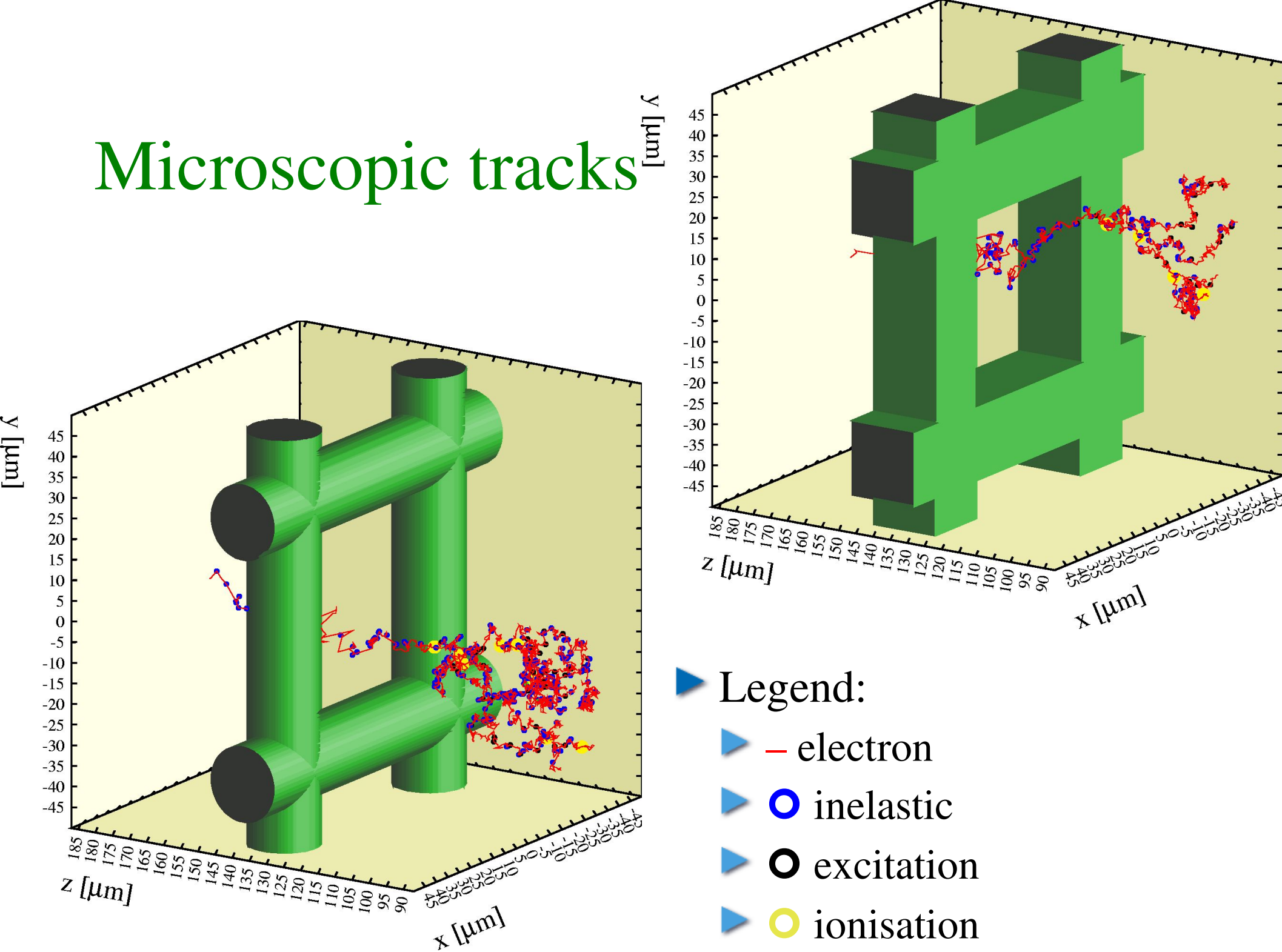
Micromegas transparency – neBEM

An update on the mesh transparency study
presented earlier by Kostas Nikolopoulos

Goal of this study

- Understanding the transparency of a Micromegas mesh:
  - What does the flux argument tell us ?
  - Is there benefit in using microscopic tracking ?
  - How sensitive is the transparency to details of geometry ?
  - Does the dipole moment in the mesh play a role ?
  - Finite elements vs boundary elements

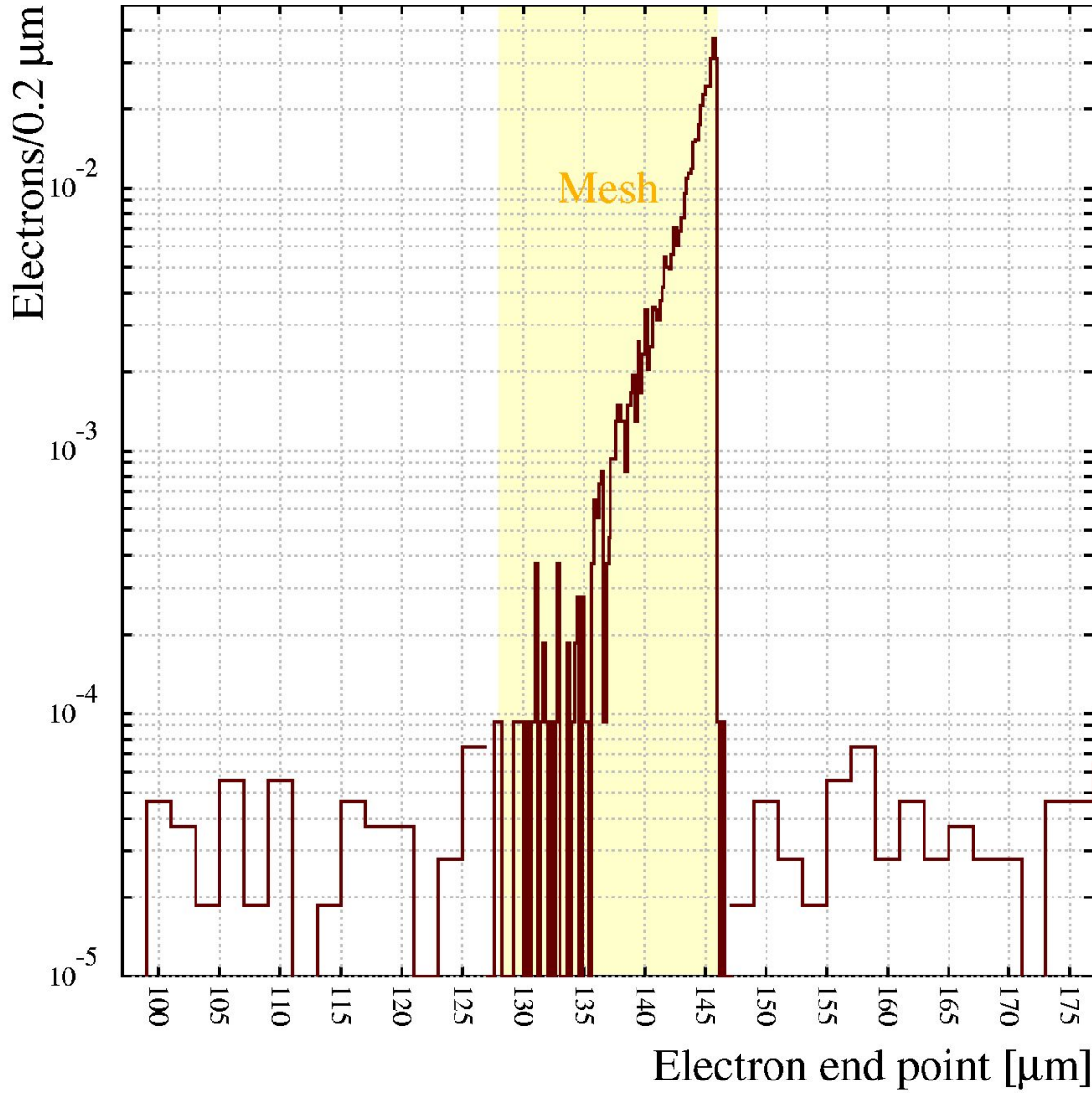
Microscopic tracks



- Legend:
  - – electron
  - inelastic
  - excitation
  - ionisation

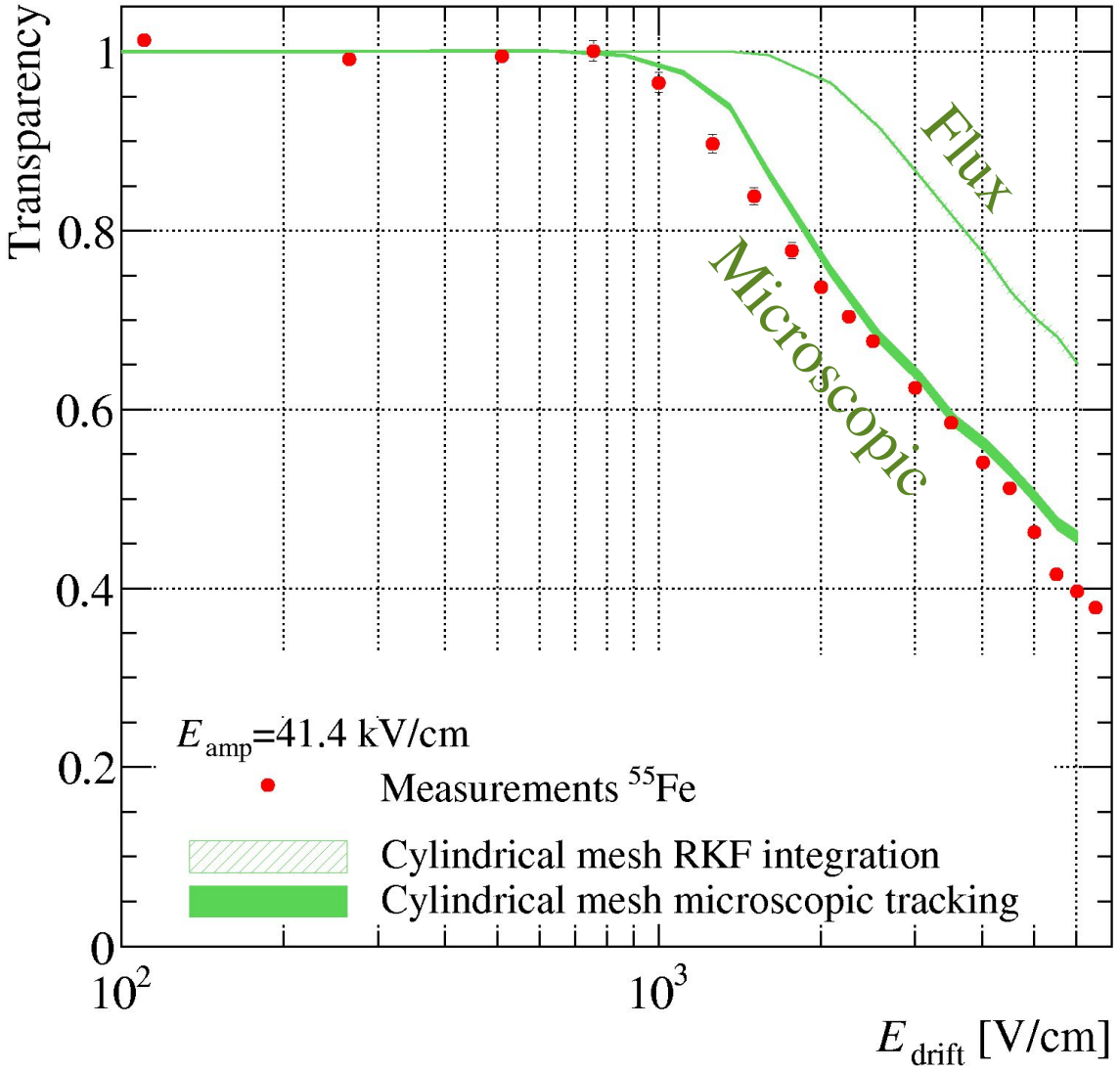
Location of losses

- Losses mainly occur at the drift surface of the mesh.
- A lesser reason for loss is attachment to CO_2.
- There is therefore no need to simulate entire avalanches.



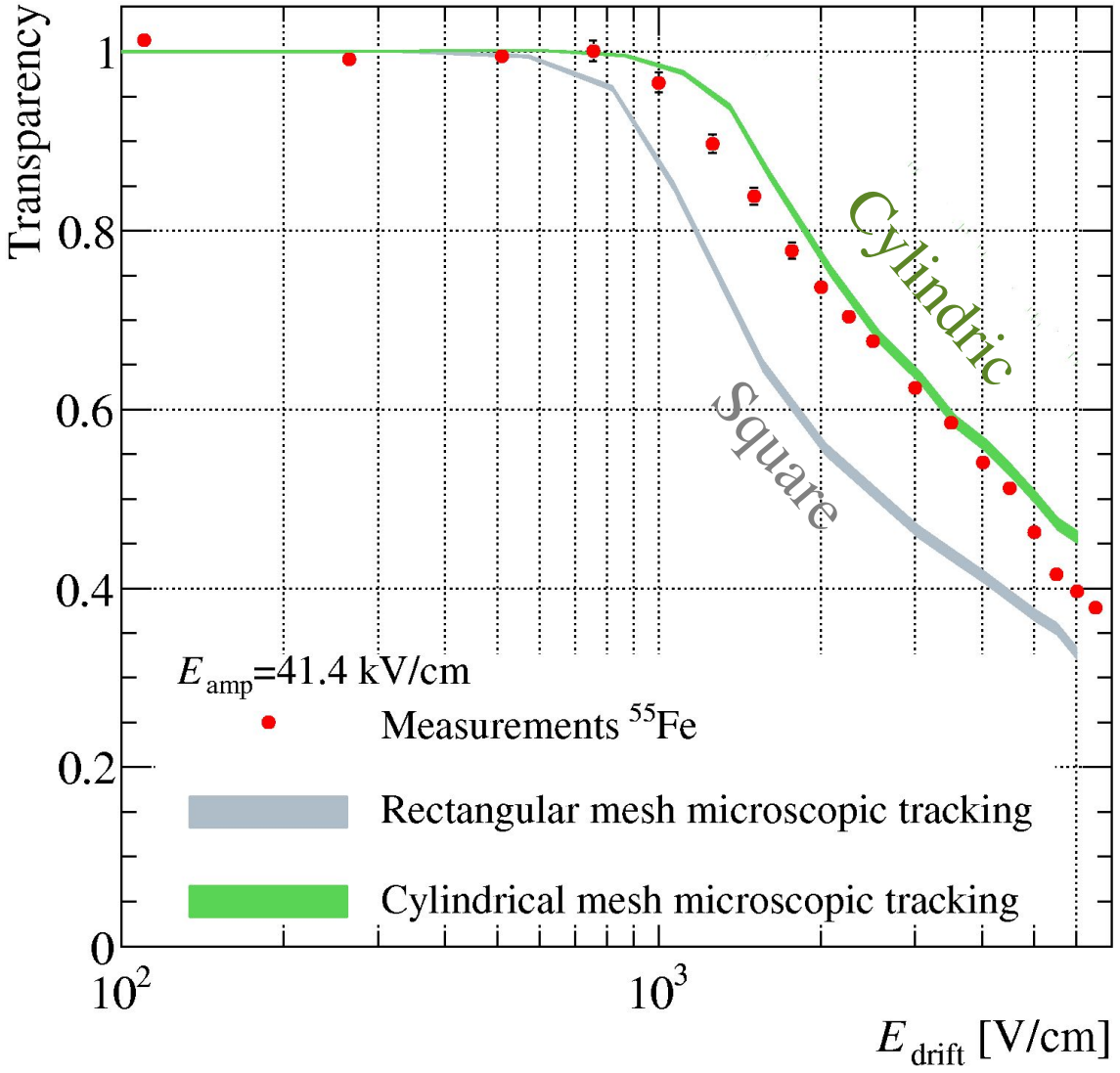
Flux vs microscopic ?

- A diffusion-free flux argument does not reproduce the data.
- The microscopic approach works.
- Calculations done using finite elements.



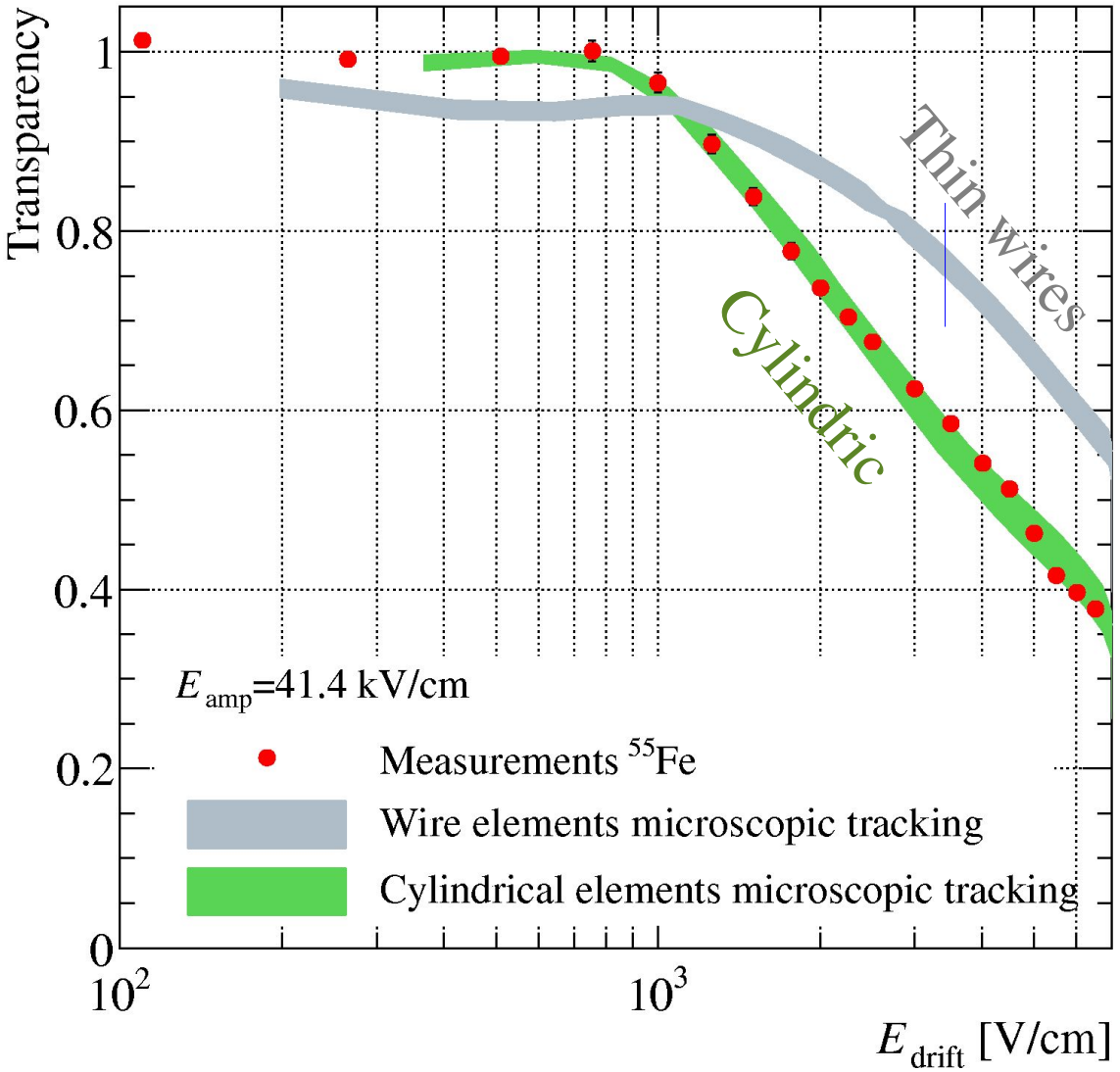
Square mesh wires ?

- Square wires are much simpler to model than cylindric wires – but this is an inadequate simplification.
- Calculations done using finite elements.



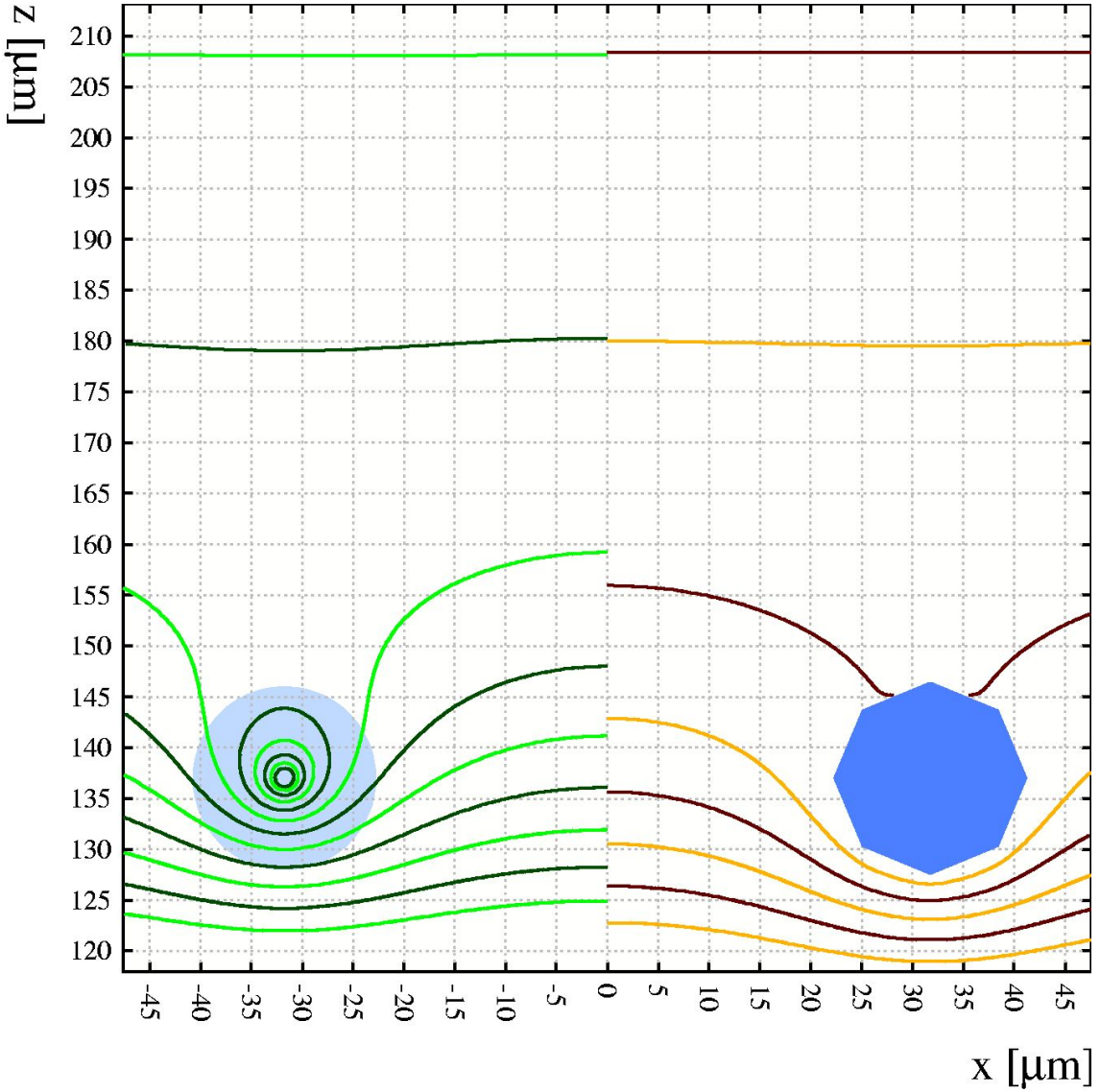
Thin-wire approximation ?

- The thin-wire approximation is usual in wire chambers – but is not adequate here.
- Calculations done using neBEM.



Dipole moment of the mesh

- Compare equipotentials at $E_{\text{drift}} = 3.3$ kV/cm: thin-wire elements overestimate the transparency by 15 %.



Boundary vs Finite elements

- The names are similar, but the methods are not ...

- Finite elements:
  - commercial programs
  - highly CPU efficient
  - closed source
  - cumbersome field maps

- Boundary elements
  - authors within RD51
  - still to optimise
  - open source
  - easy to adapt and interface

- The results are equivalent, neBEM used much more CPU time, but took less human time.

Conclusion

- Simulation of small scale devices requires that:
  - diffusion is taken into account;
  - structures are modeled without oversimplification;
  - dipole moments are included.

- Microscopic tracing, both using finite element and using boundary element fields, successfully reproduces the transparency.

- [Submitted to JINST, JINST_006P_0411]

Elastic scattering cross sections

At the request of Steve Biagi

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):

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

(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

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.]

1980s: Higher moments, high precision

- Expansion in spherical harmonics;
- An accuracy of 1 % (and better) becomes routine.

The starting point for most theoretical work is the Boltzmann equation for the electron velocity distribution function, $f(\mathbf{r}, \mathbf{v}, t)$. The latter is formally expanded in a series of spherical harmonics,

$$f(\mathbf{r}, \mathbf{v}, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f_{lm}(\mathbf{r}, v, t) Y_{lm}^{\dagger}(\hat{\mathbf{v}}), \qquad (1)$$

where $Y_{lm}(\hat{\mathbf{v}}) \equiv Y_{lm}(\theta, \phi) = P_l^{|m|}(\cos\theta)\, e^{im\phi}$, and θ, ϕ denote the polar angles of the unit velocity vector $\hat{\mathbf{v}}$ in some frame of reference.

S.L. Lin, R.E. Robson and E.A. Mason, *Moment theory of electron drift and diffusion in neutral gases in an electrostatic field,* J. Chem. Phys. **71** (1979) 3483-3498 (the "LRM" paper).

R.E. Robson and K.F. Ness, *Velocity distribution function and transport coefficients of electron swarms in gases: Spherical-harmonics decomposition of Boltzmann's equation*, Phys. Rev. A **33** (1986) 2068–2077.

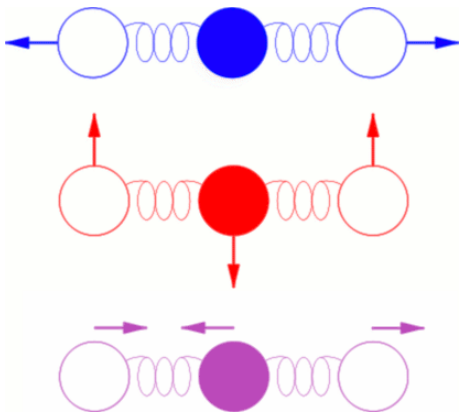
K.F. Ness and R.E. Robson, *Velocity distribution function and transport coefficients of electron swarms in gases. II. Moment equations and applications*, Phys. Rev. A **34** (1986) 2185–2209.

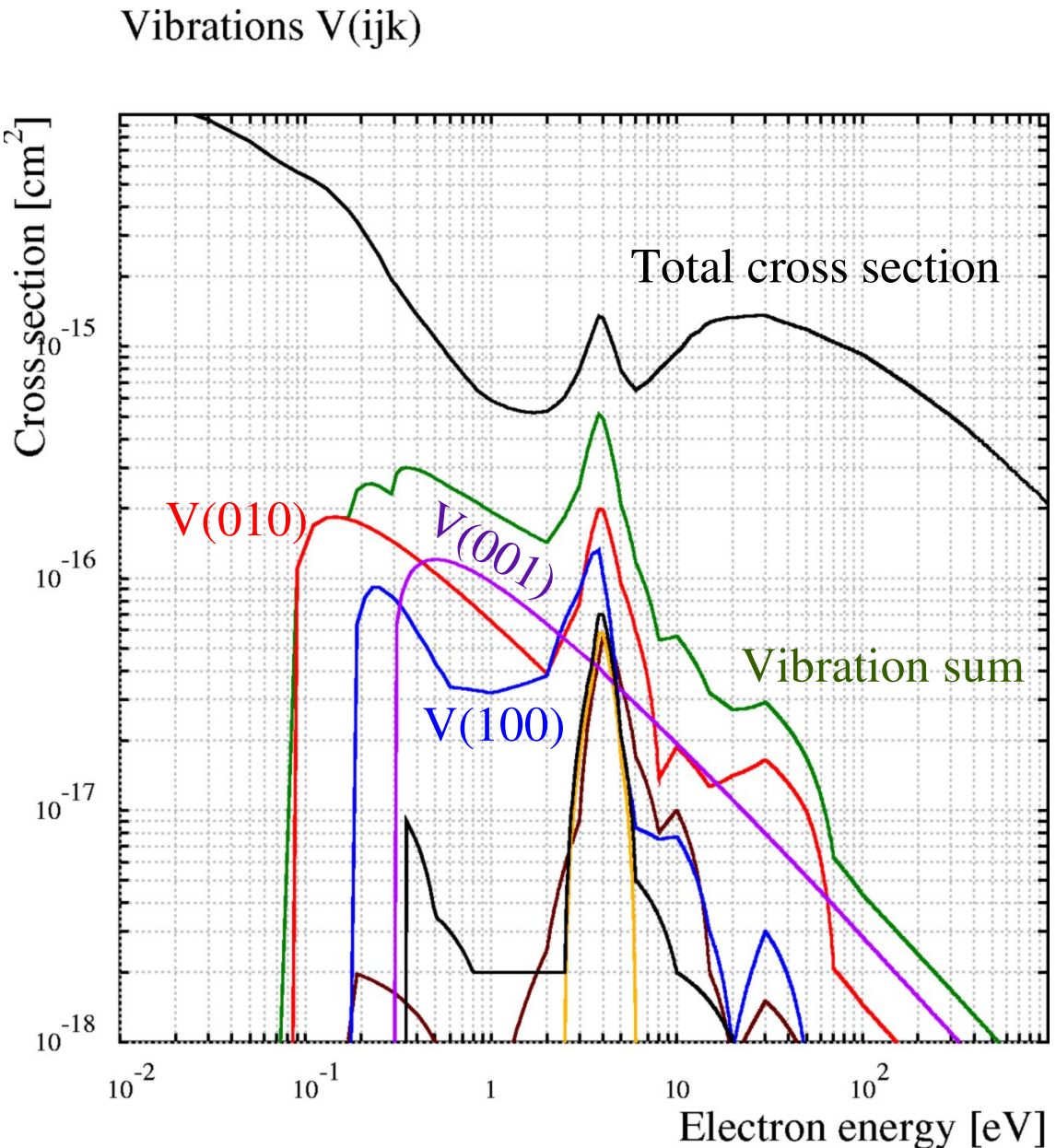
2000: Monte Carlo, Magboltz

- A large number of cross sections for 60 molecules...
  - All noble gases, *e.g.* argon:
    - elastic scattering,
    - 3 excited states and
    - ionisation.
  - Numerous organic gases, additives, *e.g.* CO_2:
    - elastic scattering,
    - 44 inelastic cross sections (vibrations, rotations, polyads)
    - 35 super-elastic cross sections,
    - 6 excited states,
    - attachment and
    - ionisation.

CO_2 – vibration modes

- CO_2 is linear:
  - O – C – O
- Vibration modes are numbered V(*ijk*)
  - *i*: symmetric,
  - *j*: bending,
  - *k*: anti-symmetric.





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. [...]”

- URL: `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
- ...

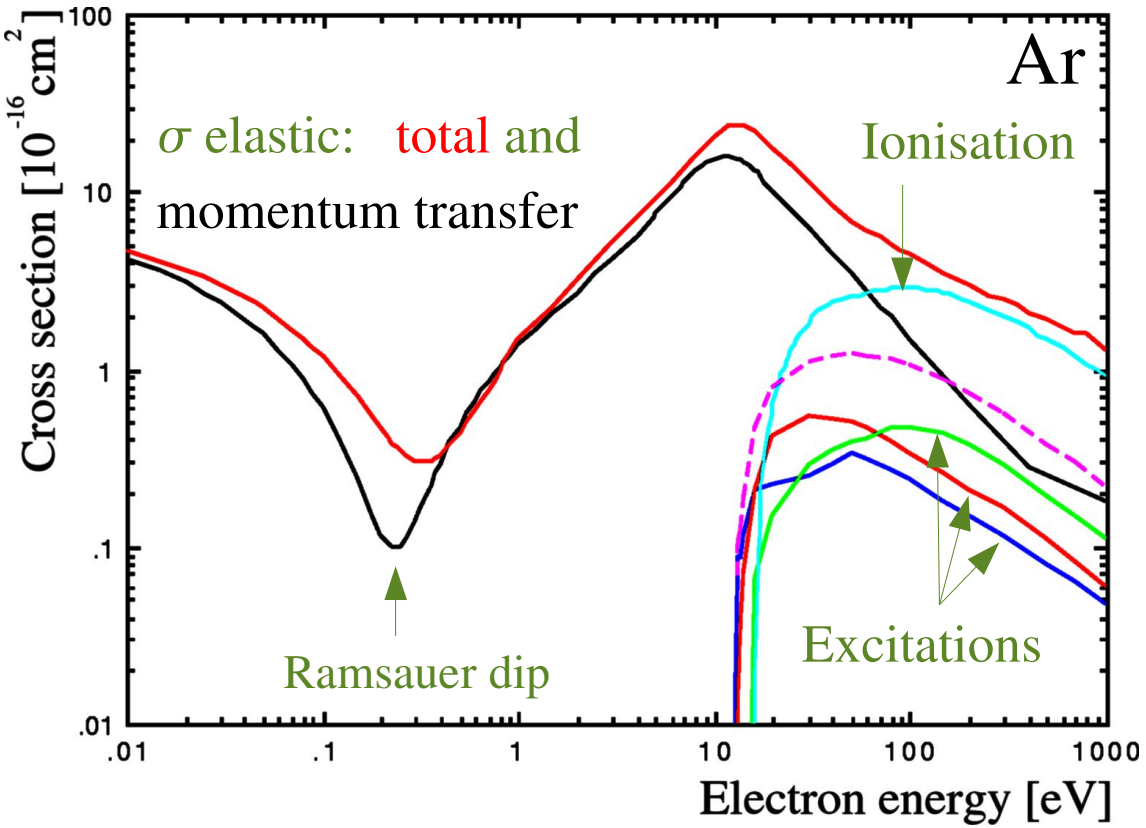
Leanne Pitchford

Michael Allan

Klaus Bartschat

Back to the basics ... elastic scattering

- Elastic scattering:
  - dominant contribution for much of the energy range that concerns us;
  - only term < 15.7 eV (ionisation threshold).
- Non-trivial structure:
  - features Ramsauer dip;
  - compare σ_{total} and σ_{mt}.



σ_{total} and σ_{mt}

- Total and momentum transfer cross section:

$$\sigma_{tot}(\epsilon) = 2\pi \int_0^{\pi} \sin\theta \, d\theta \;\; \sigma_e(\epsilon, \theta)$$

$$\sigma_{mt}(\epsilon) = 2\pi \int_0^{\pi} \sin\theta \, d\theta \;\; \sigma_e(\epsilon, \theta)(1 - \cos\theta)$$

- Special cases for σ_e:
  - isotropic: $\sigma_{mt} = \sigma_{tot}$
  - peaks forward: $\sigma_{mt} \sim 0$ no transfer
  - peaks transverse: $\sigma_{mt} \sim \sigma_{tot}$
  - peaks backwards: $\sigma_{mt} \sim 2\,\sigma_{tot}$ transfer maximal

Transport properties and σ_{mt}

- The momentum transfer cross section appears in the Boltzmann equation solved for transport parameters:

$$\frac{E^2}{3}\frac{d}{du}\left(\frac{u}{NQ_m}\frac{df}{du}\right)+\frac{2m}{M}\frac{d}{du}(u^2NQ_mf)+\frac{2mkT}{Me}\frac{d}{du}\left(u^2NQ_m\frac{df}{du}\right)+\sum_j(u+u_j)f(u+u_j)NQ_j(u+u_j)-uf(u)N_j\sum_j Q_j(u)$$

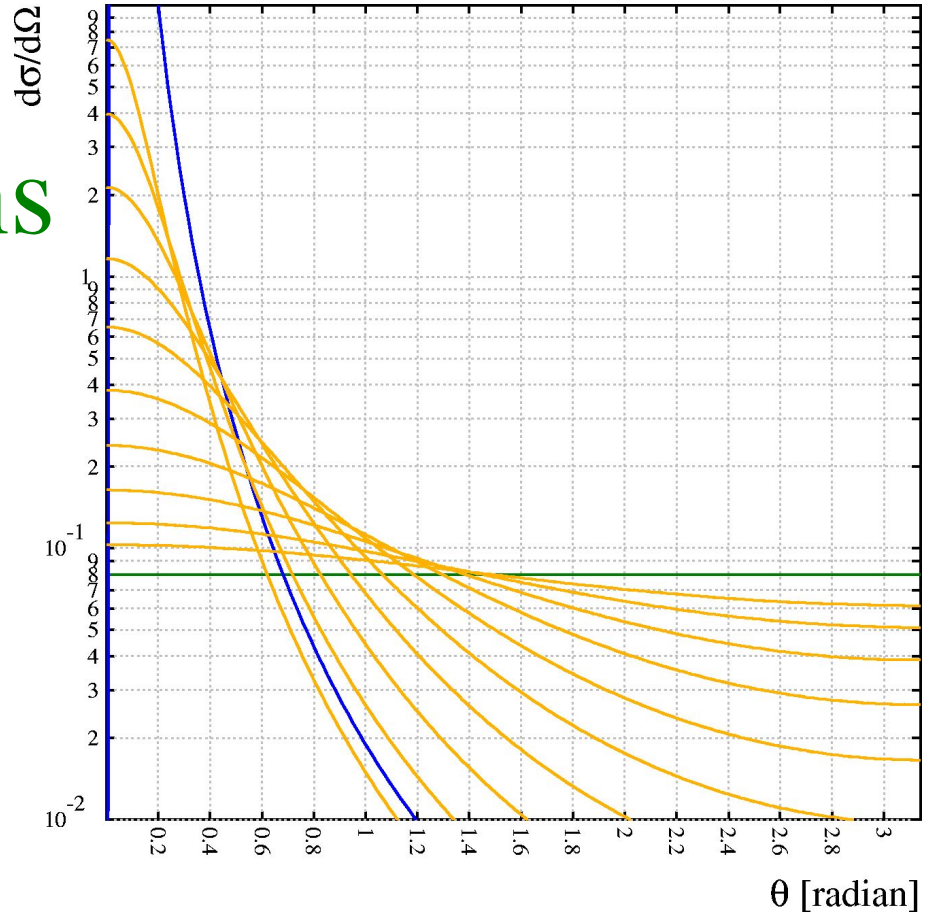
$$+\sum_j(u-u_j)f(u-u_j)NQ_{-j}(u-u_j)-uf(u)N\sum_j Q_{-j}(u)=0.$$

σ_{mt}

- Conversely, the momentum transfer cross section at low energies is traditionally derived from transport parameters (drift velocity and diffusion).

- Literature: LS Frost and AV Phelps (1962) 10.1103/PhysRev.127.1621 and later publications by the same group.

Simple cross sections



- Hard-sphere scattering:

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

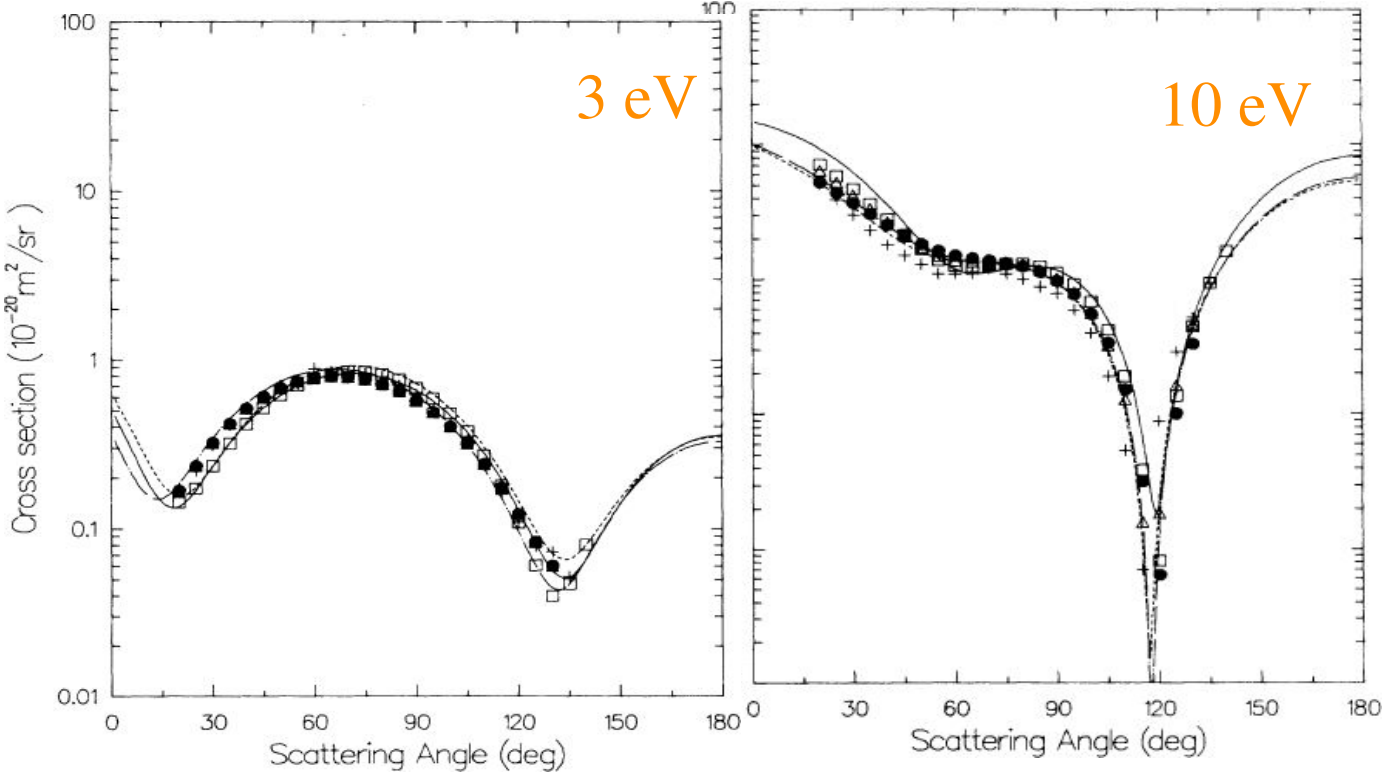
- Coulomb scattering:

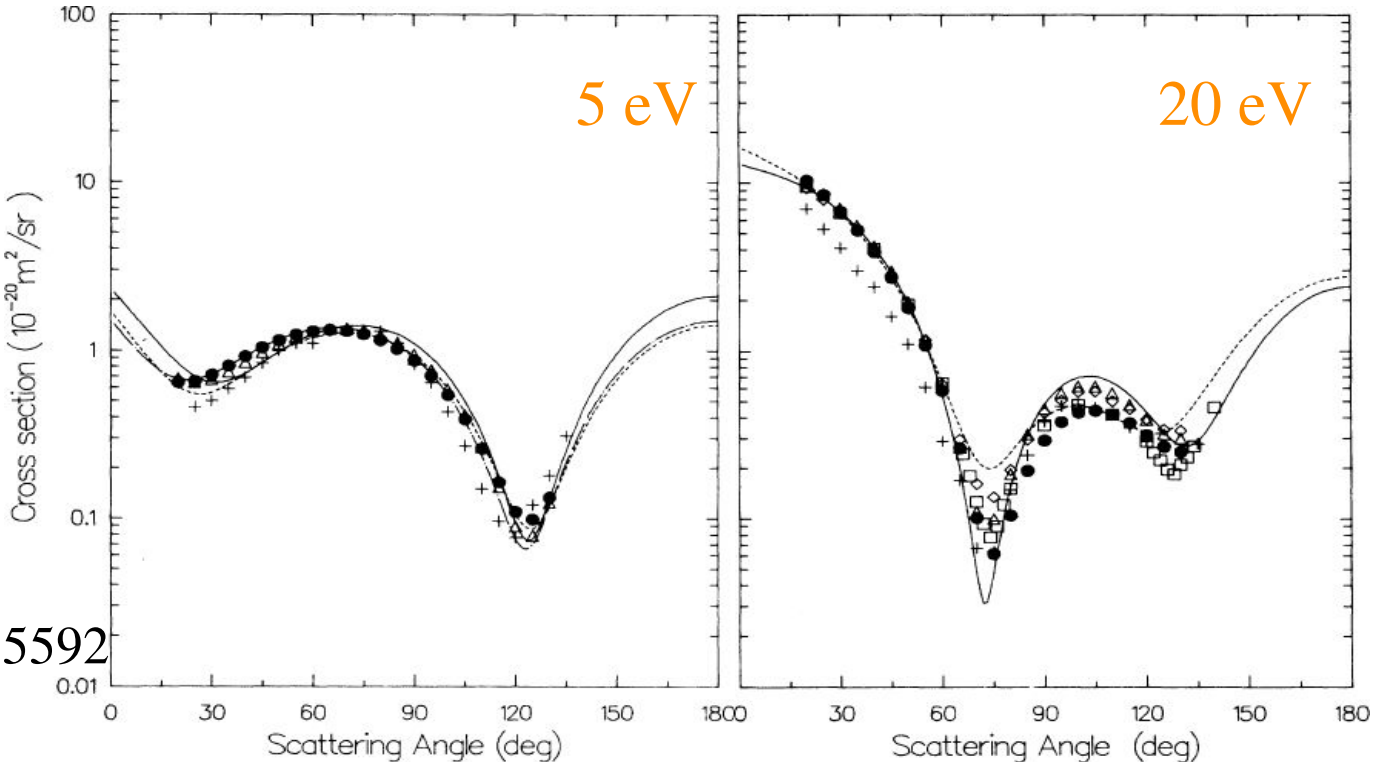
$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{1}{\sin^4(\theta/2)}$$

- Screened Coulomb scattering, 1st Born approximation:

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

Ar data





- JE Furst et al. (1989) 10.1103/PhysRevA.40.5592

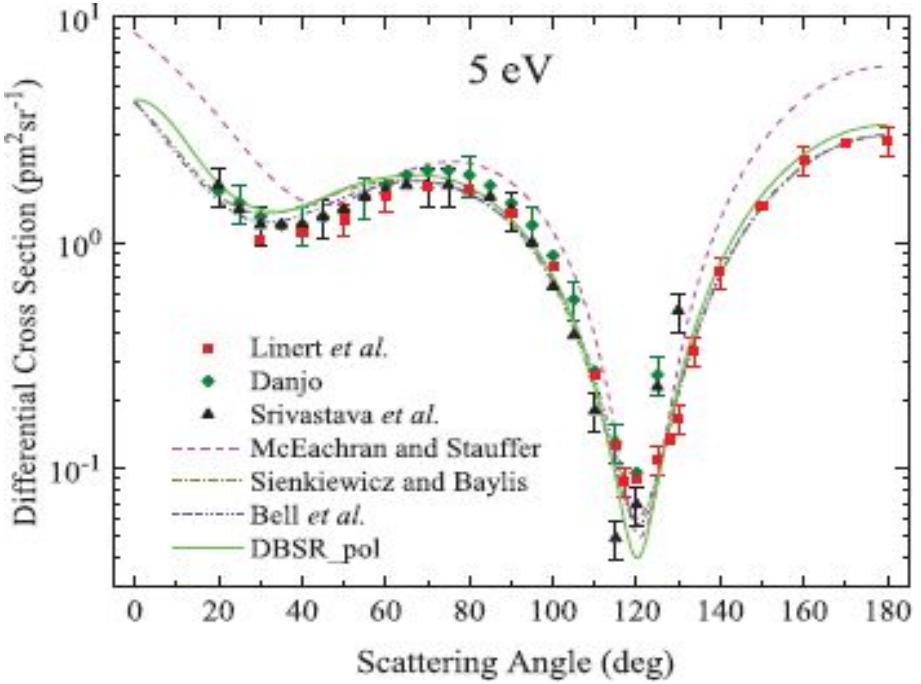
Diffraction ? Polarisation ?

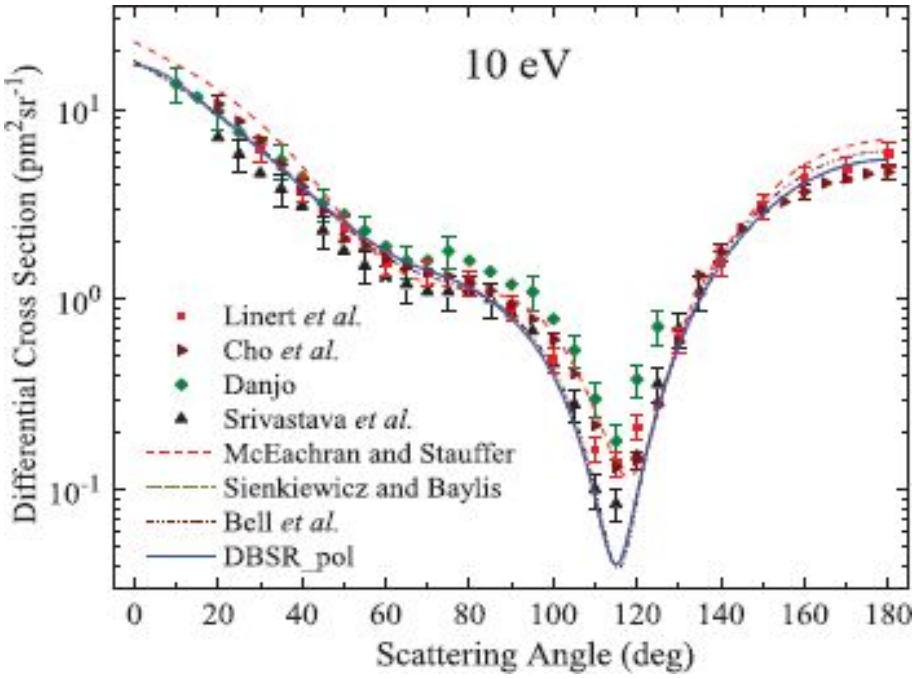
- Electron de Broglie wavelength $\lambda = h\,c\,/\,\sqrt{2}\,m_e\epsilon$
  - 1 eV: $\lambda = 1200$ pm
  - 100 eV: $\lambda = 120$ pm
  - Here, we are concerned with energies up to ~20 eV.

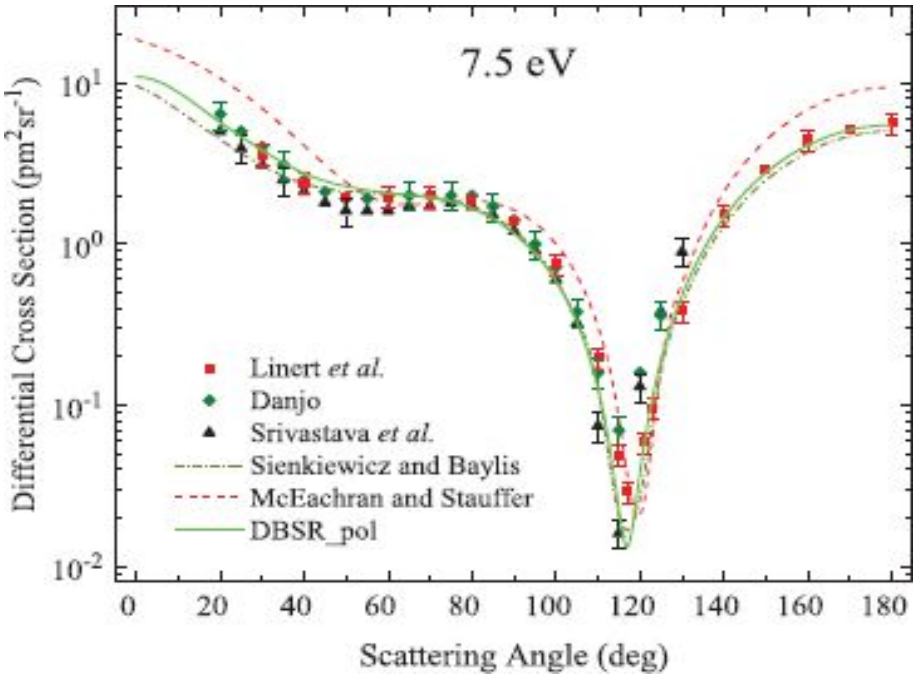
- Typical diameters (depending on definition) are smaller:
  - Ne: $r = 40 - 70$ pm
  - Ar: $r = 70 - 100$ pm
  - Xe: $r = 100 - 140$ pm

Krypton data

- Earlier data, compared with the DBSR_pol calculation



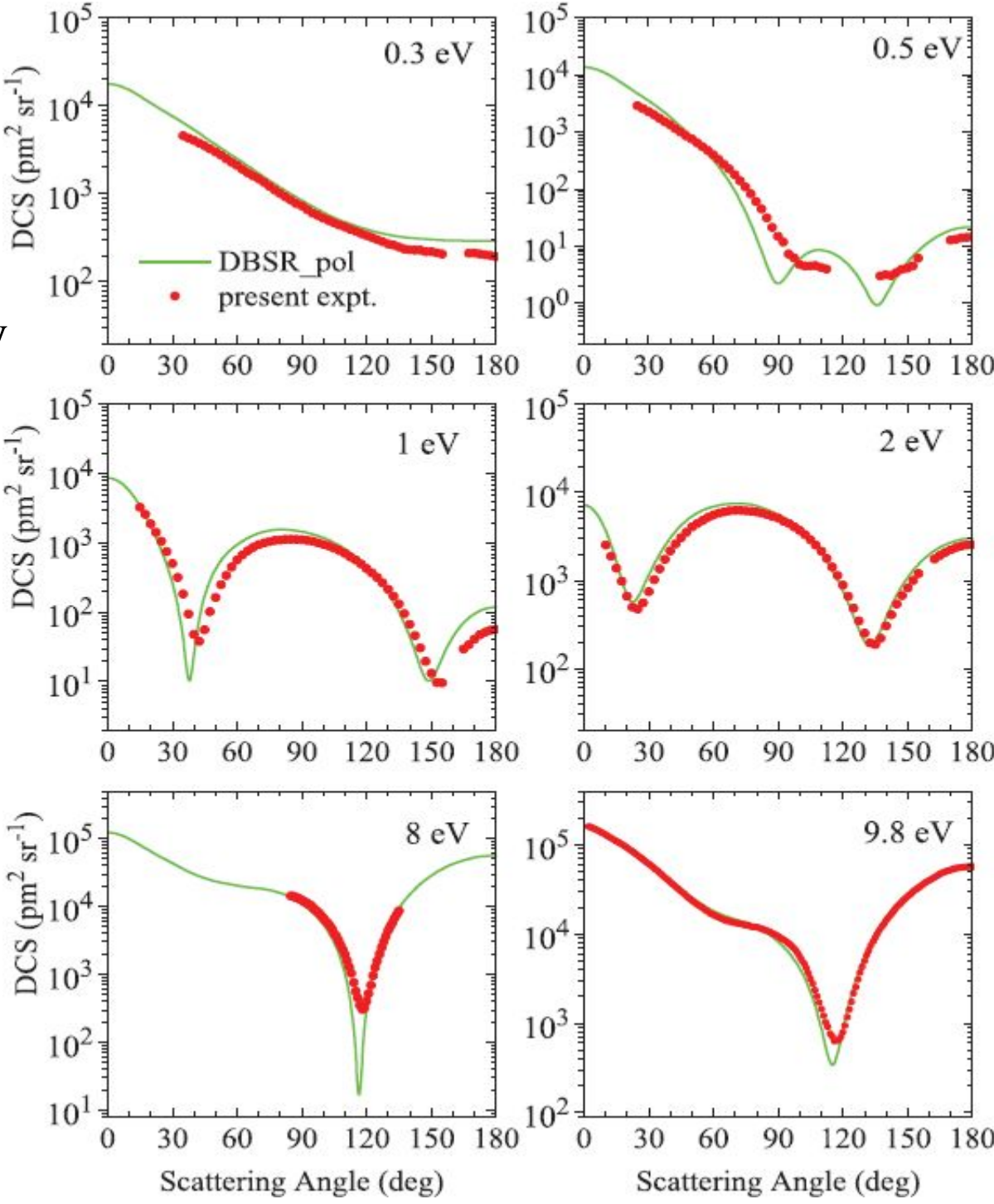




Krypton data

- A remarkable joint study with high-precision experimental data and a theoretical model has just been published:

  O. Zatsarinny et al. (2011)
  10.1103/PhysRevA.83.032713



Generating scattering angles

- Magboltz uses the following recipe:
  - Tweak the Born approximation by adding a parameter ξ:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{1}{4\pi}\frac{1+8\epsilon/\epsilon_0}{(1+4\epsilon/\epsilon_0-4\epsilon/\epsilon_0\cos\theta)^2} \rightarrow \frac{1}{4\pi}\frac{1-\xi^2(\epsilon/\epsilon_0)}{(1-\xi(\epsilon/\epsilon_0)\cos\theta)^2},$$

  - ξ is determined from $\sigma_{\mathrm{mt}} / \sigma_{\mathrm{tot}}$ both integrated over $\mathrm{d}\Omega$,
  - when ξ is known, generate a scattering angle θ according to the above differential cross section.

- Andriy Okhrimovskyy et al. (2002) 10.1103/PhysRevE.65.037402

Using this data

- Quadrupole terms and higher are not thought to affect the transport parameters at the 0.1 % level.

- Since the current target precision of Magboltz is lower than that, the principal use for now of these differential cross sections is through the ratio of the total and momentum transfer cross sections.

Plans on elastic cross sections

- It is notoriously difficult to measure absolute electron elastic cross sections – the associated uncertainties are amongst the most important in Magboltz.

- The goal is establishing a reference set of elastic cross sections at the maximum in Ar, Kr and Xe.

- Currently, the accuracy of σ_{mt} is ~ 5 % and the hope is that this will reduce to 2-3 %.