Anton Oed

(1933-2018)

Summer student

INTRODUCTION

- WHO I AM
  SUMMER STUDENT (C FABJAN)
  Rob VEENHOF / LEIDEN - NETHERLANDS
- WHAT I HAVE BEEN DOING
  WRITING A COMPUTER PROGRAM FOR
  DRIFT CHAMBER SIMULATION
- WHAT THE PROGRAM CAN DO
  - CALCULATE THE ELECTRIC FIELD AND POTENTIAL IN A DRIFT CHAMBER
  - PLOT ELECTRIC FIELD + POTENTIAL
  - CALCULATE AND PLOT DRIFT LINES AS WELL AS EQUAL-ARRIVAL-TIME CONTOURS,
  - SIMULATE THE SIGNAL ON THE SENSE WIRES DUE TO A CHARGED PARTICLE GOING THROUGH THE DC.
  - WRITE THE SIGNAL ON A FILE THAT CAN BE USED AS INPUT FOR SCEPTRE.

1st talk

NA 34 Wednesday Meeting

Wed. 29/8/84

14 oo, Conf R.

Agenda

The NEW DC - Simulation — Rob Versluis

Comments on UCAL Simulation — Yona O.

Thoughts on the U I Scient. Cal. — Richard W.

The yellow report

CERN 77-09
3 May 1977

ORGANISATION EUROPÉENNE POUR LA RECHERCHE NUCLÉAIRE
CERN EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

PRINCIPLES OF OPERATION OF MULTIWIRE PROPORTIONAL AND DRIFT CHAMBERS

F. Sauli

Lectures given in the
Academic Training Programme of CERN
1975-1976

GENEVA
1977

Stigler's law

“no scientific discovery is named after its original discoverer”

Simulation

- Target: calculation of signals in drift chambers;
- starting point: a program without a single comment, variables named VAR2, VAR10 ... and subroutines SUB3, SUB9 ...
- learned not to start from an existing program.

Ionisation

- Originally:
  - exponential spacing of clusters;
  - Landau deconvoluted to form clusters.

- Various models are now interfaced:
  - Heed, PAI — charged high-energy particles;
  - SRIM — stopping and range of ions in solids;
  - TRIM — transport of ions in matter;
  - Geant 4 interface — simulating of detectors ...

Ionisation clustering

SIGNAL SIMULATION

- MODIFIED LANDAU DISTRIBUTION

-REQUIRED

$$f'(\lambda)^{*\bar{N}} = f(\lambda)$$

IE : THE SUM OF $\bar{N}$ NUMBERS DRAWN FROM $f'(\lambda)$ IS DISTR. AS $f(\lambda)$

- THEREFORE

SINCE

$$f(\lambda) = L^{-1}\, s \log s \qquad \text{(INVERSE LAPLACE)}$$

AND

$$f'(\lambda)^{*\bar{N}} = f(\lambda)$$

WE FIND

$$f''(\lambda) = L^{-1}\, \frac{s}{\bar{N}} \log s$$

$$= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \exp\left(\frac{1}{\bar{N}} s \log s + s\lambda\right) ds$$

$$= \frac{\bar{N}}{2\pi i} \int_{c-i\infty}^{c+i\infty} \exp\left(\frac{s}{\bar{N}} \log \frac{s}{\bar{N}} + \frac{s}{\bar{N}} \left(\log \bar{N} + \bar{N}\lambda\right)\right) d\frac{s}{\bar{N}}$$

$$= \bar{N}\, f(\bar{N}\lambda + \log \bar{N})$$

- TRANSLATED TO ENERGIES

$$f'(E) = \frac{\bar{N}}{s} f\left(\frac{\bar{N}E - E_{mp}}{s} + \log \bar{N}\right)$$

Heed

Igor Smirnov

- PAI model or absorption of real photons:

  $Atom + \pi^- \rightarrow Ion^{+*} + \pi^- + e^-$ (photo-electric effect,
  $Atom + \gamma \rightarrow Ion^{+*} + e^-$ real or virtual photon)

- Decay of excited states:

  $Ion^{+*} \rightarrow Ion^{++} + e^-$ (Auger)
  $Ion^{+*} \rightarrow Ion^{+} + \gamma$ (fluorescence)
  $Ion^{+*} \rightarrow Ion^{+*}$ (Coster-Kronig)

- Processing of electrons:
  - below ionisation energy transport
  - photo- & Auger-electrons (clusters, "δ-electrons"):

  $e^- + Atom \rightarrow Ion^{+} + 2\ e^-$ (absorption of high-energy electrons)

Core formulae PAI model


Wade Allison


John Cobb

- Key: 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

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

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

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

With:

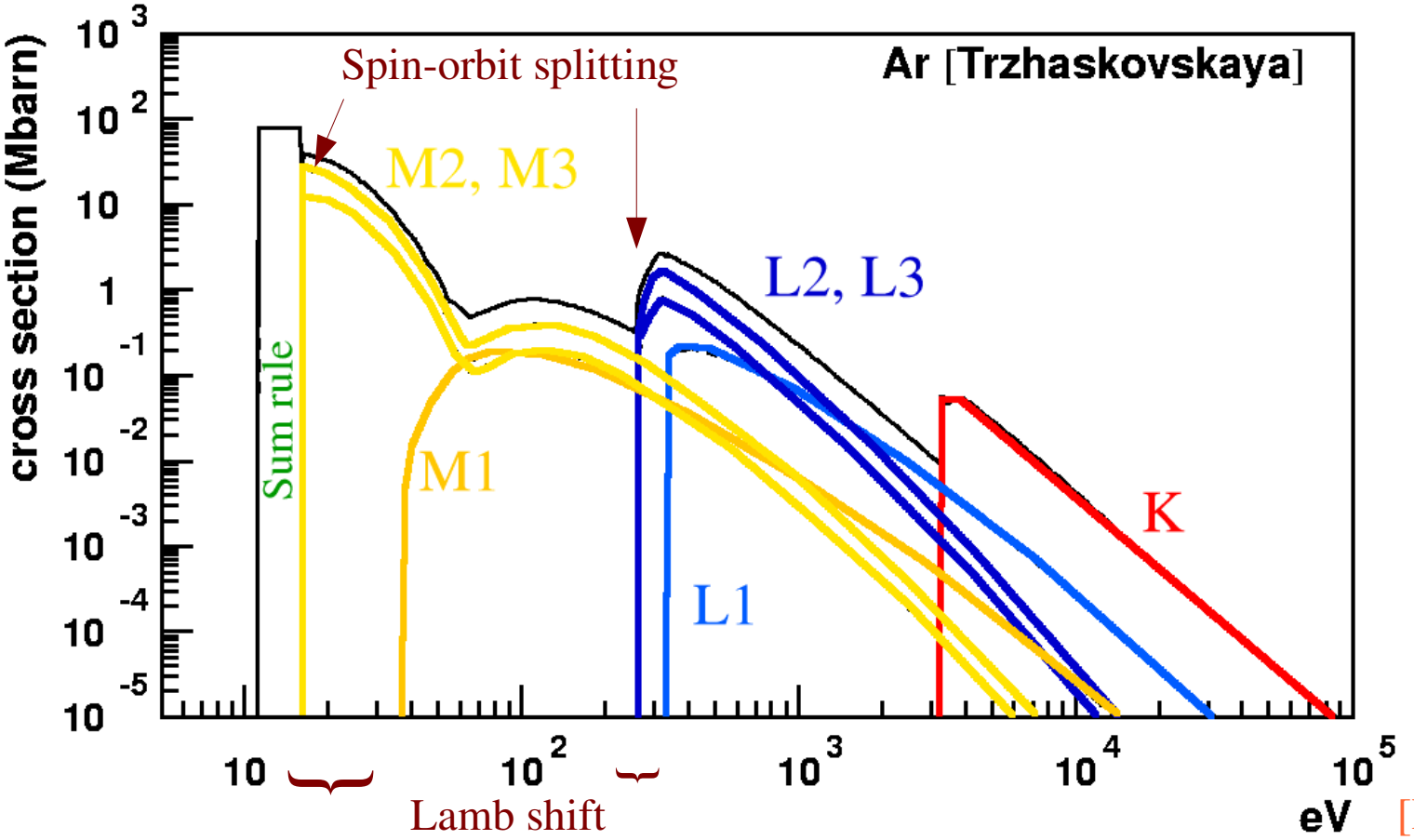
$$\epsilon_2(E)=\frac{N_e\hbar c}{EZ}\sigma_\gamma(E)$$

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

$$\theta=\arg(1-\epsilon_1\beta^2+i\,\epsilon_2\beta^2)=\frac{\pi}{2}-\arctan\frac{1-\epsilon_1\beta^2}{\epsilon_2\beta^2}$$

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

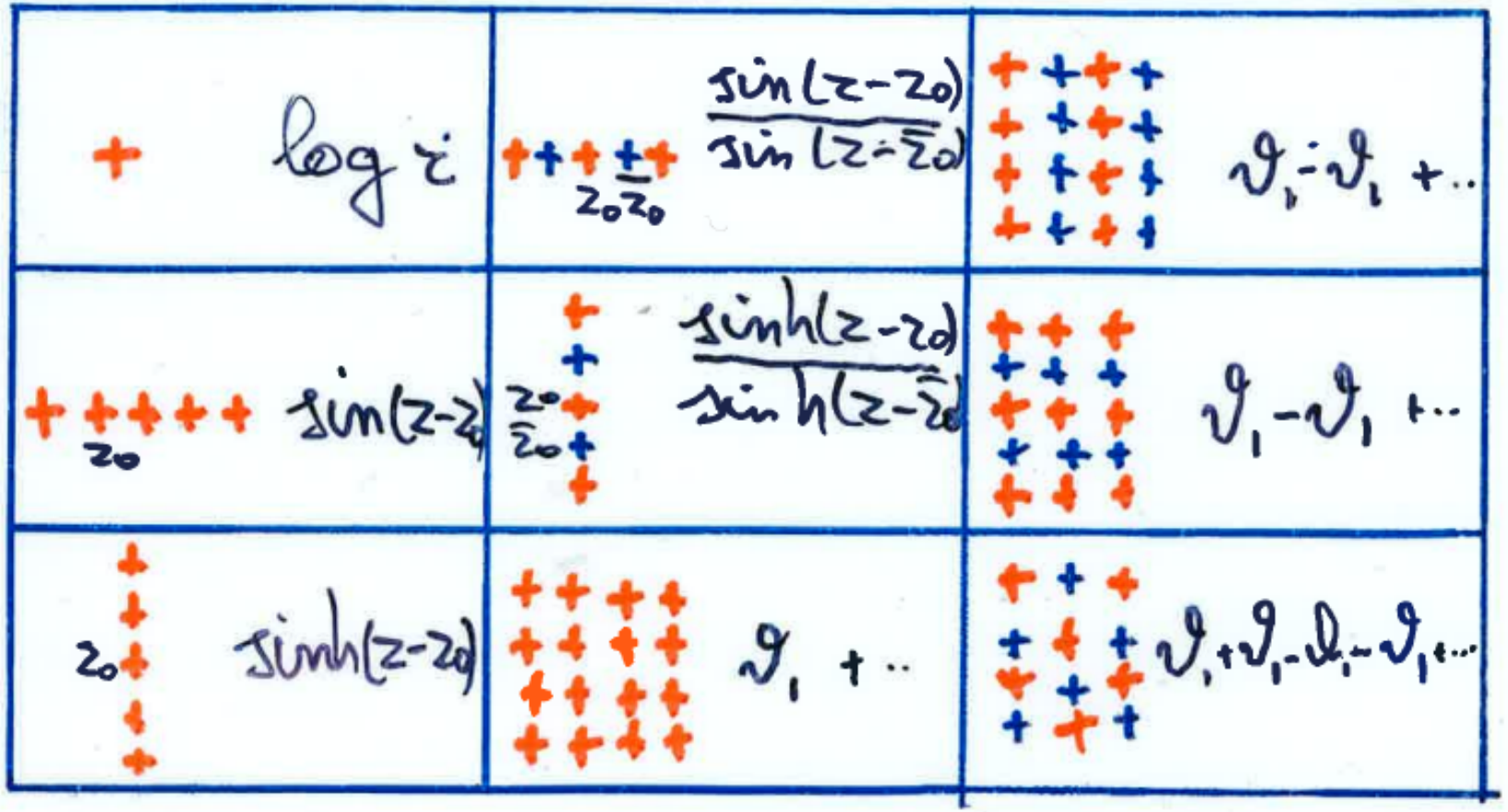
M1 = 3s
M2 = 3p 1/2
M3 = 3p 3/2

[Plot from Igor Smirnov]

Wire chamber fields

- The most common field calculations were for isolated wires, rows of wires, grids, cylinders, “infinite” planes and periodicities.
- For these, nearly exact fields can be derived for:
  - MWPC,
  - drift chambers,
  - PPC,
  - TPC
  - ...
- Applied also for e.g. wire sag calculations.
- The field wizzard in the 1980s was G.A. Erskine.

Wire chamber fields



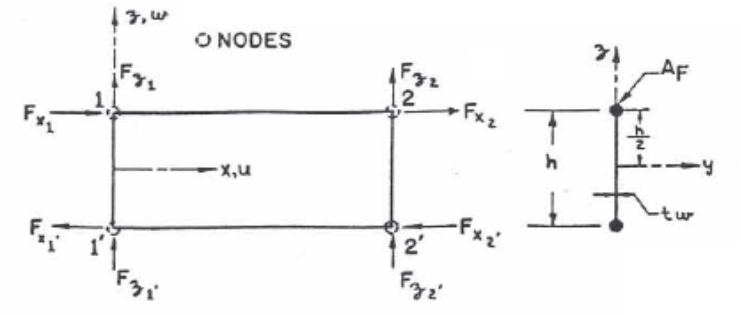
MPGDs and the mean free path

- Recall:
  - Mean free path of electrons in Ar: 2.5 μm,
- Compare with:
  - Micromegas mesh pitch: 63.5 μm
  - GEM polyimide thickness: 50 μm
  - Micromegas wire thickness: 18 μm
  - GEM conductor thickness: 5 μm
- Hence:
  - mean free path approaches small structural elements;
  - such devices should be treated at a molecular level.
- In addition, MPGDs usually have structures for which no nearly-exact (e.g. 3d structures) fields are known.

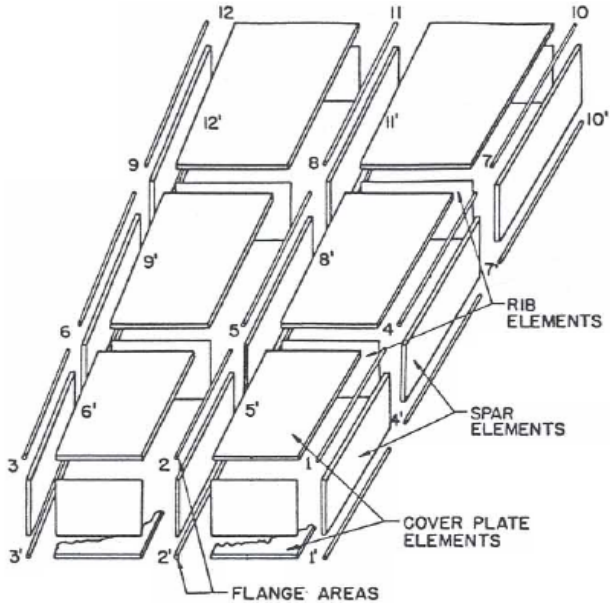
Ιωάννης Χατζι Αργύρης
(1913-2004)

Aircraft wings – finite elements

- "*Stiffness and Deflection Analysis of Complex Structures*", a study in the use of the finite element technique (then called "direct stiffness method") for aircraft wing design.

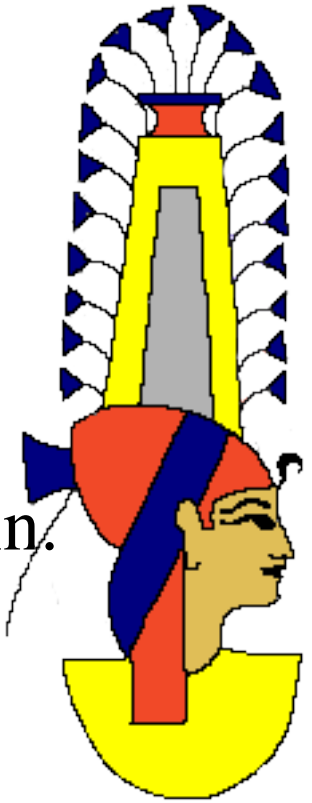


$$[K] = \frac{6EI}{Lh^2(1+4n)} \begin{bmatrix} u_1 & v_1 & w_1 & u_2 & v_2 & w_2 \\ (4/3)\ (1+n) & & & & & \\ 0 & 0 & & & & \\ -(h/L) & 0 & h^2/L^2 & & & \\ (2/3)\ (1-2n) & 0 & -(h/L) & (4/3)\ (1+n) & & \\ 0 & 0 & 0 & 0 & 0 & \\ h/L & 0 & -(h^2/L^2) & h/L & 0 & h^2/L^2 \end{bmatrix}$$



[M.J. Turner, R.W. Clough, H.C. Martin and L.J. Topp, *Stiffness and Deflection Analysis of Complex Structures*, J. Aero. Sc. **23** (1956), 805-824. MJT & LJT with Boeing.]

Boundary element methods



- Contrary to the finite element method, the elements are 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 contrast, the method poses substantial numerical challenges: non-sparse matrices and inherent singularities.

1935: Electron energy distribution

- Calculation of the electron energy distribution
  - allowing for energy loss in elastic collisions;
  - detailed balancing of energy and momentum gain (E-field, diffusion) and loss (elastic collision);
  - velocity dependent cross section;
  - use of Legendre expansion (crediting H.A. Lorentz, 1916):

$$f(x, v, \omega) = f_0(x, v) + P_1(\cos\omega) f_1(x, v) + P_2(\cos\omega) f_2(x, v) + \cdots = f_0(x, v) + (\xi/v) f_1(x, v) + \cdots .$$

(P_1, P_2: Legendre polynomials)

The function f_0 determines the random distribution in velocity, and f_1 determines the electron drift. The higher terms in the series are nearly always very small and do not correspond to any simple physical property of the distribution, but serve simply to improve the form of the distribution function.

[Philip M. Morse, W.P. Allis and E.S. Lamar, *Velocity Distributions for Elastically Colliding Electrons*, Phys. Rev. **48** (1935) 412–419]

Arthur V. Phelps
(1923 - 2012)

1962: Numerical e^- transport

- Iterative approach, allowing for inelastic cross section terms:
  - educated guess of cross sections (elastic & inelastic);
  - numerically solve the Boltzmann equation (no moments);
  - compare calculated and measured mobility and diffusion;
  - adjust cross sections.

"... more than 50,000 transistors plus extremely fast magnetic core storage. The new system can simultaneously read and write electronically at the rate of 3,000,000 bits of information a second, when eight data channels are in use. In 2.18 millionths of a second, it can locate and make ready for use any of 32,768 data or instruction numbers (each of 10 digits) in the magnetic core storage. The 7090 can perform any of the following operations in one second: 229,000 additions or subtractions, 39,500 multiplications, or 32,700 divisions. " (IBM 7090 documentation)

[L.S. Frost and A.V. Phelps, *Rotational Excitation and Momentum Transfer Cross Sections for Electrons in* H_2 *and* N_2 *from Transport Coefficients*, Phys. Rev. **127** (1962) 1621–1633.]

Magboltz: microscopic e^- transport

- A large number of cross sections for 60 molecules...
  - Numerous organic gases, additives, *e.g.* CO_2:
    - elastic scattering,
    - 44 inelastic cross sections (5 vibrations and 30 rotations + super-elastic and 9 polyads),
    - attachment,
    - 6 excited states and
    - 3 ionisations.
  - noble gases (He, Ne, Ar, Kr, Xe):
    - elastic scattering,
    - 44 excited states and
    - 7 ionisations.

LXcat

- LXcat (pronounced *elecscat*) is an open-access website for collecting, displaying, and downloading ELECtron SCATtering cross sections and swarm parameters (mobility, diffusion coefficient, reaction rates, etc.) required for modeling low temperature plasmas. [...]”

[http://www.lxcat.laplace.univ-tlse.fr/]

LXcat people

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

Art Phelps

Leanne Pitchford

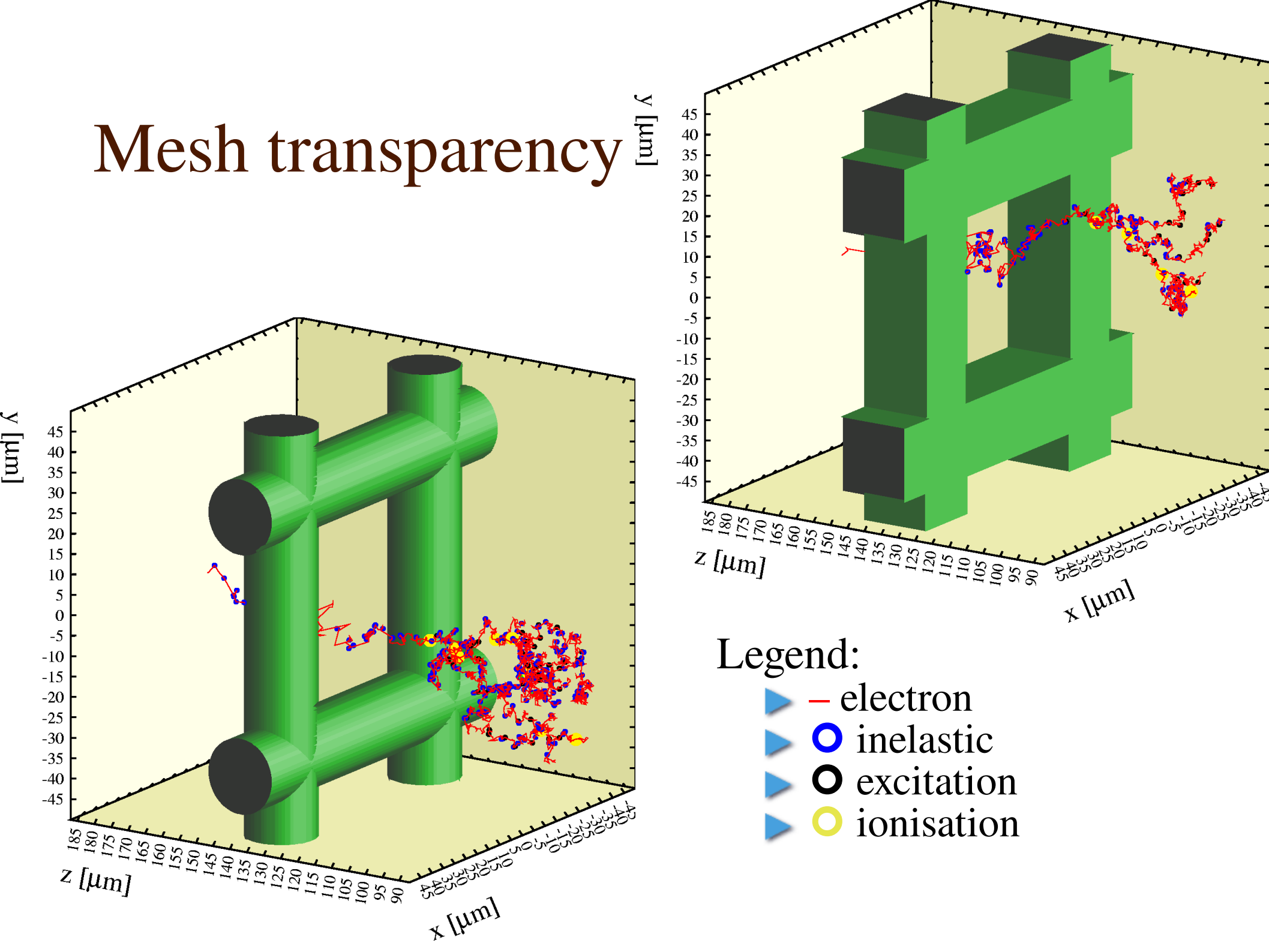
Michael Allan

Klaus Bartschat

Drift: RKF, Monte Carlo, microscopic

- RKF vs microscopic, and now obsolete, Monte Carlo;
- Beware ... in detectors such as GEM, the transparency depends on the step size. Only the natural step size leads to correct results.
- Used for e.g. transparency of meshes.
- Microscopic tracking of ions is not yet solved.

Mesh transparency

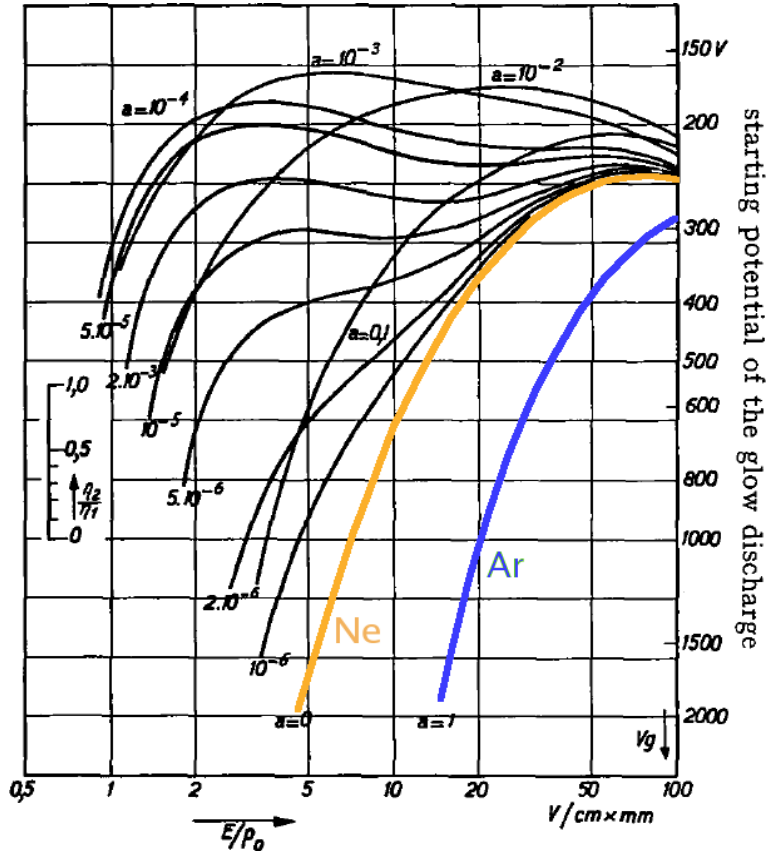


Frans Michel Penning,
photo taken around 1921
(1894-1953)

1928: Ar-Ne-Hg Penning effects

- Frans Michel Penning worked from 1924 on gas discharges at the Philips Natuurkundig Laboratorium.
- Transformation of excitations to ionisations.

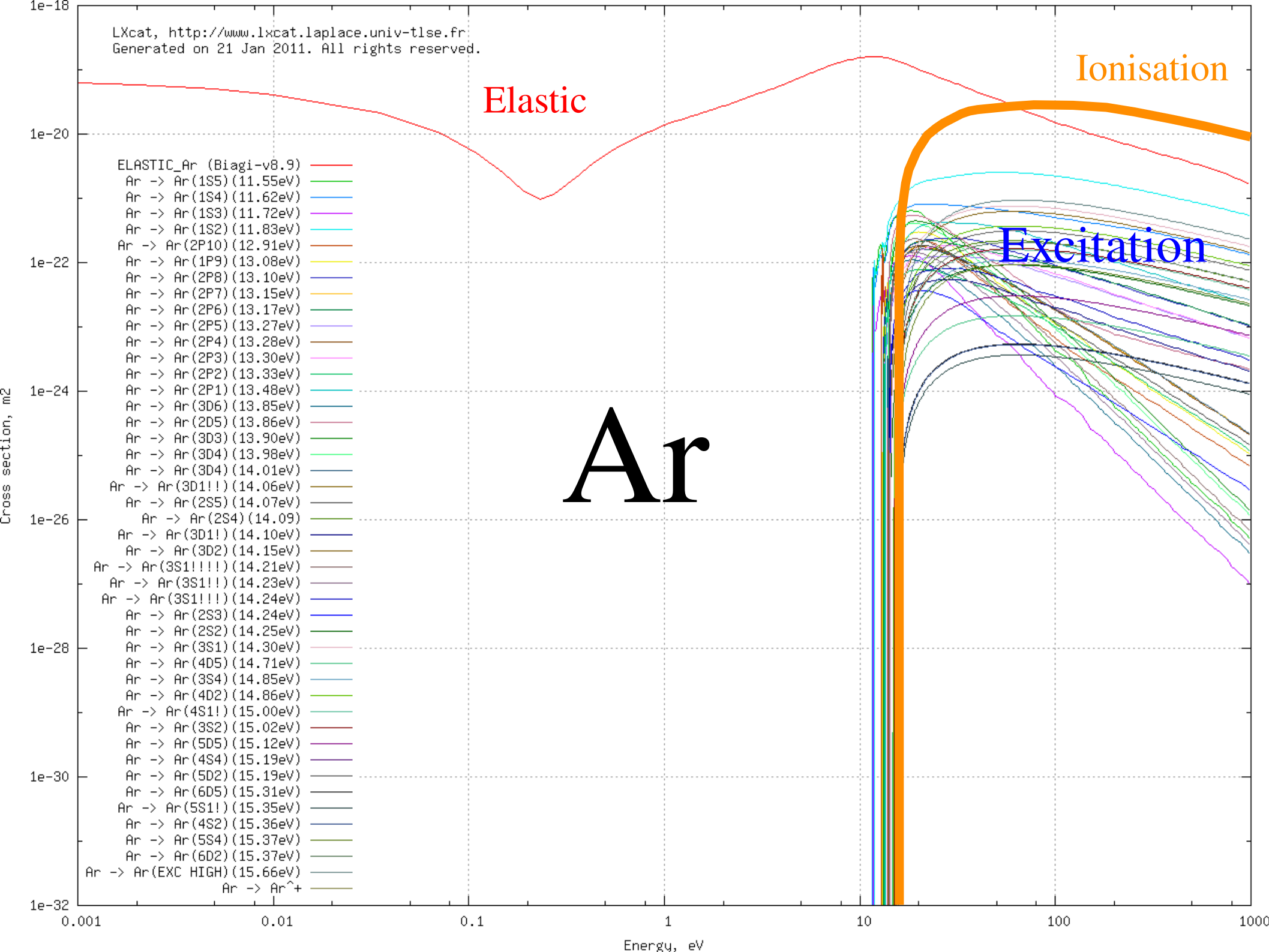
Der Einfluß sehr geringer Beimischung von Hg und Ar auf die Zündspannung V_z des Neons wurde quantitativ bestimmt. Die Erklärung wurde gefunden in der Ionisierung der Fremdatome durch die metastabilen Atome des Neons. Die notwendige Bedingung für diesen Vorgang: $V_i' < V_{met.}$ wurde geprüft bei Ne, Ar und He als Hauptgasen mit verschiedenen anderen Gasen als Beimischung und stets bestätigt gefunden. Andererseits erniedrigten immer Beimischungen, wobei $V_i' < V_{met.}$ die Zündspannung; nur NO in Ar machte eine Ausnahme von dieser Regel, was aber auf Grund des Termschemas von NO nicht zu verwundern braucht.



F. M. Penning, *Über den Einfluß sehr geringer Beimischungen auf die Zündspannung der Edelgase*, *Z. Phys.* **46** (1928) 334-348.

F.M. Penning, *The starting potential of the glow discharge in neon argon mixtures between large parallel plates: II. Discussion of the ionisation and excitation by electrons and metastable atoms*, Physica **1** (1934) 1028-1044.

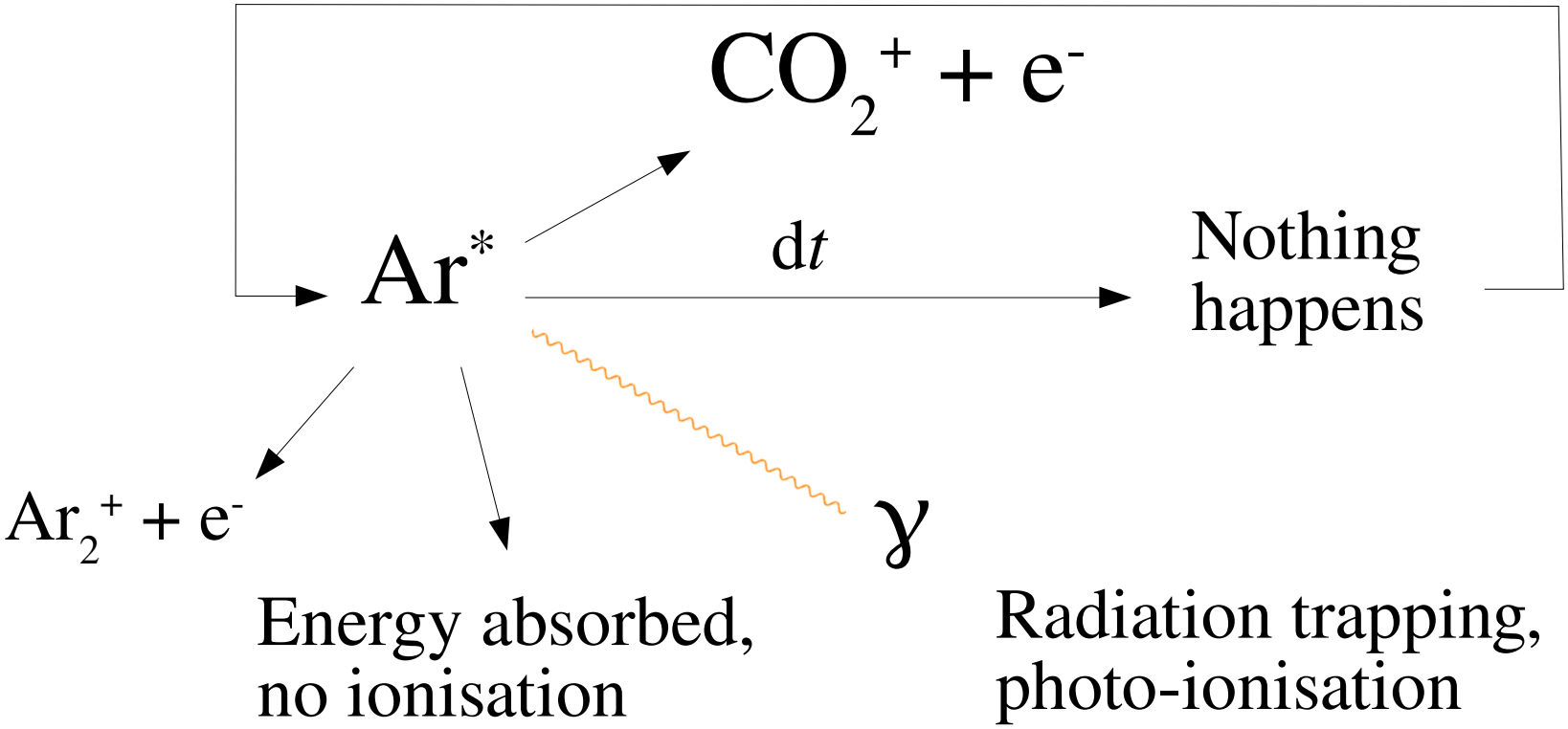
F.M. Penning, Electrische gasontladingen, Philips Technische Bibliotheek (posthumous, 1955). Translated in various languages.


LXcat, http://www.lxcat.laplace.univ-tlse.fr
Generated on 21 Jan 2011. All rights reserved.
Elastic
Ionisation
Excitation
Ar
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^+
Cross section, m2
1e-18
1e-20
1e-22
1e-24
1e-26
1e-28
1e-30
1e-32
0.001
0.01
0.1
1
10
100
1000
Energy, eV

Frans Michel Penning
(1894-1953)

Simplified Penning model

- Take small steps until the energy has been used up



Principal reactions involving CO_2

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

- CO_2: 3-body association, 7-20 ps
  - $CO_2^+ + 2CO_2 \rightarrow CO_2^+ \bullet CO_2 + CO_2$

- [For 10 % CO_2, atmospheric pressure, room temperature]

Situating cluster ions

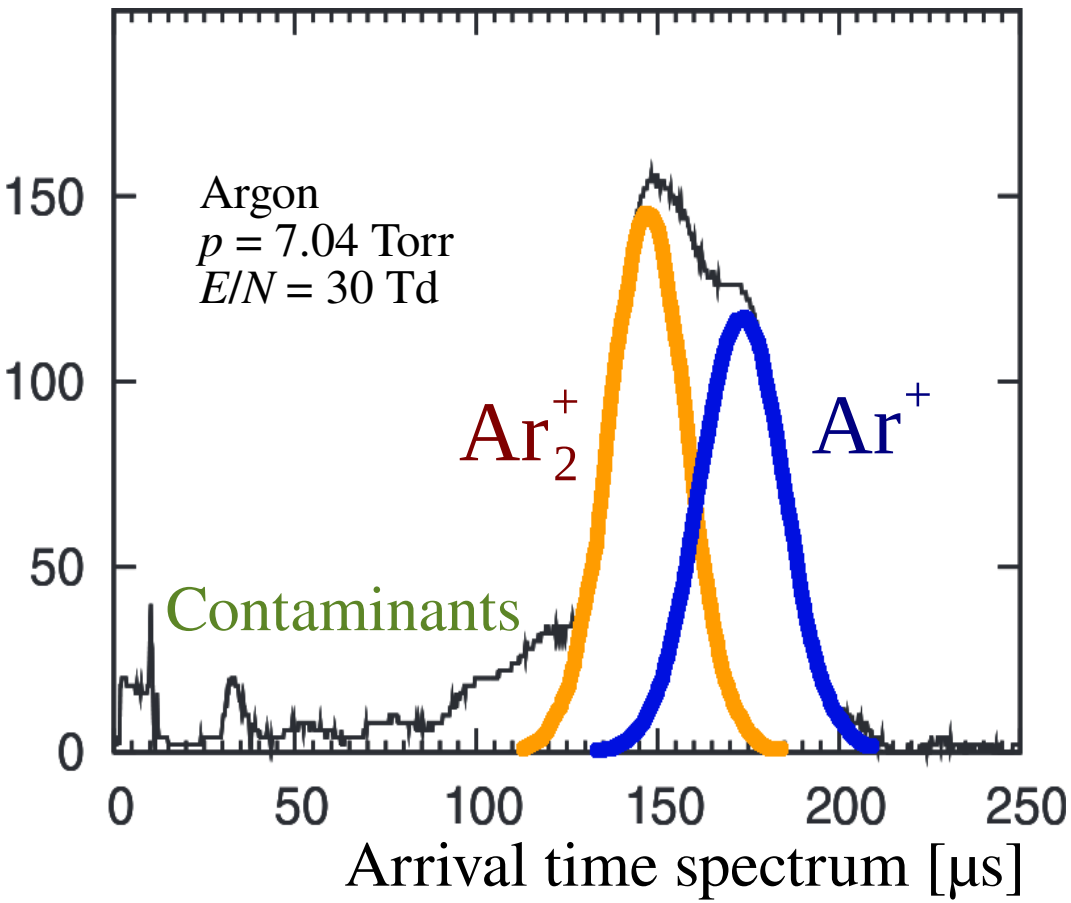
- Chemically bound molecules: 0.75 - 11.1 eV
  - covalent or ionic bond
- Cluster ions: 0.09 - 1.7 eV
  - bound by charge-induced dipole forces
  - constituents retain their identity
- van der Waals molecules: 0.0009 - 0.1 eV
  - bound by van der Waals forces
  - observed at low temperatures

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

Ions drifting in pure Ar

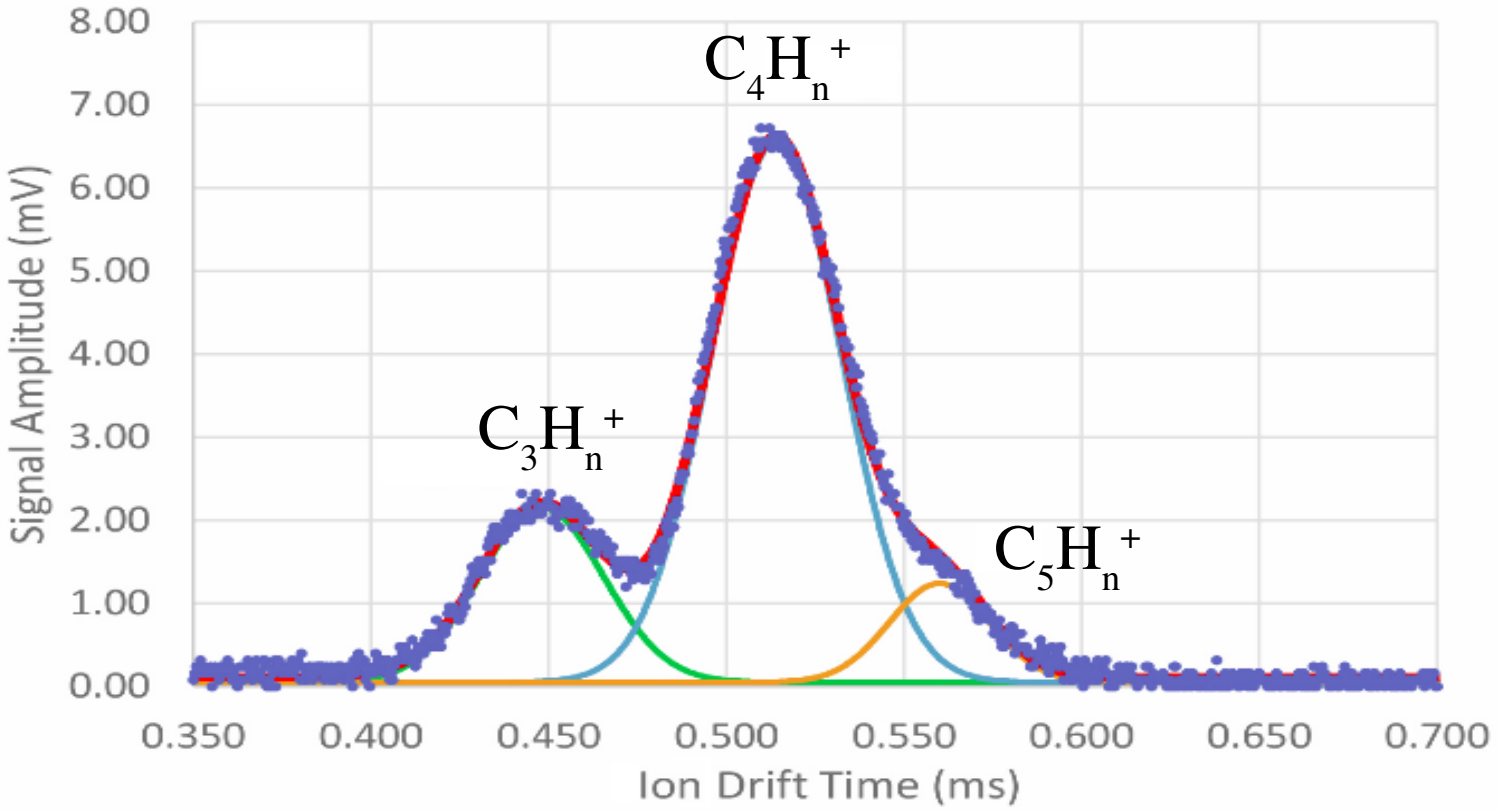
- In pure Ar, dimers are formed:
  - $Ar^+(^2P^o_{3/2}) + 2Ar \rightarrow Ar^+ \bullet Ar + Ar$ ($k = 2.3 \pm 0.1\ 10^{-31}$ cm^6/s, 7 ns)
  - Note: dimers move *faster* than ions due to $Ar \leftrightarrow Ar^+$ resonant charge exchange

[P.N.B. Neves et al. 10.1063/1.3497651]

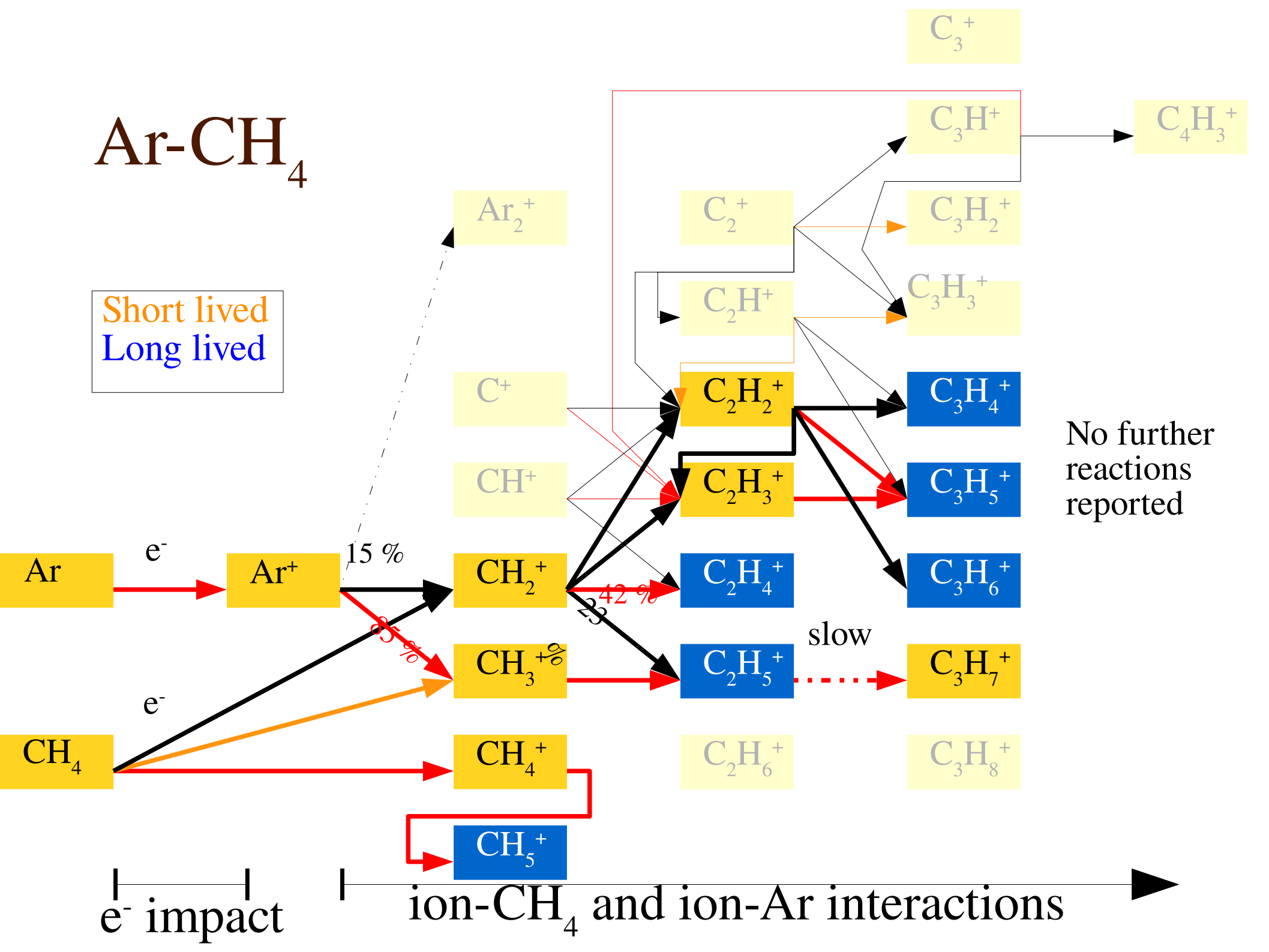


How about alkanes ?

- Ar 90 % - C_2H_6 10 %, at low pressure.
- Expect Ar^+ or $C_2H_6^+$ but ... none are seen – why ?

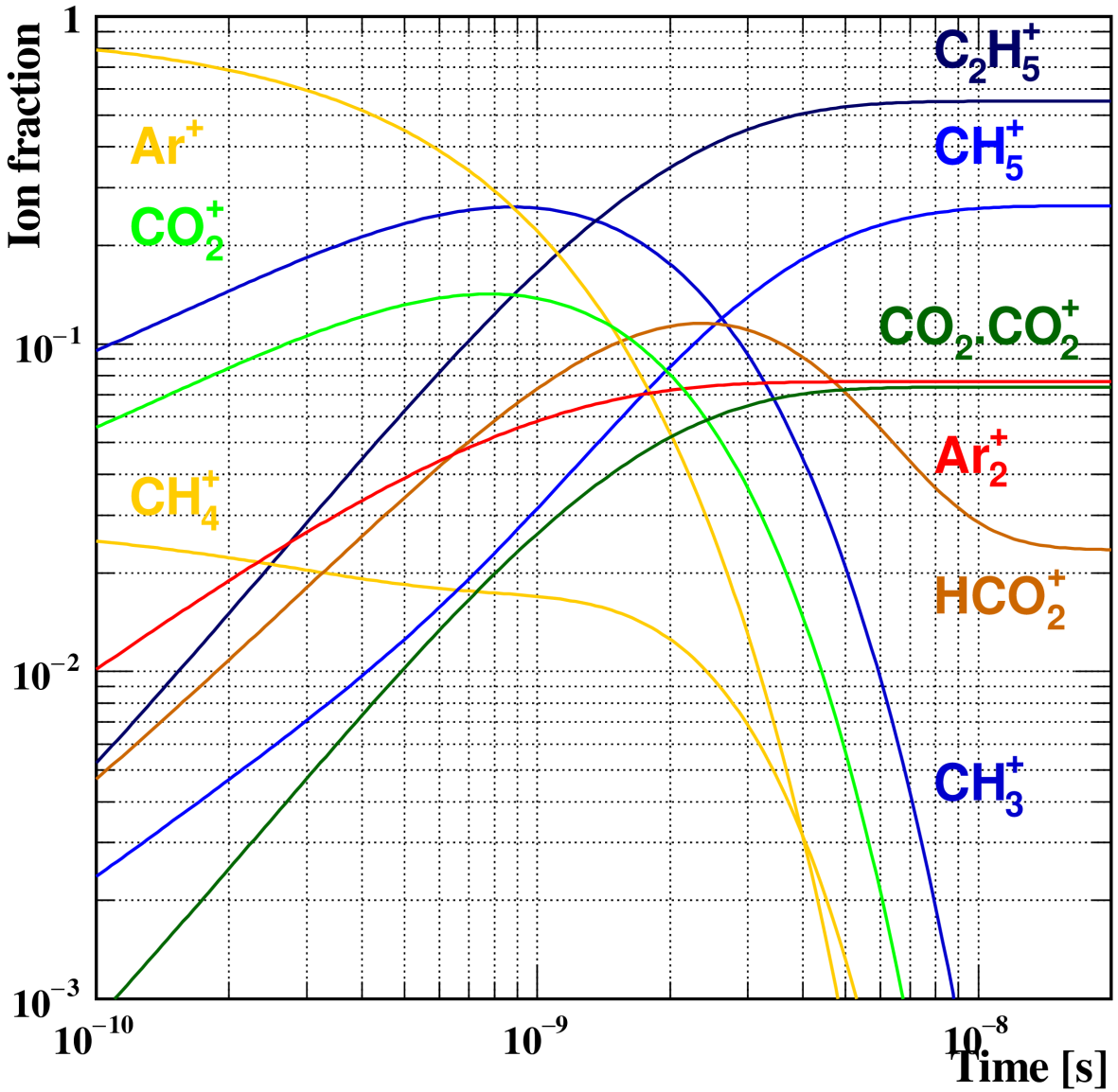


[André Cortez et al. 10.1088/1748-0221/8/12/P12012]


Ar-CH4
Short lived
Long lived
Ar
e-
Ar+
15 %
Ar2+
C+
CH+
CH2+
CH3+
CH4
e-
CH4+
CH5+
85 %
C2+
C2H+
C2H2+
C2H3+
C2H4+
C2H5+
C2H6+
42 %
23
C3+
C3H+
C3H2+
C3H3+
C3H4+
C3H5+
C3H6+
C3H7+
C3H8+
C4H3+
slow
No further reactions reported
e- impact
ion-CH4 and ion-Ar interactions

Evolution in Ar-CO_2-CH_4 (93-4-3)

- Initial ions:
  - Ar^+ →
    - CO_2^+,
    - CH_3,
    - Ar_2^+
  - CO_2^+ →
    - CH_4^+
    - $CO_2^+.CO_2$
    - HCO_2^+
  - CH_4^+ →
    - CH_5^+,
    - HCO_2^+
    - CH_3CO^+
  - CH_3^+ →
    - $C_2H_5^+$



Products after 10 ns

- $C_2H_5^+$ → $C_3H_7^+$ slow reaction, $k = 1\ 10^{-14}$

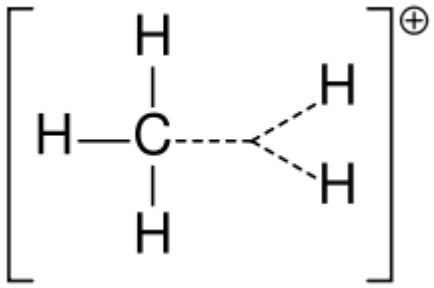
[Hiraoka & Kebarle https://doi.org/10.1063/1.431116]

- CH_5^+ → "products" slow reaction, $k = 3\ 10^{-11}$
- $CO_2 \cdot CO_2^+$ → grows to n = 3-4, reacts with CH_4 to HCO_2 ?

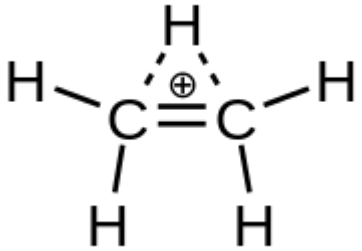
[Y. Kalkan et al. 2015 JINST 10 P07004]

- Ar^+ → Ar_2^+ drifts faster than Ar^+

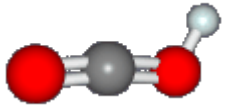
- HCO_2^+ → CH_5^+ HCO_2^+ decays at $k = 6\ 10^{-10}$



methanium

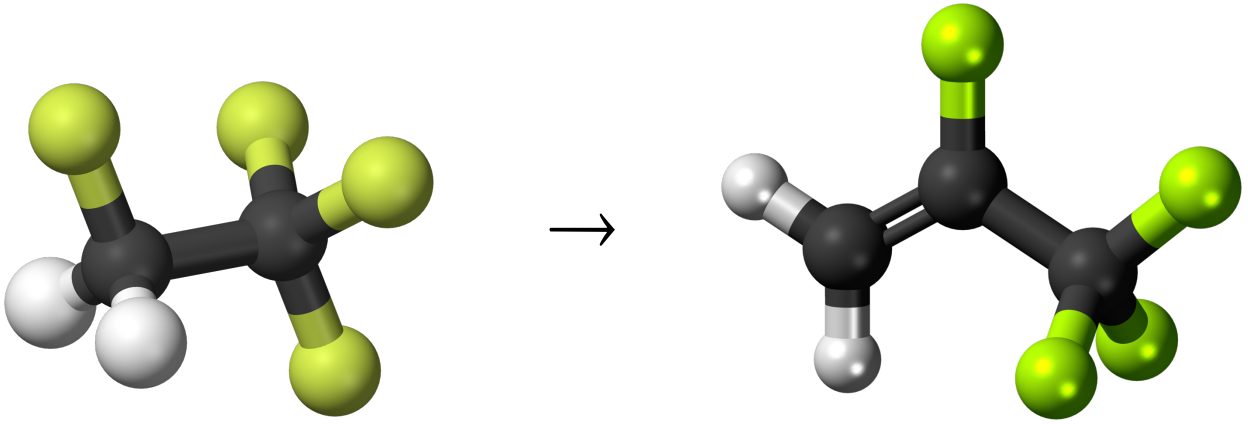


ethenium



protonated carbon dioxide

Plans



- Search for environment-friendly gases that have cross-sections making them suitable as replacements for the currently used damaging gases – Christian Franck, ETHZ and students;
- better understand and model ion mobility – collaboration with Coimbra colleagues;
- study of resistive layers – Djunes Janssens;
- study properties of dielectrics;
- study surface and space charge;
- non-equilibrium effects in avalanches.

Spare slides

Garfield++

- Josef Pellizzari tought me: don't start with C++ if you're age 40 or above;
- Garfield++ is therefore the work of the new generation;
- it is not a line-for-line translation;
- ain in keeping with current software practice, many users have provided bits and pieces;
- there is ample room for more.

Mean free path of electrons in argon

- From literature we know that:
  - Cross section of 1 atom: $\sigma \approx 1.5\ 10^{-16}$ cm^2
  - Atoms per volume: $n_0 \approx 2.7\ 10^{19}$ $atoms/cm^3$

- Mean free path for an electron ?
  - An electron hits all atoms of which the centre is less than a cross section σ radius from its path;
  - over a distance L, the electron hits $n_0\ \sigma\ L$ atoms;
  - mean free path = distance over which it hits 1 atom;

$$\lambda_e = 1/(\sigma\ n_0) \approx 2.5\ \mu m$$

  - much larger than
    - 4 nm distance between atoms, and
    - 140-600 pm typical gas molecule diameters.