MPGD simulation: models, ingredients, precision

Material properties
Fields
Electron transport
Ion chemistry

Caen, October 4th 2017

Operating principles of MPGDs:

▶ A charged particle passes through the gas and ionises molecules;

▶ the electric field in the gas volume provokes multiplication and transports the ionisation electrons and ions;

▶ the movement of electrons and ions leads to induced currents in electrodes.

Ingredients of MPGD simulation

- Ionisation
  - PAI models: Heed for low energy electrons, Geant4;
  - Degrad: extension to higher energy of Magboltz.
- Field:
  - dielectric constants, resistive layers;
  - finite and boundary element methods, meshing;
  - closed expressions, thin-wire approximation.
- Electrons in a gas:
  - electron cross sections, isotropy;
  - Penning and quenching rates.
- Ions in a gas:
  - mobility and diffusion;
  - chemistry, rate coefficients.
- Transport:
  - Runge-Kutta;
  - microscopic tracking based on cross sections;
  - Magboltz: ergodic principle, SST corrections;
  - charging-up.

Issues with ionisation

▶ PAI models (Heed, Geant 4):
  ▶ Simulate ionisation of a gas by a charged particle;
  ▶ Heed contains relaxation, not all PAI models do;
  ▶ the model as such is contested;
  ▶ the photo-absorption cross section is not well known.

▶ Degrad:
  ▶ extension of Magboltz to higher electron energy;
  ▶ naturally deals with electron scattering;
  ▶ also handles photons and minimum ionising particles;
  ▶ uses measured cross sections, does not rely on models.

▶ SRIM:
  ▶ simulates ions, closed source, interface questionable.

Basic formulae of the PAI model

▶ Key ingredient: photo-absorption cross section $\sigma_\gamma(E)$

$$\frac{\beta^2 \pi}{\alpha} \frac{d\sigma}{dE} = \frac{\sigma_\gamma(E)}{E} \log\left(\frac{1}{\sqrt{(1-\beta^2 \epsilon_1)^2 + \beta^4 \epsilon_2^2}}\right) +$$

Relativistic rise

Cross section to transfer energy E

$$\frac{1}{N\bar{h}c}\left(\beta^2 - \frac{\epsilon_1}{|\epsilon|^2}\right)\theta +$$

Черенков radiation

$$\frac{\sigma_\gamma(E)}{E} \log\left|\frac{2 m_e c^2 \beta^2}{E}\right| +$$

Resonance region

$$\frac{1}{E^2} \int_0^E \sigma_\gamma(E_1) dE_1$$

Rutherford scattering

With:
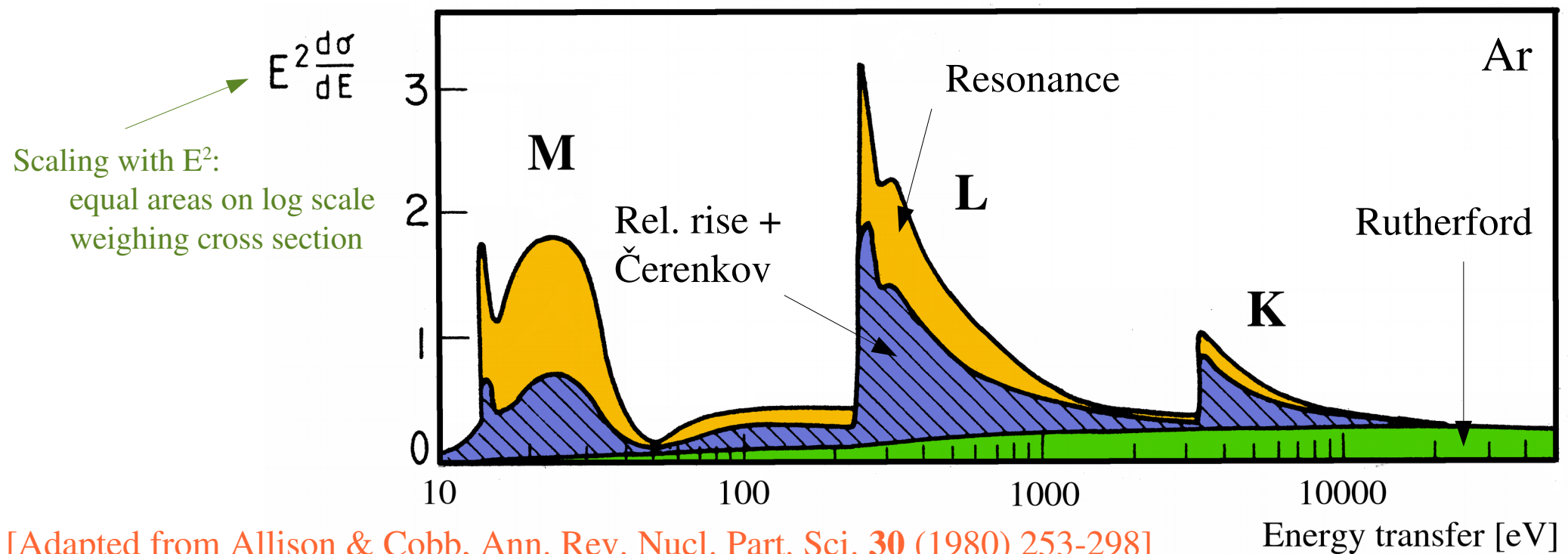
$$\epsilon_2(E) = \frac{N_e \hbar c}{EZ} \sigma_\gamma(E)$$

$$\epsilon_1(E) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{x \epsilon_2(x)}{x^2 - E^2} dx$$

$$\theta = \arg(1 - \epsilon_1 \beta^2 + i \epsilon_2 \beta^2) = \frac{\pi}{2} - \arctan \frac{1 - \epsilon_1 \beta^2}{\epsilon_2 \beta^2}$$
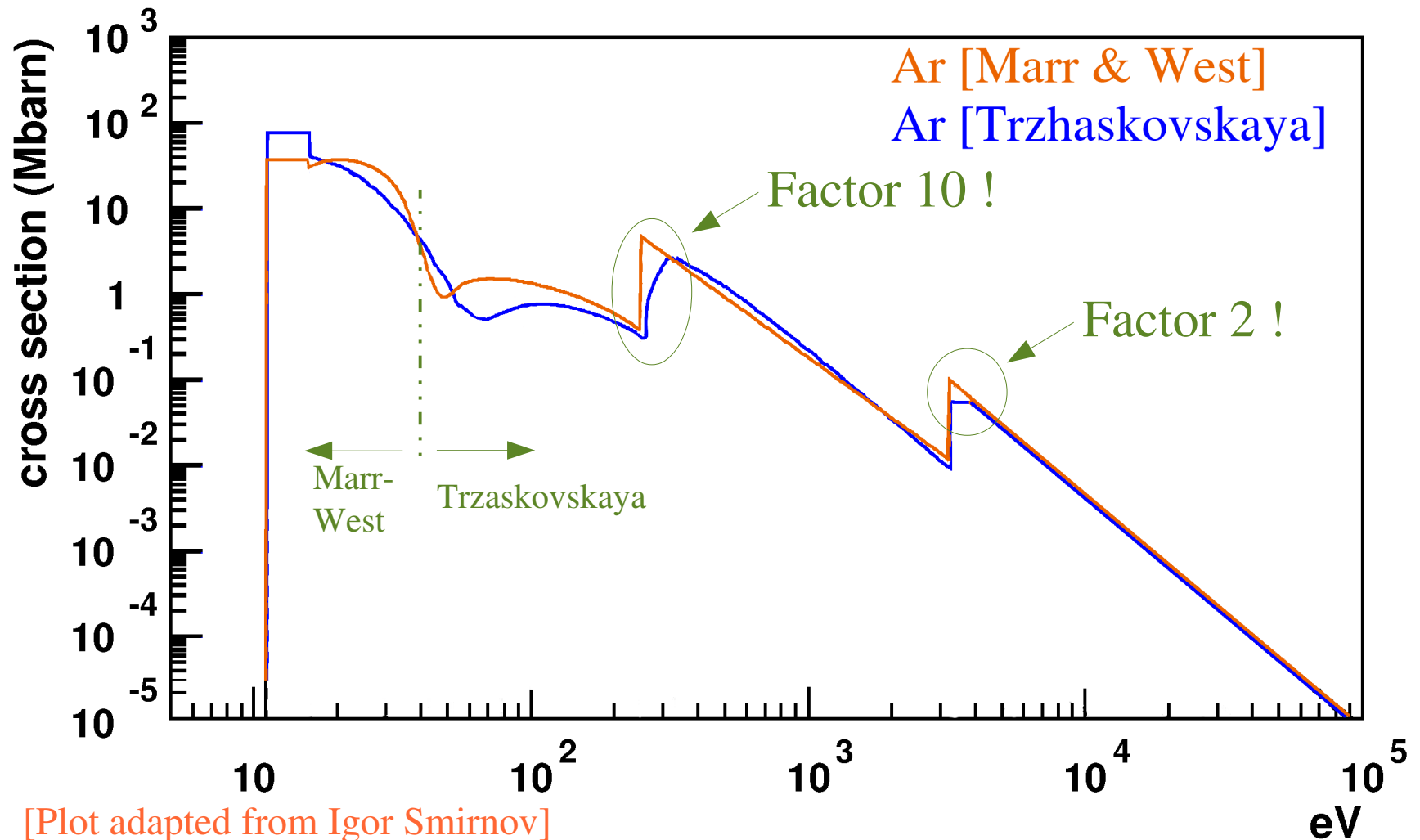
Importance of the PAI model terms

▶ All electron orbitals (shells) participate:
  ▶ outer shells: frequent interactions, few electrons;
  ▶ inner shells: few interactions, many electrons.
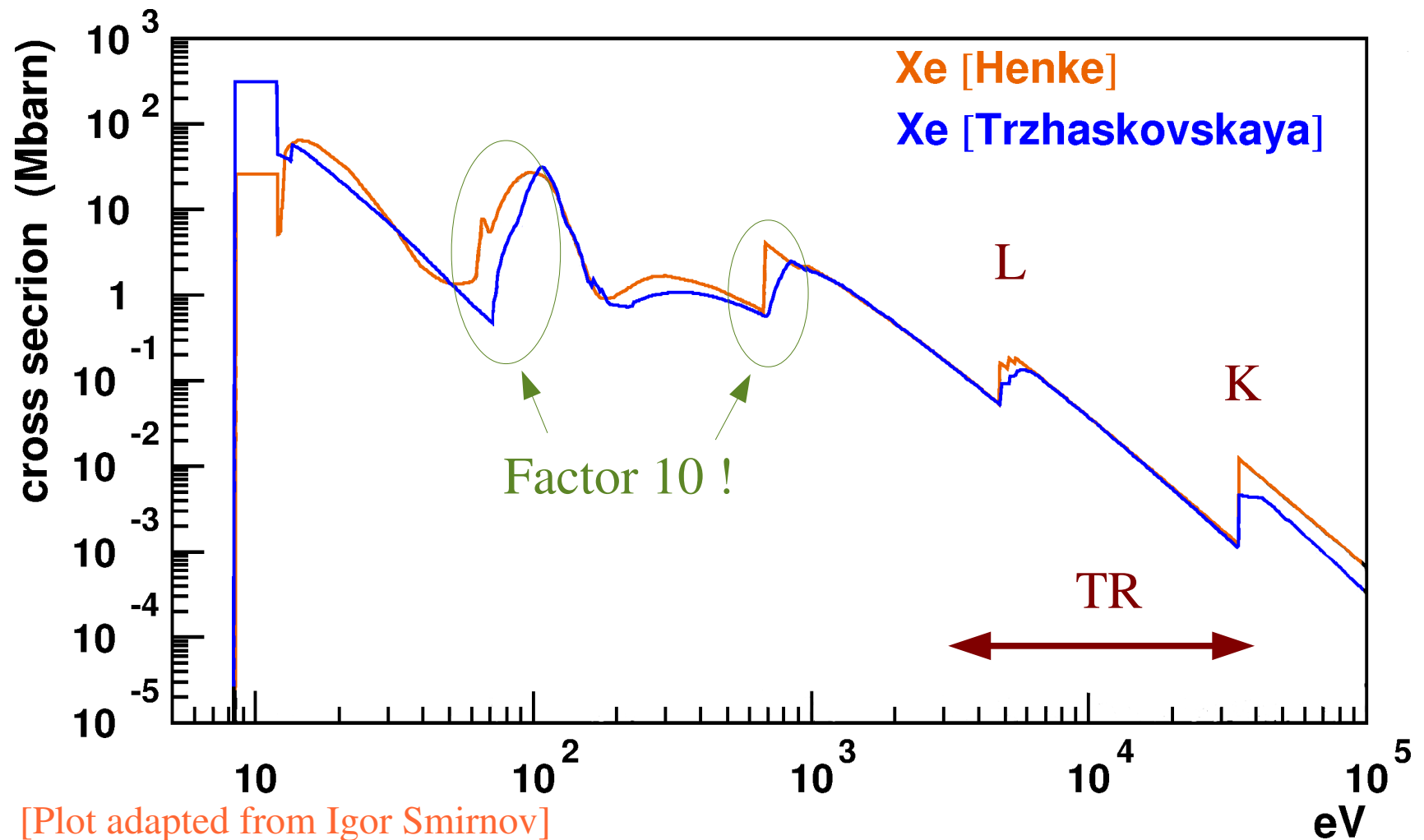▶ All terms in the formula are important.

$E^2 \frac{d\sigma}{dE}$

Scaling with E^2:
equal areas on log scale
weighing cross section

Ar

Resonance

M

L

K

Rel. rise +
Čerenkov

Rutherford

Energy transfer [eV]

How well is the cross section known ?

Disagreement at the shell borders !

cross section (Mbarn)

Ar [Marr & West]
Ar [Trzhaskovskaya]

Factor 10 !

Factor 2 !

Marr-West   Trzaskovskaya

eV

[Plot adapted from Igor Smirnov]

How well is the cross section known ?

▶ Fairly well in TR range, except at 5 keV and at 35 keV.

[Plot adapted from Igor Smirnov]

Heed: Photo-absorption in argon

▶ Argon has 3 shells, hence 3 groups of lines:

K = 1s

L1 = 2s
L2 = 2p 1/2
L3 = 2p 3/2

M1 = 3s
M2 = 3p 1/2
M3 = 3p 3/2

[Plot from Igor Smirnov]
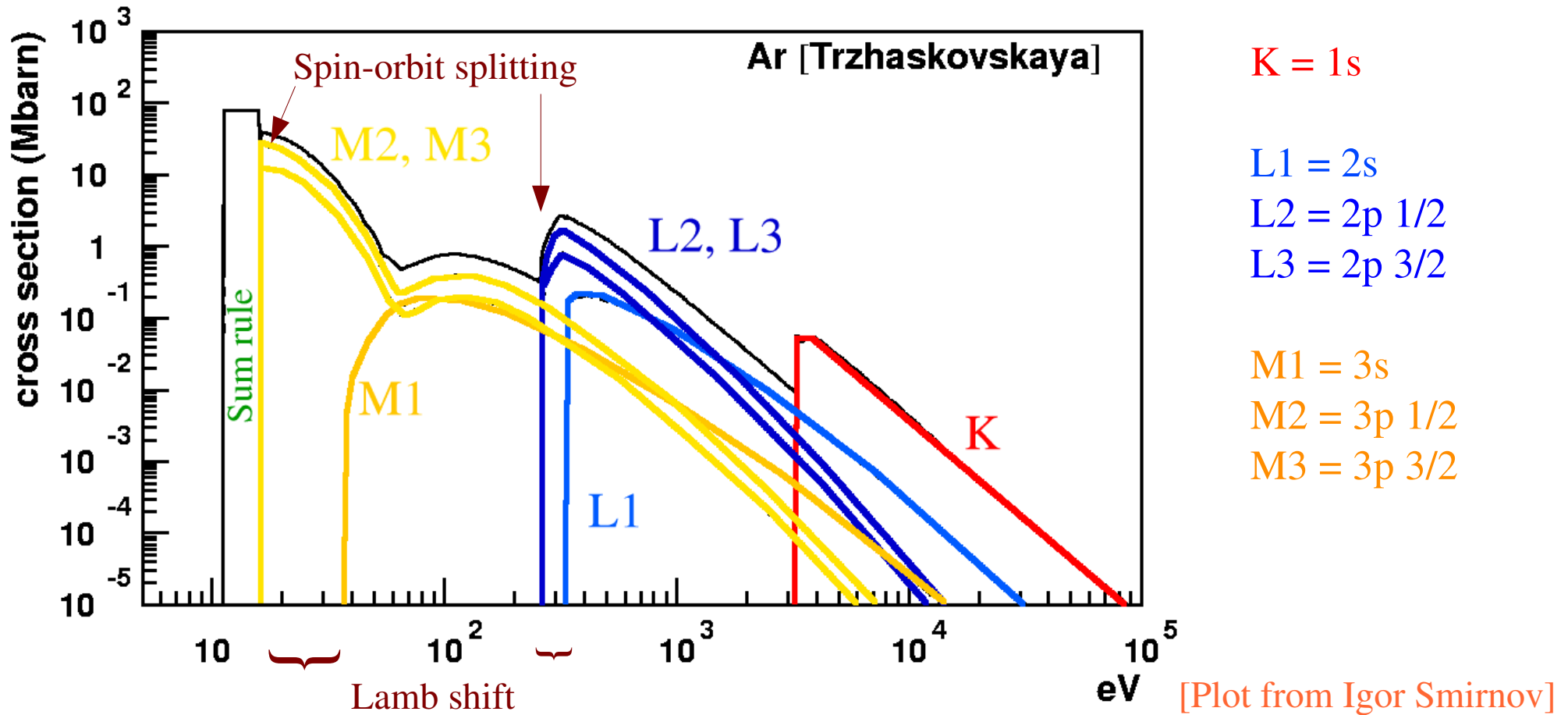
# Materials used to construct MPGDs

▶ Metals:
- treated as perfect conductors;
- not difficult: simple value boundary conditions.

▶ Perfect insulators:
- treated as zero-conductivity materials;
- transition between materials of different dielectric constant;
- break the 1st law of gas-based detectors.

▶ Resistive materials: next major challenge
- far from perfect conductor, imperfect resistor;
- charging-up, charge evacuation and "warming-up";
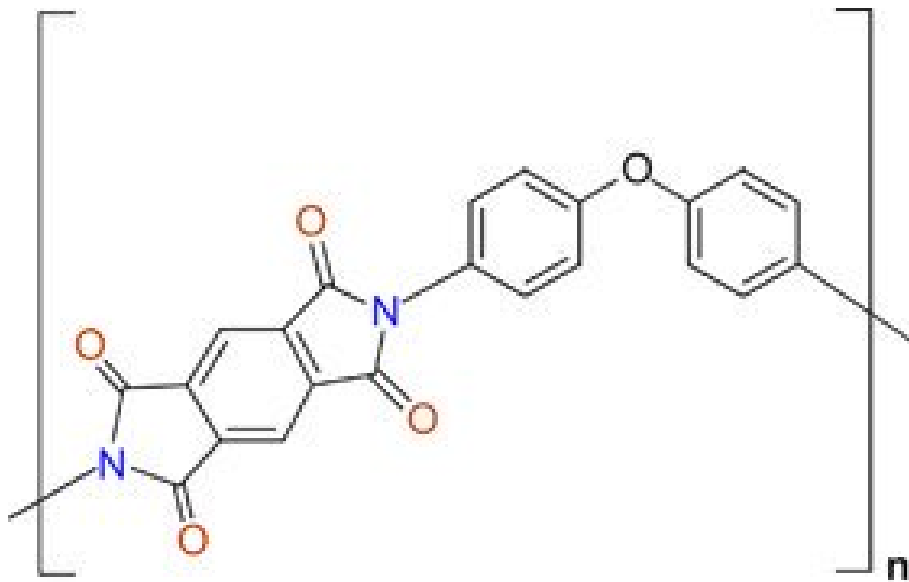- effect on signals, time-dependent weighting fields;

Dielectric media

▶ Dielectric ridge on a dielectric surface
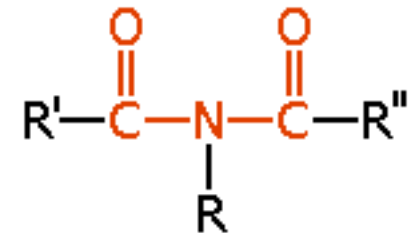

$\epsilon = 8$

$\epsilon = 4$
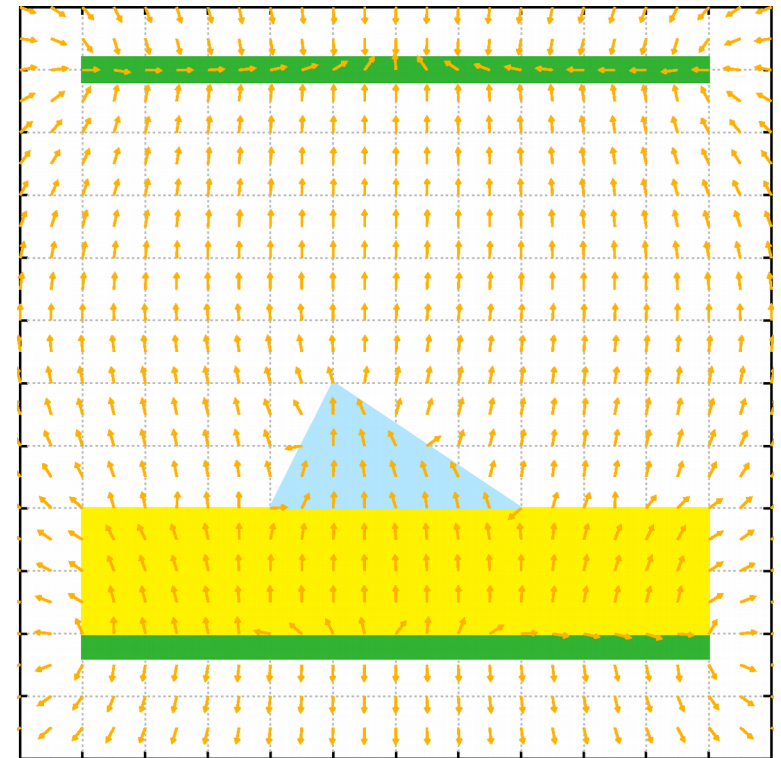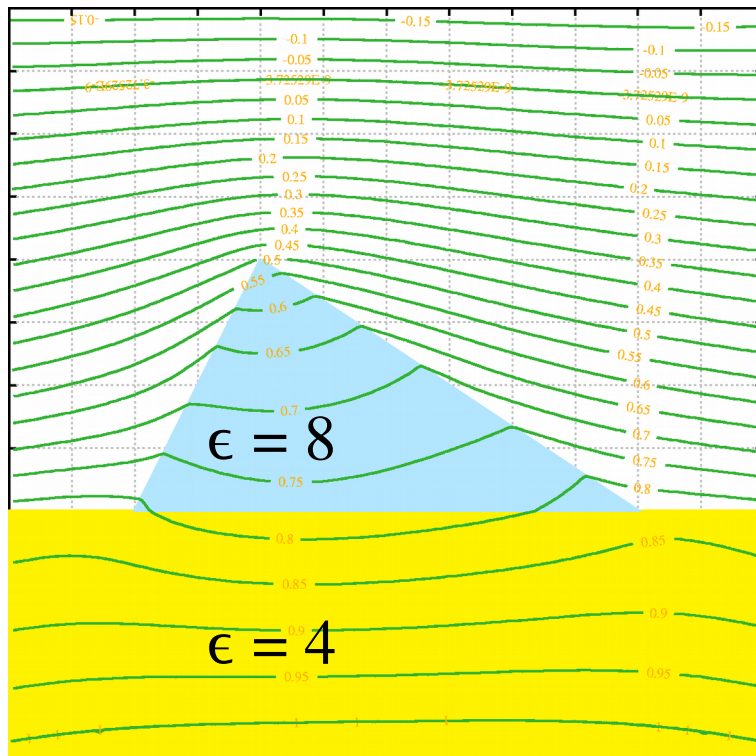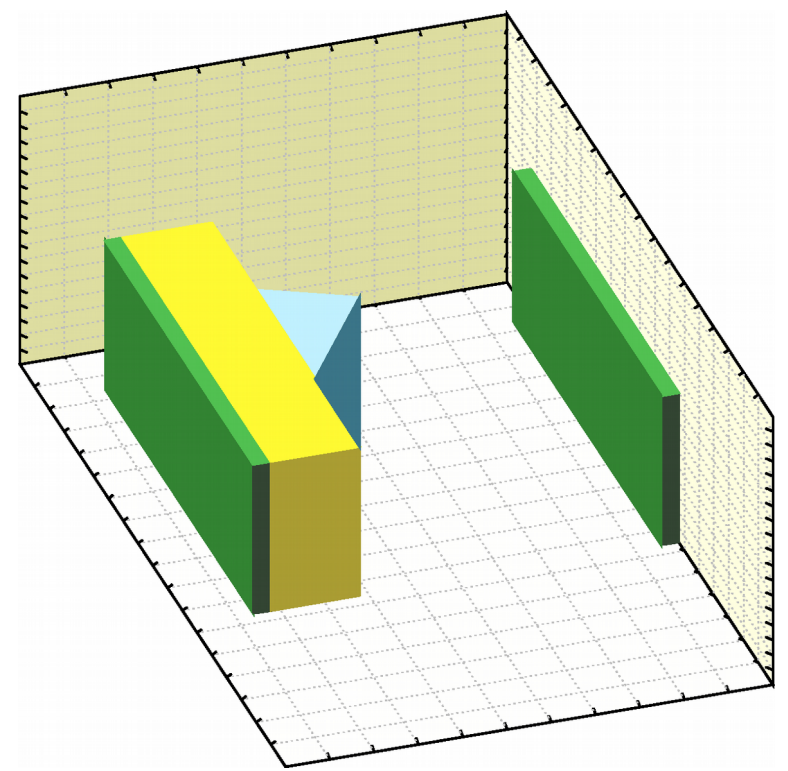
PMDA-ODA: almost perfect insulator
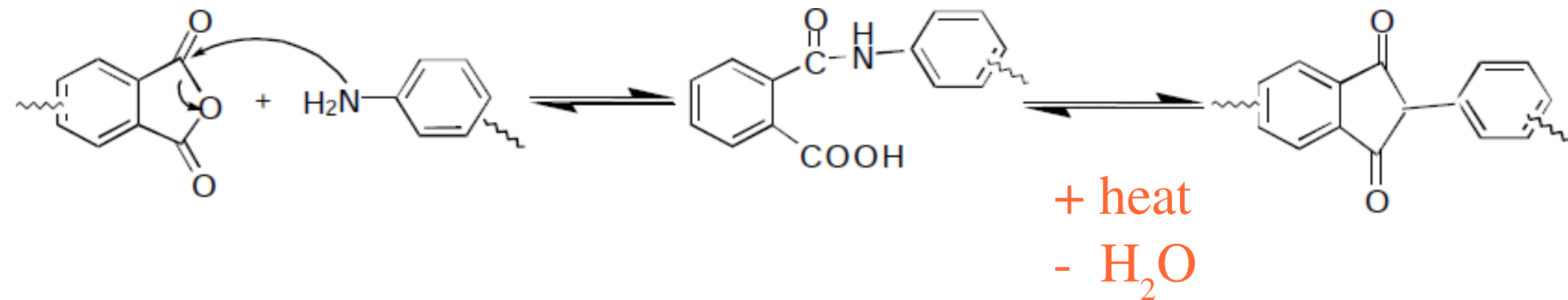
▶ Building block of a widely used polyimide:

▶ The name comes from the imide group:

PMDA-ODA reaction

▶ Sequence:
 ▶ N is attracted by the carbonyl group,
  ▶ the anhydride ring is broken and
  ▶ intermediate polyamic acid forms,
  ▶ if heated, the ring closes again between COOH and NH:

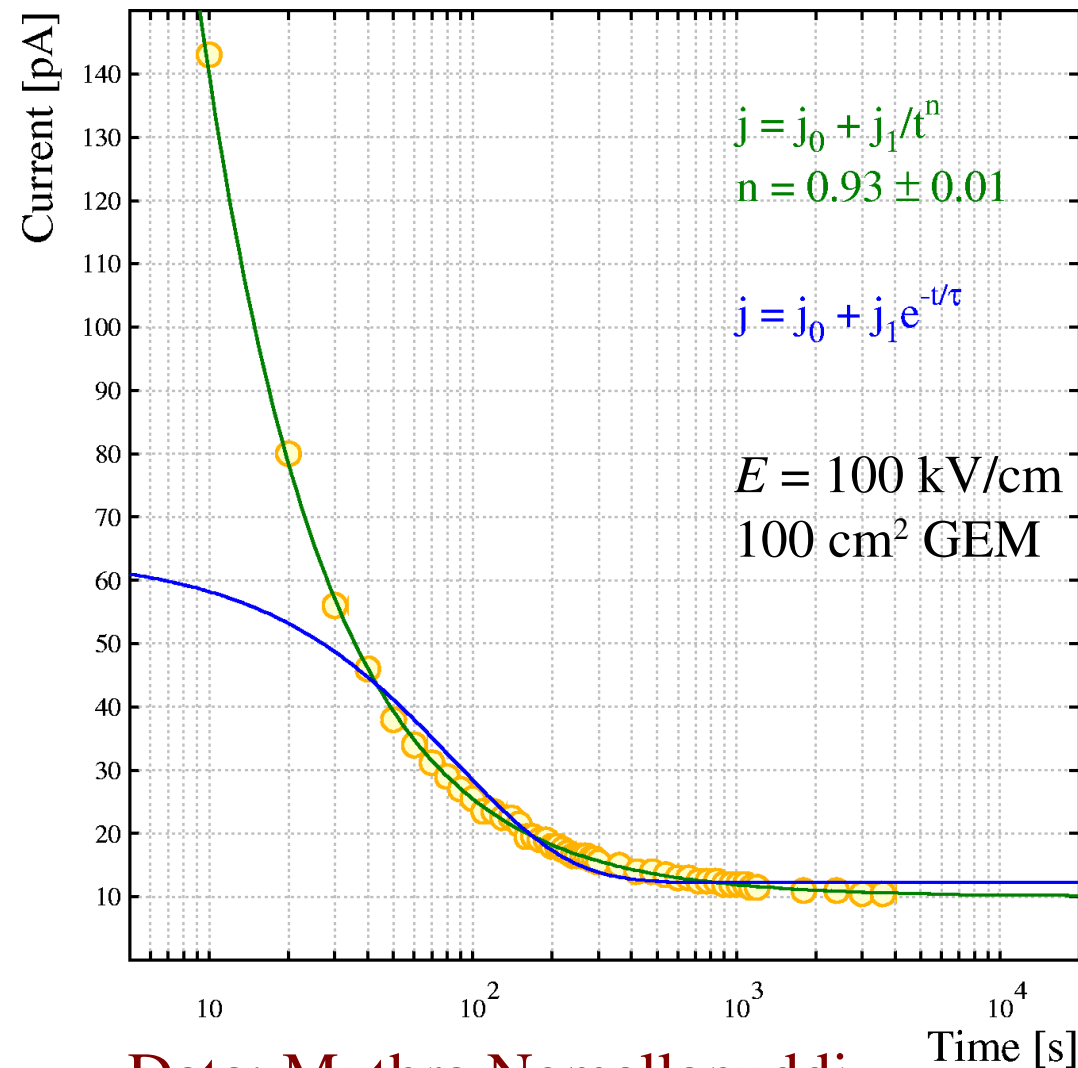+ heat

- H_2O

[From Varun Ratta, PhD thesis, Virginia Tech, 1999.]

PAA → PI vs baking temperature

- The quantity of remaining PAA depends on the baking temperature.

- The proton density therefore also varies.

[H. Oji *et al*., Memoirs of the Synchrotron Radiation Center, Ritsumeikan University, Kyoto, Japan **8** (2006) 187-188.]
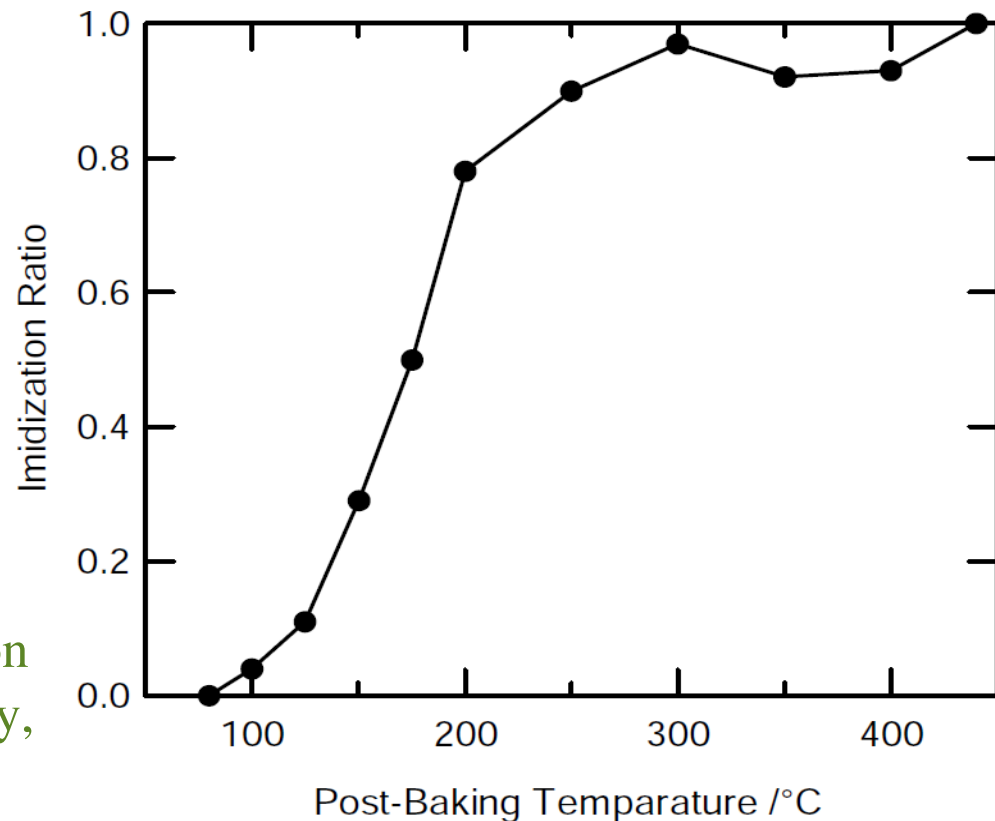
Charging-up current

- When applying voltage across a new GEM, a current flows:

  - *not* constant (i.e. not a resistor)
  - decay is *not* exponential (i.e. not a capacitor);
  - decay is *not* linear (i.e. not evacuation);

  - but a *power law* with a steady-state term.

$$j = j_0 + j_1/t^n$$
$$n = 0.93 \pm 0.01$$

$$j = j_0 + j_1 e^{-t/\tau}$$

$E = 100$ kV/cm
100 cm^2 GEM

Current [pA]

Time [s]

Data: Mythra Nemallapuddi

Rudolf Hermann Arndt Kohlrausch
(November 6th 1809, Göttingen -
March 8th 1858, Erlangen)

Kohlrausch relaxation

▶ This time dependence is known since 1854 at least.
Also known as Curie-von Schweidler behaviour.

▶ Numerous models have been proposed

H. Kliem, *Kohlrausch relaxations: new aspects about the everlasting story*, doi: 10.1109/TDEI.2005.1511096.

▶ One of the simplest models specifically assumes ions
(e.g. protons, not electrons) as charge carriers and has thin
insulating barriers between dielectric medium and electrodes.

▶ Note: Kohlrausch mentions both the power law and the stretched polynomial.
The latter model of Kliem leads to a power law.

Issues with the electric field

- Fields in wire chambers:
  - closed expressions, thin-wire approximation;
  - well-understood conditions of applicability.

- Finite elements for complicated shapes:
  - spotting the inaccuracy of FEM calculations is delicate:
  - respect of the boundary conditions is guaranteed;
  - but the "solution" does not solve the Maxwell equations.

- Boundary elements for complicated shapes:
  - the field is guaranteed to be a Maxwell solution;
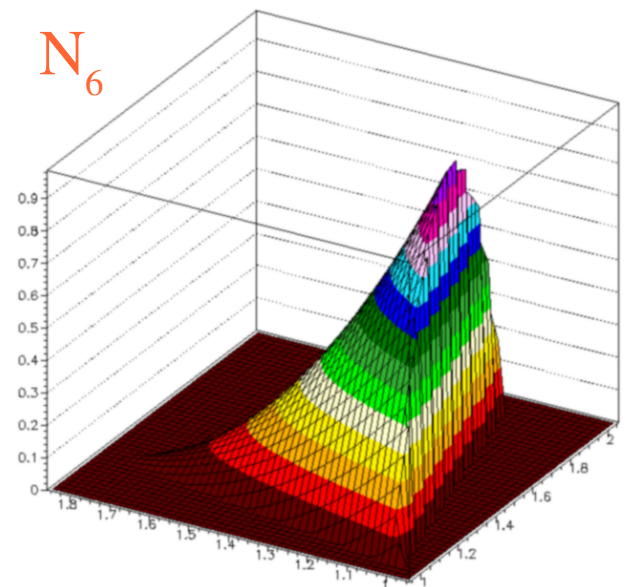 - all that can go wrong is respect of the boundary conditions.

Thin-wire approximation

- Compare:

  - left: a thin wire approximation of a Micromegas mesh,

  - right: neBEM calculation of the same (using polygon elements):
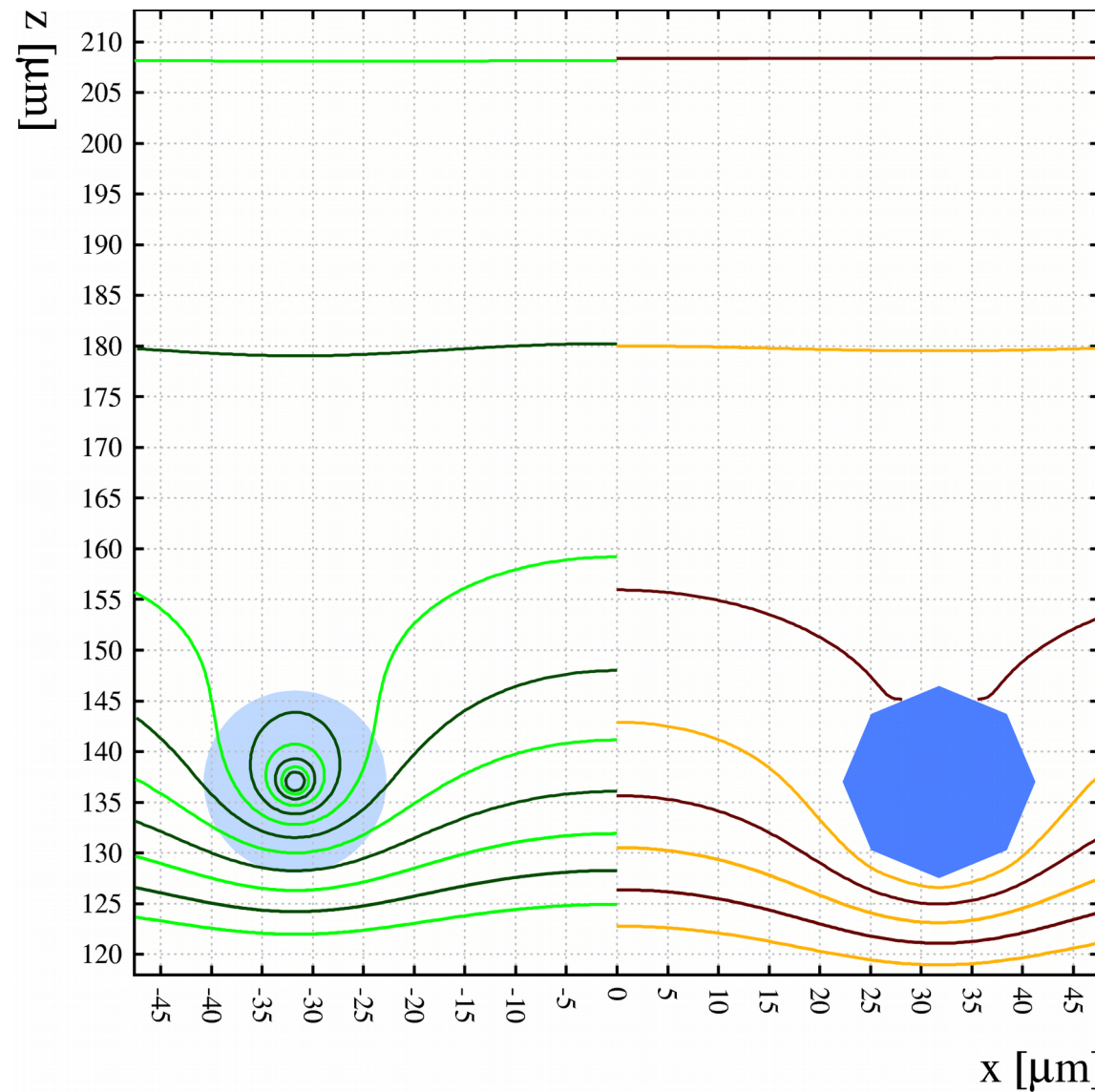
2nd Order triangle shape functions
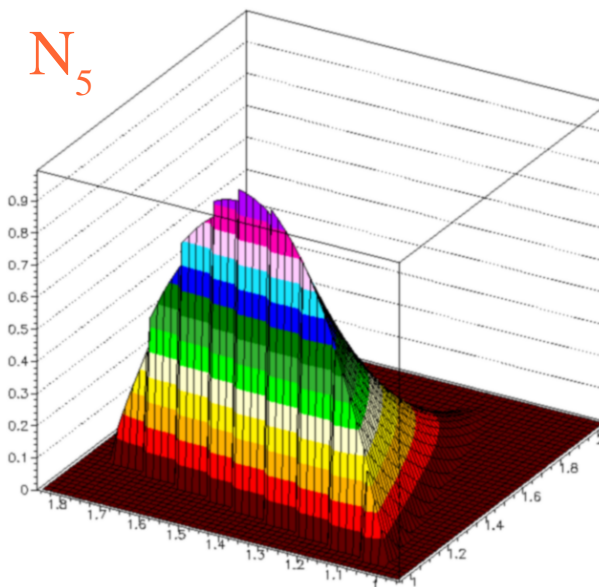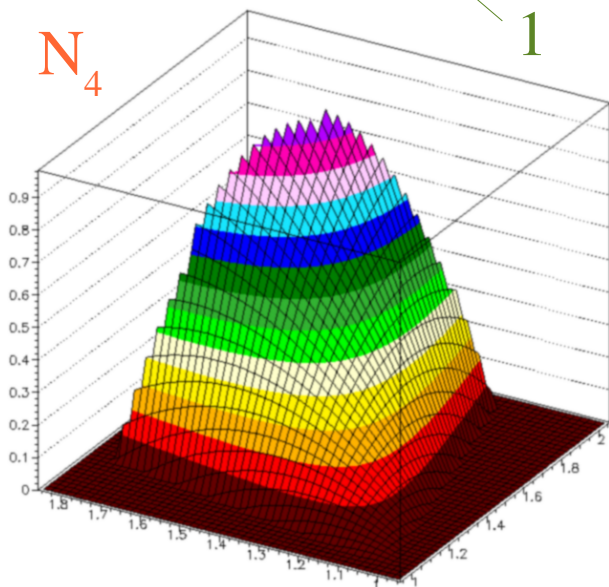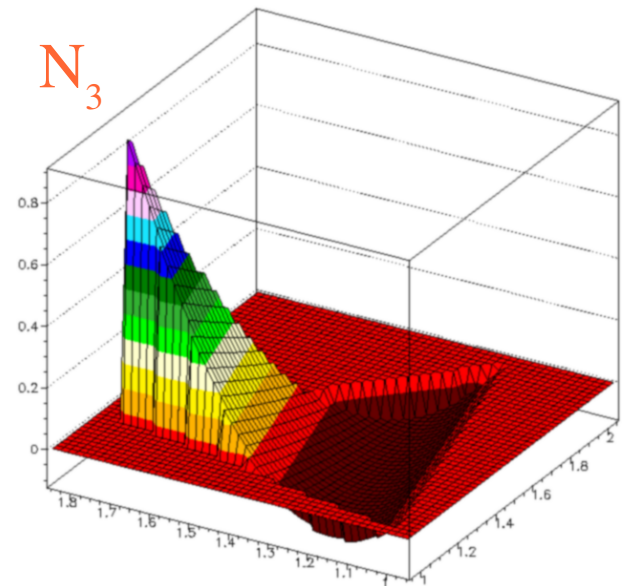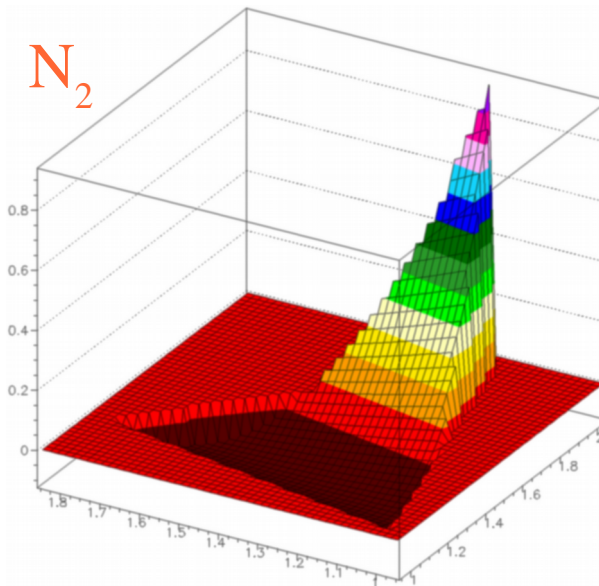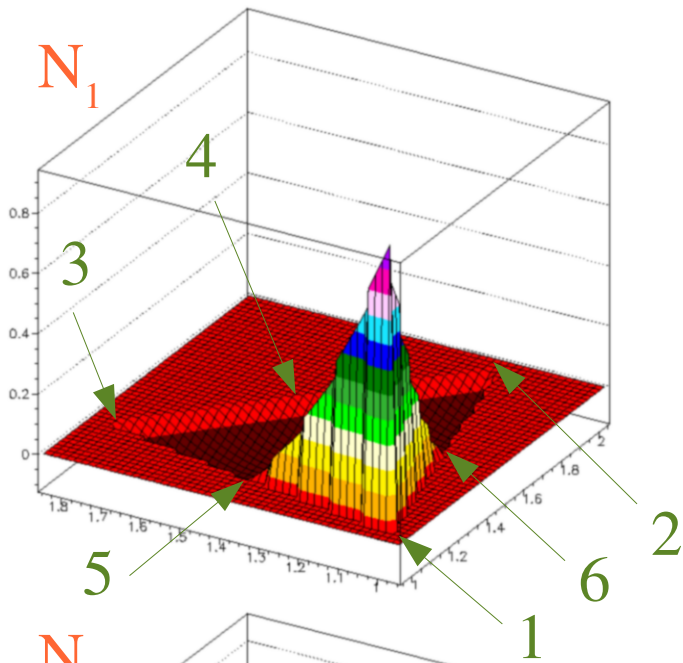
Are polynomial N_i suitable for V ?

▶ Polynomial shape functions imply a polynomial potential, here a 3.2 cm tube with a 30 μm wire at 3 kV inside:
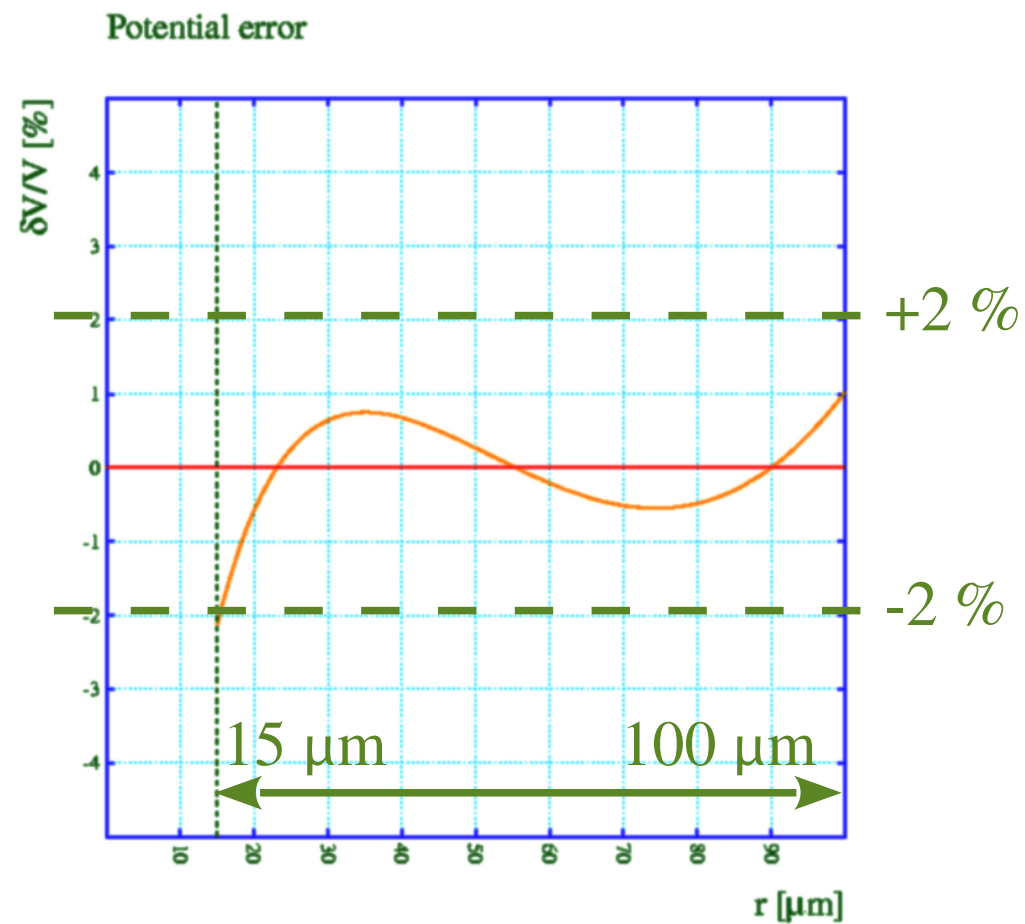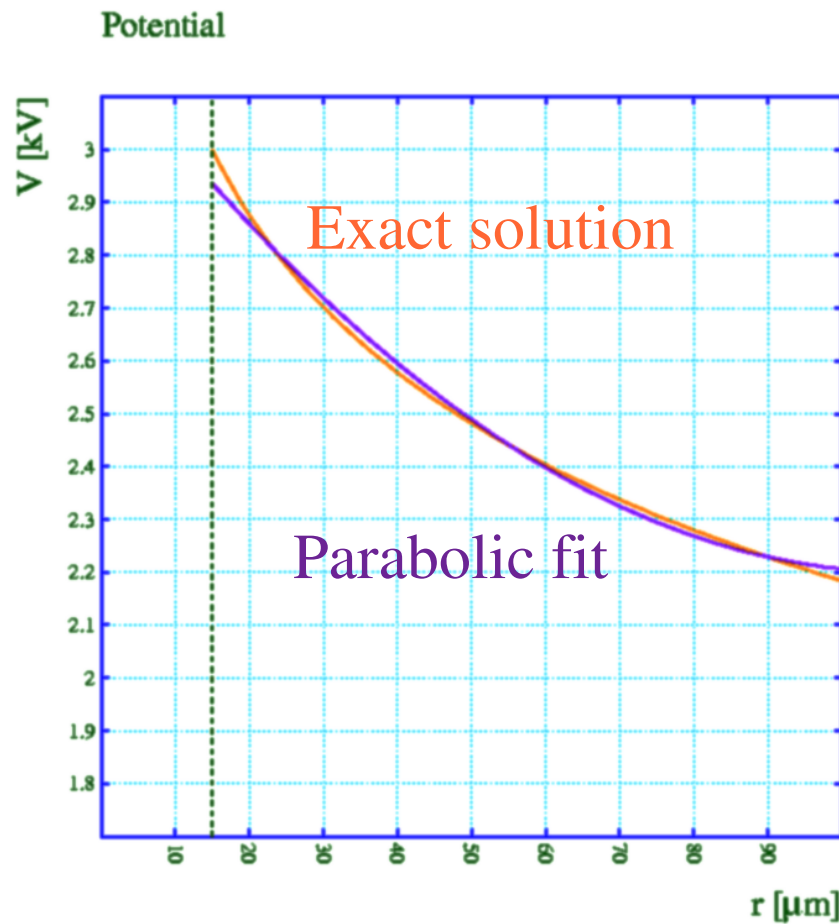
Are polynomial N_i suitable for E ?

▶ ... and a polynomial E field that is one order lower !
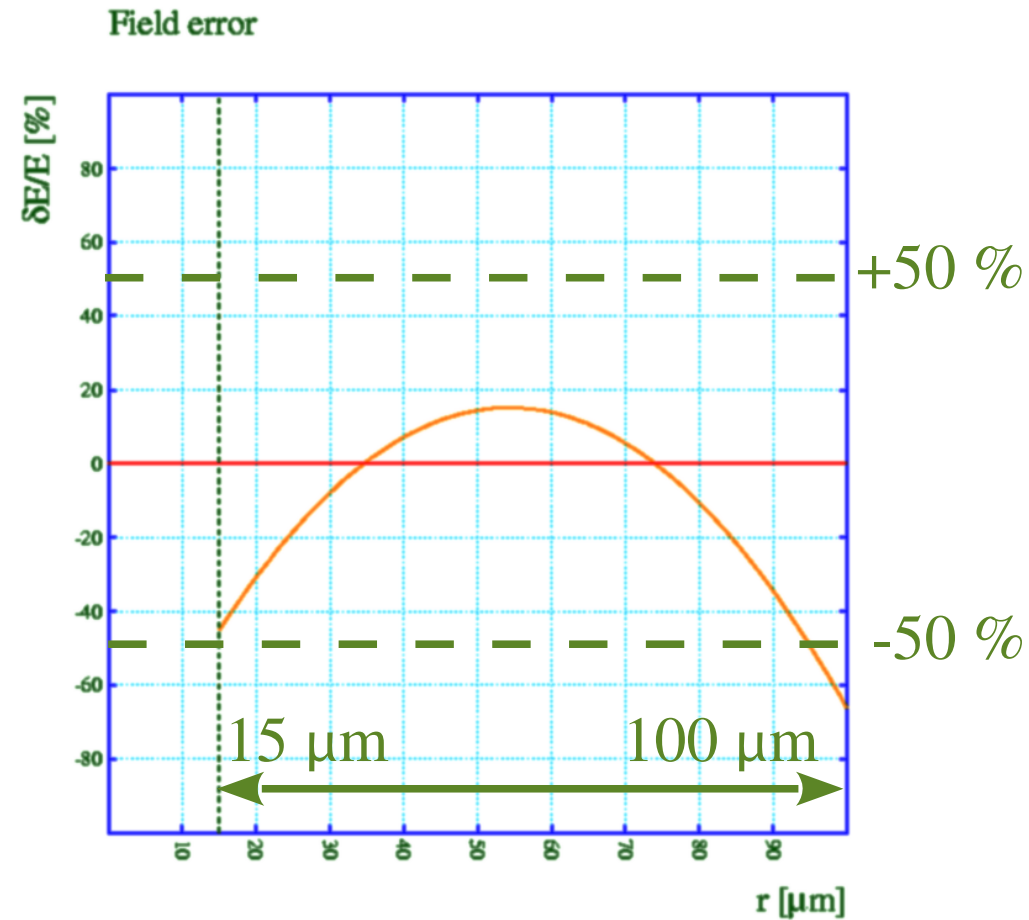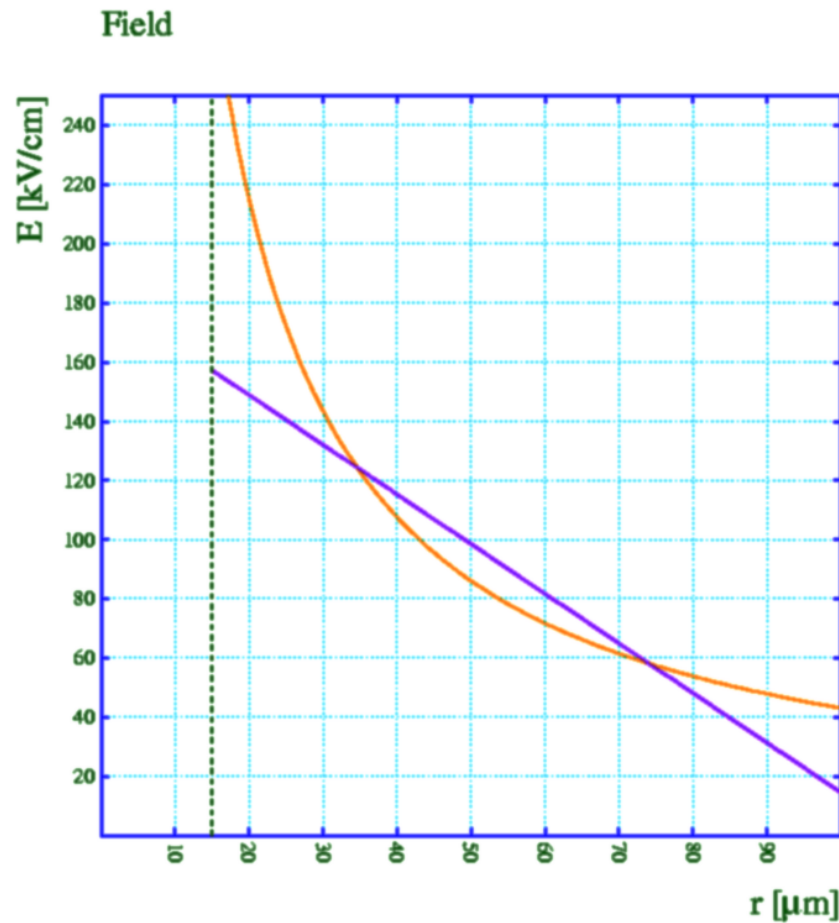
The price to pay for finite elements

▶ Finite element programs are flexible but they focus on the
   wrong thing: they solve V well, but we do not really need it:
   - ▶ quadratic shape functions do a fair job at approximating
        $V \approx \log(r)$ potentials;
   - ▶ potentials are continuous;
   - ▶ potentials and fields are not Maxwell compliant.

▶ E is what we use to transport charges, but:
   - ▶ gradients of quadratic shape functions are linear and not
        suitable to approximate $E \approx 1/r$, left alone $E \approx 1/r^2$ fields;
   - ▶ electric fields are discontinuous at element boundaries;
   - ▶ a local accuracy of ~50 % in high-field areas is not unusual.

Food for thought ...

▶ The Finite Element Method is a very useful tool which can make a good engineer better, but it can make a bad engineer dangerous. [Robert D. Cook, Professor of Mechanical Engineering University of Wisconsin, Madison]

Boundary element methods

▶ The elements are 2d surface panels located on the boundaries, not inside the problem domain. Charges are computed for the boundary elements.

▶ The field in the problem domain is calculated as the sum of Maxwell-compliant field functions, each extending over the entire problem domain. There are no discontinuities in the problem domain (only on the surface).

▶ But ... the method poses substantial numerical challenges: large non-sparse matrices and inherent singularities. The technique is time consuming.

$$\Phi = \frac{1}{2}\left(\,(z_M Y^2 - XG)(LP_1 + LM_1 - LP_2 - LM_2) + i|Y|(z_M X + G)(LP_1 - LM_1 - LP_2 + LM_2)\right.$$

$$- S_1 X \left(tanh^{-1}\left(\frac{R_1 + iI_1}{D_{11}|Z|}\right) + tanh^{-1}\left(\frac{R_1 - iI_1}{D_{11}|Z|}\right) - tanh^{-1}\left(\frac{R_1 + iI_2}{D_{21}|Z|}\right) - tanh^{-1}\left(\frac{R_1 - iI_2}{D_{21}|Z|}\right)\right)$$

$$+ \frac{2G}{\sqrt{1 + z_M{}^2}} \log\left(\frac{\sqrt{1 + z_M{}^2}D_{12} - E_1}{\sqrt{1 + z_M{}^2}D_{21} - E_2}\right) + 2Z \log\left(\frac{D_{21} - X + 1}{D_{11} - X}\right)\,\right) + C$$

where

$$D_{11} = \sqrt{(X - x_1)^2 + Y^2 + (Z - z_1)^2};\ D_{12} = \sqrt{(X - x_1)^2 + Y^2 + (Z - z_2)^2}$$

$$D_{21} = \sqrt{(X - x_2)^2 + Y^2 + (Z - z_1)^2};\ I_1 = (X - x_1)|Y|;\ I_2 = (X - x_2)|Y|$$

$$S_1 = sign(z_1 - Z);\ R_1 = Y^2 + (Z - z_1)^2$$

$$E_1 = (X + z_M{}^2 - z_M Z);\ E_2 = (X - 1 - z_M Z),$$

$$H_2 = Y^2 + GZ$$

$$LP_1 = \frac{1}{G - iz_M|Y|} log\left(\frac{(H_1 + GD_{12}) + i|Y|(E_1 - iz_M D_{12})}{-X + i|Y|}\right)$$

$$LM_1 = \frac{1}{G + iz_M|Y|} log\left(\frac{(H_1 + GD_{12}) - i|Y|(E_1 - iz_M D_{12})}{-X - i|Y|}\right)$$

$$LP_2 = \frac{1}{G - iz_M|Y|} log\left(\frac{(H_2 + GD_{21}) + i|Y|(E_2 - iz_M D_{21})}{1 - X + i|Y|}\right)$$

$$LM_2 = \frac{1}{G + iz_M|Y|} log\left(\frac{(H_2 + GD_{21}) - i|Y|(E_2 - iz_M D_{21})}{1 - X - i|Y|}\right)$$

and C denotes a constant of integration.

neBEM – the price to pay

► For computing the field at any point, neBEM sums the fields due to each element on that point.

► Evaluating the Green's functions, especially the one for triangular elements, is costly.

► For a modest doubly-periodic 1000-solid model there would be ~10^8 function evaluations. For an avalanche study we would love to have 1000. We then need to compute the field at ~10^7 points.

BEM vs FEM

▶ neBEM
  ▶ not widely used, few commercial programs;
  ▶ boundary conditions respected at collocation points;
  ▶ Maxwell compliant electric fields & potentials;
  ▶ plausible Green's functions;
  ▶ fields without discontinuities;
  ▶ fully populated influence matrix, limiting problem size

▶ FEM
  ▶ well-tested, efficient programs widely available commercially;
  ▶ boundary conditions respected on the nodes;
  ▶ polynomial potentials do not solve the Maxwell equations;
  ▶ locally linear E-fields;
  ▶ E-fields discontinuous on element boundaries;
  ▶ sparse matrix, virtually no limitations on the problem size

Electron-gas cross sections + transport

- Cross sections are obtained from
  - fits of transport data at low electron energy and
  - from electron beam measurement at higher energy.
  - Some cross sections are purely theorethical.

  - Illustrated with anisotropic scattering cross sections.

- Velocity data is generally reproduced to 1 % or better, and diffusion to better than 10 %, but the multiplication can be wrong by orders of magnitude.

  - Illustrated with the Penning effect.

LXcat people

- Art Phelps,
- Leanne Pitchford – Toulouse,
- Klaus Bartschat – Iowa,
- Oleg Zatsarinny – Iowa,
- Michael Allan – Fribourg,
- Steve Biagi
- ...

Art Phelps

Leanne Pitchford

Michael Allan

Klaus Bartschat

Magboltz: microscopic e⁻ transport

▶ A large number of cross sections for 60 molecules...

  ▶ Numerous organic gases, additives, *e.g.* CO_2:

   ▸ elastic scattering (isotropic and anisotropic),
   ▸ 44 inelastic cross sections (5 vibrations and 30 rotations + super-elastic and 9 polyads),
   ▸ attachment,
   ▸ 6 excited states,
   ▸ 11 ionisations (CO_2^+, C_K, O_K, 2 excitations, 6 dissociations),
   ▸ 64 dissociations (charged and neutral),
   ▸ 2 bremsstrahlung (C and O).

  ▶ noble gases (He, Ne, Ar, Kr, Xe), *e.g.* Ar:

   ▸ elastic scattering (isotropic and anisotropic),
   ▸ 44 excited states,
   ▸ 7 ionisations (Ar^+, Ar^{++}, Ar^{+++}, K, L1, L2, L3),
   ▸ attachment,
   ▸ bremsstrahlung.

And counting ...

Simple cross sections

▶ Hard-sphere scattering:

$$\frac{d\sigma}{d\Omega} = \frac{r^2}{4}$$

▶ Coulomb scattering:

$$\frac{d\sigma}{d\Omega} = \frac{1}{\sin^4(\theta/2)}$$

▶ Screened Coulomb scattering, 1st Born approximation:

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi} \frac{1+8\epsilon/\epsilon_0}{(1+4\epsilon/\epsilon_0-4\epsilon/\epsilon_0\cos\theta)^2}, \qquad \epsilon_0 = 27.21\,\text{eV}$$
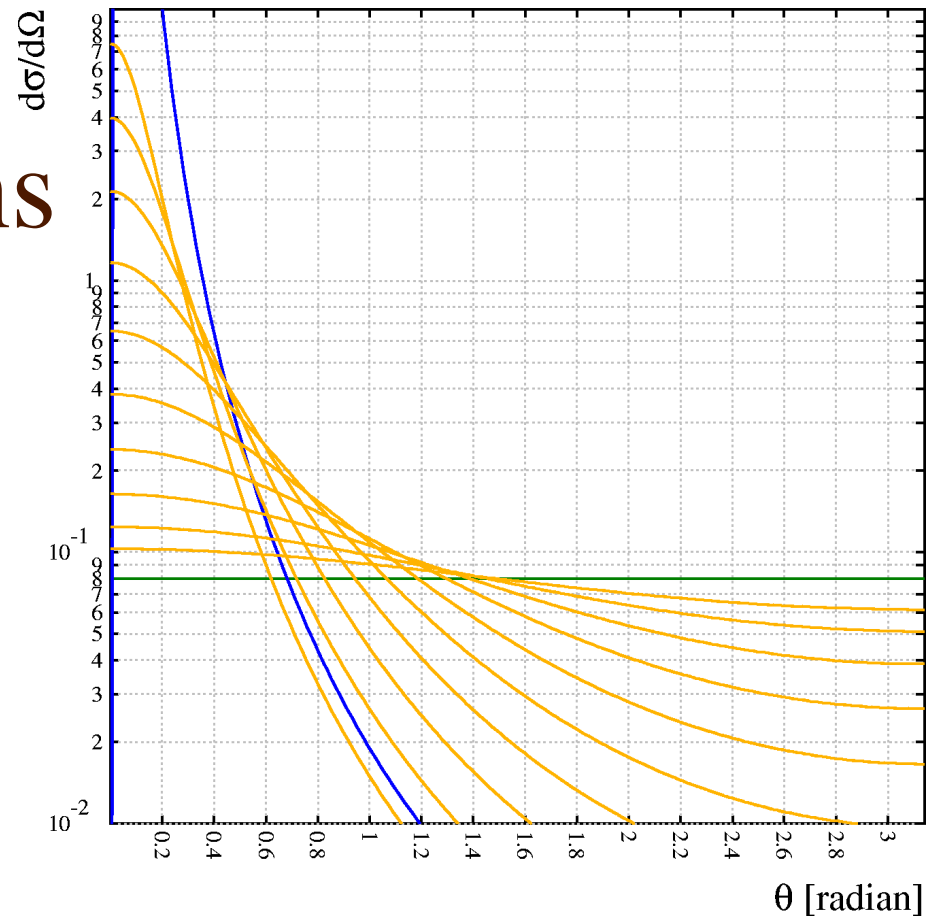
Krypton data

▶ From a joint study with high-precision data and a theoretical model.

[O. Zatsarinny et al. (2011) 10.1103/PhysRevA.83.032713]
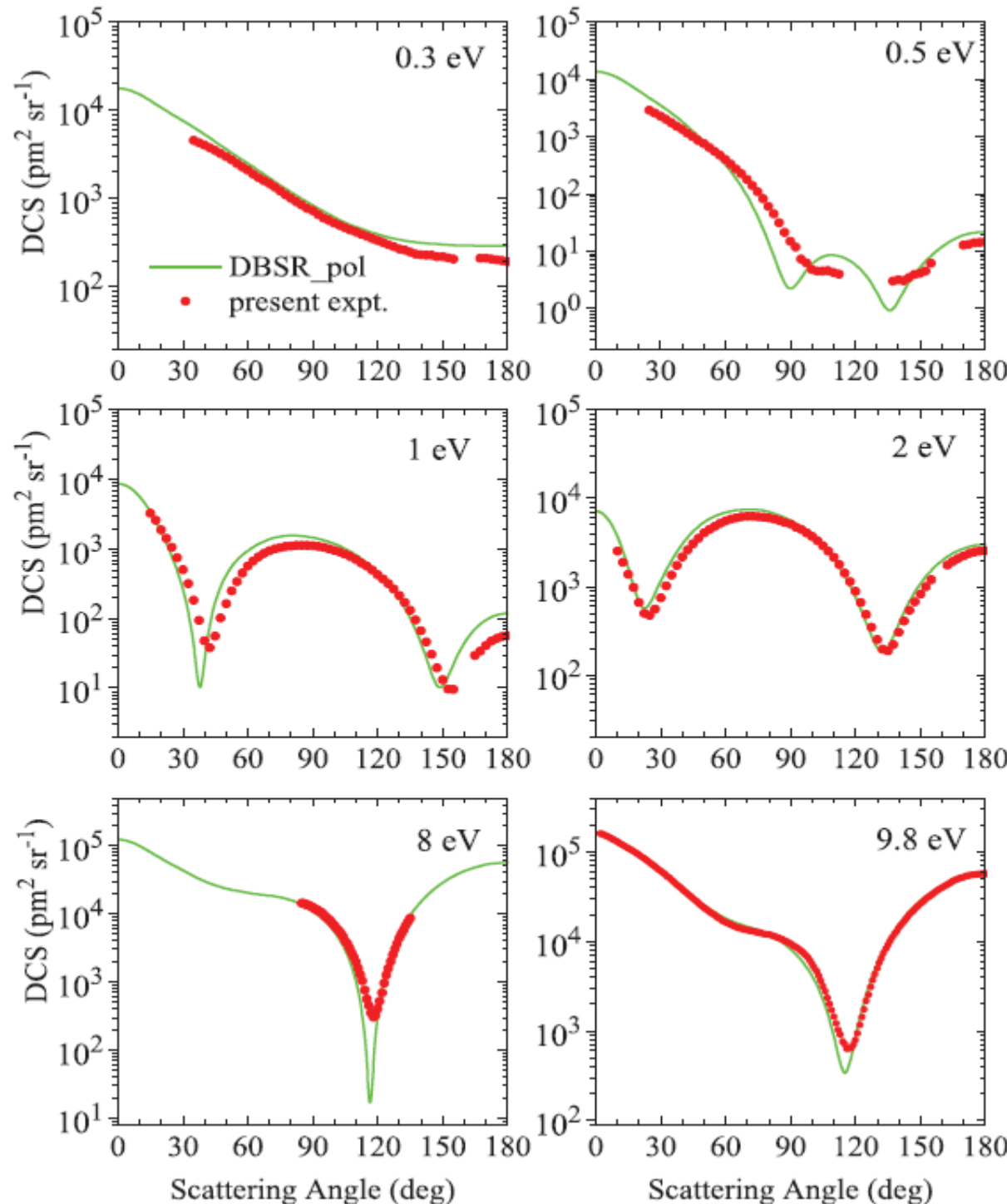
Reason for structure

▶ Elastic Scattering:
"Away from Feshbach resonances, the most important effect for elastic scattering is the polarization of the target by the projectile."

▶ "[...] DBSRpol model only included the $4s^2\,4p^6$ ground state with total electronic angular momentum $J = 0$ and a single pseudostate with $J = 1$ [...]"

[O. Zatsarinny, K. Bartschat and M. Allan 10.1088/1742-6596/388/1/012008]

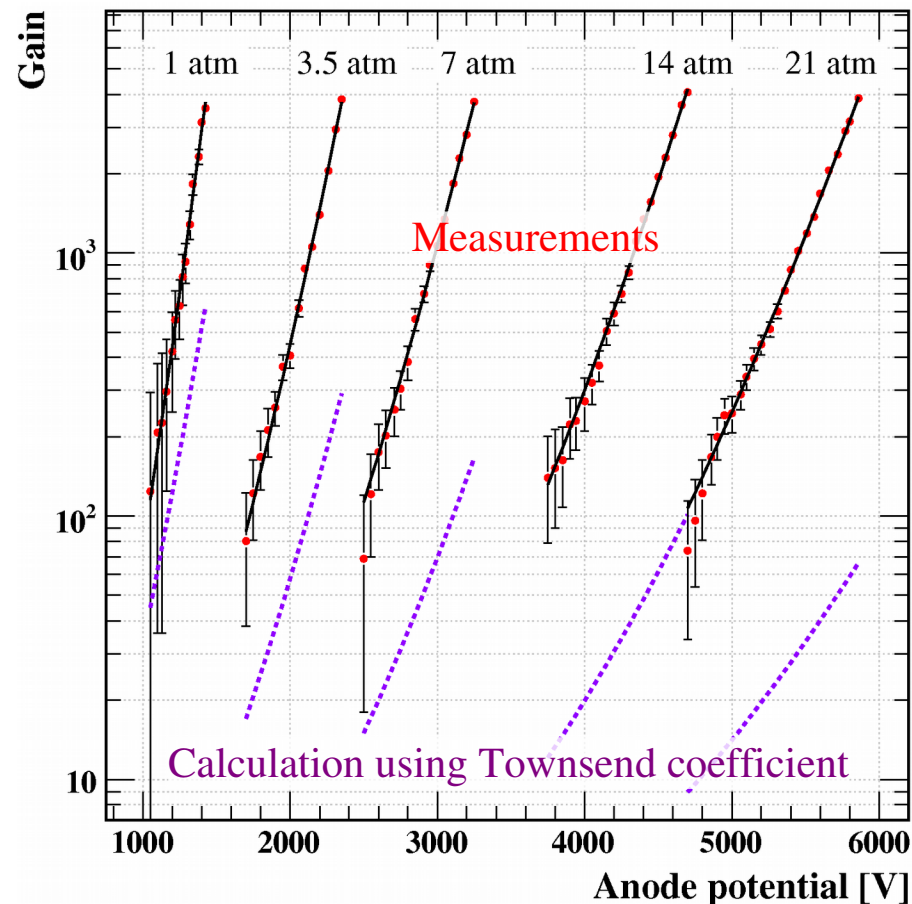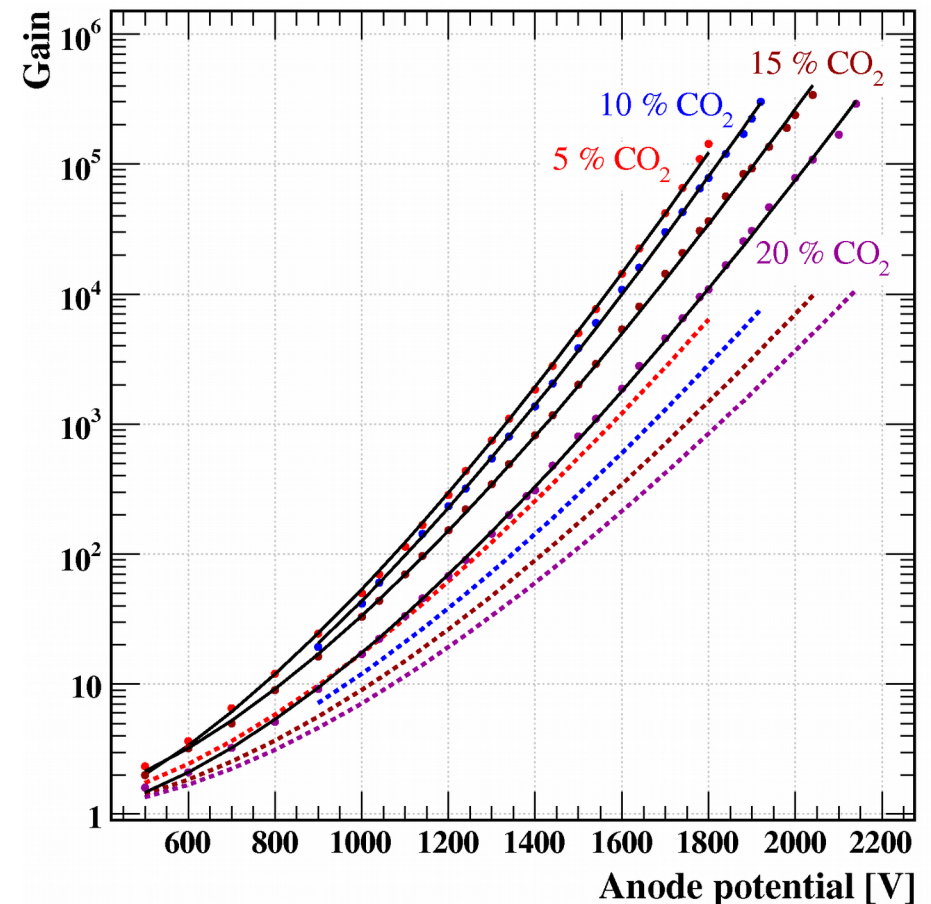# Electrons: Penning parameter

- The Magboltz Townsend coefficients do not reproduce the gas gain.

- Probably due to charge transfer from excited noble atoms to quencher gas molecules, and the subsequent ionisation of the quencher.
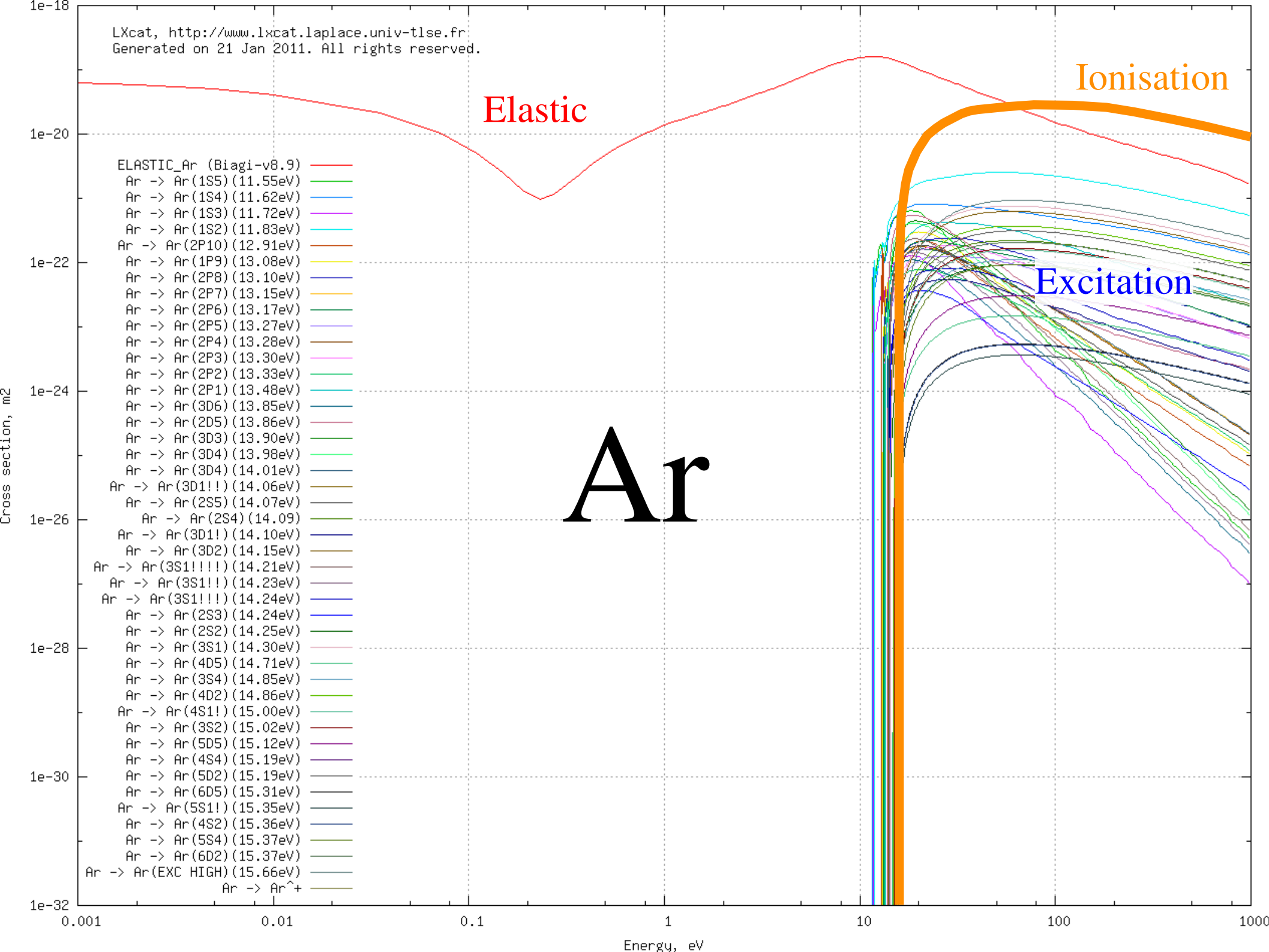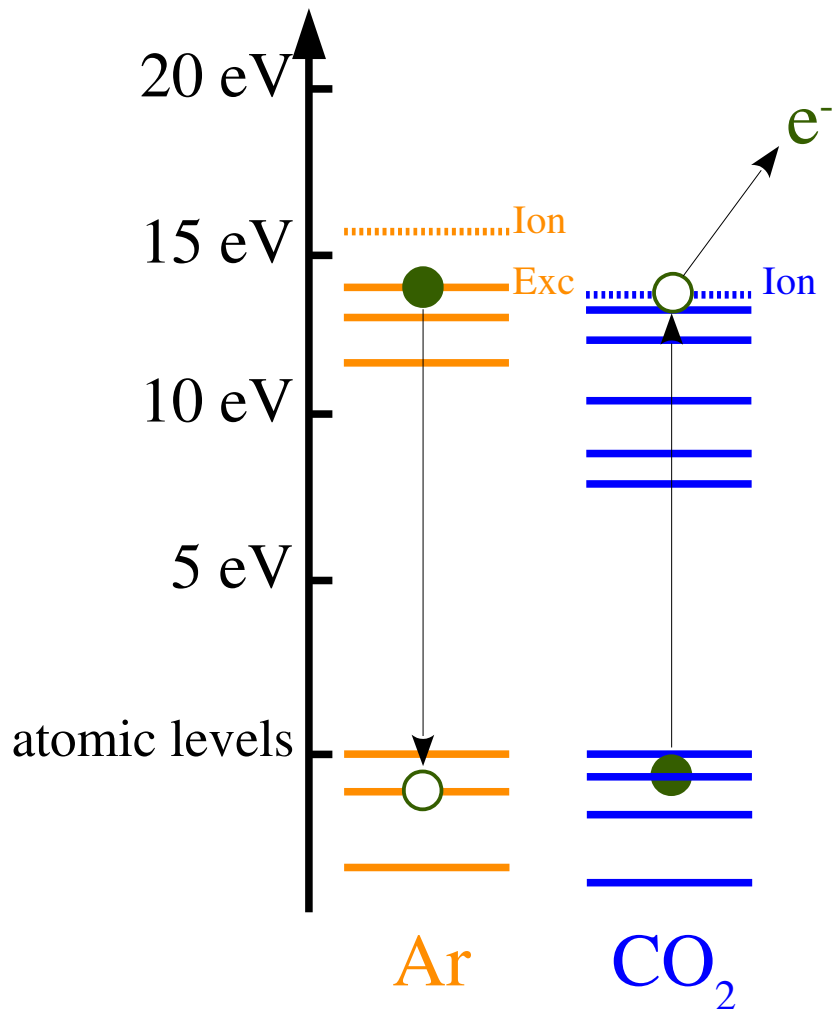
Magnitude of Penning effect

▶ Ar - CH$_4$

▶ Ar - CO$_2$

Elastic

Ionisation

Excitation

Ar

Cross section, m2

Energy, eV

ELASTIC_Ar (Biagi-v8.9)
Ar -> Ar(1S5)(11.55eV)
Ar -> Ar(1S4)(11.62eV)
Ar -> Ar(1S3)(11.72eV)
Ar -> Ar(1S2)(11.83eV)
Ar -> Ar(2P10)(12.91eV)
Ar -> Ar(1P9)(13.08eV)
Ar -> Ar(2P8)(13.10eV)
Ar -> Ar(2P7)(13.15eV)
Ar -> Ar(2P6)(13.17eV)
Ar -> Ar(2P5)(13.27eV)
Ar -> Ar(2P4)(13.28eV)
Ar -> Ar(2P3)(13.30eV)
Ar -> Ar(2P2)(13.33eV)
Ar -> Ar(2P1)(13.48eV)
Ar -> Ar(3D6)(13.85eV)
Ar -> Ar(2D5)(13.86eV)
Ar -> Ar(3D3)(13.90eV)
Ar -> Ar(3D4)(13.98eV)
Ar -> Ar(3D4)(14.01eV)
Ar -> Ar(3D1!!)(14.06eV)
Ar -> Ar(2S5)(14.07eV)
Ar -> Ar(2S4)(14.09)
Ar -> Ar(3D1!)(14.10eV)
Ar -> Ar(3D2)(14.15eV)
Ar -> Ar(3S1!!!!)(14.21eV)
Ar -> Ar(3S1!!)(14.23eV)
Ar -> Ar(3S1!!!)(14.24eV)
Ar -> Ar(2S3)(14.24eV)
Ar -> Ar(2S2)(14.25eV)
Ar -> Ar(3S1)(14.30eV)
Ar -> Ar(4D5)(14.71eV)
Ar -> Ar(3S4)(14.85eV)
Ar -> Ar(4D2)(14.86eV)
Ar -> Ar(4S1!)(15.00eV)
Ar -> Ar(3S2)(15.02eV)
Ar -> Ar(5D5)(15.12eV)
Ar -> Ar(4S4)(15.19eV)
Ar -> Ar(5D2)(15.19eV)
Ar -> Ar(6D5)(15.31eV)
Ar -> Ar(5S1!)(15.35eV)
Ar -> Ar(4S2)(15.36eV)
Ar -> Ar(5S4)(15.37eV)
Ar -> Ar(6D2)(15.37eV)
Ar -> Ar(EXC HIGH)(15.66eV)
Ar -> Ar^+

Direct vs Exchange ionisation
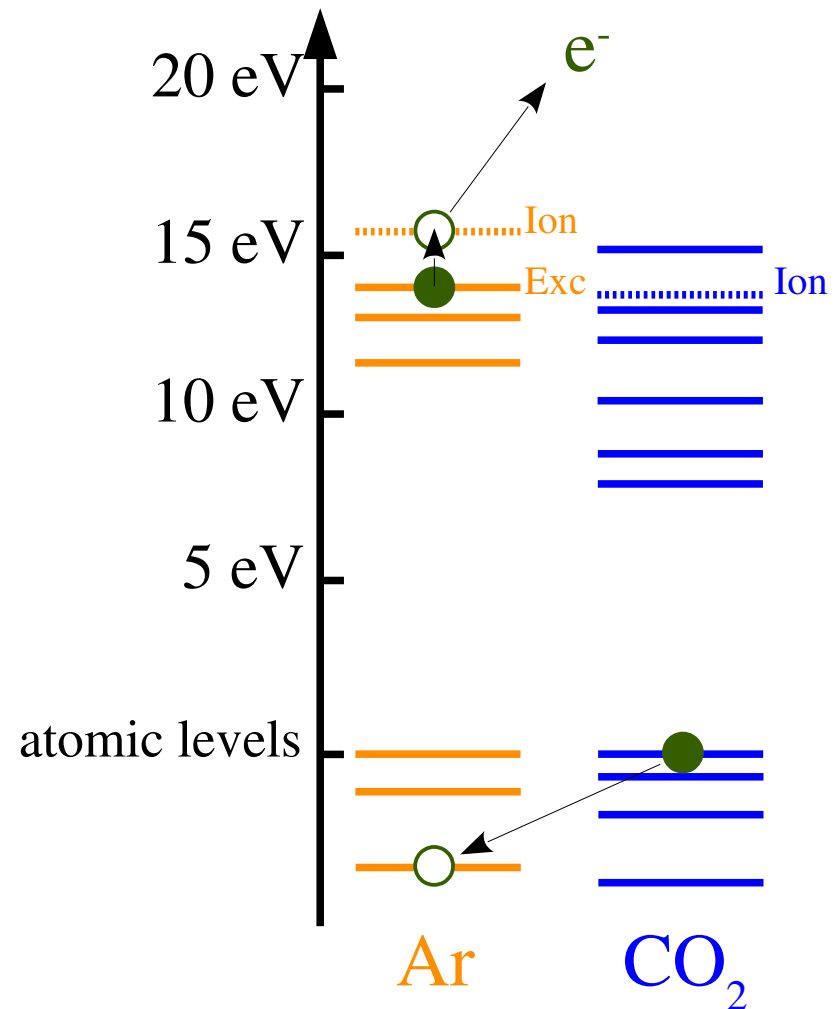
Simple Penning model

▶ Let A be a noble gas and B a quencher, A^* is excited with excitation energy > ionisation energy of B^+.

▶ In a time step, A^* produces $n\,\mathrm{d}t$ electrons:
  ▶ A^* collides with B and transfers its excess energy, or
  ▶ A^* decays and radiatively ionises B

$$n \;=\; pc\frac{f_{B^+}}{\tau_{A^*B}} + \frac{f_\mathrm{rad}}{\tau_{A^*}}$$

▶ A^* can try again if A^* neither collides + ionises, nor decays. The probability is:

$$1 - \frac{\mathrm{d}t}{\tau_\mathrm{P}}, \qquad \frac{1}{\tau_\mathrm{P}} \;=\; pc\frac{f_{B^+}}{\tau_{A^*B}} + \frac{1}{\tau_{A^*}}$$

$p \;=\;$ pressure
$c \;=\;$ quencher fraction
$f_{B^+} \;=\;$ transfer probability in collision
$f_\mathrm{rad} \;=\;$ radiative lifetime
$\tau_{A^*B} \;=\;$ collision time

[Ö Şahin et al., 2010 JINST 5 P05002]

Simple Penning model (cont'd)

▶ Summing to get the number of electrons from A^*:

$$r(p,c) = n\,\mathrm{d}t + n\,\mathrm{d}t\left(1 - \frac{\mathrm{d}t}{\tau_P}\right) + n\,\mathrm{d}t\left(1 - \frac{\mathrm{d}t}{\tau_P}\right)^2 + \dots$$

$$= n\,\tau_P$$

Nothing happened
in the first step

▶ $r(p,c)$ is the fraction of the excitation frequency to be added to the ionisation frequency in order to correct the Townsend coefficient for the Penning effect.
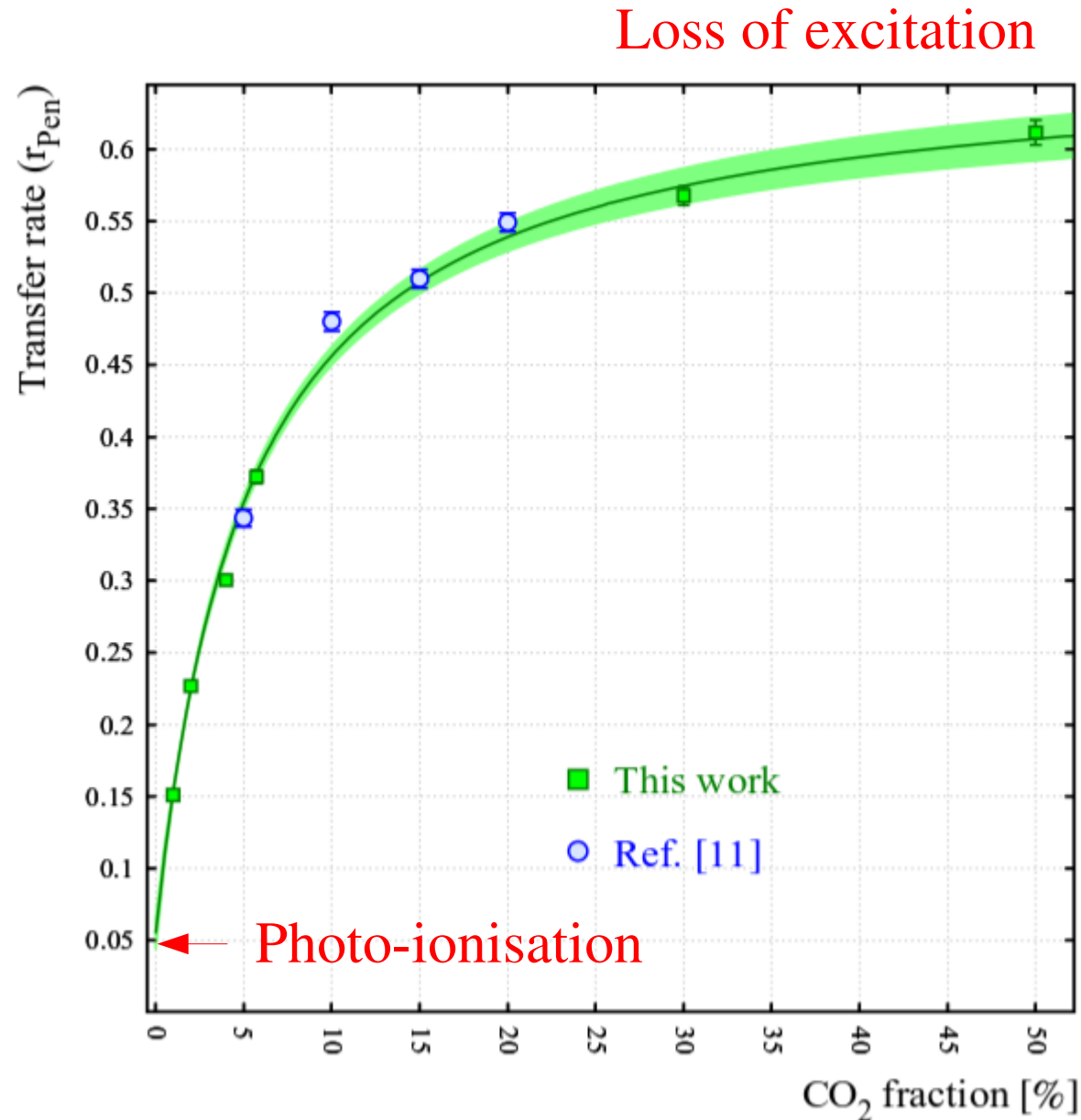
▶ There are only two a priori unknown parameters:
  ▶ f_{rad}: the radiative ionisation probability
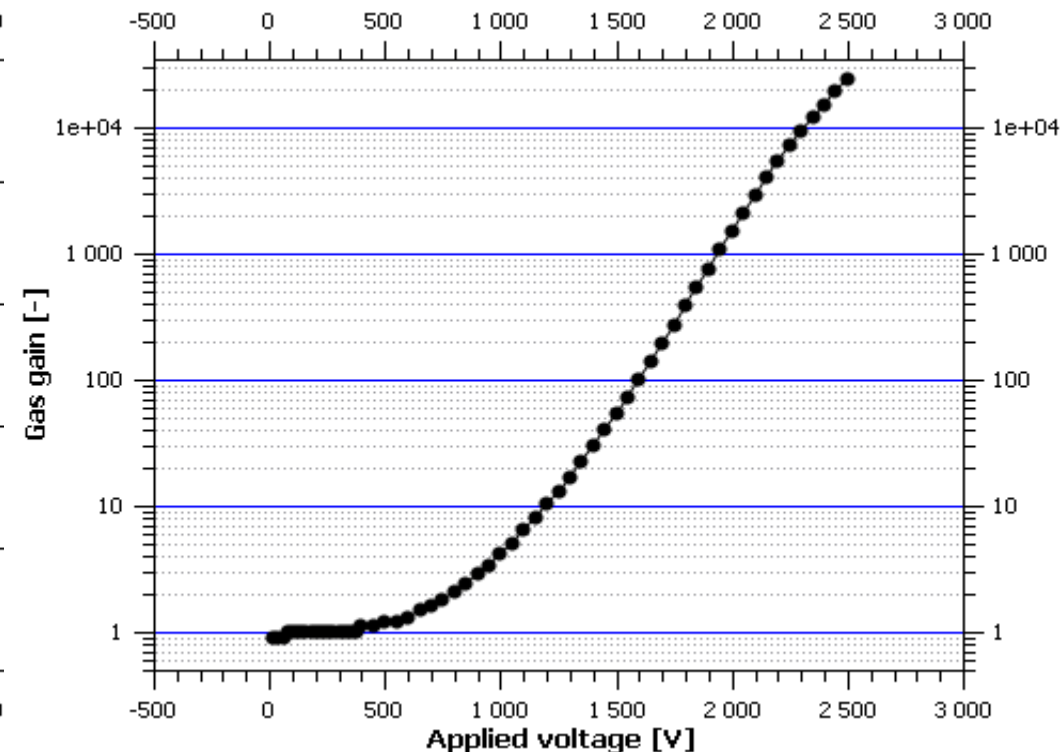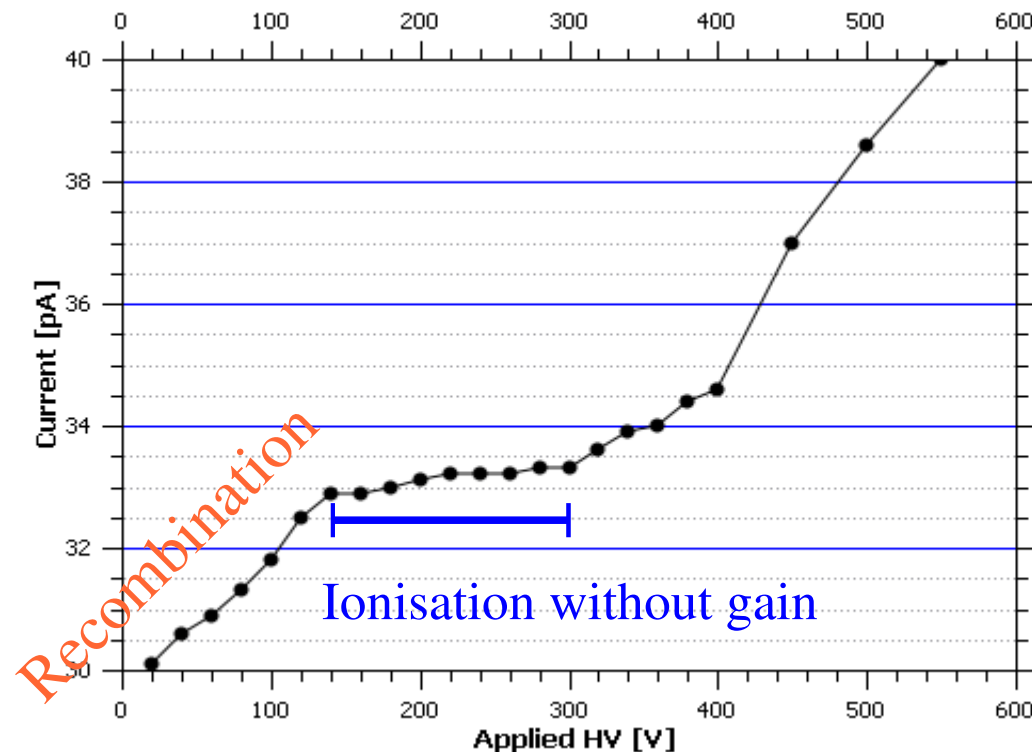 ▶ f_B+: the collisional transfer probability

Ar-CO$_2$ transfer rates

► Penning parameter fits with data from Tadeusz Kowalski et al. 1992 and 2013.

► At $p = 1070$ hPa.

[10.1016/0168-9002(92)90305-N, 10.1016/j.nima.2014.09.061]

Loss of excitation

Photo-ionisation

Kraków: 5 orders of magnitude !

▶ Current reference is taken at the ionisation level.

▶ Main source of error: ~5 %.

Ions chemistry: rate constants

▶ I thought that the signal ions in Ar-CO_2 are Ar^+ ions.

▶ Ar^+ ions have a mobility in Ar of 1.5 cm^2/V.s, in agreement with the measurements.

$$\text{But} \quad ... \quad IP_{Ar^+} > IP_{CO_2^+} \ !$$

▶ Ions transfer charge, combine, break up in nsec.

▶ Rate constants are found in the literature, typically 10-30 %.

▶ Difficulties:

   ▶ not all reactions relevant for us have been measured;

   ▶ our measurements suffer from the lack of a mass spectrometer.
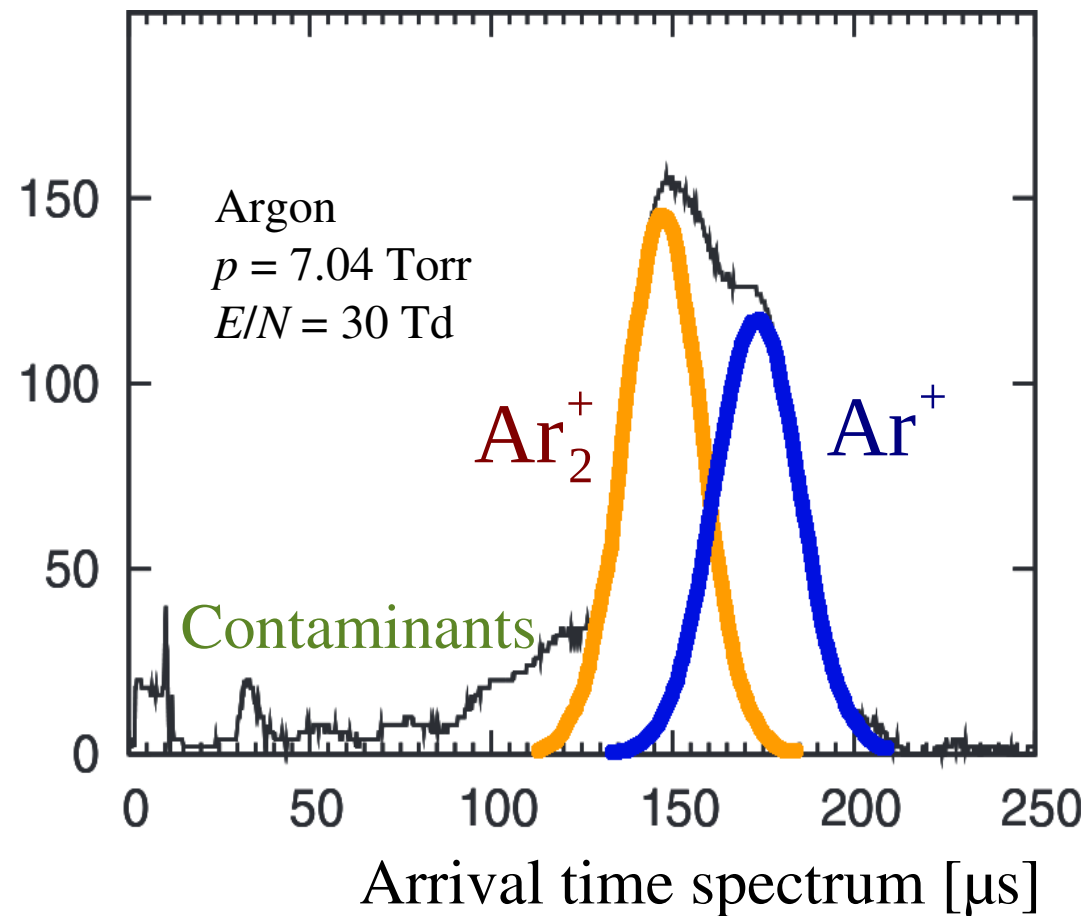
Ions drifting in pure Ar

▶ In pure argon, dimers are formed:

   ▶ $Ar^+(^2P^o_{3/2}) + 2Ar \rightarrow Ar^+ \cdot Ar + Ar$
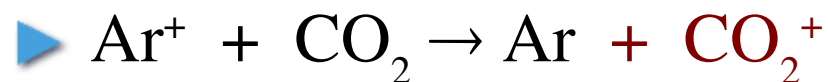   ($k = 2.3 \pm 0.1 \; 10^{-31}$ cm^6/s, 7 ns)
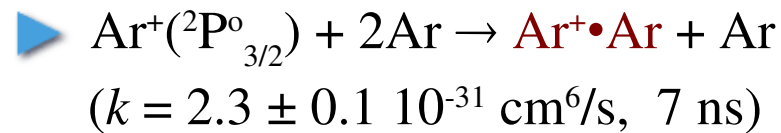
   ▶ Note: dimers move *faster* than ions due to $Ar \leftrightarrow Ar^+$ resonant charge exchange.
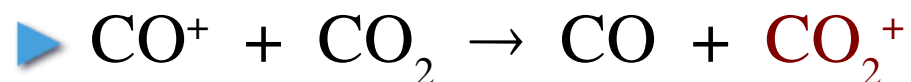
[PNB Neves et al. 10.1063/1.3497651]

Argon
$p = 7.04$ Torr
$E/N = 30$ Td

Ar_2^+ Ar^+

Contaminants

Arrival time spectrum [µs]

Clustering reactions involving CO_2

- Ar^+: charge exchange, $\tau \approx 0.85$ ns
  - $Ar^+ + CO_2 \rightarrow Ar + CO_2^+$

- Ne^+: charge transfer in 2-steps, $\tau \approx 8$ ns
  - $Ne^+ + CO_2 \rightarrow Ne + CO^+ + O$
  - $CO^+ + CO_2 \rightarrow CO + CO_2^+$
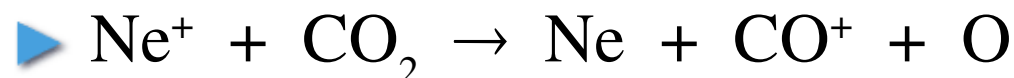
- CO_2: 3-body association, 7-20 ps or 0.7-2.0 ns
  - $CO_2^+ + 2CO_2 \rightarrow CO_2^+ \bullet CO_2 + CO_2$
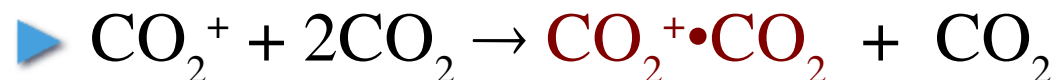
- [For 10 % CO_2, atmospheric pressure, room temperature]

Situating cluster ions

▶ Chemically bound molecules: 0.75-11.1 eV
  ▶ covalent or ionic bond

▶ Cluster ions: 0.09-1.7 eV
  ▶ bound by charge-induced dipole forces;
  ▶ constituents retain their identity.

▶ van der Waals molecules: 0.0009-0.1 eV
  ▶ bound by van der Waals forces;
  ▶ observed at low temperatures.

[B.M. Smirnov, "Cluster Ions and Van Der Waals Molecules," CRC press]

Ions drifting in Ar-CO$_2$ and Ne-CO$_2$

▶ Neither CO$_2^+$, Ar$^+$ nor Ne$^+$ but CO$_2^+\bullet$(CO$_2$)$_n$

Ar-CH$_4$

Short lived
Long lived

No further
reactions
reported

e$^-$ impact

ion-CH$_4$ and ion-Ar interactions
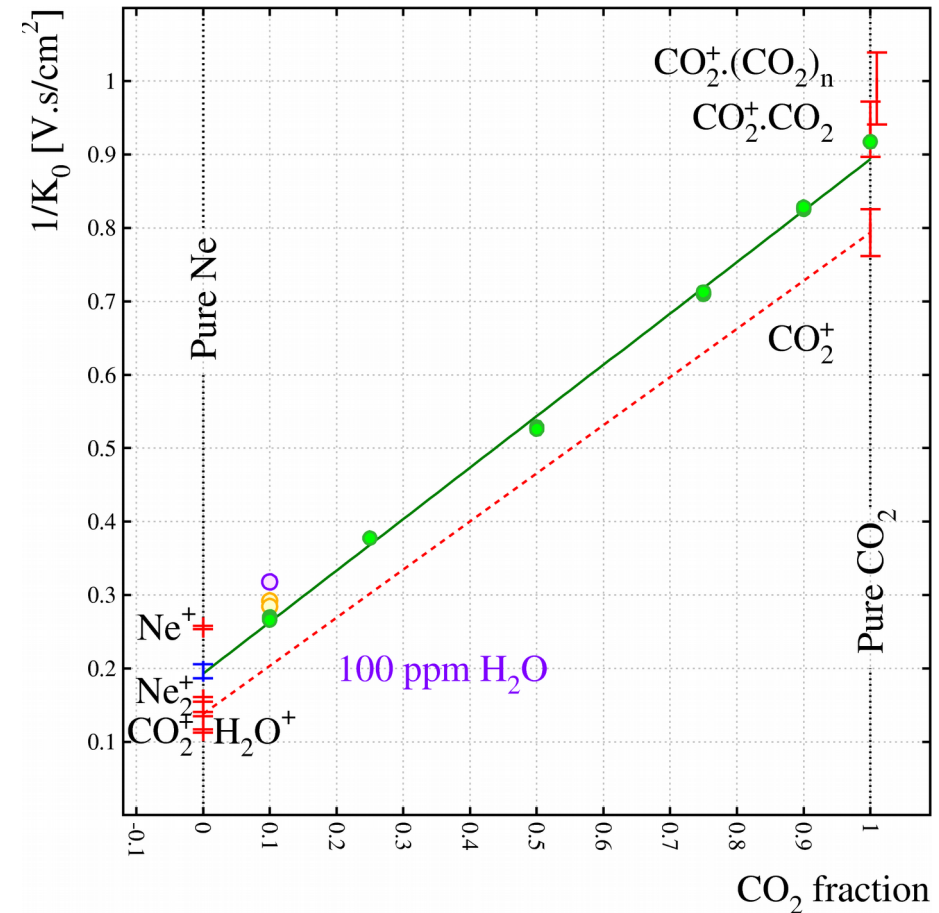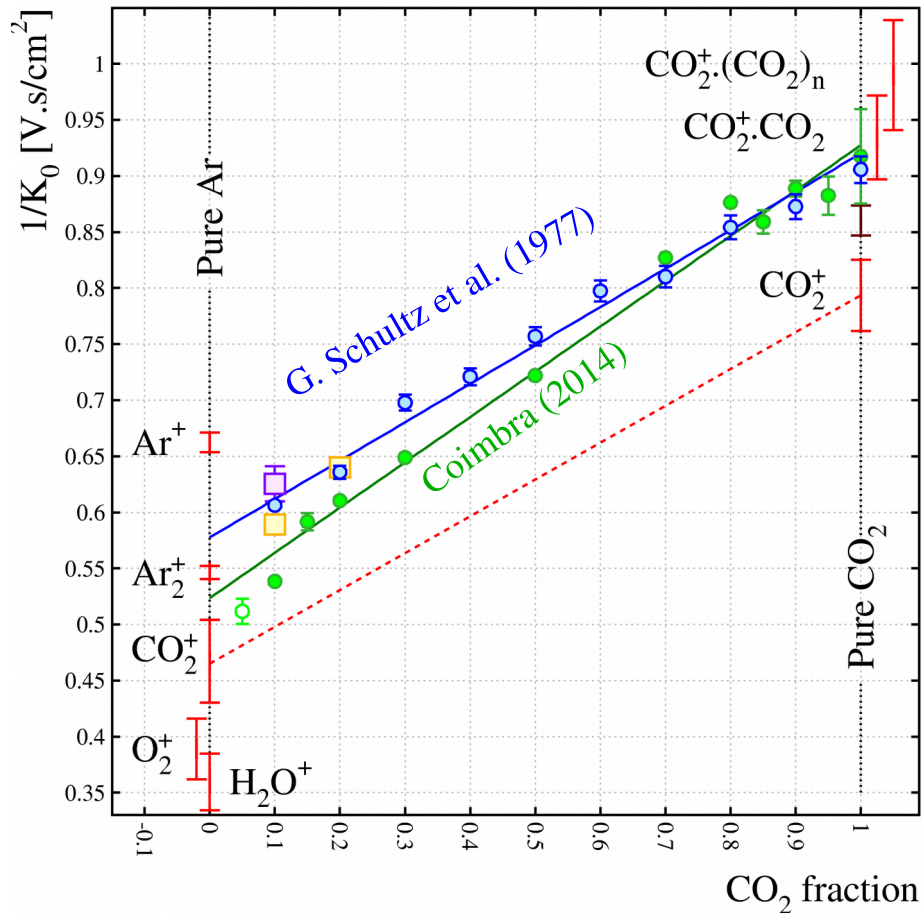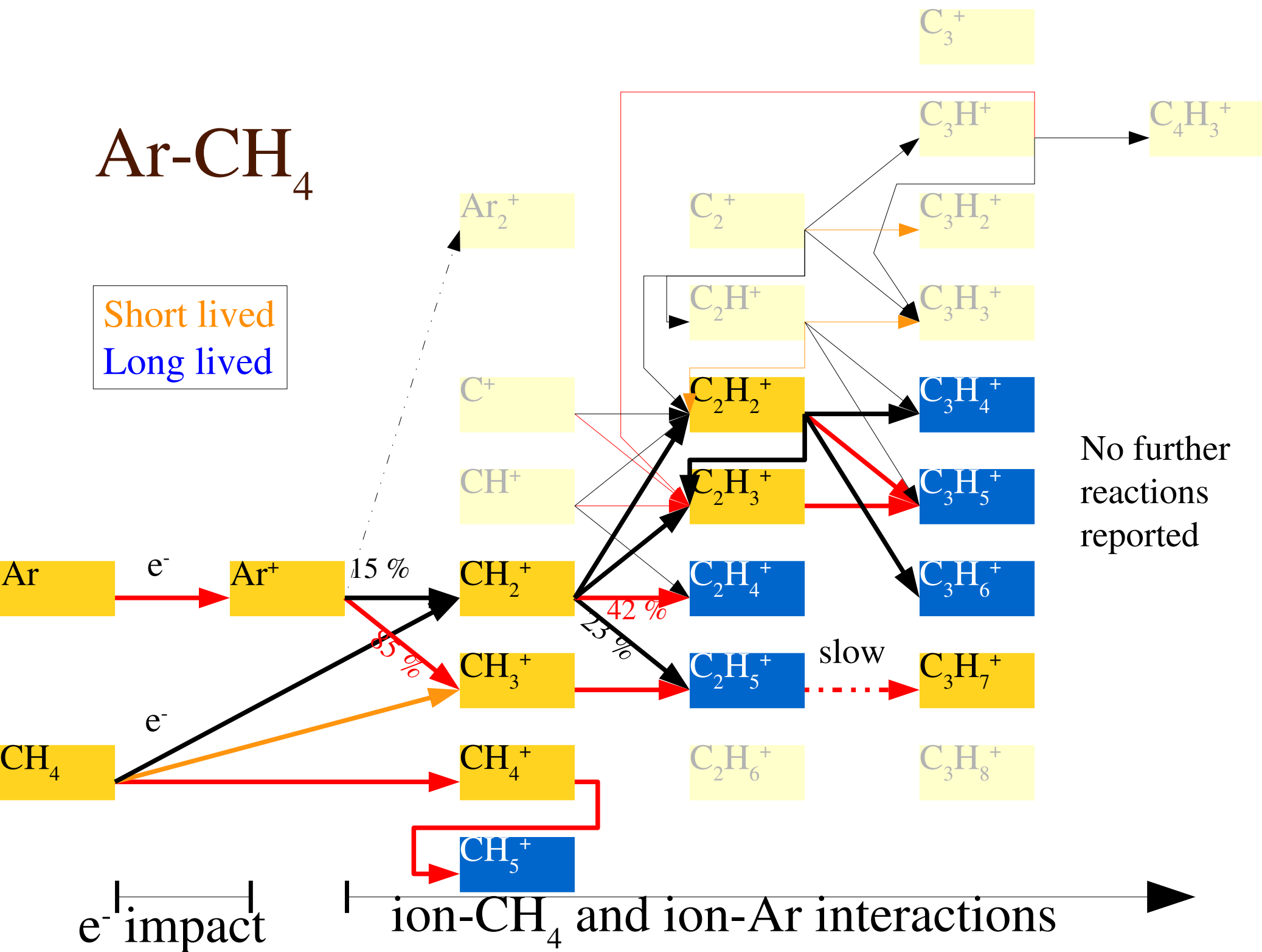
Atlas TRT signal

- **Data**:
  - Xe-CF_4-CO_2 70/20/10
  - V_w=1530 V
  - r_w = 15 μm, r_t = 2 mm
- **Fit**:
  - i_0 manually adjusted
  - t_0 = 24 ns, equivalent to
  - μ = 0.15 cm²/V.s

Electron signal

Ion tail
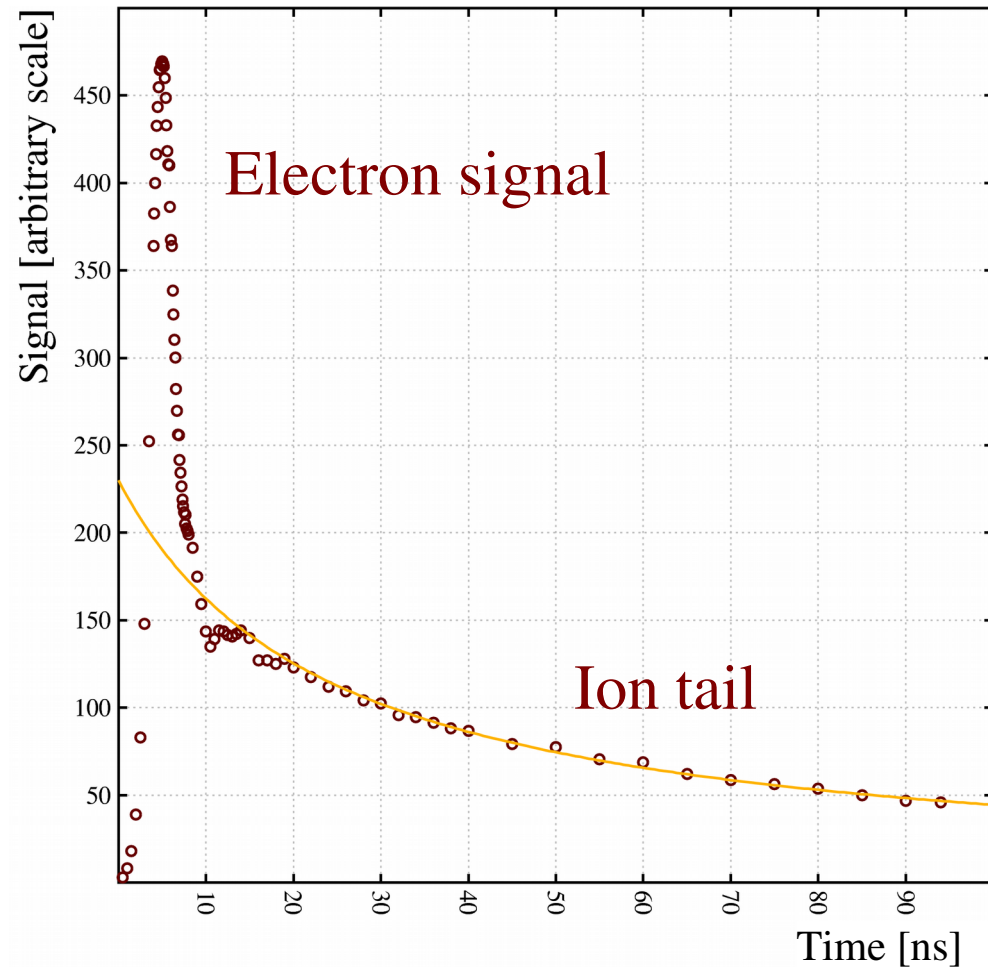
Mobility of ions in Xe

▶ $E/N = 10$ Td, extrapolated from higher E/N where needed (Xe^+).

▶ Polarisation limit assuming $\alpha_{Xe} = 4.01$ D.

▶ Xe_2^+ and Xe_3^+ are below the polarisation limit.

[From the H.W. Ellis et al. compilations except Xe^+ and Xe_2^+, which are from P.N.B. Neves, 10.1063/1.3497651]
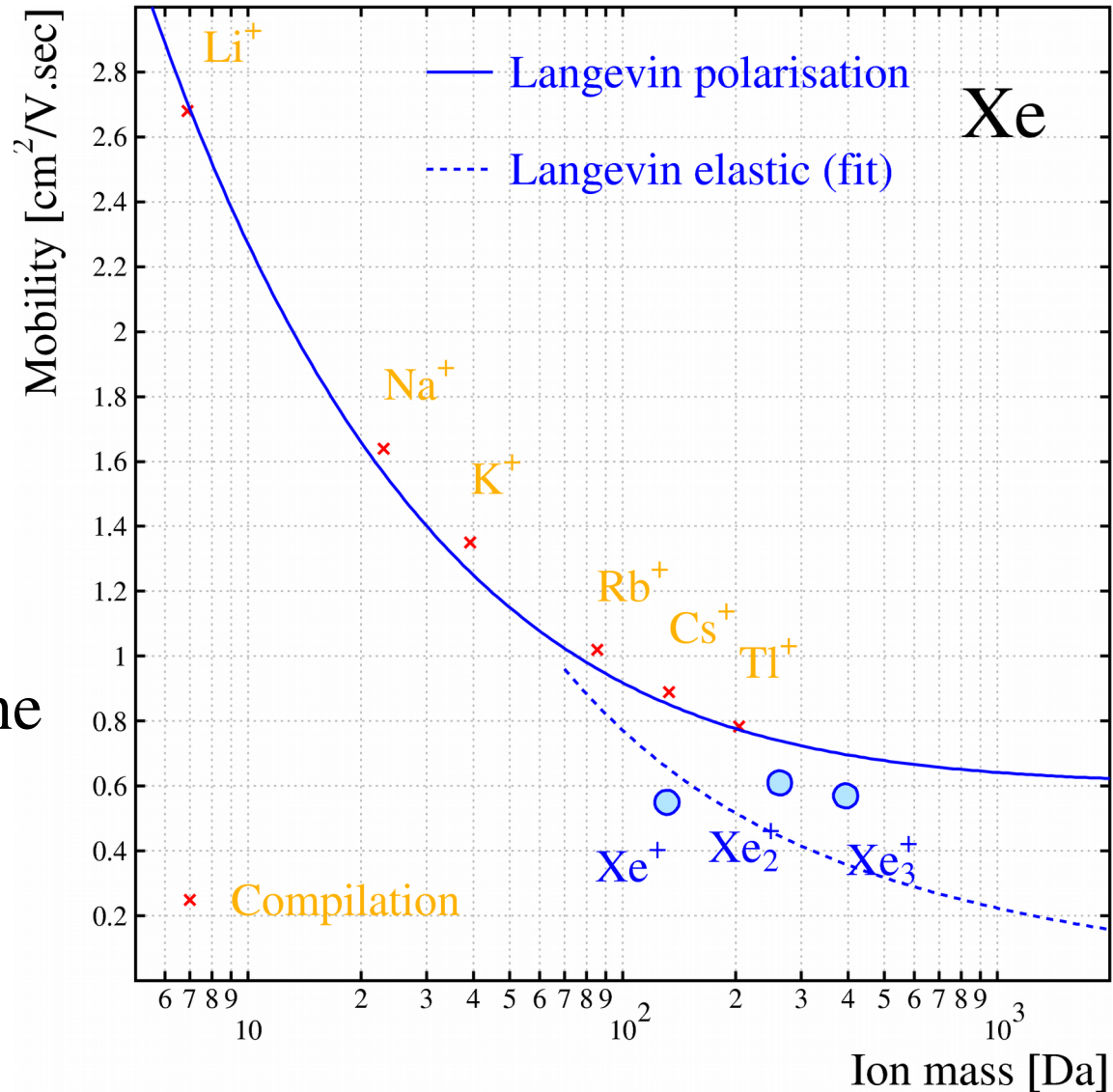
Ionisation in Xe-CF$_4$-CO$_2$ (70-20-10)

	Ion	Energy [eV]	Rate [GHz]	Fraction
Xe	Xe$^+$	12.12984	53.75	95.5 %
CF$_4$	CF$_3^+$	15.70	1.24	2.2 %
	CF$_2^+$	21.47	0.01399	
CO$_2$	CO$_2^+$	13.776	1.072	1.9 %
	CO$_2^{+*}$	17.314	0.09423	
	CO$_2^{+*}$	18.077	0.05669	
	O$^+$	19.07	0.02739	
	CO$^+$	19.47	0.02597	

Magboltz 11.2bis,
$E = 100$ kV/cm
1 atm, 20 C

Reactions in Xe-CF$_4$-CO$_2$

$\blacktriangleright$ $Xe^+ + Xe + M \rightarrow Xe_2^+ + M$ $k = 2.0 \pm 0.2 \ 10^{-31}$

[A.P. Vitols and H.J. Oskam, Phys. Rev. A **8** (1973) 1860-1863.]

$\blacktriangleright$ $CO_2^+ + CO_2 + M \rightarrow CO_2 \cdot CO_2^+ + M$ $k = 2.4 \ 10^{-28}$

[B.M. Smirnov, Cluster Ions and Van Der Waals Molecules]

$\blacktriangleright$ $CO_2^+ + Xe \rightarrow CO_2 + Xe^+$ $k = 6.0 \ 10^{-10} \pm 30 \ \%$
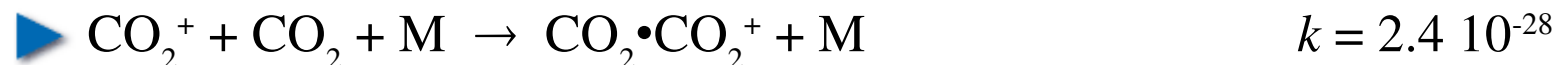
[V.G. Anicich and W.T. Huntress Jr., Astrophys. J. Suppl. **62** (1986) 553-672.]

Evolution of $Xe\text{-}CF_4\text{-}CO_2$ (70-20-10)

- Initial ion mix for 100 kV/cm;

- Xe^+ and Xe_2^+ dominate from 10 ns on, Xe_n^+ for $n > 2$ are not shown: rates are not known.

- CF_3^+ is an avalanche product; with its low IP, it does not react;

- CF_4^+ is not produced, CF_4 has a high IP, is not attacked by ions.

- CO_2^+ transfers to Xe^+ and rapidly forms clusters.
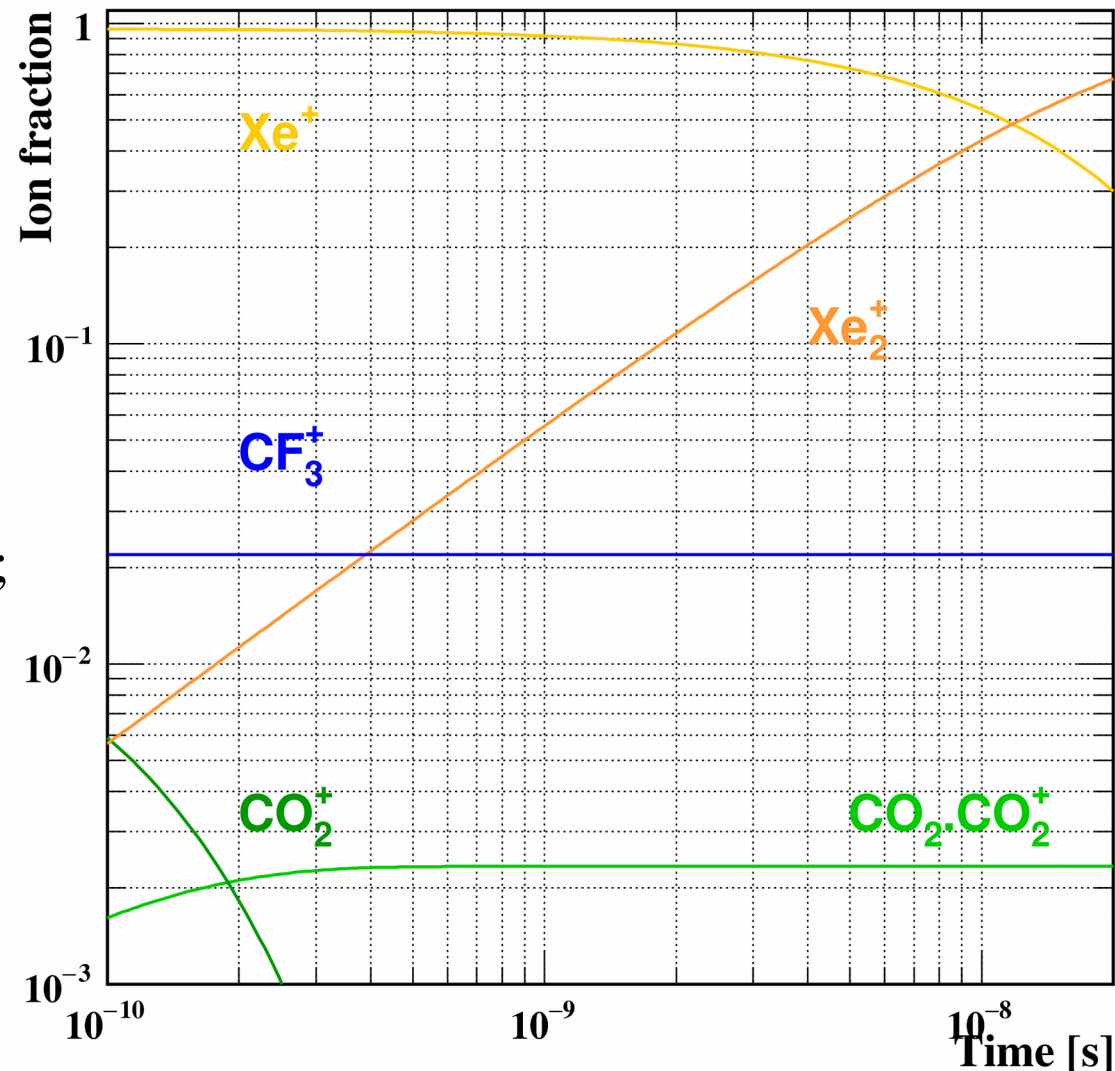
Evolution of $Xe\text{-}CO_2\text{-}C_2H_6$ (70-27-3)

- Initial ion mix for 100 kV/cm;

- CO_2^+ rapidly forms clusters due to the large CO_2 fraction;

- CO_2 does not affect the dominance of C_xH_y over Xe.

- Xe_n^+ for $n > 2$ are not shown because rates are not known.
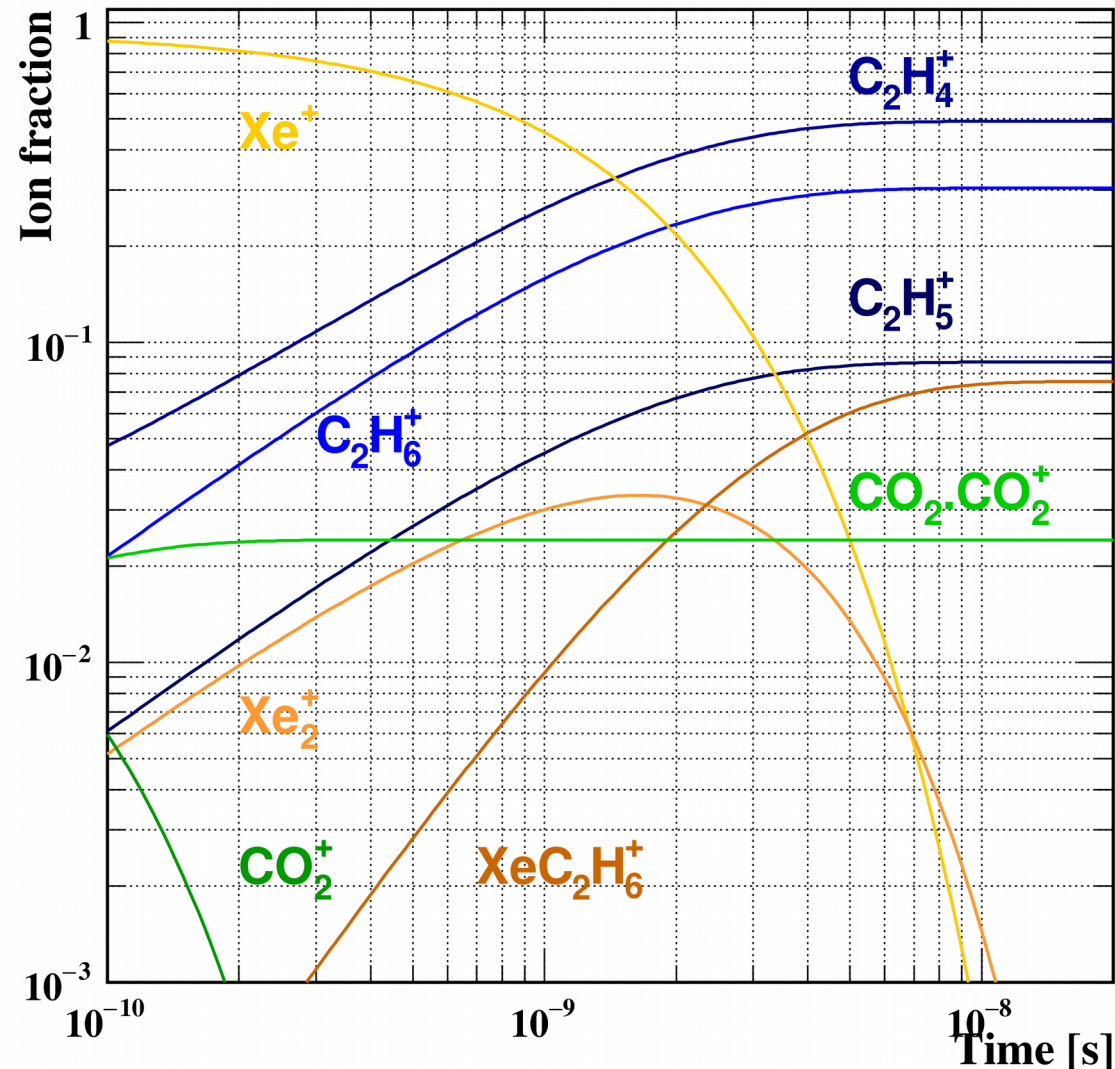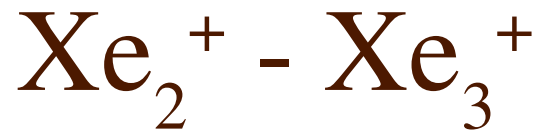
Xe_2^+ - Xe_3^+

▶ We have not found the rate comstant for Xe_3^+ production in the literature, but H. Helm has measured:

$$K_e = \frac{[Xe_2^+][Xe][Xe]}{[Xe_3^+][Xe]} = \frac{k_r}{k_f} = 2.8 \pm 0.5 \; 10^{18}$$

▶ where k_f is the rate coefficient for the transformation of Xe_2^+ to Xe_3^+, and k_r the rate for the reverse reaction.

▶ Given that $[Xe_3^+] / [Xe_2^+] = 3.6 \pm 0.6 \; 10^{-19} \; N$, the ratio of concentrations is 9.7 ± 1.6 at 293 K, atmospheric pressure and zero field.

[H. Helm, 10.1103/PhysRevA.14.680]

Mobility and stability of small Xe_n^+

▶ Mobilities are known for the smallest Xe clusters;
▶ these are remarkably stable;
▶ ΔH for $n \geq 5$ clusters is nearly constant at ~0.1 eV.

Xe_n^+	Mass	$\mu\ (E = 0, T{=}300\ K)$	$\Delta H\ n\text{-}1 \rightarrow n$	References
	[Da]	[cm²/V.s]	[eV]	
Xe^+	131.293	0.55	-	Helm, Viehland-Mason
Xe_2^+	262.586	0.61	1.05 (5 %)	NIST, Helm 1976
Xe_3^+	393.879	0.57	0.29 (5 %)	NIST, Helm 1976
Xe_4^+	525.172	?	0.26 (3 %)	NIST, Hiraoka
Xe_5^+	656.465	?	0.11 (5 %)	NIST, Hiraoka

[Kenzo Hiraoka et al. 10.1063/1.457751, M. Amarouche et al. 10.1063/1.454267]

Large Xe$_n$ clusters

▶ Much larger clusters, with a typical size of 10^4, have been observed.

▶ They are produced by "supersonic adiabatic expansion through a nozzle."

▶ A topic of current investigation in RD51.

Tracking techniques

- Devices much larger than the electron mean free path:
  - if diffusion can be neglected, Runge Kutta integration;

- devices with structural elements at the micron scale:
  - electron tracking at the molecular level;

- ions:
  - cross sections for microscopic ion tracking not available, and anyhow not practical: $\lambda_{gas-ion} \sim 50$ nm;
  - Monte Carlo based on measured diffusion and mobility;
  - chemistry remains to be implemented.

Single avalanche

▶ **Diffusion diminishes on passing the mesh.**

▶ **Circles indicate**
  ▶ **excitation,**
  ▶ **ionisation and**
  ▶ **attachment.**
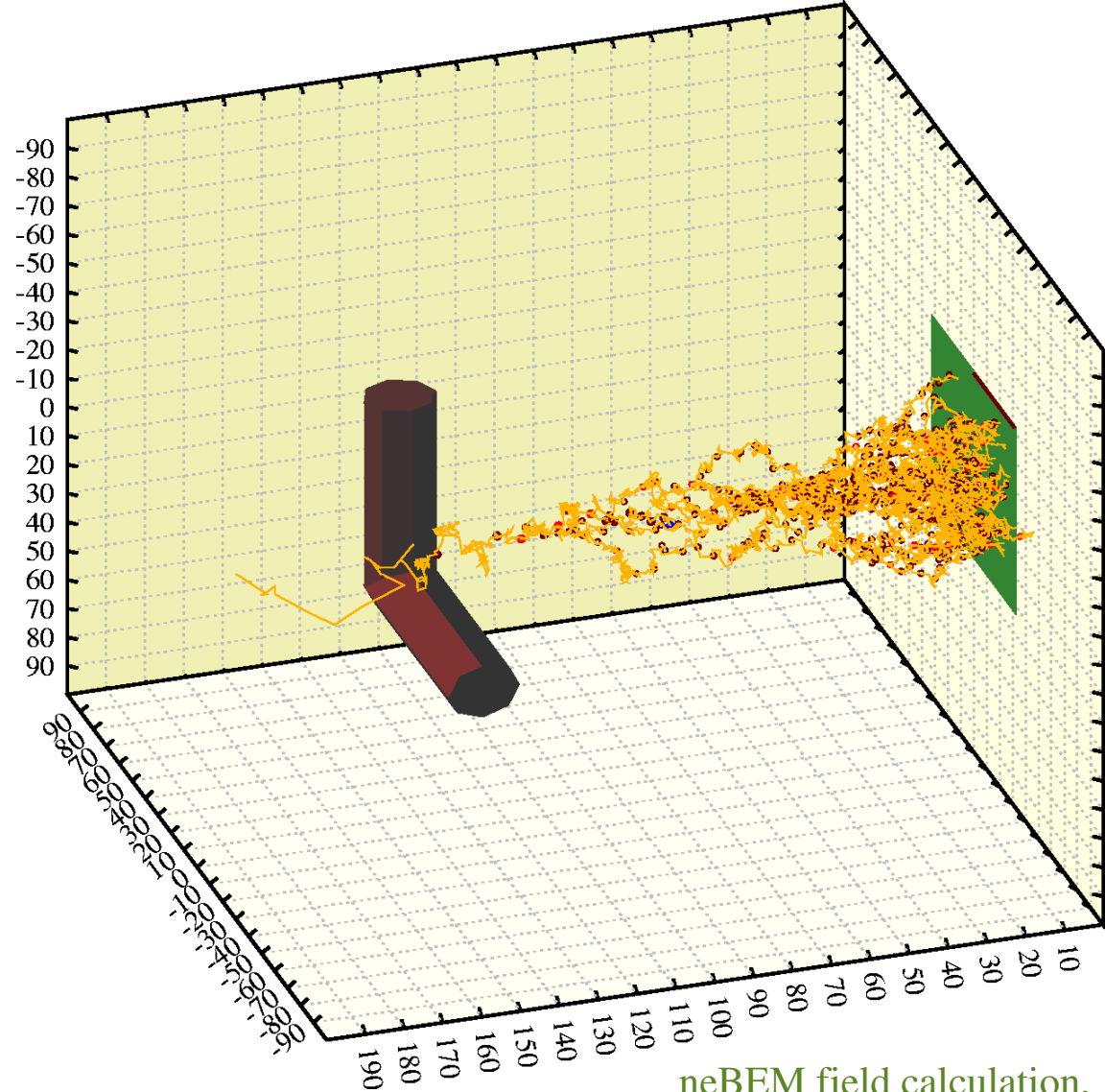
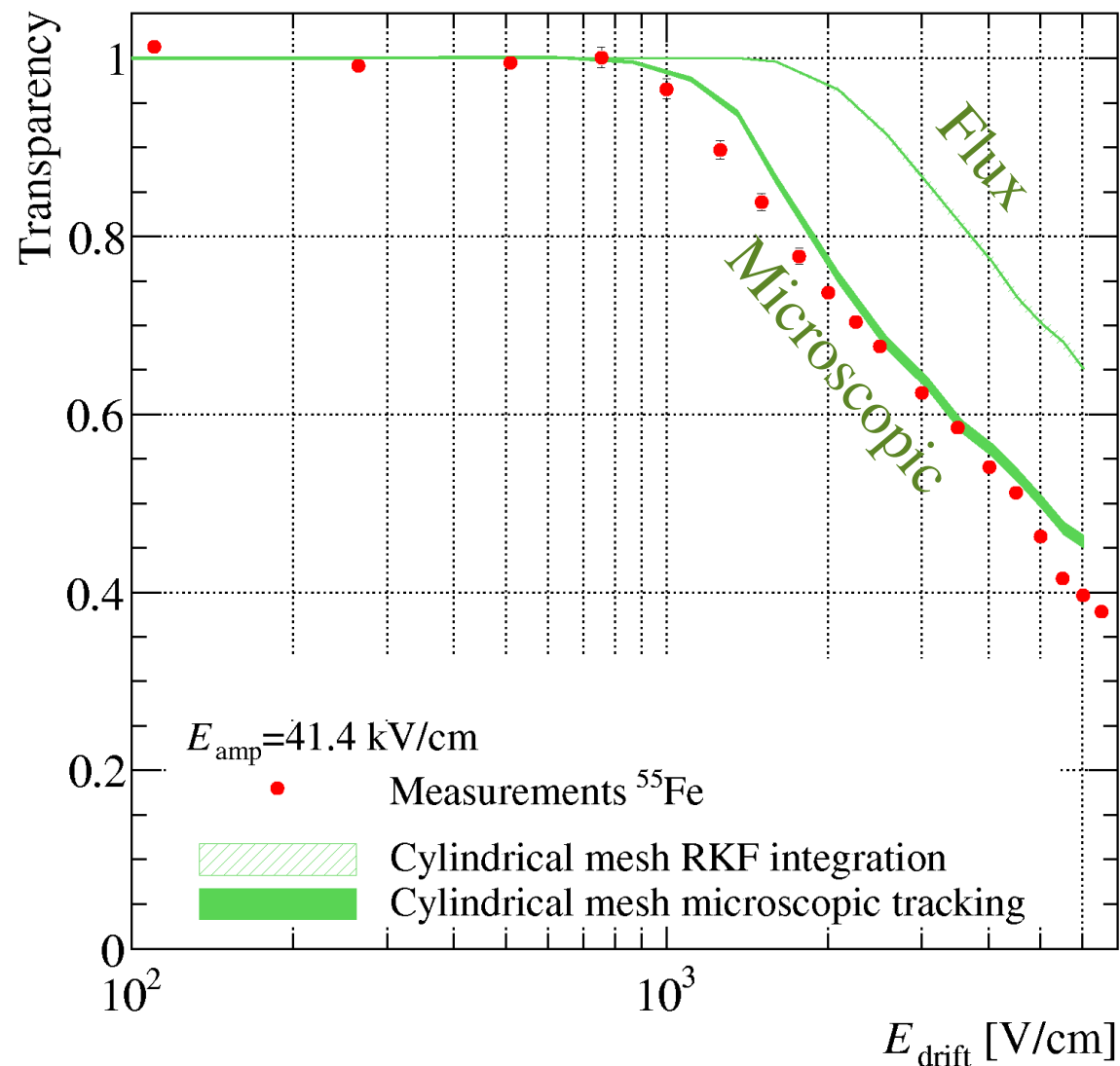neBEM field calculation, double-periodic structure
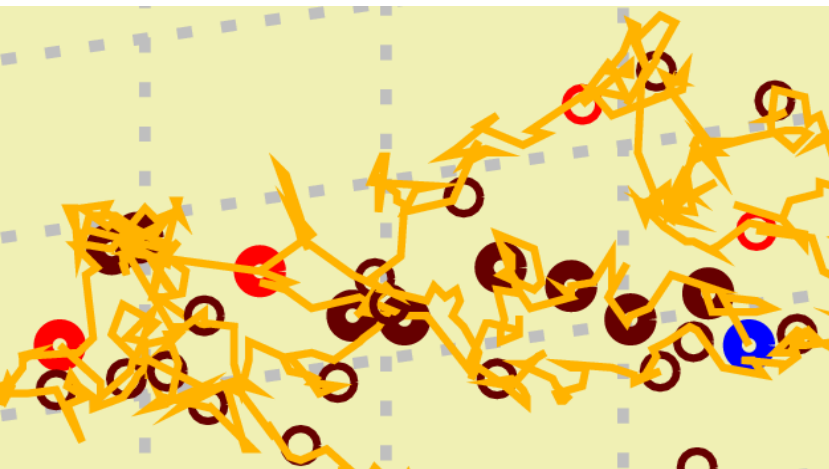

```
&SIGNAL
sel p q (s)
window 0 0.000005
area -0.0100 -0.0100 0    0.0100 0.0100 0.0200    view -3*x-2*y+z=0 rot 180 3d
int-par mc-coll 10

Call plot_drift_area
Global delay = 0
Call microscopic_avalanche(0, 0, 0.0190, ...
    `plot-electron, signal, abort-100, mark-excitation, mark-ionisation, mark-attachment`, ...
    100, 1, ...
    0, 0, 0, edist, rates, n_e, n_i, delay)
Call plot_drift_line
Call plot_end
```

Flux vs microscopic ?

▶ A diffusion-free flux argument does not reproduce the data ...

▶ but the microscopic approach works.

Field calculations: finite elements.

Plot axes: Transparency vs E_{drift} [V/cm]. Curves labelled *Flux* and *Microscopic*.

E_{amp}=41.4 kV/cm

• Measurements ^{55}Fe

▨ Cylindrical mesh RKF integration

▬ Cylindrical mesh microscopic tracking

Summary of uncertainties

▶ Ionisation:
- ▶ PAI: factor of 10 at shell edges of the photo-absorption cross section.

▶ Material properties:
- ▶ dielectric constants known to a few percent (manufacturer);
- ▶ conductivity known to an order of magnitude, not pure resistors;
- ▶ properties depend strongly on humidity, temperature, surface treatment ...

▶ Fields:
- ▶ finite elements: larger for E than V, poor near charges, error-prone;
- ▶ boundary elements: depends on discretisation;
- ▶ general resistive layers remain to be implemented.

▶ Electron transport:
- ▶ electron velocity: better than 1 % for reasonable settings;
- ▶ electron diffusion: worse;
- ▶ avalanche gain: orders of magnitude in Penning mixtures;
- ▶ attachment: several-body reactions.

▶ Ion transport:
- ▶ signal ions can be C_xH_y, $CO_2^+ \bullet (CO_2)_n$, Xe^+_n, Ar_2^+, Ne_2^+ ...
- ▶ not all rate constants relevant for us are available.