ELECTRON, ION AND ATOM COLLISIONS LEADING TO ANOMALOUS DOPPLER BROADENING IN HYDROGEN AND HYDROGEN RARE GAS MIXTURES

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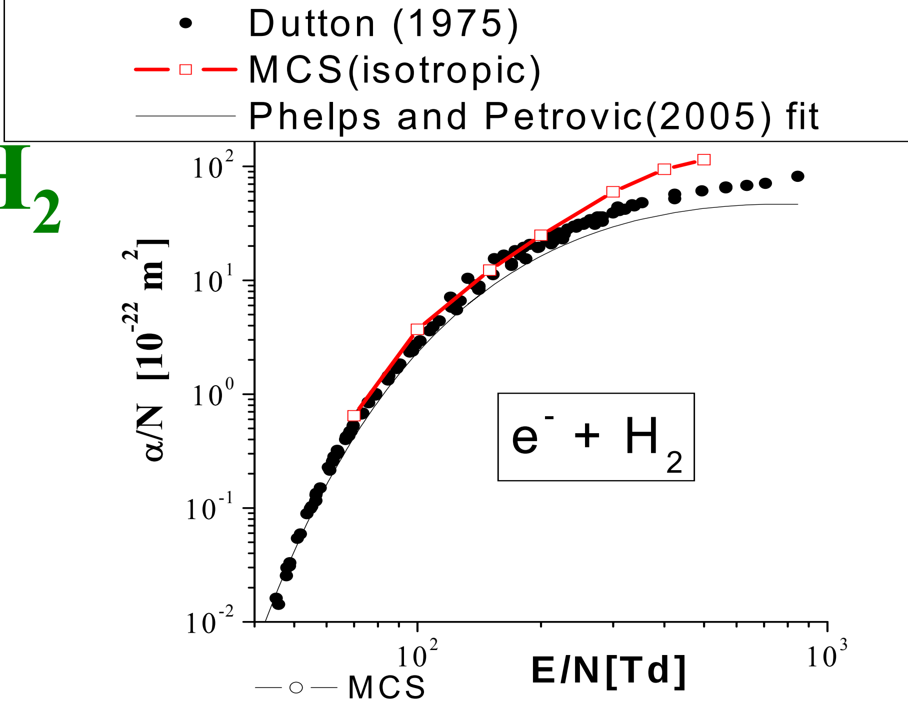
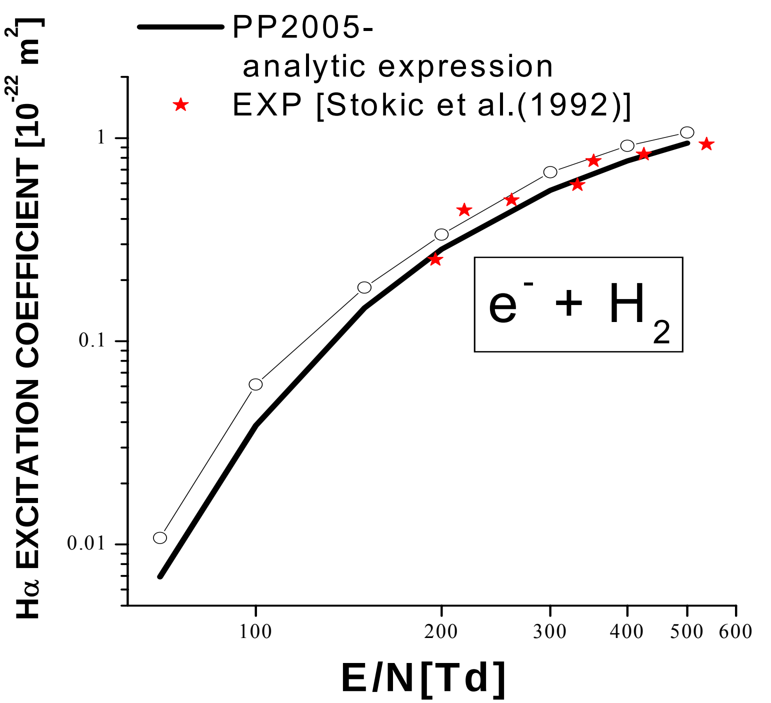
Cross section set for electron scattering on H_2

- ***Table E. Processes for electron scattering on H_2. Isotropic scattering.***

No	Process	Threshold [eV]
1)	elastic scattering	0.000
2)	J=0→J=2	0.044
3)	J=1→J=3	0.073
4)	Vibrational excitation (v=1)	0.516
5)	Vibrational excitation (v=2)	1.000
6)	Vibrational excitation (v=3)	1.500
7)	$B^3\Sigma$ excitation	8.900
8)	$B^1\Sigma$ excitation	11.300
9)	$C^3\Pi$ excitation	11.750
10)	$A^3\Sigma$ excitation	11.800
11)	$C^1\Pi$ excitation	12.400
12)	$G^1\Sigma$ (v=2) excitation	13.860
13)	$D^3\Pi$	14.000
14)	DISS. EXC.(N=2) Lyman α	15.000
15)	RYDBERG SUM	15.200
16)	IONIZATION (Rapp and EG)	15.400
17)	DISSOC.EXC (N=3) Ha	16.600

Electron impact dissociative ionization is included by introducing branching of 7 % to ionization cross section.



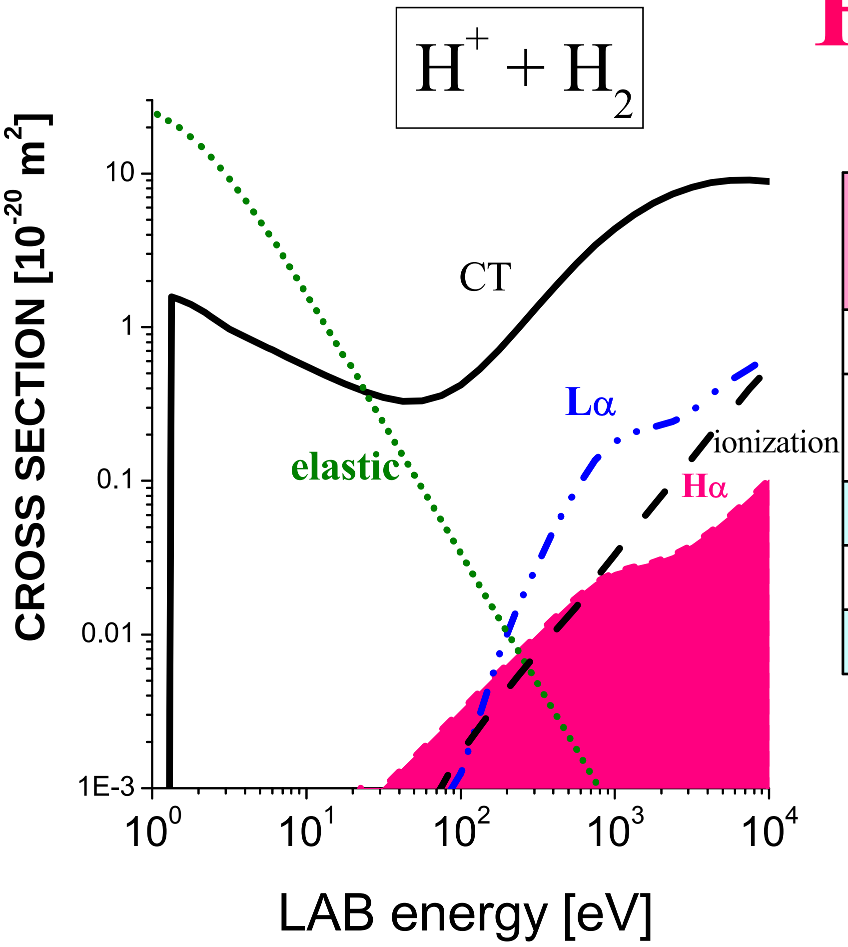


Heavy particle cross sections

- These cross sections (PP2005) are based on Phelps (1990) data and are modified to fit spatial excitation and Doppler broadened profile of Hα excitation in Townsend discharge by his multibeam method.

PP2005 – Phelps and Petrovic (2005)

$H^+ + H_2$ cross sections

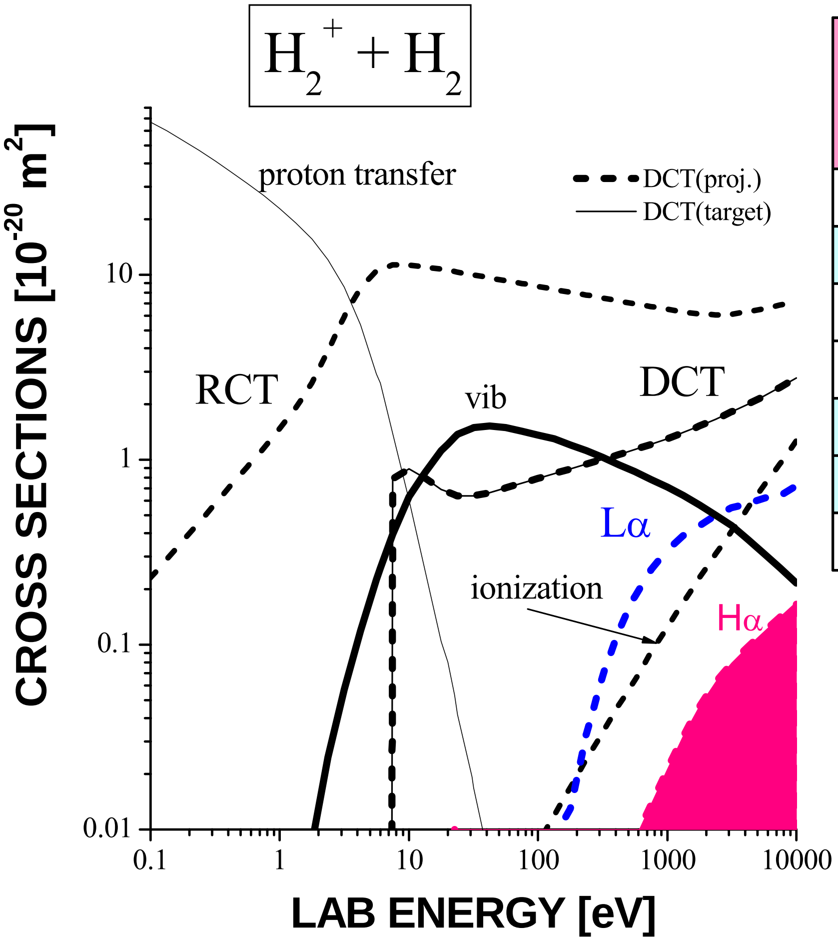


No	Process by product	Anisotropy	CMS threshold [eV]	LAB threshold [eV]
1)	elastic scattering (an)	Isotropic	0	0
2)	CT (an) Prod. of slow H_2^+ ,fast H	Forward	0.66667	1.0
3)	Lyman α....[P1990]	Forward	11.9	17.85
4)	Hα production (an)	Forward	13.3333	20.0
5)	ionization [P1990]$	Forward	15.4	23.1

Vib-Vibrational excitation cross section is sum of
v=0-1,0-2,0-3 transitions,
from P1990 and is used only in P2006.

an – analytic cross section (PP2005).
$ - production of H_2^+
P1990 – A.V. Phelps, J.Phys.Chem.Ref.Data,**19**(3) (1990).
CT – charge transfer

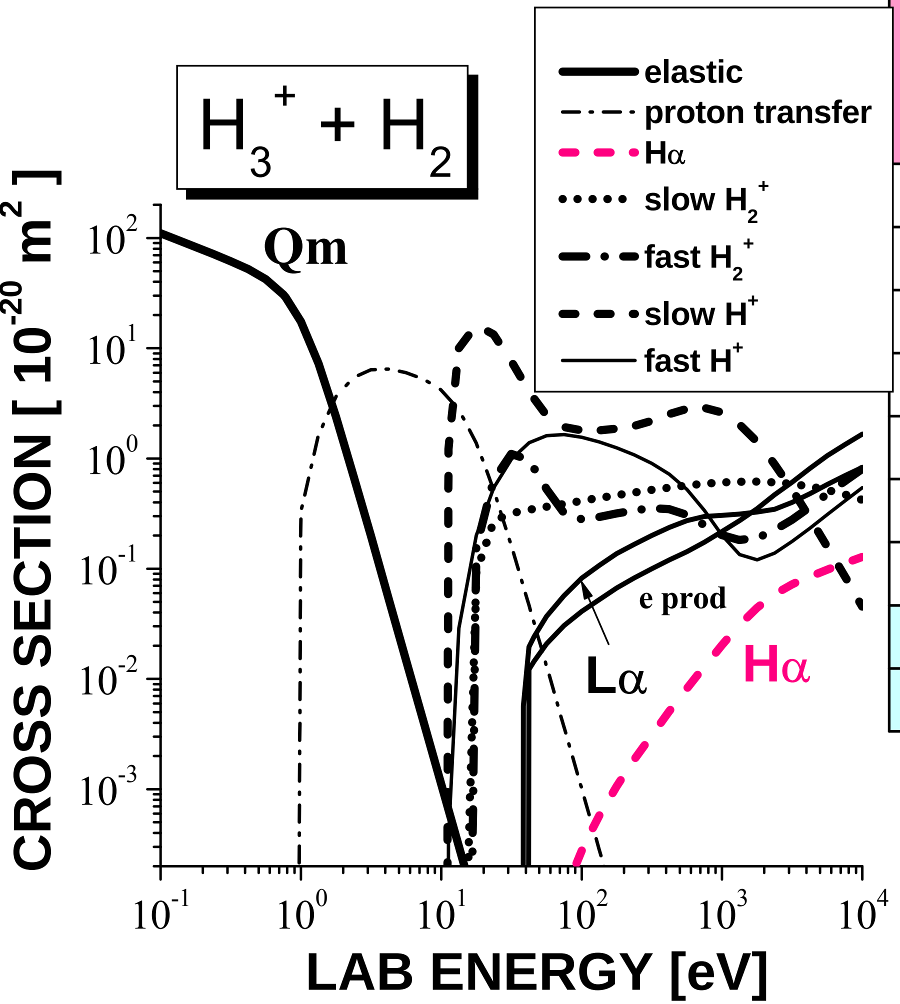
$H_2^+ + H_2$ cross sections



No	Process by product	Anisotropy	CMS threshold [eV]	LAB threshold [eV]
1)	$H_3^+ + H$ (an)	Isotropic	0	0
2)	$H_2(v=1)$ [P1990]	Forward	0.516	1.032
3)	DCT proj (an)	Forward	3	6
4)	DCT target (an)	Forward	3	6
5)	Lyman α [P1990]	Forward	11.3	22.6
6)	e- prod. [P1990]$	Forward	15.4	30.8
7)	H_α excitation (an)	Forward	10	20

an – analytic cross section (PP2005),
$ - production of H_2^+,
P1990 – A.V. Phelps, J.Phys.Chem.Ref.Data,**19**(3) (1990),
RCT – resonant charge transfer,
DCT - dissociative charge transfer.

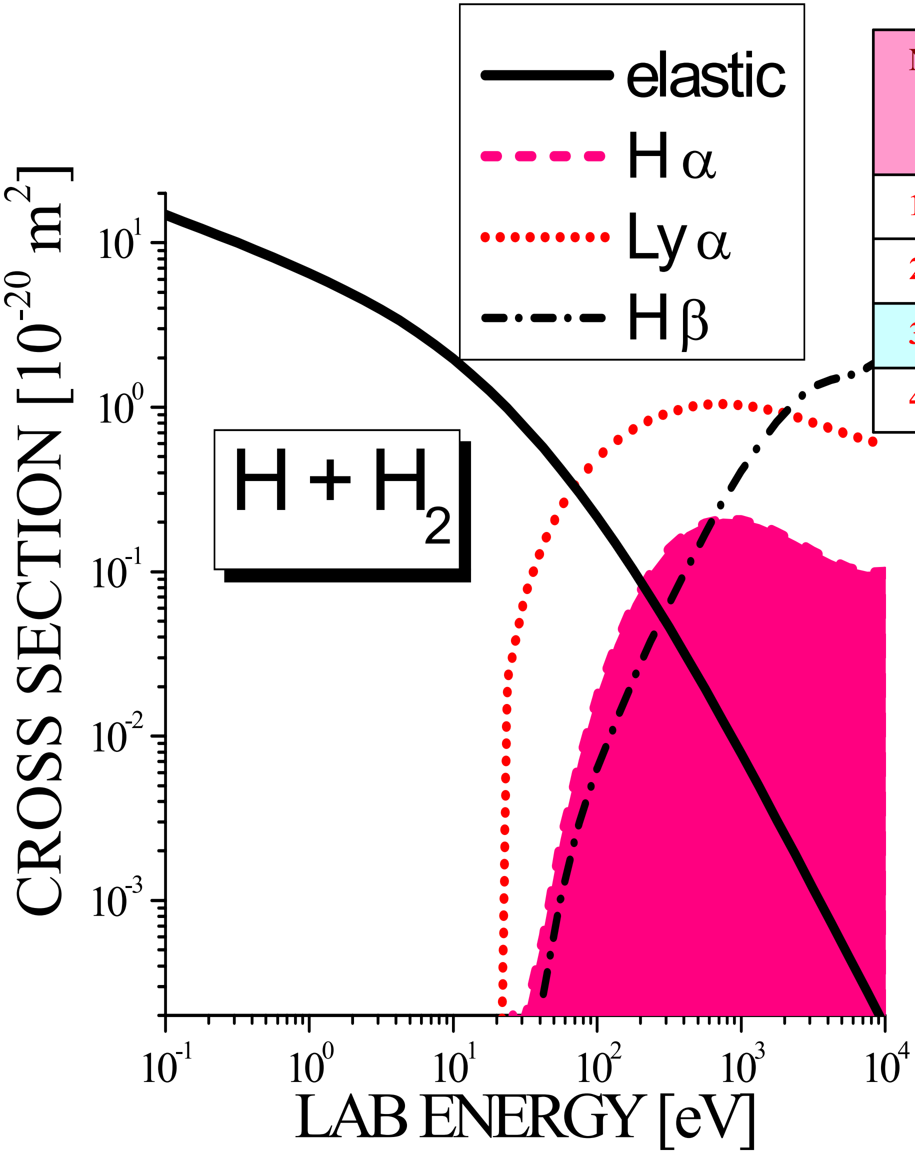
$H_3^+ + H_2$ cross sections



No	Process by product	Aniso-tropy	CMS Thres-hold [eV]	LAB Thres-hold [eV]
1)	elastic scattering (an)	Isotropic	0	0
2)	Proton transfer (an)	Backward	0.312	0.78
2)	fast H_2^+ (an)	Forward	6.2	15.5
3)	fast H^+ (an)	Forward	4.4	11
4)	fast H_2 + slow H^+ (an)	Backward	4.4	11
5)	fast H + slow H_2^+ (an)	Backward	6.2	15.5
6)	H_α excitation (an)	Forward	18.32	45.8
7)	Lyman α [P1990]	Forward	15.4	37
8)	e- prod. (e-,H_2^+) [P1990]	Forward	14.8	38.5

an – analytic cross section -PP2005.
P1990 – A.V. Phelps, J.Phys.Chem.Ref.Data,19(3) (1990).

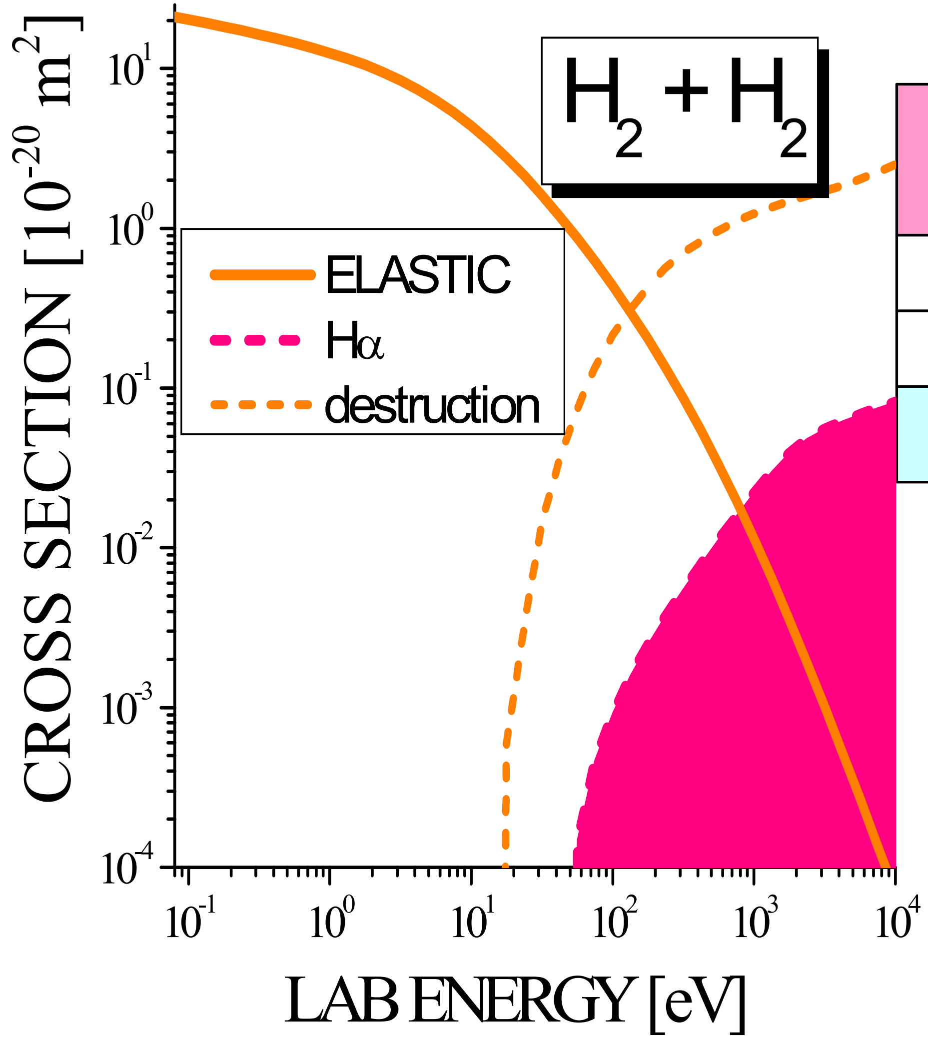
(fast)H + H_2 cross sections



No	Process by product	Anisotropy	CMS threshold [eV]	LAB threshold [eV]
1)	elastic scattering (an)	Isotropic	0	0
2)	Hα excitation (an)	Forward	17.333	26.0
3)	Hβ excitation [P1990]	Forward	17.000	25.5
4)	Lα excitation (an)	Forward	12.000	18.0

an – analytical cross section (PP2005).
P1990 – A.V. Phelps, J.Phys.Chem.Ref.Data,**19**(3) (1990).

(fast)H_2 + H_2 cross sections



No	Process by product	Anisotropy	CMS threshold [eV]	LAB threshold [eV]
1)	elastic scattering (an)	Isotropic	0	0
2)	Hα excitation (an)	Forward	22.90	45.8
3)	H_2 destruction [(f)H formation] [P1990]	Forward	4.4781*	8.9562

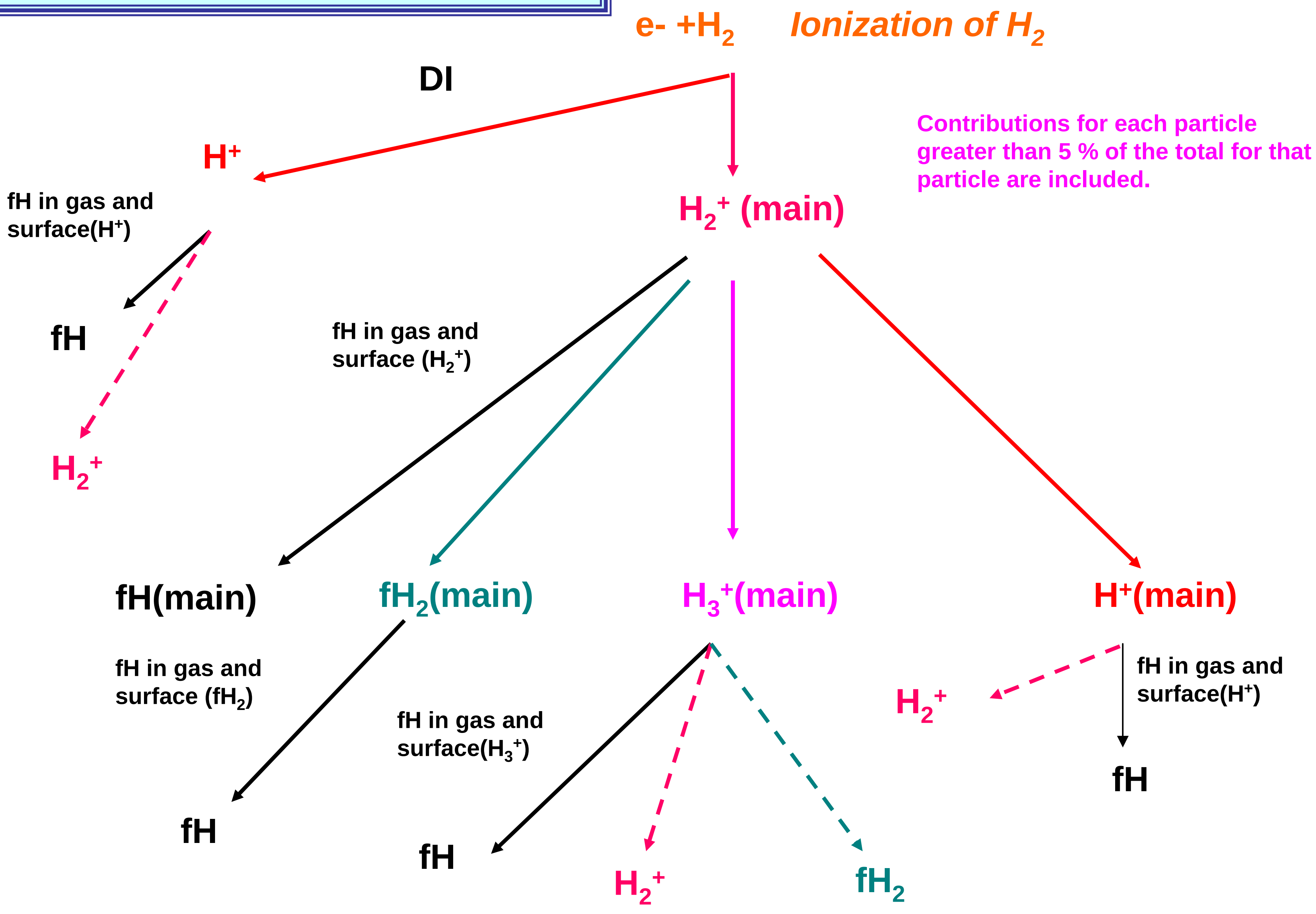
an – analytic cross section (PP2005).
P1990 – A.V. Phelps, J.Phys.Chem.Ref.Data,**19**(3) (1990).
* E.W. Mc Daniel, 1989, Atomic Collisions, Electron and Photon Projectiles, p.655. Cross section for H2 destruction is tabulated from 17.78 eV. Cross section is linearly extrapolated to 0 at 8.9562 eV. It is assumed that destruction proceeds via projectile dissociation.

Modeling heavy particle refl. on surface

1. Each charged particle born in the discharge (H^+,H_2^+,H_3^+) is **neutralized** at the surface.
2. **H^+, H_2^+ and H_3^+** form one, two and three **H atoms** upon reflection from the surface, respectively, with 2/3 of the incoming energy per particle, and 50 % probability of escape
3. Impact of **fast H** results only in backward reflection; impact of **fast H_2** produces two **H atoms** with 2/3 of incoming energy per particle, alaso with 50 % probability of escape
4. H atoms are followed backward ONLY if they have kinetic energy sufficient to excite **Hα**.
5. Fast H atoms are **backscattered diffusely** (cosine distribution).
6. Anode is assumed to be a perfect absorber for all particles (Ra=0).

Ra, Rc – reflection coefficients for heavy particles at anode and cathode respectively.

Monte Carlo Code



e- +H_2 *Ionization of H_2*

DI

Contributions for each particle greater than 5 % of the total for that particle are included.

H^+

fH in gas and surface(H^+)

fH

H_2^+

H_2^+ (main)

fH in gas and surface (H_2^+)

fH(main)

fH_2(main)

H_3^+(main)

H^+(main)

fH in gas and surface (fH_2)

fH

fH in gas and surface(H_3^+)

fH

H_2^+

fH_2

H_2^+

fH in gas and surface(H^+)

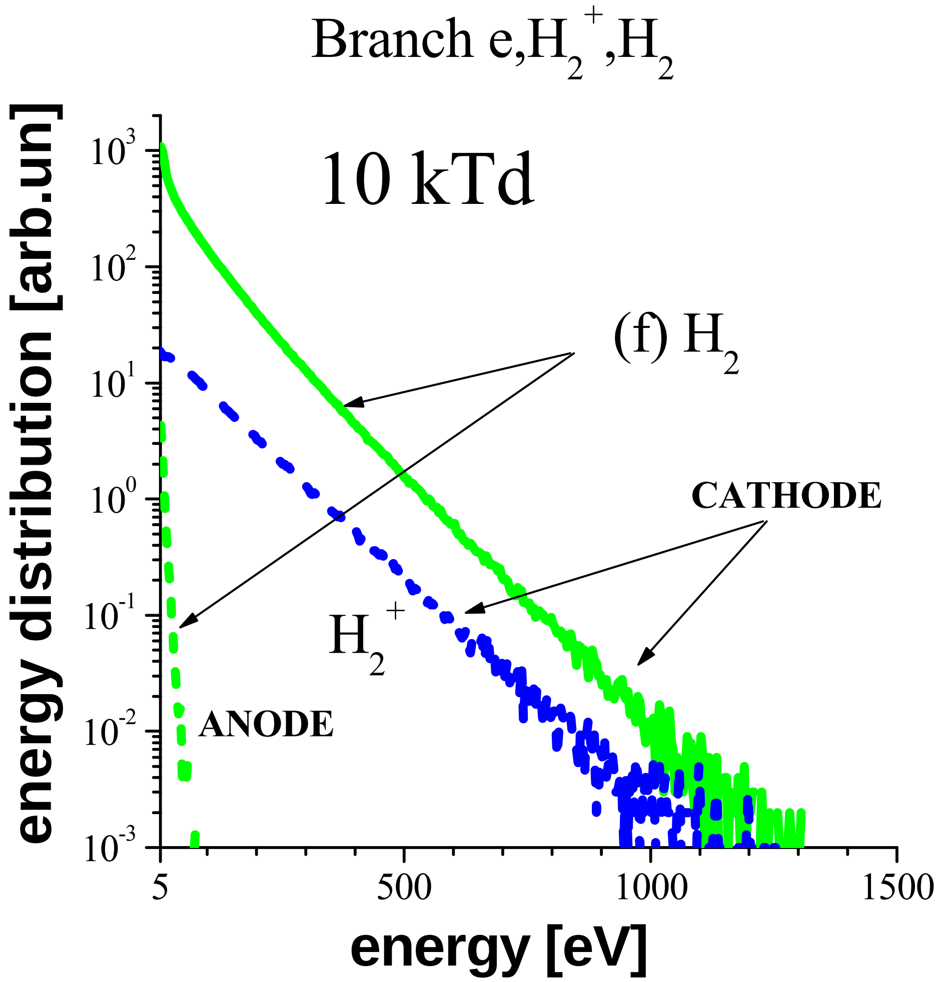
fH

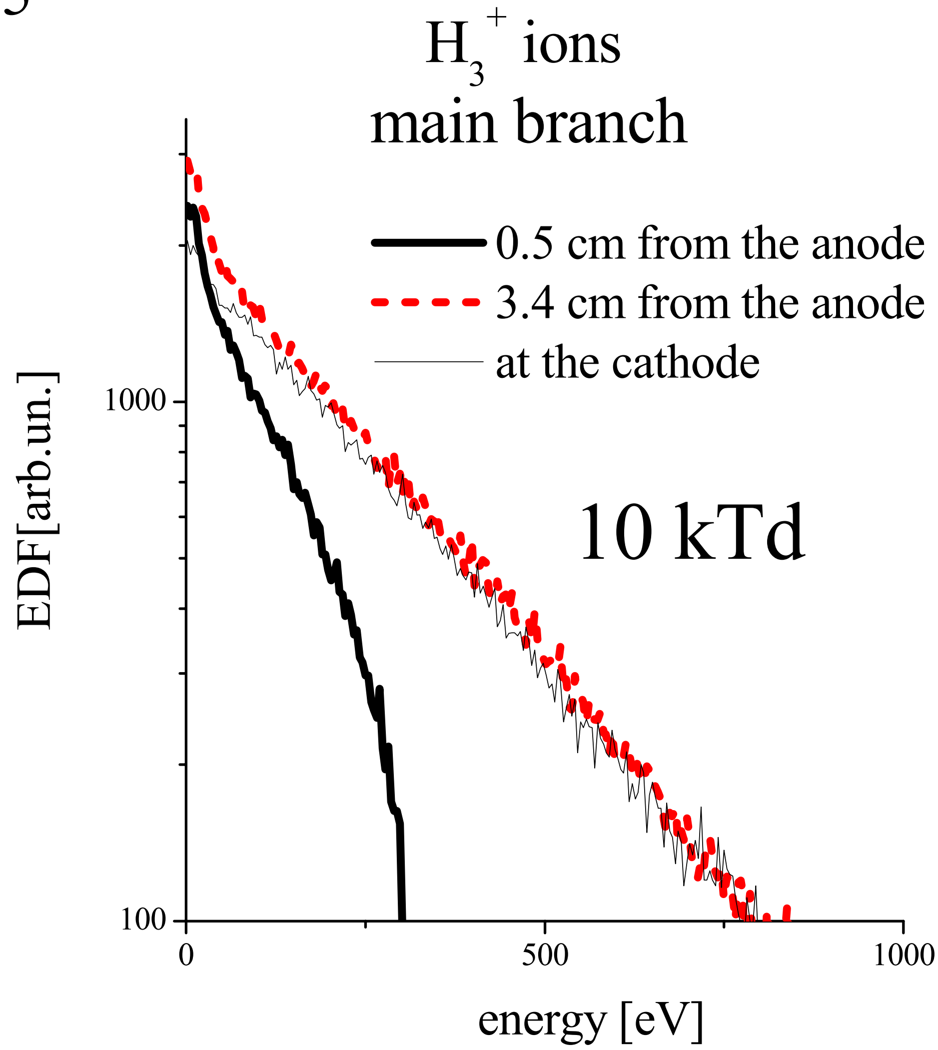
Monte Carlo Simulation RESULTS

E/N=10 kTd, E=609.5 V/cm, p=185 mTorr,d=3.9 cm

Heavy particle *membrane* energy distributions of particles approaching the cathode and the anode

H_2^+ ions and (f)H_2 PP2005



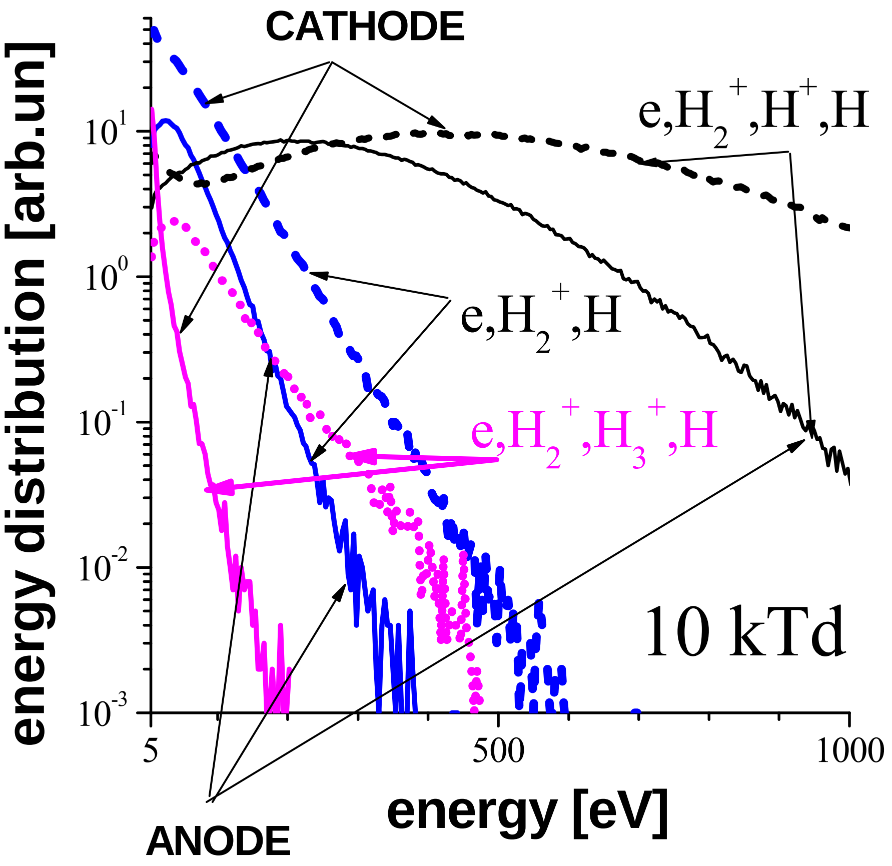


MOST IMPORTANT CONTRIBUTION – FAST H ATOMS

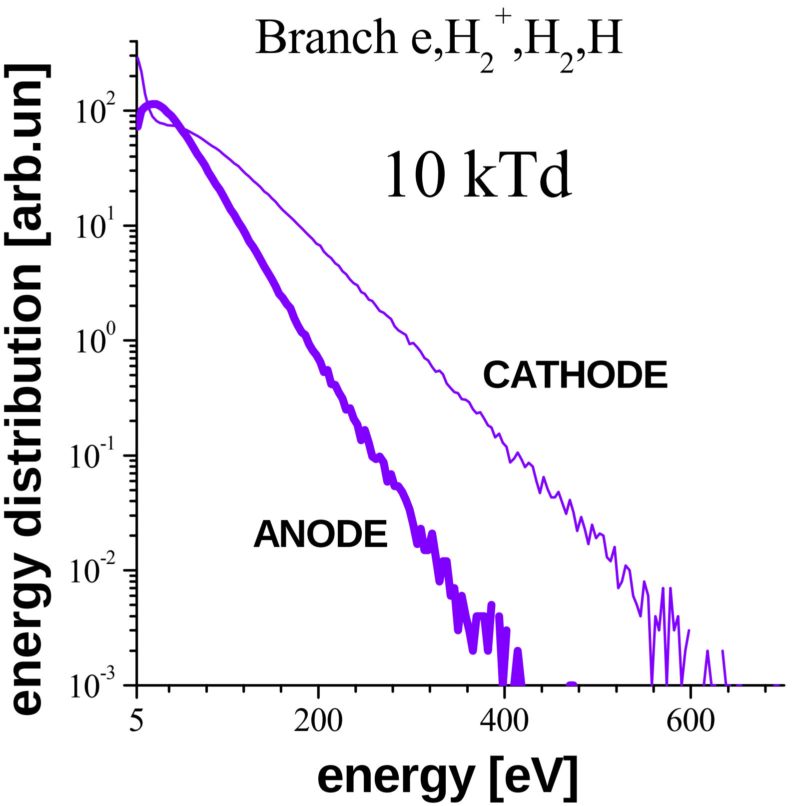
MEMBRANE ENERGY DISTRIBUTION OF fast H ATOMS ARRIVING TO THE ELECTRODES

PP2005

ionic contributions to (f)H



(f)H$_2$ contribution to (f)H



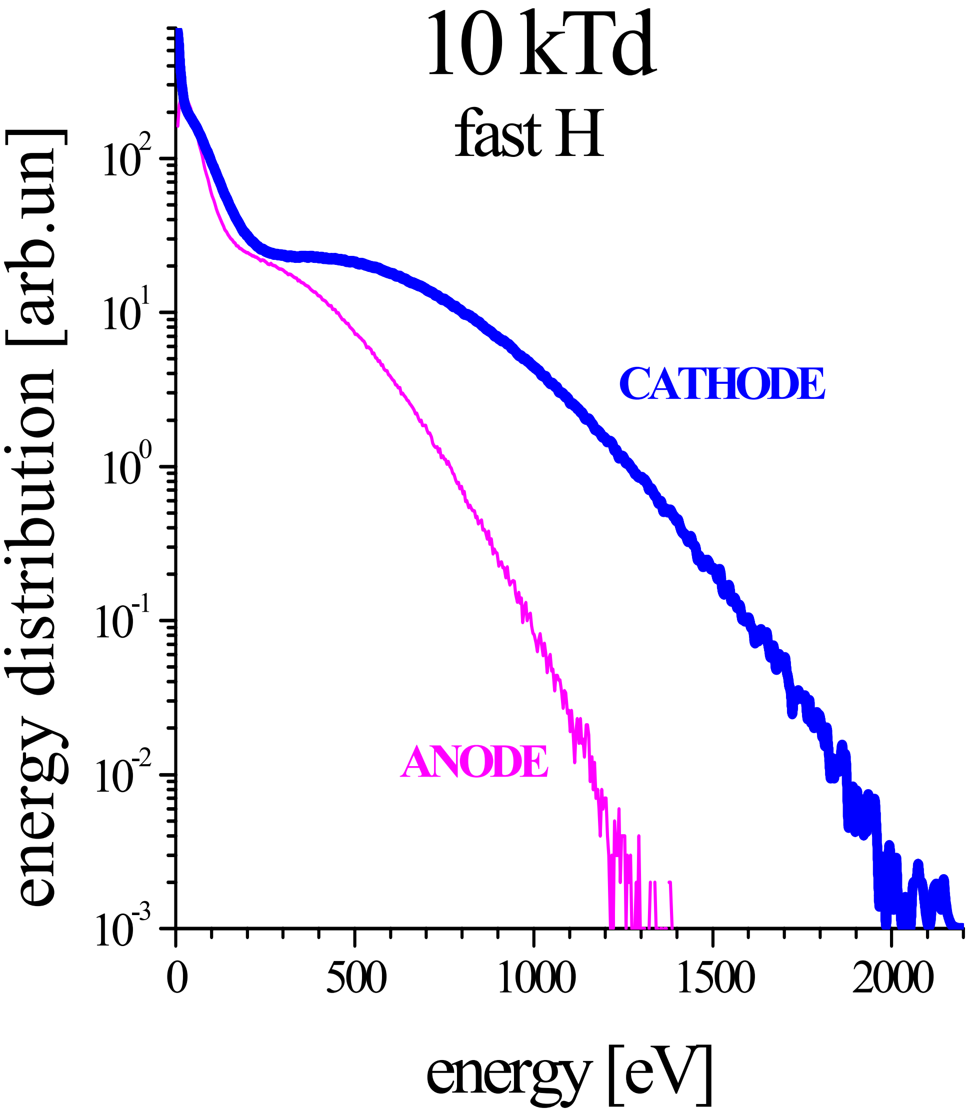
MEMBRANE ENERGY DISTRIBUTION OF fast H ATOMS ARRIVING TO THE ELECTRODES

Contribution of all particles to (f)H energy distribution

EDF is shaped by

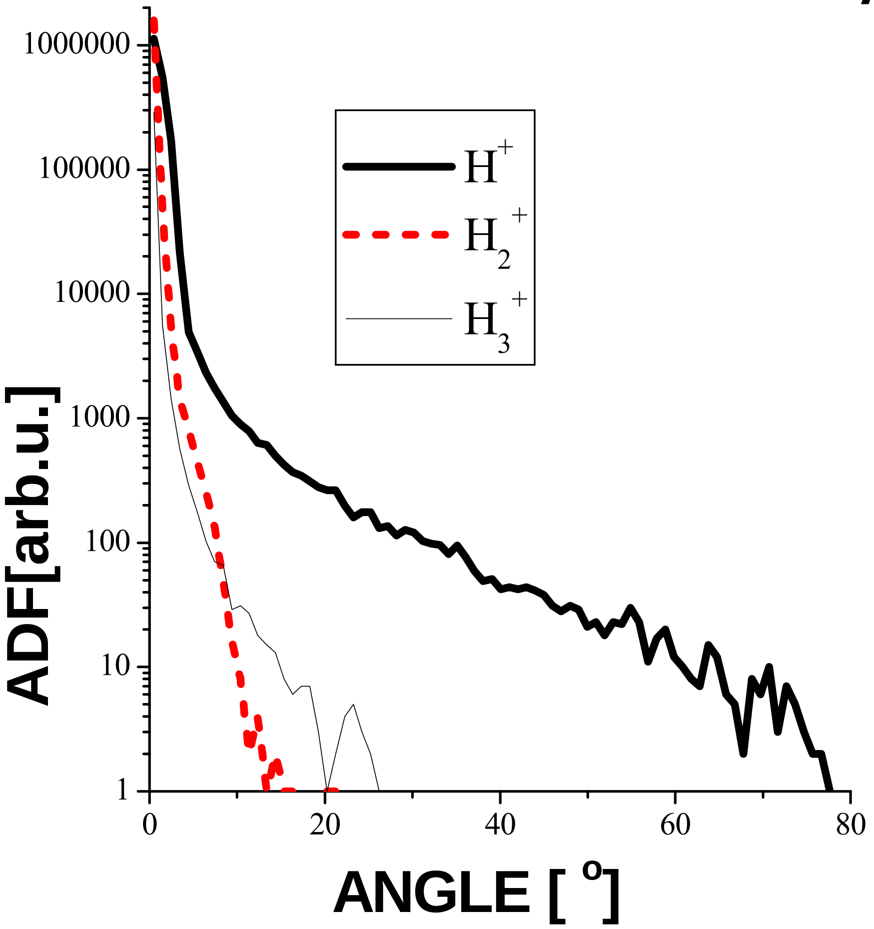
*H^+ ions at high energy

*H_2^+ and H_3^+ ions at moderate and low energy



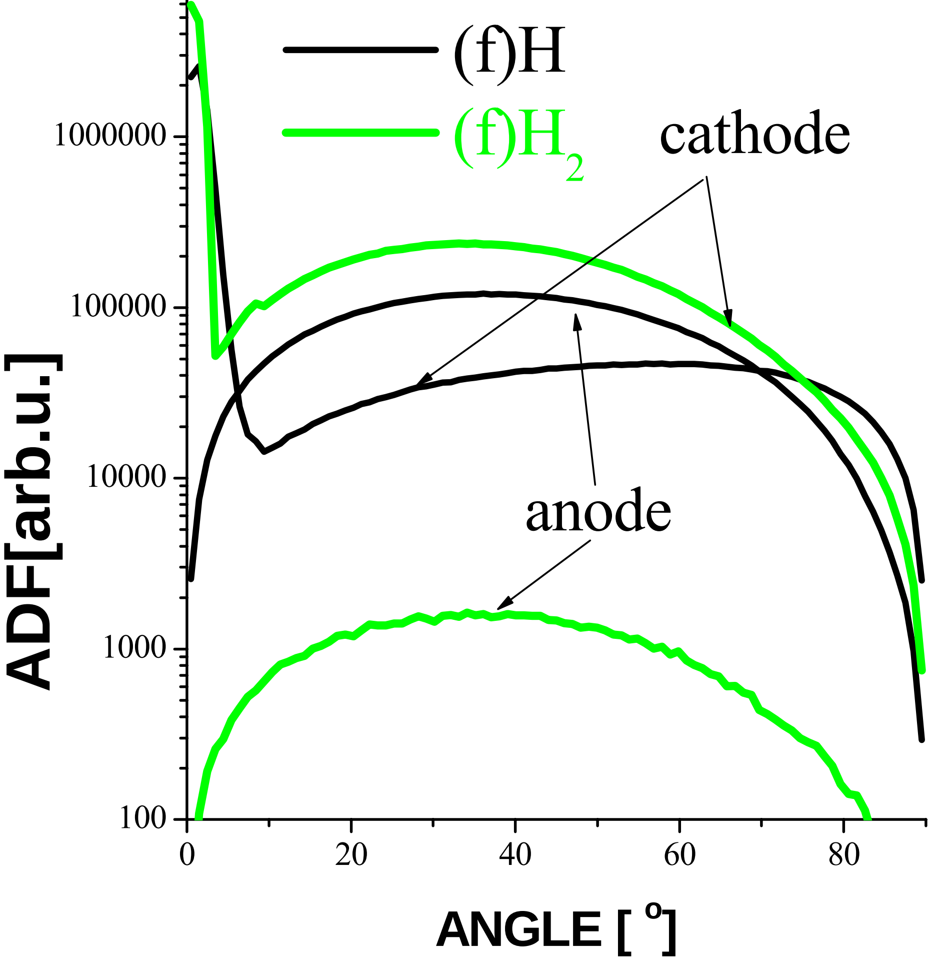
ANGULAR DISTRIBUTION OF PARTICLES AT THE ELECTRODES

CHARGED PARTICLES FORWARD PEAKED AT THE CATHODE



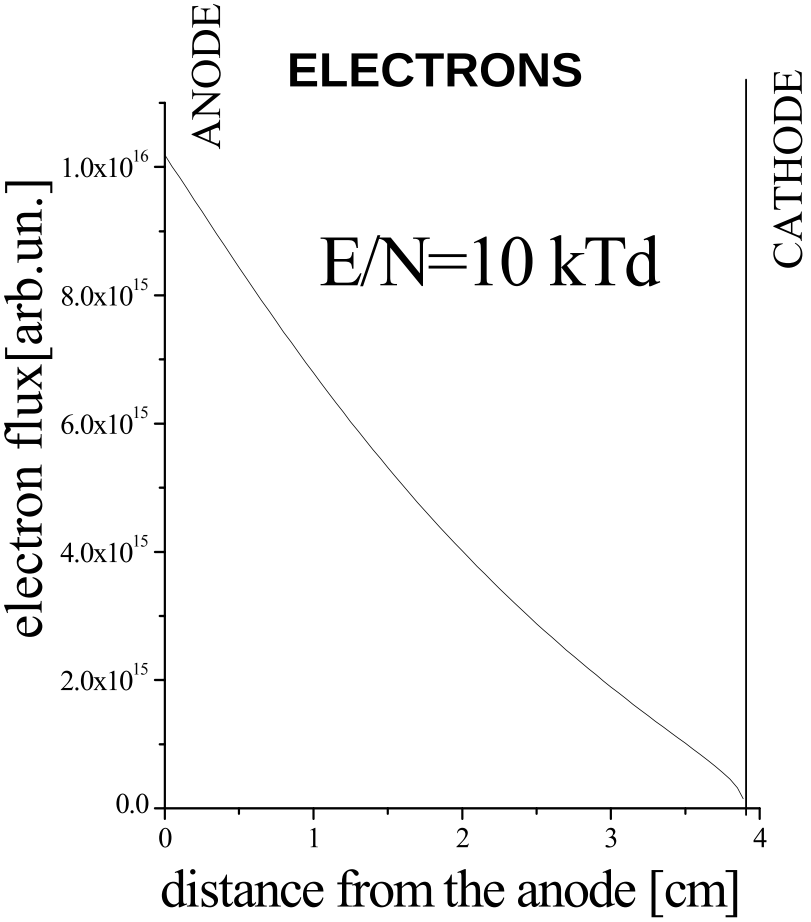
no angular dependence of reflection coefficient
PP2005

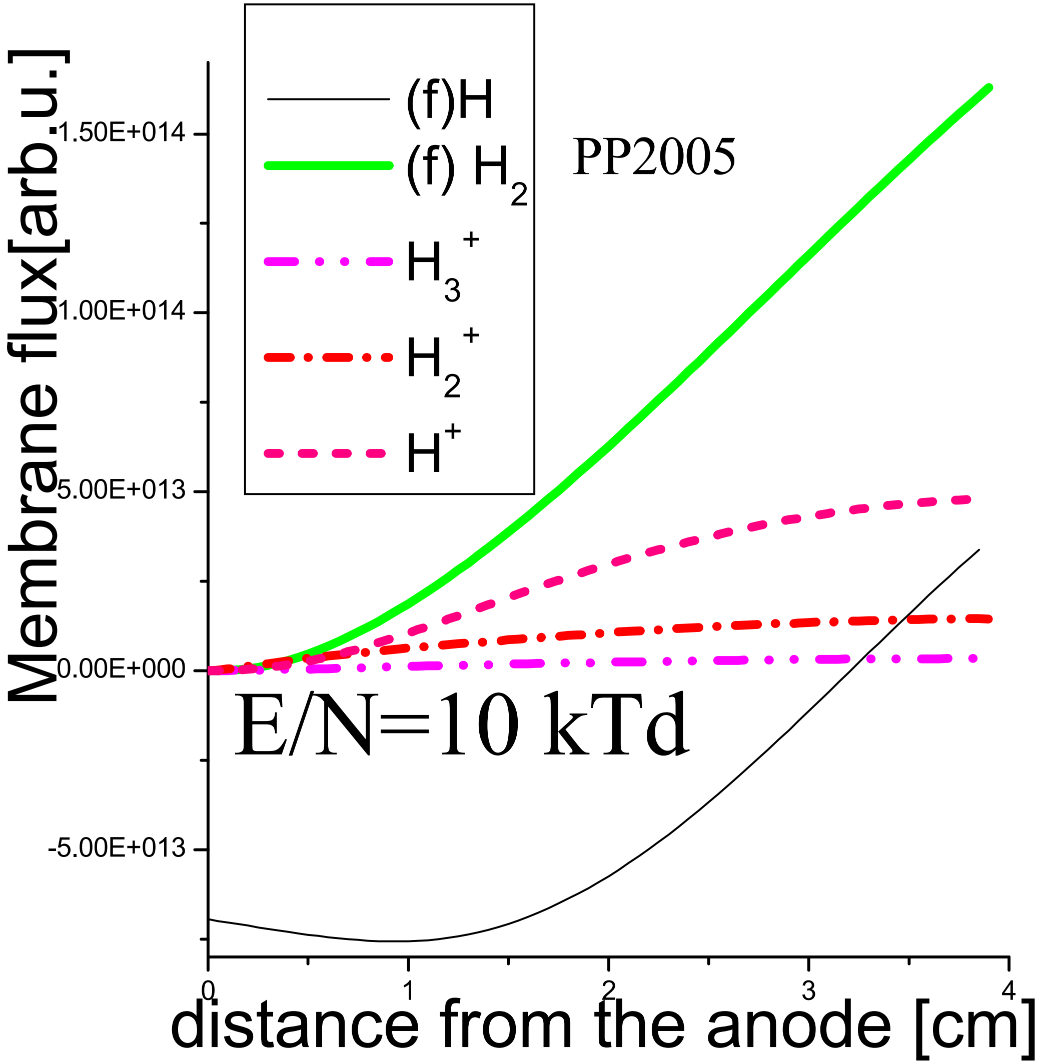
(fn) FORWARD PEAKED AT THE CATHODE ISOTROPICALLY ARRIVING AT THE ANODE



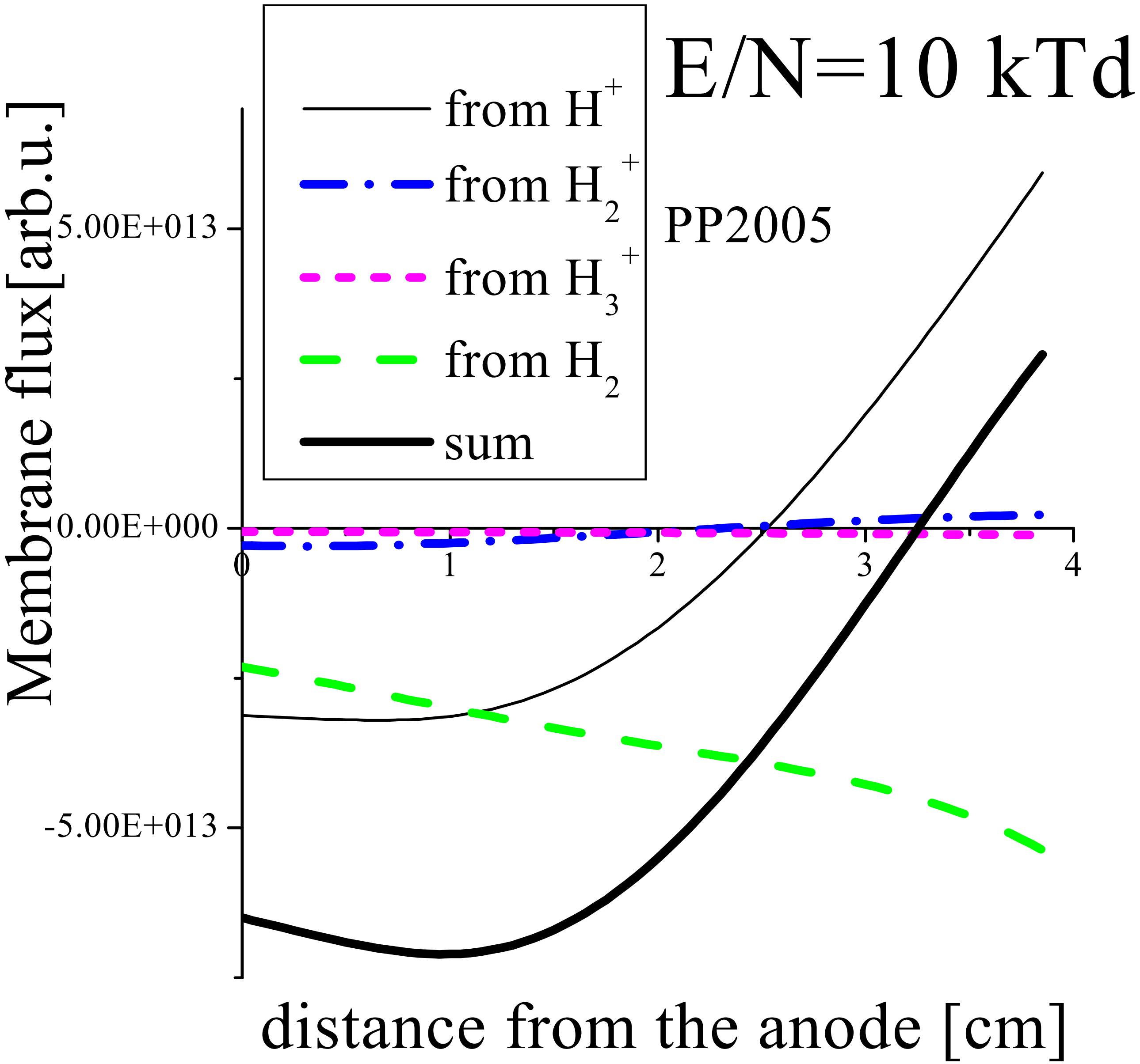
no angular dependence of reflection coefficient
PP2005

Particle fluxes





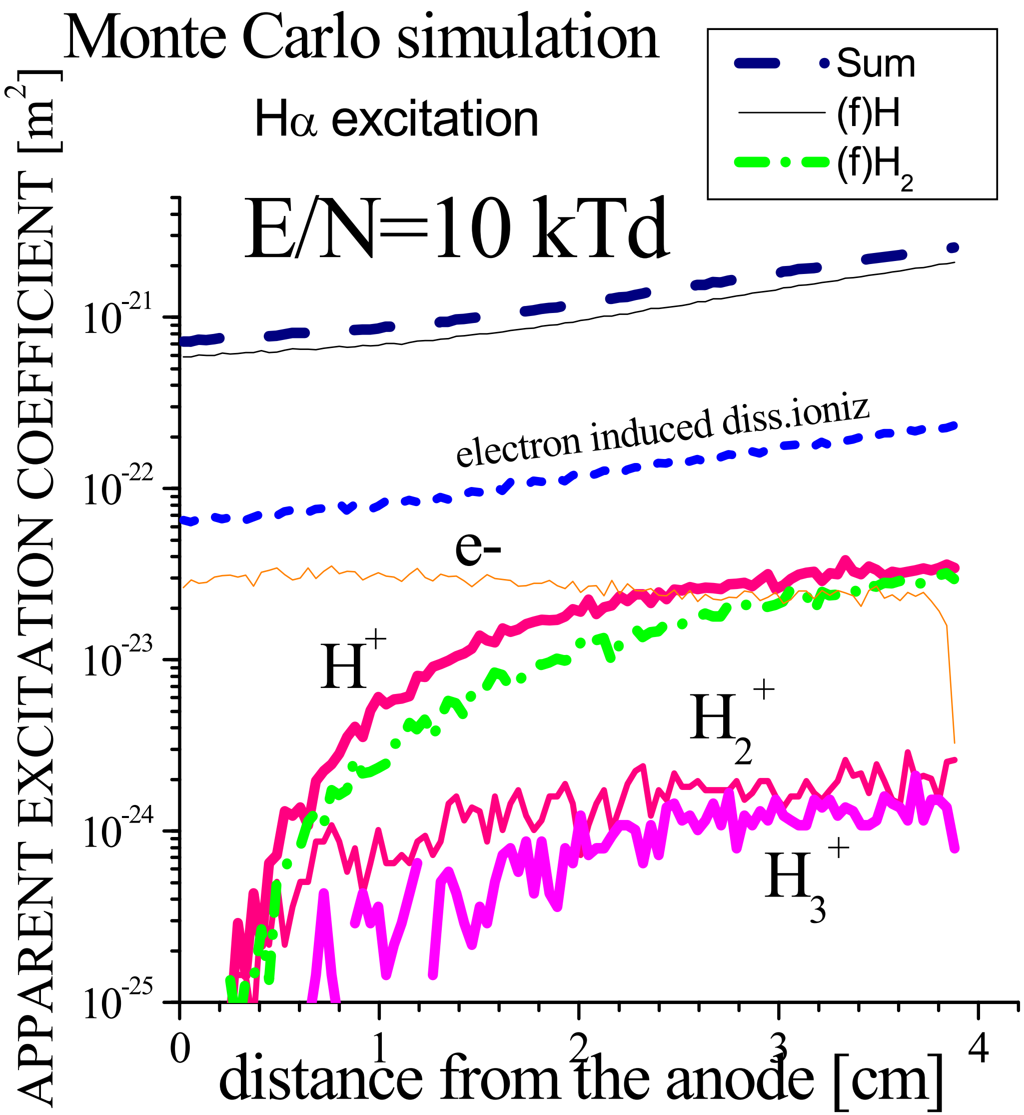
Contribution to (f)H Particle fluxes



Membrane flux a) of (f)H atoms as a function of distance for PP2005.

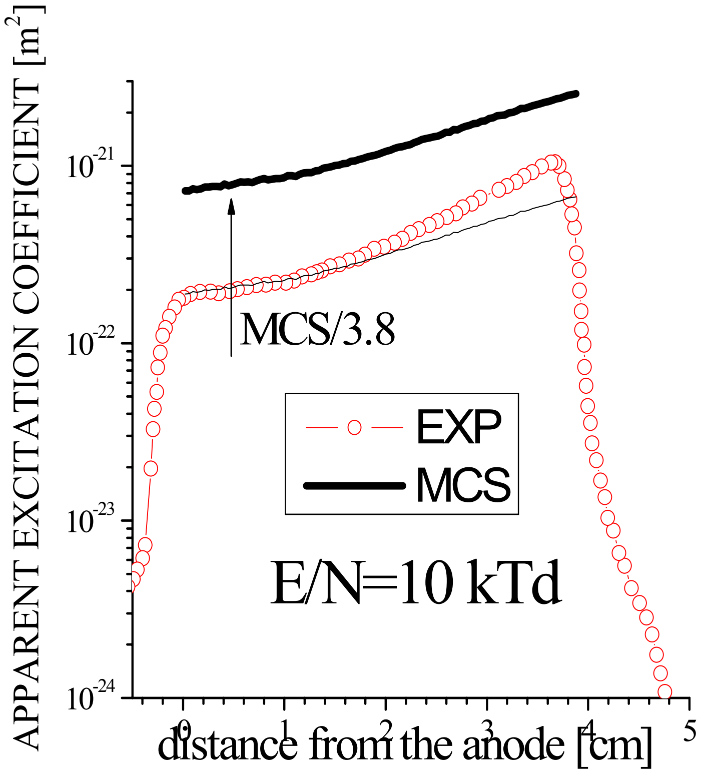
Contributions to spatial profile

for 1000000 initial electrons



PP2005

Comparison with experiment



EXP Hα Doppler profile detection

- Wavelength change for λ=656.28 nm line due to the atom emitter velocity is

$$\Delta\lambda = 0.03041\sqrt{\varepsilon[eV]}\ [nm]$$

excited atom energy

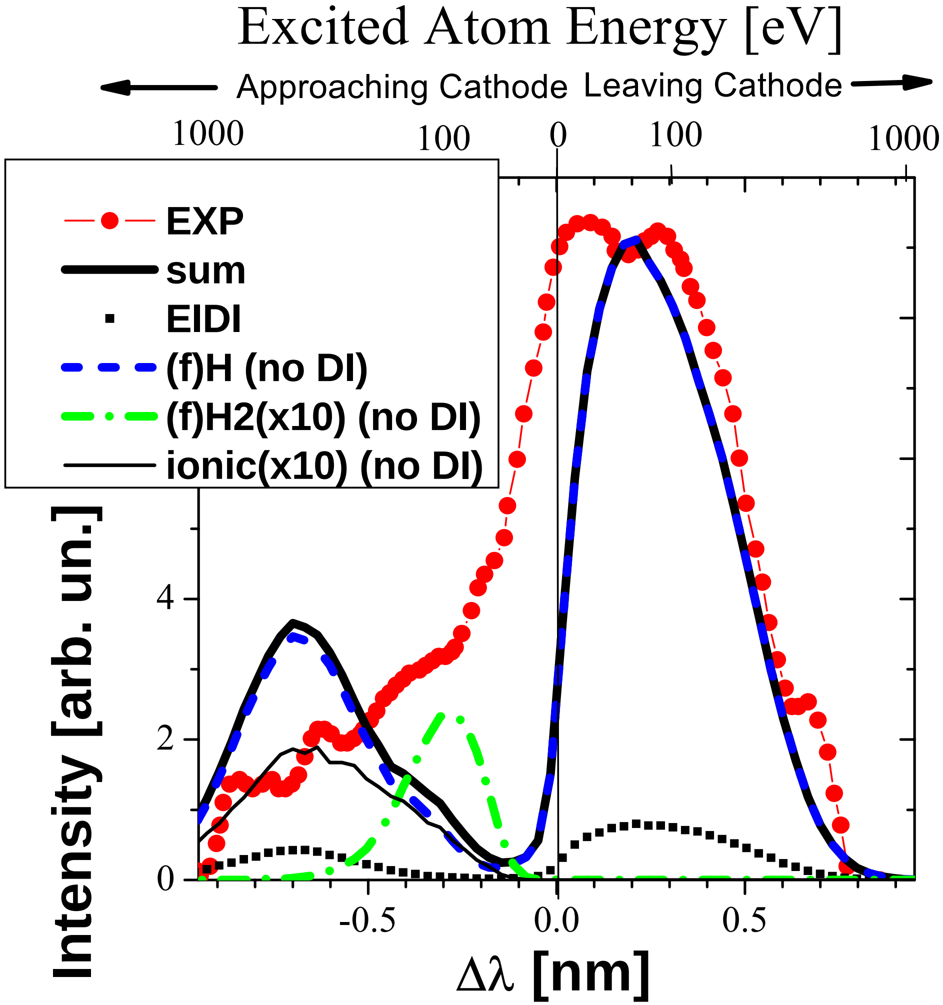
- For 100 eV : Δλ=0.304 nm
- For 1000 eV: Δλ=0.962 nm

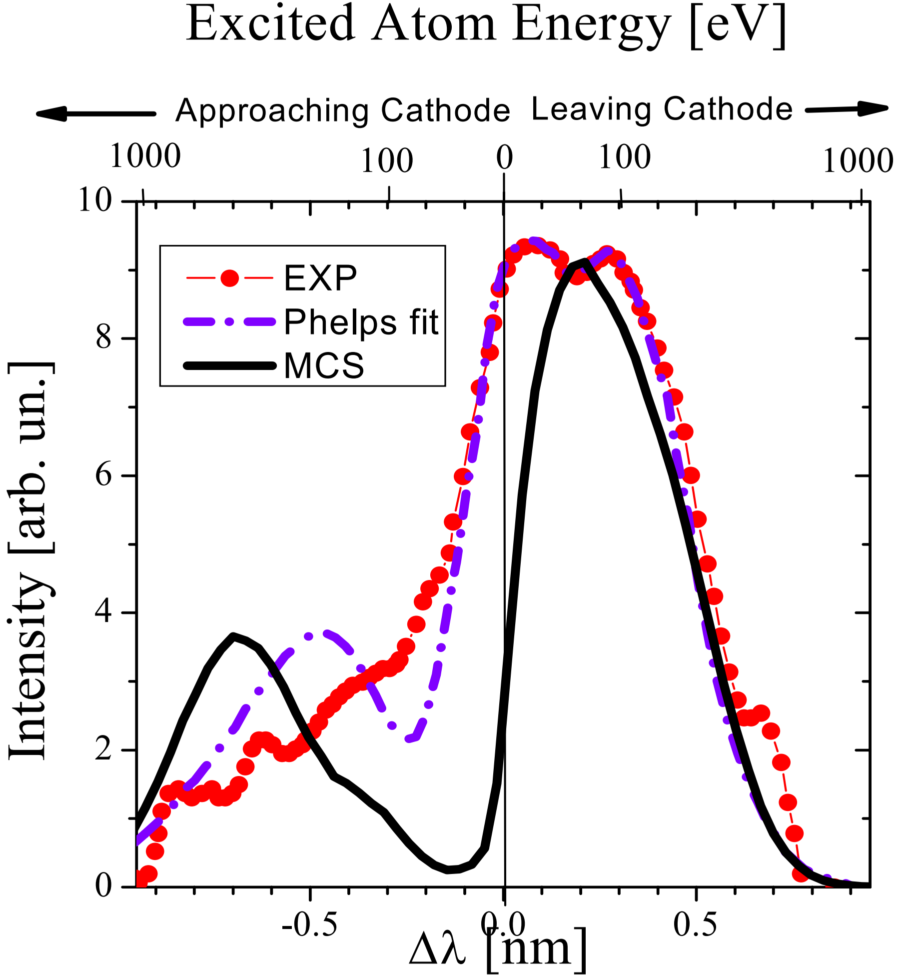
Spectral resolution is 0.24 nm that

gives the energy of excited species 62.3 eV

WHY SO POOR – well think of the current necessary to maintain the Townsend discharge conditions: i.e. 1-5 max 10 μA

Contributions to Doppler profile and comparison with EXP





Spectr. profiles for the $H\alpha$ line observed parallel to the axis of low-pressure, low current H_2 discharge at E/N=10 kTd (N=0.6095 10^{16} cm^{-3}). **DI** – contribution from H^+ produced in electron dissociative ionization,

fast H (noDI)- contribution of all fast H according to the scheme without DI,

sum - effect all particles according to the scheme

Phelps fit, **EXP** from Petrović et al., Phys.Rev. Lett. (1992) (Fig 1 a)

ionic (no DI) – contribution of H+,H2+, H3+ ions without .DI, **fast H2(noDI)** – contribution from fast H2 without DI

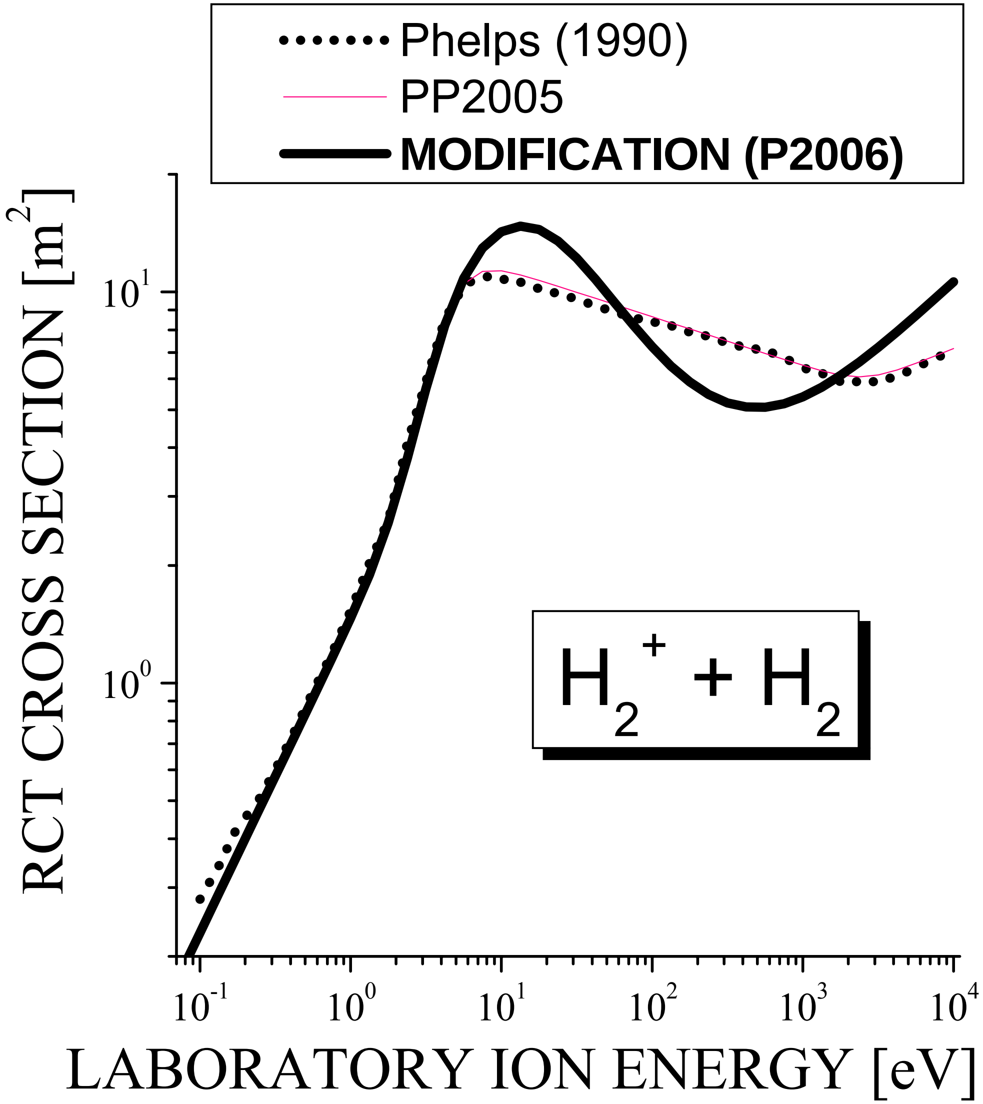
How good is present (PP2005) model?

- MCS results fit experimental spatial excitation and Doppler broadened profile of Hα excitation
- Absolute spatial emission is about 4 times larger than EXP!!! Can we improve that?

by making a more realistic model?

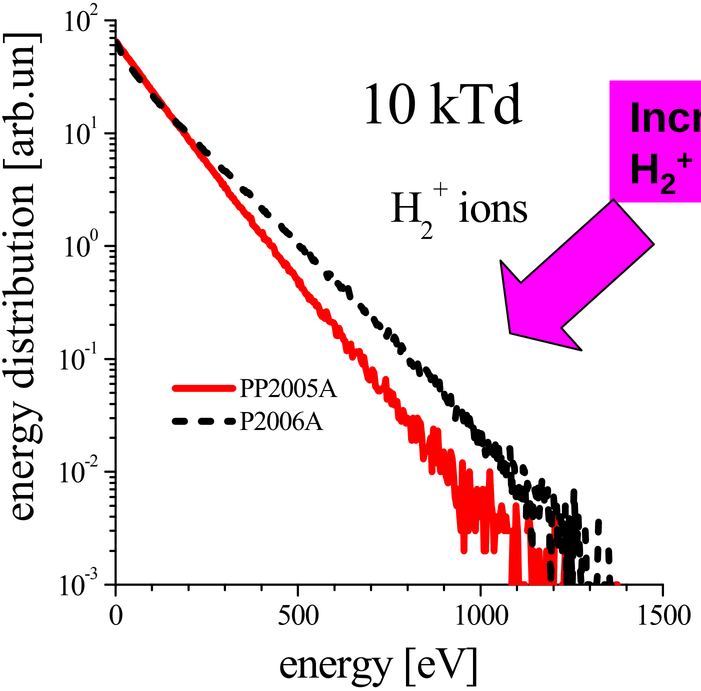
1st- will modify H_2^++H_2 cross section set:

shape of
resonant charge transfer (RCT)
cross section for H_2^+ on H_2



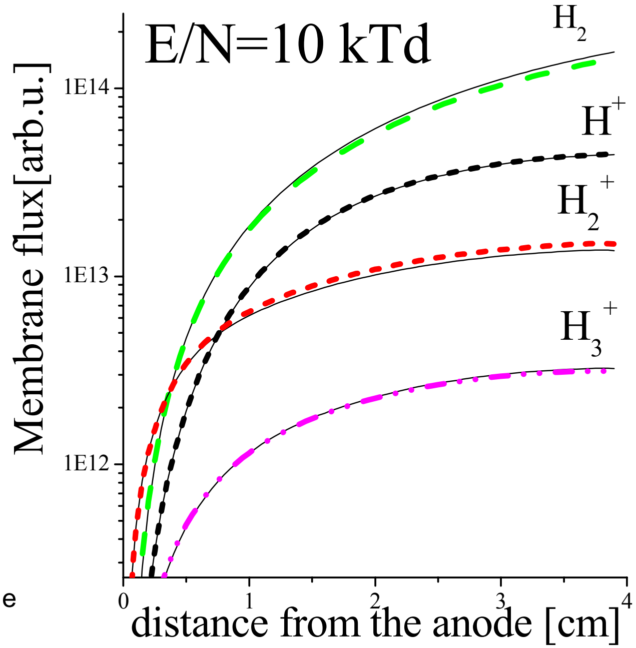
Effect of modification of the shape of RCT cross section for $H_2^+ + H_2$

EDF at the cathode

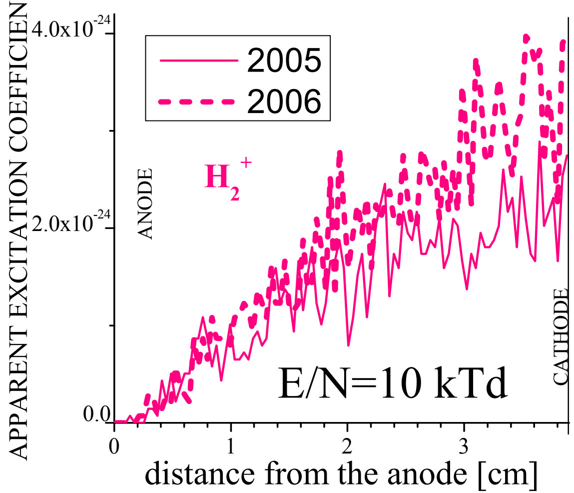


Increase of the high energy H_2^+ ions

Decrease of (f)H_2 flux
Increase of H_2^+ flux



Hα excitation
in Townsend hydrogen discharge

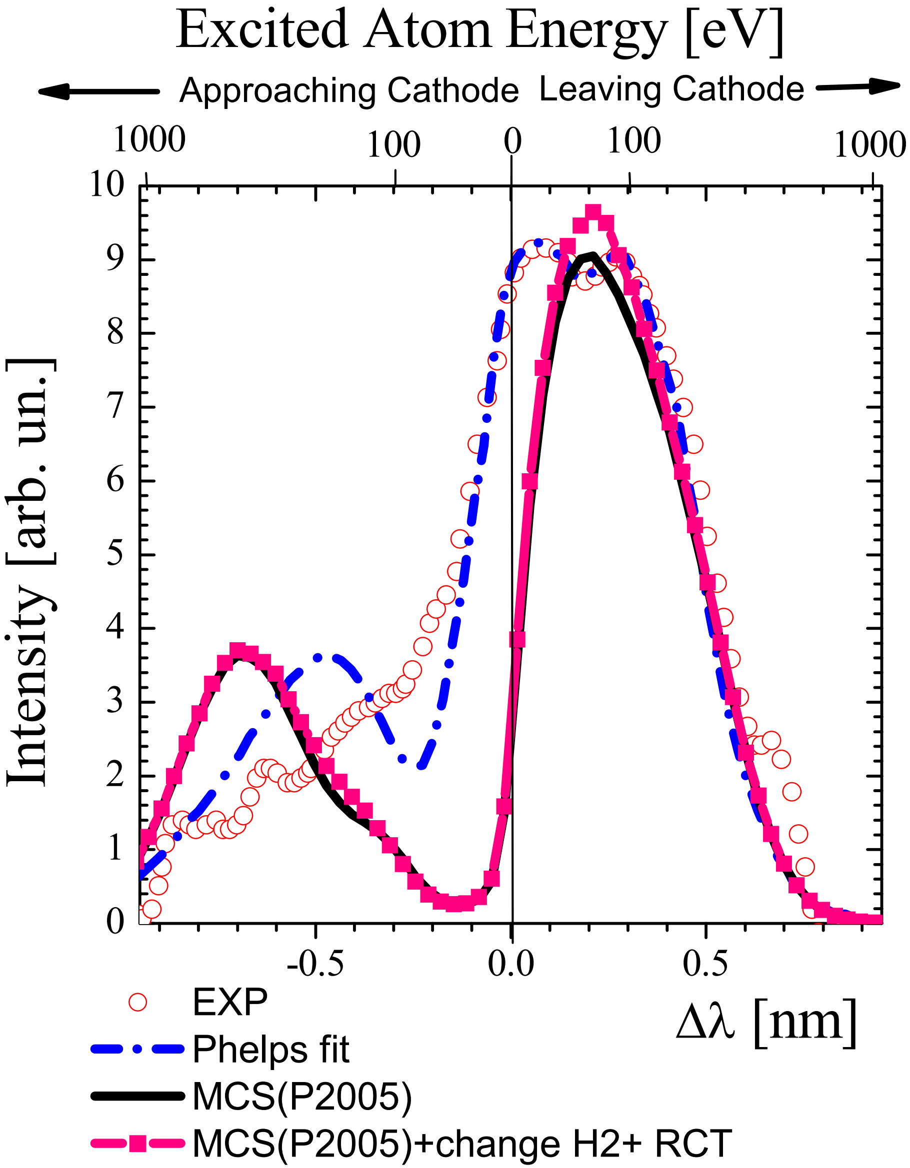


Increase of H_2^+ induced **Hα** emission intensity close to the cathode

Effect of modification of shape of RCT cross section for $H_2^+ + H_2$ on Doppl.profile

- slightly changed "direct" profile,

  -increased "backward" profile due to the inreased number of (f)H produced by higher energy H_2^+ ions and faster H_2 than in previous model (PP2005)

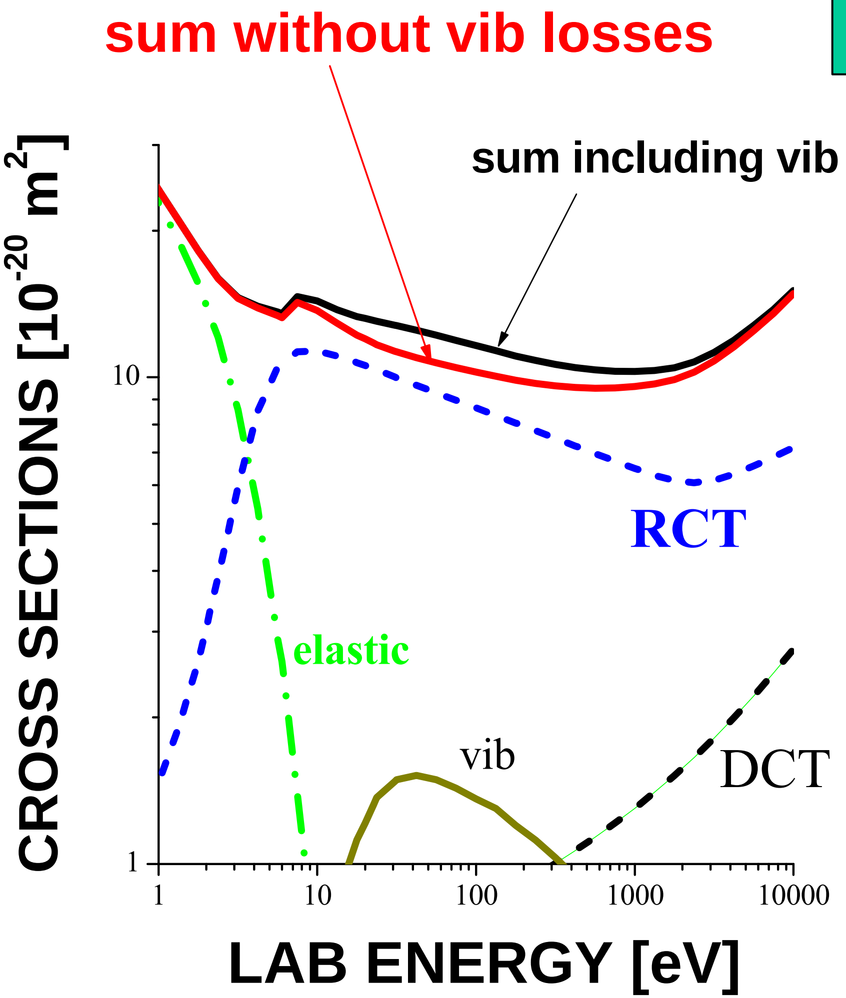


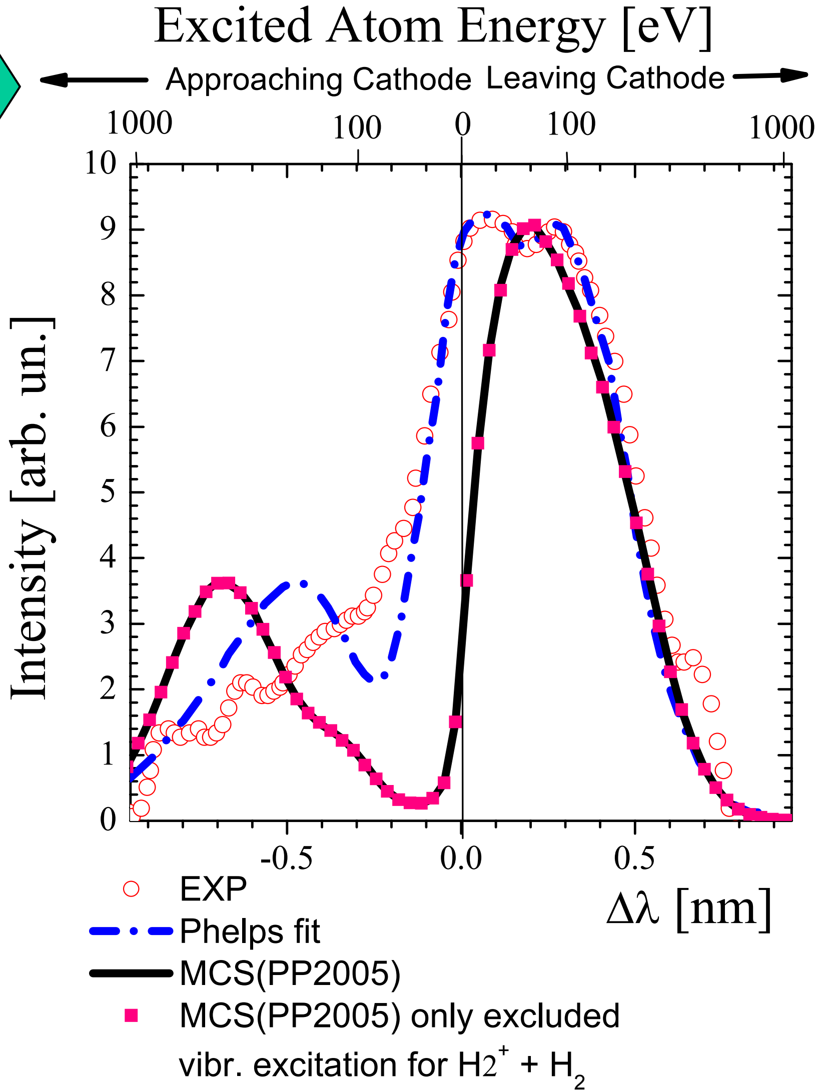
2^{nd} –will modify $H_2^+ + H_2$ cross section set:

exclude vib. losses from

H_2^+ on H_2 cross section set

INSIGNIFICANT

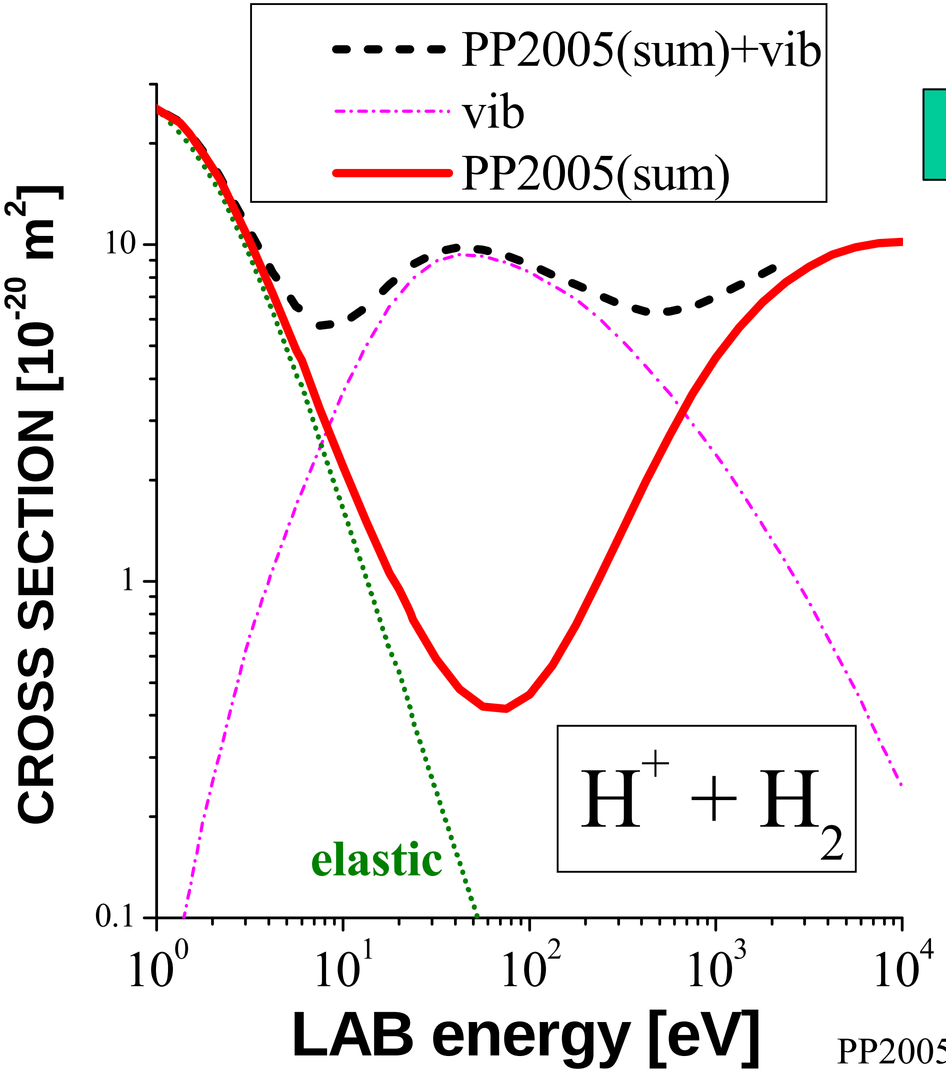


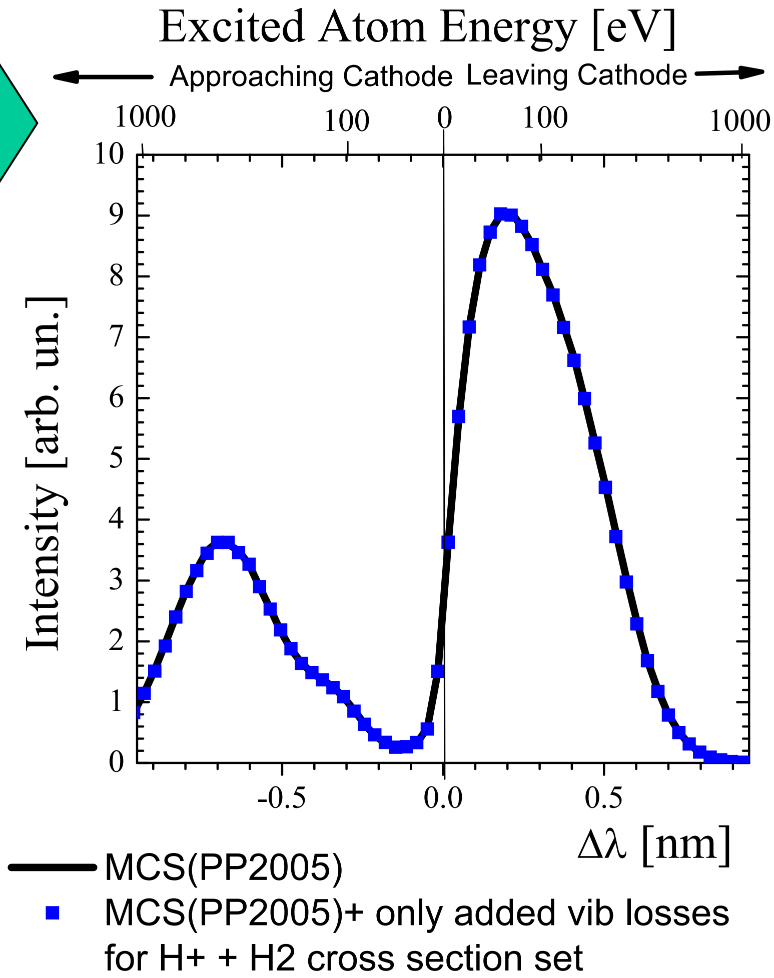


3rd:Will modify $H^+ + H_2$ cross section set:

include vibrational losses for H^+ on H_2

INSIGNIFICANT





PP2005(sum)-sum of PP2005 cross sections

Vib-sum of vibrational v=0,1,2 cross sections

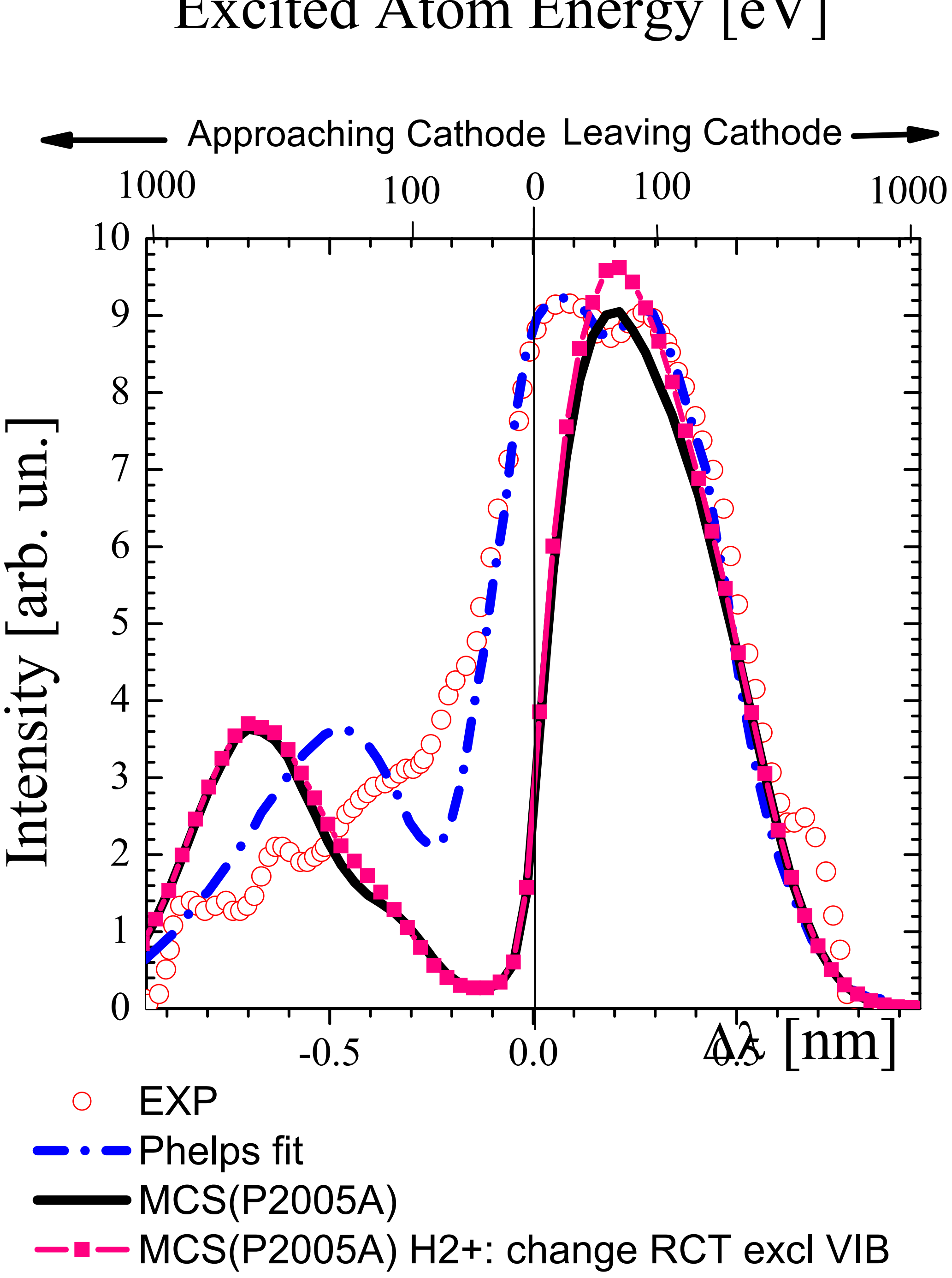
Effect of ALL MODIFICATIONS OF the CROSS SECTION SET:

- shape change for RCT cross sct. for $H_2^+ + H_2$
- excluding vib. excitation from $H_2+ + H_2$ cross sct.
- adding vib excitation to H^+ scattering model

(appears to bi insignificant at these E/N)

On Hα Doppler broadened line profile.

IS SMALL AT VERY HIGH E/N



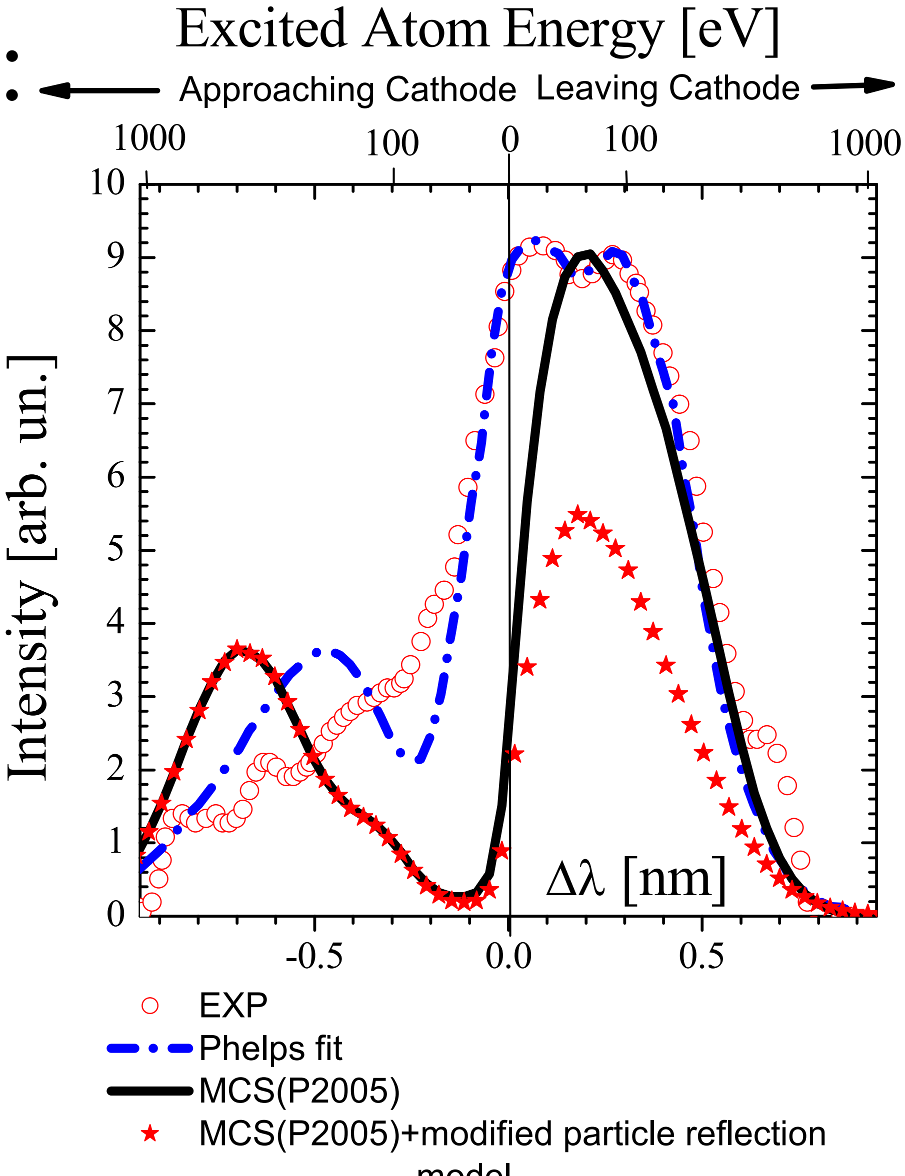
4th: will modify particle reflection model at the surface:

- Constant reflection coefficient (0.5) become energy dependent

$$R = \frac{0.6}{\left(1 + \sqrt{\frac{E[\mathrm{eV}]}{3000}}\right)^3}$$

- energy of the reflected particles instead of being 2/3 of incoming energy per particle now is uniformly distributed up to incoming energy per particle.

Effect of modification of particle reflection model at the cathode on Doppler broadened line profile:

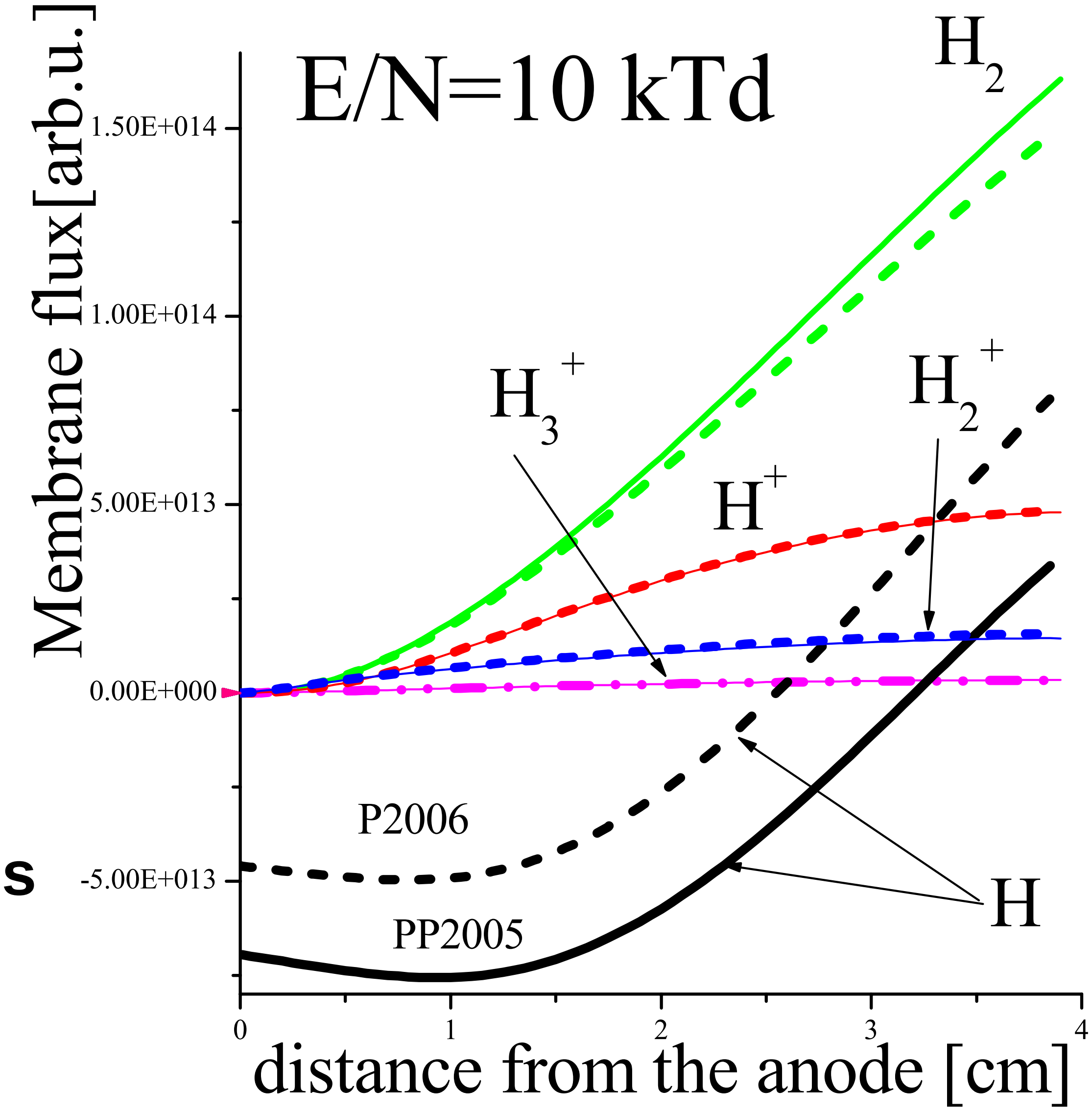


Peak due to the (f)H atom reflection leaving the cathode dropped for about 40 %

Spatial profile remained of the same shape! **Agreement** between modeling results and experiment **IMPROVED**! (see next slides).

FINAL COMPARISON OF THE RESULTS FOR TWO SCATTERING MODELS

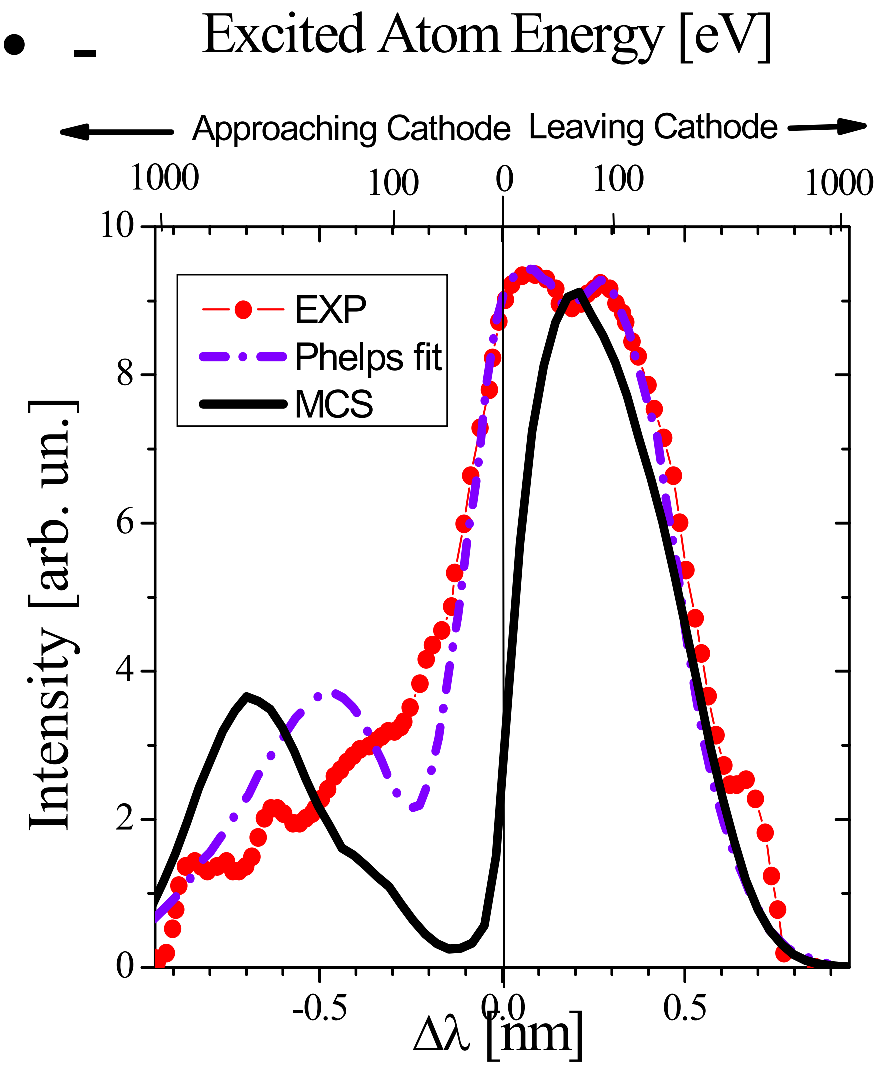
Particle fluxes for 2 scattering models

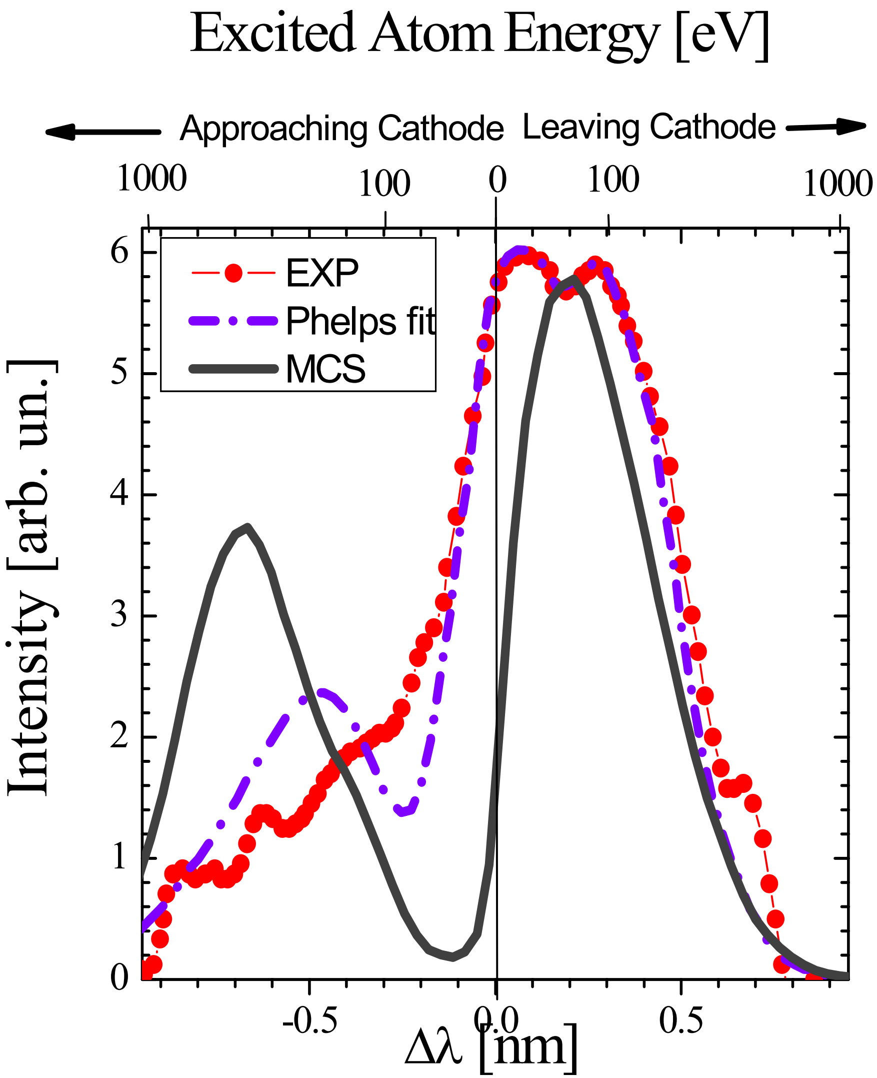


PP2005 - Solid lines
PP2006 - dashed lines

Doppler profile for 2 scattering models

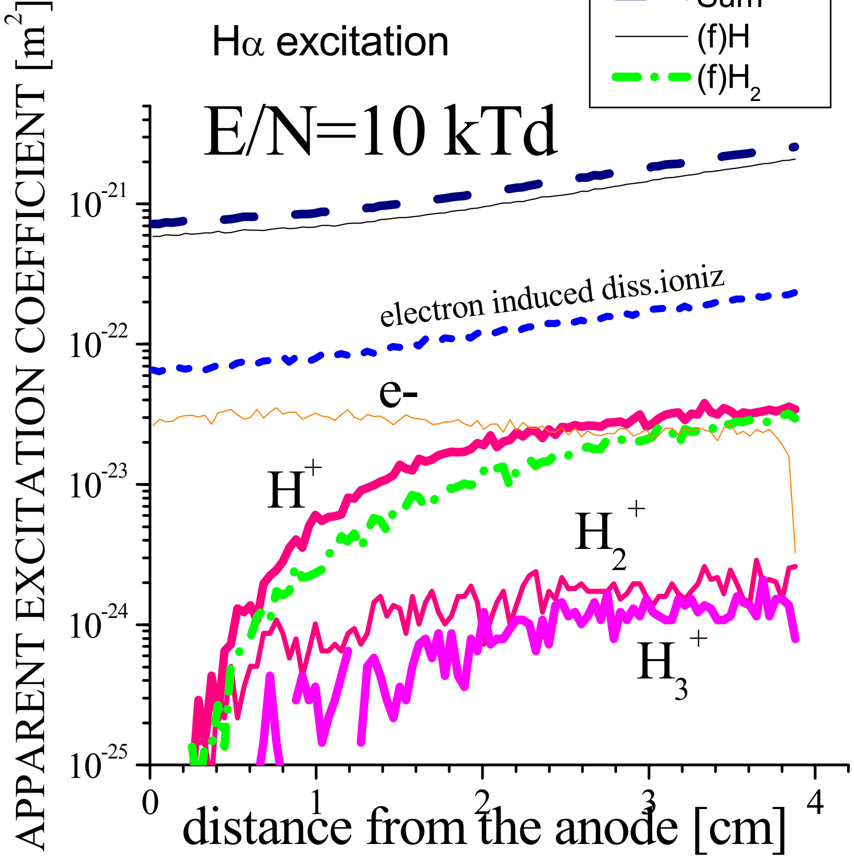
- –

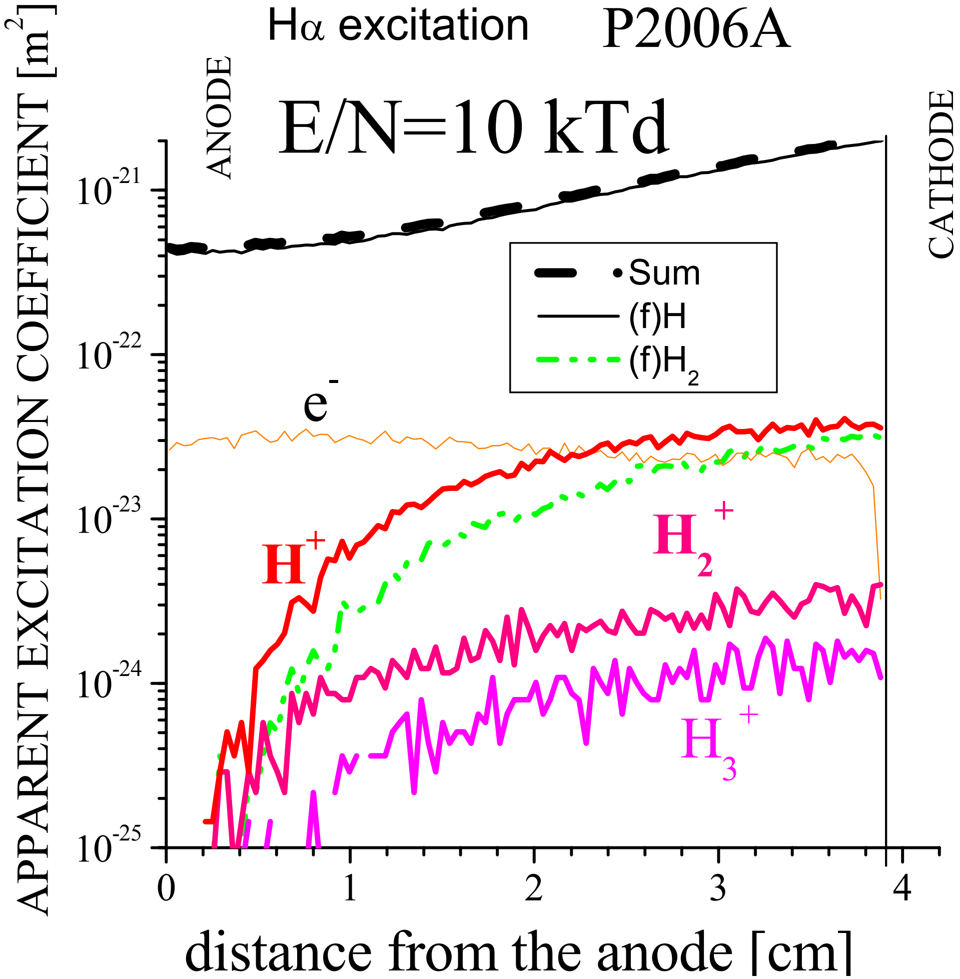




Spatial dependence of Hα emission for 2 scattering models

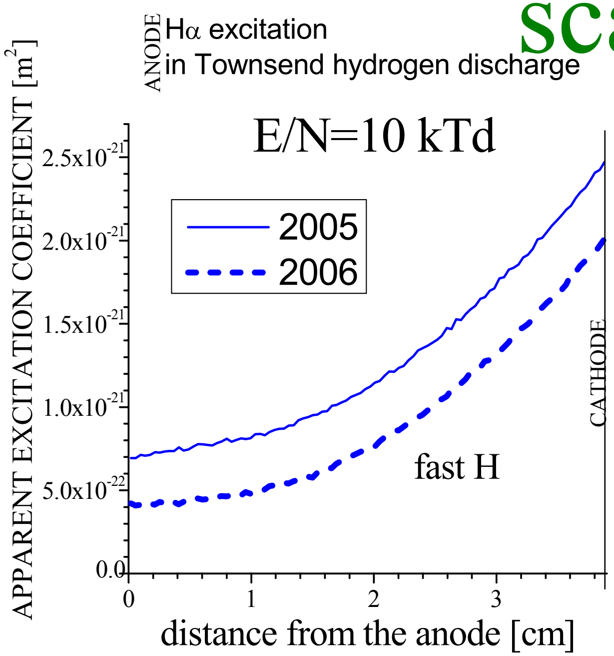
- Monte Carlo simulation

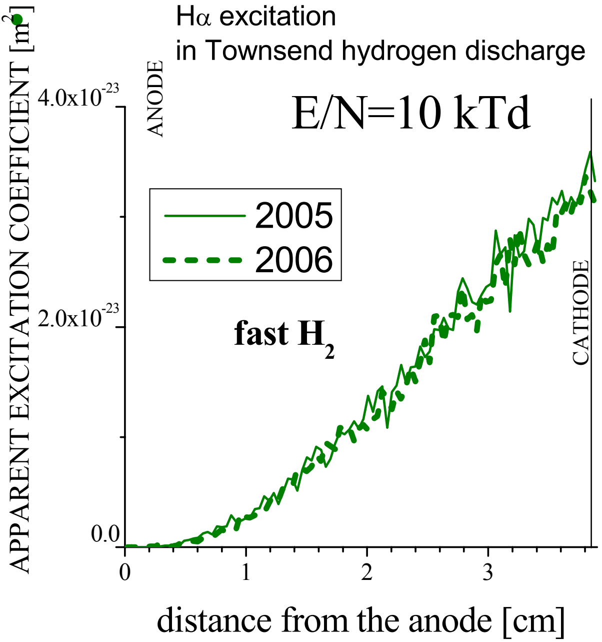


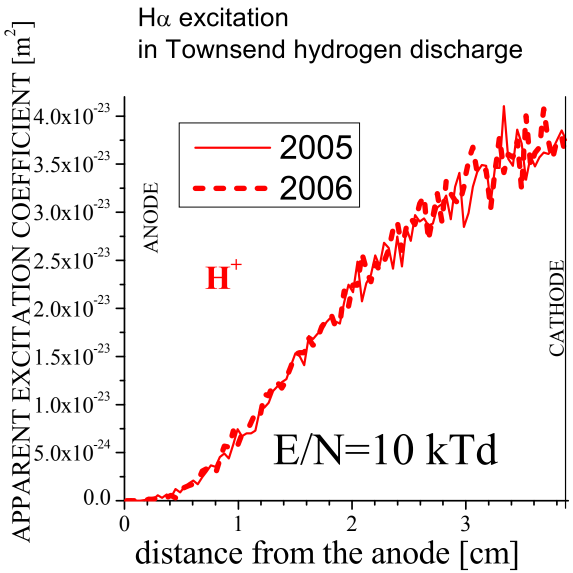


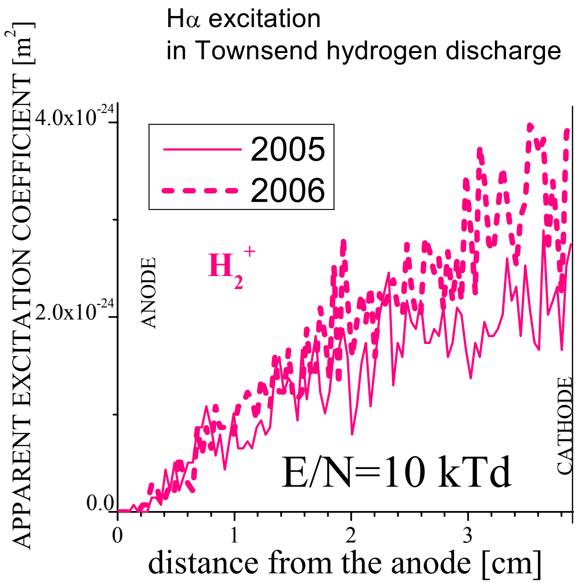
Contributions to spatial emission for 2 scattering models

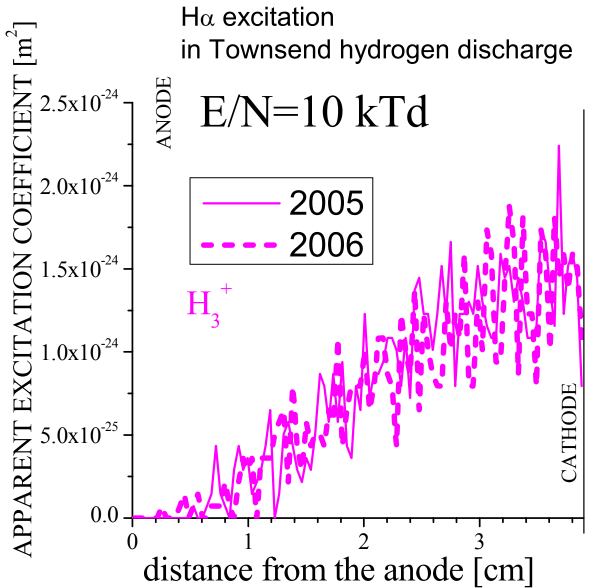
PP2005 - Solid lines
PP2006 - dashed lines





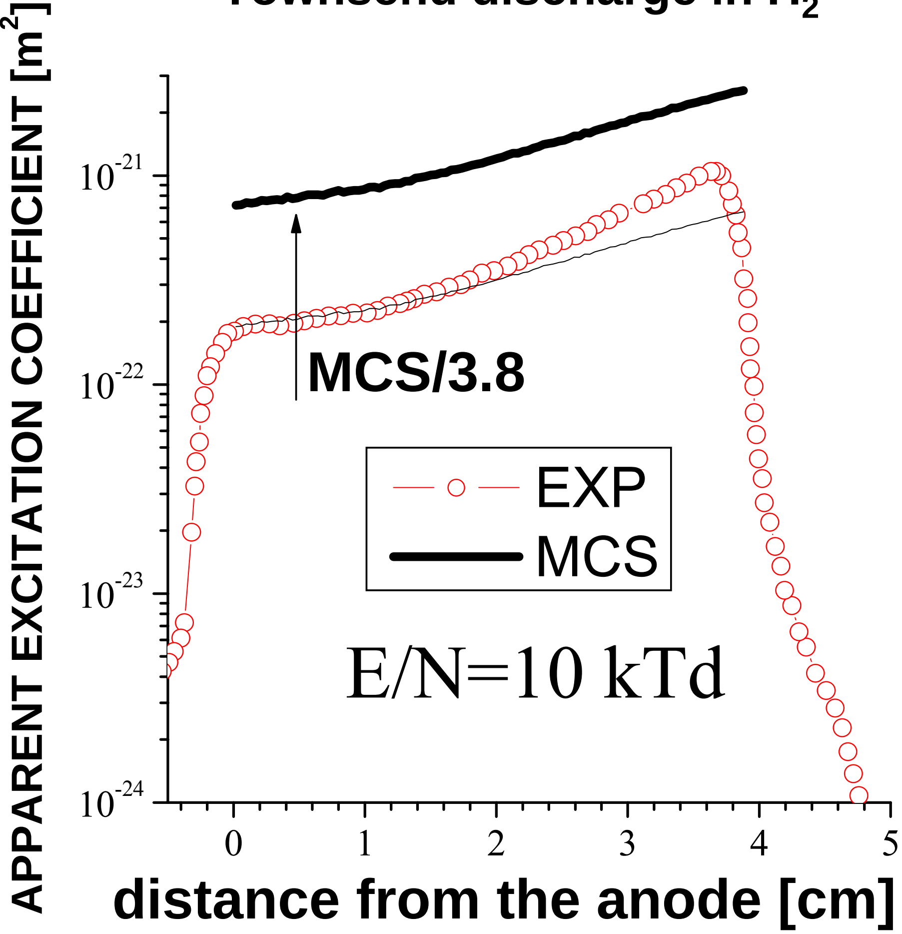




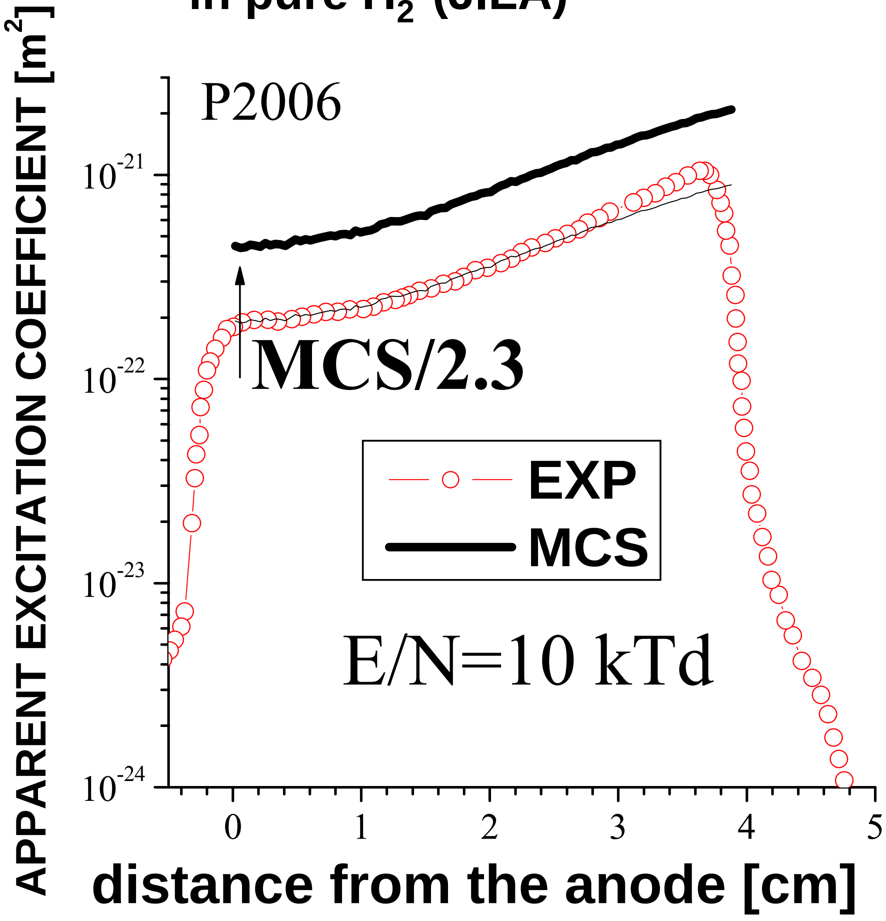


Comparison of Monte Carlo results with an experimental spatial profile for 2 scattering models

MCS-Monte Carlo simulation of Townsend discharge in H_2



EXP: Townsend discharge in pure H_2 (JILA)



for 1000000 electrons

We also analyzed

- **Effect of reflection coefficient dependence with incident angle with model PP2005,**
- **How all vibrational losses affect results obtained by model PP2005,**
- **Effect of electron anisotropy in collisions leading to singlets and ionization.**

So to conclude

- **Basic physics of the process is included in the model,**

- **Details of the model still require some fine tuning,**

- **Two key issues:**
  - **Too few collisions of ions in MC**
  - **Exact model of reflection.**

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