Multiple electron scattering in ion-atom and electron-solid collisions

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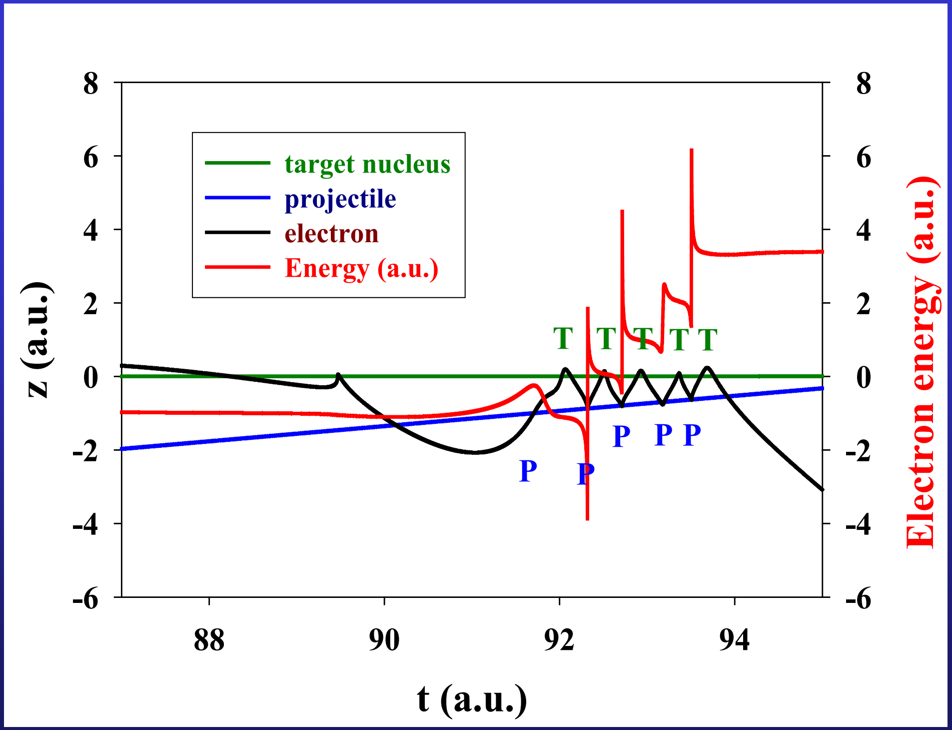
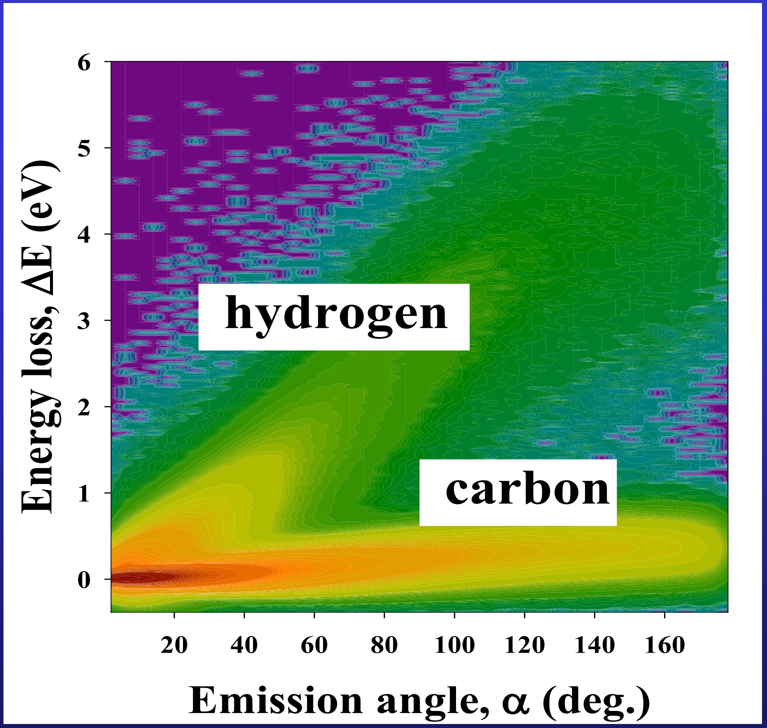
SPIG 2020





Outlook

Fermi-shuttle type multiple electron scattering in atomic collisions

Basic idea --- Why? ---History
Classical Trajectory Monte Carlo method -- a method of the analysis
The present level of understanding -- Examples
Summary

Monte Carlo simulation of electron spectra backscattered elastically from solid sample

Why? --- Background and motivation
Monte Carlo simulation
Results
- Energy loss and angular correlation pattern
- Energy loss distributions
- Single and multiple scattering

Summary

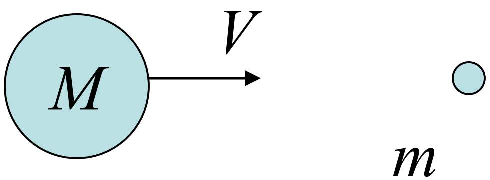
Part I:

Fermi-shuttle type multiple electron scattering in atomic collisions

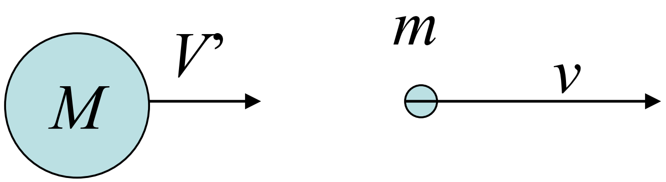
Ping-pong game: heavy paddle – light ball

Elastic scattering:

Before:



After:



Momentum conservation: $MV = MV' + mv$

Energy conservation: $\frac{1}{2}MV^2 = \frac{1}{2}MV'^2 + \frac{1}{2}mv^2$

$$V' = V\frac{1 - m/M}{1 + m/M}$$

$$v = 2V\frac{1}{1 + m/M}$$

The final velocity of the light particle in the **laboratory frame**

Large energy gain

Energy gain in ping-pong game

Projectile velocity (V)

$$E_V = 0.5\, m_e V^2$$

kicks:	**1**	**2**	**3**	**4**	**5**
ball velocity:	**2V**	**4V**	**6V**	**8V**	**10V**
ball energy:	**4** E_V	**16** E_V	**36** E_V	**64** E_V	**100** E_V

Why?

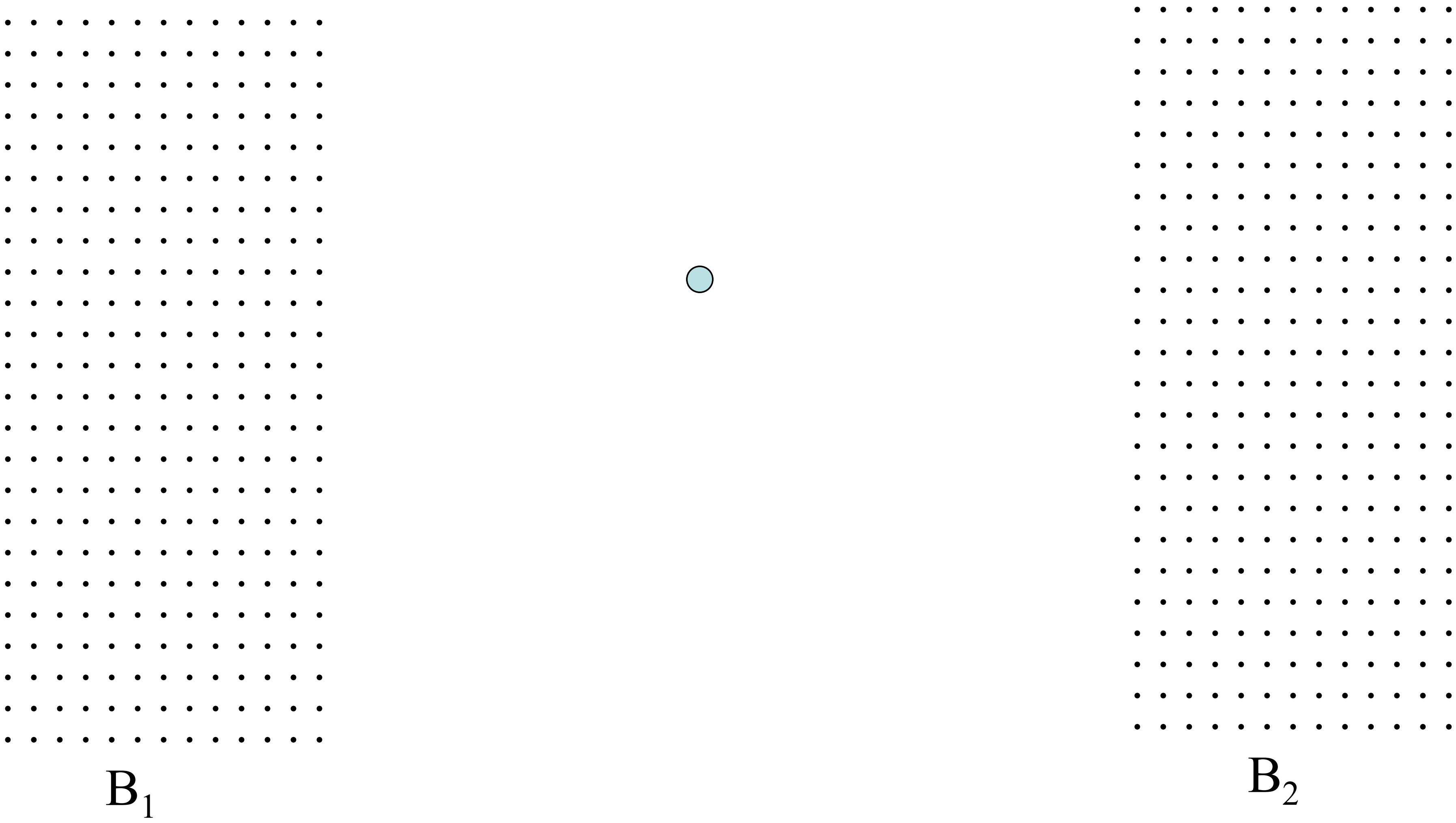
- Basic research - fundamental physics
- Hot electrons

  astrophysics
  ion-beam technology

- Technological importance

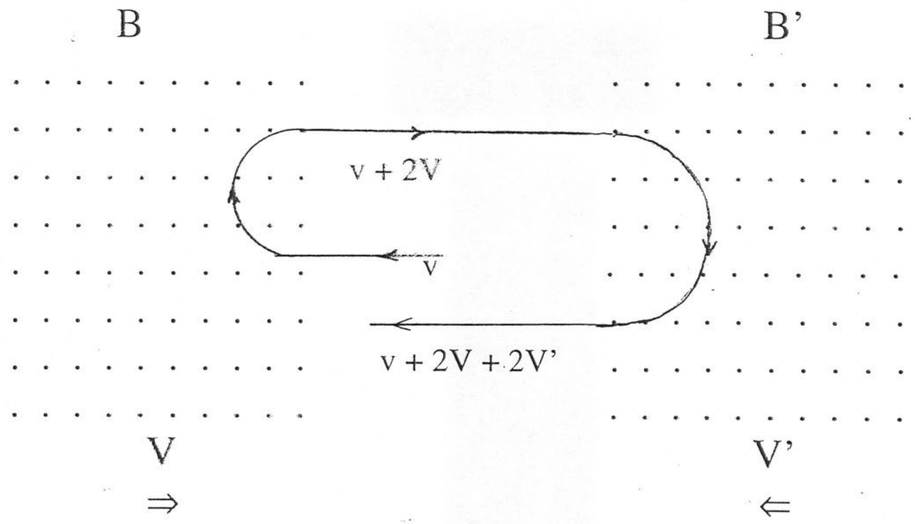
  plasma physics
  fusion
  analytical methods – medical application

Charge particles in moving magnetic fields



Pioneer: E. Fermi, Phys Rev. 75 (1949)

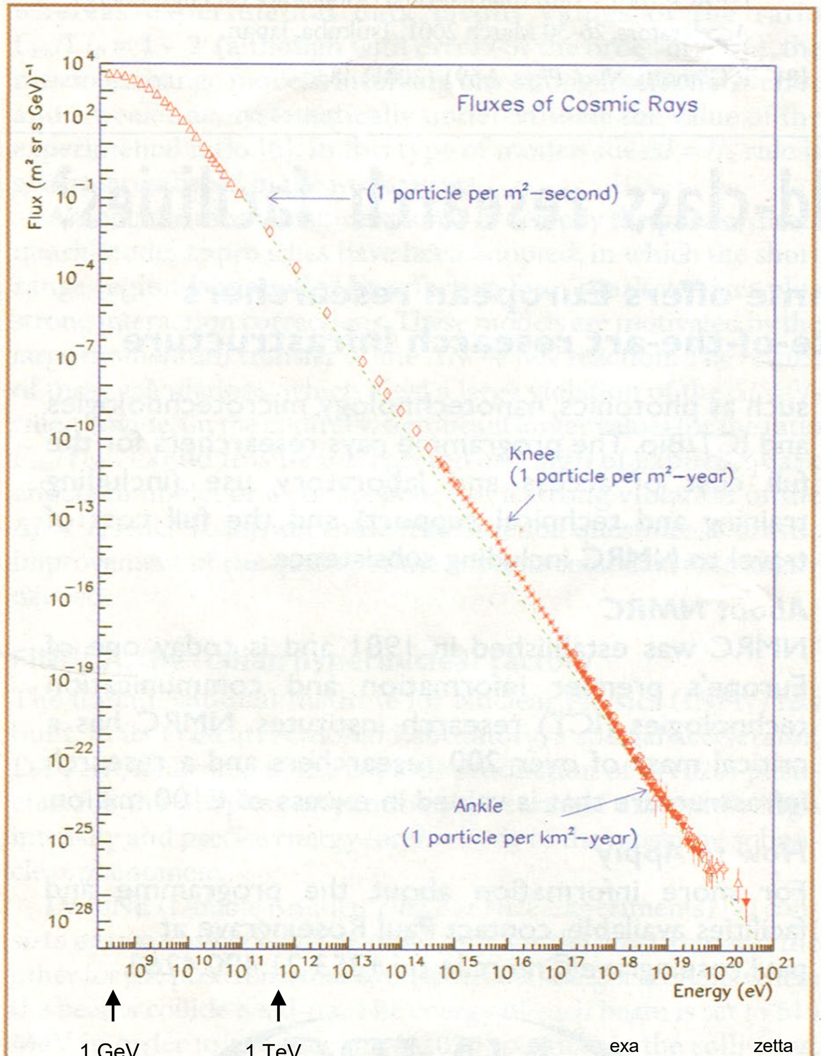
A possible origin of cosmic rays (energetic charged particles):



Typical values:

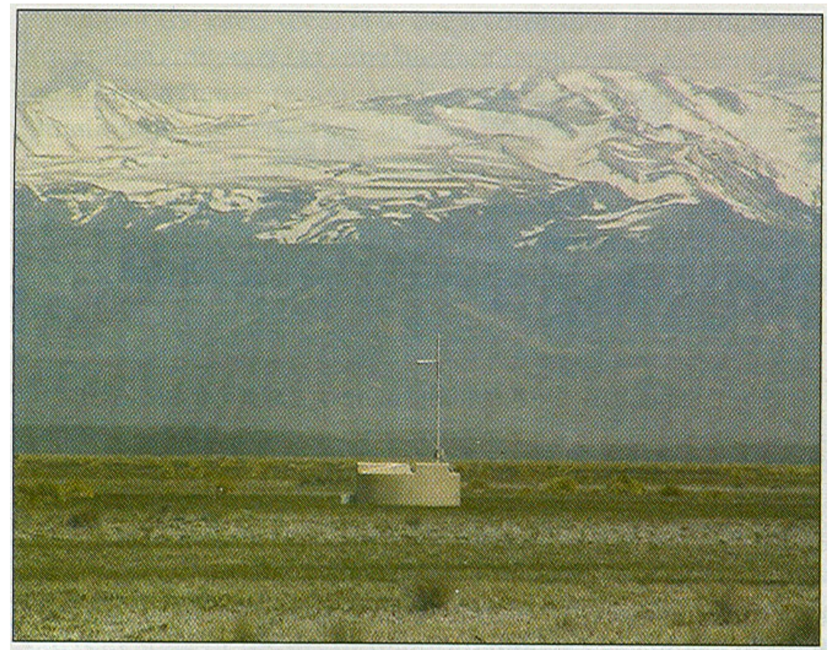
B: ~ 10^{-5} gauss
V: ~ 30 km/s
E-gain: ~ 10 eV / reflection (in the nonrelativistic regime)
Number of collisions: ~ 10^{8}
Minimum injection energy: ~ 200 MeV (for protons)
Final energy: 1-2 GeV

Energy distribution of the cosmic particles (particle / (m^2 sr s GeV))



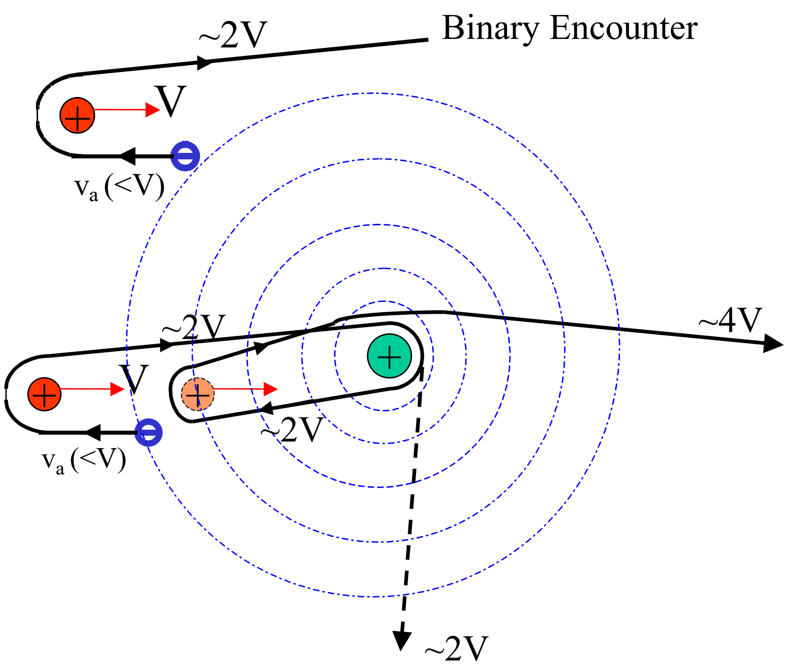
▲ **Fig. 1:** The all-particle spectrum of cosmic rays (from S. Swordy). The arrows and values between parentheses indicate the integrated flux above the corresponding energies.

Pierre Auger project - Argentina
1600 detectors in 3000 km^2

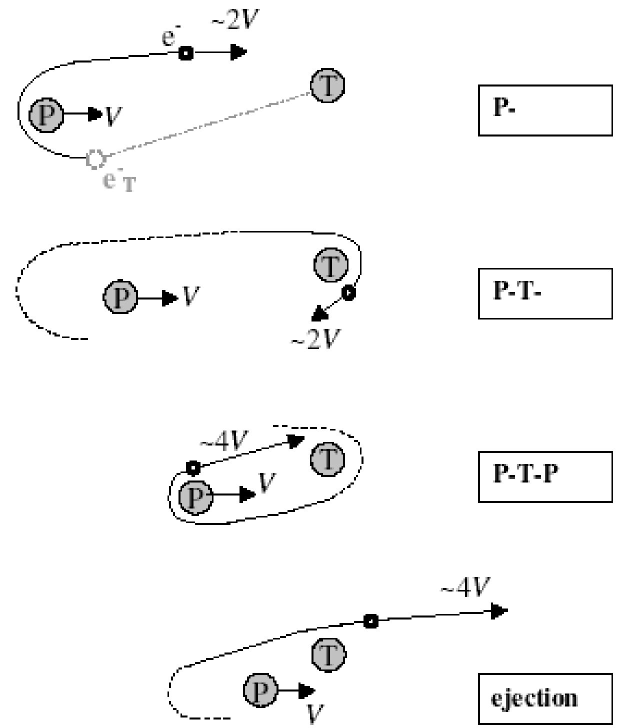


Source: M. Boratav, Probing theories with Cosmic rays Europhysics News, September/October (2002), 162

Mechanism



Movie



Start with: target ionization: projectile ionization (loss):

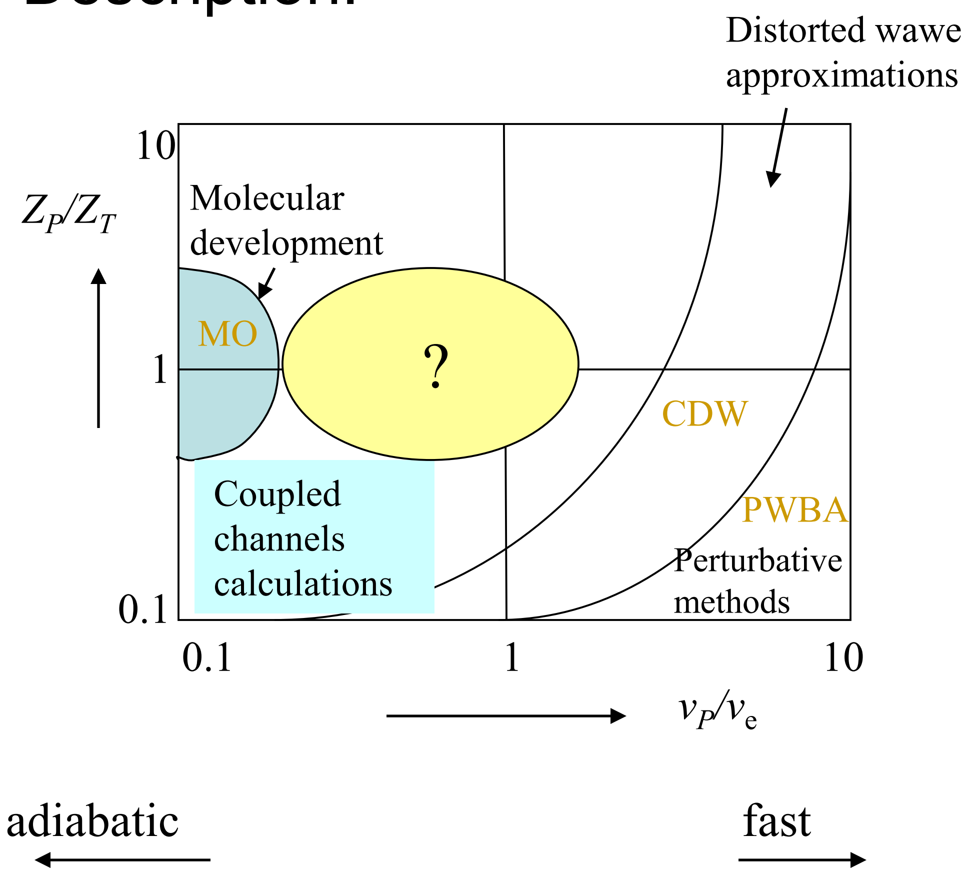
*v*e= 2V, 4V, 6V,… or V, 3V, 5V, …

References:

1. B. Sulik *et al*., Phys. Rev. Lett. **88**, 73201(2001),
2. B. Sulik, K. Tőkési, Advances in Quantum Chemistry **52** (2007) 253.

Ionization in ion-atom collisions

Description:

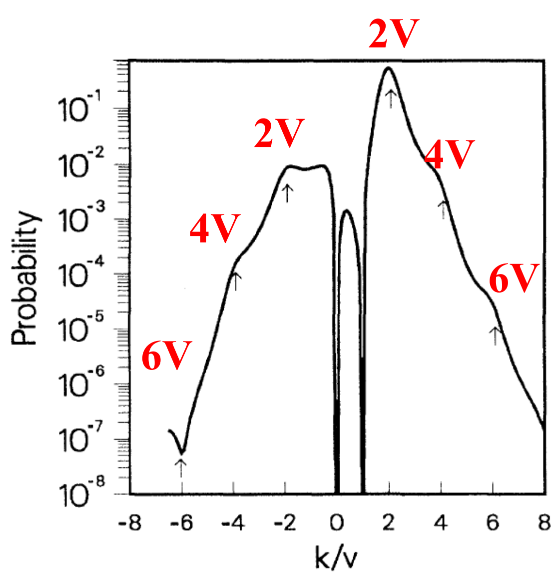


Non-perturbative models:

Classical (CTMC)

Exact quantum models, e.g., one dimensional „scattering” on a delta potential

Surprise (Wang et al.,1991):

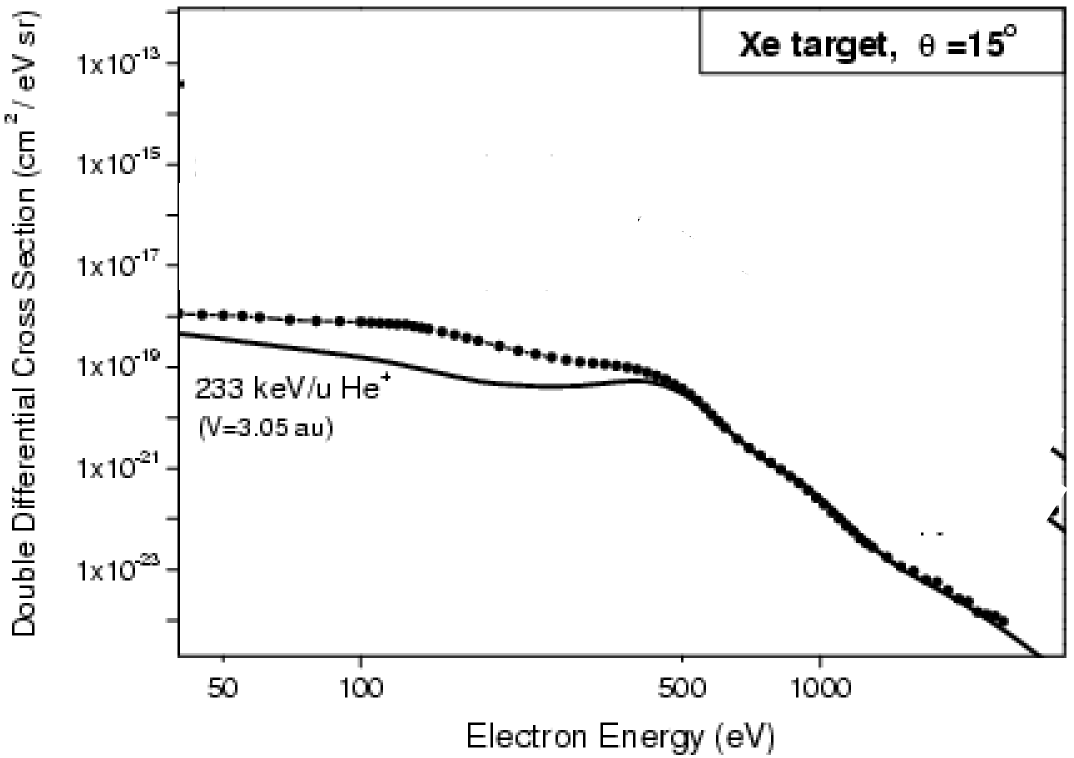


Observation of the Fermi-shuttle process in the double-differential electron spectra. Separation of multiple scattering components.

1st order Born theory is excellent for light ion impact at high electron energies.

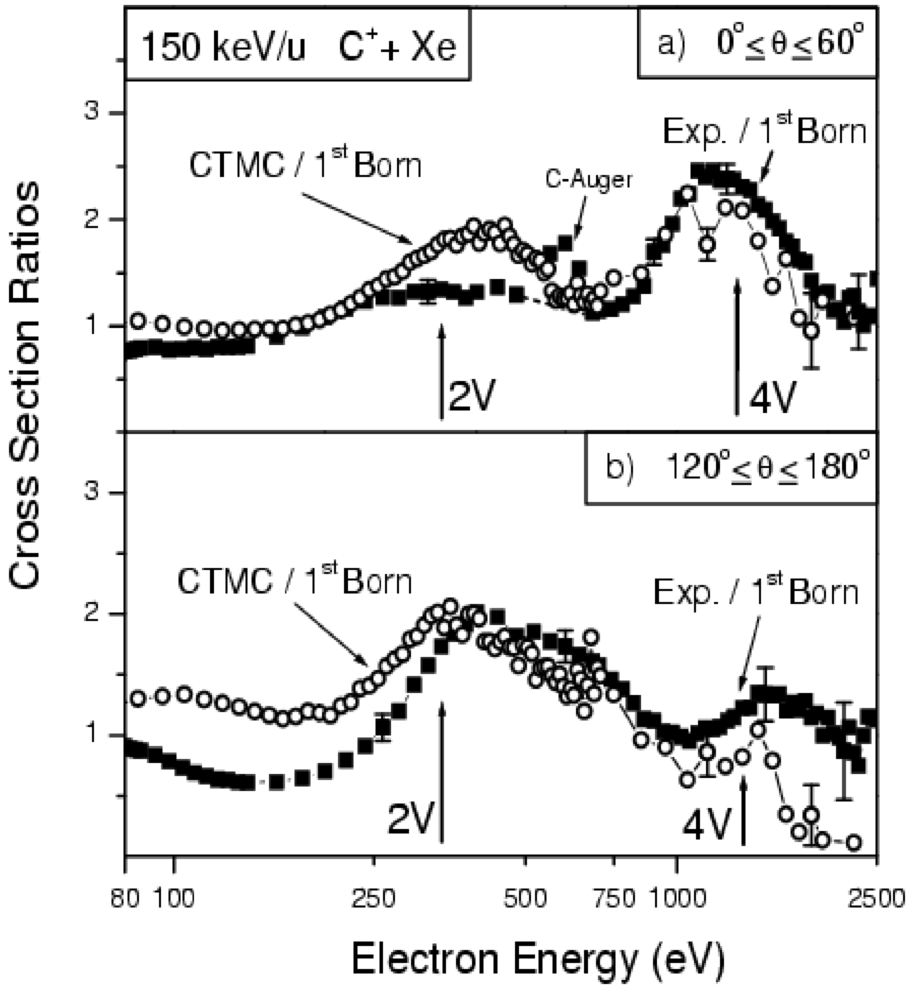
Higher-order process is on the background of 1st order processes

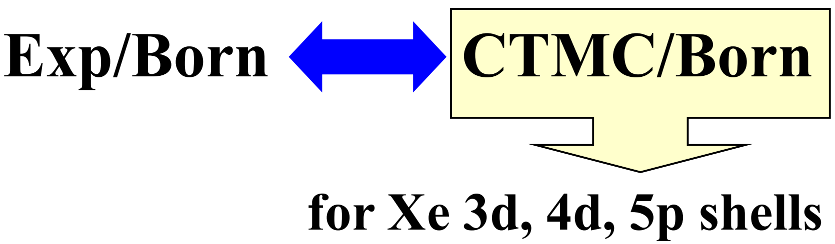
For carbon ions we have extra yields above the first order calculations, centered at 4 *V*



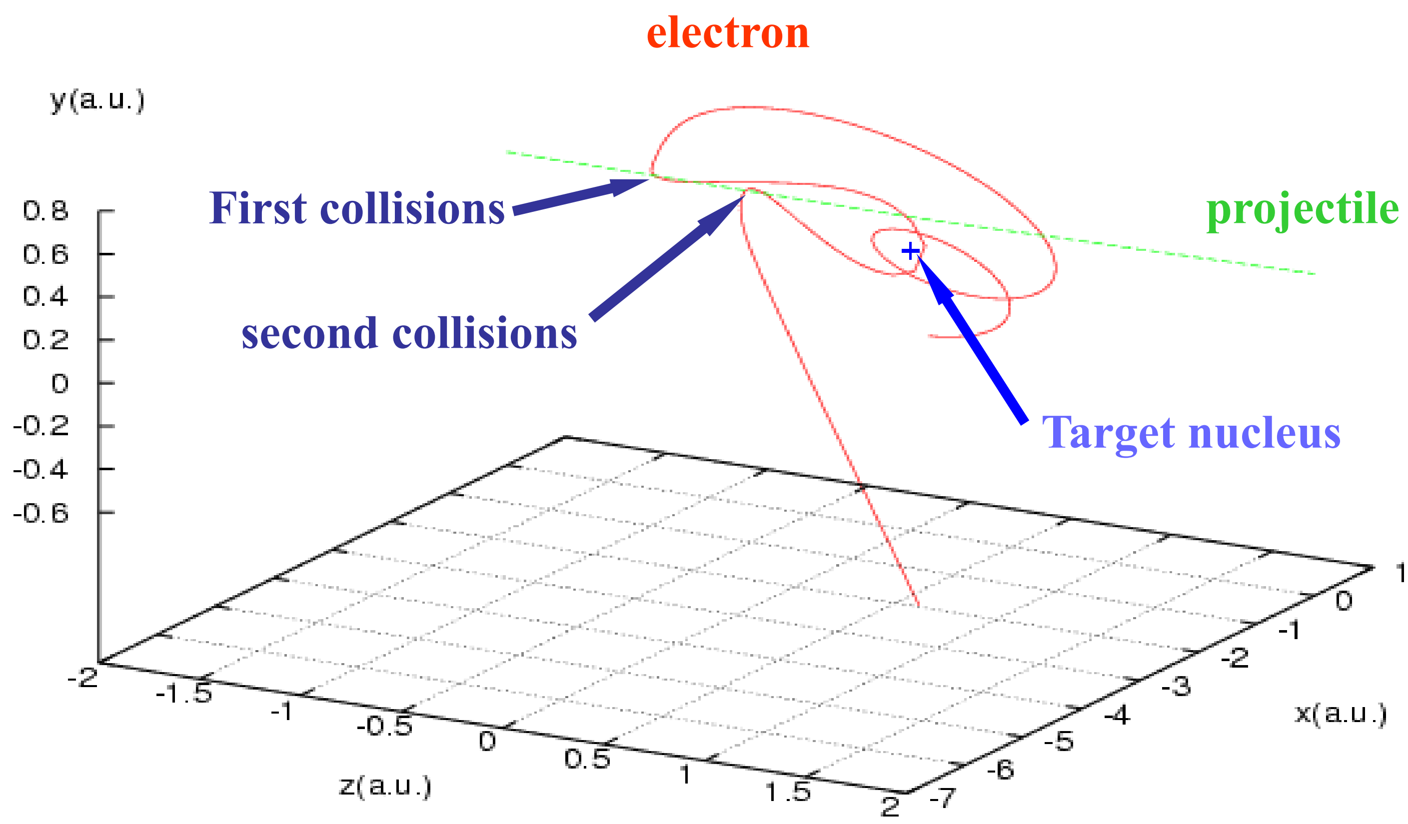
Key for identification: kinematics

Integrated cross sections in forward and backward angles





Example


electron
y(a.u.)
First collisions
second collisions
projectile
Target nucleus
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
z(a.u.)
1
0
-1
-2
-3
-4
-5
-6
-7
x(a.u.)

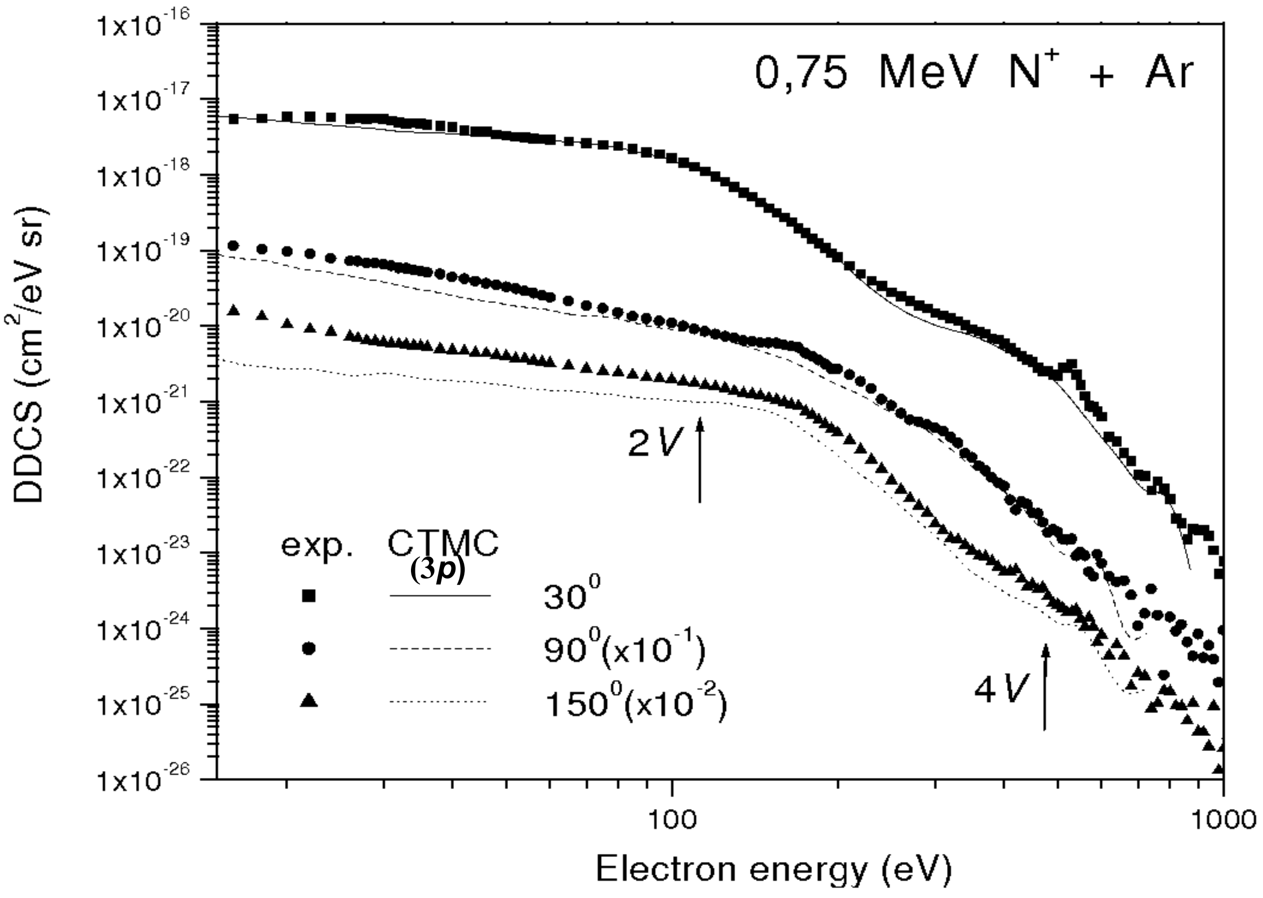
1.8 MeV (150 keV/u) C^+ + Xe

Statistics for ping-pong

Energy window: 1100-1500 eV

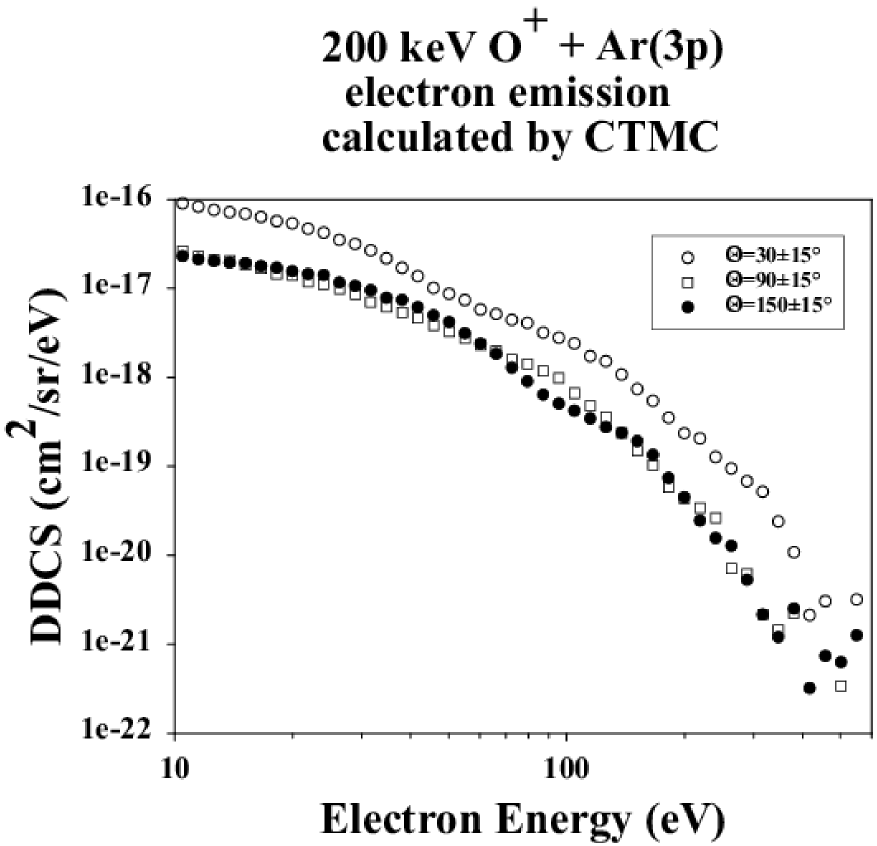
Sub-shell	0-30 degree *forward emission*		150-180 degree *backward emission*	
	events	P-T-P	events	P-T-P-T
3d	45	84%	29	90%
4d	80	80%	26	65%
5p	21	71%	4	75%

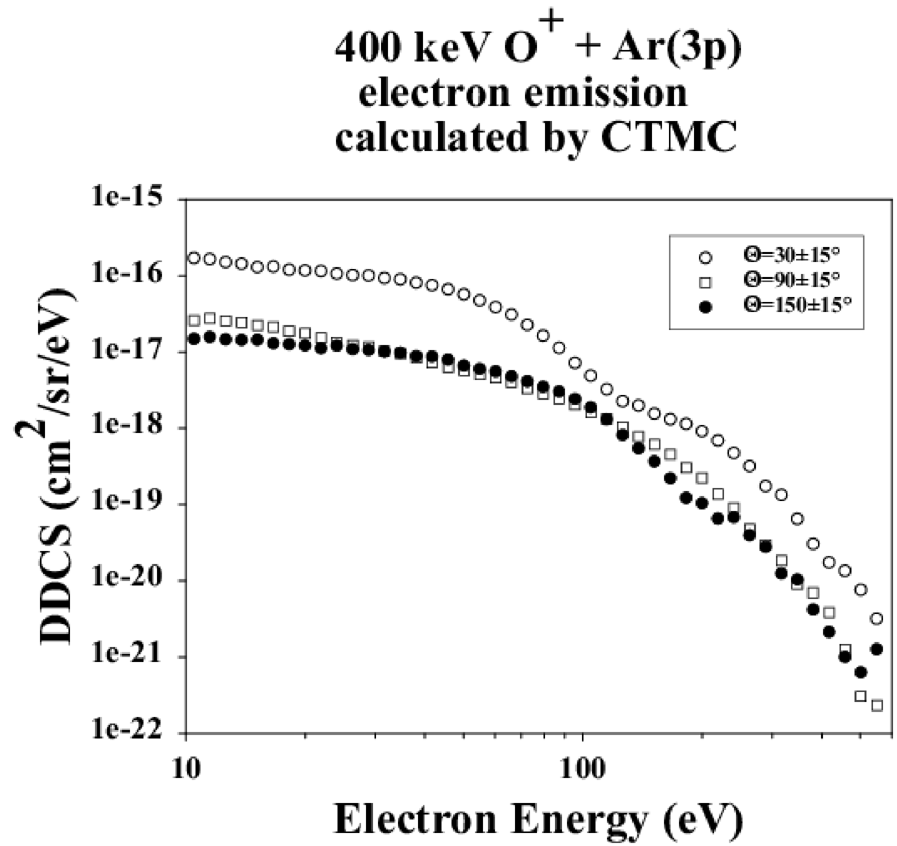
Somewhat higher ion impact energies – 2
Absolute cross sections



85% P-T-P and P-T-P-T

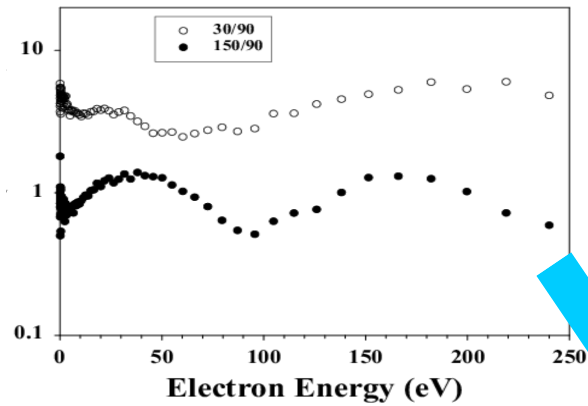
CTMC results



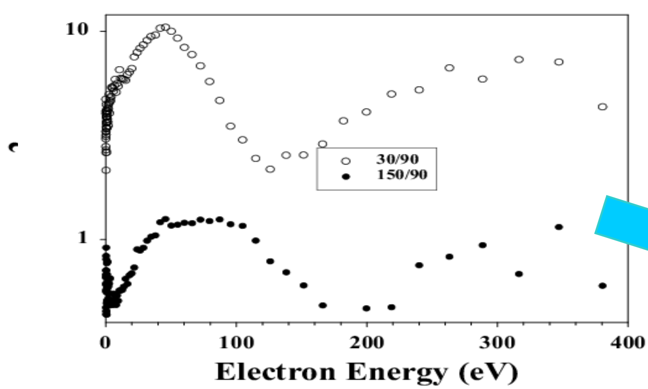


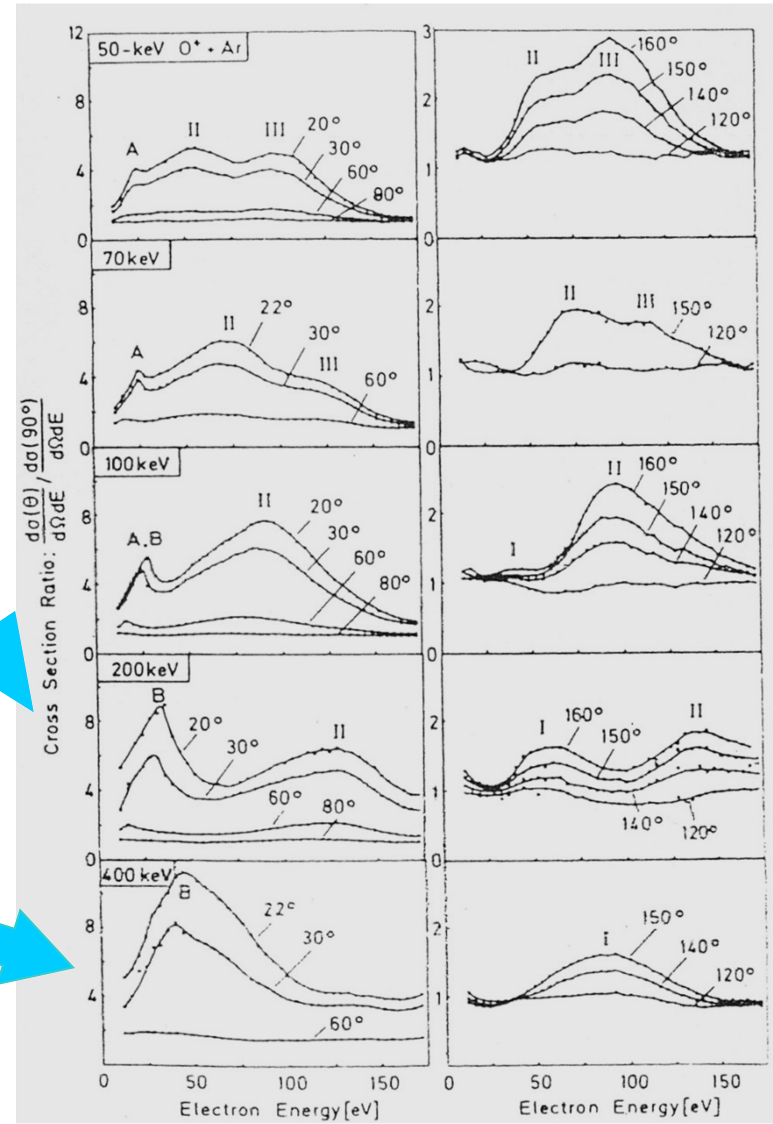
CTMC results - ratios

200 keV O^+ + Ar(3p)
electron emission
calculated by CTMC



400 keV O^+ + Ar(3p)
electron emission
calculated by CTMC



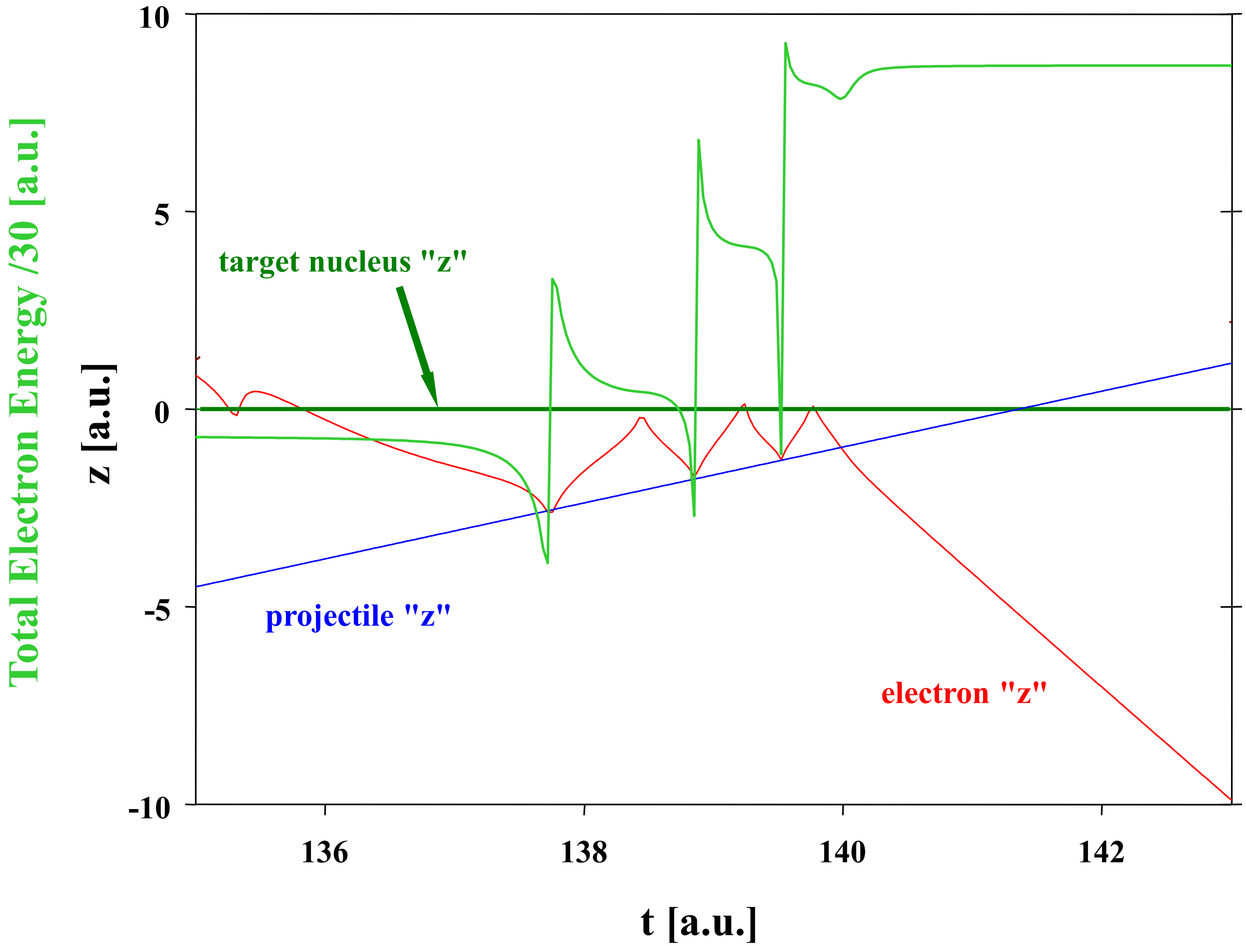


CTMC trajectories

200 keV O^{+} + Ar(3p)

$E_{electron}$ =260 eV, θ=155^{o}

b=0.91 a.u.

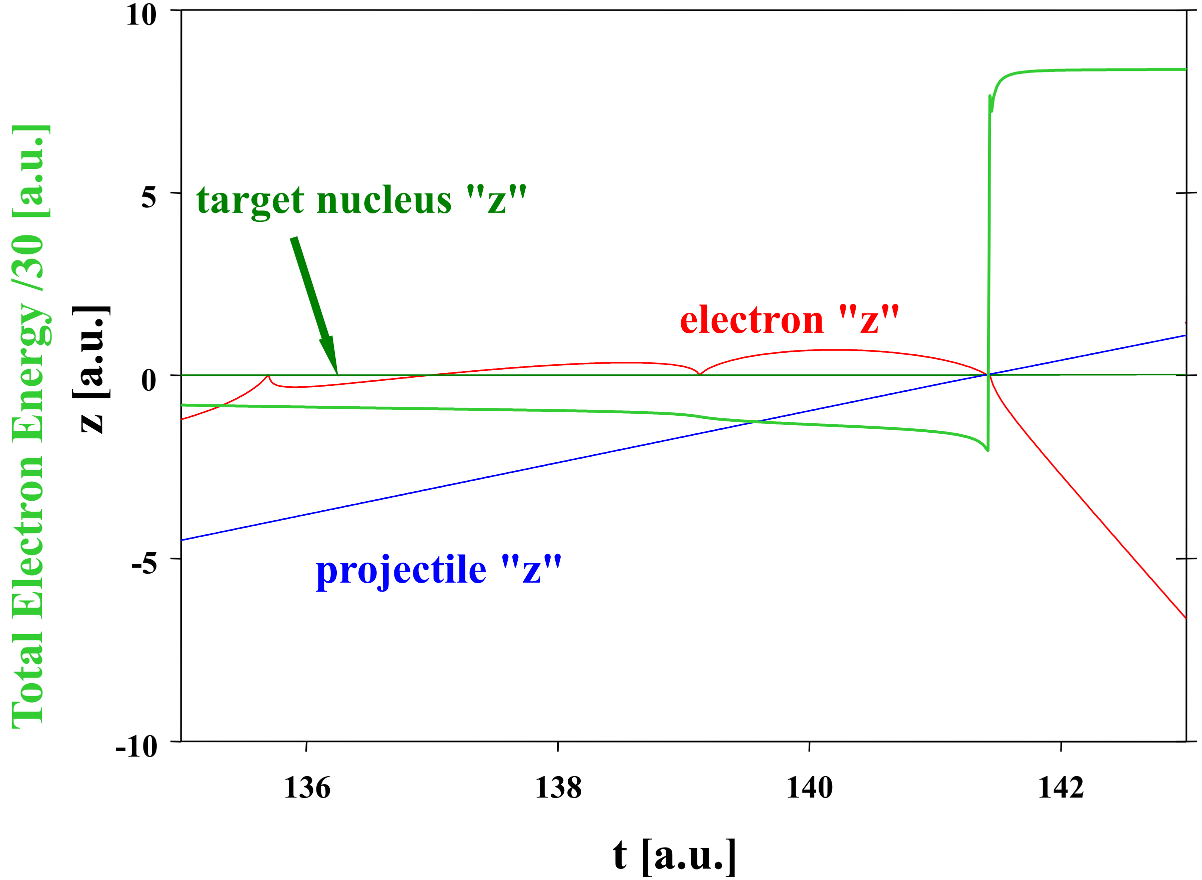


CTMC trajectories

200 keV O^+ + Ar(3p)

$E_{electron}$=250 eV, θ=155°

b=0.07 a.u.



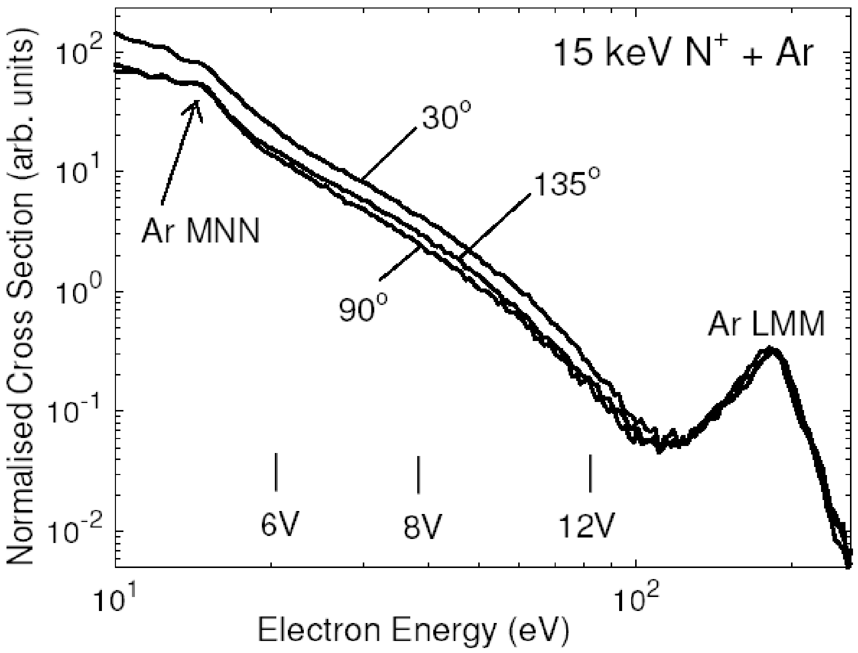
Estimated ratio: < 10%
(by sampling)
(for E_e > 100 eV)

The majority of events looks to be accelerating scattering (or – with other words – non-adiabatic quasimolecular development)

Slow ion impact (>98% ping-pong)

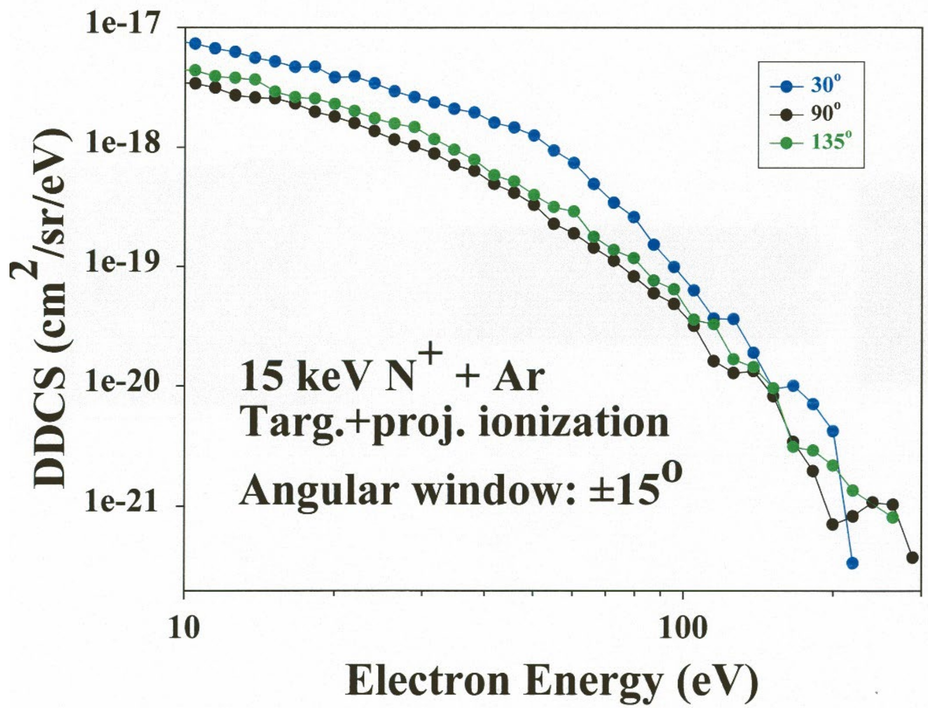
Experiment

HMI Berlin



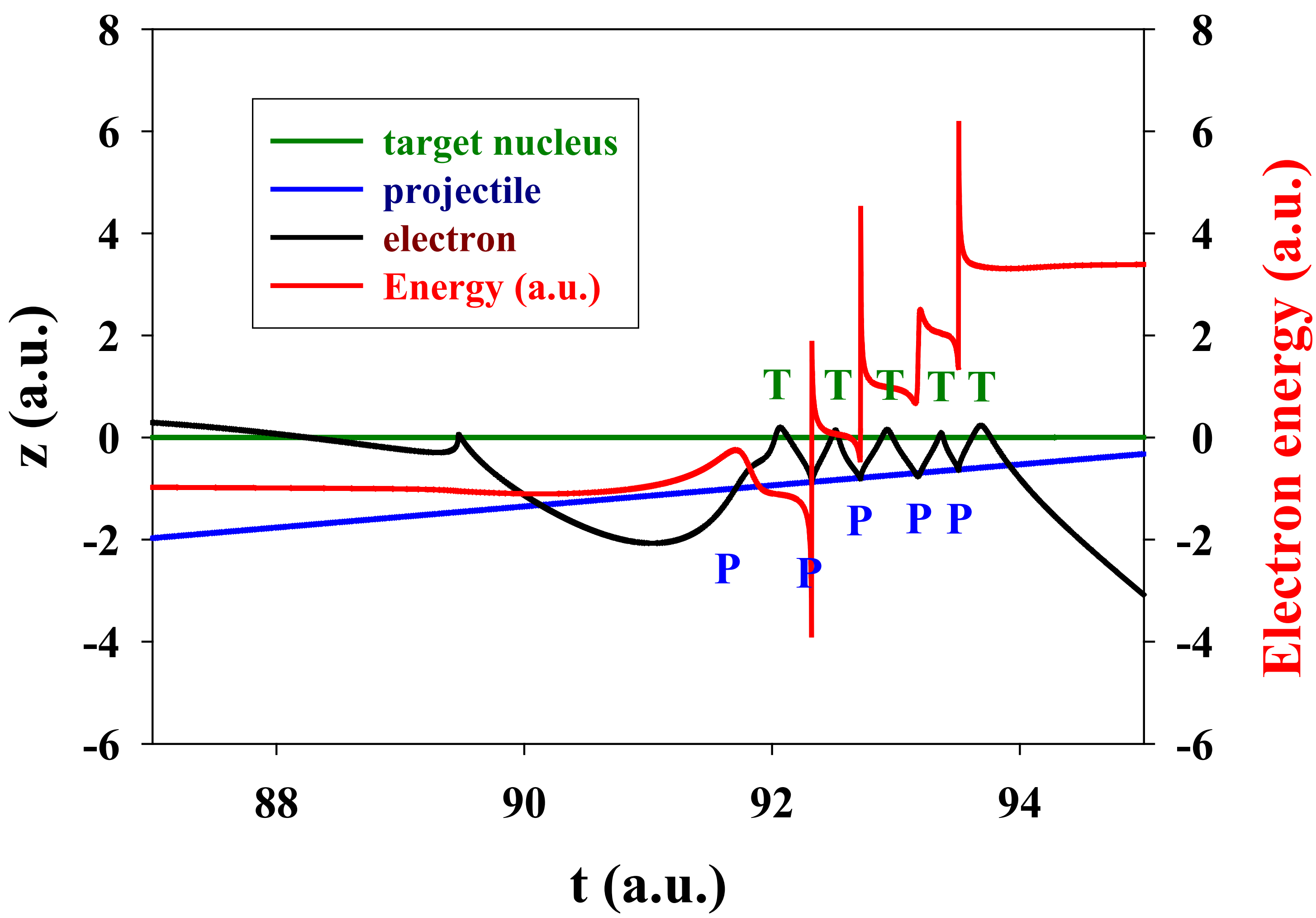
CTMC

Debrecen



Long ping-pong game (15 keV N^+ + Ar)

P-T-P-T-P-T-P-T-P-T



Conclusions

- CTMC reproduce different experiments for collisions of slow, singly charged ions (1-30 keV/u) with atoms.

- A method for analysing the CTMC „events" has been developed.

-Fermi-shuttle multiple scattering is significant or dominant for slow collisions.

Electron emission in low energy ion-matter interactions might be governed by multiple scattering.

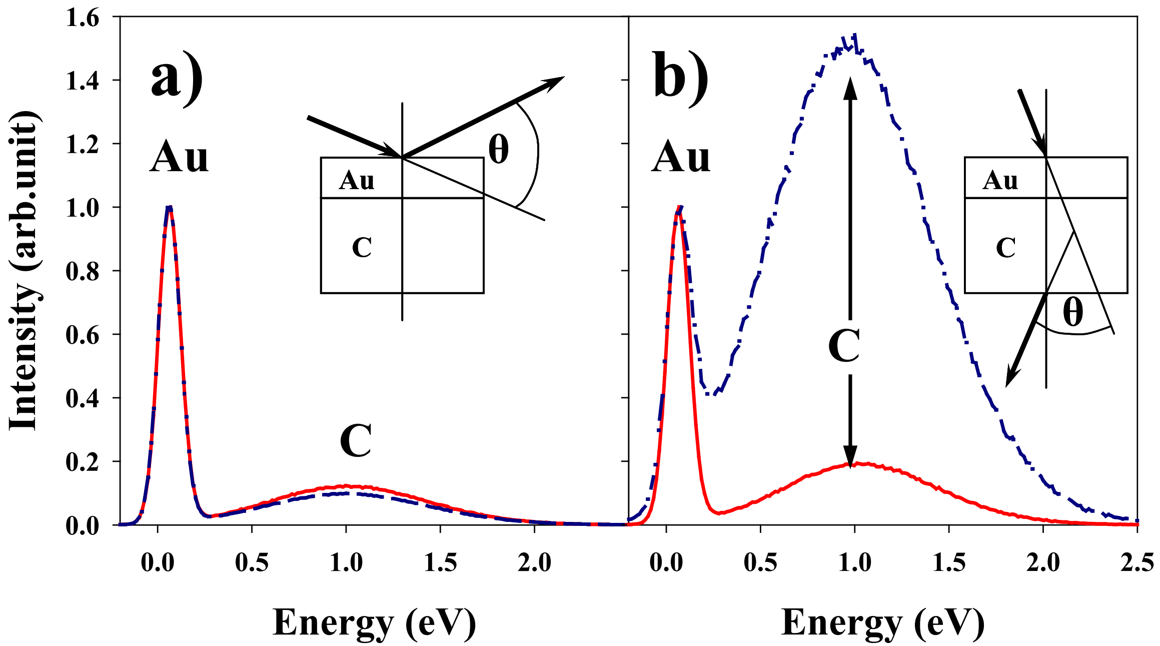
Part II:

Monte Carlo simulation of electron spectra backscattered elastically from solid sample

The influence of multiple scattering

Double layers

Multicomponent samples



Why?

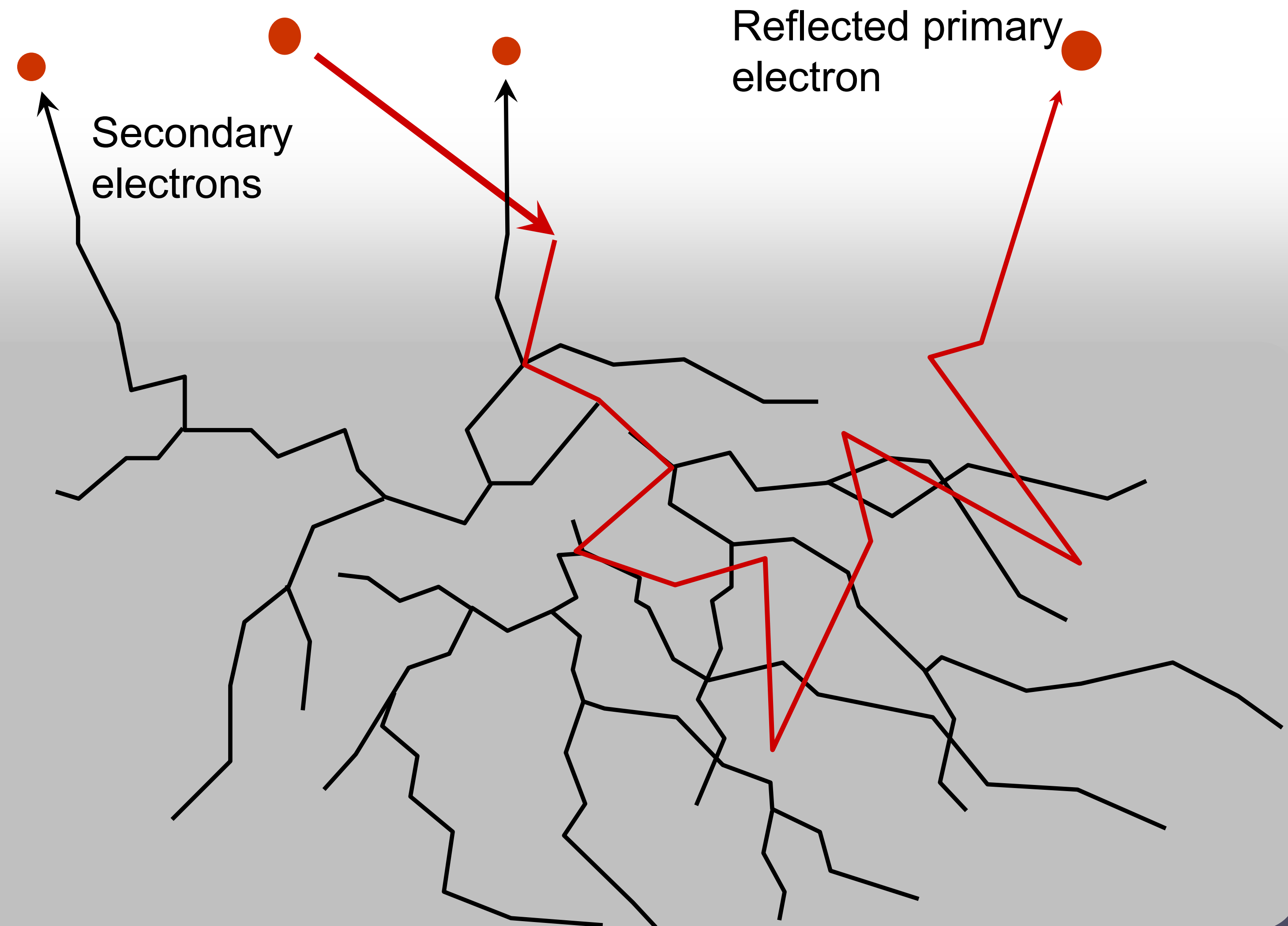
We take an advantage that the energy of the elastically backscattered electrons is shifted from the primary values due to the energy transfer between the primary electron and the target atoms (recoil effect).

Application for quantitative analysis

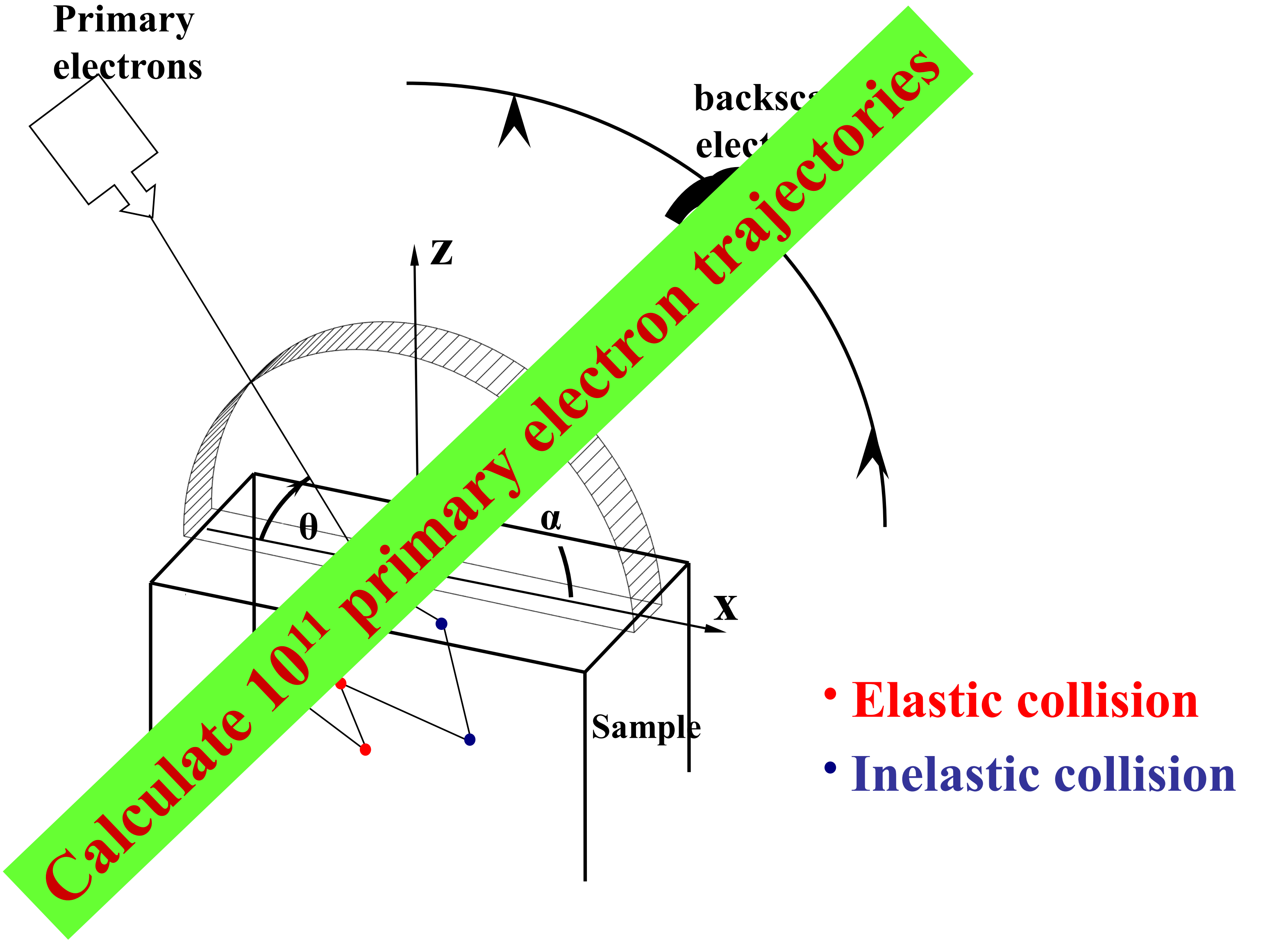
- hydrogen cell → new energy source

- measuring in nano-scale

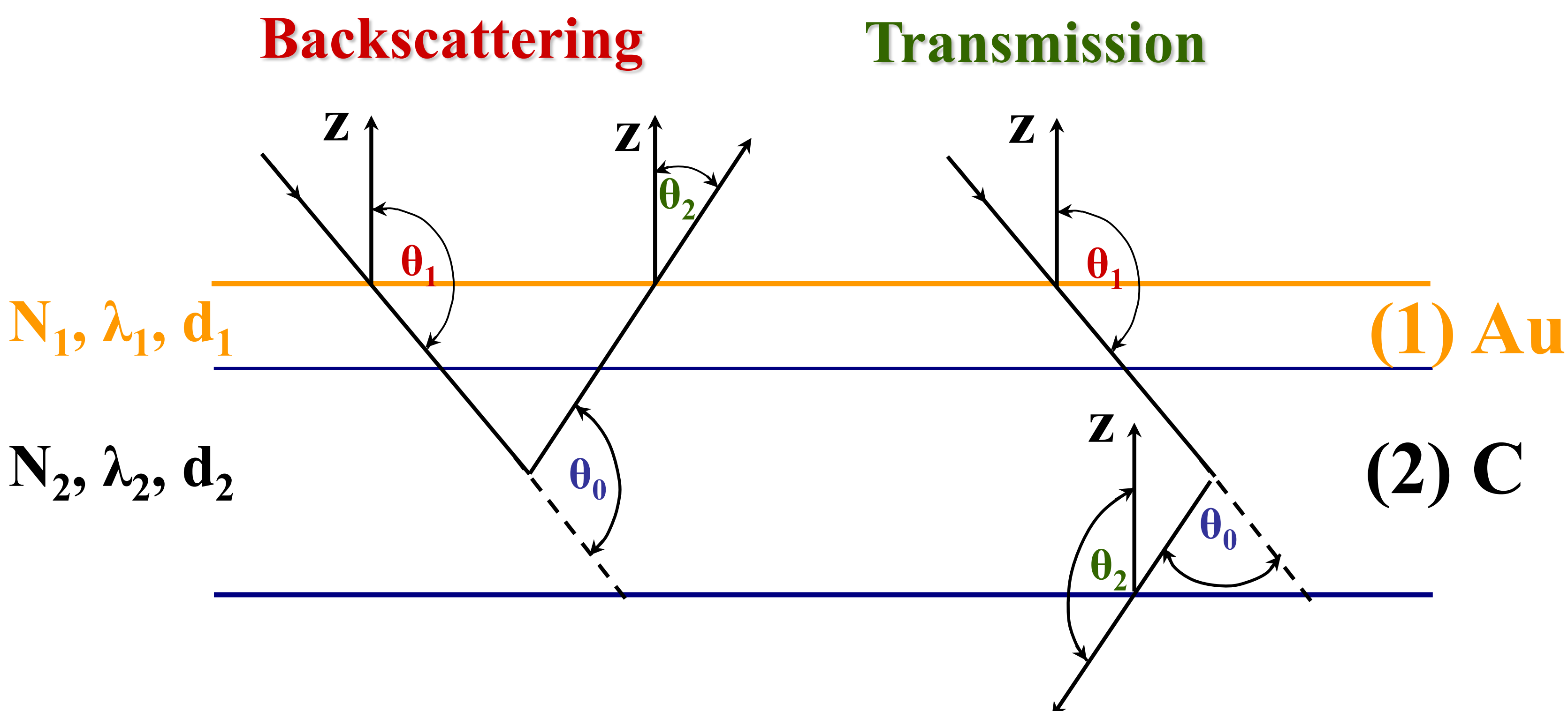
Scenario



Schematic view of the geometric configuration of the calculation.



Scattering Geometry



$dP_1(1)$
$dP_1(2)$

$$dP_1(1) = g e^{d_1/(\lambda_1 \cos\theta_2)} e^{d_2/(\lambda_2 \cos\theta_2)} \left[1 - e^{d_1/(\lambda_1 g \cos\theta_1)}\right] \lambda_1 N_1 \frac{d\sigma_1}{d\Omega}(\theta_0) d\Omega,$$

$$dP_1(2) = g e^{d_1/(\lambda_1 \cos\theta_1)} e^{d_2/(\lambda_2 \cos\theta_2)} \left[1 - e^{d_2/(\lambda_2 g \cos\theta_1)}\right] \lambda_2 N_2 \frac{d\sigma_2}{d\Omega}(\theta_0) d\Omega,$$

where $$g = \frac{\cos\theta_2}{\cos\theta_2 - \cos\theta_1}$$

Monte Carlo simulation

- Monte Carlo simulation of electron transport in solids is based on the stochastic description of scattering processes.
- Electron penetration is approximated by a classical zigzag trajectory.
- In our simulations both the elastic and inelastic scattering events were taken into account.
- For the case of the first inelastic collision the calculations were stopped.
- Particular values of scattering angles of electrons in an individual event are realized by random numbers following the angular differential elastic cross sections of carbon and gold.

Energy loss due to elastic scattering

$$E_r = \frac{2mE_0}{M_l}\left(1+\frac{E_0}{2mc^2}\right)\left[1-\cos\theta_0+\sqrt{\frac{M_l\varepsilon_l}{m\varepsilon_0}\left(1-\frac{E_0}{2mc^2}\right)}\left(\cos\theta_l-\cos\theta_0\cos\theta_l-\sin\theta_0\sin\theta_l\cos\varphi_l\right)\right]$$

- m and E_0 are the mass and kinetic energy of the electron
- θ_0 is the scattering angle
- $l = 1,2$ denotes the kind of atom taking part in the collision
- M_l, ε_l are the mass and kinetic energy of the atom
- θ_l és φ_l characterizes the direction of motion of the atom with respect to the velocity of the electron before the scattering event

Monte Carlo simulation of electron spectra backscattered elastically from double-layer sample at relativistic energy

Background

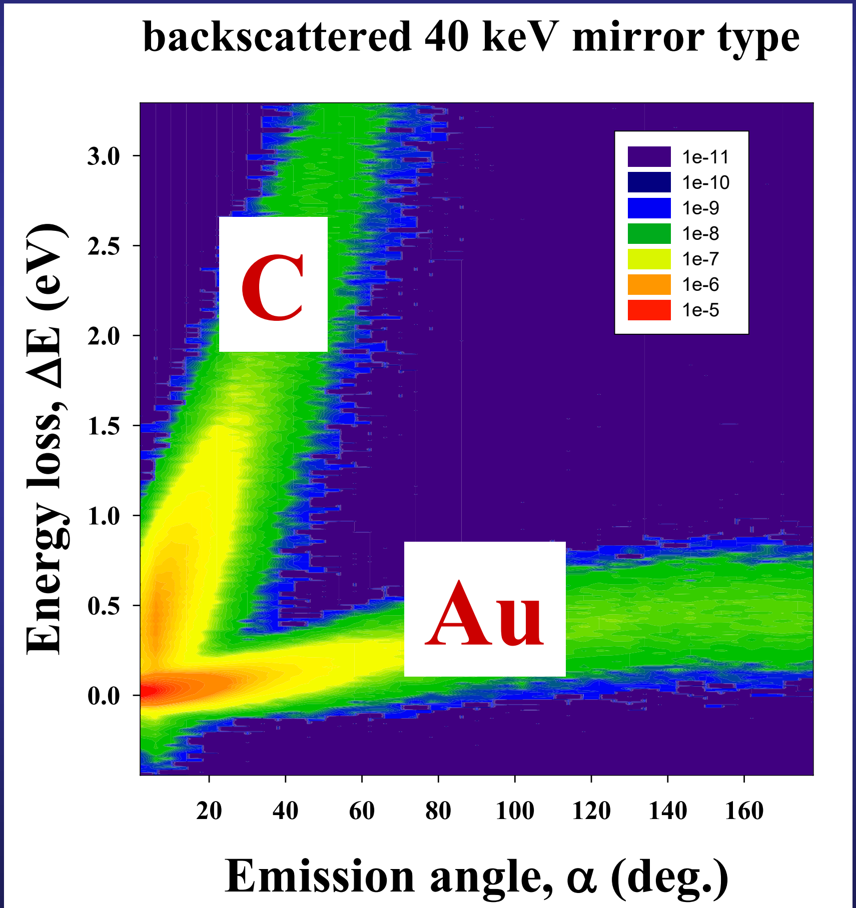
• Studies of Electron Rutherford Backscattering (ERBS) are in the centre of interest.
elastic scattering of electrons (3-40 keV)
- good energy resolution (< 1eV)

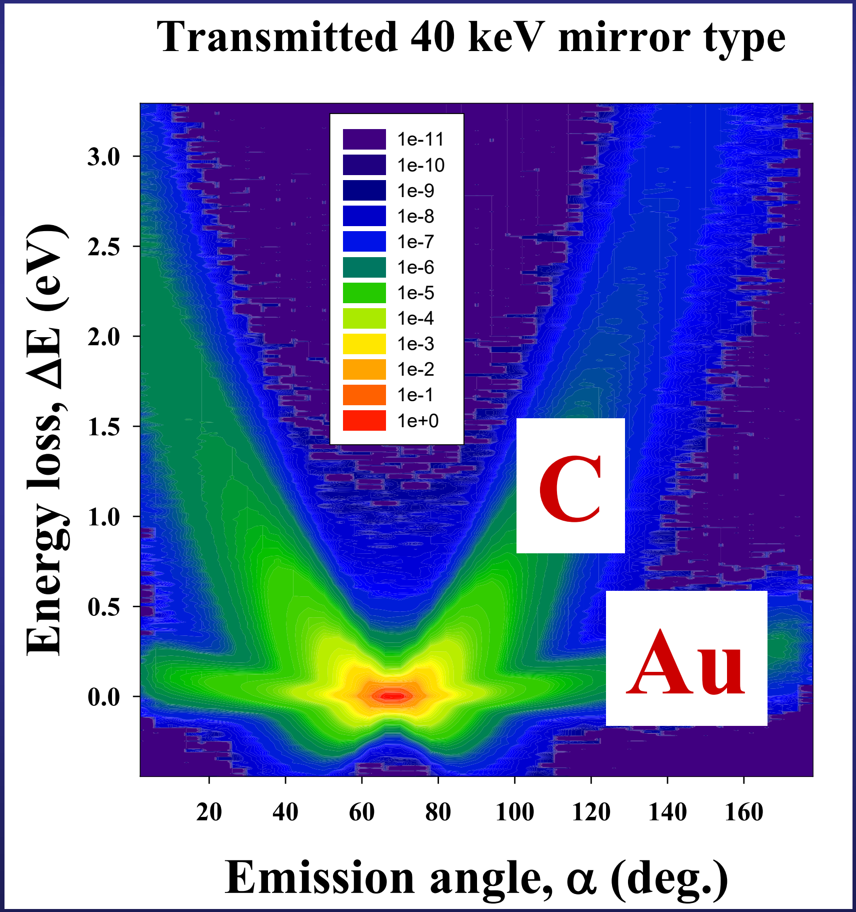
Motivation

• Accurate Monte Carlo simulation for double-layer system.
• Effects of the multiple and „mixed" scatterings to the elastic peak.

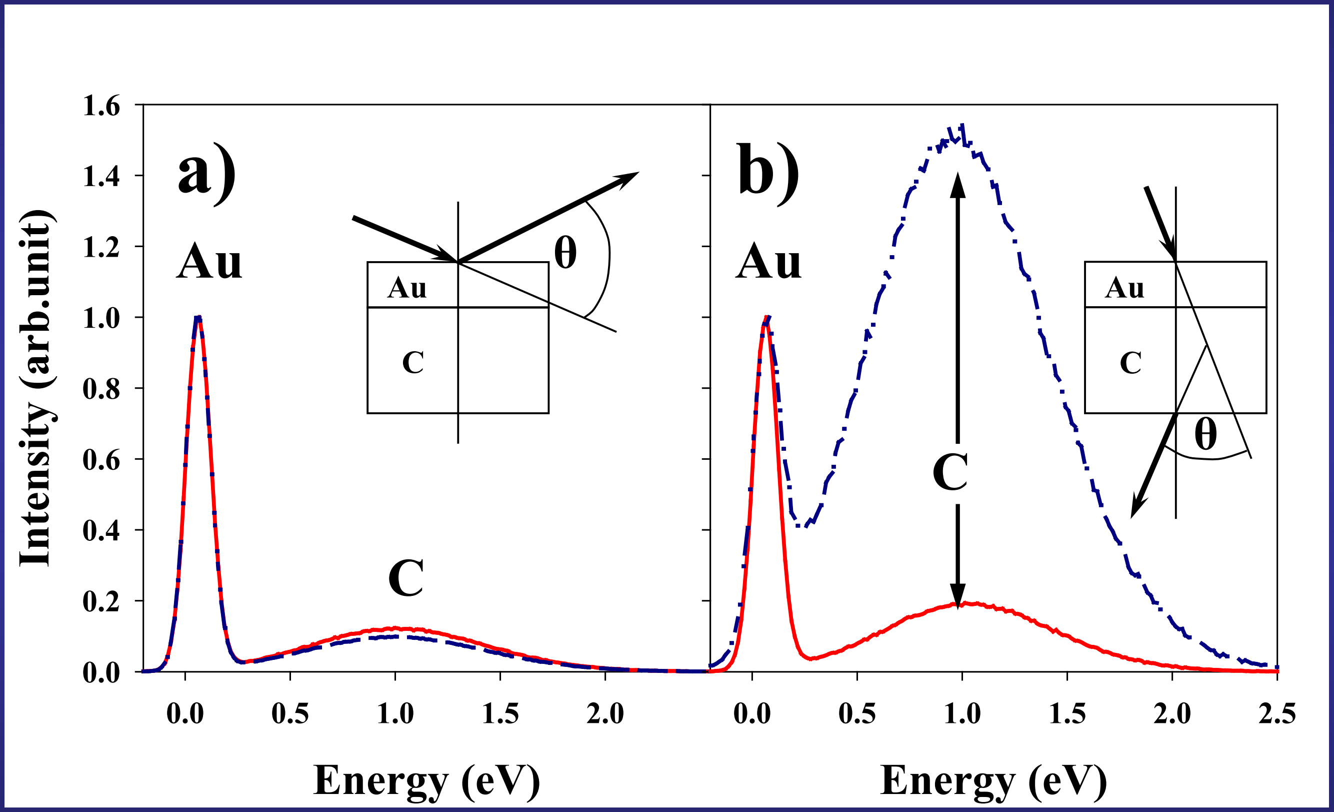
• peak intensities - estimate of the thickness layer
• FWHM of the peak – average kinetic energy of the electrons in solid
• accurate peak shape – final state interaction

Contour plot (blue: minimum intensity, red: maximum intensity) of the electron intensity of elastically scattered electrons from Au-C double-layer Au - 1Å, C- 90 Å.





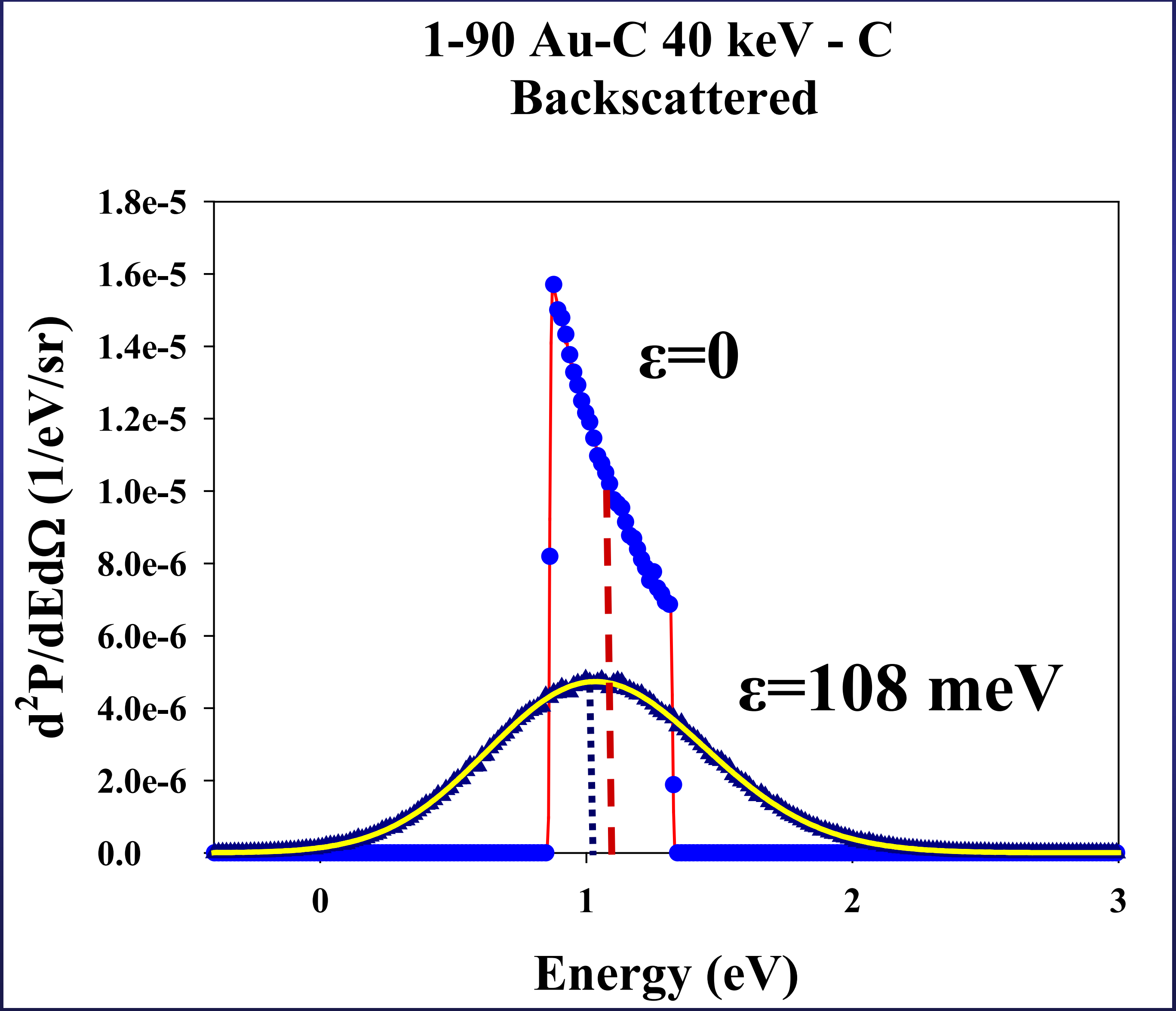
Energy loss distributions at 40 keV primary energy θ_0 =44.3° and $\Delta\Omega$=±5° solid angle



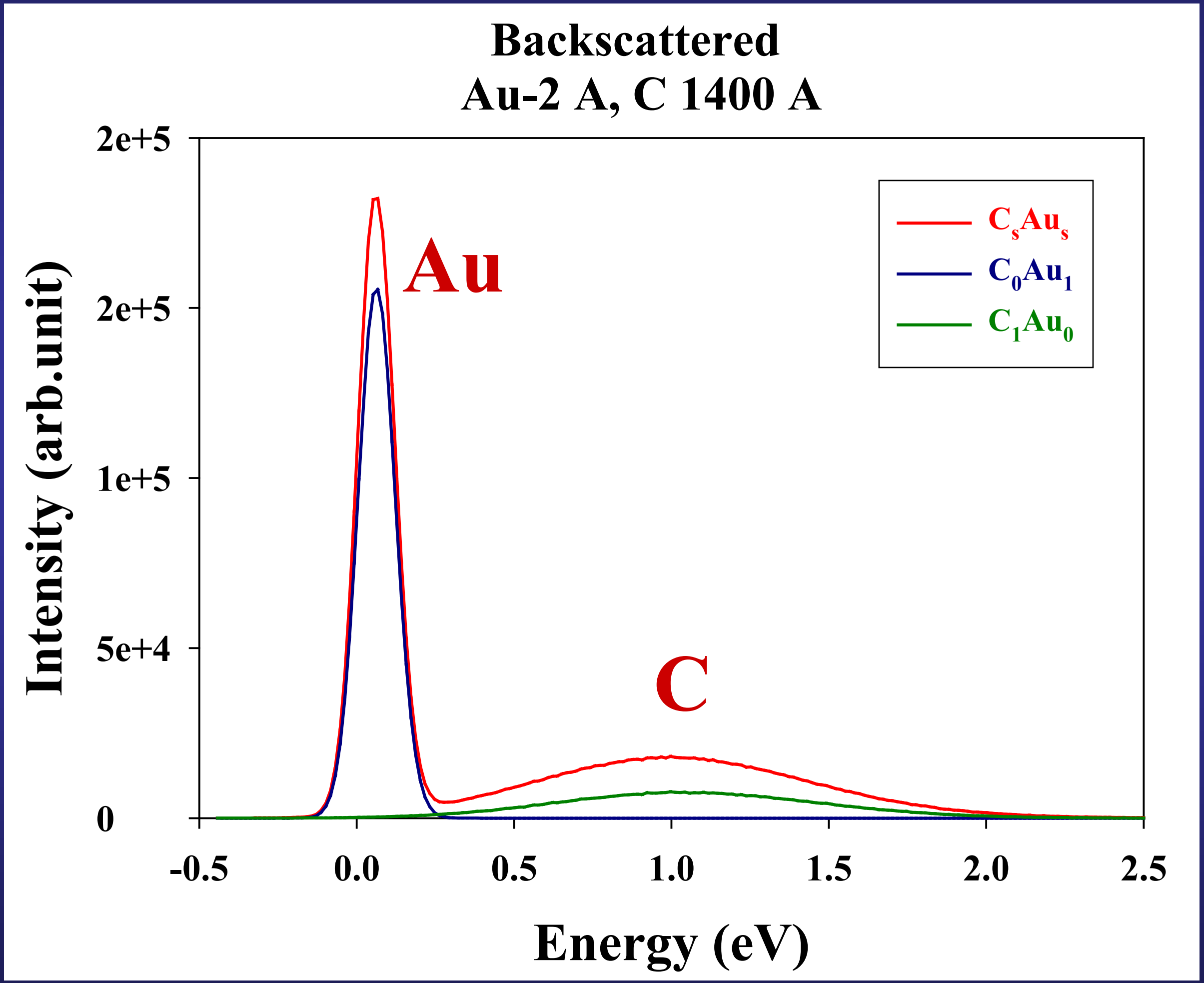
Solid line : Au – 1 Å, C – 90 Å

Dashed line: Au – 2 Å, C – 1400 Å

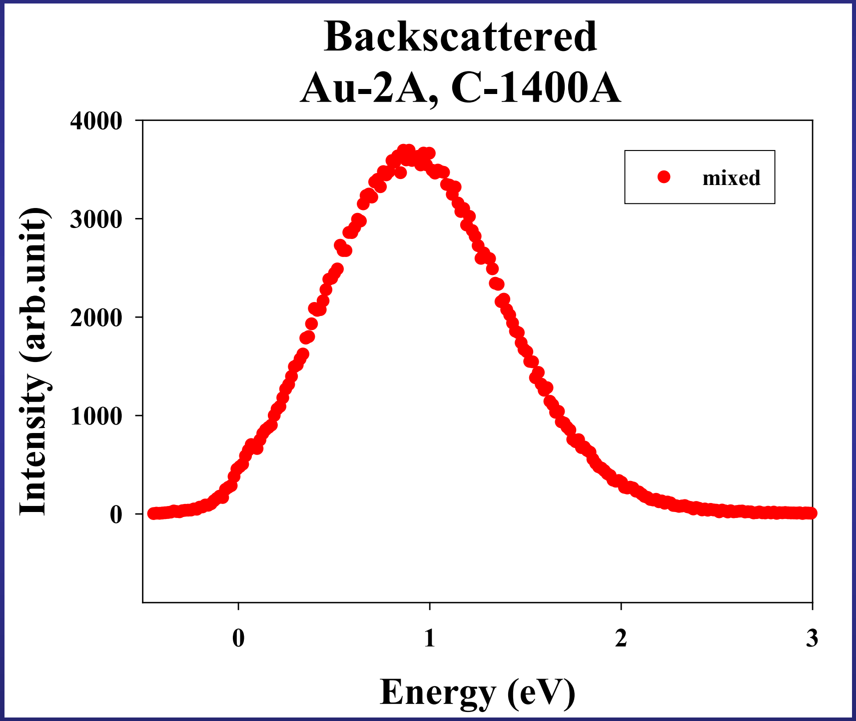
Single scattering on carbon

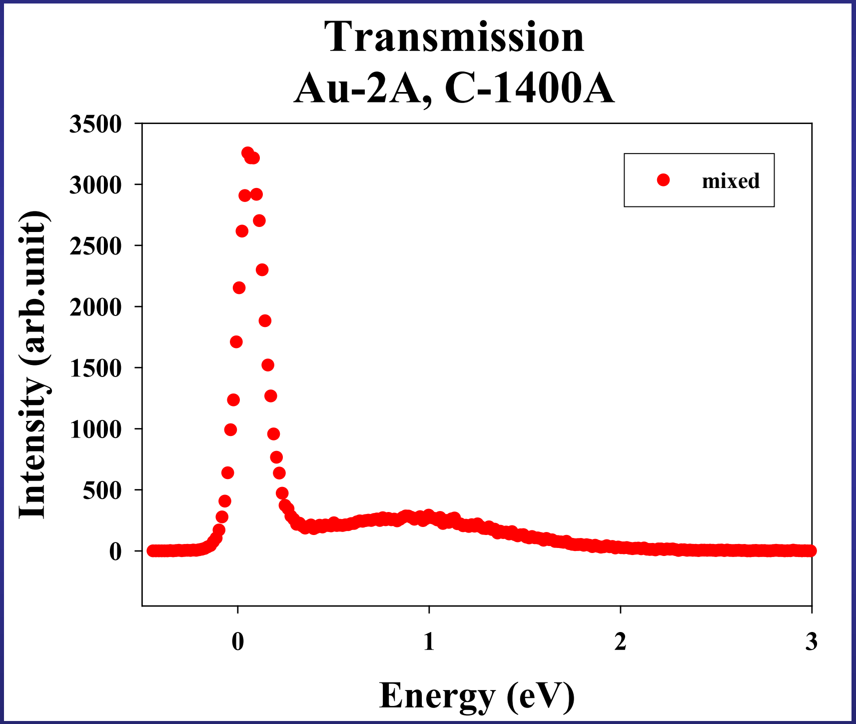


Partial energy loss distributions at 40 keV primary energy θ_0 =44.3° and ΔΩ=±5° solid angle



Multiple scattering on different components (C^iH^j i≥1, j≥1) at 40 keV primary energy





Partial Elastic scattering yields - I

Geometry [sample] (Å)	Peaks / Sum	Single scattering (%)	Multiple scattering	
			Same atomic mass (%)	Different atomic mass (%)
Reflection $\begin{bmatrix} Au-1 \\ C-90 \end{bmatrix}$	Au	49.35	3.98	(≤ 0.1)
	C	29.07	11.84	(~ 5.7)
	Σ	**78.42**	**15.82**	**5.76**
Reflection $\begin{bmatrix} Au-2 \\ C-1400 \end{bmatrix}$	Au	50.10	8.03	(≤0.1)
	C	16.87	15.88	(~ 9.1)
	Σ	**66.96**	**23.91**	**9.13**
Transmission $\begin{bmatrix} Au-1 \\ C-90 \end{bmatrix}$	Au	35.86	0.83	(6.11)
	C	47.32	8.33	(1.54)
	Σ	**83.19**	**9.16**	**7.65**
Transmission $\begin{bmatrix} Au-2 \\ C-1400 \end{bmatrix}$	Au	0.68	0.03	(7.32)
	C	7.11	79.98	(4.87)
	Σ	**7.79**	**80.02**	**12.19**

Elastic peak intensities

Test of the Monte Carlo simulation

Geometry [sample] (Å)	$P_1(C) / P_1(Au)$			$P_{mono}(C)/P_{mono}(Au)$ Monte Carlo	P(C)/P(Au) Monte Carlo	$\frac{P(C)/P(Au)}{P_1(C)/P_1(Au)}$
	Θ_0=44.3° (dΩ)	Integrated (ΔΩ)	M[illegible] Carlo ([illegible]Ω)			
Reflection $\begin{bmatrix} Au-1 \\ C-90 \end{bmatrix}$	0.5939	0.5895	[illegible].589 (1)	0.767 (2)	0.875 (3) 0.883 (16)	1.48 1.50
Reflection $\begin{bmatrix} Au-2 \\ C-1400 \end{bmatrix}$	0.3417	0.3365	0.337 (1)	0.563 (1)	0.720 (2) 0.730 (8)	2.14 2.17
Transmission $\begin{bmatrix} Au-1 \\ C-90 \end{bmatrix}$	1.3071	1.3[illegible]	1.320 (5)	1.517 (5)	1.336 (6) 1.343 (10)	1.01 1.02
Transmission $\begin{bmatrix} Au-2 \\ C-1400 \end{bmatrix}$	10.167	[illegible]0	10.43 (24)	122 (2)	11.45 (14) 12.75 (41)	1.12 1.25

Elastic peak positions

Single scattering:

$E_0 = 40keV$ $E_{r0}(C) = 1080meV$

$\Theta_0 = 44.3°$ $E_{r0}(Au) = 66meV$

$E_{r0}(C) - E_{r0}(Au) = 1014meV$

Geometry [sample] (Å)	$E_{r0}(C) - E_{r0}(Au)$ [meV]		
	Single scattering	Mono atomic scattering	Sum of the scatterings
Reflection $\begin{bmatrix} Au-1 \\ C-90 \end{bmatrix}$	984 (1)	968 (1)	952 (1) (-6.1%)
Reflection $\begin{bmatrix} Au-2 \\ C-1400 \end{bmatrix}$	988 (1)	965 (1)	940 (1) (-7.3%)
Transmission $\begin{bmatrix} Au-1 \\ C-90 \end{bmatrix}$	977 (1)	974 (1)	970 (1) (-4.3%)
Transmission $\begin{bmatrix} Au-2 \\ C-1400 \end{bmatrix}$	968 (3)	926 (2)	910 (2) (-10.3%)

Elastic peak widths

Single scattering:

E

$E_0 = 40\text{keV}$

Θ

$\Theta_0 = 44.3°$ $\rightarrow \Delta E_r(Au) = 149$ meV

ε(

$\bar{\varepsilon}(Au) = 40$ meV

Geometry [sample] (Å)	ΔE_r (C) [FWHM ; meV]		
	Single scattering	Mono atomic scattering	Sum of the scatterings
Reflection $\begin{bmatrix} Au-1 \\ C-90 \end{bmatrix}$	966 (2)	979 (2)	1006 (2) (+4.1%)
Reflection $\begin{bmatrix} Au-2 \\ C-1400 \end{bmatrix}$	970 (2)	996 (2)	1034 (2) (+6.6)%
Transmission $\begin{bmatrix} Au-1 \\ C-90 \end{bmatrix}$	959 (2)	963 (2)	985 (3) (+2.7%)
Transmission $\begin{bmatrix} Au-2 \\ C-1400 \end{bmatrix}$	954 (5)	1020 (4)	1061 (4) (+11.2%)

Quantitative analysis of the hydrogen peak in the spectra of electrons backscattered from polyethylene

Background

• Observation of the hydrogen peak is a challenging if not impossible task in conventional electron spectroscopy.

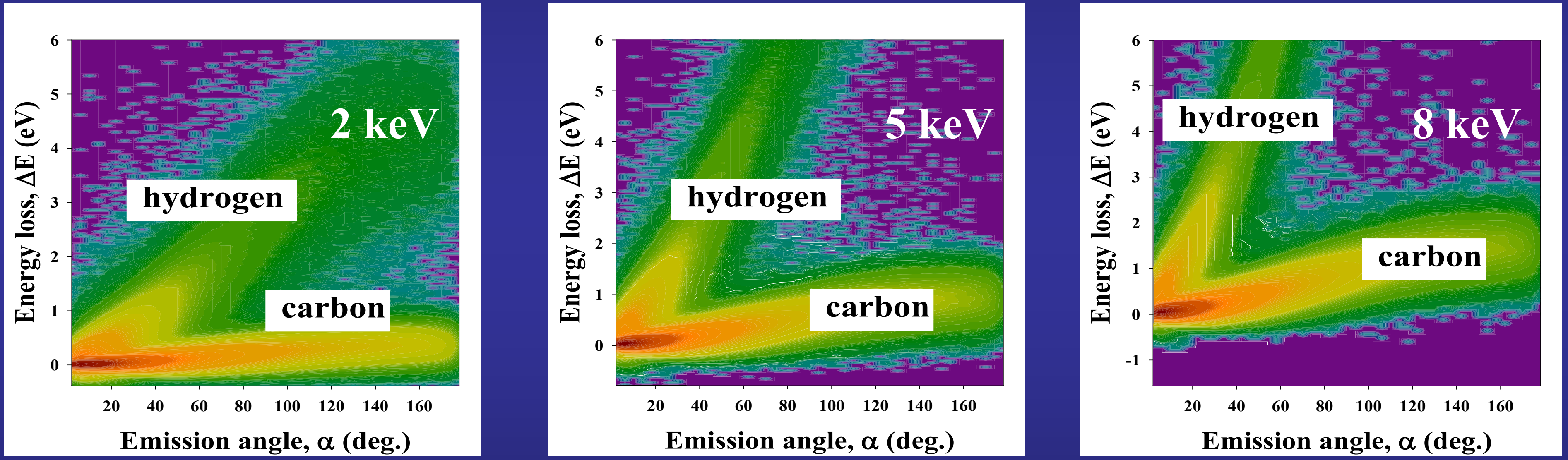
• Hydrogen was observed earlier in formvar film in high energy electron scattering experiments using transmission geometry.

Motivation

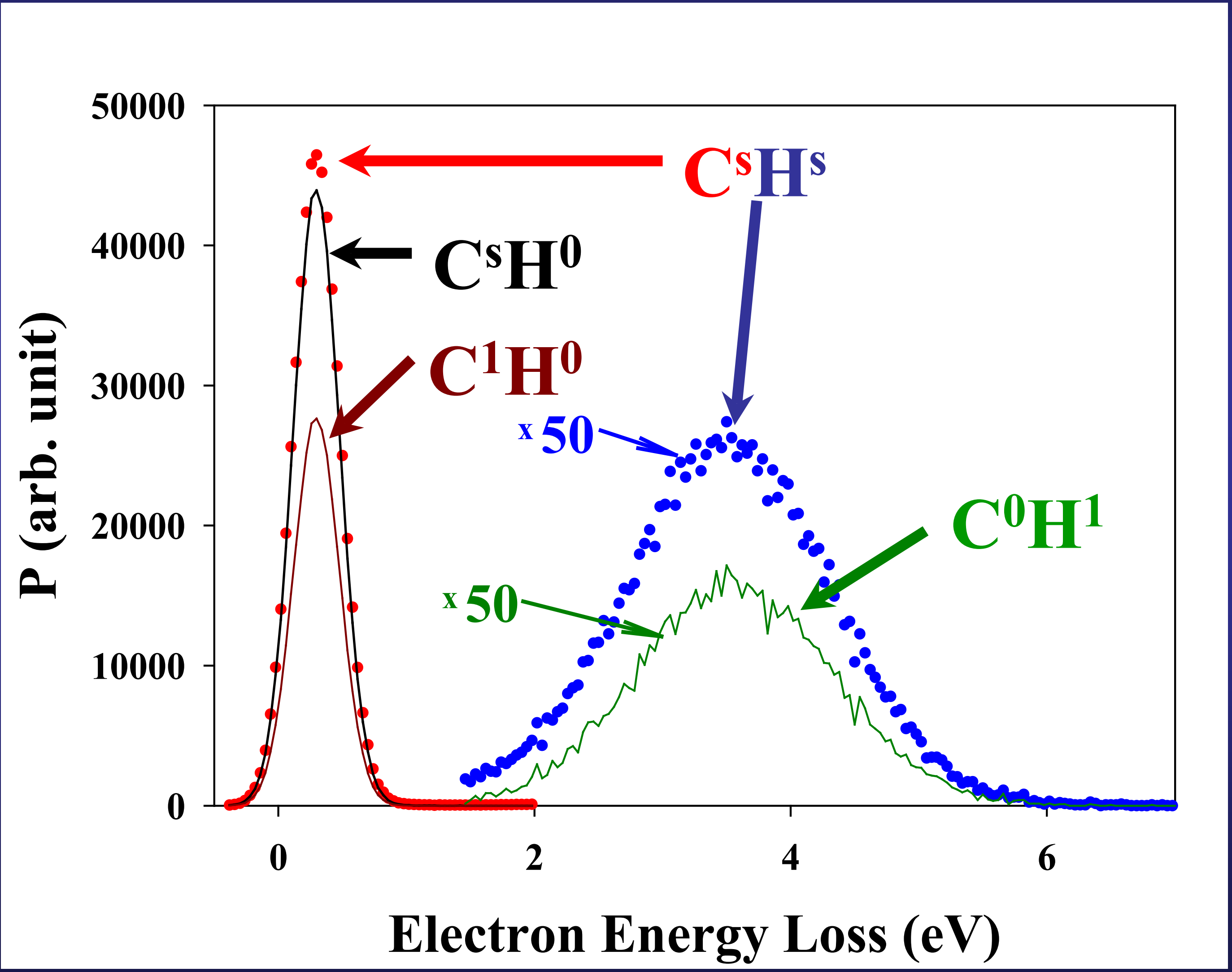
• An alternative way for the detection of hydrogen is shown.

• The spectra of electrons backscattered elastically from polyethylene (CH2)n is used.

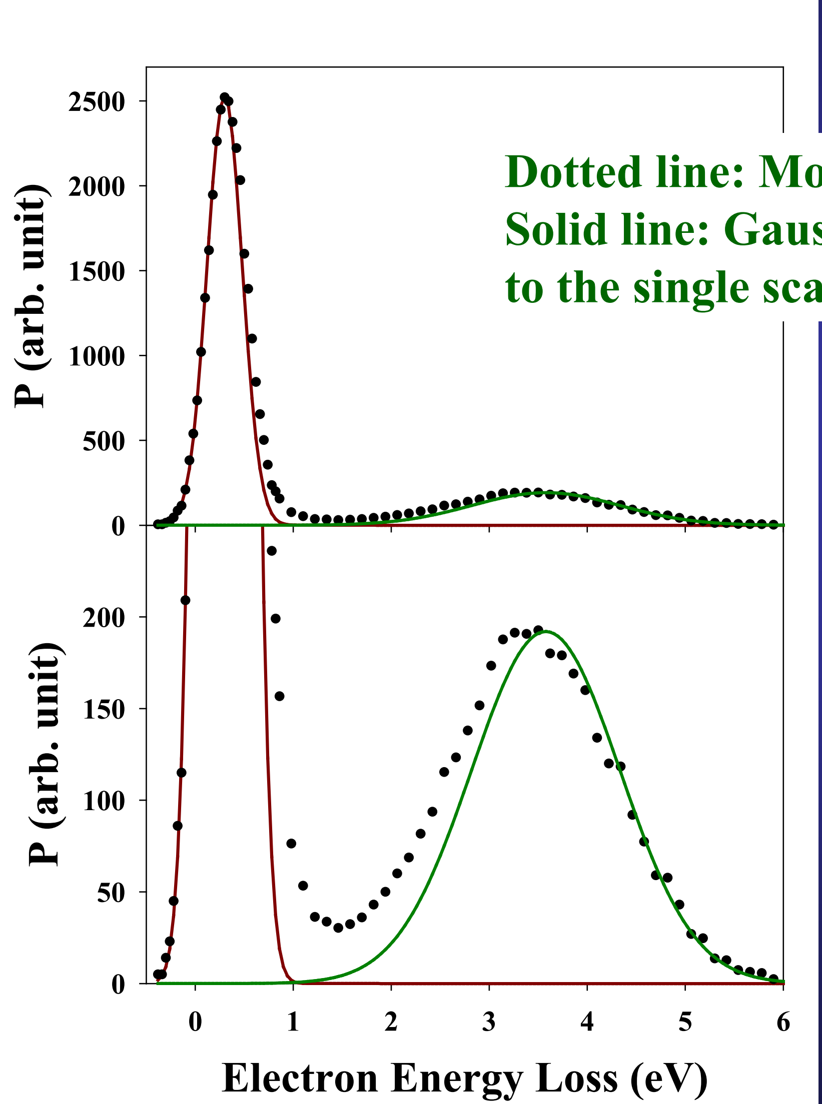
Contour plot (blue: minimum intensity, red: maximum intensity) of the electron intensity backscattered elastically from polyethylene.



Energy loss distributions at 2 keV primary energy θ =130° and $\Delta\Omega$=±5° solid angle

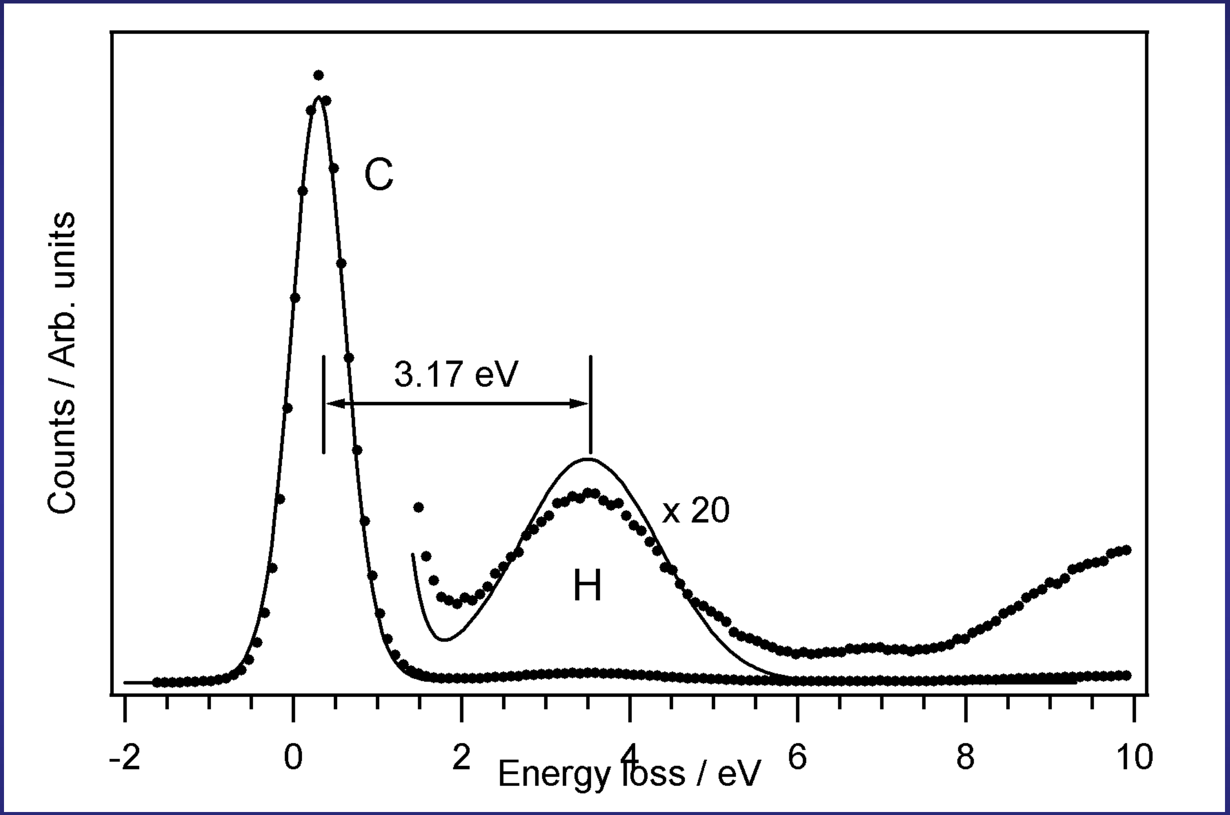


Multiple scattering on different components (C^iH^j i≥1, j≥1) at 2 keV primary energy



Dotted line: Monte Carlo simulation
Solid line: Gaussian peak corresponding to the single scattering contribution

Comparison with experiment



The energy distribution of electrons backscattered elastically from polyethylene at $\theta = 130^o$. The primary electron energy was 2 keV. Dotted line: measurement, solid line: MC simulation.

CONCLUSIONS

- The high energy resolution elastic peak electron spectroscopy is applicable for quantitative analysis.
- The relative hydrogen content can be estimated by the observation of the well separated *H* elastic peak.
- The single scattering model can be used for thin samples and transmission geometry.
- However, the multiple scatterings, depending on the primary electron energy and geometry, modify the measurable data (distance between the elastic peaks, FWHM, yields), therefore for more precise analysis the contribution of mixed multiple electron scattering has to be taken into account – Monte Carlo simulation.

THANK YOU FOR YOUR ATTENTION!