Electron scattering: cross sections for plasma modeling

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Data Center for Plasma Properties

NFRI, Gunsan, 03.12.2014

Electrical discharges

- Discharges:

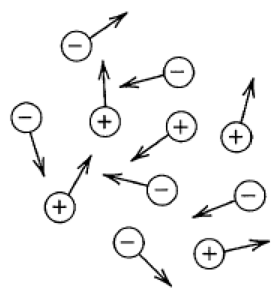
  Are driven by voltage or current sources

  Charged particle collisions with neutral particles are important

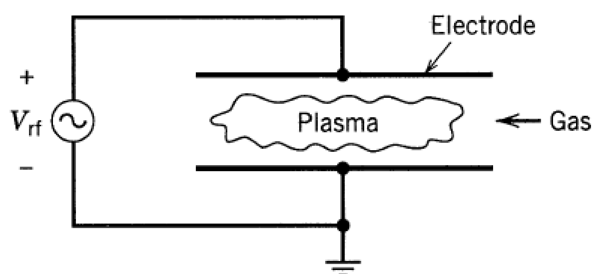
  There are boundaries at which surface losses are important

  Ionization of neutrals sustains the plasma in the steady state

  The electrons are not in thermal equilibrium with the ions



(a)

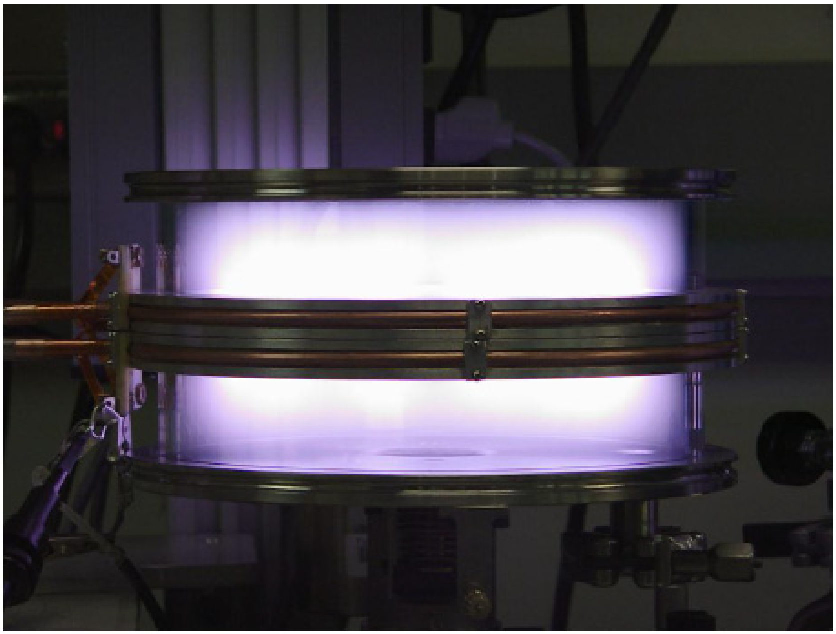


(b)

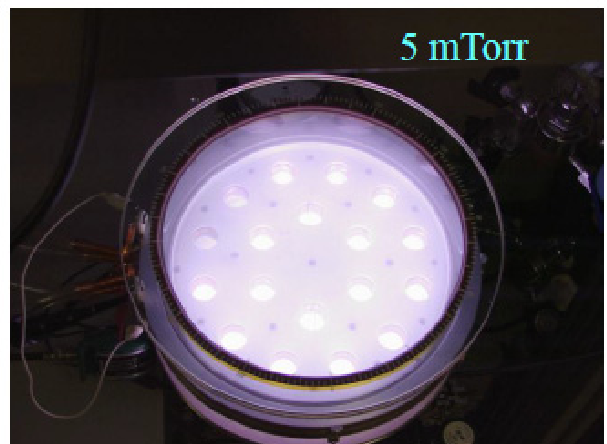
Michael A. Lieberman, 2003

Plasma etching

Xenon, 400 kHz, 10 mTorr, 400 W



V. Godyak, PEUG, Santa Clara, 2003



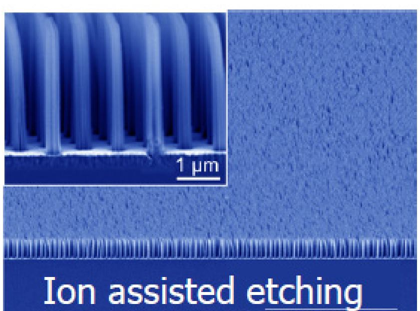
other plasmas

Ane Aanesland
Laboratoire de Physique des Plasmas
CNRS – Ecole Polytechnique
France

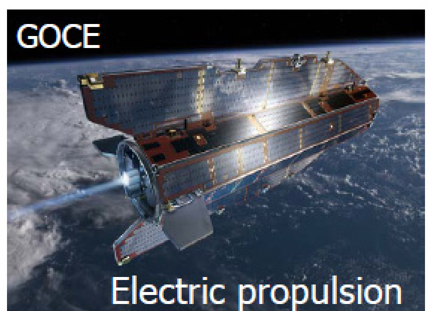
Electrons – Pros & Cons

Electrons required for plasma **generation** and beam **neutralization**

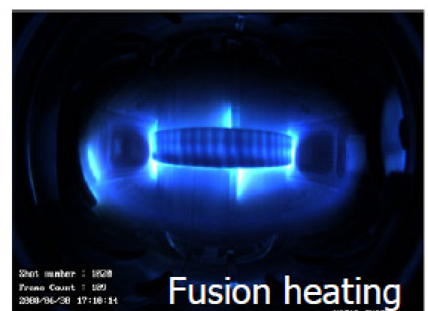
Electrons cause problems by surface and differential **charging** and slow ion-electron **recombination**



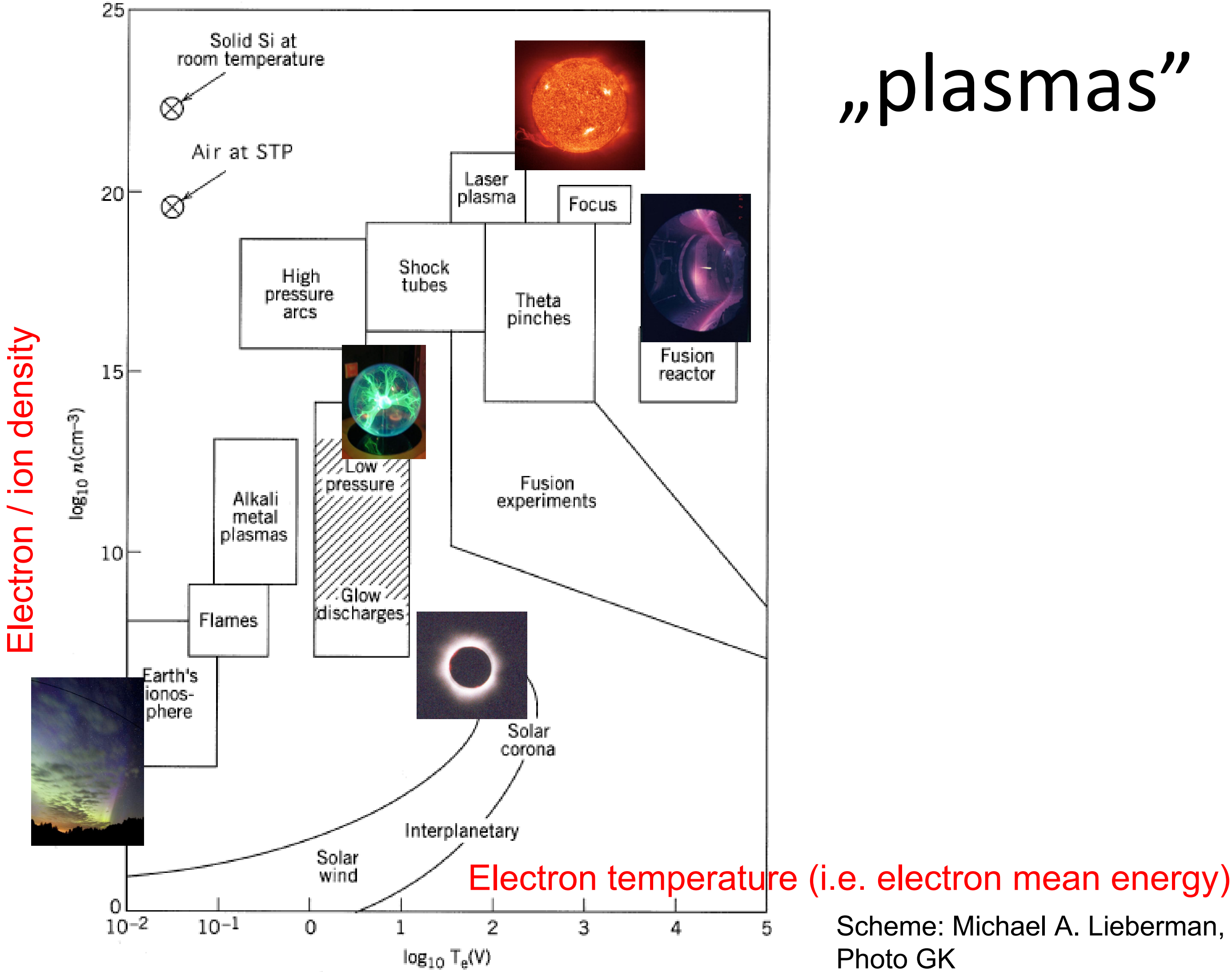
Ion assisted etching



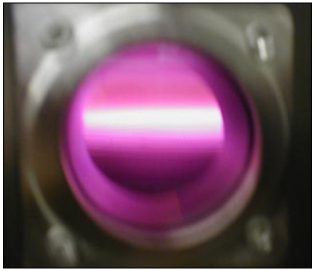
Electric propulsion


Fusion heating

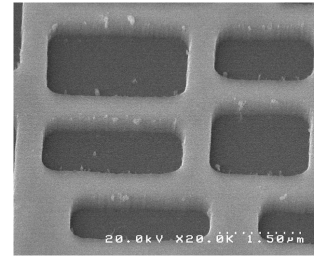
„plasmas”



Scheme: Michael A. Lieberman, 2003
Photo GK



Plasma etching

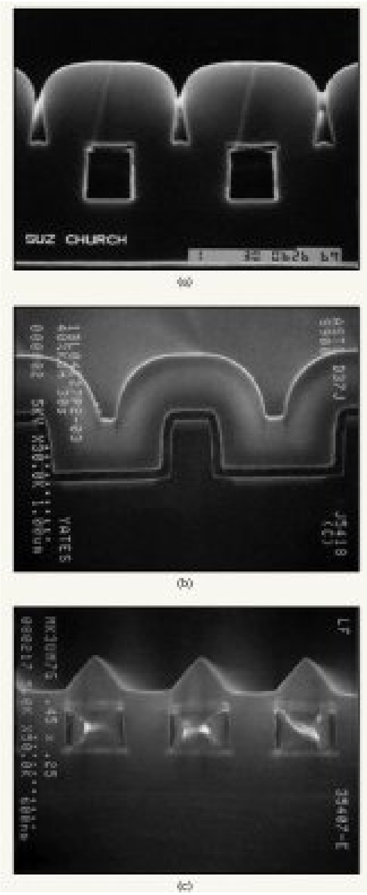


Material	Etch Gases	Reactive Species	By-product
Aluminum	Boron Trichloride and Chlorine	Free chlorine	AlC13
Polyimide	Oxygen	Monatomic oxygen and/or ozone	CO and H20
Polysilicon	CF4 / 8% SF6 or Chlorine	Free fluorine or free chlorine	SiF4 or SiCl4
Silicon dioxide	Freon 14 and Freon 23	CF3	SiF4 and CO
Silicon nitride	Freon 14 (CF4) / 8% O2 or Sulfur Hexafluoride	Free fluorine	SiF4 and N2

Plasma deposition

Table 1 Typical electron-impact reactions of silane molecules in an rf plasma discharge. The asterisk (*) refers to electronic excited state. From [1].

Reactant	Reaction products	Enthalpy of formation (eV)
$e^- + SiH_4 \longrightarrow$	$SiH_2 + H_2 + e^-$	2.2
	$SiH_3 + H + e^-$	4.0
	$Si + 2H_2 + e^-$	4.2
	$SiH + H_2 + H + e^-$	5.7
	$SiH^* + H_2 + H + e^-$	8.9
	$Si^* + 2H_2 + e^-$	9.5
	$SiH_2 + 2H_2 + 2e^-$	11.9
	$SiH_3 + H + 2e^-$	12.3
	$Si+ + 2H_2 + 2e^-$	13.6
	$SiH+ + H_2 + H + 2e^-$	15.3



Plasma-assisted chemical vapor deposition of dielectric thin films for ULSI semiconductor circuits
D. R. Cote, S. V. Nguyen, A. K. Stamper, D. S. Armbrust, D. Tobben, R. A. Conti, and G. Y. Lee

IMB J. Res. Develop. 43, 1/2, 1999

Plasma deposition

C_2F_6/H_2 C_2H_2/Ar Ar/CH_4

Selected Applications 377

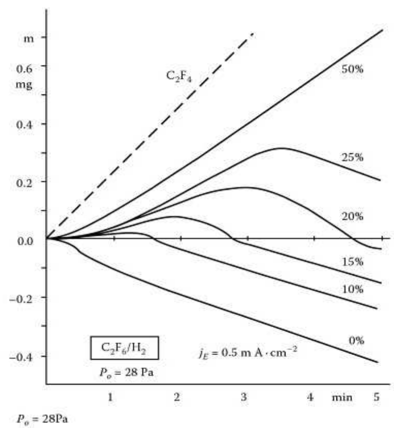


FIGURE 8.50 Polymer deposition and etching of Si measured on a Si substrate positioned on the powered electrode of a 50 kHz discharge in closed C_2F_6/H_2 discharges in relation to the discharge time for various H_2 admixtures ($p_o = 28$ Pa, $j = 0.5$ mA).

400 Nonthermal Plasma Chemistry and Physics

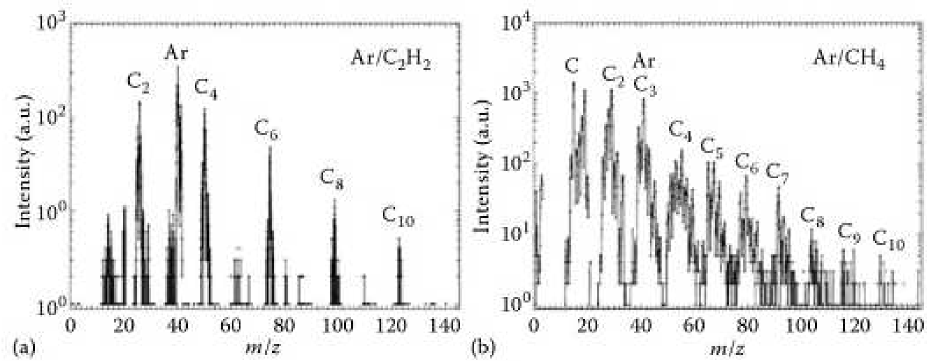


FIGURE 8.64 Ion mass spectra of Ar/C_2H_2 (a) and Ar/CH_4 (b) rf-discharges. (From Do, H.T. et al., *Contrib. Plasm. Phys.*, 45, 378, 2005.)

$$C_2F_6 + H_2 + e^- \rightarrow (C_xF_yH_z)_n + e^- + \ldots$$

$$C_2H_2 + Ar + e^- \rightarrow C_{10} + Ar + e^- \ldots$$

Nonthermal Plasma Chemistry and Physics, ed. J. Meichsner, M. Schmidt, R. Schneider, H.E. Wagner
CRC Press, Taylor & Francis Group, Boca Raton, 2013

Modeling gas discharges

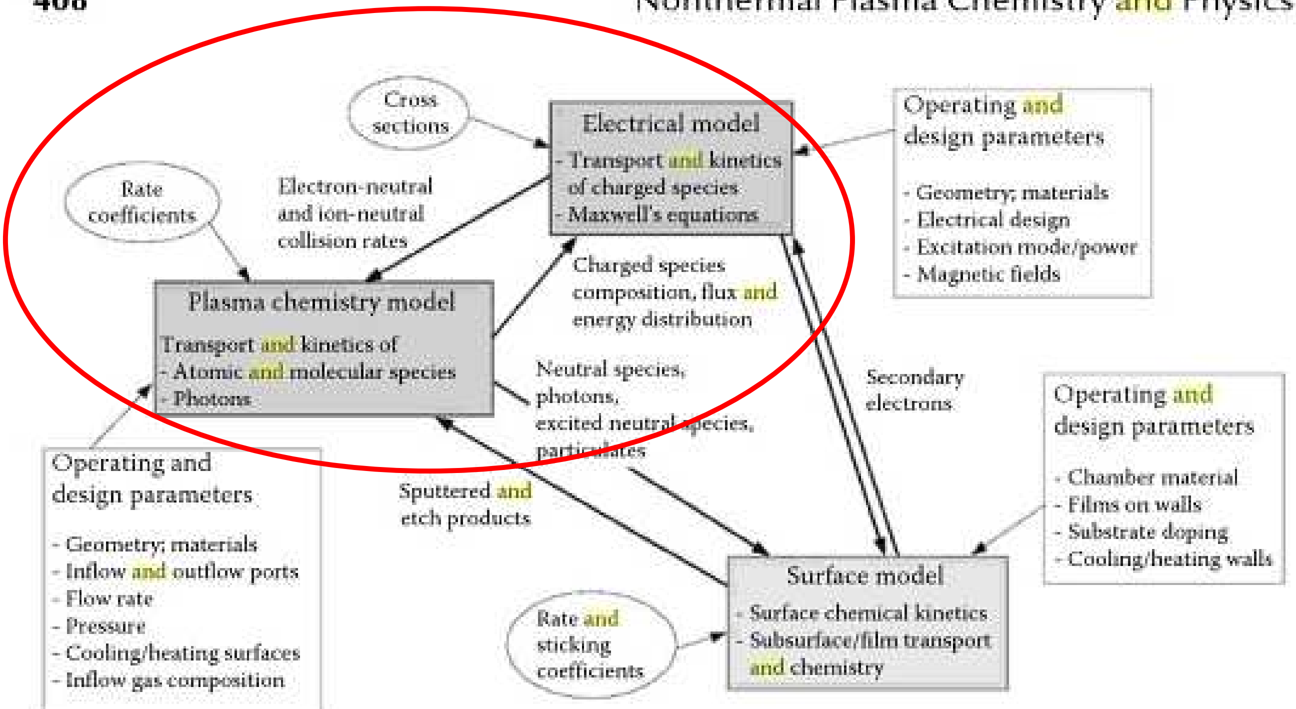


FIGURE 9.1 Components of plasma modeling. (From Graves, D.B., *IEEE Trans. Plasma Sci.*, 22, 31, 1994.)

Meichnser et al., *Non-thermal plasma chemistry and physics*, Taylor & Francis (2013)

1. Total cross section

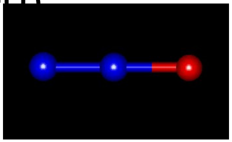
$$I = I_0 \exp(-\sigma n l)$$

2. Partial cross sections:

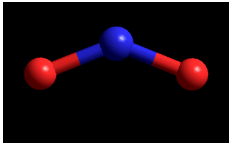
elastic scattering $e^- + A \rightarrow e^- + A$

rotational excitation $e^- + CH_4\ (J=0) \rightarrow e^- + CH_4\ (J=2)$

vibrational excitation $e^- + AB\ (v=0) \rightarrow e^- + AB\ (v>0)$



electron attachment (dissociative) $e^- + AB \rightarrow A^- + B$



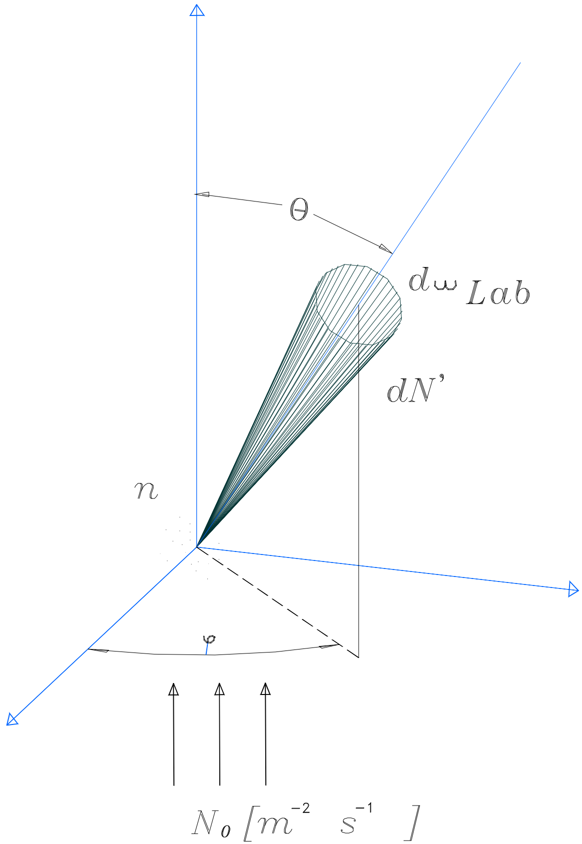
electronic excitation $e^- + A \rightarrow e^- + A^*$

neutral dissociation $e^- + AB \rightarrow A + B + e^-$

ionization $e^- + A \rightarrow A^+ + 2e^-$

dissociative ionization $e^- + AB \rightarrow A + B^+ + 2e^-$

Definition: differential cross section



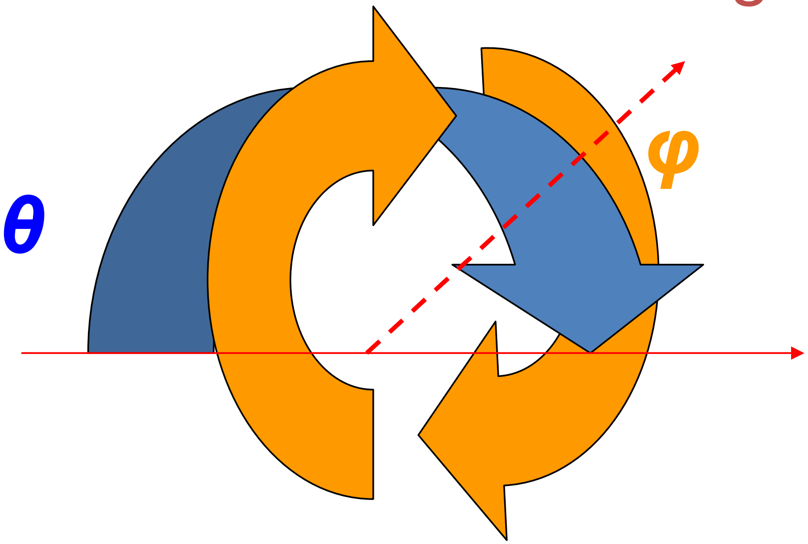
$$\frac{d\sigma}{d\omega} = \frac{dN'}{nN_0}$$

units

$$\left[\frac{N'}{nN_0}\right] = \frac{1/s/sr}{1/m^3}\frac{1}{1/(m^2 s)} = 1/(m^2 sr)$$

DCS = number of particles scattered into a given angle [in $1/(m^2sr)$]

Differential → integral cross section



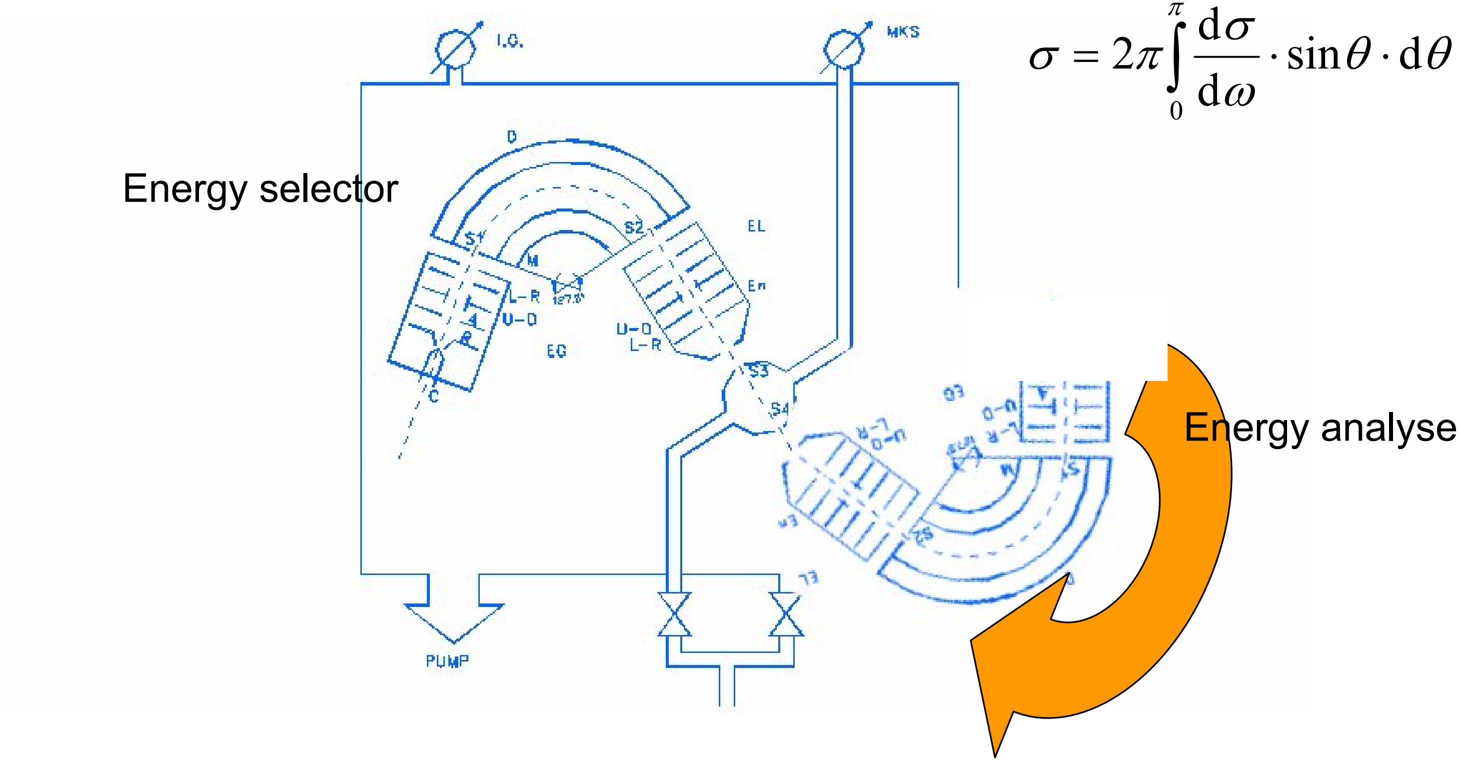
$$\sigma = \int_{4\pi} \frac{d\sigma}{d\omega} d\omega = \int_0^{2\pi}\int_0^{\pi} \frac{d\sigma}{d\omega} d\theta d\varphi$$

cylindric symmetry:

$$\sigma = 2\pi \int_0^{\pi} \frac{\mathrm{d}\sigma}{\mathrm{d}\omega} \cdot \sin\theta \cdot \mathrm{d}\theta$$

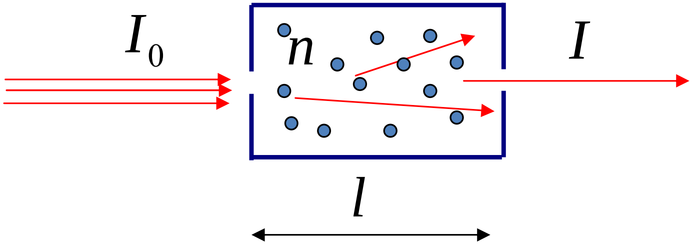
Differential → integral cross sections

$$\sigma = 2\pi \int_0^{\pi} \frac{\mathrm{d}\sigma}{\mathrm{d}\omega} \cdot \sin\theta \cdot \mathrm{d}\theta$$



Measurements require normalization (we do not know *n* and *N*) !

Total cross section = attenuation of the beam



de Beer – Lambert law: $I = I_0 \exp(-\sigma n l)$

$$\sigma = -\frac{1}{nl} \ln \frac{I}{I_0}$$

We need to measure only: I, I_0, n, l
(n we get from p and T)

Total (absolute) measurements: I, I_0, p, T, L

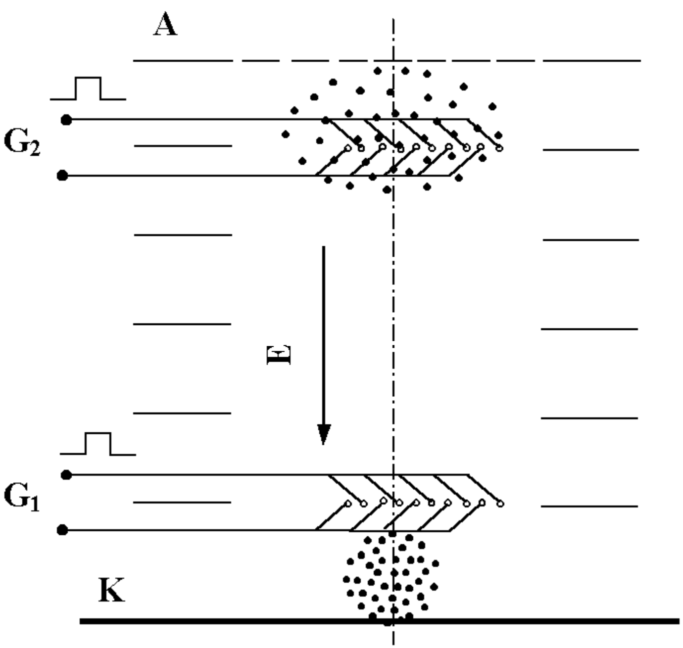
- declared errors: “**a few** per cent”

(1% pressure, 1% temperature, <1% scattering path ….)

other errors: “a few more per cent”:
- energy resolution
- angular acceptance
- inelastic scattering discrimination
- normalizations (e.g. scattering path length)
- current stability and/or intensity

Electron-drift measurements → momentum transfer cross sections

$$\frac{\partial}{\partial t} n_e(\mathbf{r},t) = -w\frac{\partial}{\partial z} n_e(\mathbf{r},t) + D_T\left[\frac{\partial^2}{\partial x^2} n_e(\mathbf{r},t) + \frac{\partial^2}{\partial y^2} n_e(\mathbf{r},t)\right] + D_L \frac{\partial^2}{\partial z^2} n_e(\mathbf{r},t)$$



$$w = -\left(\frac{2}{m}\right)^{1/2} \frac{eF}{3N}\int_0^\infty \frac{E}{\sigma_m(E)} \frac{df_0(E)}{dE} dE$$

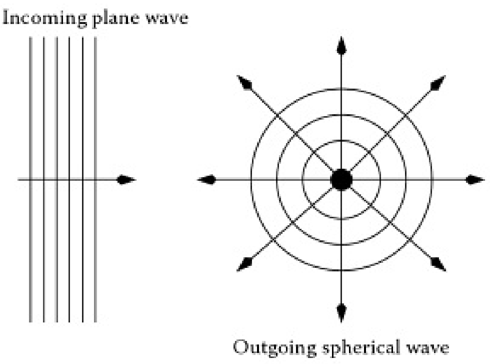
$$D_T = \left(\frac{2}{m}\right)^{1/2} \frac{1}{3N}\int_0^\infty \frac{E}{\sigma_m(E)} f_0(E) dE$$

W. Roznerski, J. Mechlińska-Drewko

Electron – atom scattering theory

$$\Phi = e^{ikz} + \frac{f(\theta)}{r} e^{ikr}$$

$$\frac{d\sigma}{d\omega} = |f(\theta)|^2$$



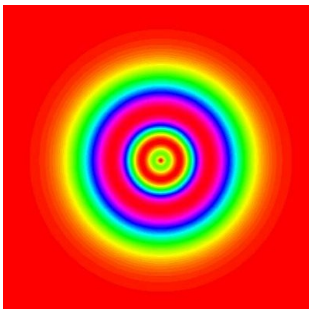
„Partial waves”, i.e. with different orbital momentum *L: s*, *p*, *d* etc.

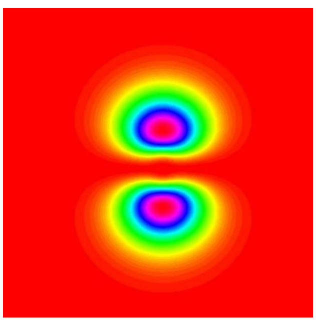
$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)\left[\exp(2i\delta_l) - 1\right] \cdot P_l(\cos\theta)$$

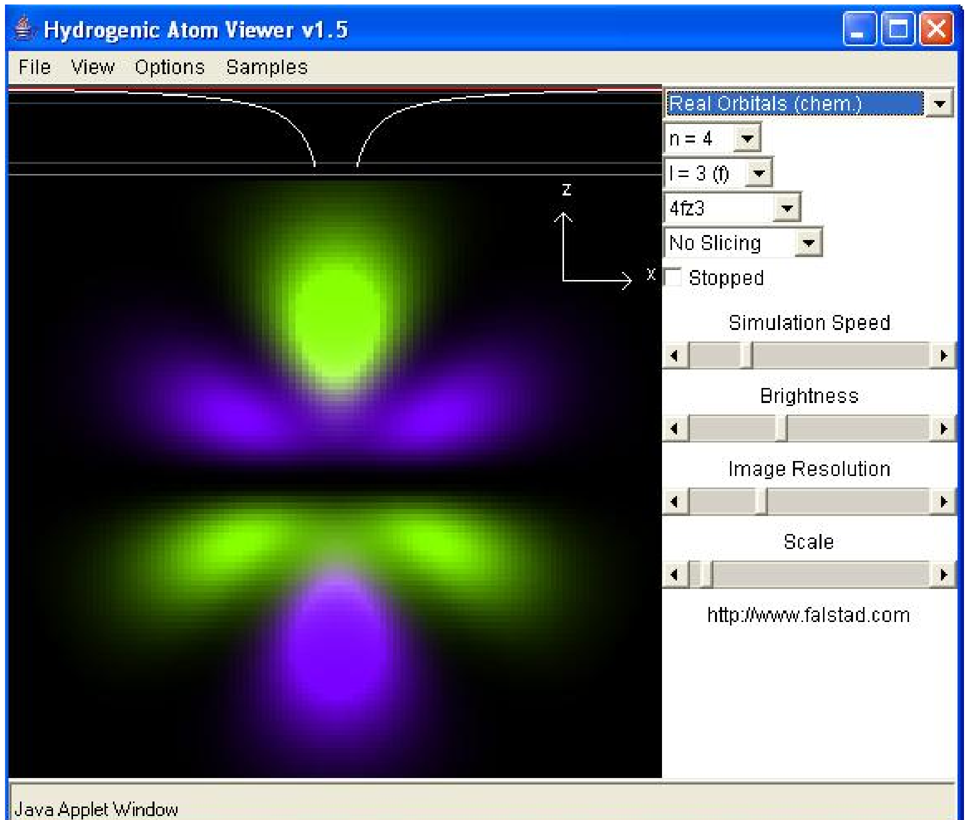
$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \cdot \sin^2 \delta_l$$

orbitals *s*, *p*, *d* etc.

- $P_l(\cos\theta)$ are the same „spherical harmonic functions” that appear in atomic hydrogen orbitals, like *f*-orbital shown here







Electron – atom (elementary) scattering theory

$$\frac{d\sigma}{d\omega} = \left|f(\theta)\right|^2$$

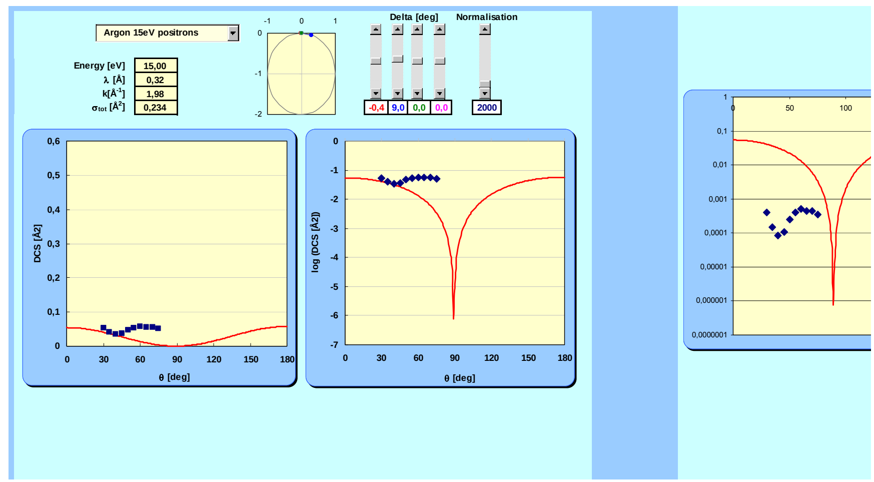
$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[\exp(2i\delta_l) - 1\right]\cdot P_l(\cos\theta)$$

$$\frac{d\sigma}{d\theta}(\theta) \propto \cdot[P_l(\cos\theta)]^2$$

$$[P_0(\cos\theta)]^2 = 1$$

$$[P_1(\cos\theta)]^2 = (\cos\theta)^2$$

$$[P_1(\cos\theta)]^2 = [\frac{1}{2}(3\cos\theta^2 - 1)]^2$$

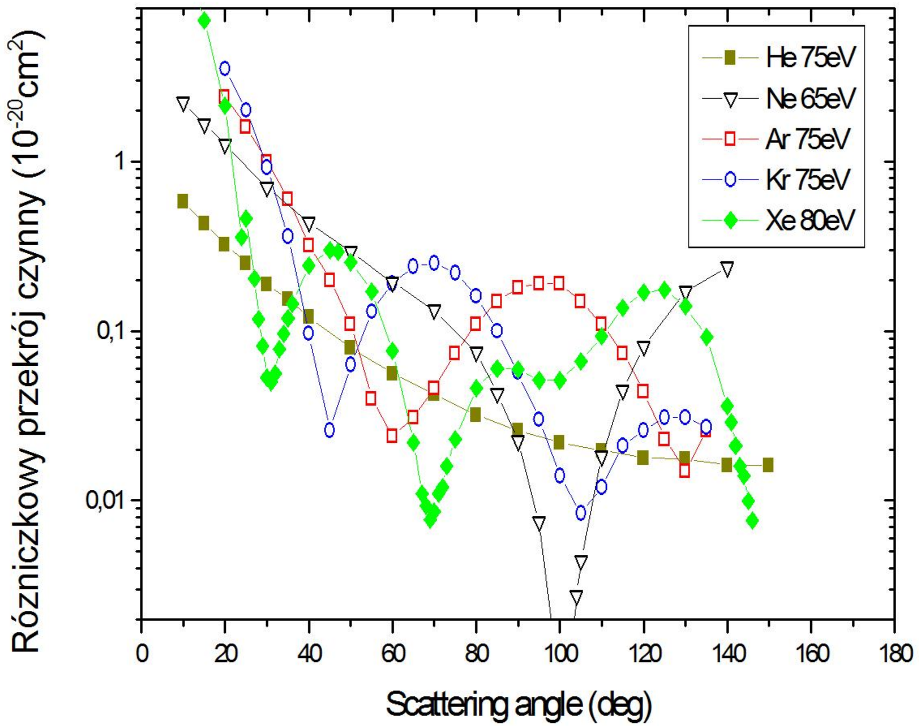


H. Nowakowska

so, we can expect that DCS are complicated functions of θ

Electron – atom scattering experiment

$\sigma(\theta) \propto \cdot[P_l(\cos\theta)]^2$ we can expect that DCS are complicated functions of θ



Electron – atom scattering experiment

$$\sigma(E) \propto \cdot \sum_l [P_l(\cos\theta, E)]^2$$ we can expect that ICS are complicated functions of E

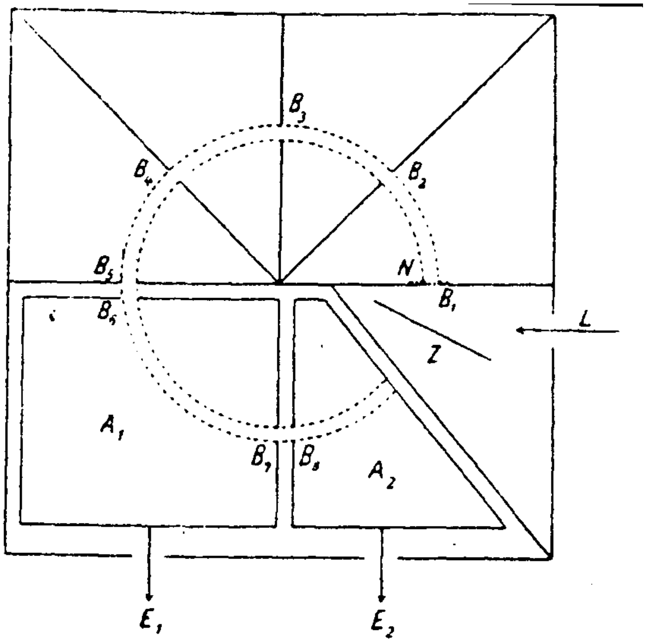
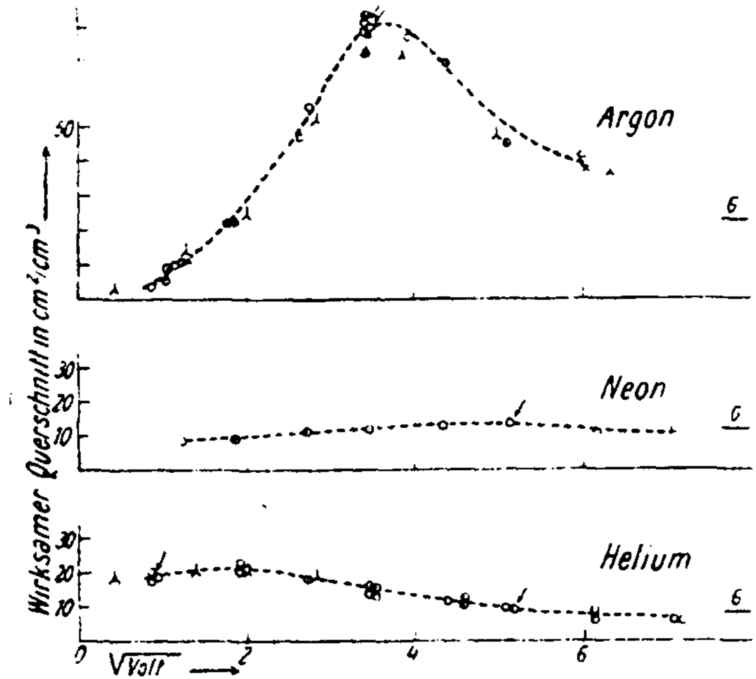
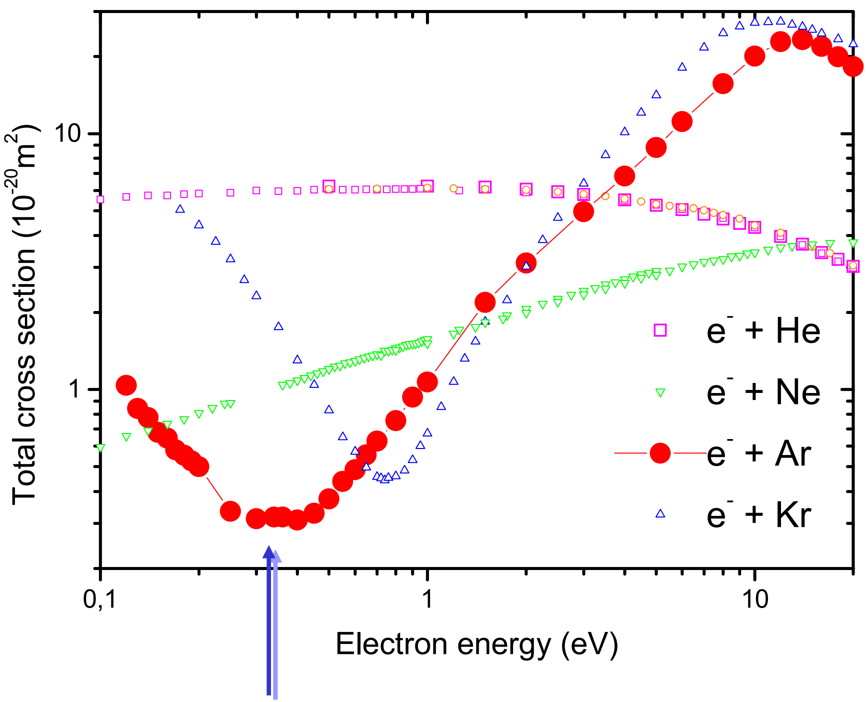


Fig. 1.

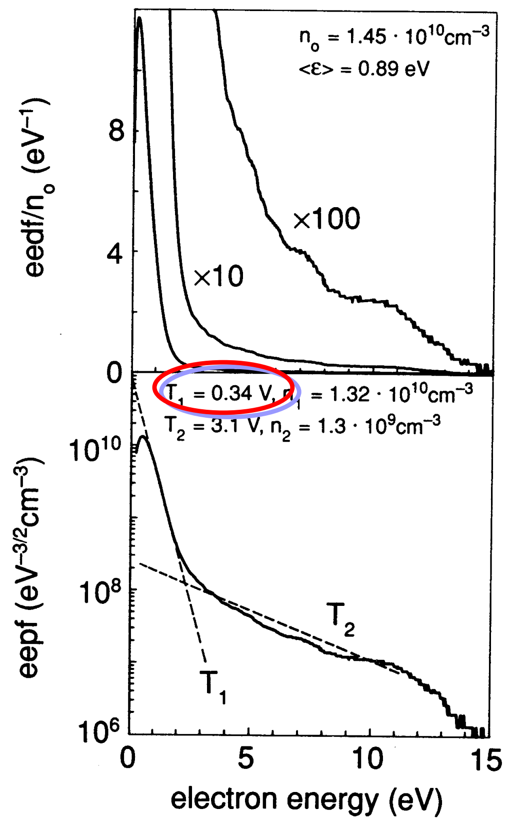


Carl Ramsauer, Gdansk, 1921

Plasma temperature ← integral cross sections

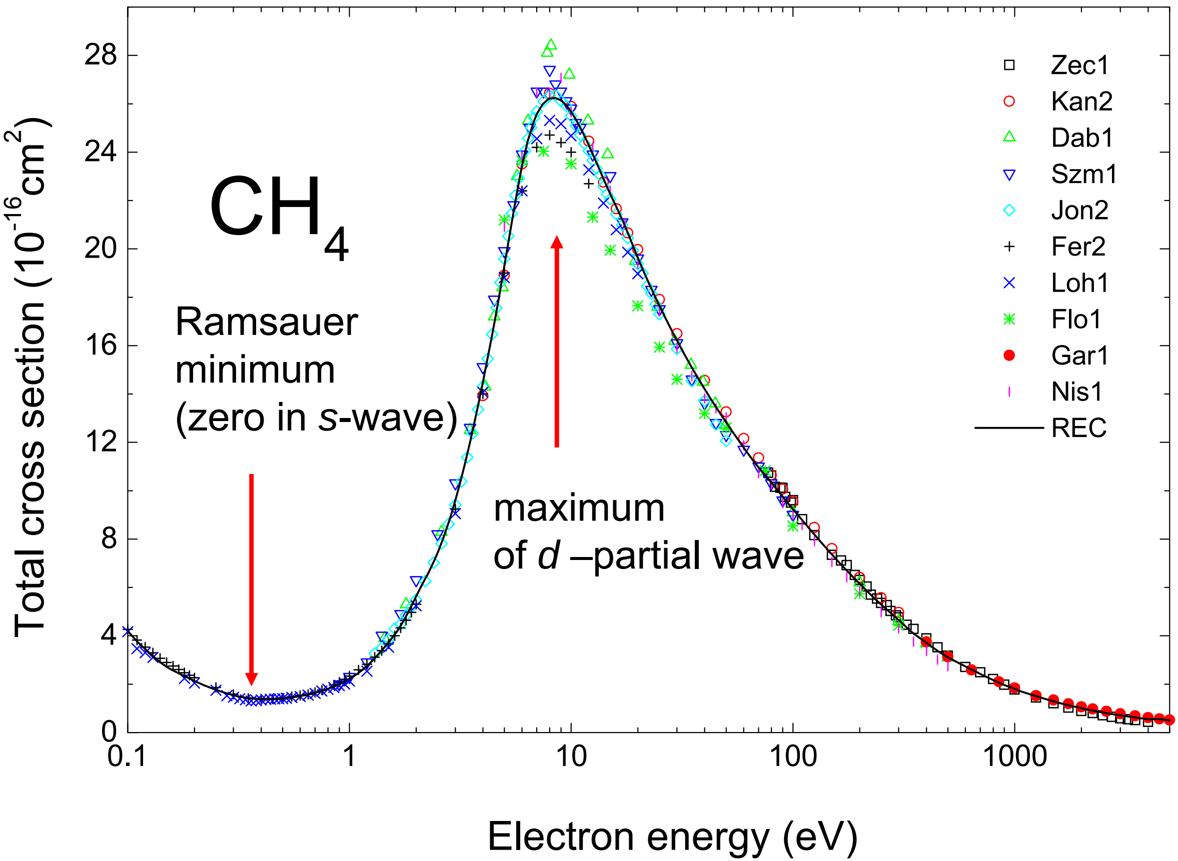


Ramsauer
minimum
(zero in *s*-wave)

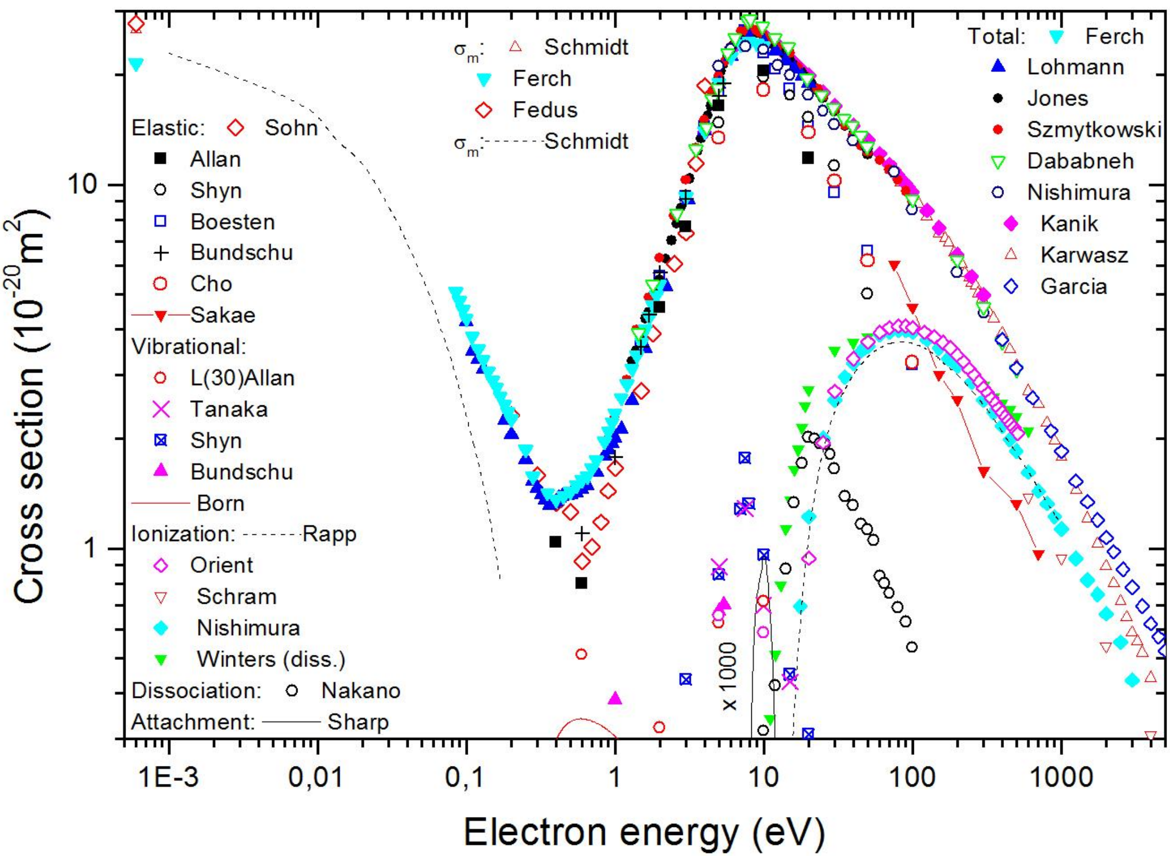


V. Godyak, Sendai 2006

Total cross section: CH_4

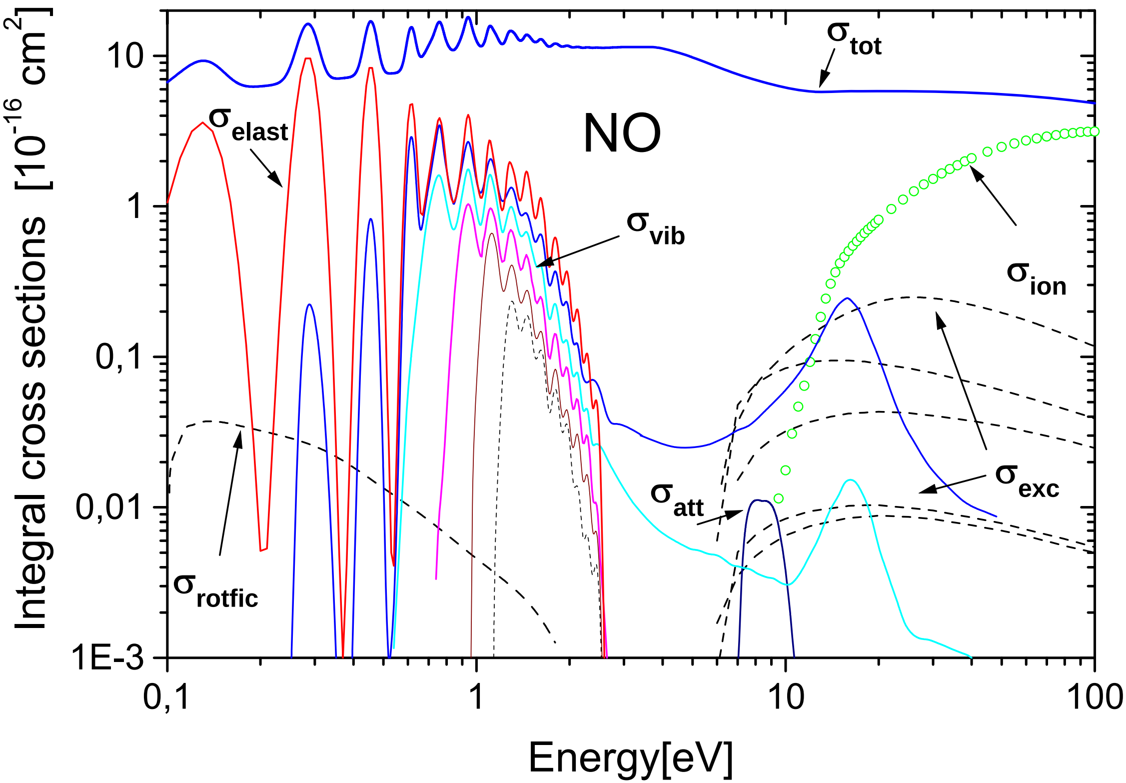


Integral cross sections for CH_4



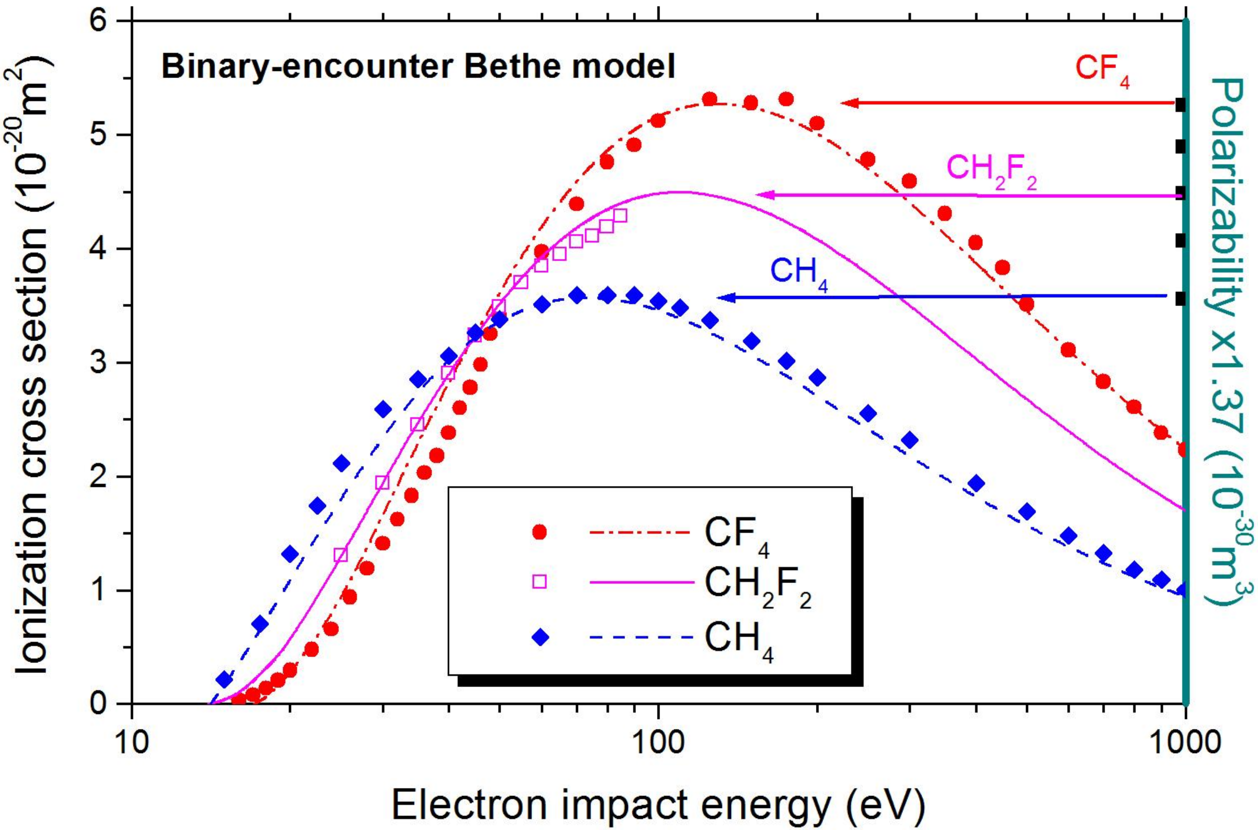
G. Karwasz, R. S. Brusa, A. Zecca, Riv. Nuovo Cimento, 2001

NO – overlapping resonances



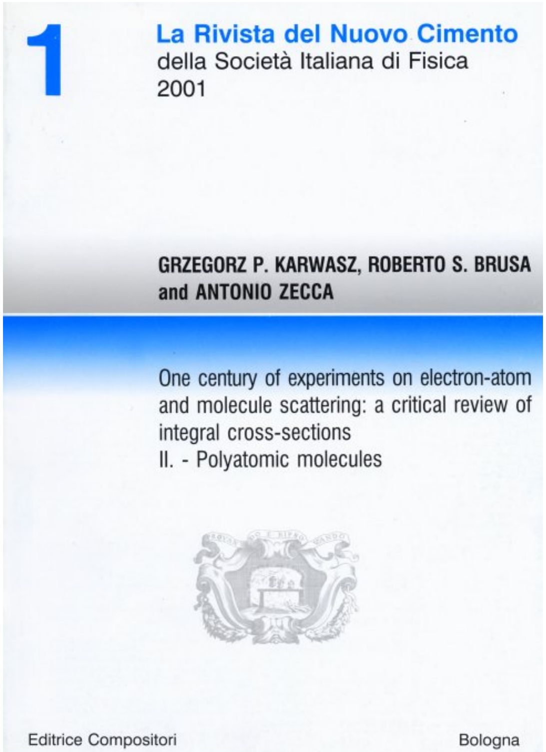
Karwasz & collaborators, Chem. Phys. Lett. 350 (2001) 318

Ionization – experiment and models



Karwasz, Mozejko, Mi-Young Song, Int. J. Mass. Spectr. 2014

Reviews, experiments, theories...



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La Rivista del Nuovo Cimento
della Società Italiana di Fisica
2001

GRZEGORZ P. KARWASZ, ROBERTO S. BRUSA and ANTONIO ZECCA

One century of experiments on electron-atom and molecule scattering: a critical review of integral cross-sections
II. - Polyatomic molecules

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