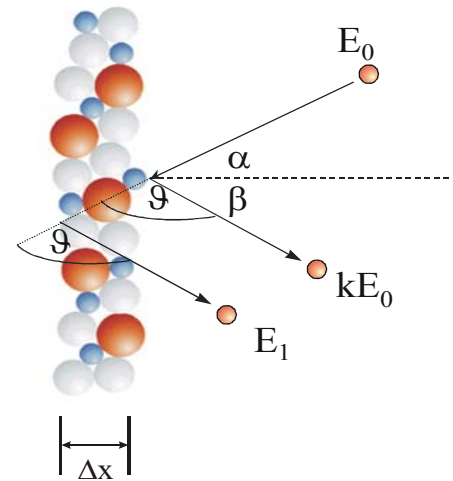
March 2006

Johannes Kepler University Linz
Institute of Experimental Physics
Department of Atomic Physics and Surface Science



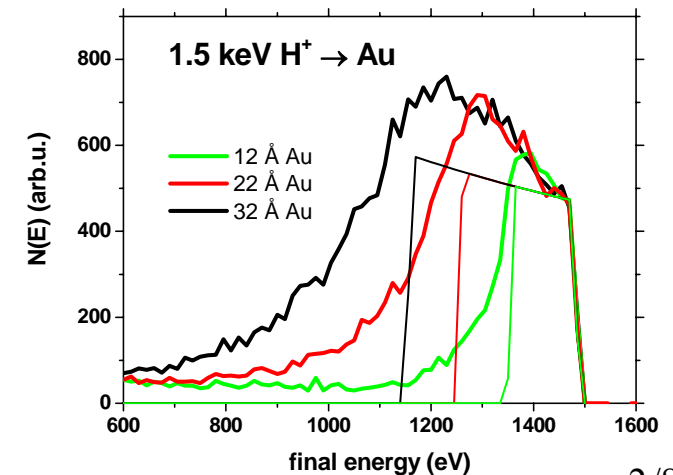
Overview:

- **Low energy ion scattering:**
 - RBS, MEIS (high energies)
 - LEIS (low energies)



- **Quantitative analysis surface**
 - structure
 - composition

- **Quantitative analysis of nanometer layers**
 - composition, depth profiles
 - depth resolution
 - mass resolution



Contents:

ion scattering: RBS ↔ LEIS

- scattering by nuclei → scattered yield
- interaction with target electrons → slowing down

Low energy ion scattering (LEIS)

- Electrostatic analyzer: ESA-LEIS
- Time-Of-Flight: TOF-LEIS

ESA-LEIS:

- instrumentation → static ESA-LEIS
- ions detected → ion fraction P+
- noble gas ions:
 - neutralisation → surface sensitivity
- applications: quantitative surface analysis → examples

TOF-LEIS (Time-of-flight)

- instrumentation → static TOF-LEIS
- ions and neutrals detected
 - surface structure analysis
 - neutral spectrum: shape, depth information
 - depth resolution → depth analysis → applications

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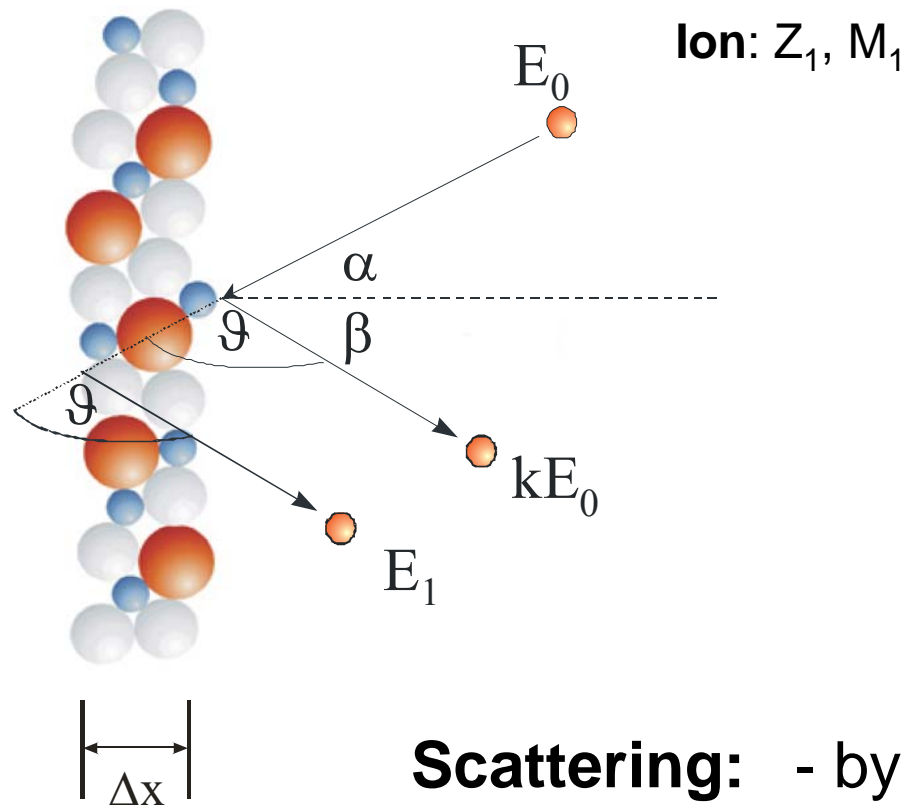
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Ion scattering:

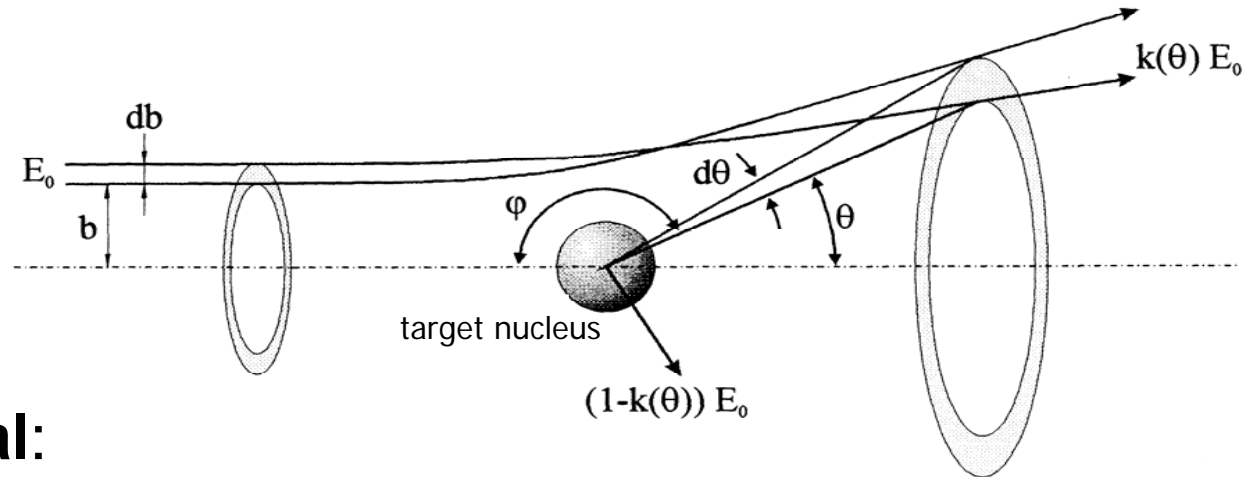
Target: Z_{i2}, M_{i2}



Ion: Z_1, M_1

Scattering: - by target nuclei
- by target electrons

Scattering by target nuclei



Scattering potential:

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \Phi(r/a)$$

$\Phi(r/a)$... screening function
(electronic screening of nucleus)

Impact parameter $b \leftrightarrow \theta$ → Scattering cross section $d\sigma/d\Omega$
→ Scattering probability dp

$$dp = ndx (d\sigma/d\Omega)$$

Scattering potential

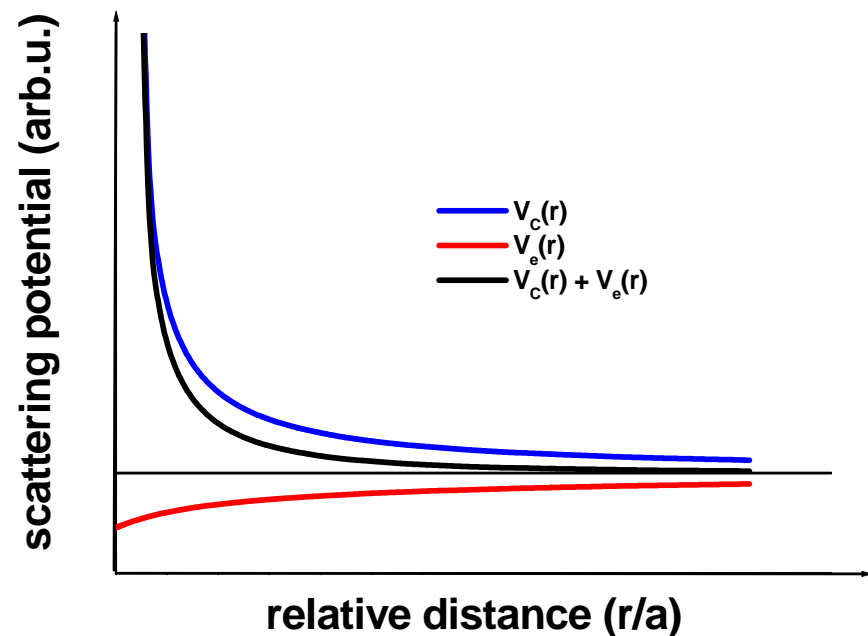
Scattering **point charge** by **point charge**: $V_C(r) = Z_1 Z_2 e^2 / r$ (Coulomb)

Scattering **dressed charge** by **neutral atom**:

$$V(r) = \underbrace{V_C(r)} + \underbrace{V_e(r)} = V_C(r) \cdot \underbrace{\Phi(r/a)}$$

interaction with: **nucleus** **electrons**
interaction is: **repulsiv** **attractive**

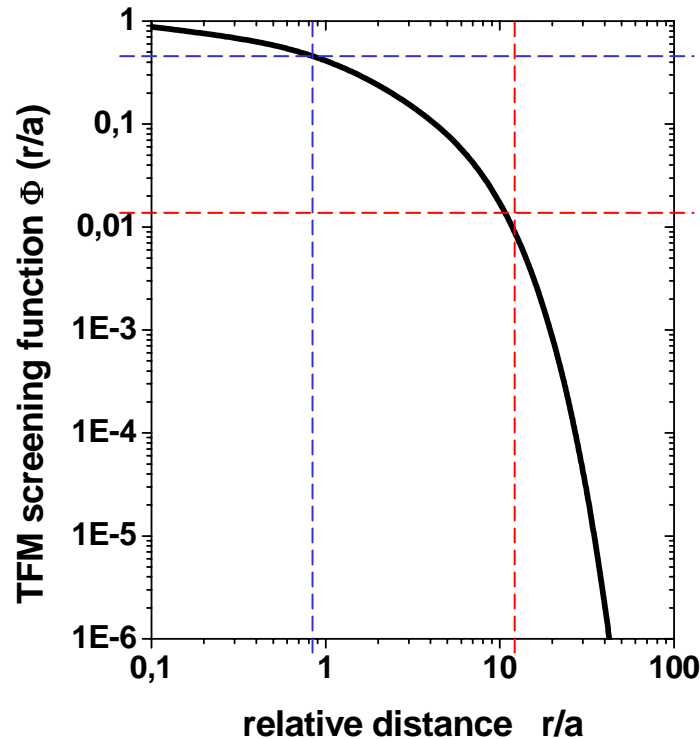
screening function



Screening function $\Phi(r/a)$ (Thomas-Fermi-Molière)

$$V(r) = V_C(r) \cdot \Phi(r/a)$$

$$\Phi\left(\frac{r}{a}\right) = \sum_{i=1}^3 b_i \exp(-c_i r/a) \quad \text{with} \quad a = \frac{0.8852 \cdot a_0}{\sqrt[3]{(\sqrt{Z_1} + \sqrt{Z_2})^2}}$$



screening length $a \approx 0.2 \text{ \AA}$

Limiting cases:

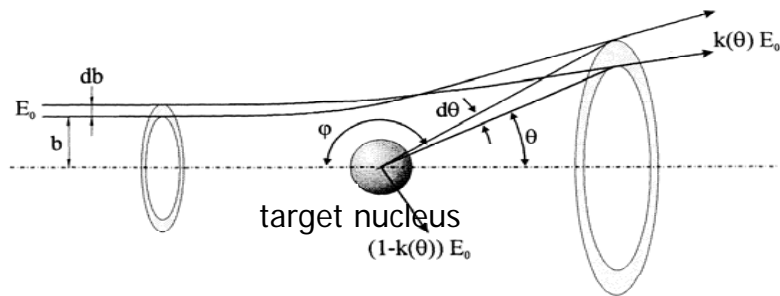
$$\Phi(r/a \rightarrow 0) = 1$$

$$\Phi(r/a \rightarrow \infty) = 0.$$

in any case: $\Phi(r/a) \leq 1$

Scattering cross section $d\sigma/d\Omega$

$V(r) = V_C(r) \rightarrow$ Rutherford cross section

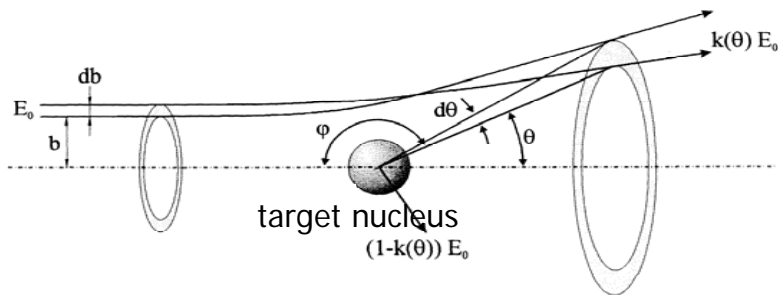


$$\frac{d\sigma_R}{d\Omega} = \left(\frac{Z_1 Z_2 e^2}{4 E \sin^2 \frac{\theta}{2}} \right)^2$$

Scattering cross section $d\sigma/d\Omega$

$V(r) = V_C(r) \rightarrow$ Rutherford cross section

$$\frac{d\sigma_R}{d\Omega} = \left(\frac{Z_1 Z_2 e^2}{4 E \sin^2 \frac{\theta}{2}} \right)^2$$



$$V(r) = V_C(r) \cdot \Phi(r/a) \rightarrow 2 \pi b db \equiv d\sigma = \left| \frac{d\sigma(\theta, E)}{d\Omega} \cdot \underbrace{2 \pi \sin\theta d\theta}_{d\Omega} \right|$$

\rightarrow relevant quantity is

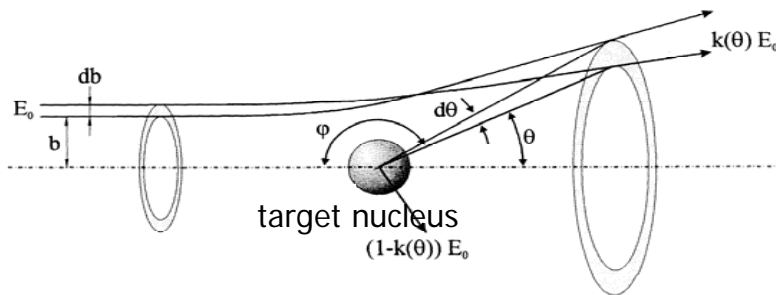
$$\frac{d\sigma}{d\Omega} = - \frac{b}{\sin\theta} \frac{db}{d\theta}$$

[from $b(\theta)$]

Scattering cross section $d\sigma/d\Omega$

$V(r) = V_C(r) \rightarrow$ Rutherford cross section

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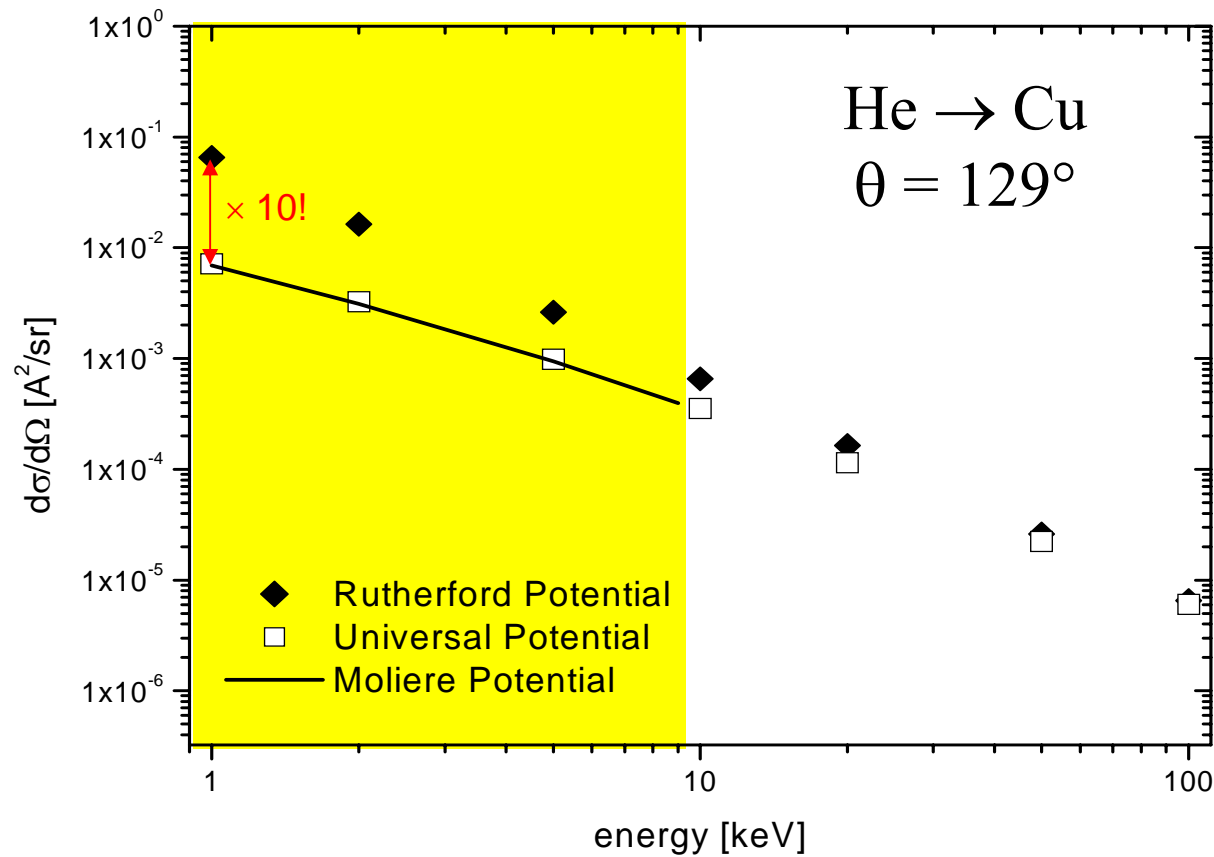


$$V(r) = V_C(r) \cdot \Phi(r/a) \rightarrow 2 \pi b db \equiv d\sigma = \left| \frac{d\sigma(\theta, E)}{d\Omega} \cdot \underbrace{2 \pi \sin\theta d\theta}_{d\Omega} \right|$$

\rightarrow relevant quantity is $\frac{d\sigma}{d\Omega} = - \frac{b}{\sin\theta} \frac{db}{d\theta}$ [from $b(\theta)$... or $\theta(b)$]

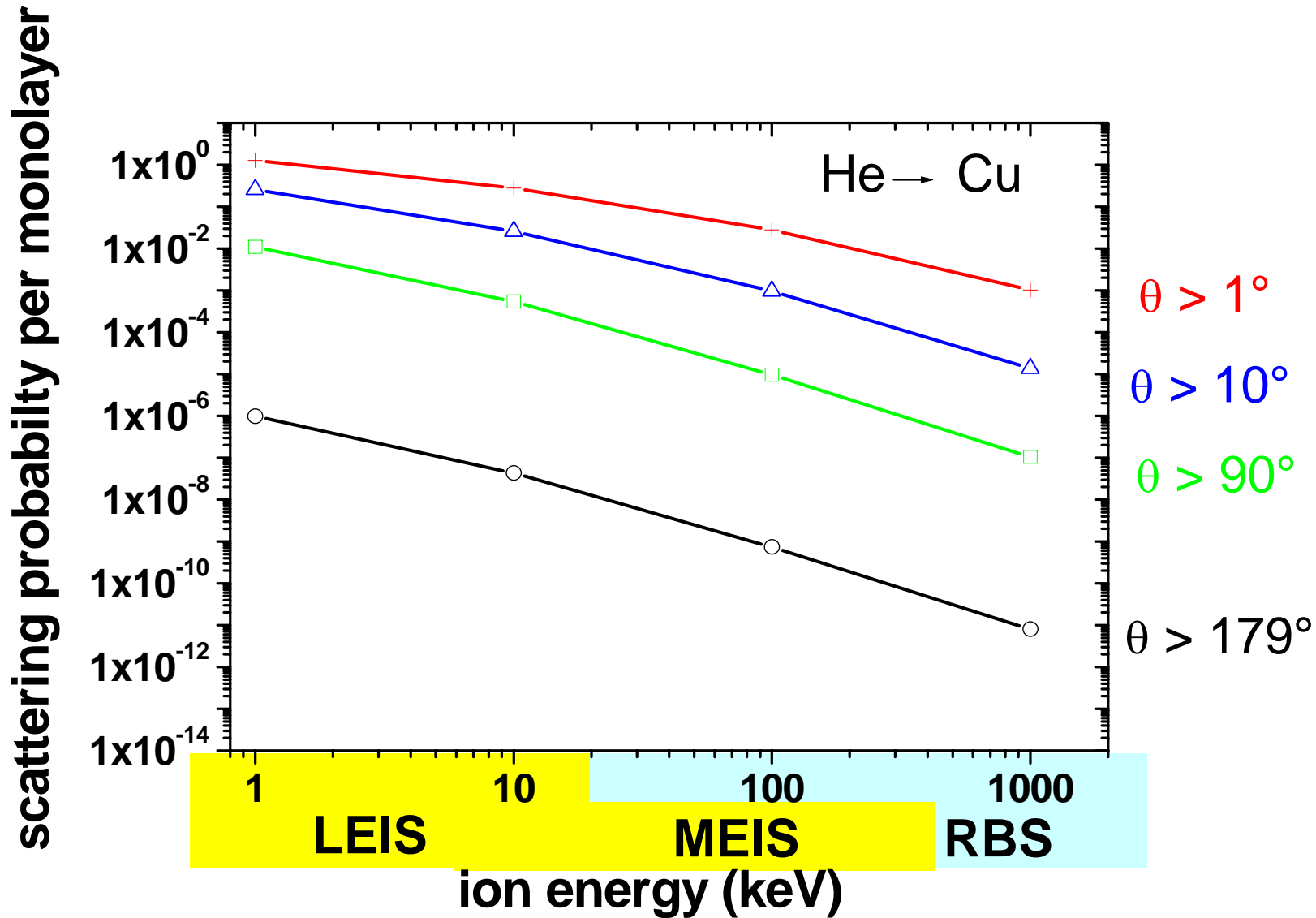
$db/d\theta$ is obtained from $\theta(b) = \pi - 2 \int_{R_{\min}}^{\infty} \frac{b dr}{r^2 \sqrt{1 - \frac{b^2}{r^2} - \frac{V(r)}{E}}} \text{ (scattering integral)}$

Scattering cross section



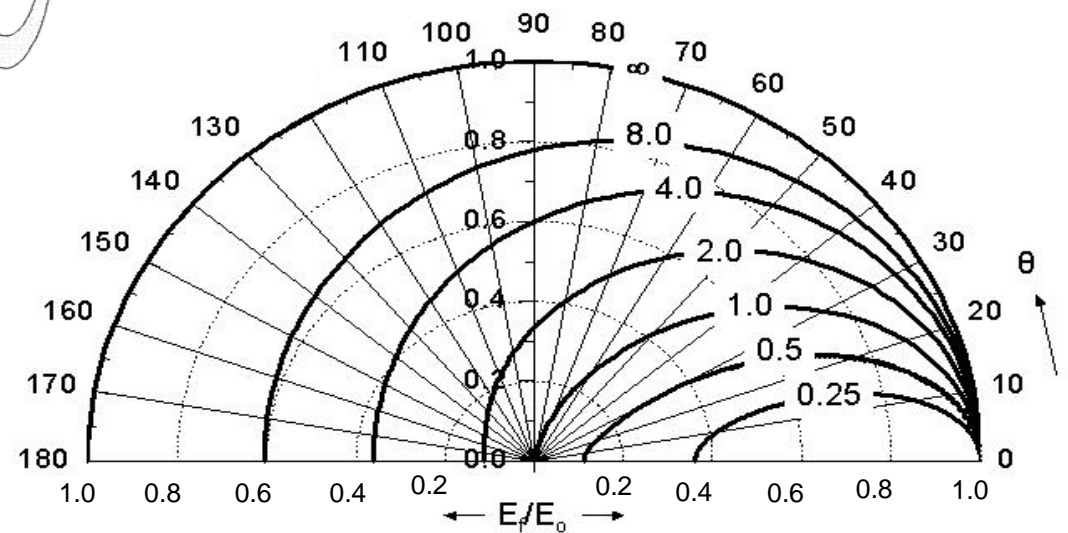
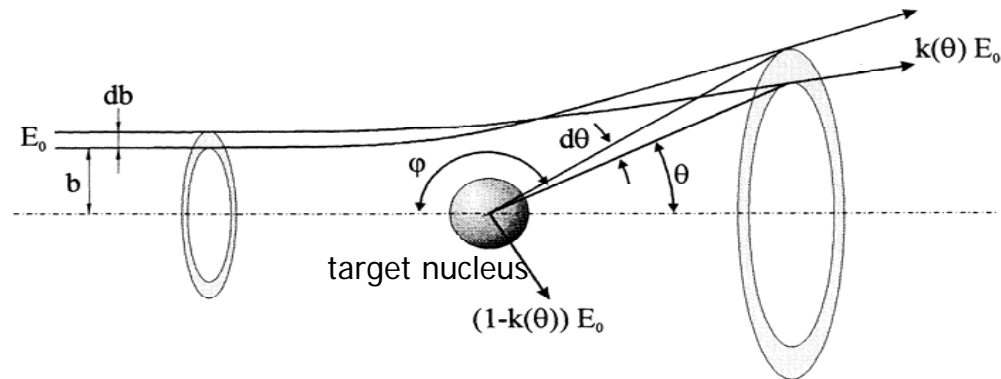
There are different models for $\Phi(r/a)$: Thomas-Fermi-Molière
universal potential
etc.

Integral scattering probability:



Collisional energy loss (binary collision)

kinematic factor: $k \equiv \frac{E_1}{E_0} = \left\{ \frac{\left[1 - (M_1 / M_2)^2 \sin^2 \theta \right]^{1/2} + (M_1 / M_2) \cos \theta}{1 + (M_1 / M_2)} \right\}^2$ for $M_1 \leq M_2$



Interaction with target electrons

- kinematics: electron's mass $M_2 \ll M_1$

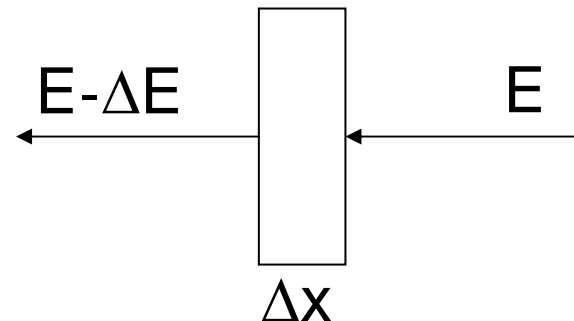
Interaction with target electrons

- kinematics: electron's mass $M_2 \ll M_1$
 - scattering angle negligible
 - small energy losses per collision
 - BUT with high probability**

Interaction with target electrons

- kinematics: electron's mass $M_2 \ll M_1$
 - scattering angle negligible
 - small energy losses per collision
BUT with high probability
- **Continuous slowing down („friction force“)**
- **Stopping Power:**

$$S = \lim_{\Delta x \rightarrow 0} \frac{\Delta E}{\Delta x} \equiv dE/dx$$

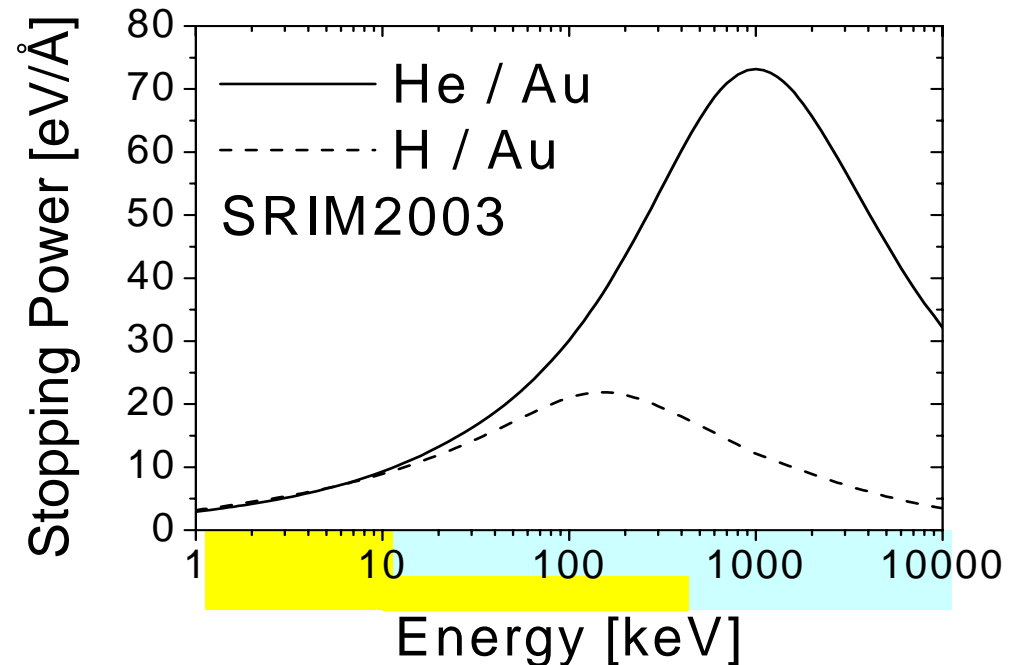


Stopping Power

- Energy loss dE per path length dx : $S = dE/dx$
- Stopping cross section: $\varepsilon = S / n = dE / ndx$

$$\text{RBS: } S \propto \frac{Z_2}{v^2} \ln\left(\frac{2 m_e v^2}{I}\right)$$

LEIS: $S \propto v$ (like friction force)



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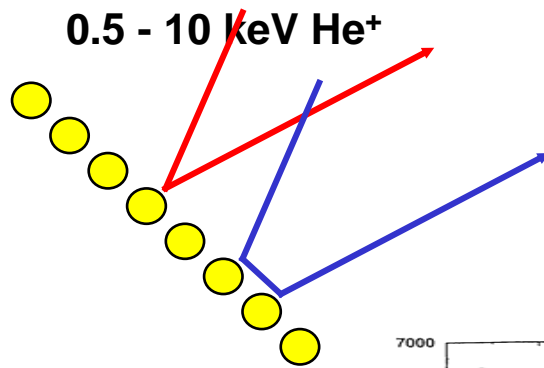
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ESA-LEIS (electrostatic analyser used)



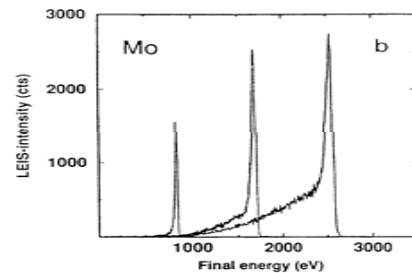
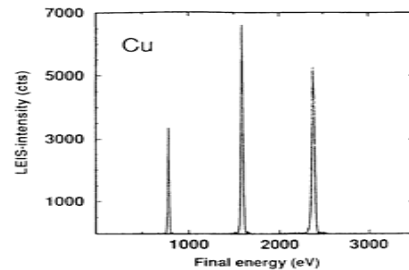
ESA → detection of scattered ions

→ sensitive for outermost atomic layer

usually:

binary collisions dominate

double collisions negligible



TOF-LEIS (time-of-flight analyser used)

→ detection of scattered neutrals + ions

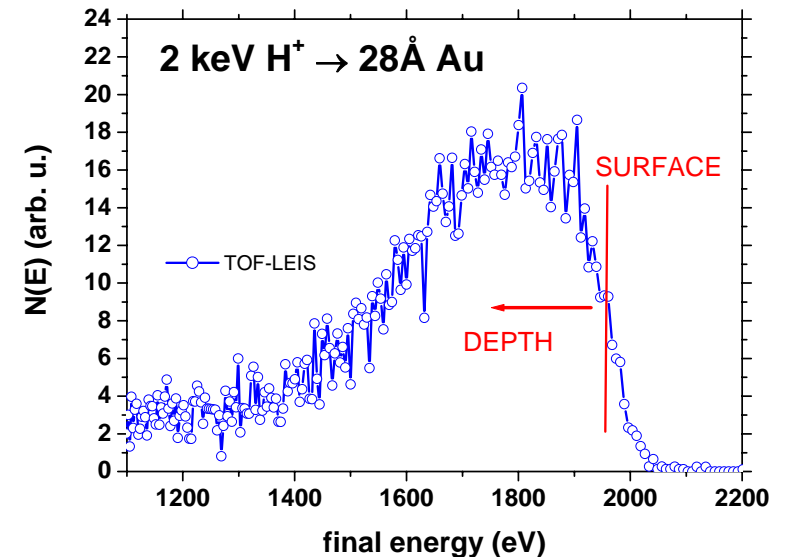
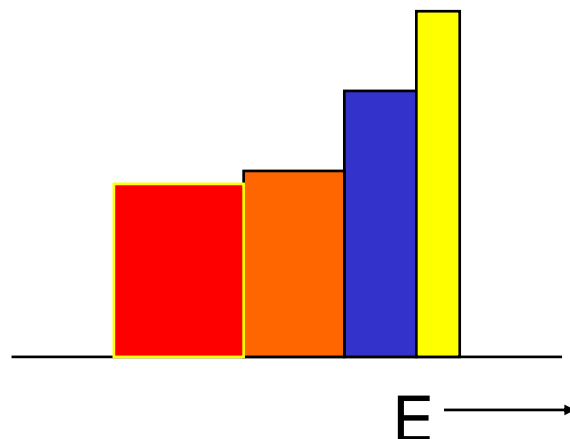
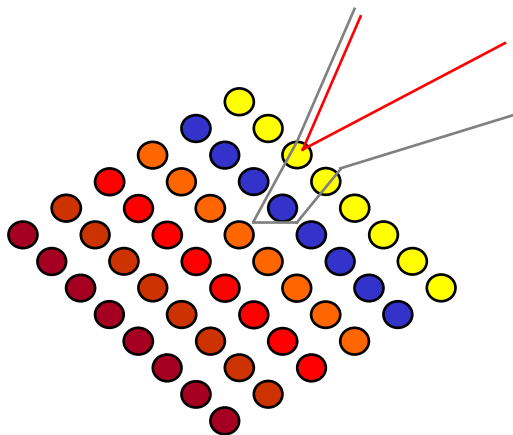
→ no surface sensitivity

like RBS at low energies

→ but: no single scattering!

→ information about nm-layers

0.5 - 10 keV H⁺, He⁺



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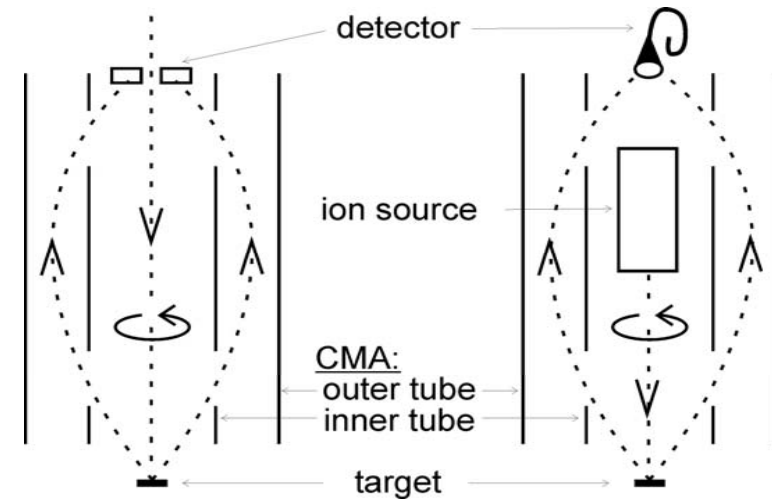
TOF-LEIS (Time-of-flight)

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ESA-LEIS Instrumentation:

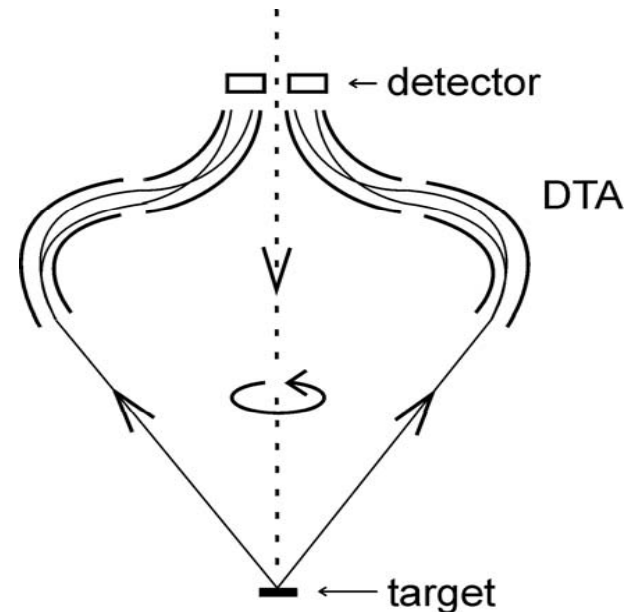
Cylindrical Mirror Analyzer (CMA):

only ions with $E_f \in [E, E + dE]$
are transmitted, with $dE \propto E$



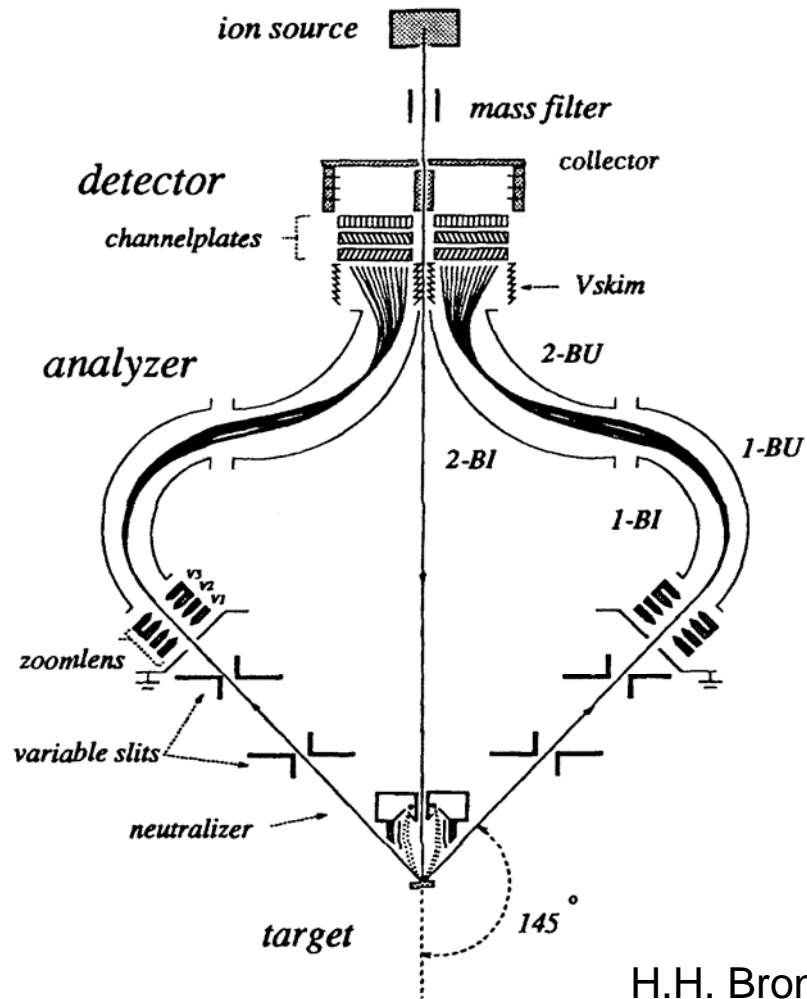
Double Toroidal Analyser (DTA):

ions with $E_f \in [E_{\min}, E_{\max}]$
are transmitted simultaneously



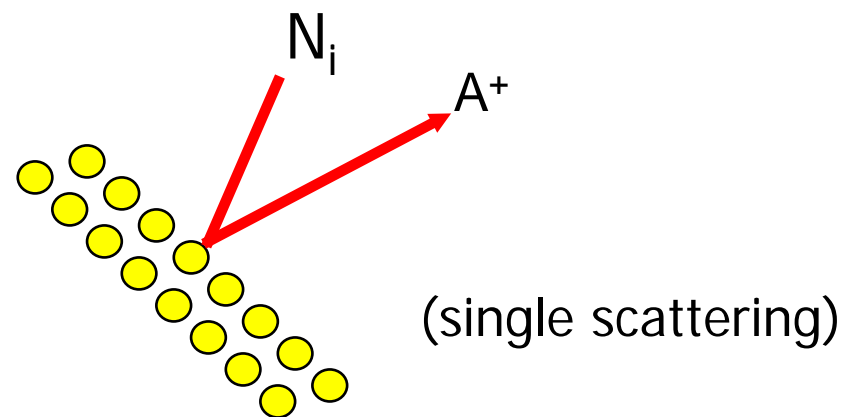
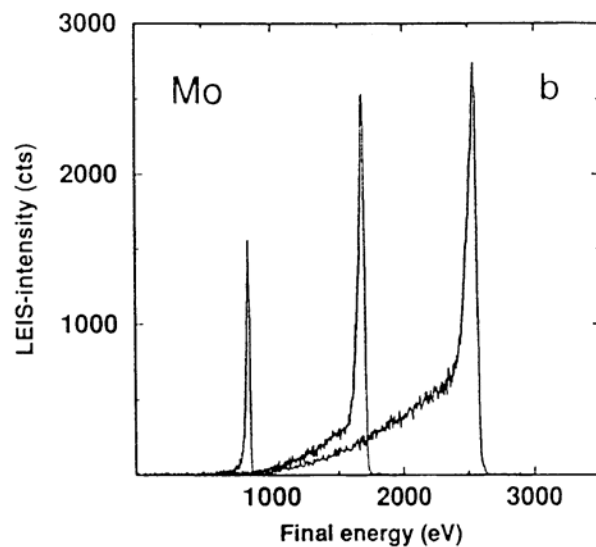
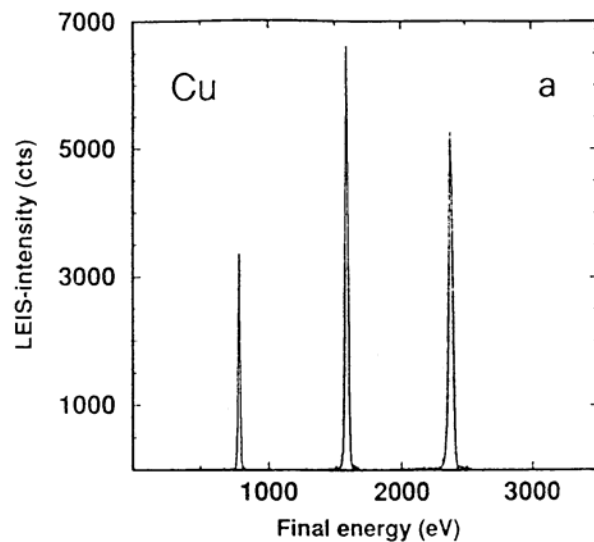
ESA-LEIS Instrumentation (static LEIS):

CALIPSO



H.H. Brongersma, Eindhoven university

$^4\text{He}^+$ ion spectra (ESA)



$$A^+ = \underbrace{\frac{N_i}{\cos \alpha}}_{\# \text{ proj.}} \cdot \underbrace{\frac{d\sigma}{d\Omega}}_{\# \text{ atoms/area}} \cdot (nd)_0 \cdot \Omega \cdot P^+ \cdot T_+$$

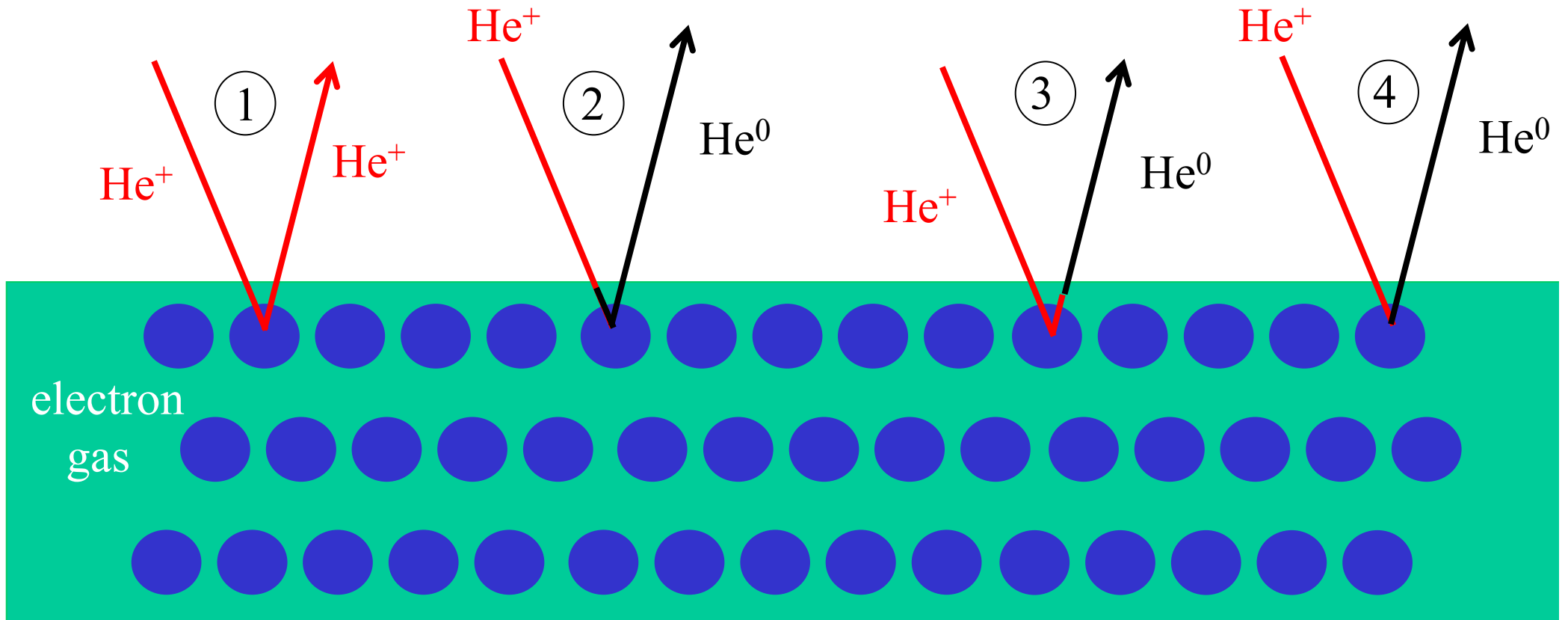
$$P^+ = N_+ / [N_+ + N_0] \dots \text{ion fraction}$$



$$A^+ = \frac{N_i}{\cos \alpha} \cdot \frac{d\sigma}{d\Omega} \cdot (nd)_0 \cdot \Omega \cdot P^+ \cdot \eta_+$$

ion yield A^+ depends on:

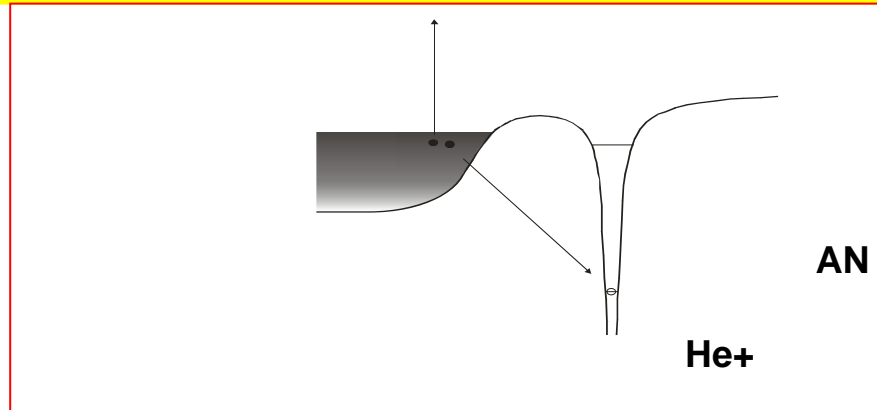
- + N_i ... number of ions
- + α ... angle of incidence
- 0 $d\sigma/d\Omega$... scattering cross section
- ? P^+ ... ion fraction
- + Ω ... solid angle
- + η_+ ... detection efficiency for ions

Neutralization in LEIS:



- (1) (2) (3) : Auger neutralization or resonant neutralization
 (4) : collision induced neutralization 
 reversed path: collision induced ionization 

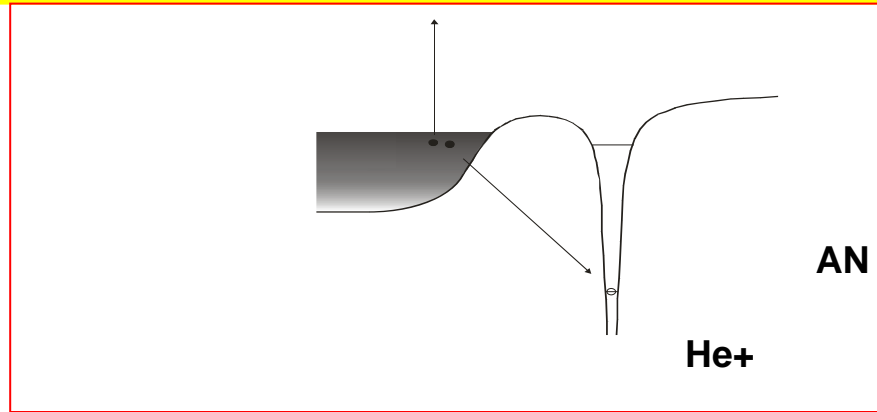
Ion fraction P^+ : neutralisation mechanisms



important for He^+ !

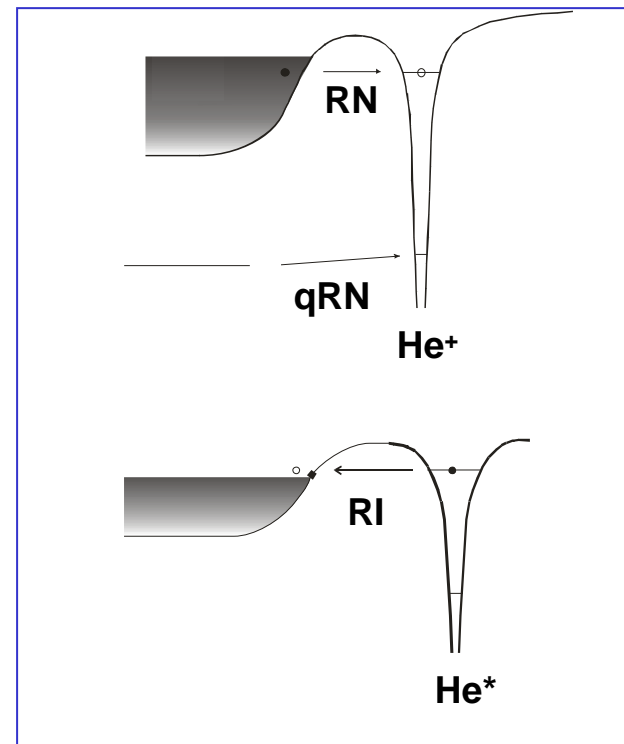
- Auger neutralisation (AN)

Ion fraction P^+ : neutralisation mechanisms



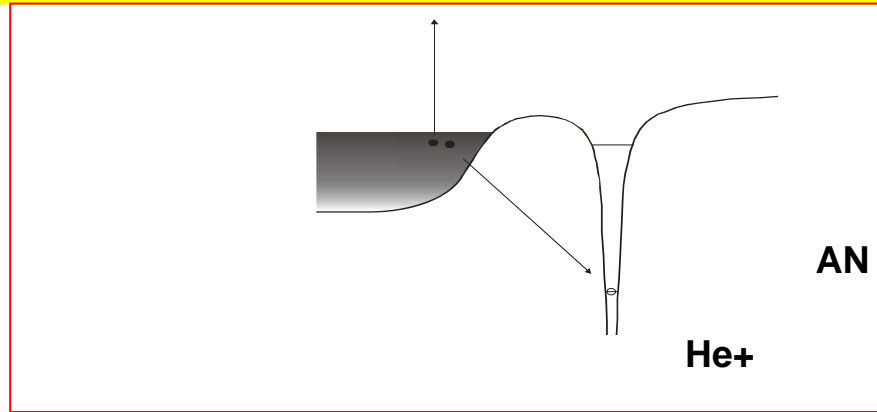
important for He^+ !

- Auger neutralisation (AN)
- Resonant neutralisation RN (ionization RI)



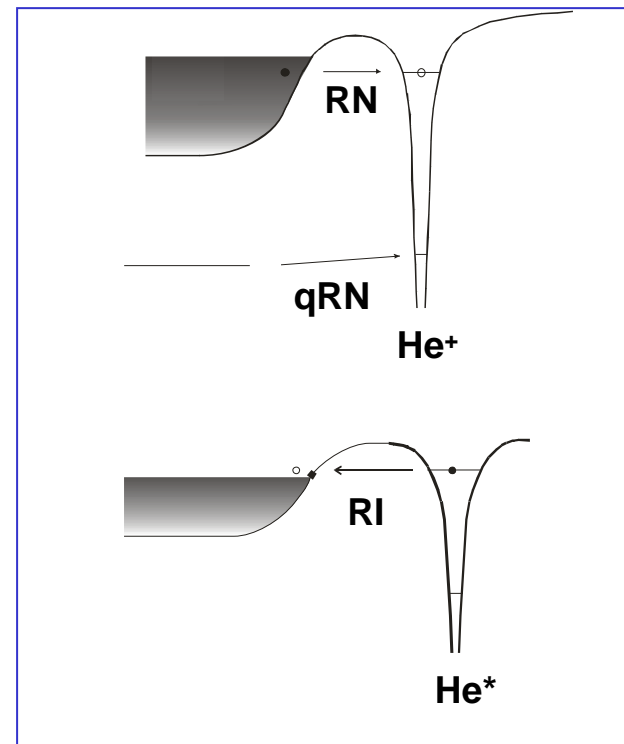
in
general
not
for
 He^+ !

Ion fraction P^+ : neutralisation mechanisms

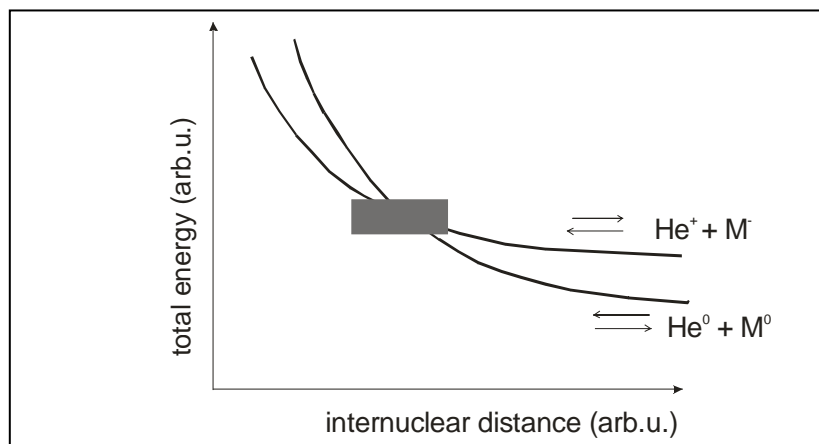


important for He^+ !

- Auger neutralisation (AN)
- Resonant neutralisation RN (ionization RI)
- collision induced charge exchange important for He^+



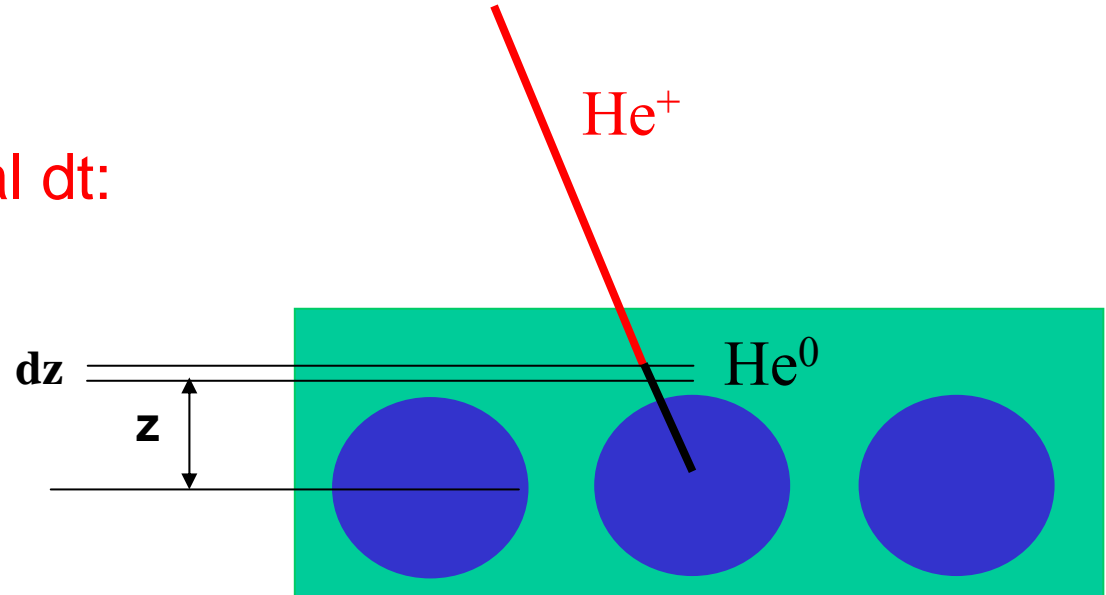
in
general
not
for
 He^+ !



Auger neutralisation on incoming path:

decrease of P^+ in time interval dt :

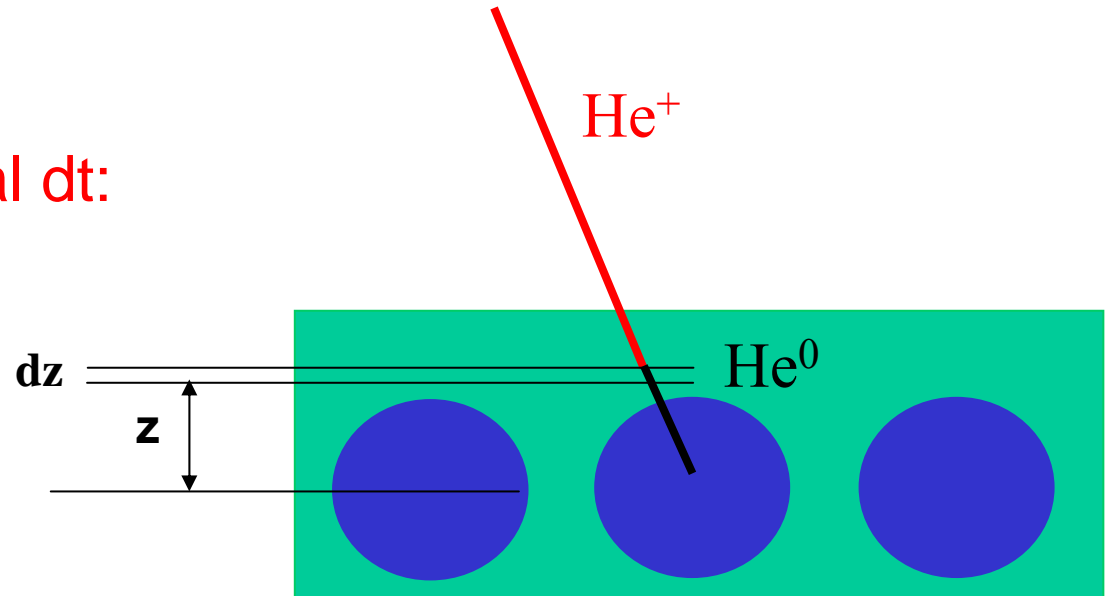
$$dP^+ = - P^+ \cdot \underbrace{\Gamma_A}_{\substack{\text{neutralization} \\ \text{probability} \\ \text{in } [z, z + dz]}} dt$$



Auger neutralisation on incoming path:

decrease of P^+ in time interval dt :

$$dP^+ = - P^+ \cdot \underbrace{\Gamma_A}_{\substack{\text{neutralization} \\ \text{probability} \\ \text{in } [z, z + dz]}} dt$$



→ fraction of surviving ions:

$$P^+ = \exp\{-\int dt \Gamma_A(z)\} = \exp\{-\int dz \Gamma_A(z) dt/dz\} \approx \exp(-v_c/v_{\perp})$$

$$v_c = \int dz \Gamma_A(z)$$

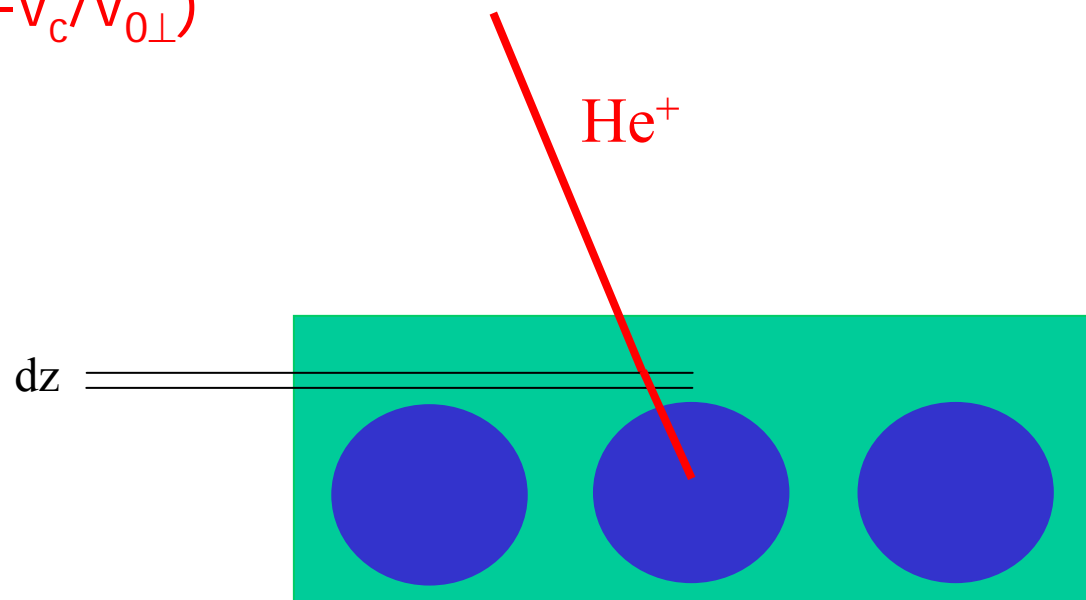
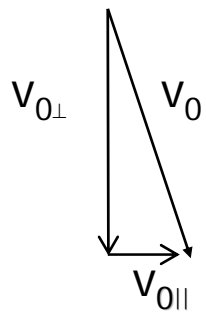
$$v_{\perp} = 1/v_{0\perp}$$

$$P^+ \approx \exp(-v_c/v_{0\perp})$$

Auger neutralization on in- and outgoing path

survival probability on the way in: P_{in}^+

$$P_{in}^+ = \exp(-v_c/v_{0\perp})$$



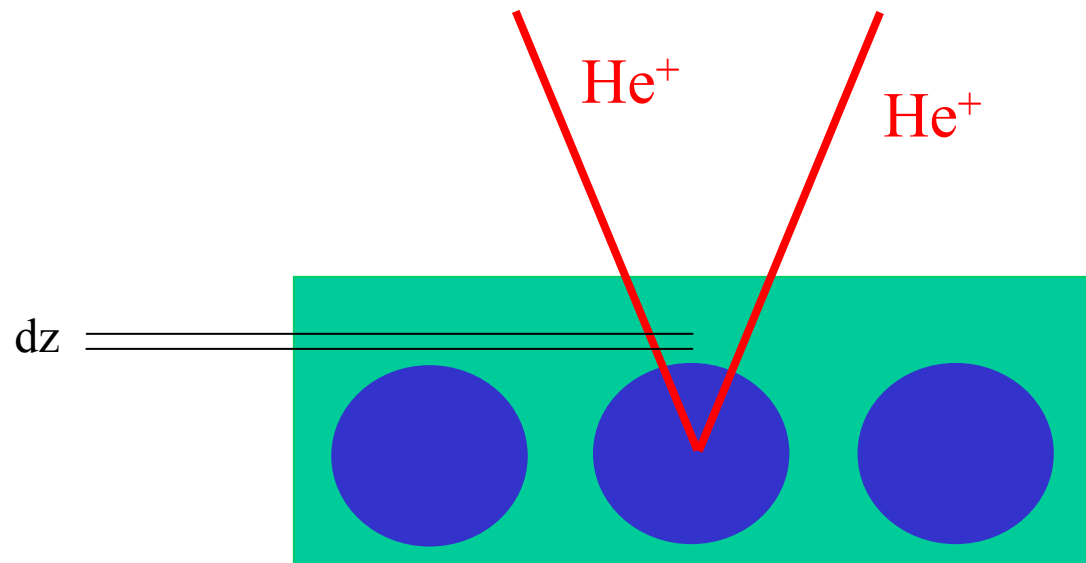
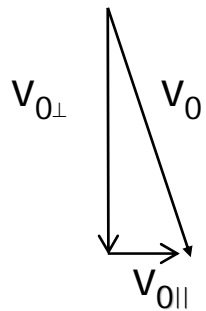
Auger neutralization on in- and outgoing path

survival probability on the way in: P_{in}^+

on the way out: P_{out}^+

$$P_{in}^+ = \exp(-v_c/v_{0\perp})$$

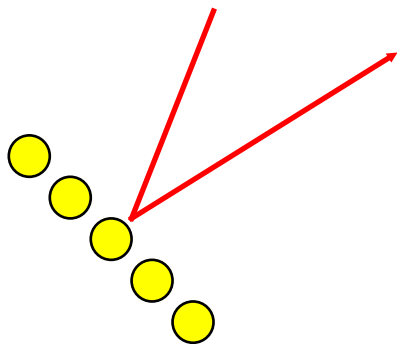
$$P_{out}^+ = \exp(-v_c/v_{f,\perp})$$



Probability to survive in charge state He⁺

premise: no resonant neutralization (He⁺!)

no collision induced charge exchange ($E < E_{th}$)



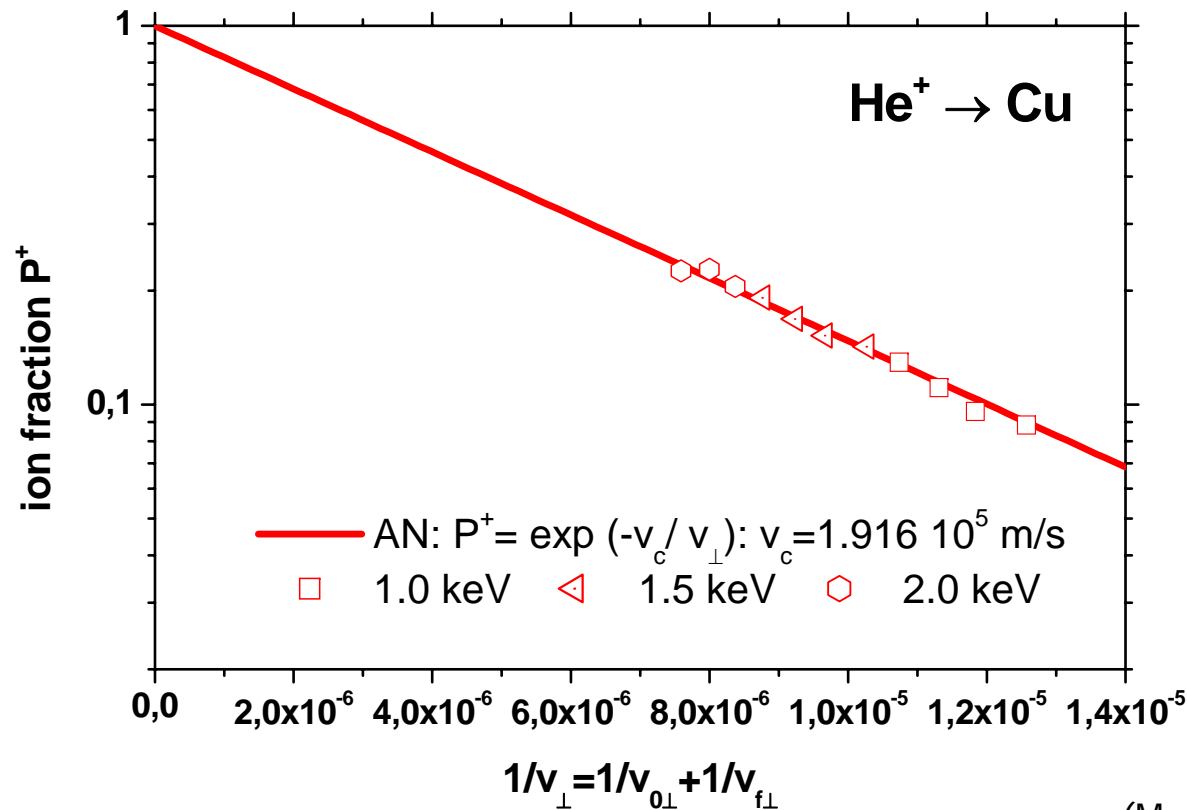
$$P^+ = P_{in}^+ \cdot P_{out}^+$$

survival probability

$$P^+ = \exp[-v_c(1/v_{0\perp} + 1/v_{f\perp})] \quad \dots \text{ pure AN}$$

Example: ${}^4\text{He} \rightarrow \text{Cu}$

$E < E_{\text{th}}$: $P^+(v_{\perp})!$... ion fraction depends only on v_{\perp}



variation of v_{\perp} via

- variation of energy
- variation of geometry

→ one single curve!!

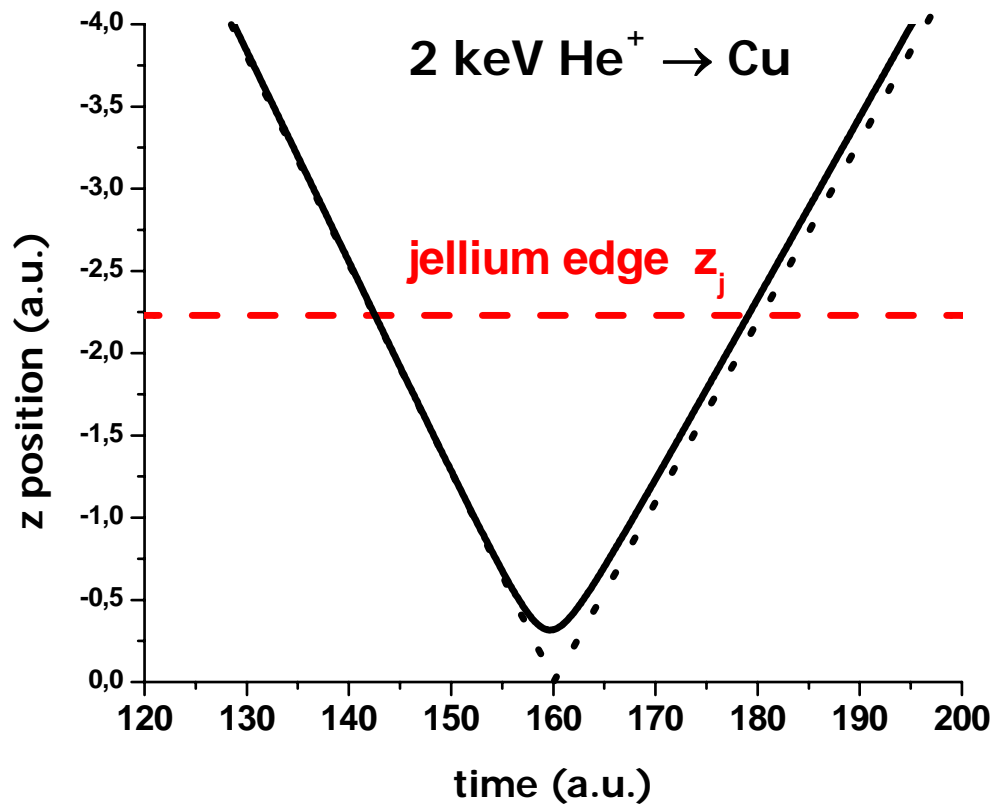
→ **Auger neutralization**

(M. Draxler 2002)

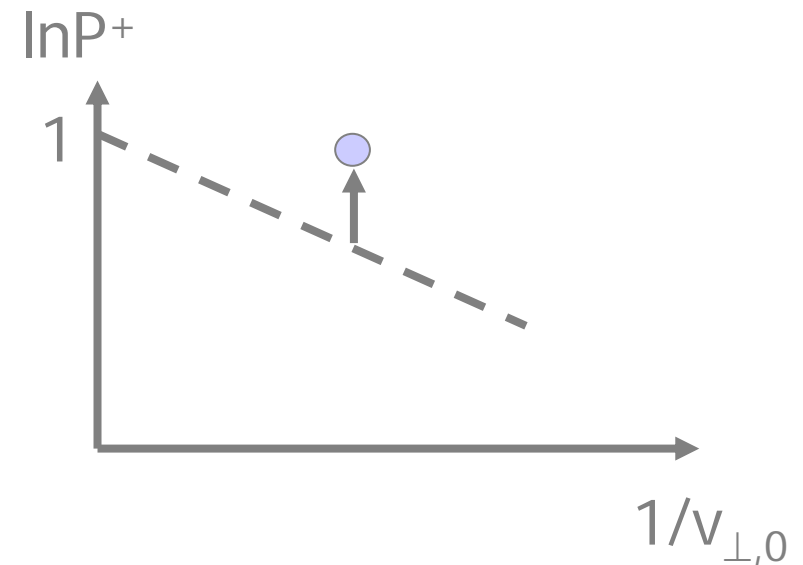
Trajectory effects

$$P^+ = e^{-\int dt \Gamma_A(z)} \approx e^{-\Delta t \Gamma_A}$$

$$\Delta t < 2z_j/v_{\perp}$$

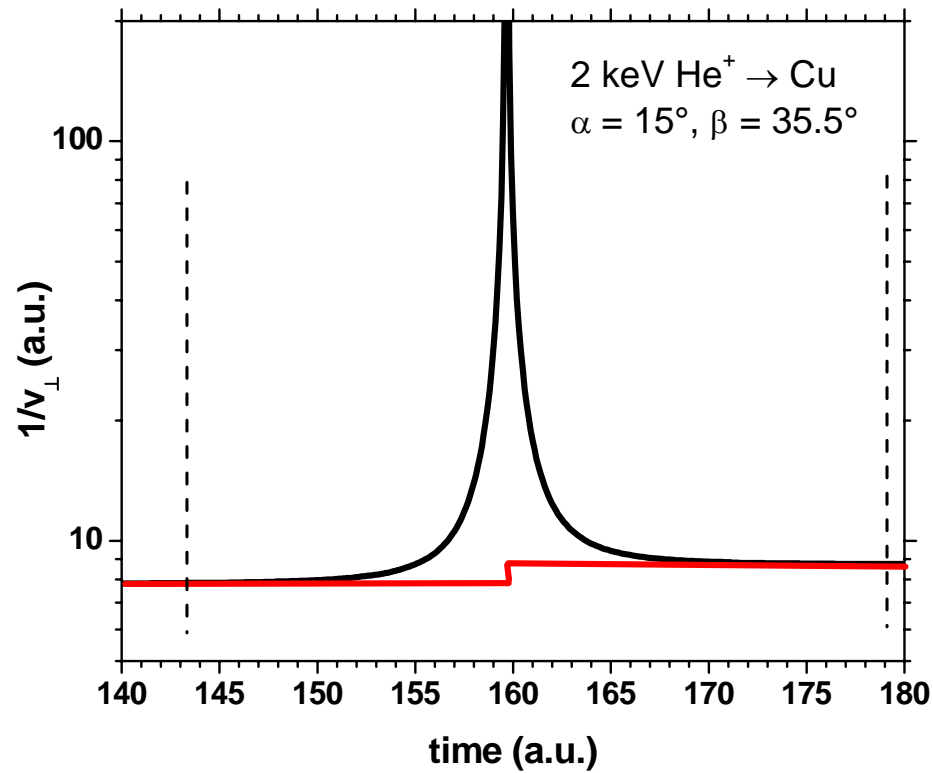


$$P^+ > e^{-v_c/v_{\perp}}$$

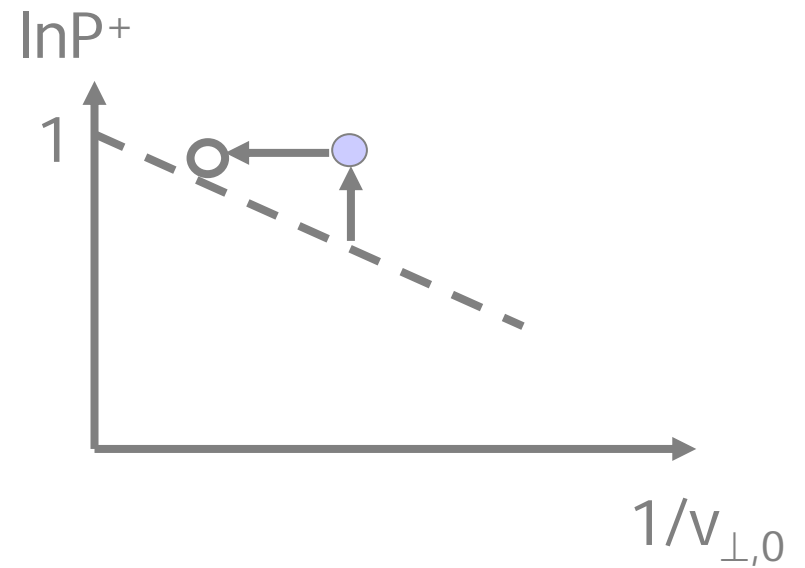


(Valdés 2004)

Trajectory effects



$$\left\langle \frac{1}{v_{\perp}} \right\rangle > \frac{1}{v_{\perp,0}}$$



Consequences?

interaction time shorter, $\langle v_{\perp} \rangle$ smaller

$$P^+ = \exp\left[-\int_{z_{\min}}^{z_{\text{jellium}}} dz \Gamma(z)/v_{\perp}(z)\right] = \exp[-\langle 1/v_{\perp} \rangle \cdot v_{c, \text{eff}}]$$

P^+ from experiment: a priori correct (hopefully)

$1/v_{\perp}$ is larger than estimated by $1/v_{\perp,0}$

v_c results too large

$$P^+ = \exp[-f_{\text{corr}} \cdot v_c / v_{\perp}]$$

$$f_{\text{corr}} = \frac{\langle 1/v_{\perp} \rangle}{1/v_{\perp,0}} \cdot \frac{v_{c, \text{eff}}}{v_c}$$

f_{corr} small correction?

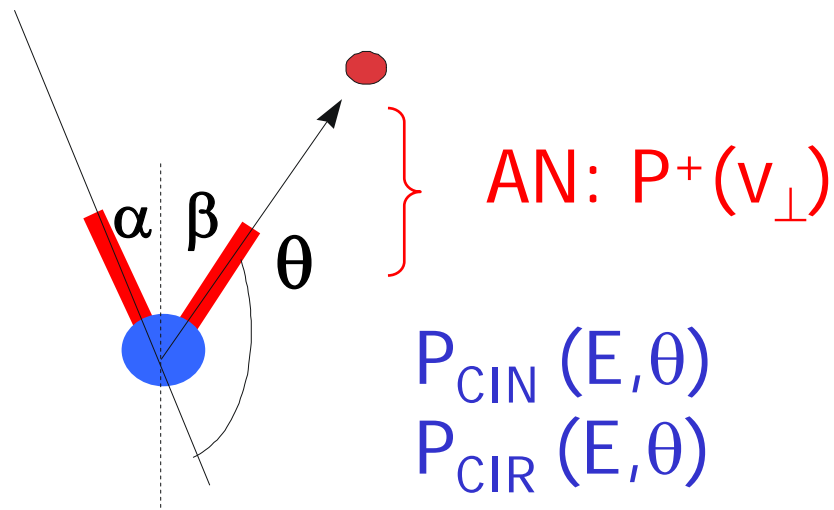
Auger neutr. \leftrightarrow collision induced processes

- projectiles: noble gas ions (e.g., He^+)

Auger neutralization AN

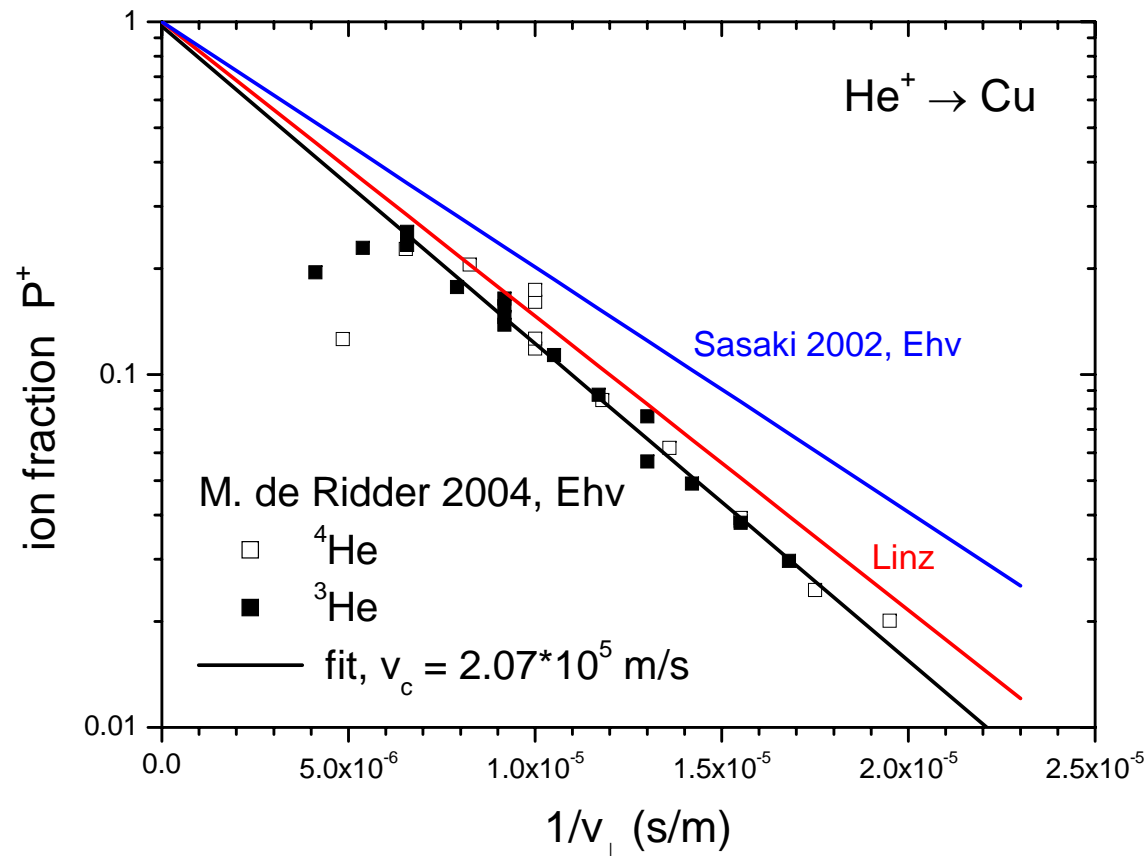
collision induced neutralization CIN

collision induced reionization CIR



Comparison Eindhoven – Linz:

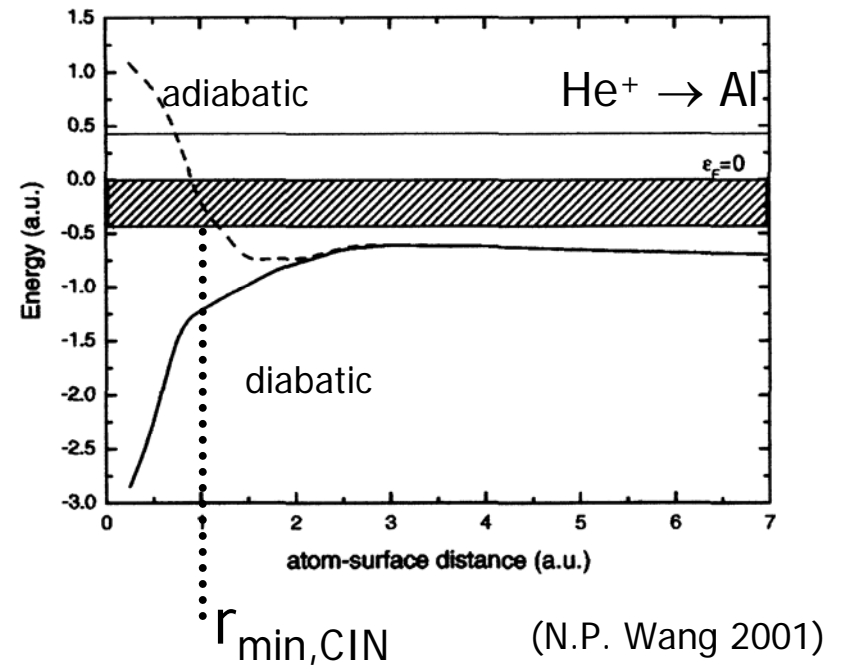
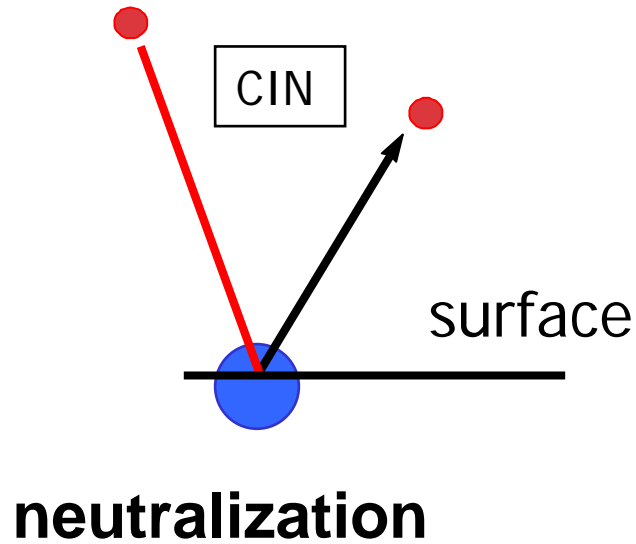
Eindhoven group: variation of energy



De Ridder & Linz:
good quantitative
agreement!

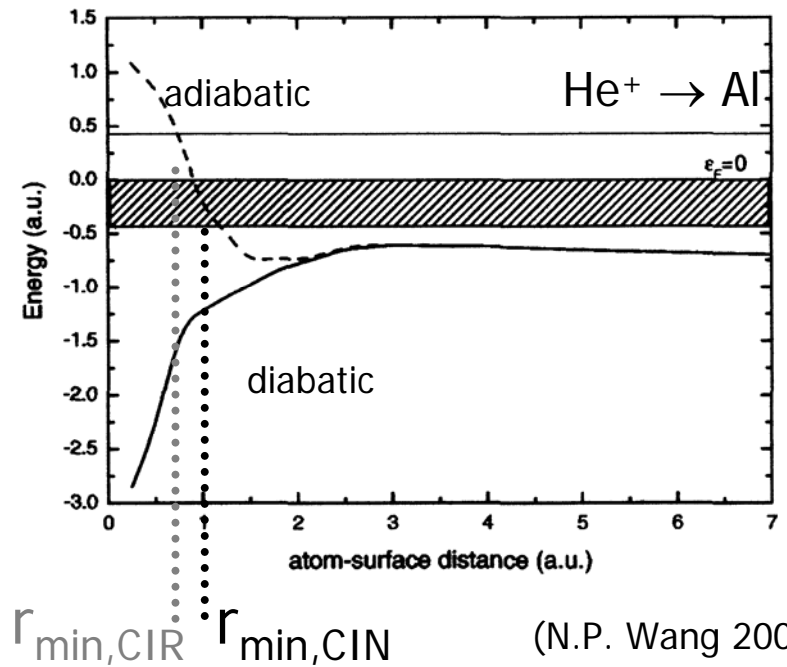
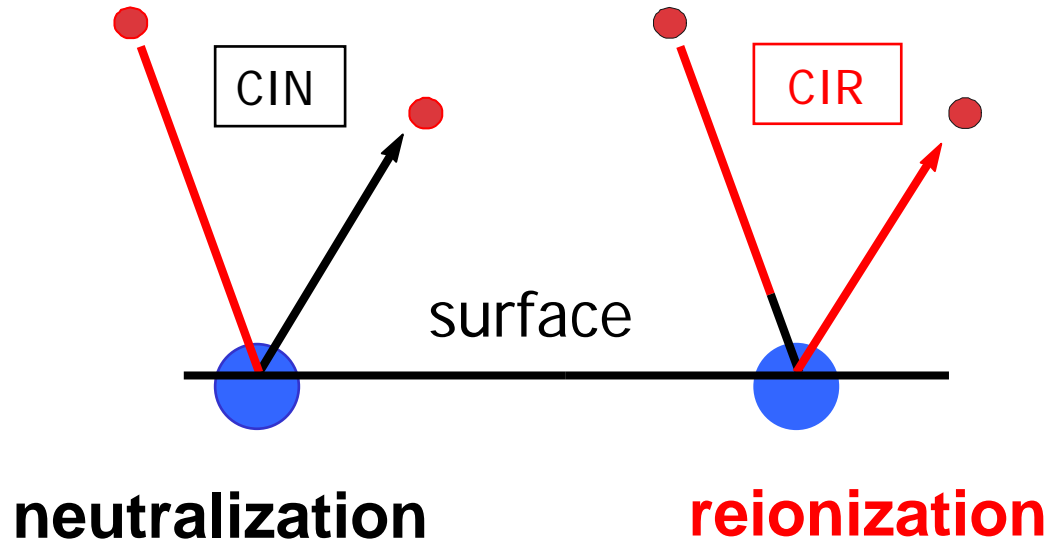
Collision induced processes

$r < r_{\min} \rightarrow$ overlap of orbitals \rightarrow electron promotion



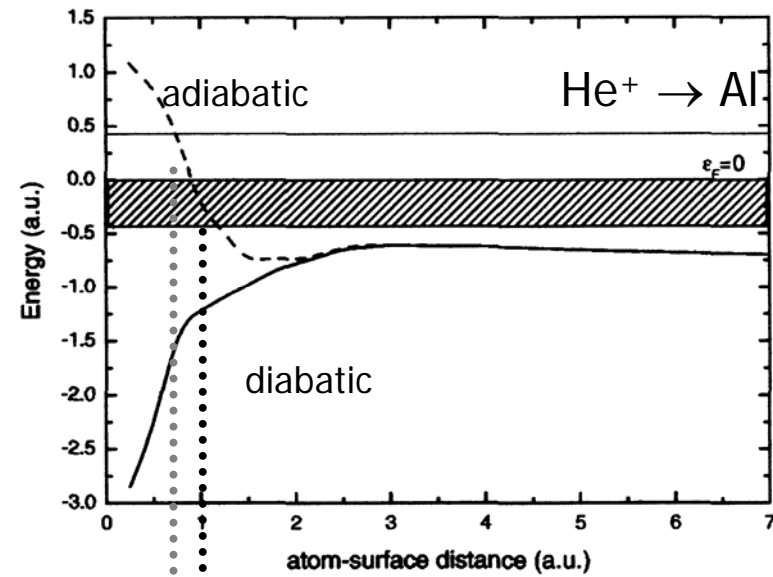
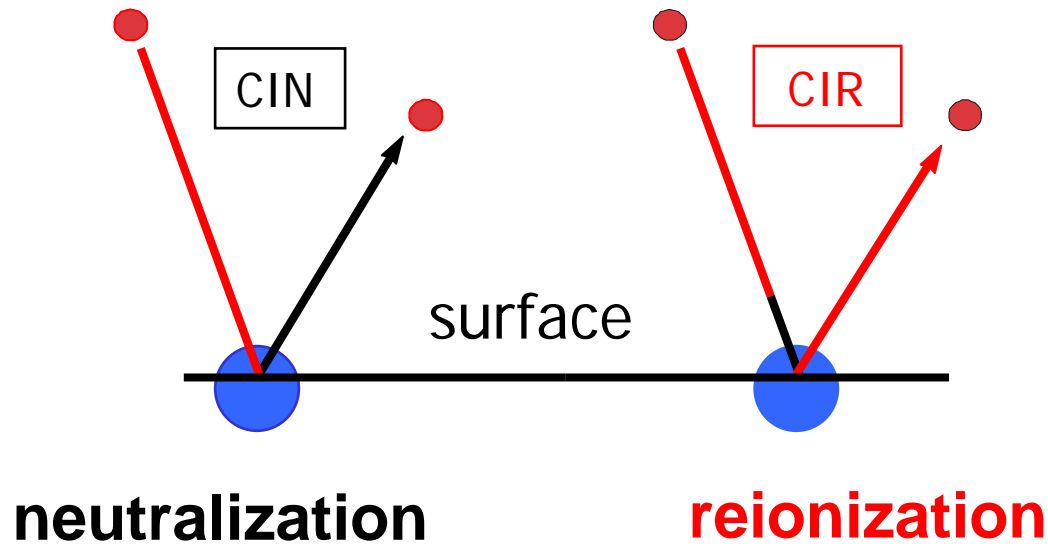
Collision induced processes

$r < r_{\min} \rightarrow$ overlap of orbitals \rightarrow electron promotion



Collision induced processes

$r < r_{\min} \rightarrow$ overlap of orbitals \rightarrow electron promotion



$r_{\min,CIR}$ $r_{\min,CIN}$ (N.P. Wang 2001)

$r < r_{\min} \leftrightarrow E > E_{th}$	{	Cu: $r_{\min} \approx 0.1 \text{ \AA}$	$\leftrightarrow E_{th} \approx 2 \text{ keV}$
		Au: $r_{\min} \approx 0.3 \text{ \AA}$	$\leftrightarrow E_{th} \approx 1.5 \text{ keV}$
		Al: $r_{\min} \approx 0.5 \text{ \AA}$	$\leftrightarrow E_{th} \approx 0.4 \text{ keV}$

Neutralisation \leftrightarrow ion fraction P^+

$$\text{ion fraction } P^+ = N_+ / (N_+ + N_0)$$

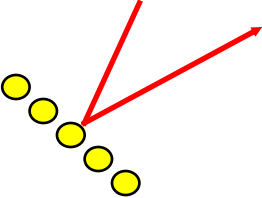
{ survivals
reionised projectiles

AN: $P^+(-v_c/v_\perp)$

collision: $P_{\text{CIN}}(E, \theta)$, $P_{\text{CIR}}(E, \theta)$

Neutralisation \leftrightarrow ion fraction P^+

$E > E_{th}$:


$$P^+ = P_{in}^+ \cdot (1 - P_{CIN}) \cdot P_{out}^+$$

survivals

Neutralisation \leftrightarrow ion fraction P^+

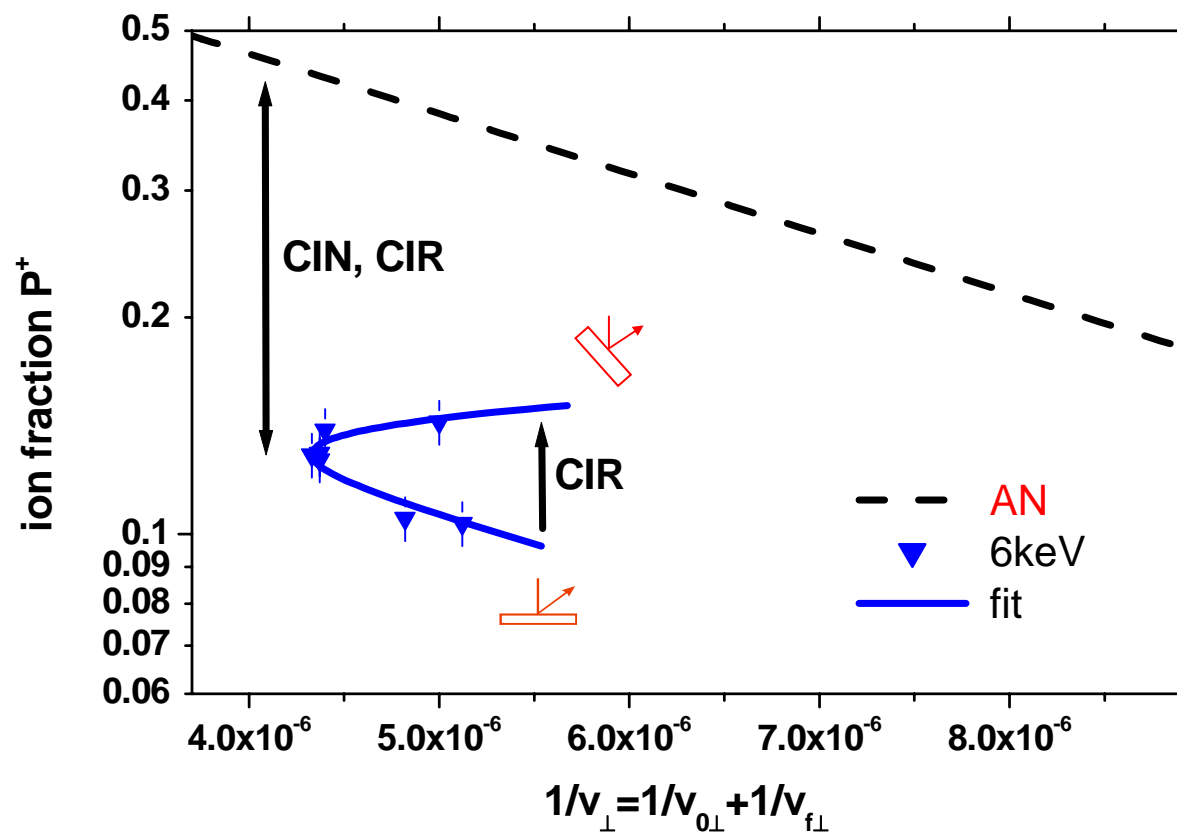
$E > E_{th}$:

$$P^+ = \underbrace{P_{in}^+ \cdot (1 - P_{CIN})}_{\text{survivals}} \cdot P_{out}^+ + \underbrace{(1 - P_{in}^+) \cdot P_{CIR}}_{\text{reionised projectiles}} \cdot P_{out}^+$$

$$P^+ = P^+(E, \theta, \mathbf{v}_{\perp}) \rightarrow P^+(\alpha) \text{ @ given } E, \theta$$

${}^4\text{He} \rightarrow \text{Cu}$

$$E > E_{\text{th}}: P^+(\mathbf{v}_{\perp}, \alpha)$$



fixed energy \leftrightarrow
 $P_{\text{CIN}}, P_{\text{CIR}}$ constant

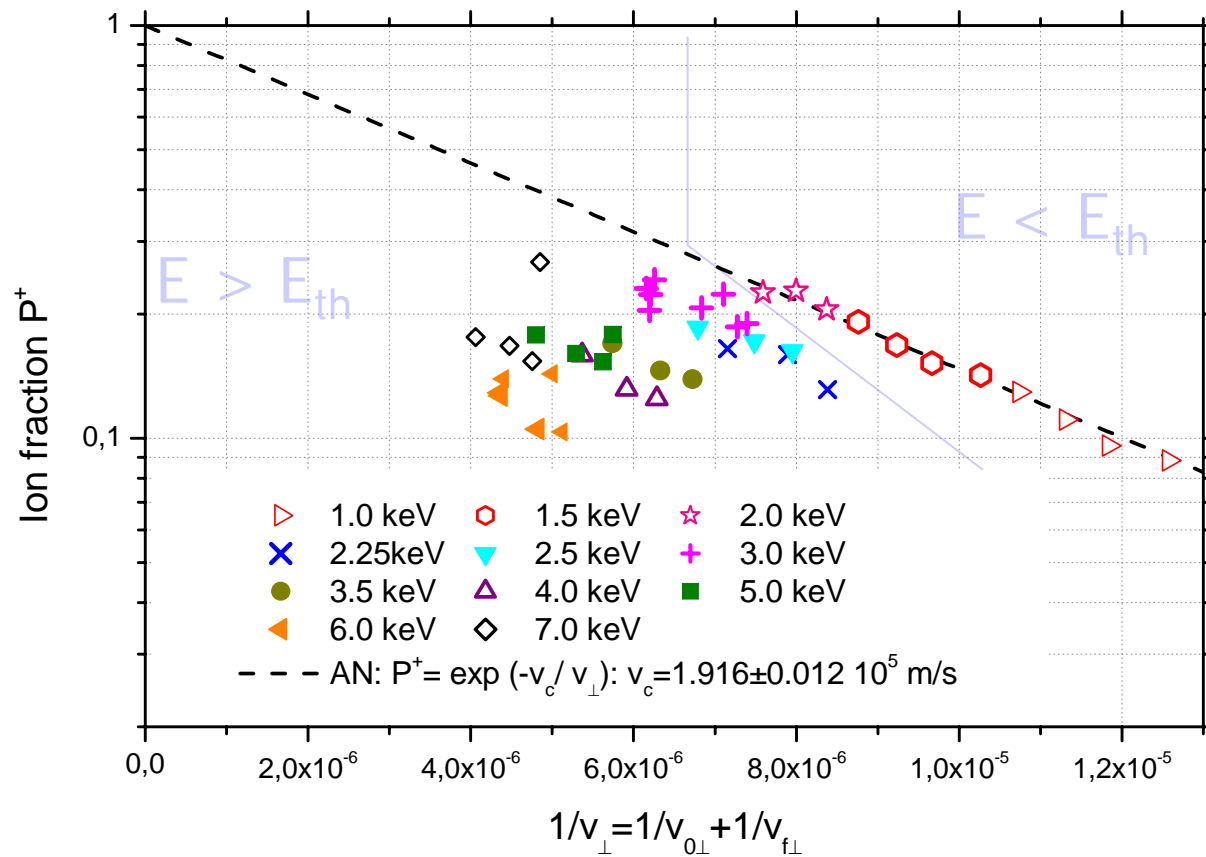
variation of v_{\perp} by variatio
of geometry

\rightarrow ‚boomerang‘ shape

$\rightarrow P_{\text{CIN}} > P_{\text{CIR}}$

(M. Draxler 2004)

${}^4\text{He} \rightarrow \text{Cu}$



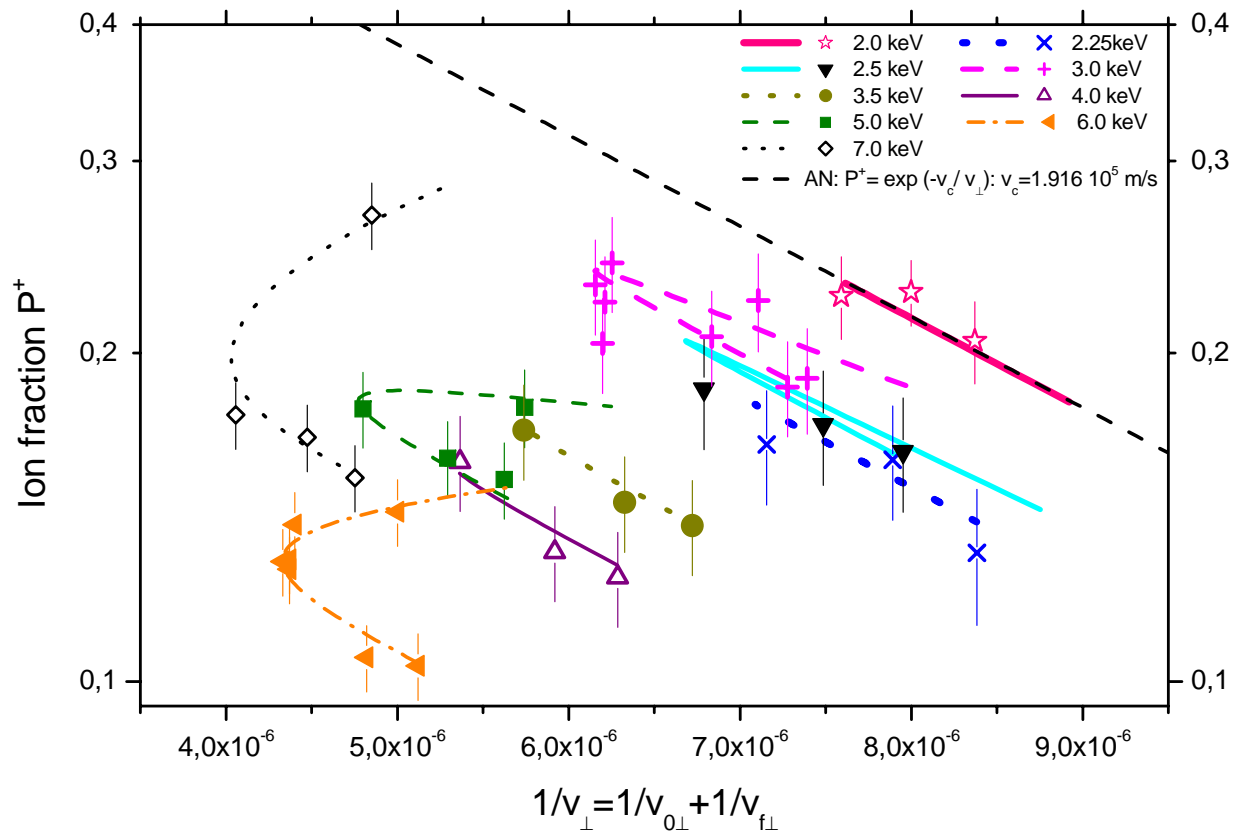
$$E < E_{th}: P^+(v_\perp)$$

$$E > E_{th}: P^+(v_\perp, \alpha)$$

(M. Draxler 2002)

${}^4\text{He} \rightarrow \text{Cu}$

High energy regime in more detail:



variation of v_{\perp} by

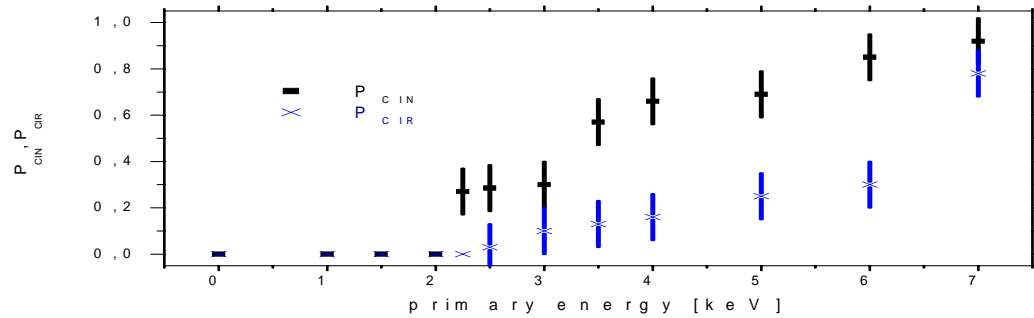
- variation of energy
- variation of geometry

→ AN

→ CIN, CIR

→ $P_{\text{CIN}} \gg P_{\text{CIR}}$

$P_{CIN}(E), P_{CIR}(E)$



$$P_{CIN} > P_{CIR}$$

$P_{CIN} \uparrow, P_{CIR} \uparrow$ with $E \uparrow$

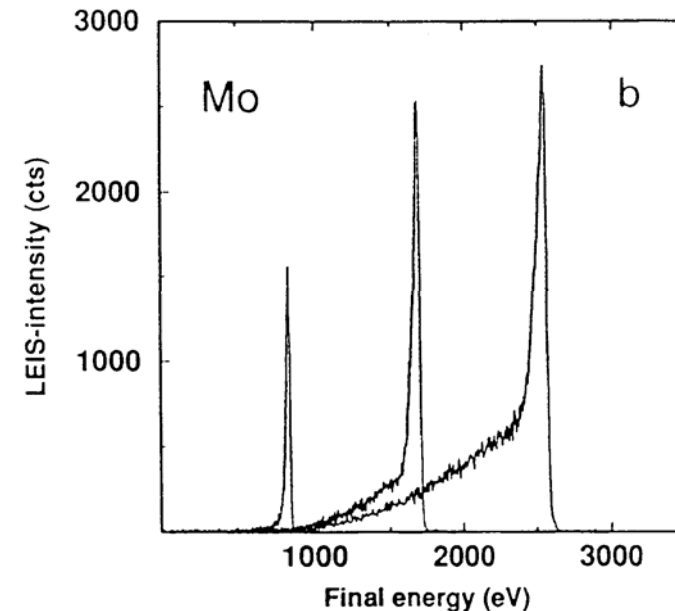
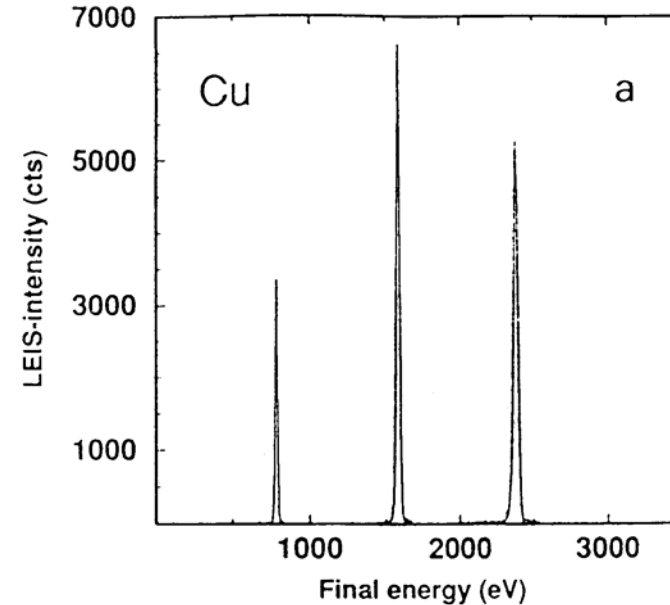
P_{CIN}, P_{CIR} at higher E ?

(M. Draxler 2002)

Shape of ion spectra

Cu: threshold for reionization is high ($E_{th} = 2.1$ keV)
→ no reionization background for $E < 3$ keV

Mo: threshold for reionization is low ($E_{th} = 0.4$ keV)
→ reionization background down to $E < 1$ keV

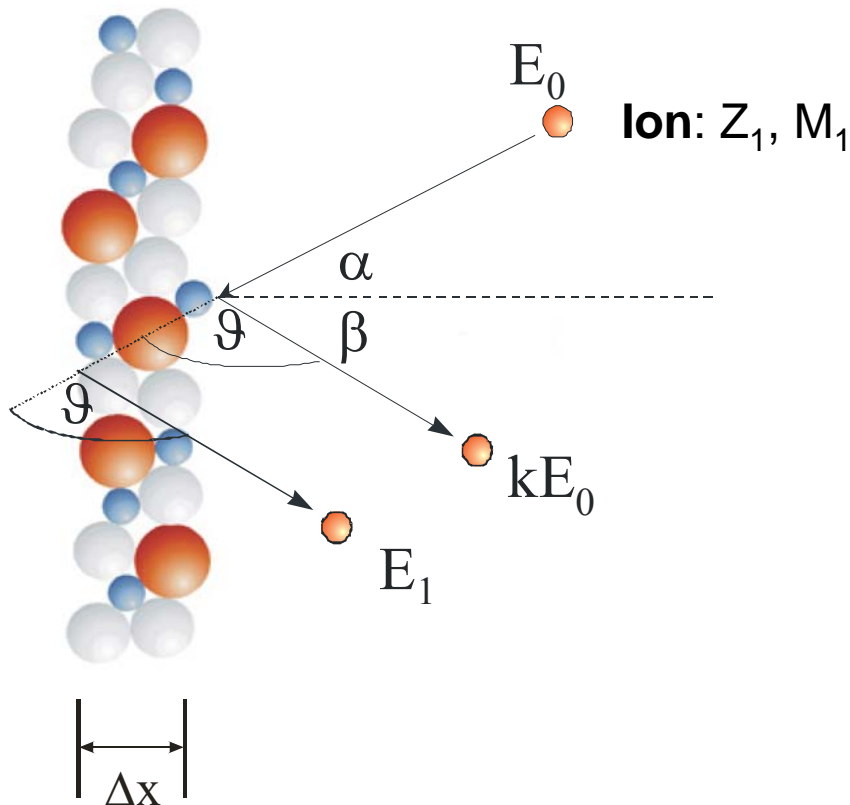


Applications: surface composition analysis

(concentrations c_j of j atoms, j = „dark blue“, „light blue“ and „red“)

$$A_j^+ = \frac{N_0}{\cos \alpha} \cdot \frac{d\sigma_j}{d\Omega} \cdot (nd)_{j,0} \cdot \Omega \cdot P_j^+ \cdot \eta_+ = c_j S_j$$

Target: Z_{j2}, M_{j2}



Quantitative surface composition analysis

Surface concentration of element j

basis:
$$A_j^+ = \frac{N_0}{\cos \alpha} \cdot \frac{d\sigma_j}{d\Omega} \cdot (nd)_{j,0} \cdot \Omega \cdot P_j^+ \cdot \eta_+ = c_j S_j$$

sensitivity factor for element j

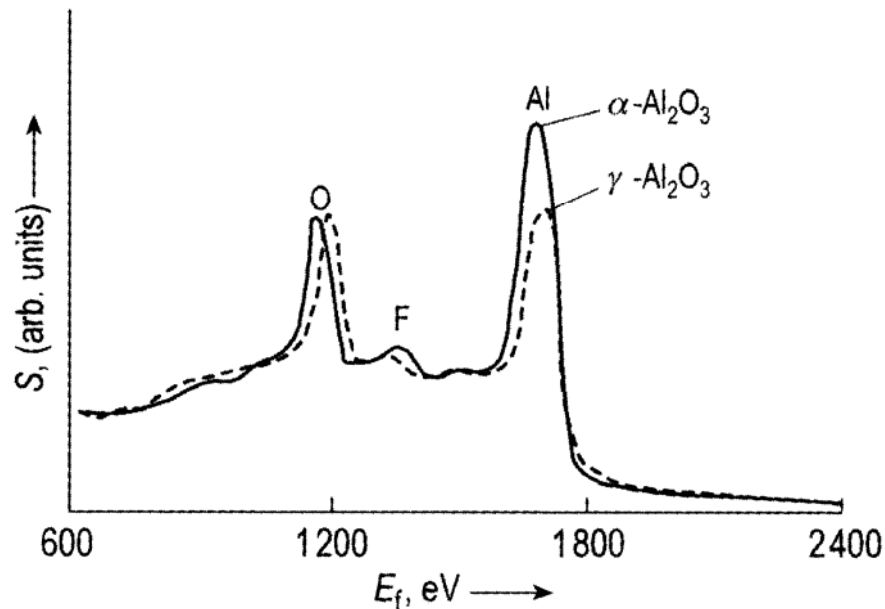
Main question: does P^+ depend on surface composition?
 \leftrightarrow are there „matrix effects“?

No matrix effects \leftrightarrow S_i does not depend on other elements present in the surface.

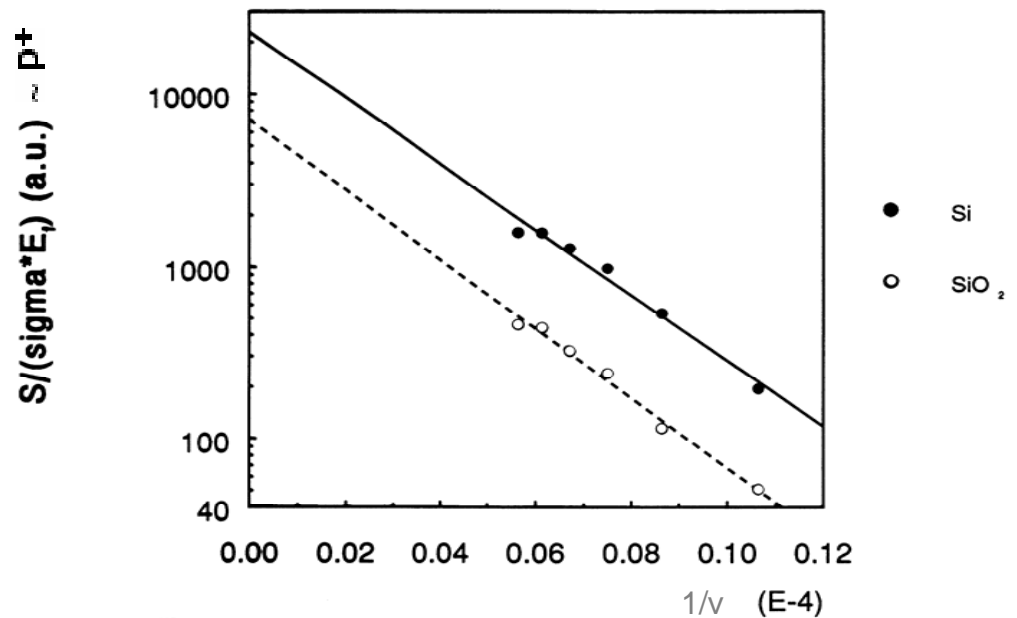
How to prove the absence of matrix effects?

Quantitative LEIS: Usually NO Matrix effects (\leftrightarrow P^+ does not depend on chemical environment)

.... not even in oxides (SiO_2 , Al_2O_3)!



(G.C. van Leerdam, 1991)

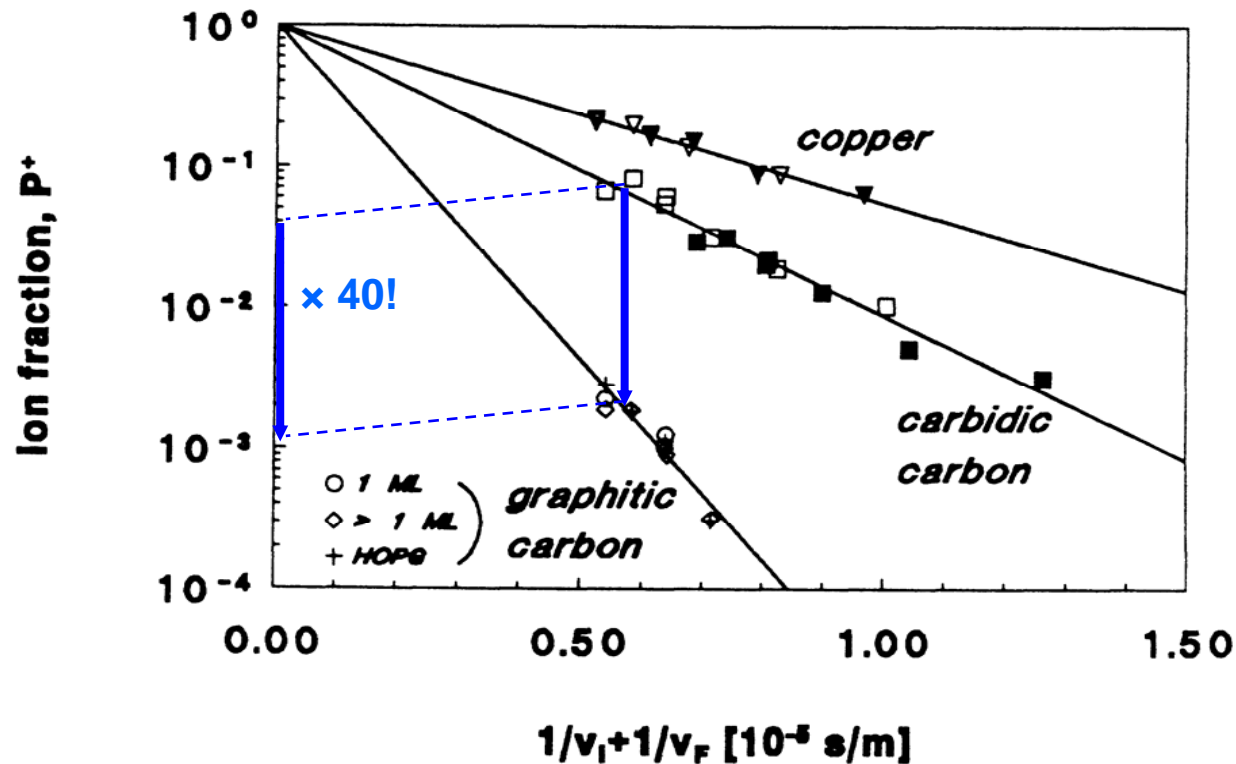


(J.P. Jacobs, 1991)

...but sometimes P^+ does depend on chemical state

... for instance: Carbon (graphitic - carbidic)

→ yield is dependent on binding partner.



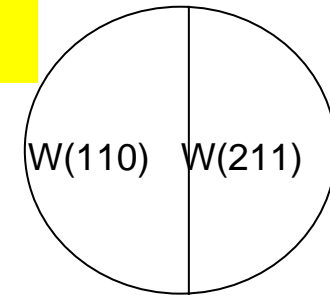
(L.C.A. van den Oetelaar, 1994)

Summary charge exchange processes

- ✓ model system to study P^+
- ✓ „local“ \leftrightarrow „non-local“ neutralisation in LEIS
- ✓ P^+ is a rather complex quantity
- ? Is P^+ well behaved?

What about quantitative surface composition analysis?

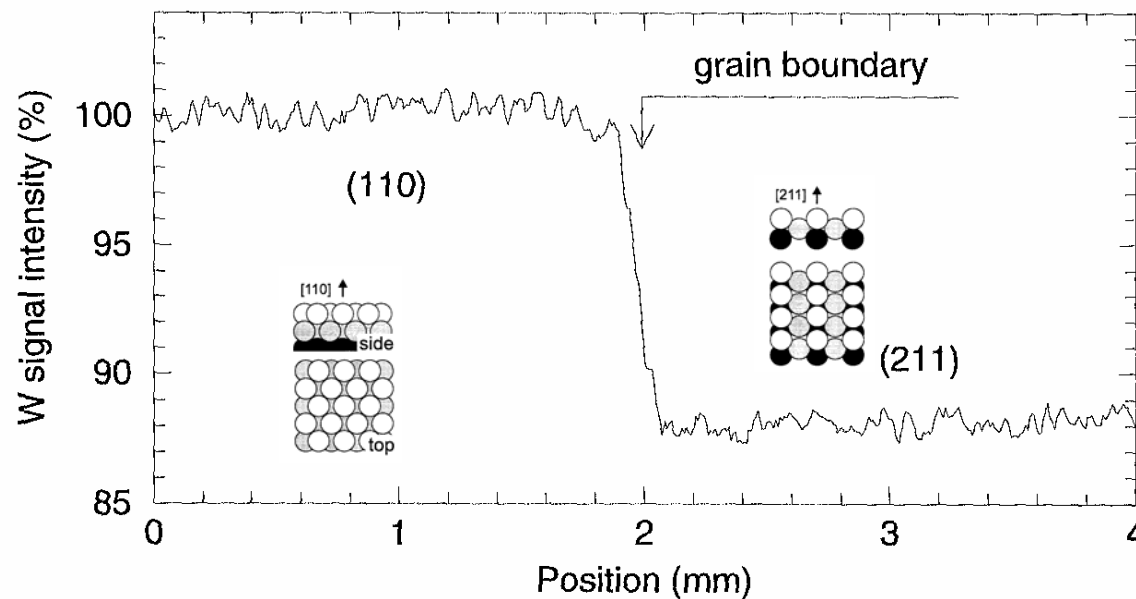
He⁺ → bicrystal W(110), W(211)



surface atoms/cm²: $n_{211}/n_{110} = 0.58$

signal ratio : $n_{211}/n_{110} = 0.88$

→ different neutralisation or deeper layers contributing



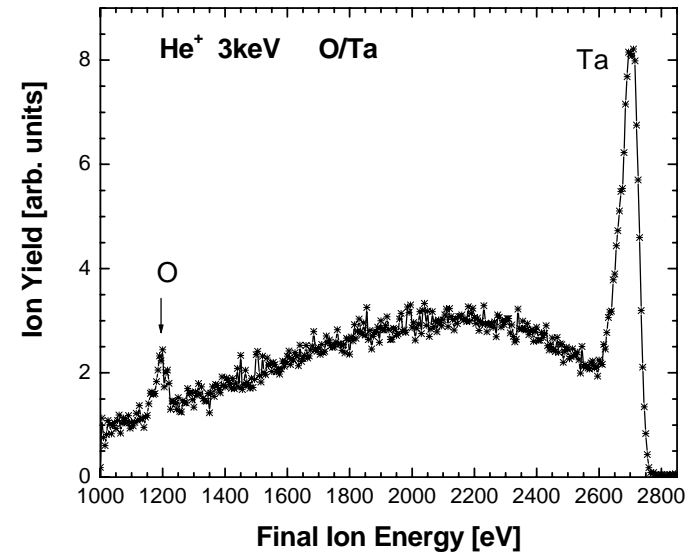
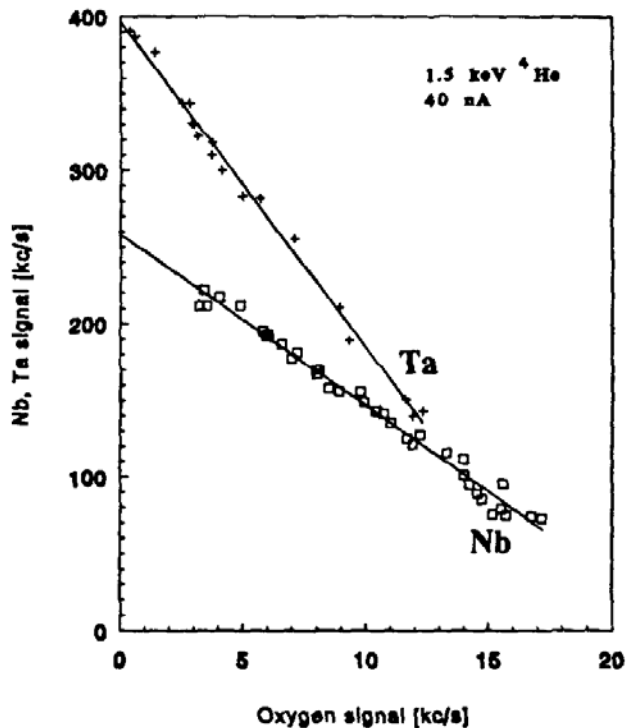
Cortenraad (2000)

Two elements (O, W) in the surface

$$c_O + c_{Ta} = 1$$

$$A_O^+ = c_O S_O$$

$$A_{Ta}^+ = c_{Ta} S_{Ta}$$



$$\rightarrow \frac{A_O^+}{S_O} + \frac{A_{Ta}^+}{S_{Ta}} = 1?$$

→ is plot A_{Ta}^+ vs. A_O^+ linear?

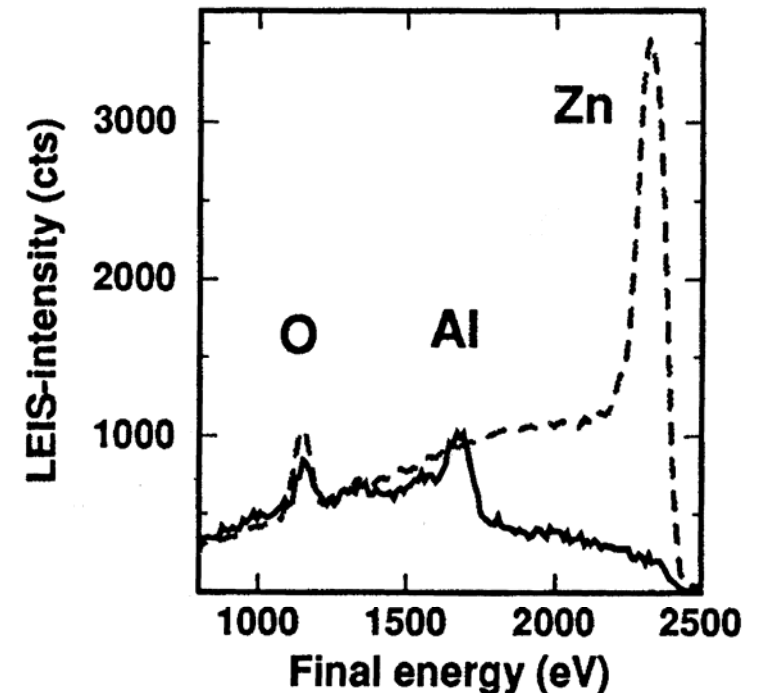
→ indeed no matrix effects!

Application: surface composition of a spinel

ZnAl_2O_4 zinc aluminate spinel*)

LEIS is sensitive to Zn (see ZnO)

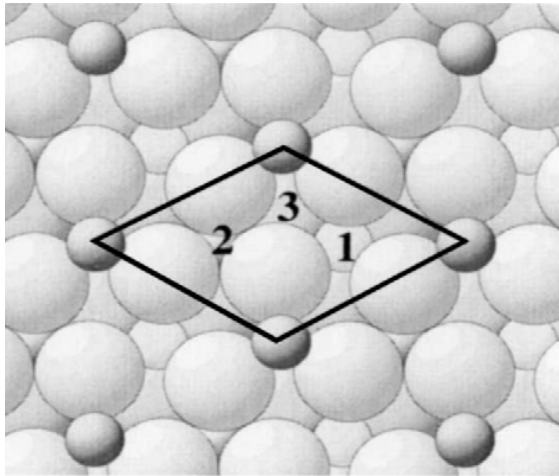
no Zn visible in spinel surface!



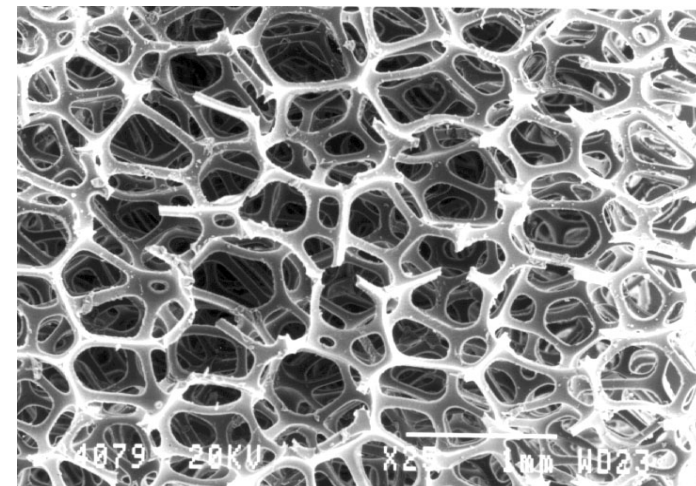
*) as bulk ceramic: used as a structural and high-temperature material.
with high-surface area: useful as catalysts and catalytic supports

Influence of surface roughness?

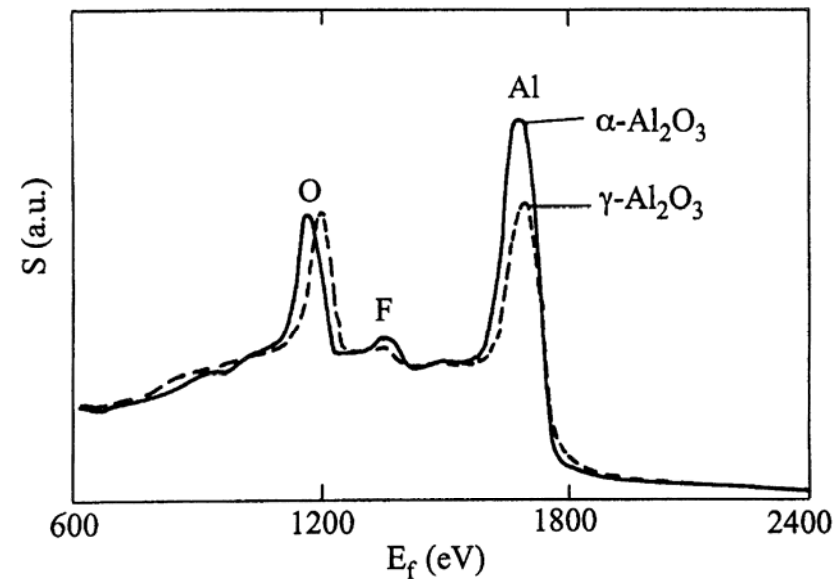
α Al₂O₃



γ Al₂O₃

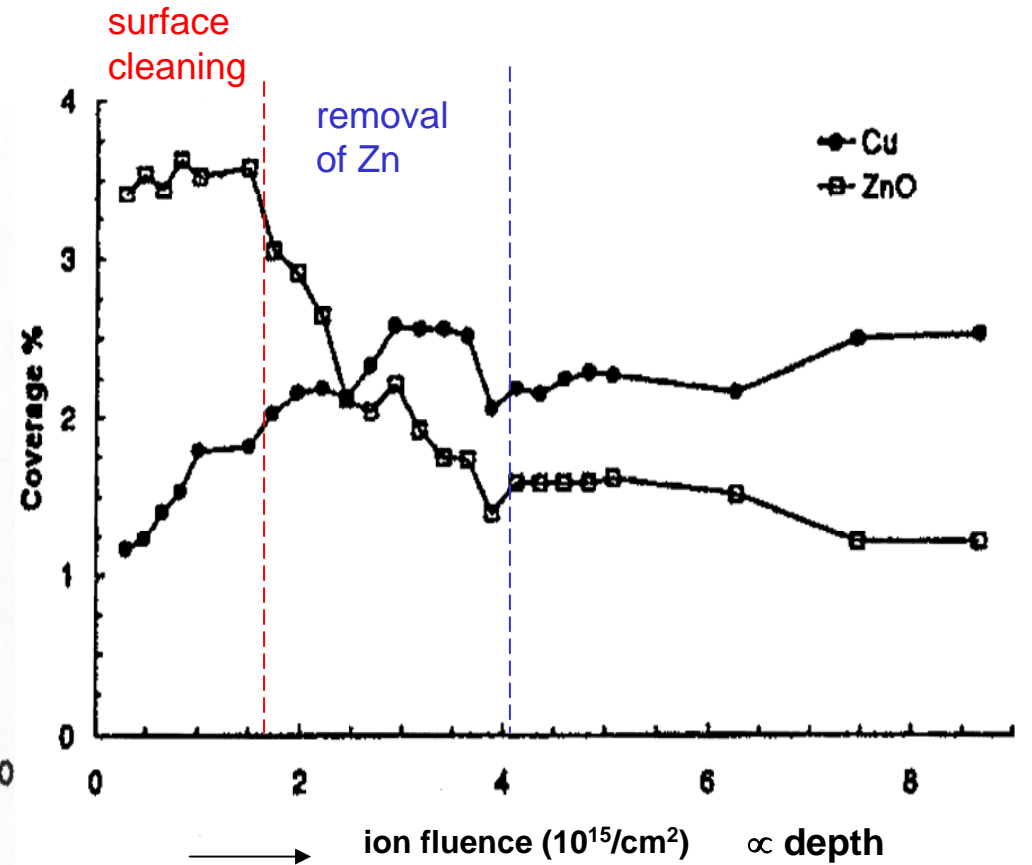
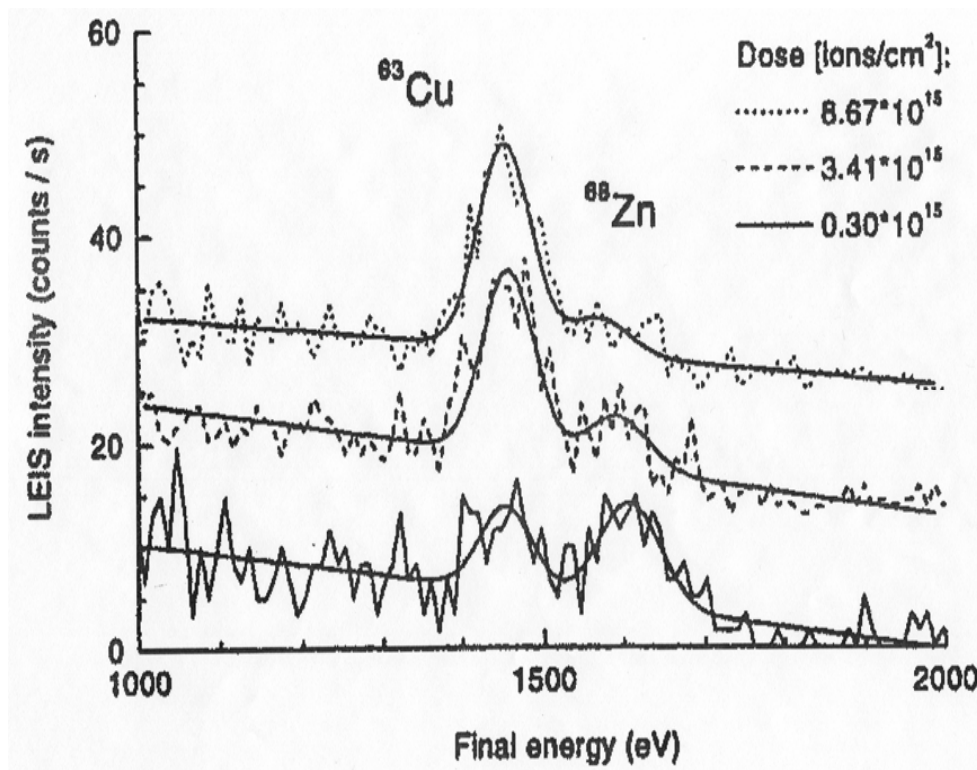


LEIS analysis for surface composition:



Analysis of a real Cu/ZnO/SiO₂ catalyst

ceramic sponges are easily destroyed by ion bombardment → static LEIS: quantitative surface composition is possible!



Contents:

ion scattering: RBS \leftrightarrow LEIS

- scattering by nuclei \rightarrow scattered yield
- interaction with target electrons \rightarrow slowing down

Low energy ion scattering (LEIS)

- Electrostatic analyzer: ESA-LEIS
- Time-Of-Flight: TOF-LEIS

ESA-LEIS:

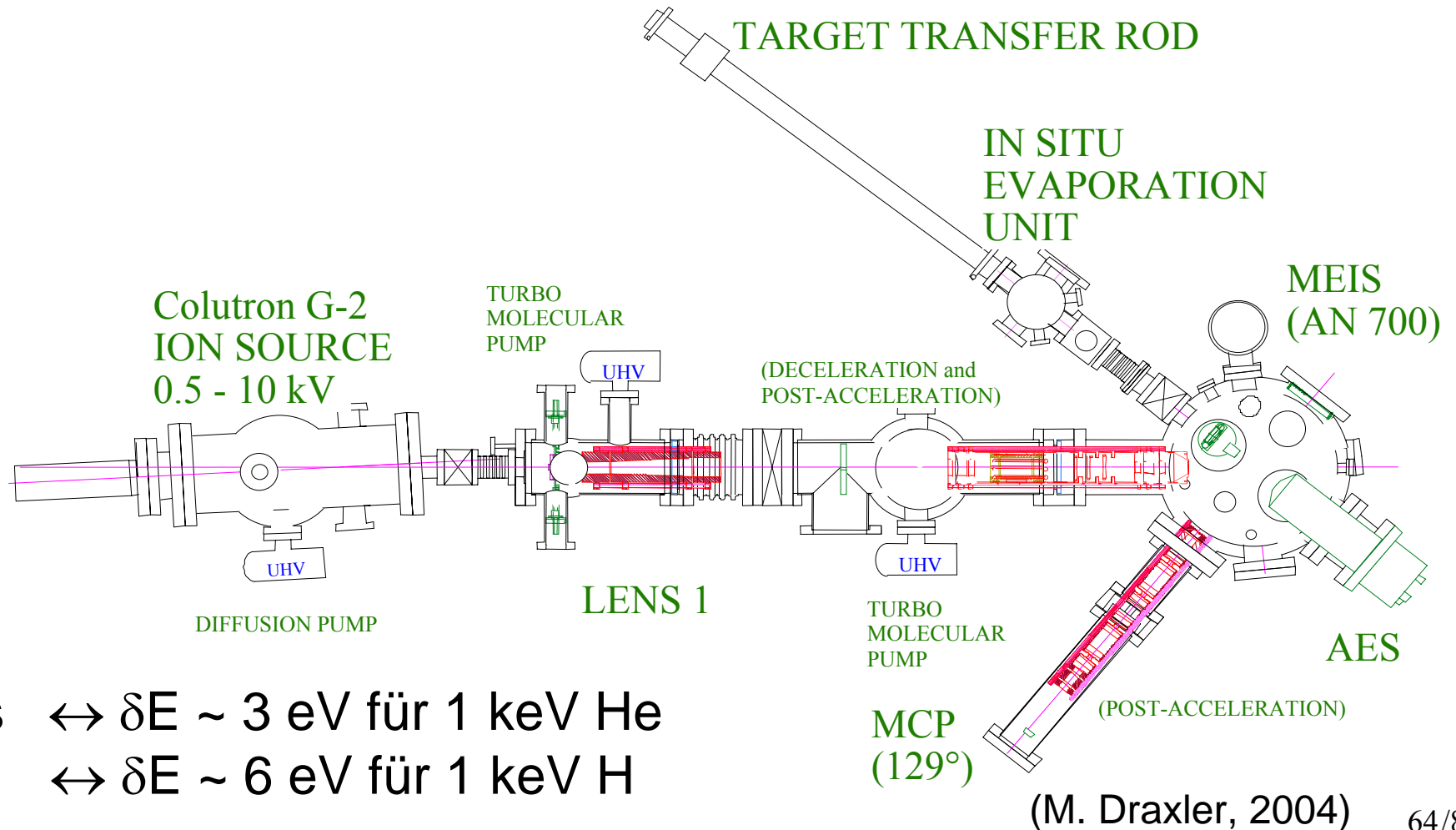
- instrumentation \rightarrow static ESA-LEIS
- ions detected \rightarrow ion fraction P^+
- noble gas ions:
 - neutralisation \rightarrow surface sensitivity
- applications: quantitative surface analysis \rightarrow examples

TOF-LEIS (Time-of-flight)

- instrumentation \rightarrow static TOF-LEIS
- ions and neutrals detected
 - surface structure analysis
 - depth resolution \rightarrow depth analysis \rightarrow applications
 - neutral spectrum: shape, depth information

Static TOF-LEIS - ACOLISSA

Advantages: - fluence $< 10^{12}$ ions/cm²
 - ions and/or neutrals

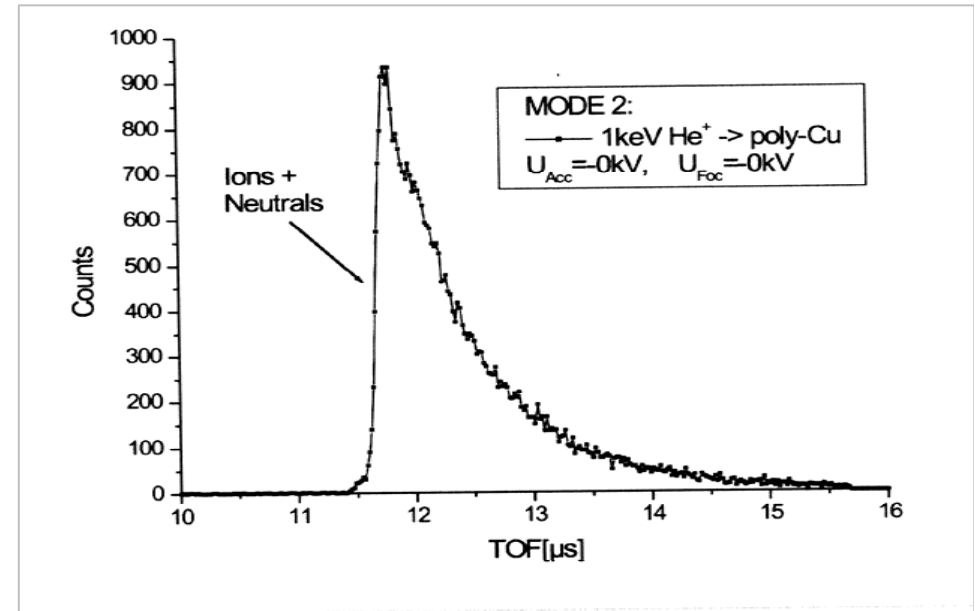


$\delta t \sim 5$ ns $\leftrightarrow \delta E \sim 3$ eV für 1 keV He
 $\leftrightarrow \delta E \sim 6$ eV für 1 keV H

(M. Draxler, 2004)

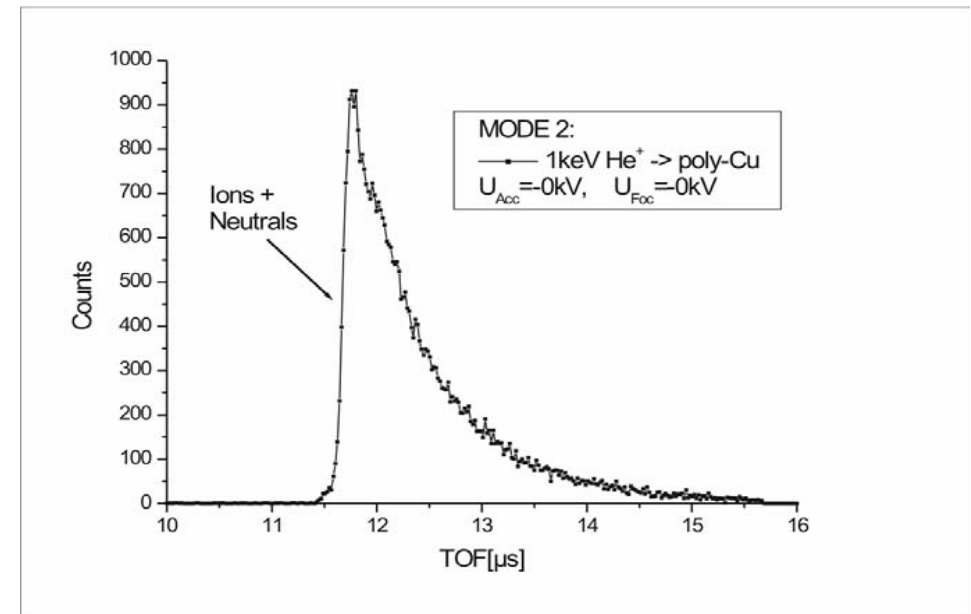
Static TOF-LEIS

no post-acceleration
→ ions + neutrals

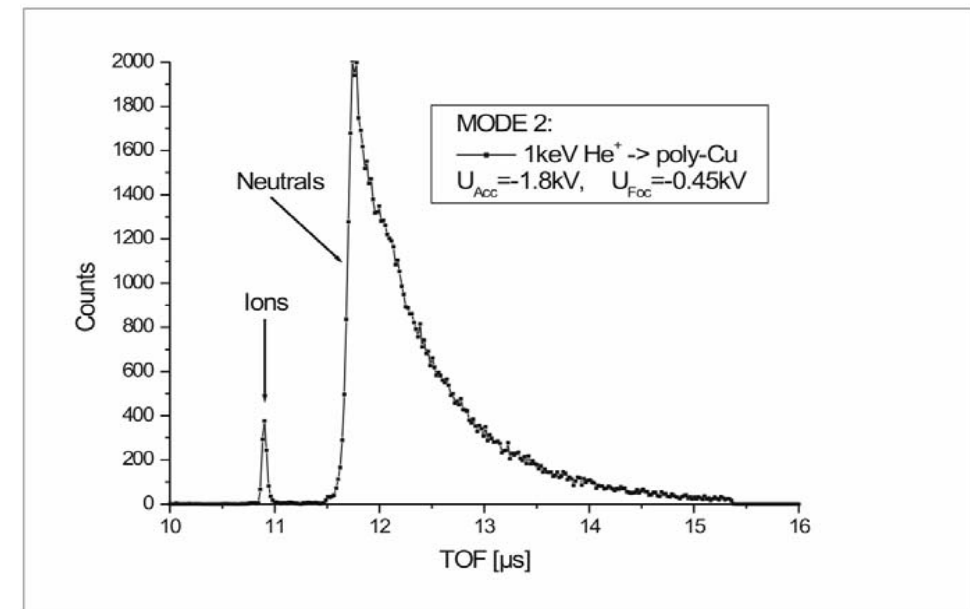


Static TOF-LEIS

no post-acceleration
→ ions + neutrals



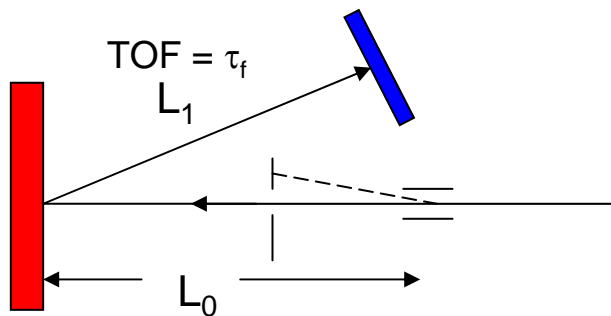
with post-acceleration
→ ions / neutrals separated



(M. Draxler, 2002)

Conversion TOF spectrum → energy spectrum

Classical mechanics: $E_f = (M/2)v_f^2 = (M/2) \cdot (L_1/\tau_f)^2$



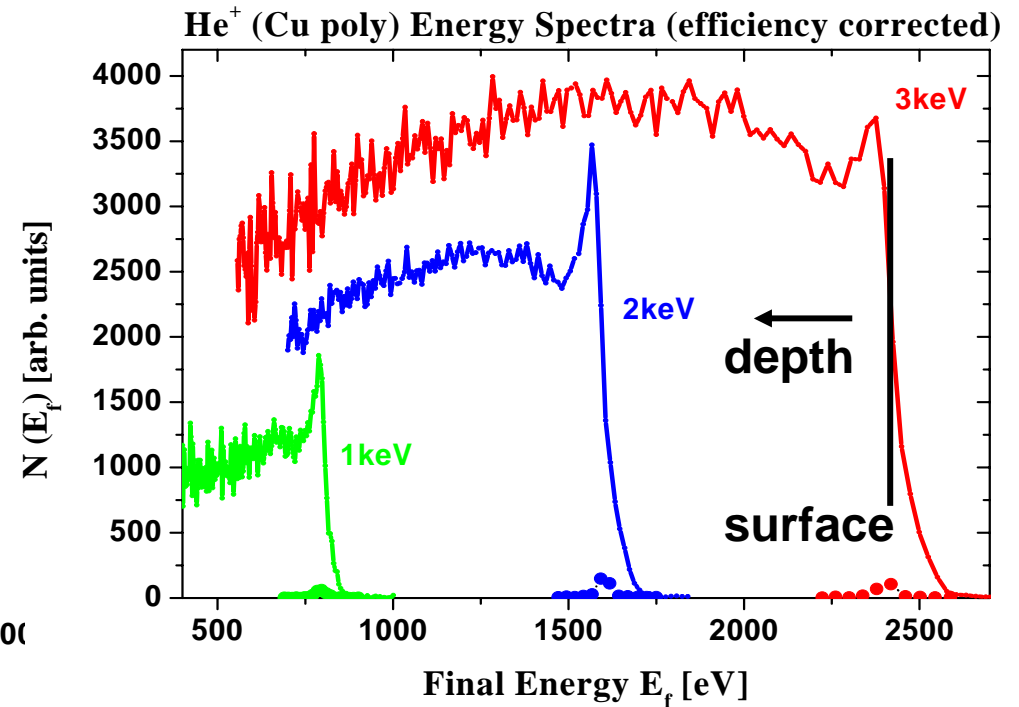
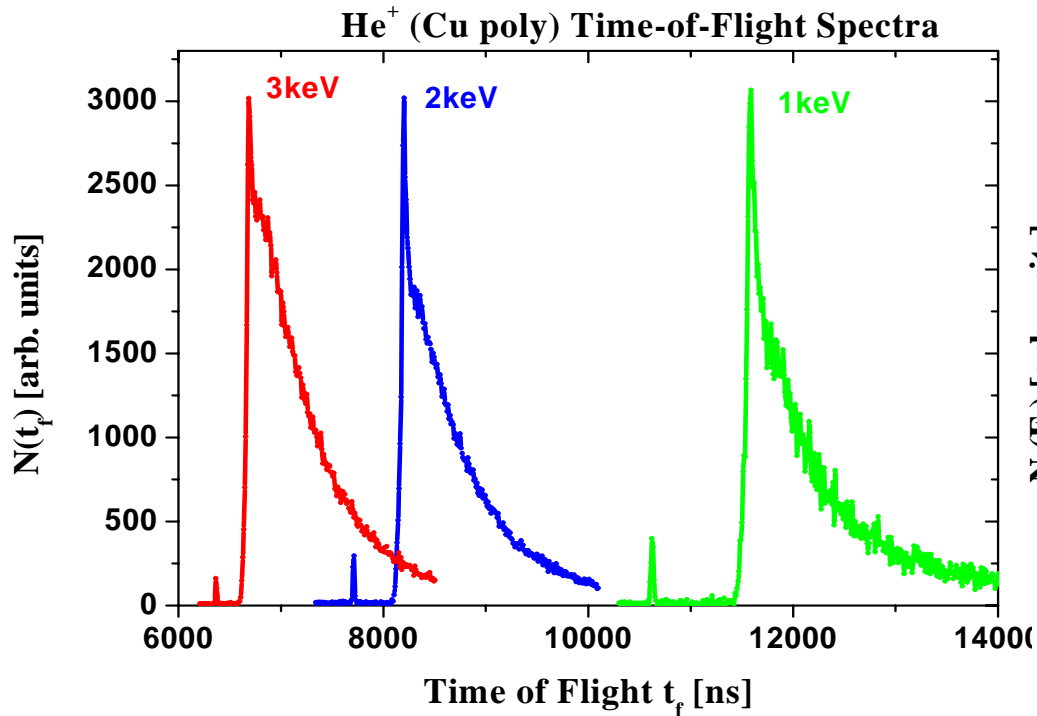
$$\frac{dE_f}{d\tau_f} = -2 \frac{M}{2} \frac{L_1^2}{(\tau_f)^3} = -2 \frac{E}{\tau_f}$$

particle conservation: $N(E_f)dE_f = N(\tau_f)d\tau_f$

particles in
one energy-
channel dE

particles in one
TOF channel dτ_f

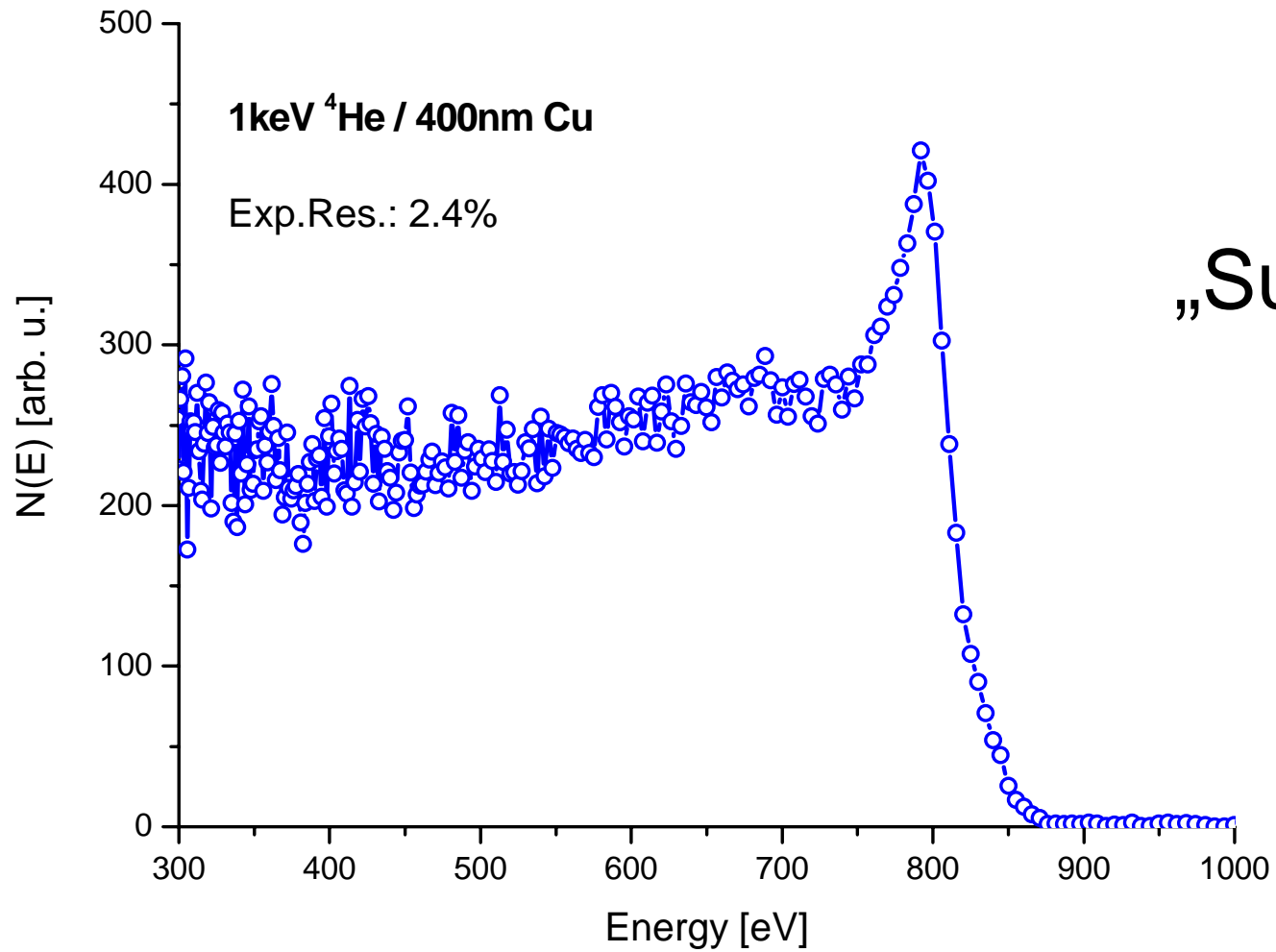
Conversion TOF spectrum → energy spectrum



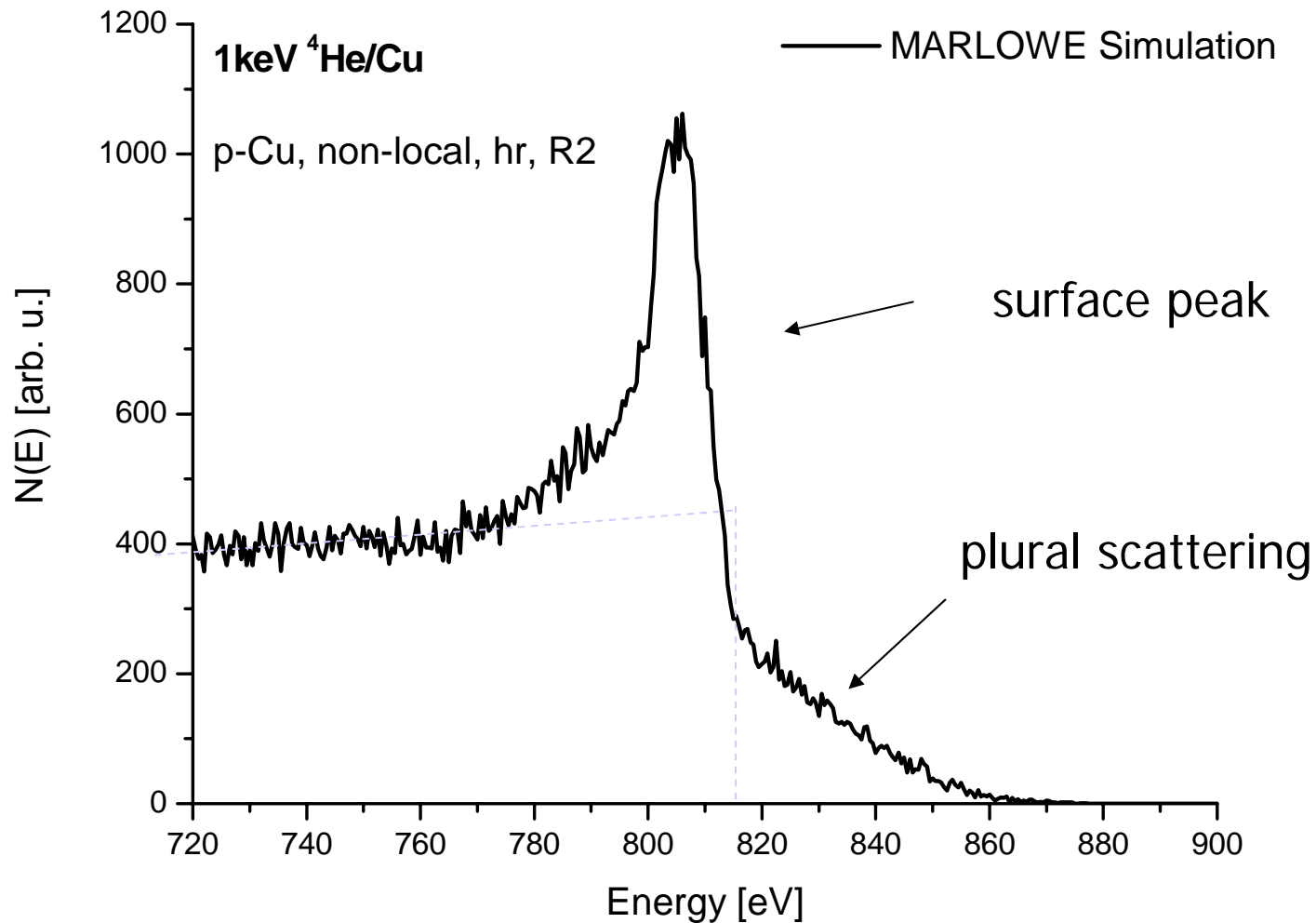
ions: surface peak (As in ESA spectra)

neutrals: much higher intensity than in ion spectrum
neutral spectrum has a surface peak,
contains also information from deeper layers

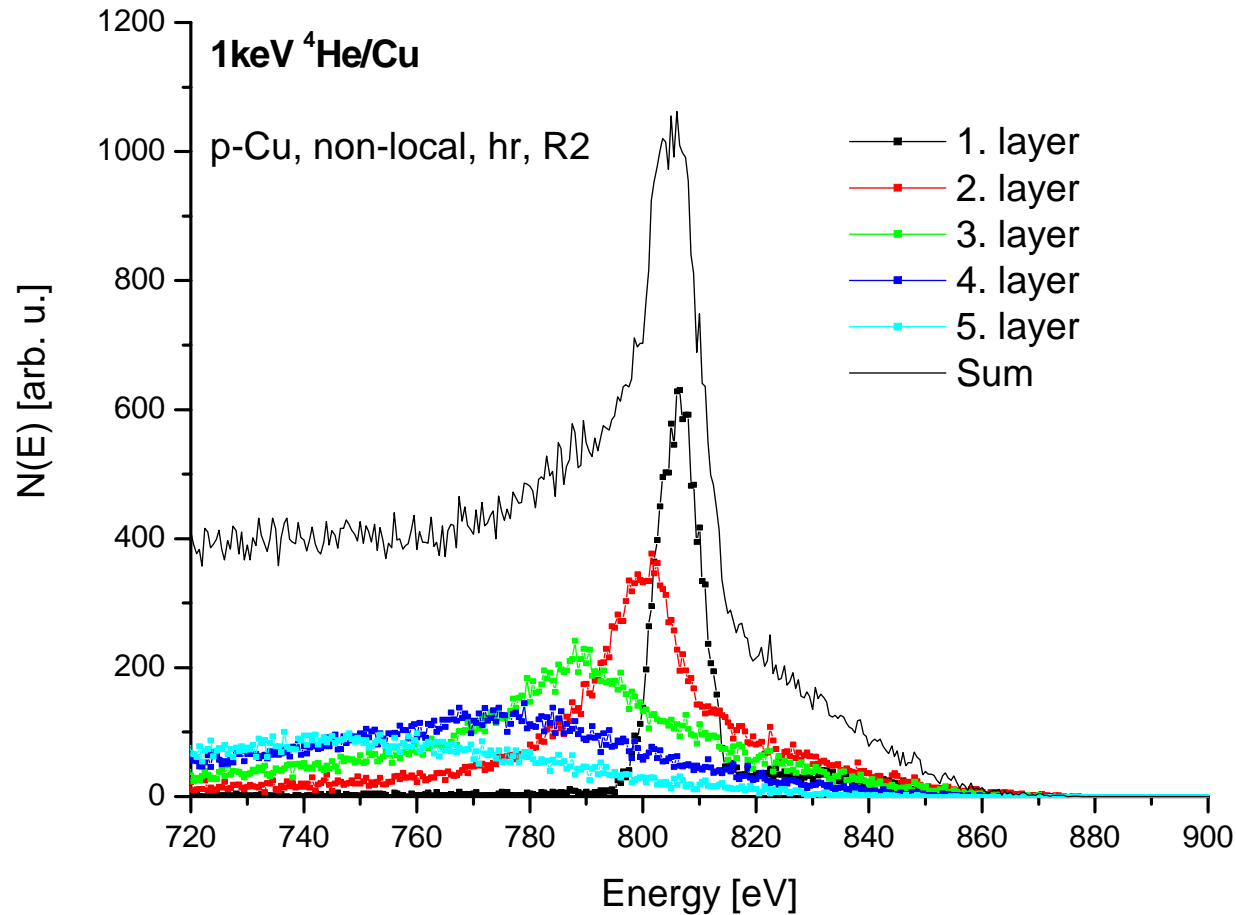
Energy spectrum



MARLOWE-simulation (Monte-Carlo)

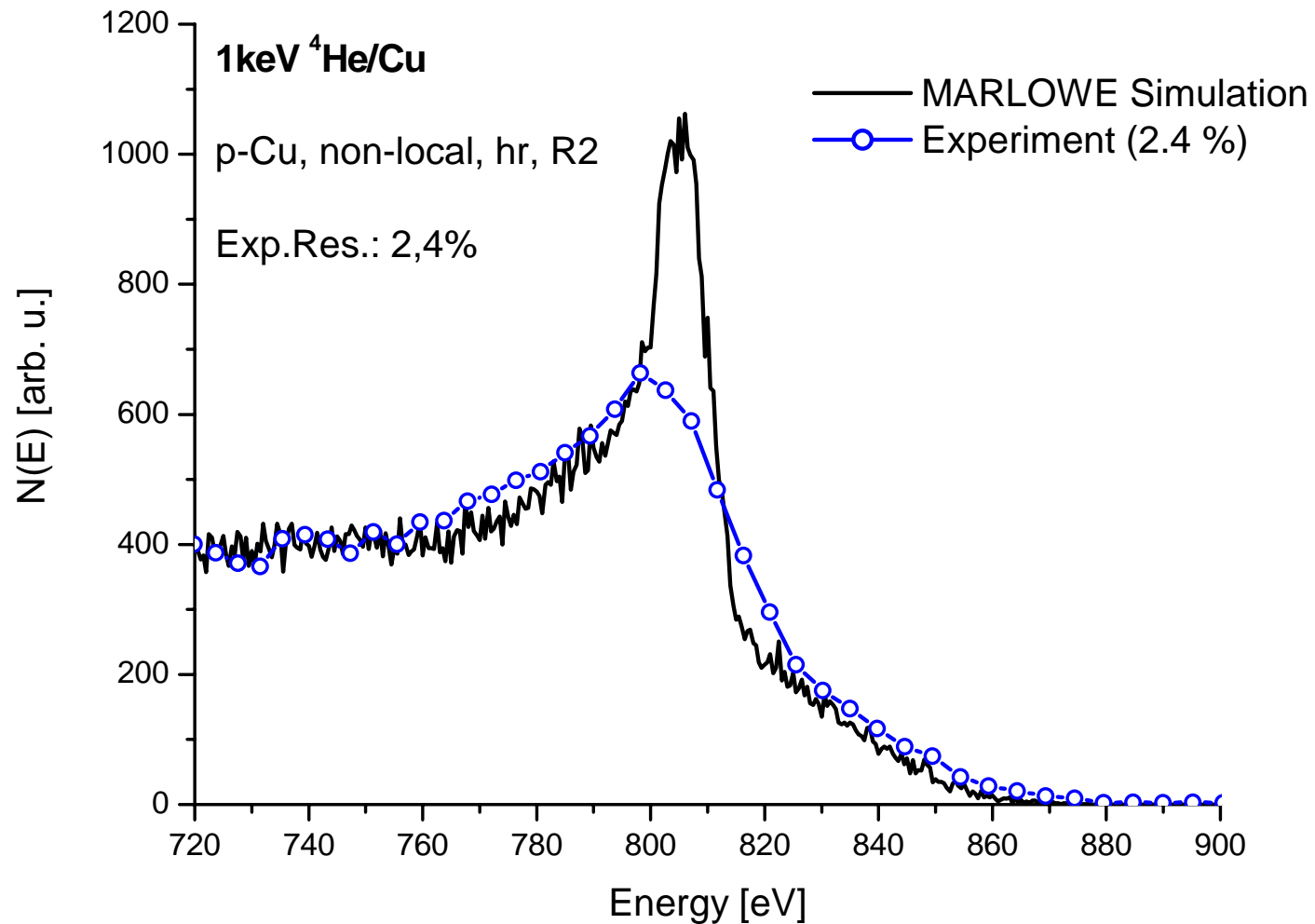


Explanation of surface peak:

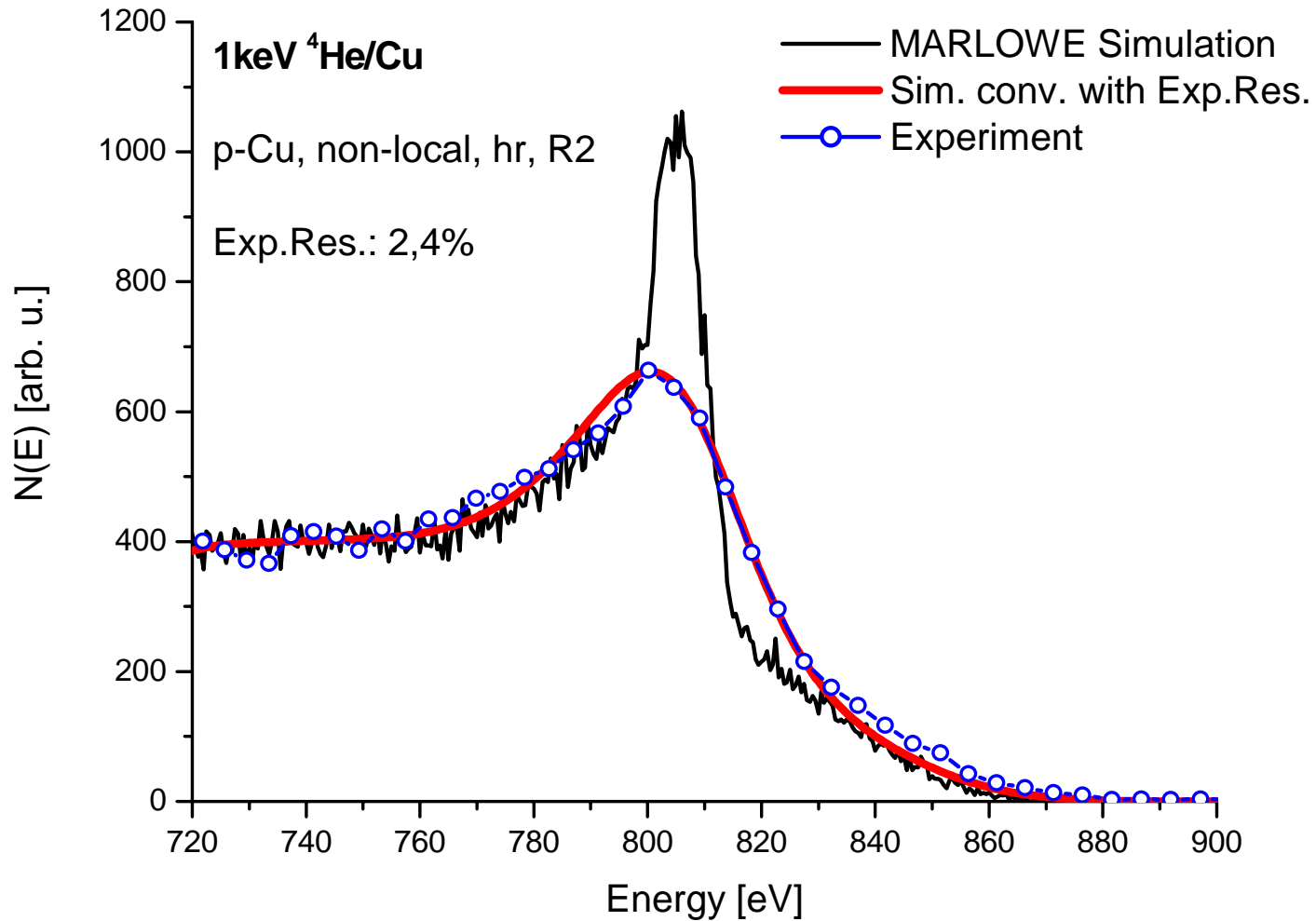


Surface peak due to (1) single scattering → multiple scattering
(2) shift of deeper layers due to stopping power

Experiment vs. simulation

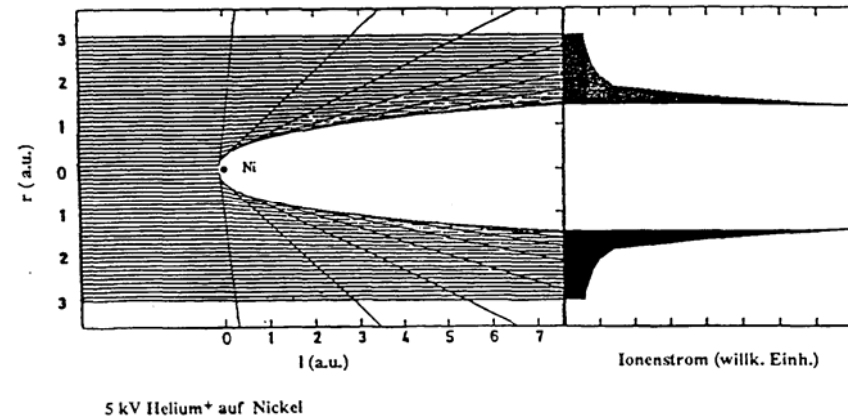


Experiment vs. simulation

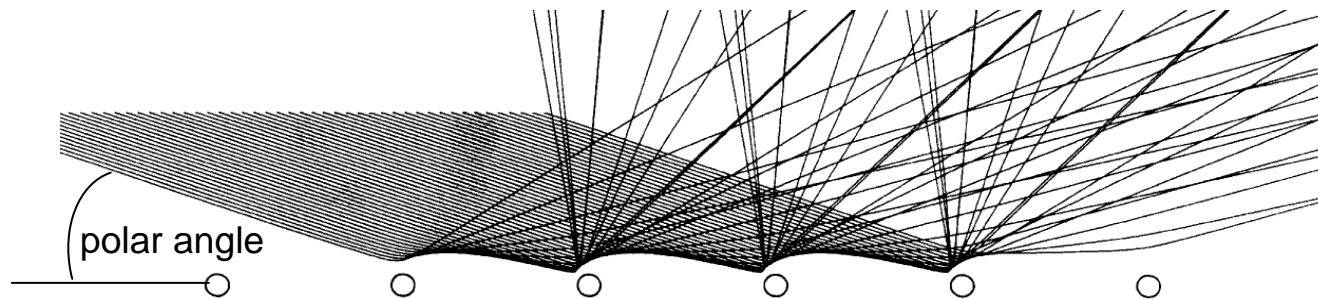


Surface structure analysis: $^4\text{He}^+$ \rightarrow Cu crystal

Channeling \rightarrow flux enhancement:

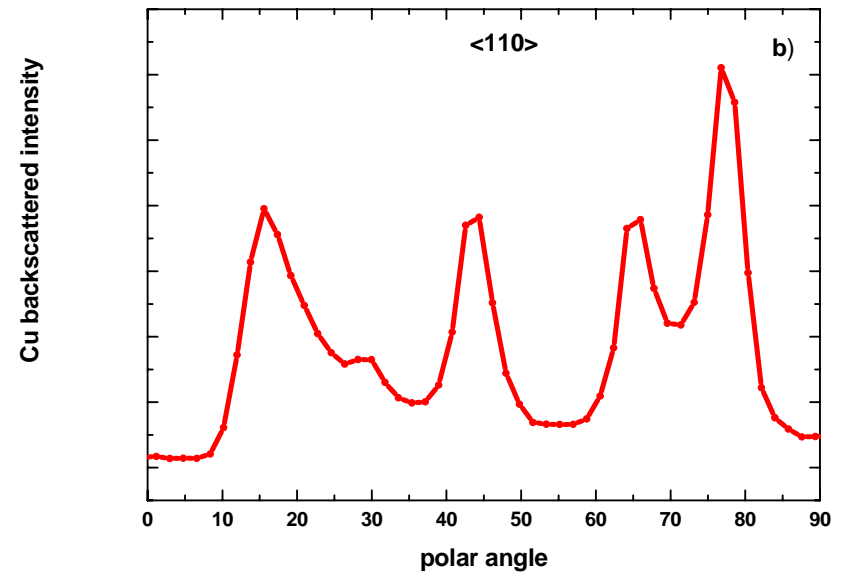
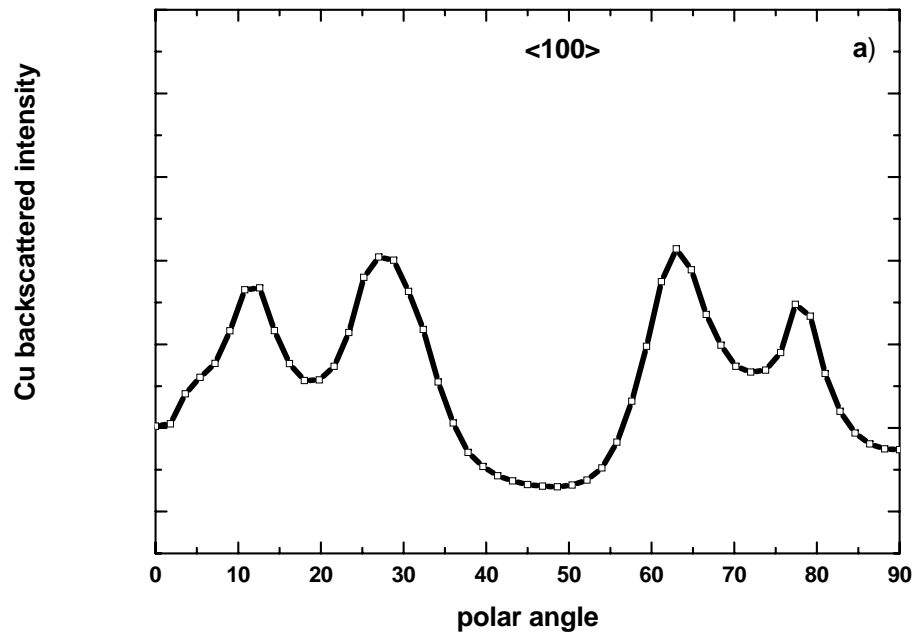


Focussing collisions at certain angles \rightarrow intensity peaks:



Surface structure analysis: $^4\text{He}^+$ \rightarrow Cu crystal

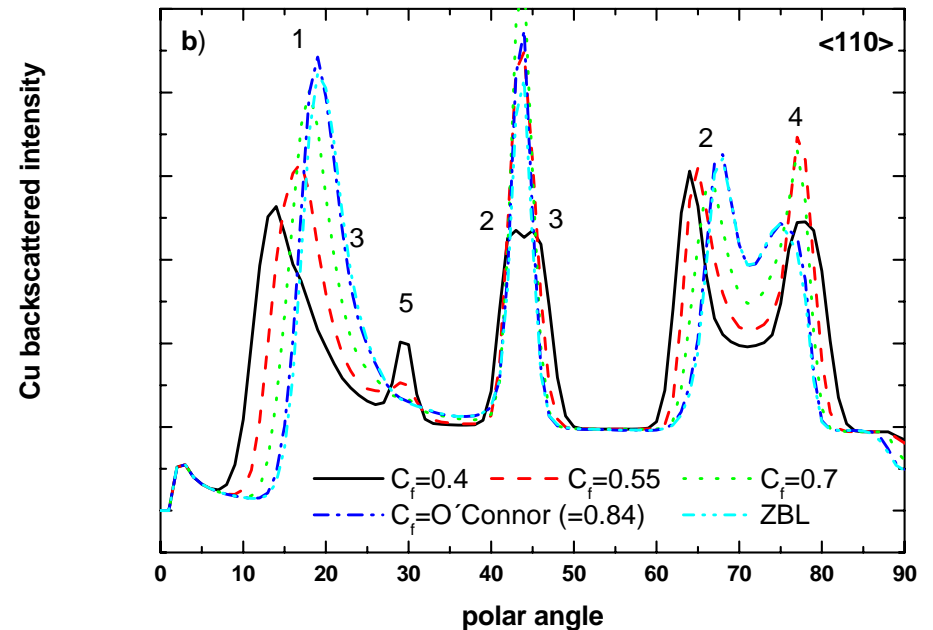
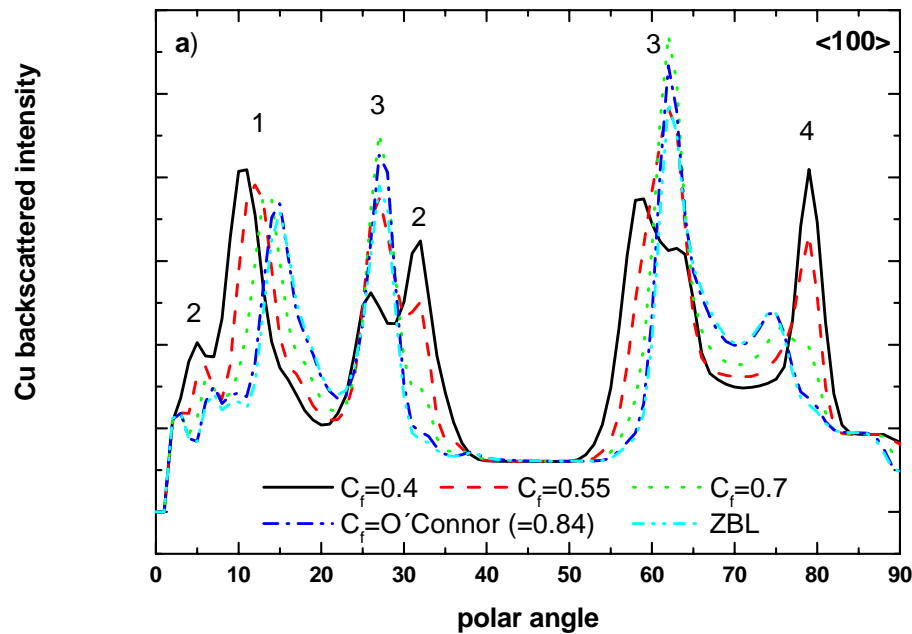
experiment: 179° scattering @ 3 keV



(Draxler 2005)

Surface structure analysis: $^4\text{He}^+ \rightarrow \text{Cu}$ crystal

Comparison experiment - Monte-Carlo simulations:

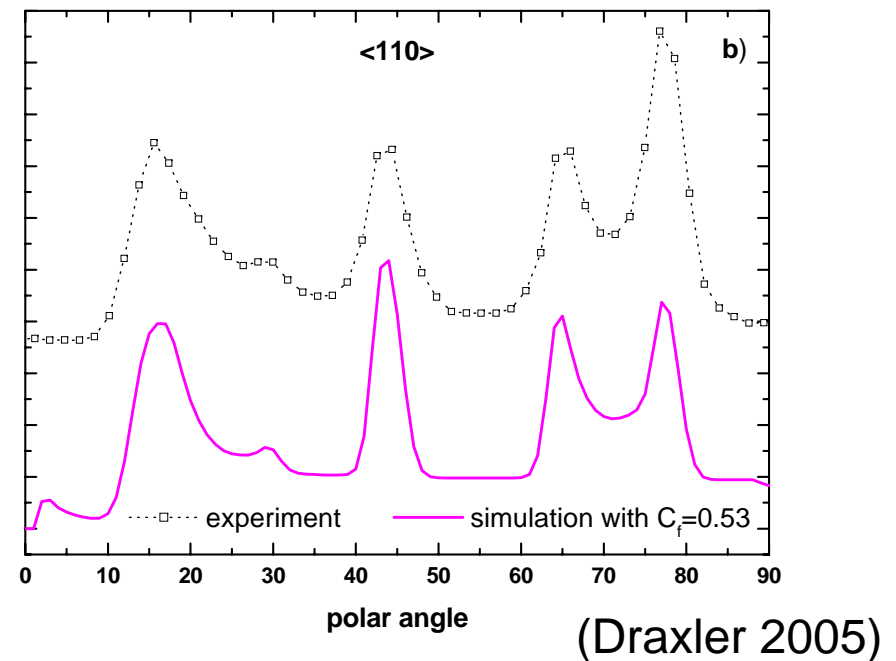
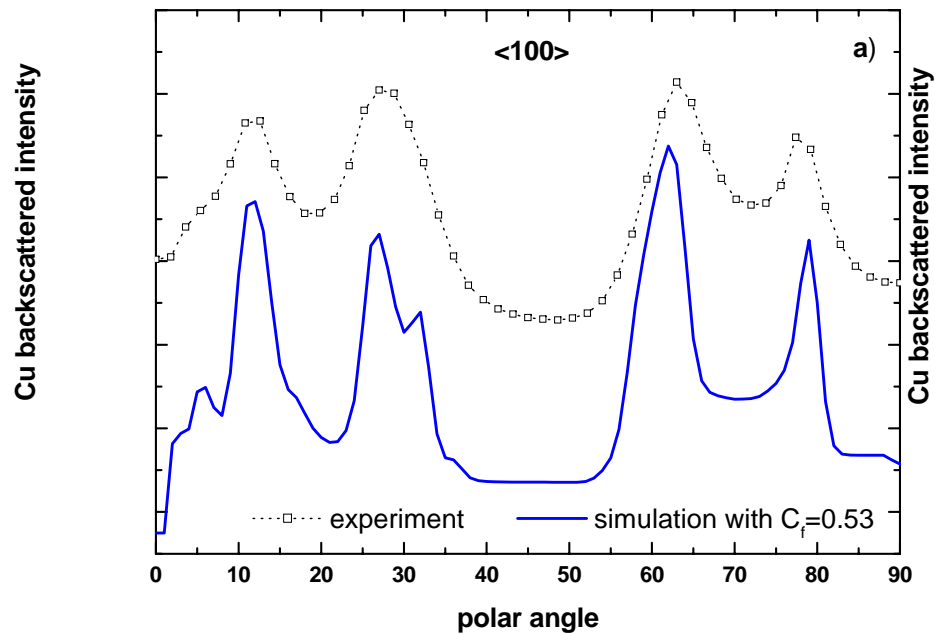


(Draxler 2005)

→ channeling is sensitive to the scattering potential
 (screening length $a = C_f \cdot a_{\text{TFM}}$)

Surface structure analysis: $^4\text{He}^+ \rightarrow \text{Cu}$ crystal

Comparison experiment - Monte-Carlo simulations:



- information on scattering potential (screening length $a \approx a_{\text{TFM}}/2$)
- information on the scattering cross section

Time resolution \leftrightarrow depth resolution

time resolution $\delta\tau$ \leftrightarrow energy resolution δE \leftrightarrow depth resolution δx

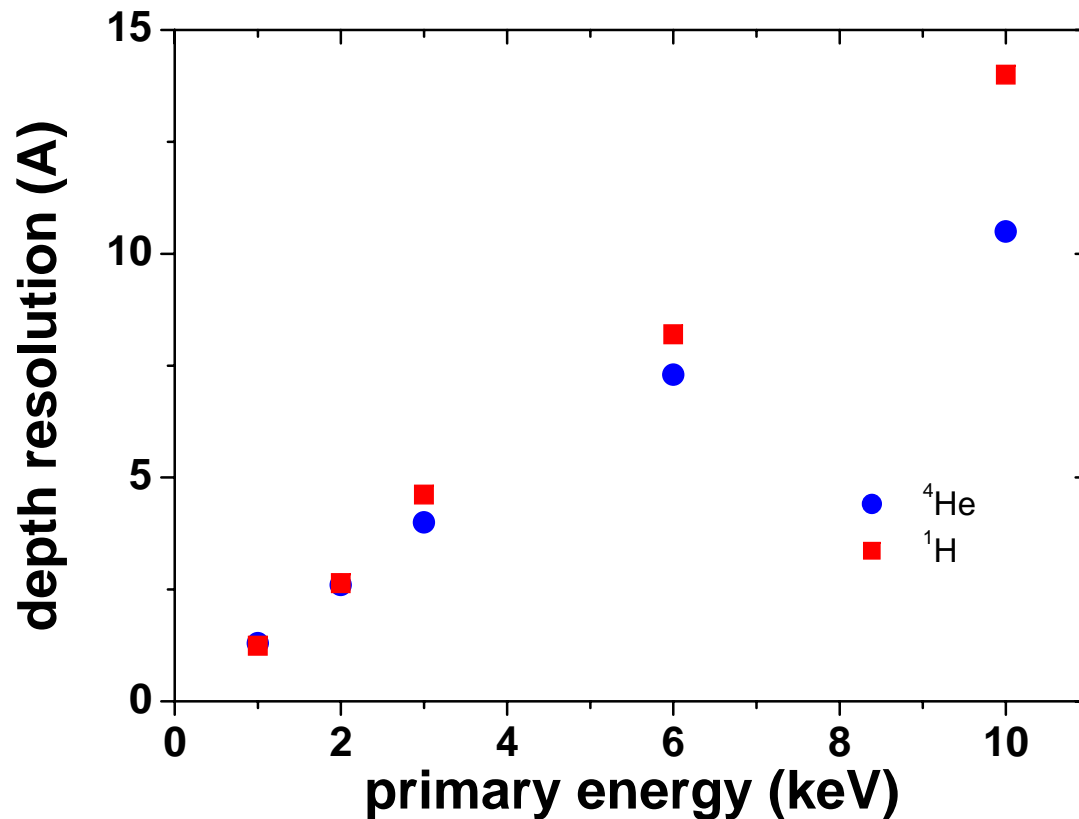
$$\delta E = 2E\delta\tau/\tau \quad (\text{similarly as in RBS})$$

typ. example: $dt = 10\text{ns}$, $L_1 = 0.67\text{ m}$

$$1\text{ keV He}^+: \tau_f = 3.4\ \mu\text{s} \rightarrow dt/\tau_f = 0.3\%$$

Depth resolution in LEIS

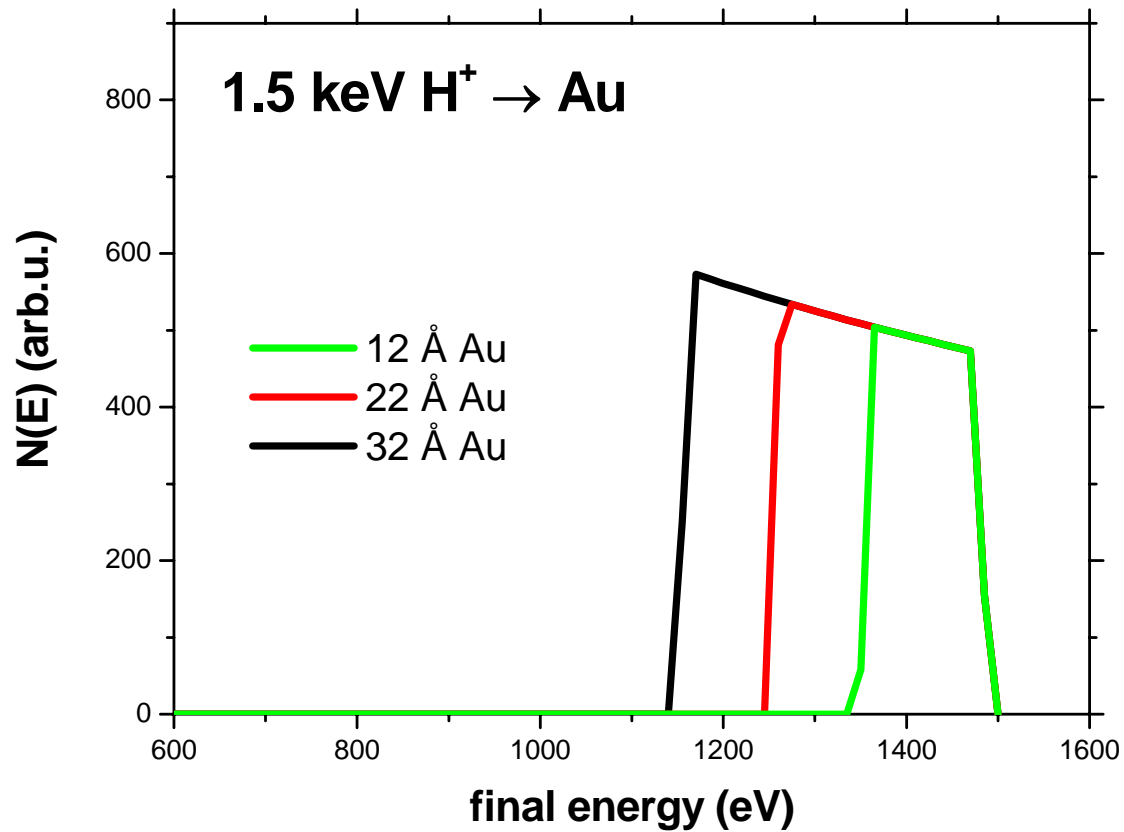
$\delta\tau = 10$ ns, $\alpha = \beta = 25^\circ$, SRIM stopping:



larger $\Delta x \rightarrow$ higher E!

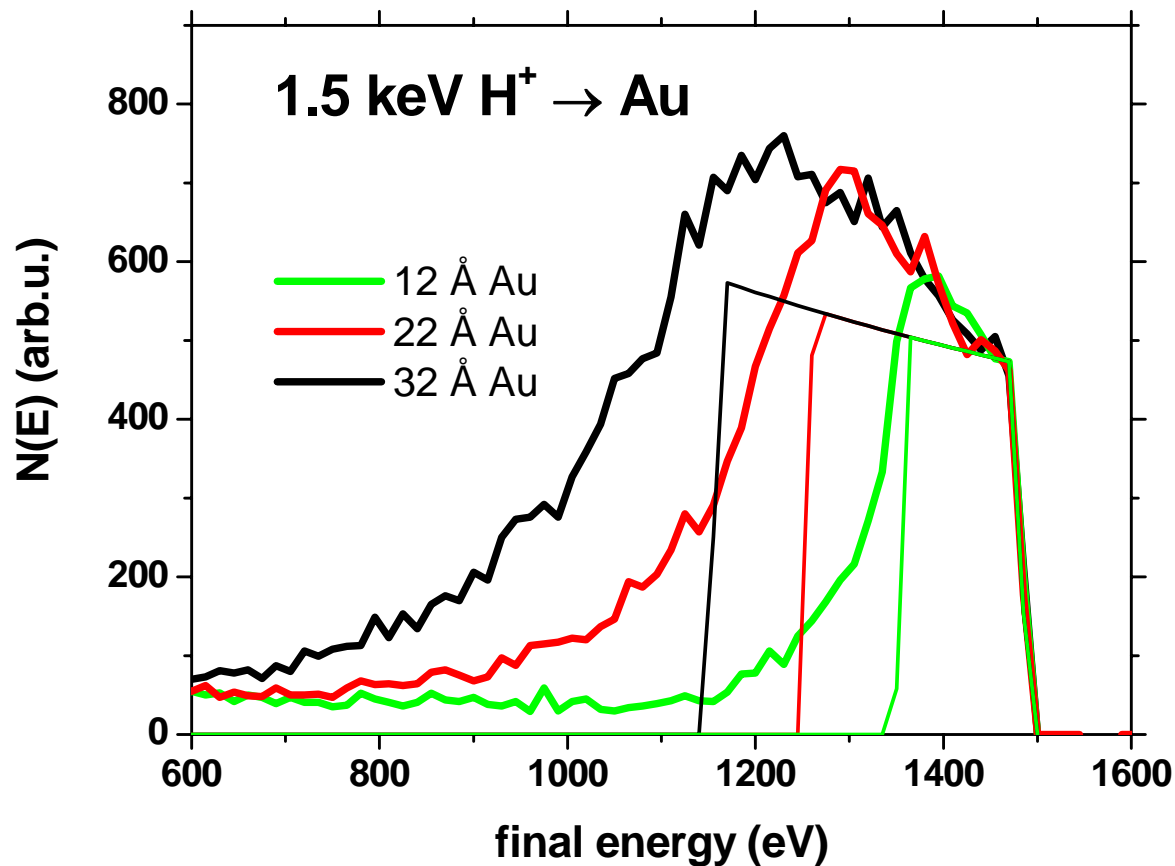
LEIS: spectrum width \leftrightarrow depth

single scattering model: $\Delta E_{\text{LEIS}} \propto \Delta X$



multiple scattering ???

TRBS simulation of LEIS:



TRBS:

- ✓ Monte-Carlo
- ✓ amorphous target
- ✓ dE/dx (non-local)
- ✓ multiple scattering

multiple scattering

- low energy edge
- plateau height

Application to nm layers

how to keep multiple scattering low?

use protons as projectiles (low Z_1)
use 'high' energies (rather 5 keV than 500 eV)

how to optimize depth resolution?

use low energies ($\delta x \propto E$)

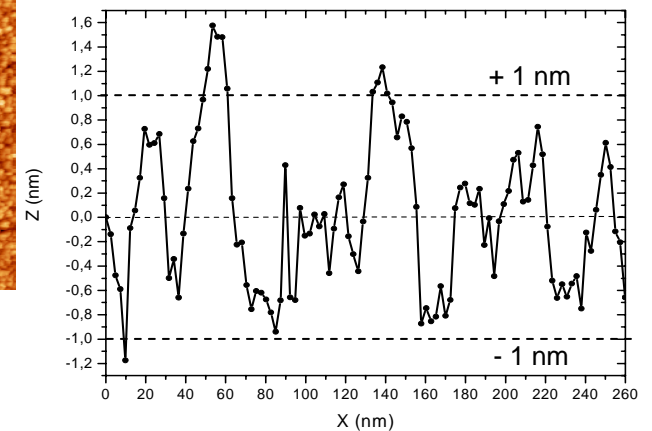
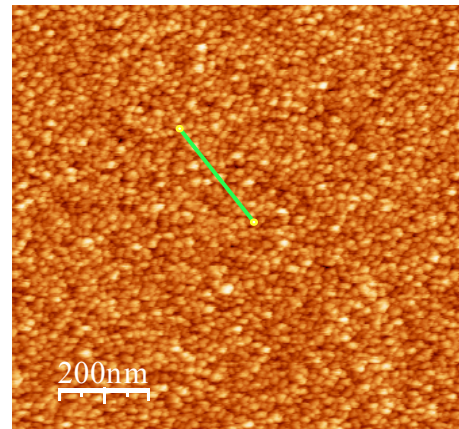
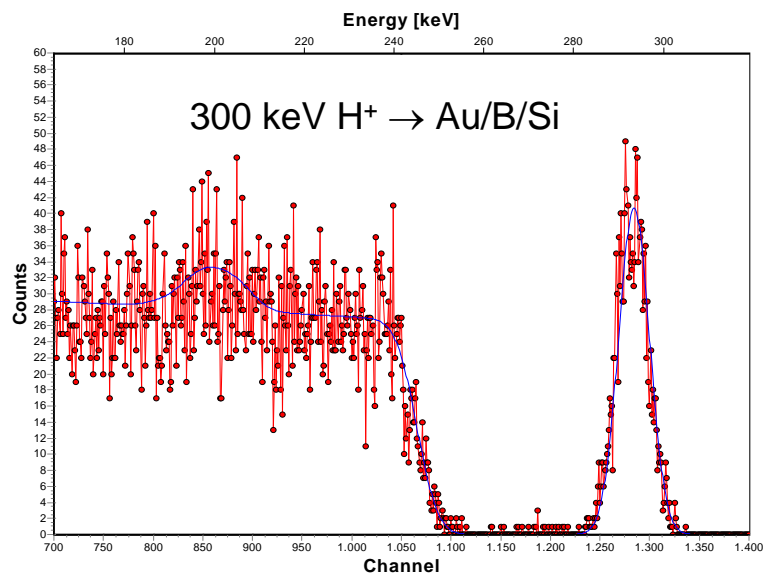
→ compromise resolution ↔ multiple scattering

2.6nm Au/B – thickness inhomogeneity

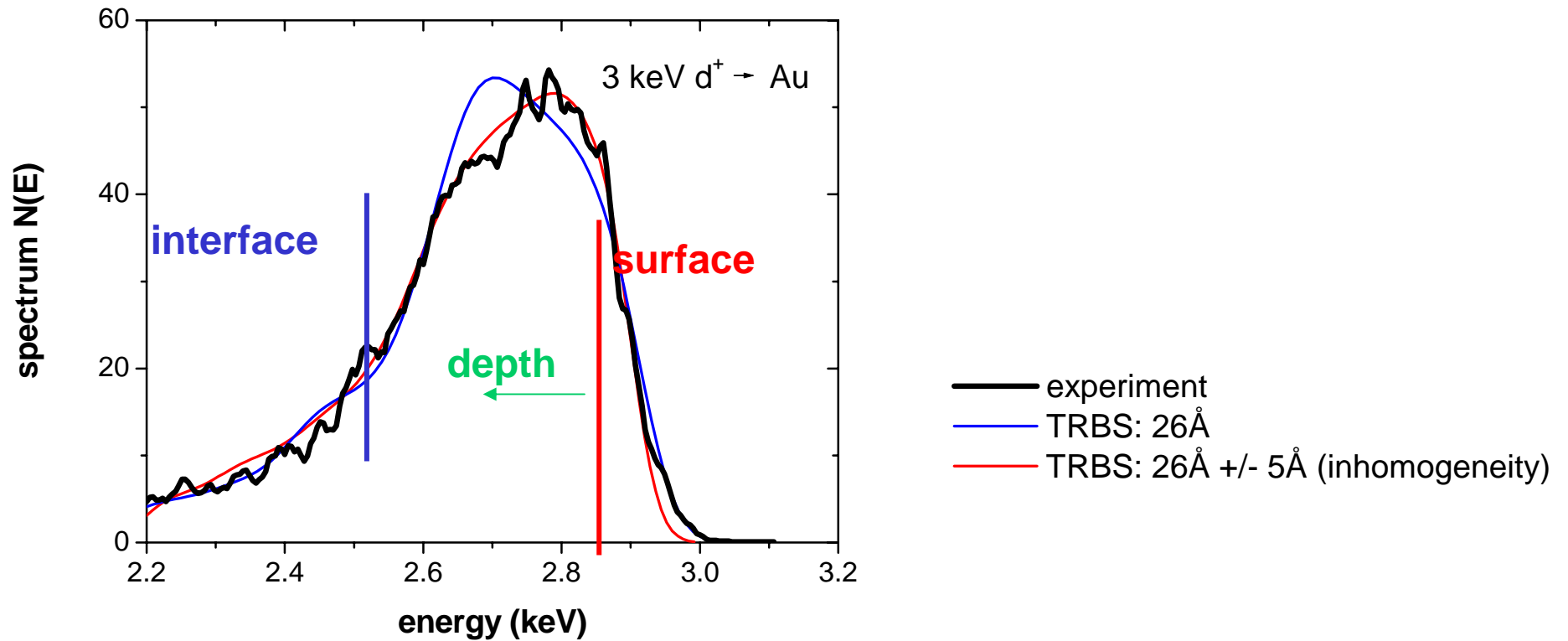
Au evaporated onto B substrate

RBS for thickness (SIM-NRA): $26\text{\AA} \pm 5\%$

atomic force microscopy for
surface inhomogeneity: $\pm 5\text{\AA}$



3 keV H⁺ → 2.6nm Au/B



LEIS quantitative for nm layers !?

Ga/Si(111) (evaporated in situ, quartz reading: 6Å)

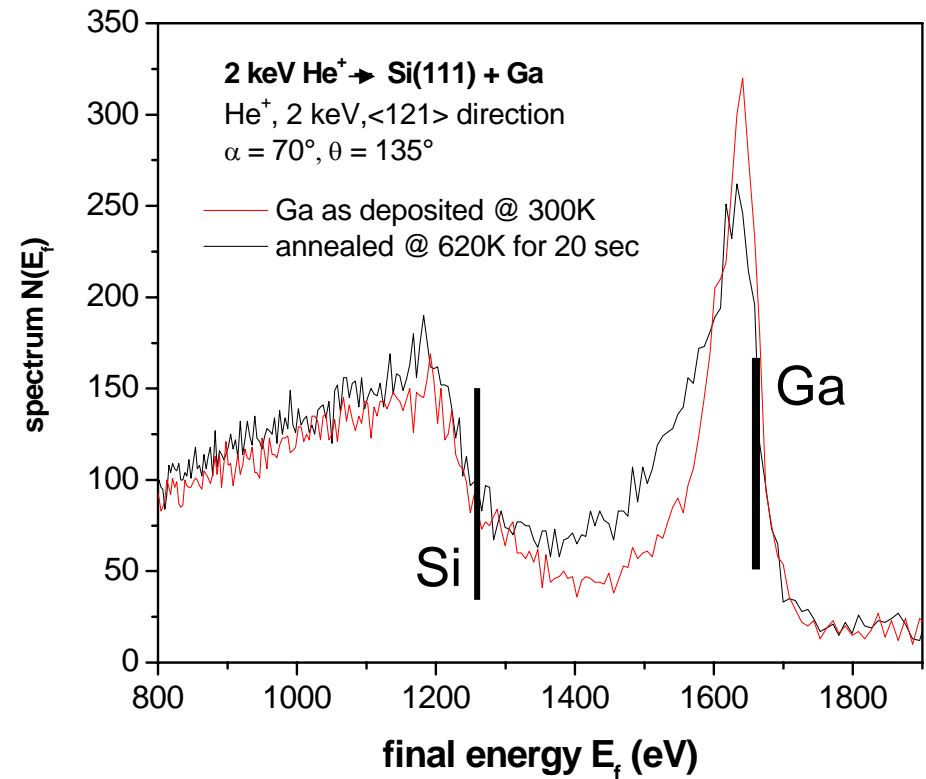
2 keV He⁺ for structure analysis: ~ 20Å (comparison to TRBS)

→ annealing → broadening of Ga peak (change in topography):

- either thickening of clusters or
- diffusion into Si

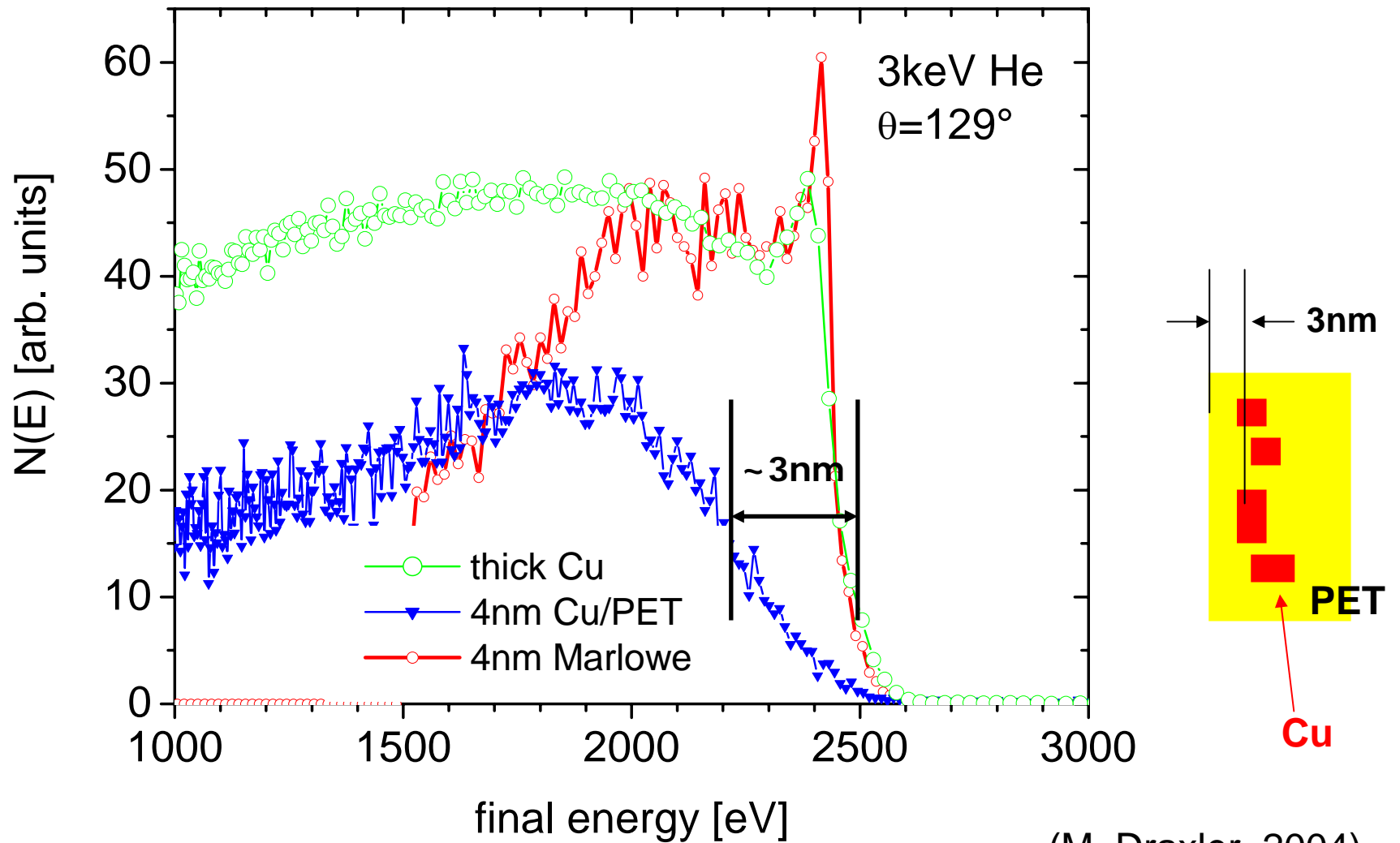
→ sharp Si edge with and w.o. annealing

→ major part of Si is free of Ga



(M. Kolibal 2005)

Technical application: Cu/PET



(M. Draxler, 2004)

Summary:

- **ESA-LEIS & TOF-LEIS:**
 - **single crystals**
 - surface structure
 - surface composition
 - neutralization
 - **thin films**
 - surface composition
 - neutralization
 - growth modes

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Thank you

Quantitative LEIS

↔ **Matrixeffects in P⁺?**

$$\text{Is } Y_{A^+} = c_A \cdot \eta_A?$$

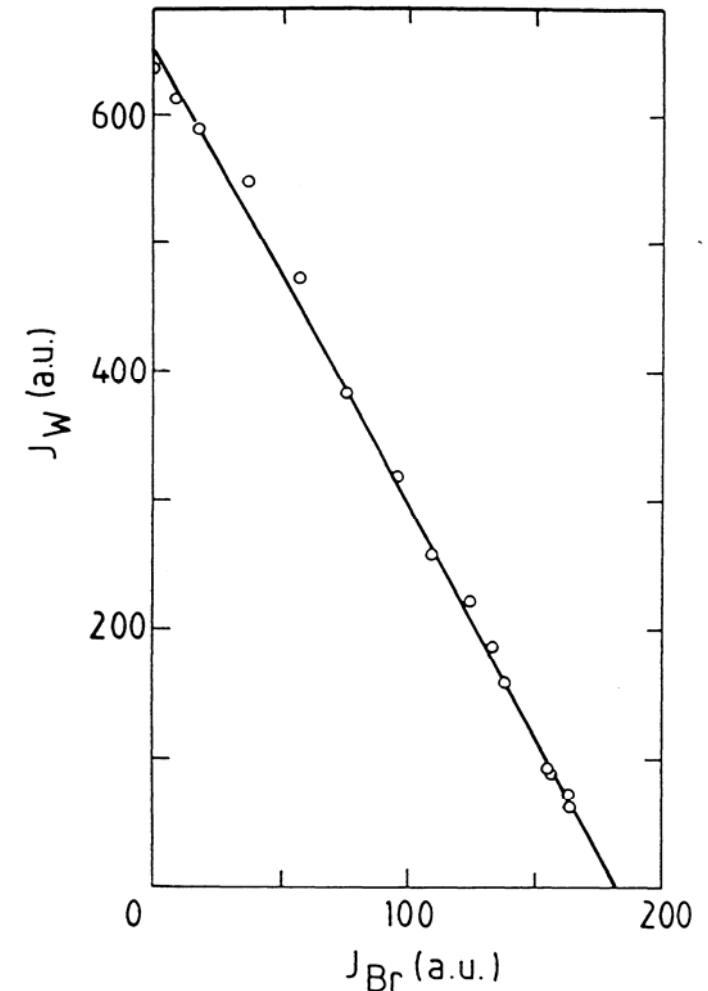
Element A Concentration c_A
 Sensitivity factor η_A

Test: Adsorption of Br on W

$$\theta_{\text{Br}} + \theta_{\text{W}} = 1$$

$$c_{\text{Br}} + c_{\text{W}} = 1$$

$$Y_{\text{W}^+}/\eta_{\text{W}} + Y_{\text{Br}^+}/\eta_{\text{Br}} = 1$$



(H.H. Brongersma, 1981)⁸⁹