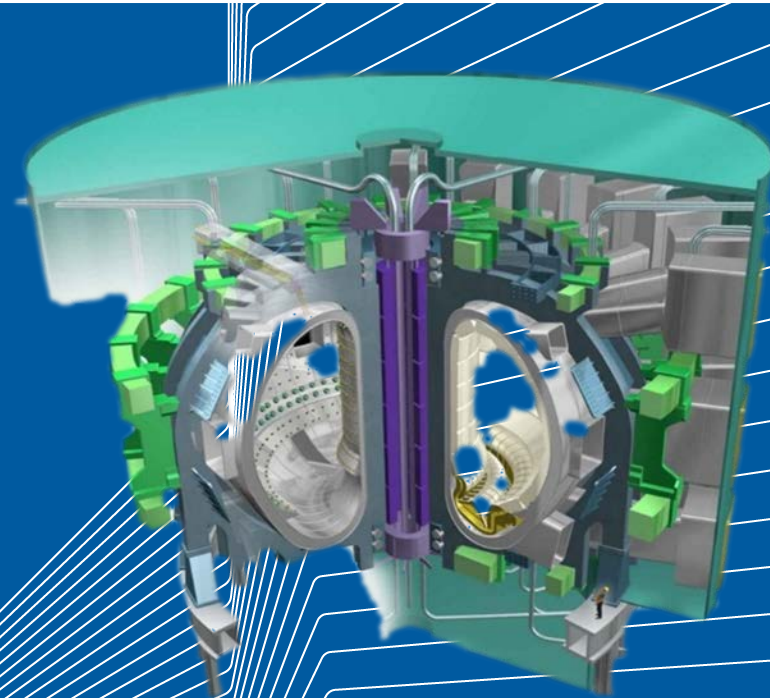


Spectroscopy in Magnetic Confined Fusion Plasmas

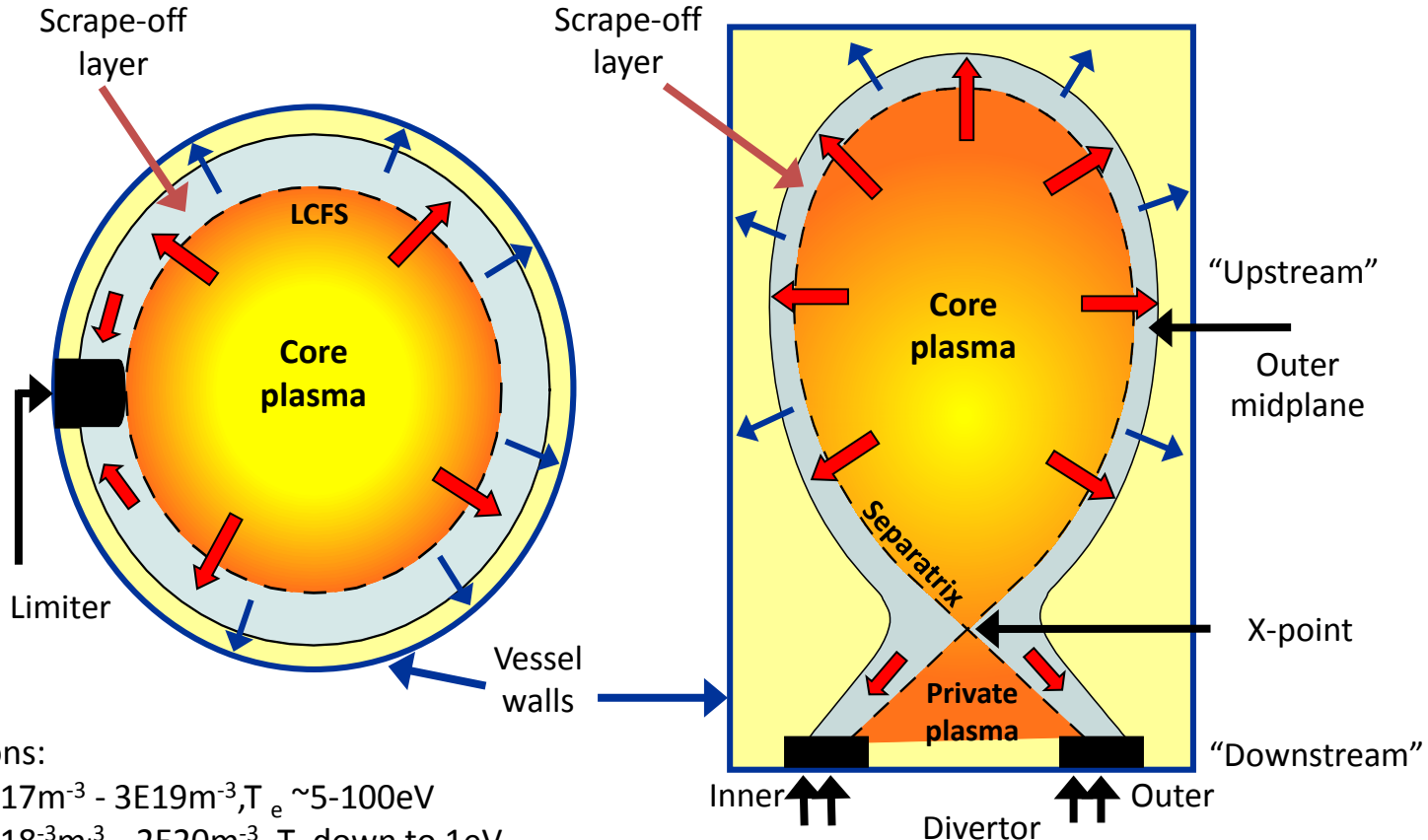
PART II

Sebastijan Brezinsek

Institut für Energie und Klimaforschung - Plasmaphysik
Forschungszentrum Jülich



Regions of Interest

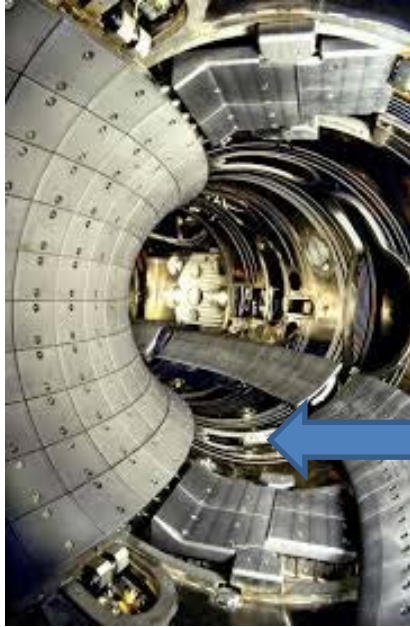


Typical conditions:

FAR SOL: $N_e \sim 3 \times 10^{17} \text{m}^{-3} - 3 \times 10^{19} \text{m}^{-3}$, $T_e \sim 5-100 \text{eV}$

Divertor: $N_e \sim 1 \times 10^{18} \text{m}^{-3} - 2 \times 10^{20} \text{m}^{-3}$, T_e down to 1eV

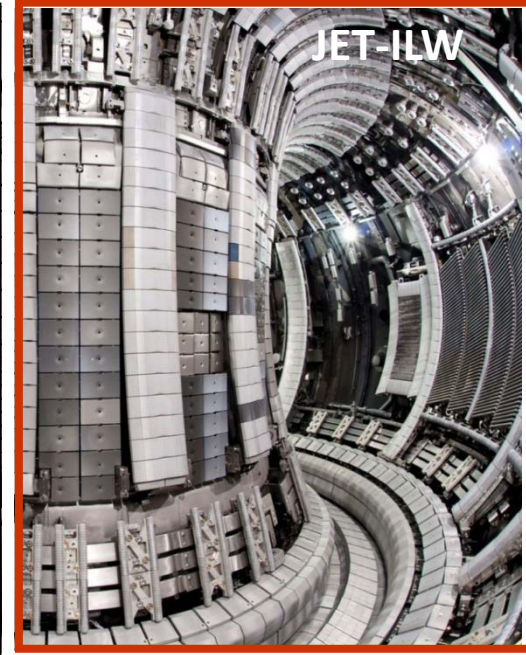
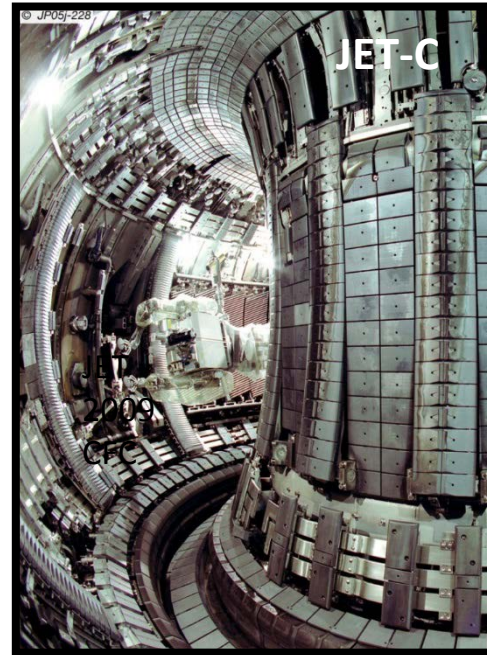
Example Facilities



TEXTOR shutdown 31.12.2013

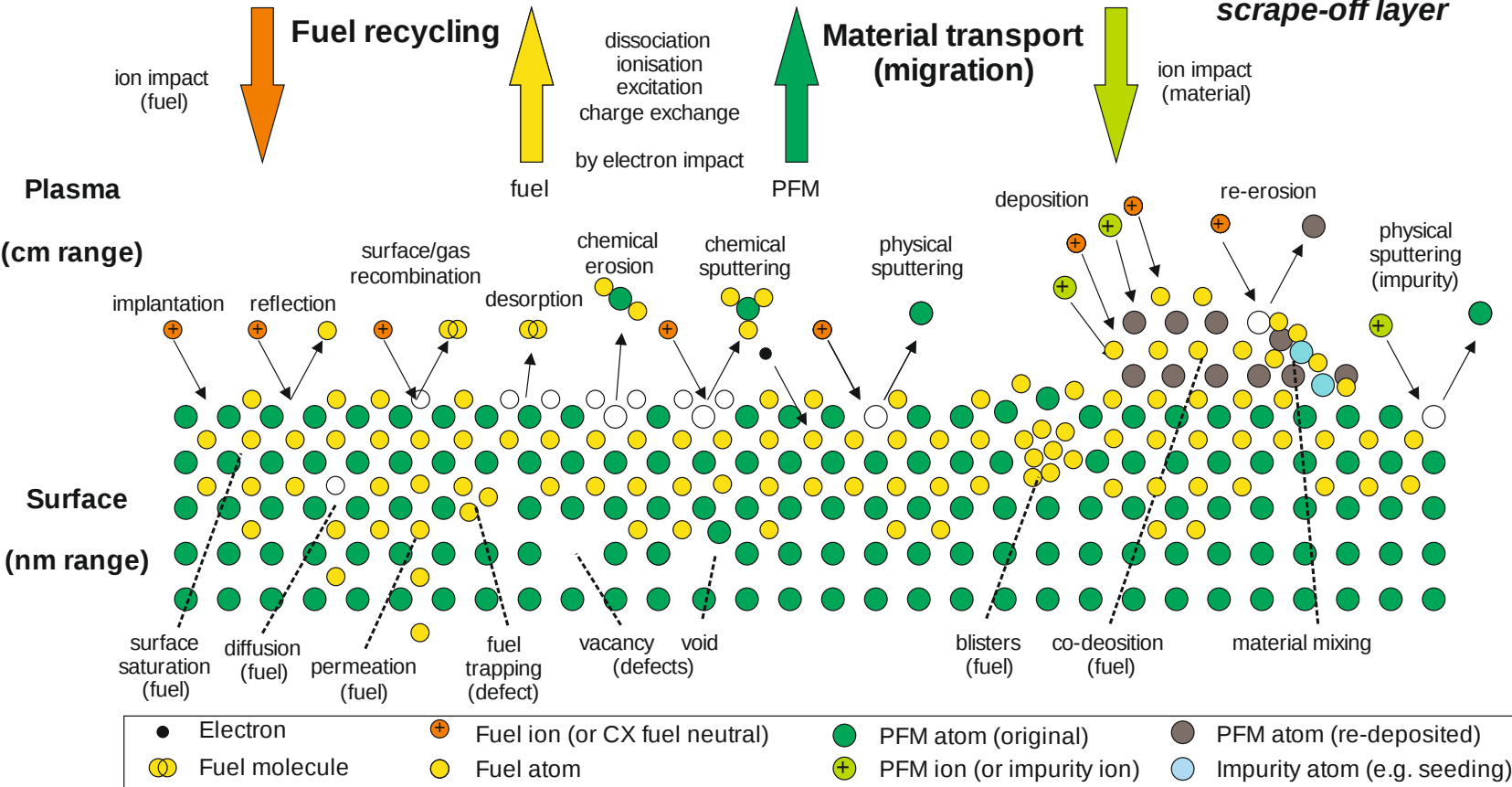
LOCK
for PSI
studies

$R \sim 1.75\text{m}$ $B_t \sim 2.8\text{ T}$ $P_{\text{aux}} \sim 8\text{MW}$
 $a \sim 0.46\text{m}$ $I_p \sim 0.8\text{MA}$ $V_p \sim 10\text{m}^3$



$R \sim 3\text{m}$ $B_t: 3.45\text{ T}$ $P_{\text{aux}} \sim 40\text{MW}$
 $a \sim 1.25\text{m}$ $I_p: \sim 5\text{MA}$ $V_p \sim 100\text{m}^3$

Plasma-Surface Interaction Processes



Processes to be measured - studied – predicted – controlled - understood:

- Plasma composition (fuel and impurities)
- Erosion, transport, and deposition/mixing
- Impurity source distribution and its strength
- Energy angular distribution of sputtered particles
- Penetration depth and radiation distribution
- Fuelling, recycling, and retention/release
- Plasma conditions
- Ionisation /recombination regime in divertor

Input needed for ITER, Reactor in view of operation (radiation/dilution), plasma fueling (fuel cycle), nuclear safety (retention/dust), lifetime (erosion /modification)

Spectroscopy is one of the view methods which permit in-situ access to PSI processes in fusion plasmas as well as plasma conditions at most critical regions

- Introduction
- **Spectroscopic techniques**
- Hydrogen (and isotopes) spectroscopy
- Beryllium hydride spectroscopy
- Tungsten spectroscopy
- Hydrocarbon and carbon spectroscopy

Mainly passive spectroscopy:

- Determination of particle fluxes
 - Fuel recycling flux (e.g. D, H, D₂, HD, H₂)
 - Intrinsic impurity flux (C, W, O ...)
 - Extrinsic impurity flux (Ar, Ne, N ...)
 - Energy and velocity distribution
 - Zeeman-splitting analysis
 - Molecule characterisation
 - Ro-vibrational population
 - Dissociation chain
 - Plasma parameter determination
 - Balmer-line ratios $\Rightarrow T_e$
 - Stark broadening $\Rightarrow n_e$
 - Charge-exchange recombination
 $\Rightarrow T_i$ and n_i
- and many more

Mainly active spectroscopy:

- Local plasma parameters (atomic beams)
- Population of energy levels (**LIF**)
- Impurity concentrations (CXRS - NBI)
- Fuel content and impurity composition of layers (LASER ablation & desorption)
- Molecular densities (CRDS - LASER)

USUALLY:

$\Rightarrow$ ionising plasma conditions
and no opacity

$\Rightarrow$ only divertor can enter recombination
and opacity can play a role

Line emission

$$\varepsilon = \frac{1}{4\pi} n_A^* A_{ij}$$

$$n_A^* \sum_{k \leq i} A_{ik} = n_A n_e \langle \sigma_{Exg} \nu_e \rangle$$

with Γ as branching ratio:

$$\Gamma = A_{ik} / \sum_{k \leq i} A_{ik}$$

$$I_{tot} = \Gamma \frac{h\nu}{4\pi} \int_{r_1}^{r_2} n_A(r) n_e(r) \langle \sigma_{Exg} \nu_e \rangle dr$$

Spectroscopy: From Photons to Particles II

$$\Phi_A = \frac{4\pi}{\Gamma} \frac{I_{tot}}{h\nu} \frac{\langle \sigma_I \nu_e \rangle}{\langle \sigma_{Exg} \nu_e \rangle} = 4\pi \frac{I_{tot}}{h\nu} \frac{S}{XB}$$

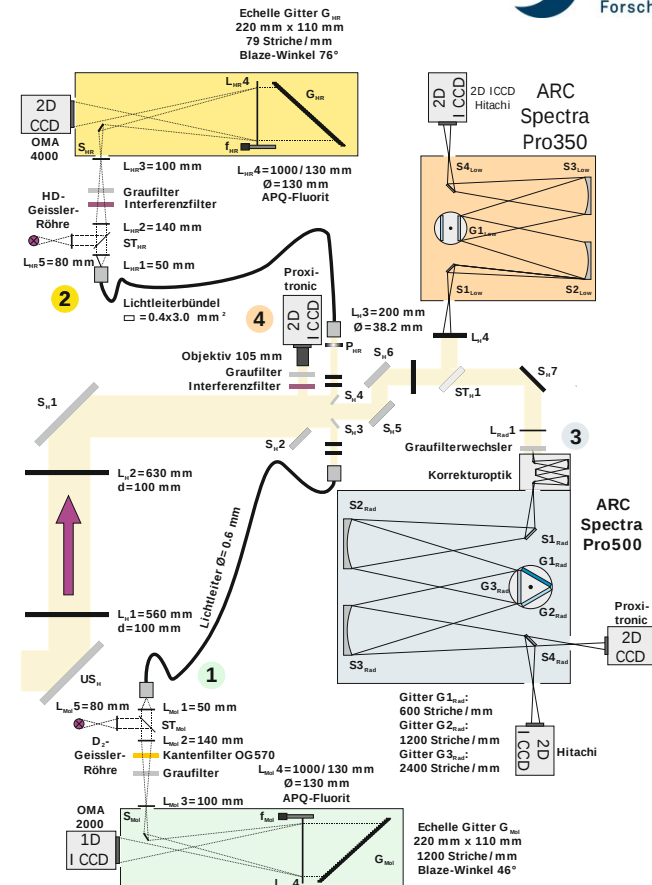
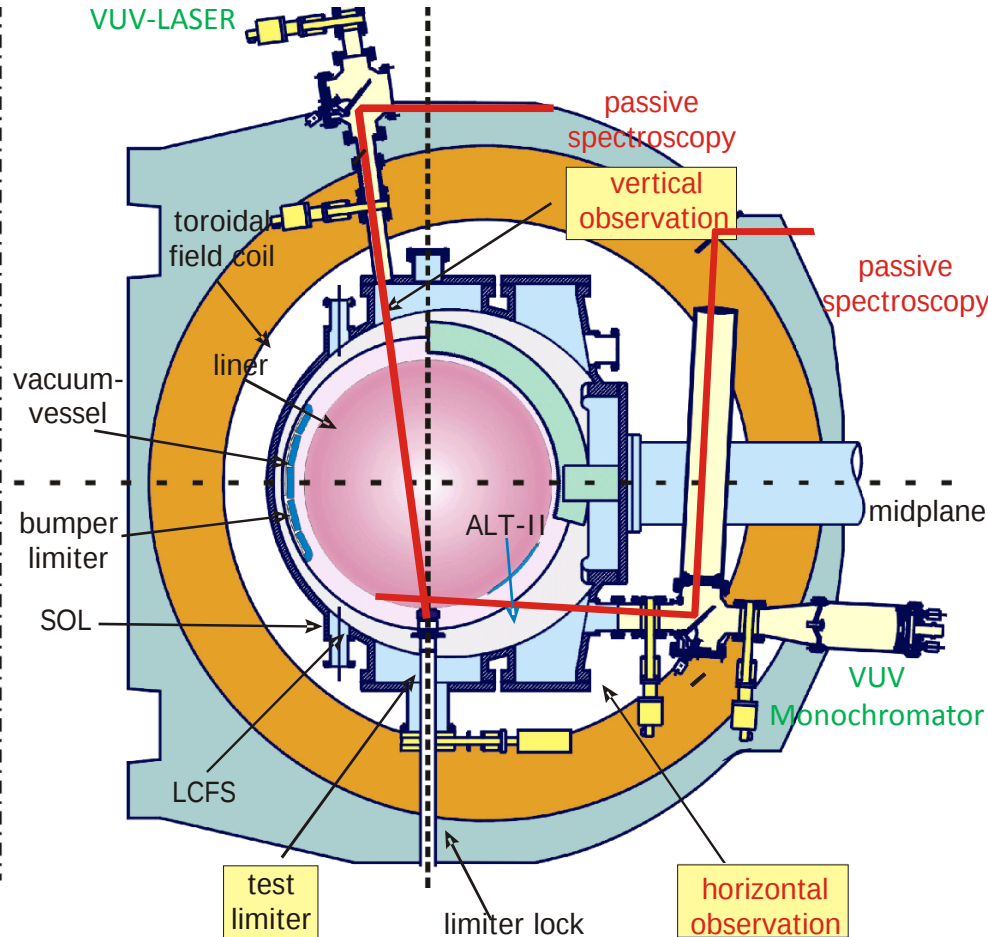
In case of molecular emission:
D/XB with „D“ for Decay =>
Dissociation + Ionisation

the expression S/XB has to be obtained
by calculations (including CRM's) or
experimentally

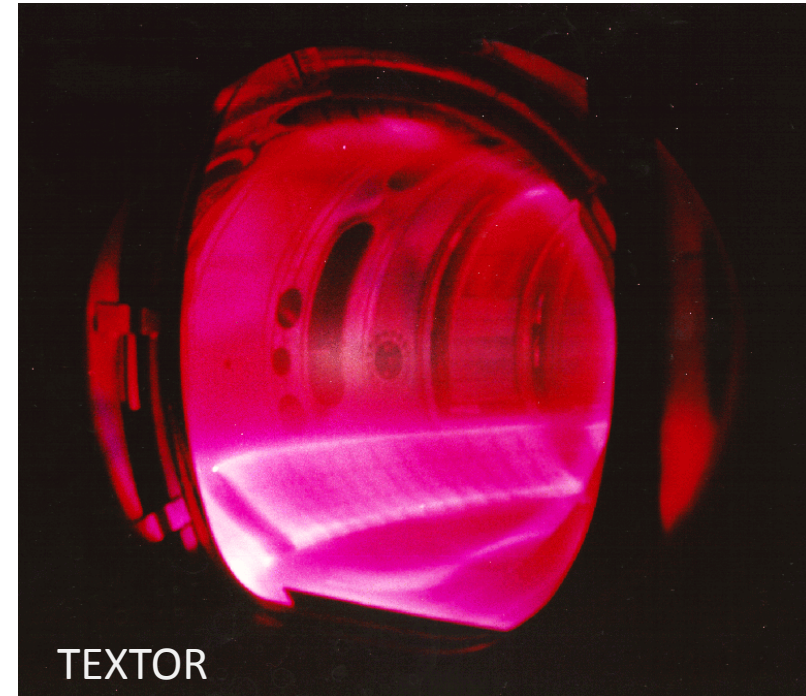
$$\frac{\langle \sigma_I \nu_e \rangle}{\Gamma \langle \sigma_{Exg} \nu_e \rangle} = \frac{\Phi_A}{4\pi (I_{tot} / h\nu)}$$

(OPEN) ADAS – „ionisation events per photon

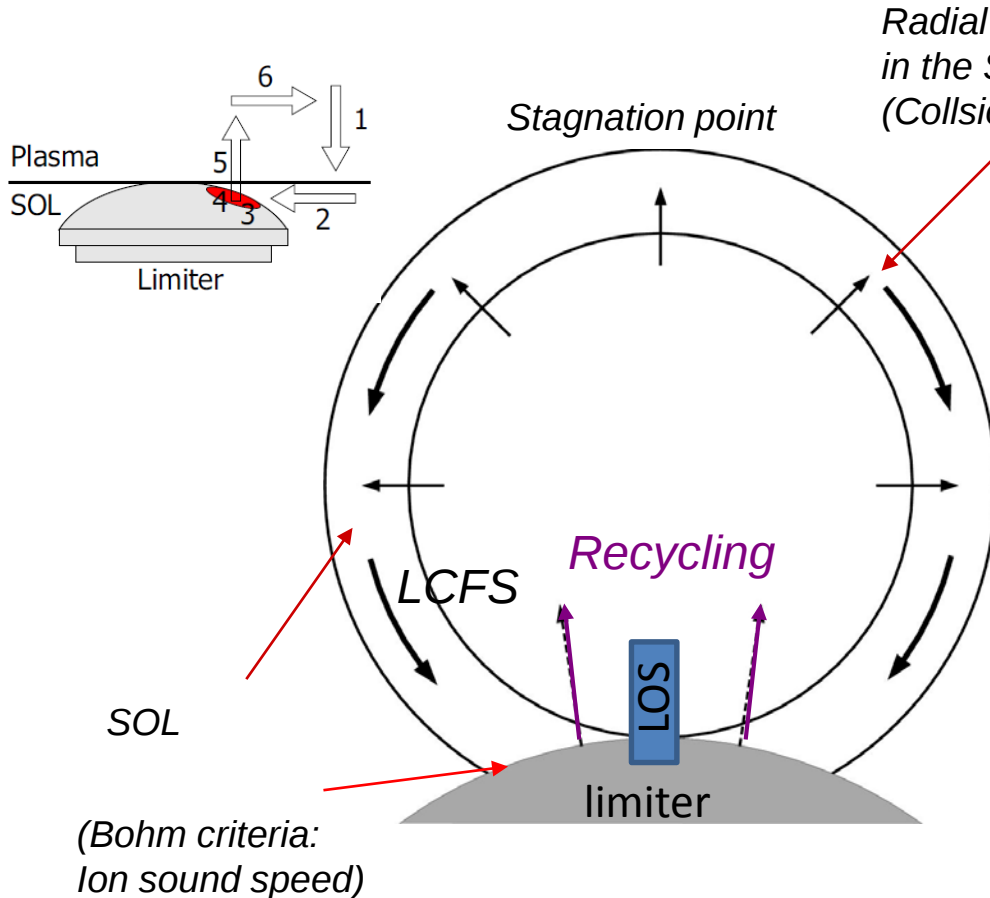
Experiments: Lock Systems in TEXTOR



- Introduction
- Spectroscopic techniques
- **Hydrogen (and isotopes) spectroscopy**
- Beryllium hydride spectroscopy
- Tungsten spectroscopy
- Hydrocarbon and carbon spectroscopy

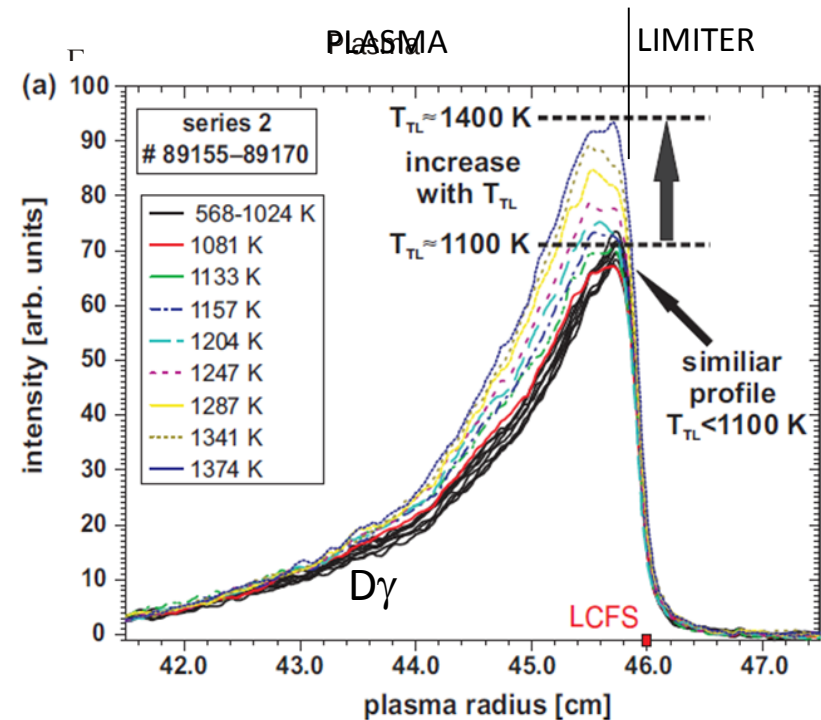


Arrangement / Neutrals Penetration

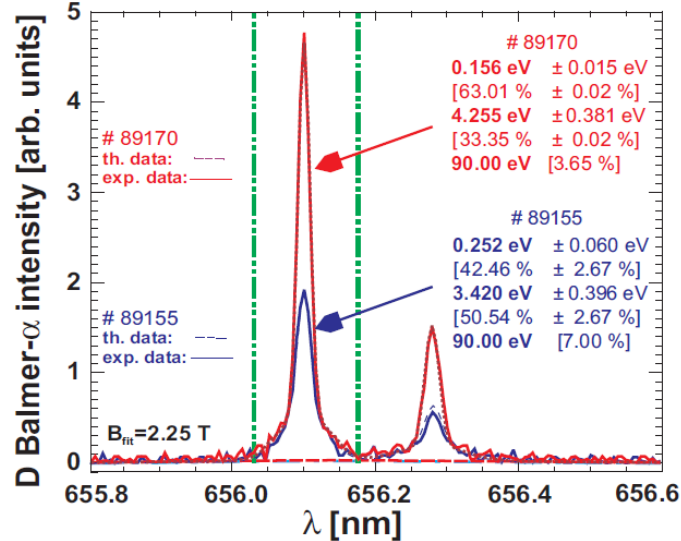


Radial transport
in the Scrape-Off Layer
(Collisions, Drifts)

“Identical” plasma in T_e and n_e ,
but photon flux changes with T_{surf}

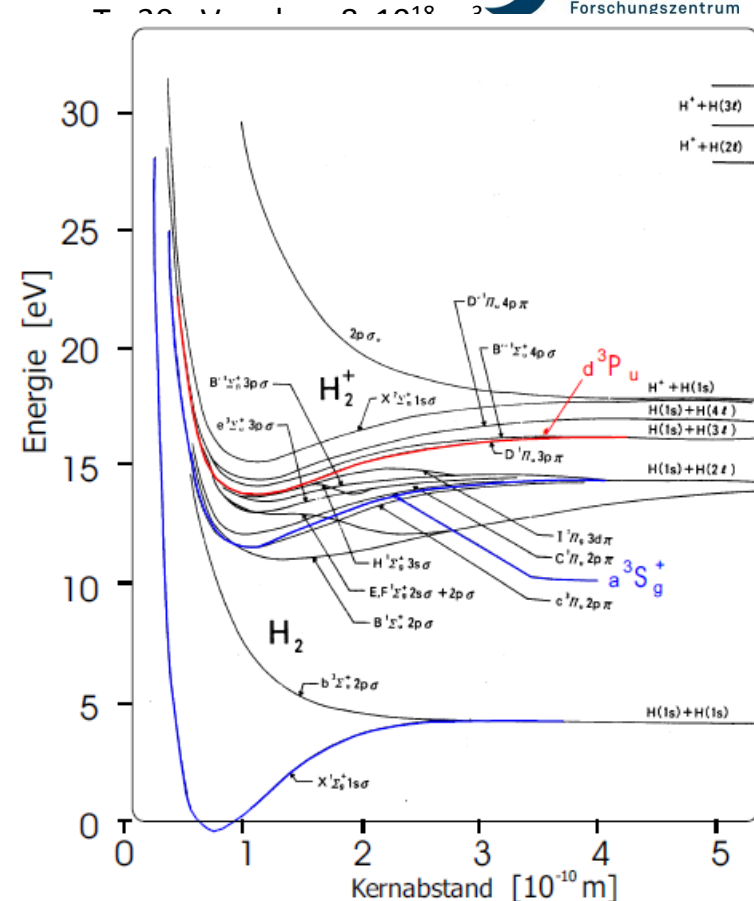


Atomic Line Shape Analysis



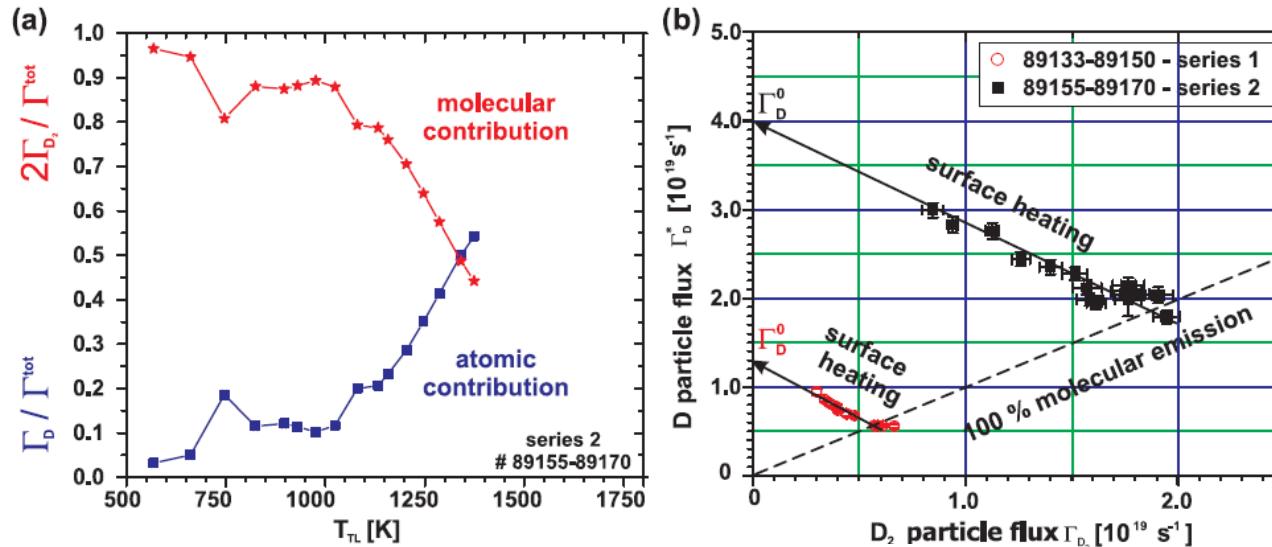
- Zeeman-Splitting analysis reveals: very cold atoms (0.2eV)
- Molecules start from surface: Franck-Condon energy 2.2eV expected

- Change of D_2 destruction mechanism at low T_e
- Destruction path via D_2^+ only dominates above 15eV
- Destruction path via D_2 dissociation dominates below 10 eV



Composition of Recycled Deuterium

- High D^+ flux to the wall ($10^{24} D^+ s^{-1}m^{-2}$), surface saturation, and almost 100 % recycling
- Thermal release of D_2 from the (graphite) wall and some reflected fast particles
- Destruction chain depends on local plasma conditions and surface temperature $\Rightarrow$ atoms at high T_{surface}

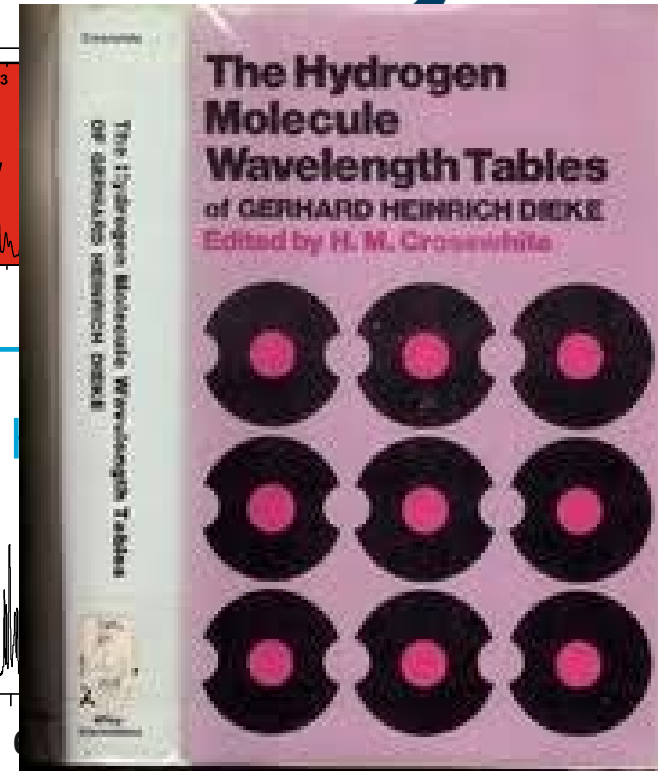
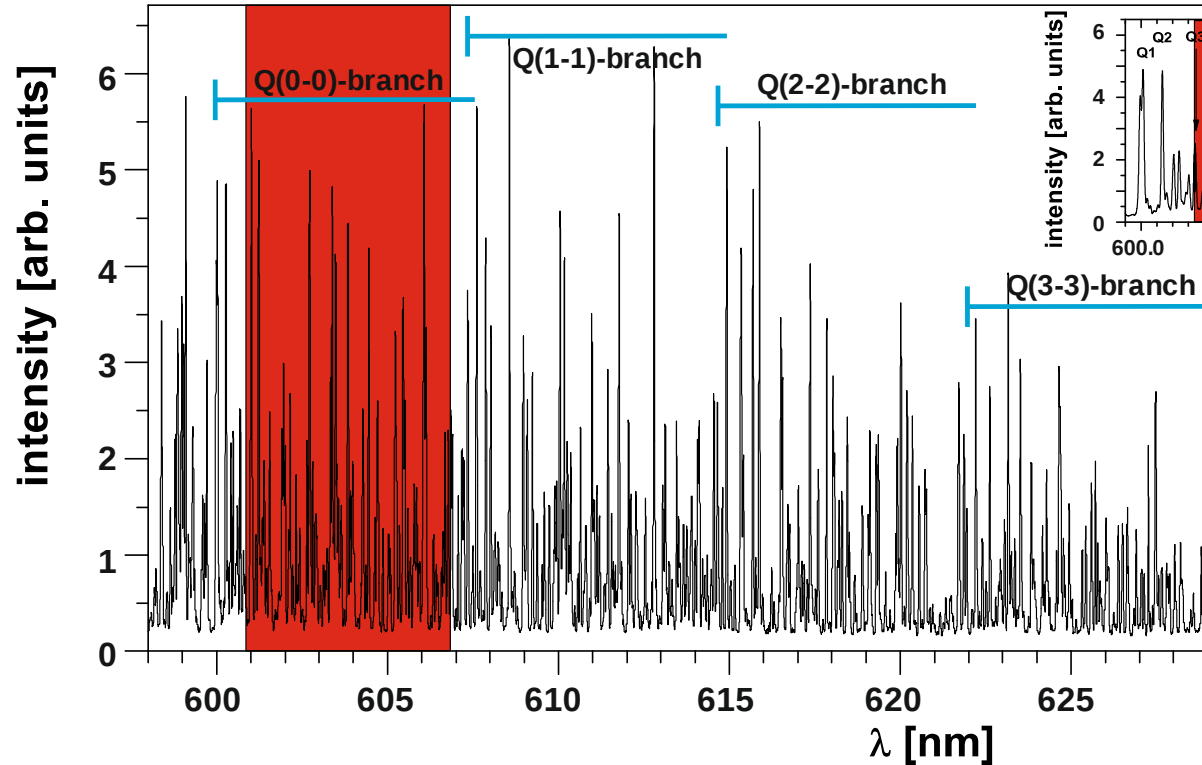


TEXTOR:

Series	Discharge	$n_e [10^{18} m^{-3}]$	$T_e [eV]$	$T_i [eV]$	$T_{\text{TL}} [K]$
1	89133-50	2.8	77	120	620-1380
2	89155-70	5.2	42	150	570-1390

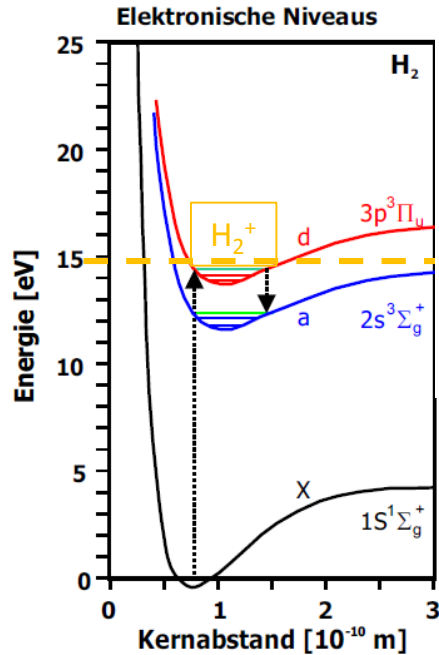
S. Brezinsek
PPCF2002

Measurement of D₂ in TEXTOR



Needs analysis and conversion to total molecular flux
from rotational to vibrational to electronic transition....

Fulcher Band: $3p\ ^3\Pi_u \rightarrow 2s\ ^3\Sigma_g^+$

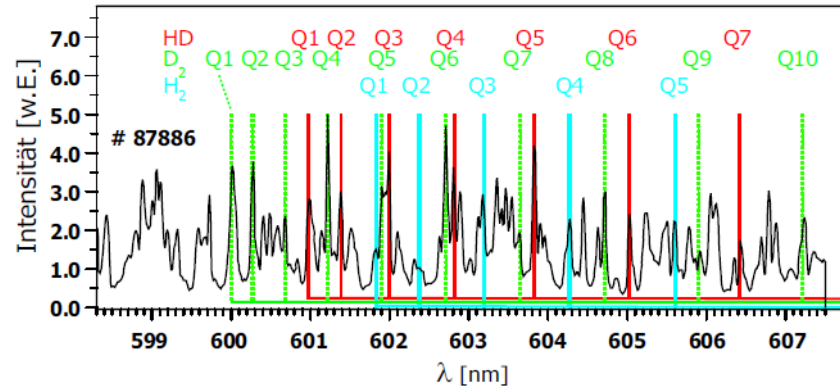
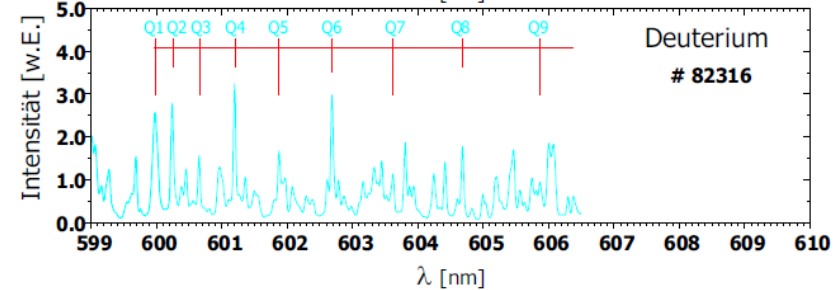
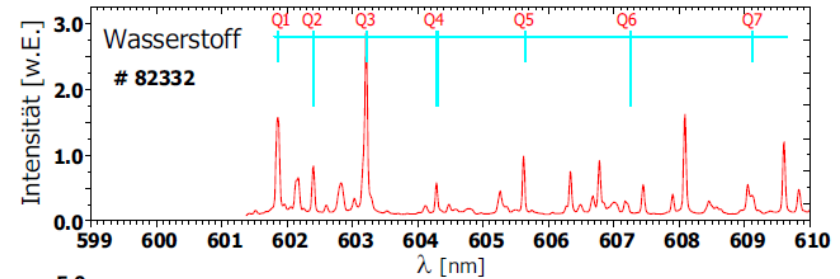


Fulcher-Bande: $3p\ ^3\Pi_u \rightarrow 2s\ ^3\Sigma_g^+$

$d\ ^3\Pi_u \rightarrow a\ ^3\Sigma_g^+$

Hund's case (b)

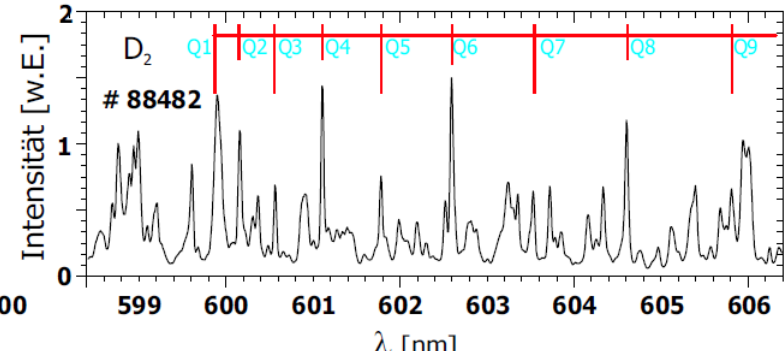
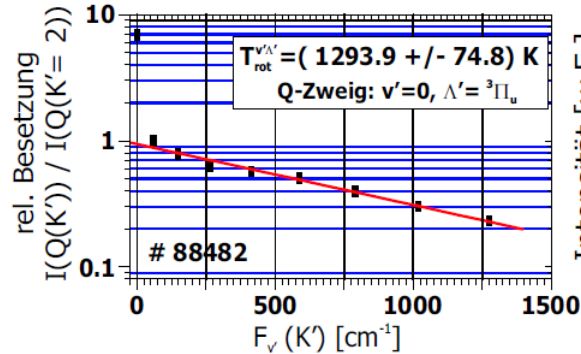
- Electronic transition of highly excited hydrogen molecules
- Direct visibility of the impact of nuclear spin! Multiplicity!



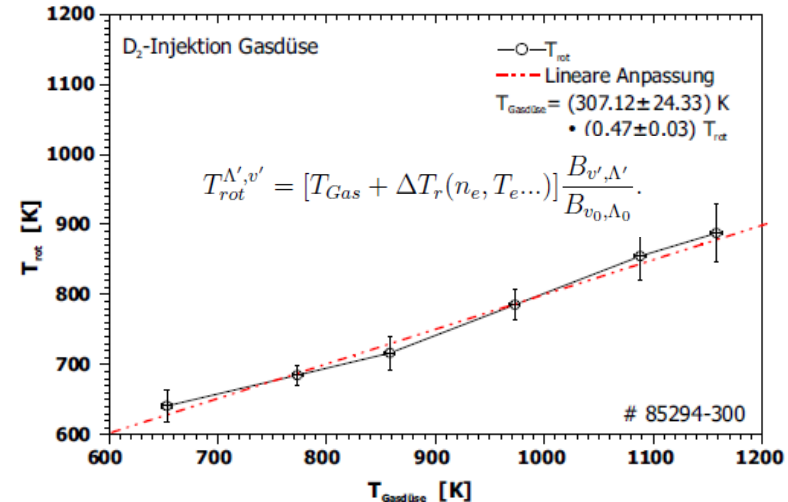
Rotational Population Temperatures

Optical rules applied
P, Q, R branches

Hönl-London Factors



- Rotational and vibrational population according to Boltzmann distribution
- D_2 (injections) for plasma diagnosis (or calibration) otherwise D_2 recycling flux
- T_{rot} and T_{vib} also used for diagnosis of plasmas
- Additional parameter determined by surface properties: $T_{surface}$ / vibrational excitation



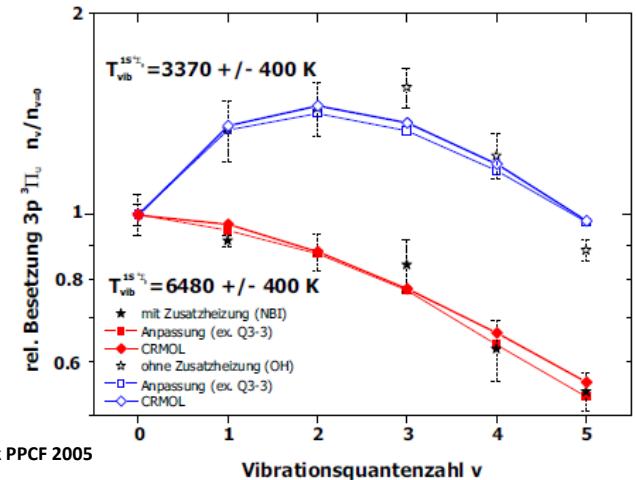
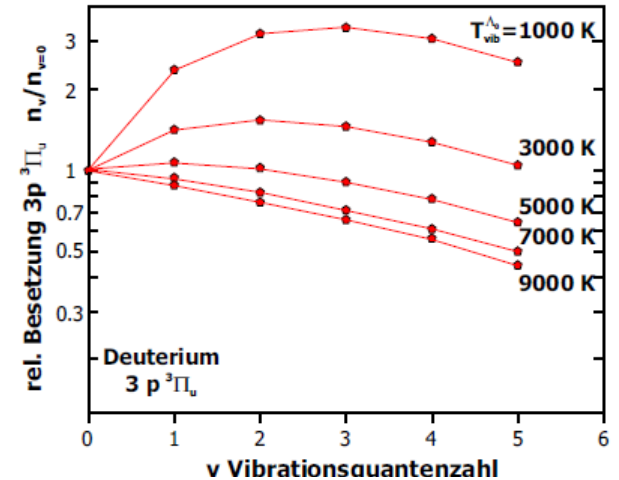
Vibrational Population Temperatures

Optical rules applied

Main diagonals called Fulcher- α bands

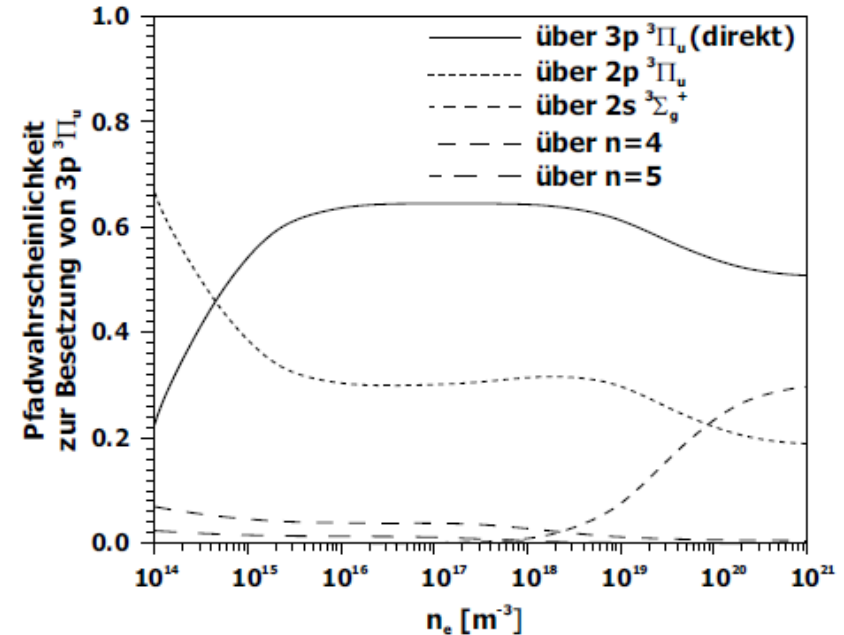
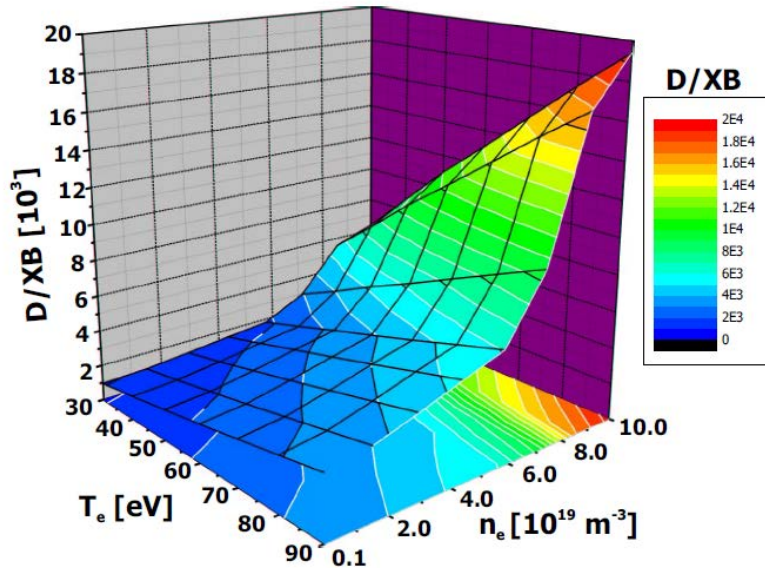
Franck-Condon Factors for transfer upper state to ground state population

- Population in upper state can be determined and linked to ground state
- CRM connects excited state with ground state: reproduce “plasma part”
- Surface materials can impact on initial distribution: e.g. C, a-C:H layers, Ta
- Responsible reactions: Eley-Rideal etc.



Photon Efficiency and Population of $3p\ ^3\Pi_u$

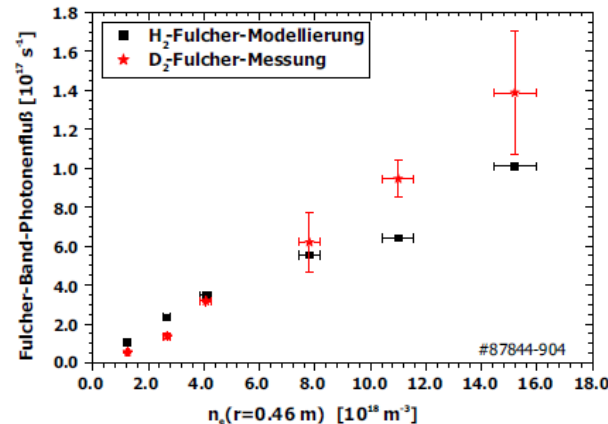
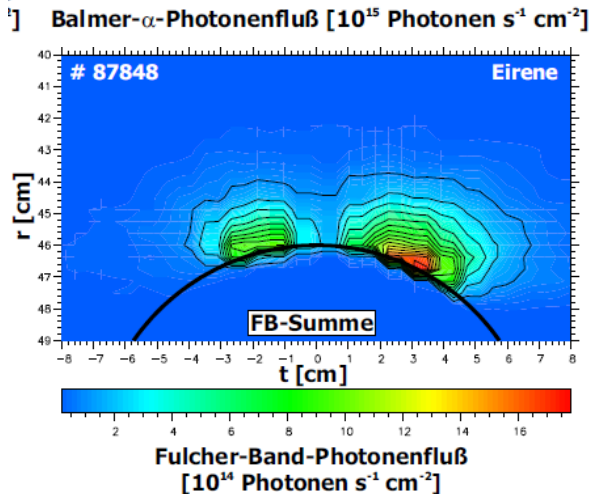
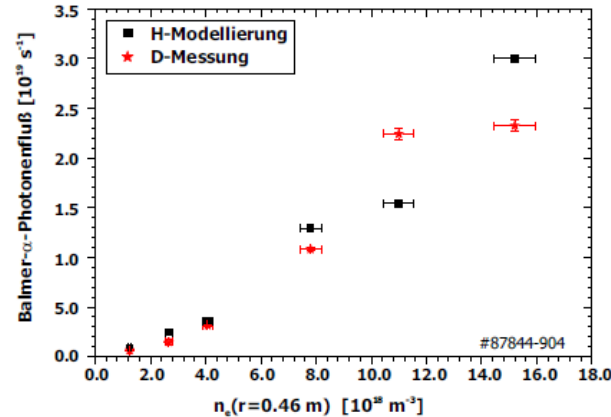
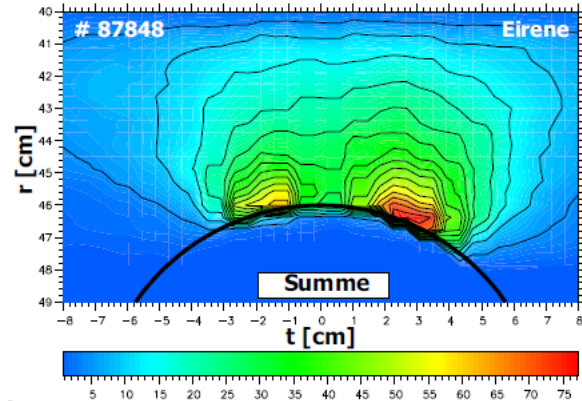
- CRM for hydrogen and deuterium exist meanwhile (e.g. in EIRENE)
- Electronically and vibrationally resolved data available



- At the time of work – benchmark by local injection of D_2 and measurement and analysis

- Simulate spectrum => determine T_{rot} (all vib states) => determine T_{vib} => n tot estimation

Comparison with EIRENE Code

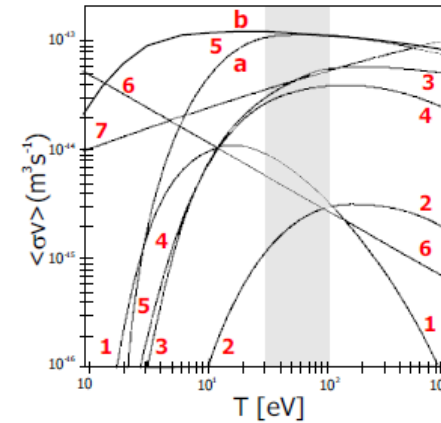
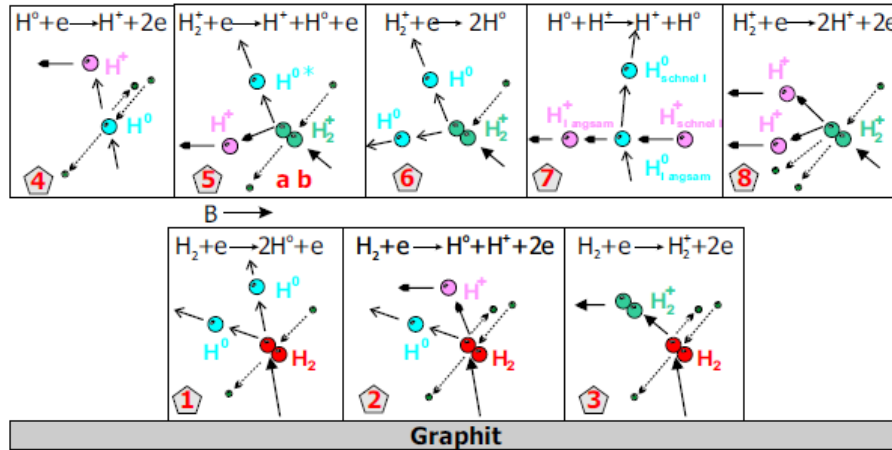


- Good agreement in easy ionizing plasma conditions
- Assuming thermal molecules at start
- Recently D_2 recycled at W showed different behavior

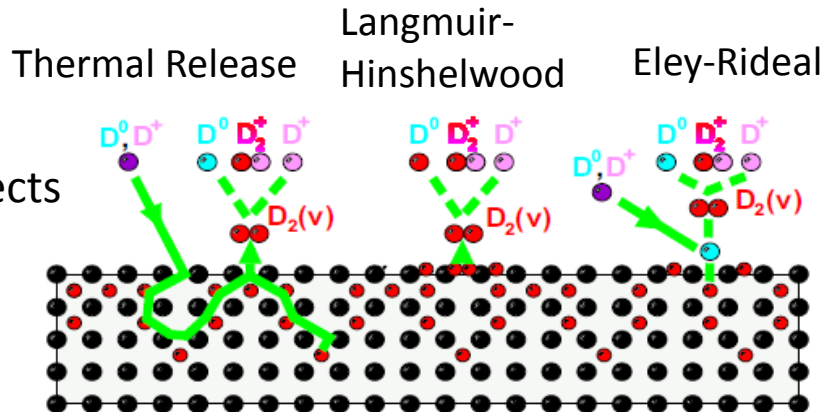
- Next challenge: recombining plasmas

Destruction Path for Hydrogen Molecules

Plasma



Surface effects

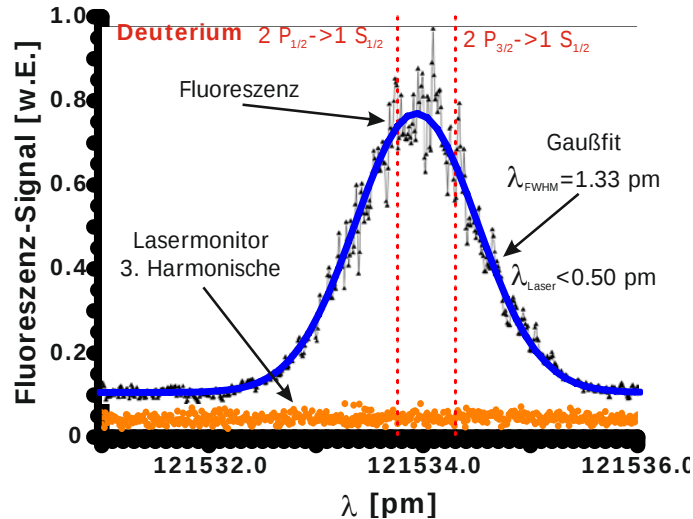


Full set in EIRENE
JUEL-4105 Report

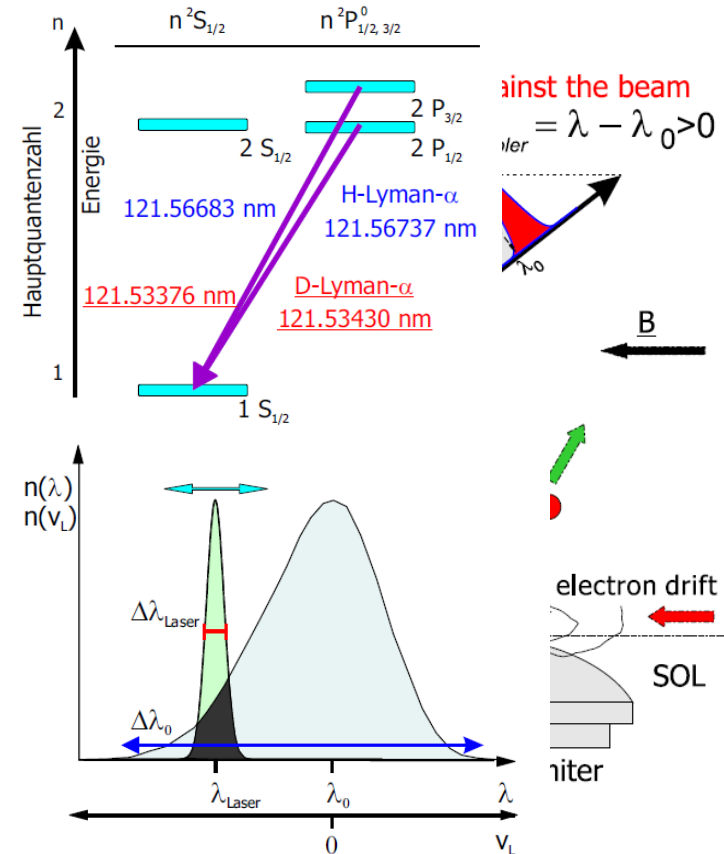
www.eirene.de

Cold Atoms? Independent Proof via LIF on Ly- α

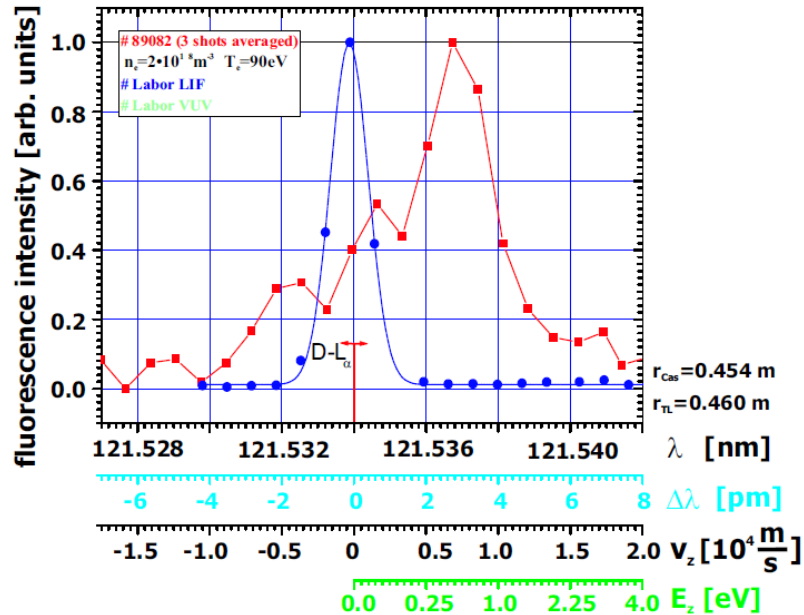
Lyman- α laser by frequency tripling: Ar/Kr



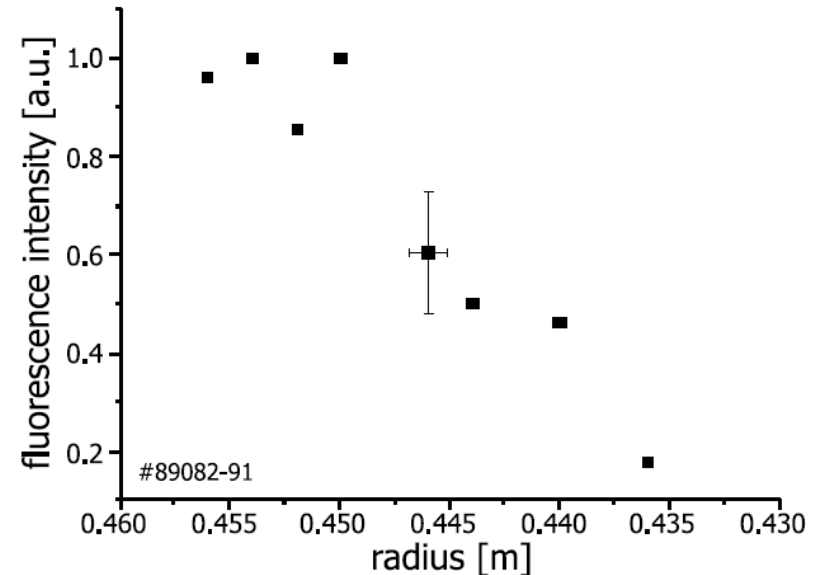
Measure population and energy of atoms in ground state of deuterium



Cold Atoms? Confirmed by LIF on Ly- α



Cold atoms - but method is very, very costly ...

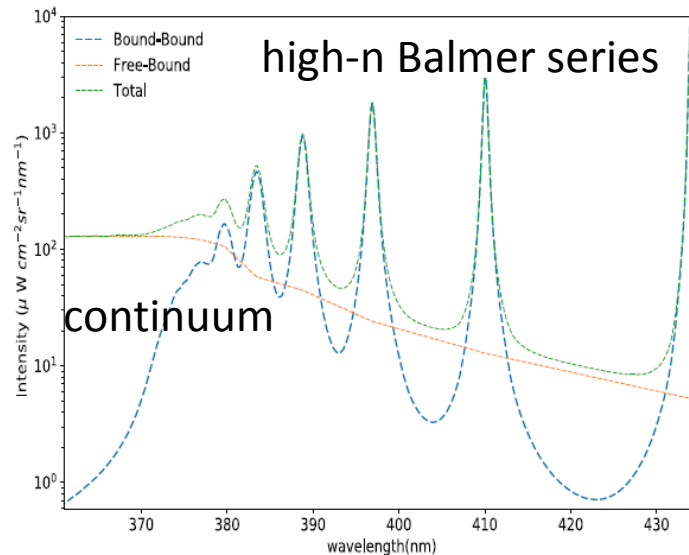
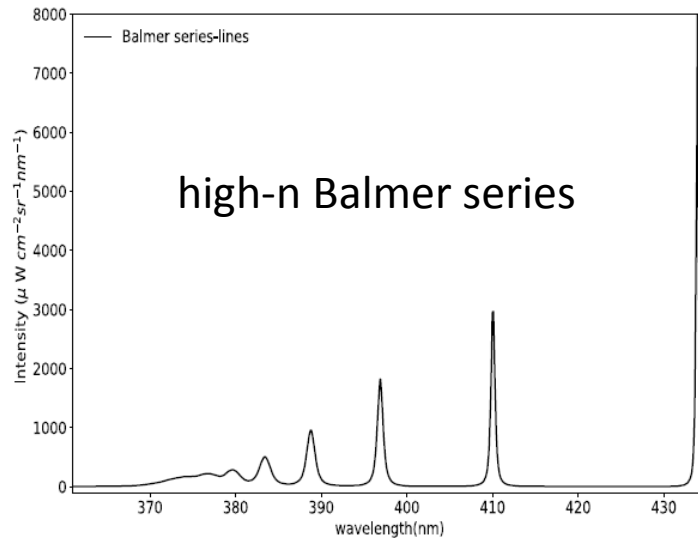


Penetration depth as expected ...

N_e and T_e in Recombining D Plasmas

Transfer to complex recombining plasmas

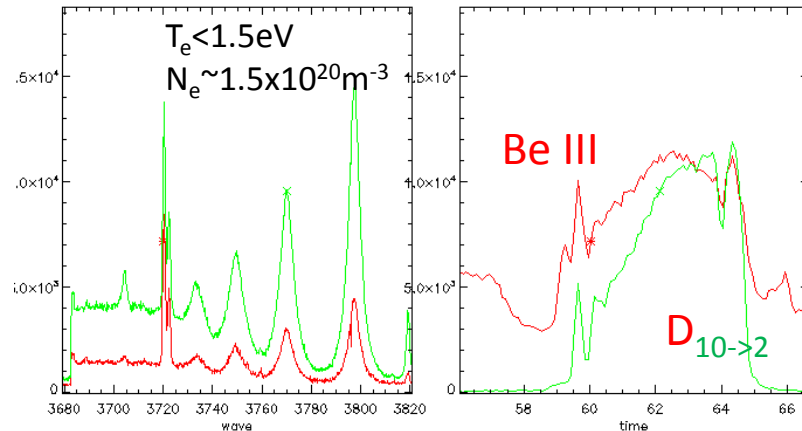
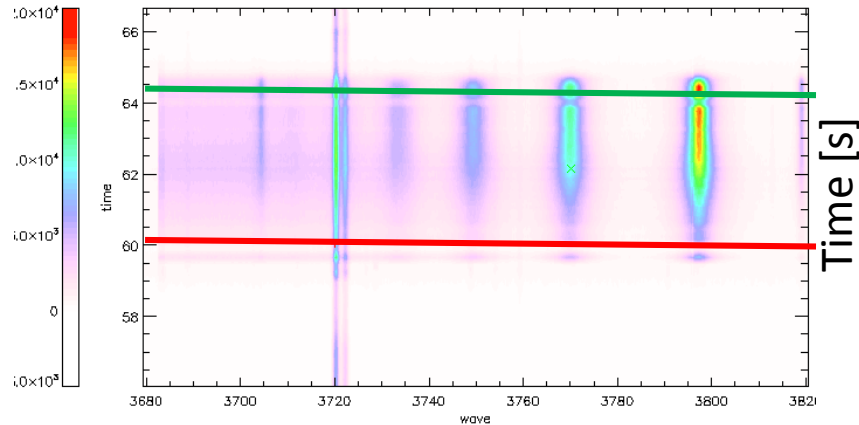
- Balmer and Paschen series recombination used and analysed (compared with ADAS data)
- Line ratio provides T_e , “continuum jump” analysis (Terry et al.)
- Stark broadening for n_e determination (Poetzel et al.)



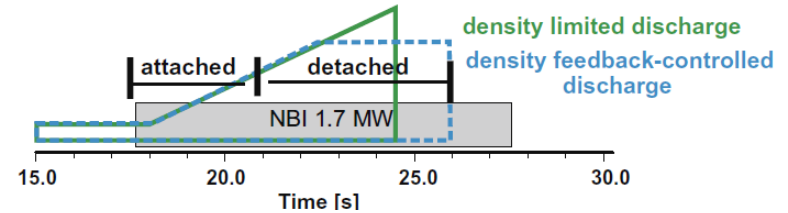
Koubiti 2019

$$N_e = 8 \times 10^{20} m^{-3}, T_e = 1.1 eV$$

JET Divertor: Recombining D Plasmas (JET-ILW)



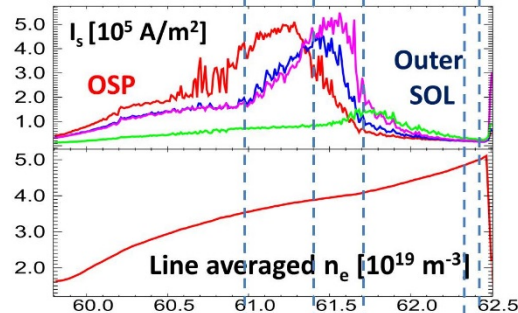
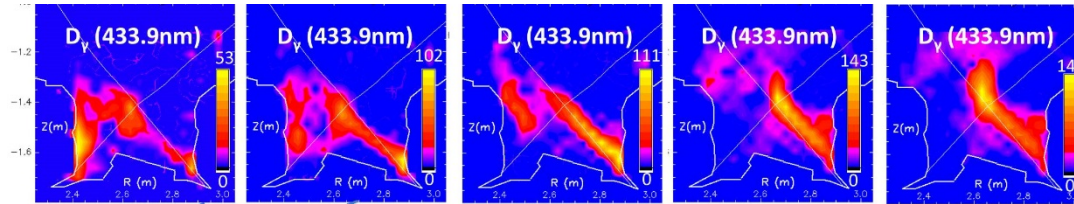
Density ramp



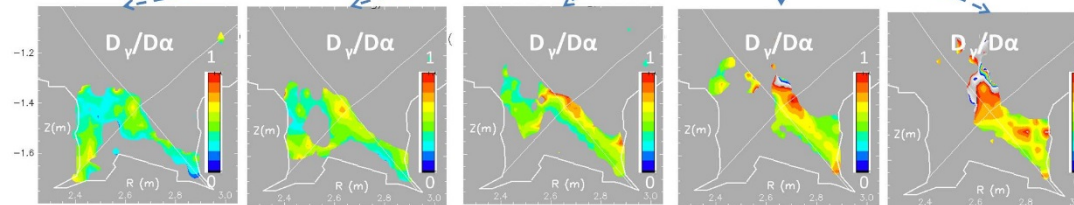
- Provides T_e and n_e from volume recombination in front of target plate
- Detachment indicator

- Issue Ly- α radiation insufficient to explain radiation in these plasmas
 - Revisiting data and new diagnostics to check for opacity effects in JET
- (B. Lomanowski et al.)

JET Divertor: Recombining D Plasmas



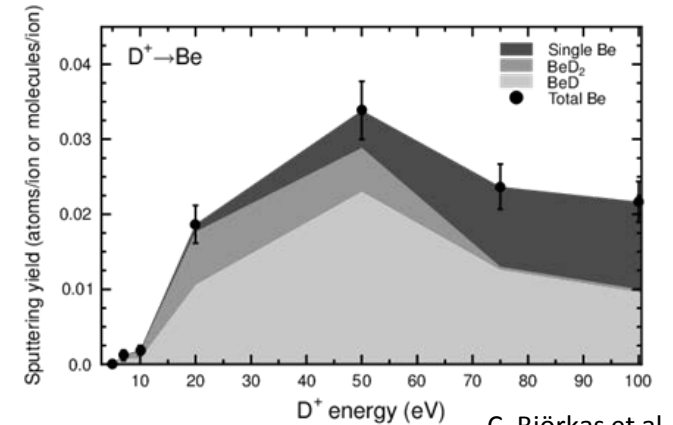
A. Huber et al.



- Interference filtered data used to obtain 2D distribution
- Full detachment at inner divertor leg observed
- Control of ionization front position possible (TCV)

- Multiple cameras with interference filters used to obtain spatially resolved T_e
- Most suitable D_γ over D_α

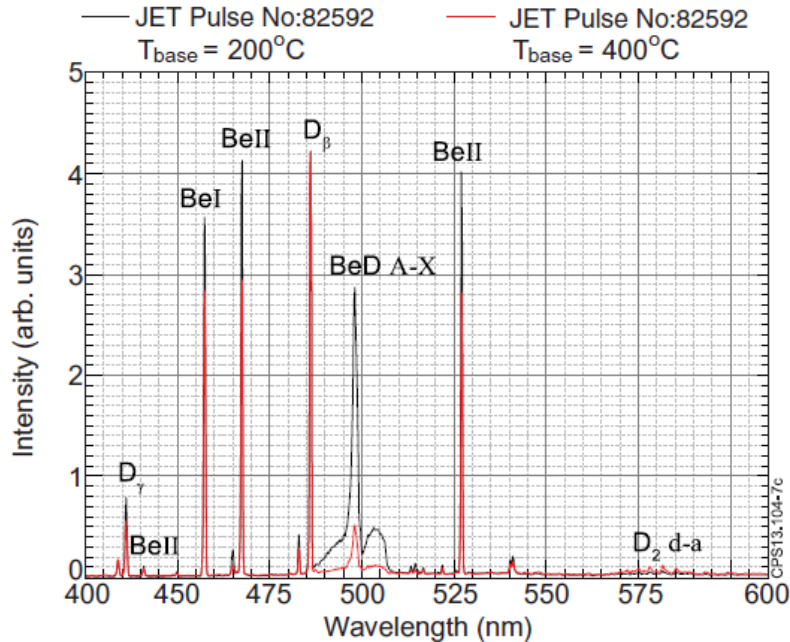
- Introduction
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- Beryllium hydride spectroscopy
- Hydrocarbon spectroscopy
- Tungsten spectroscopy



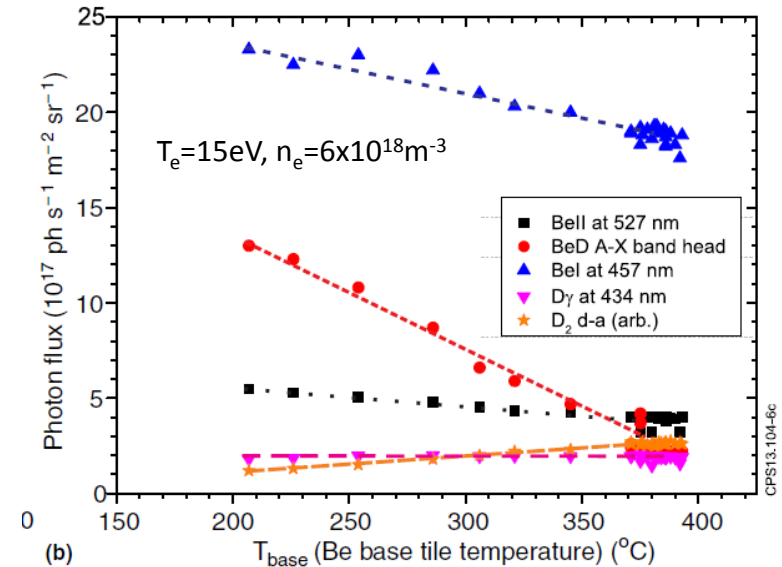
Beryllium Hydride Formation

Chemical (assisted physical) sputtering also observed in JET-ILW at the Be limiters

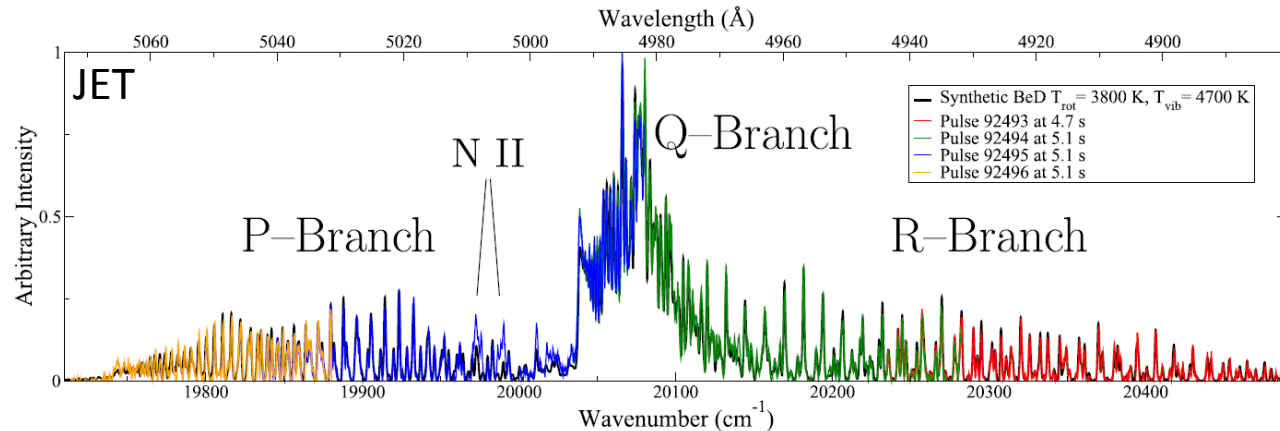
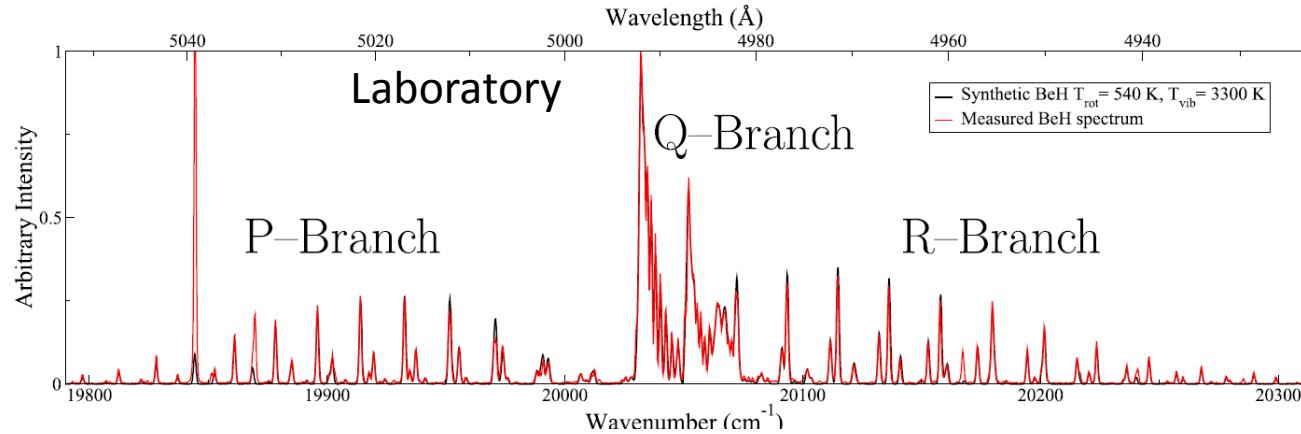
- Identical limiter discharges with temperature scan
- BeD observed and decays with T_{surf}
- D_2 increases with T_{surf} (desorption)
- Ratio of Be I and Be II fluxes provide dissociation chain information: 25% via BeD^+ formation



S. Brezinsek NF 2014



Beryllium Hydride Spectroscopy Modelling

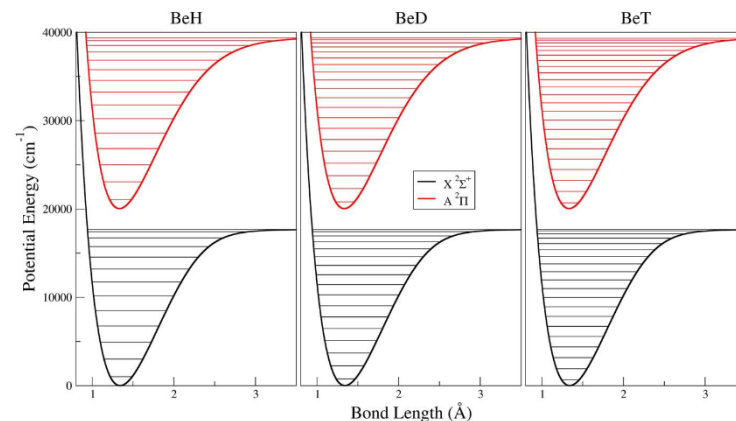
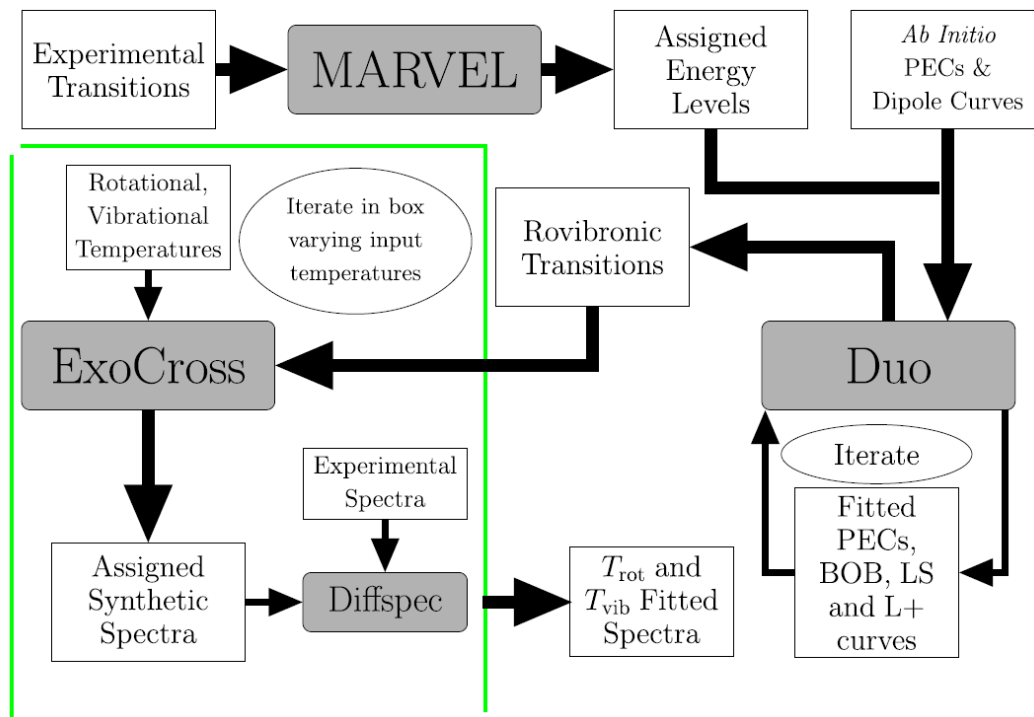


Darby-Lewis 2018

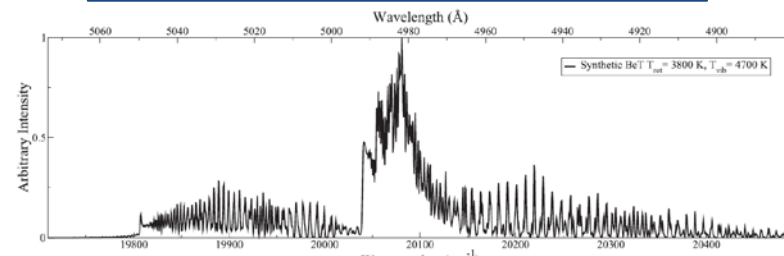
<http://exomol.com/>

Beryllium Hydride Synthetic Spectra

State-of-the-art procedure to assign energy levels and calculate rovibronic transitions

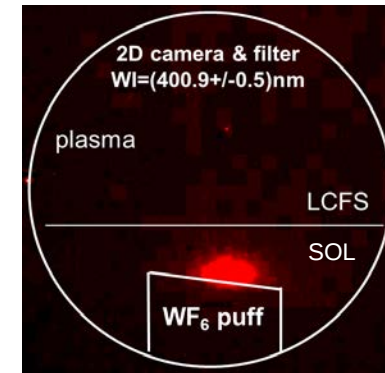


BeT A-X spectrum prediction for JET

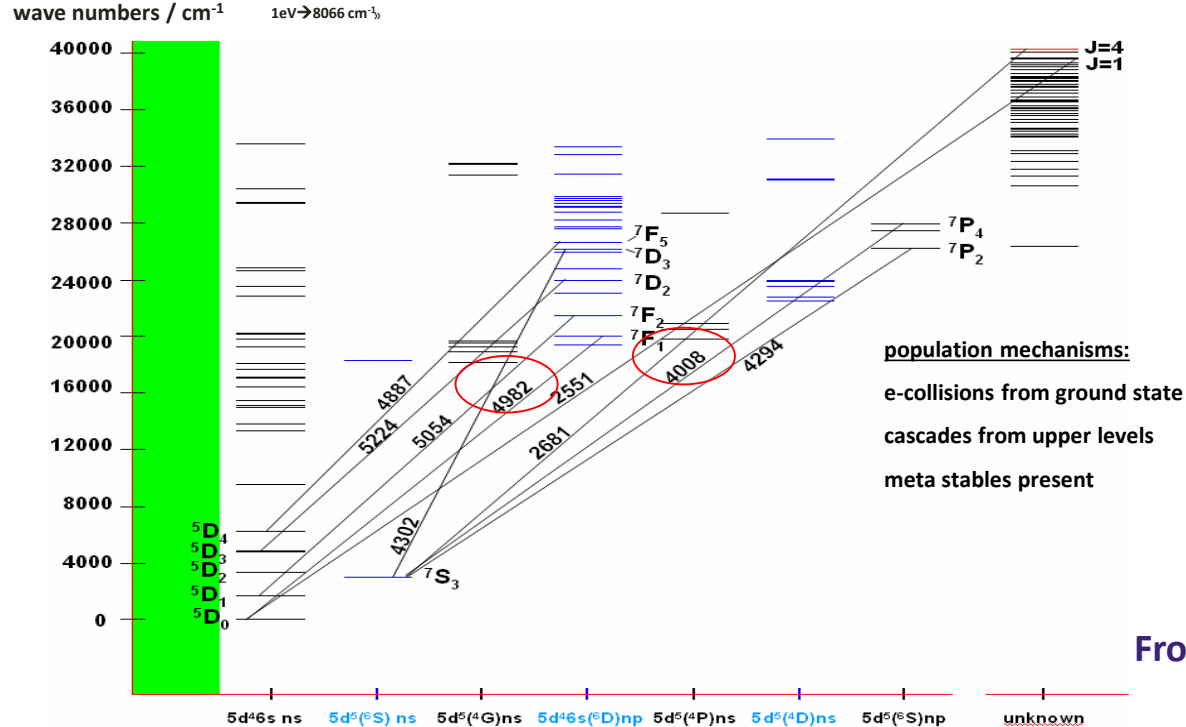


- Introduction
- Spectroscopic techniques
- Hydrogen (and isotopes) spectroscopy
- Beryllium hydride spectroscopy
- Tungsten spectroscopy
- Hydrocarbon spectroscopy

TEXTOR W calibration



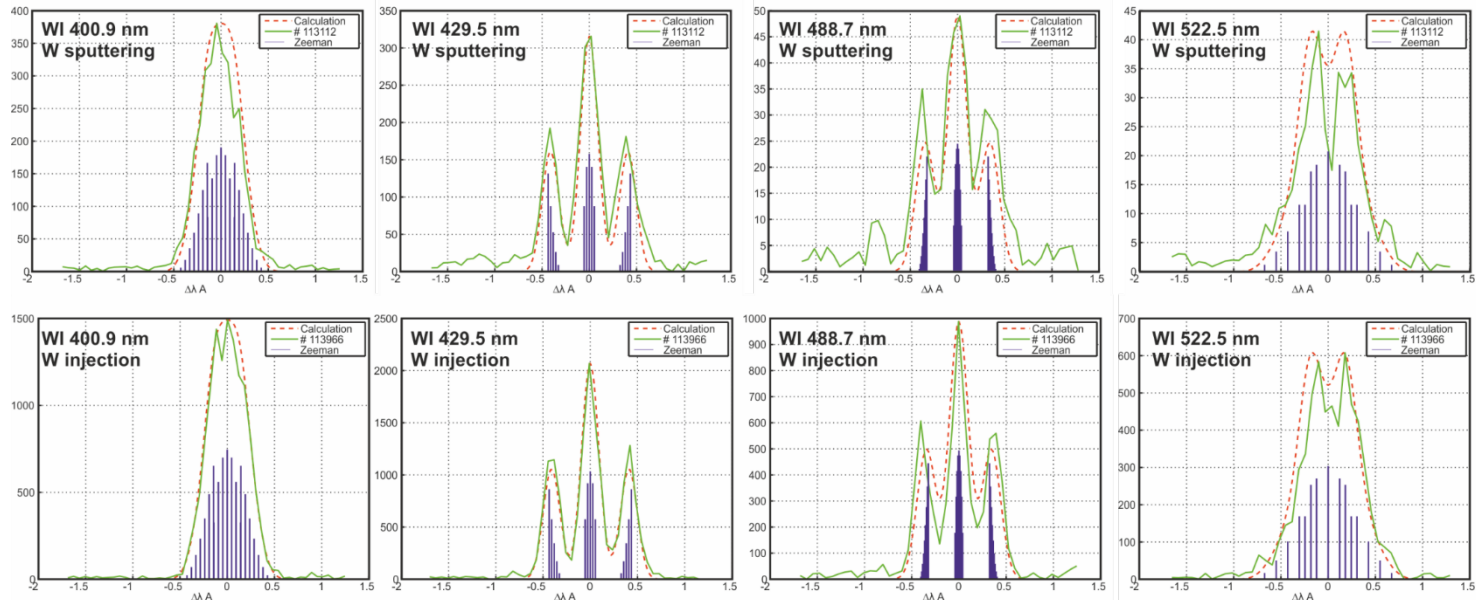
Level Diagram of Neutral W



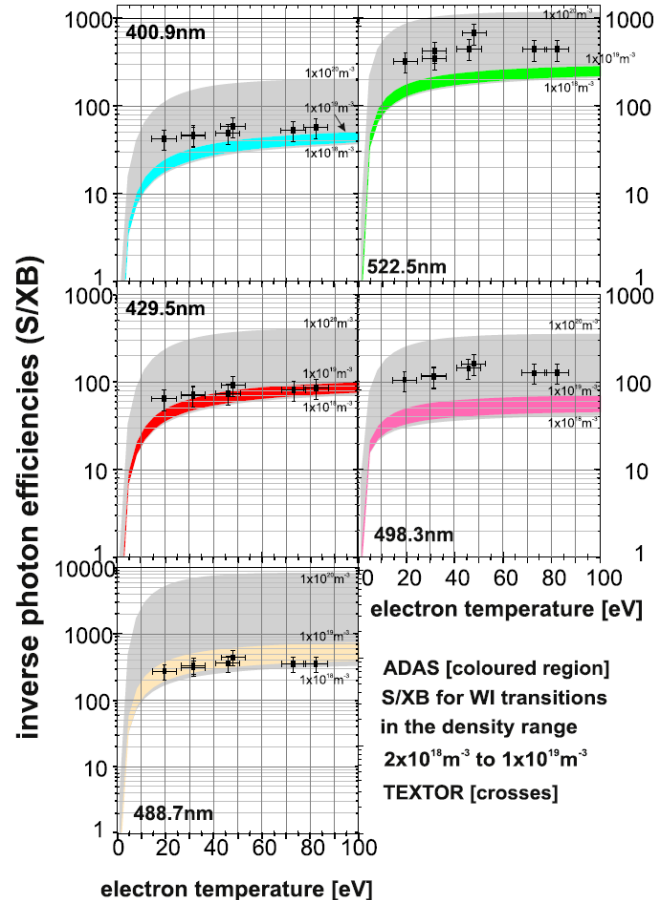
- Prominent transitions in the visible spectral range
- Definition of an artificial ground state ^5D population (T_w) in earlier times [Beigman et al.]

Injected W and Sputtered W: WI emission

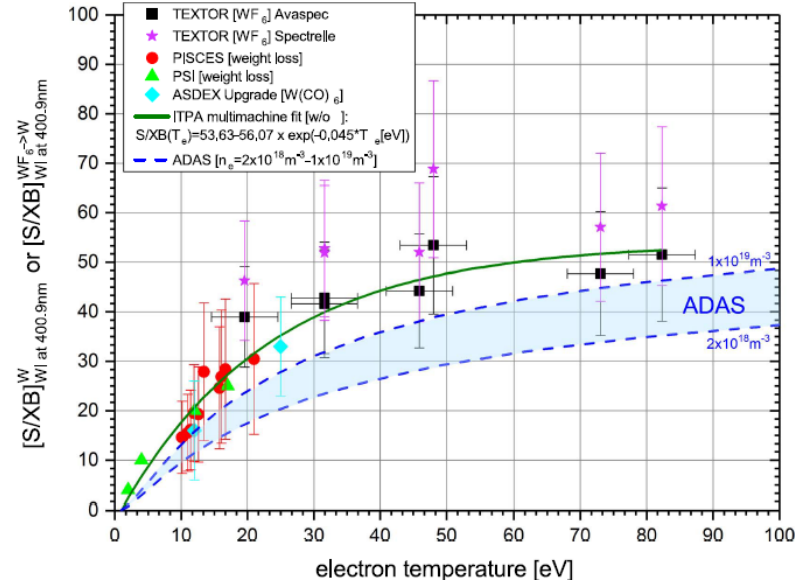
- Calibration of W lines with WF₆ injection (dissociation at about $T_e \sim 0.1\text{eV}$)
- W from WF₆ dissociation representative for W from sputtering?
 - No difference in line shape of different WI and WII lines
 - Lines and ratios of WI lines comparable in sputtered and injected W
 - WII lines measured and quantified in WF₆ injections



Photon Efficiencies: Experiment and ADAS

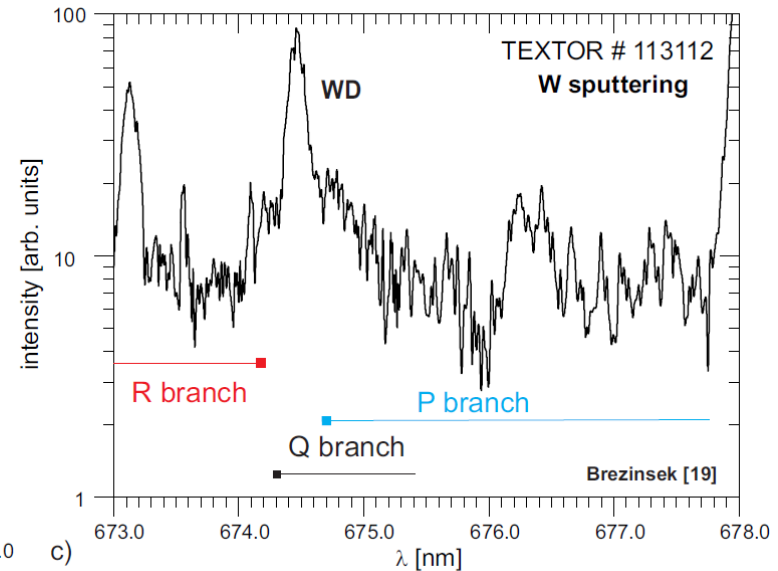
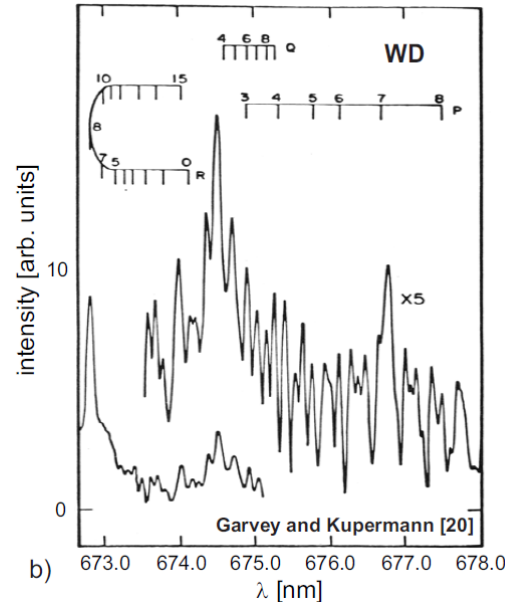
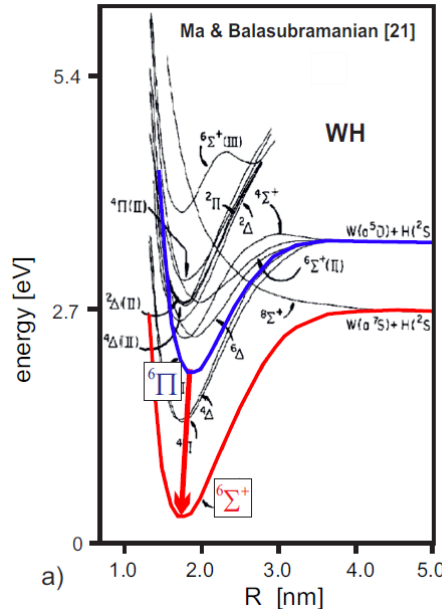
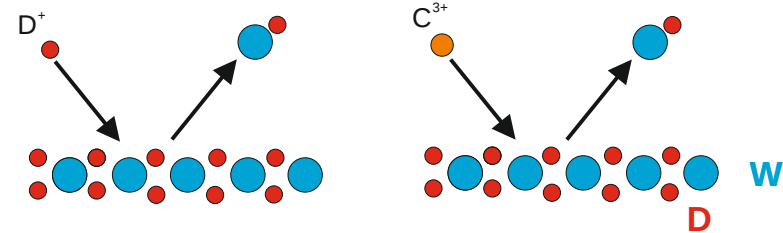


- Experimental data is “effective” assuming WF_6 dissociation is complete
- Experimental data in general in good agreement with ADAS (lower)
- Largest deviation for the “lowest” ground state transition ($\lambda=498.3\text{nm}$)
- ADAS considers only “real” ground state populated (no T_W ?)



Tungsten Hydride: : ${}^6\Pi$ - ${}^6\Sigma^+$ Transition

- Observation of WD molecule at very high D^+ fluxes (10^{23} ions $s^{-1}m^{-2}$) on cold W surfaces (<600K)
- Chemically Assisted Physical Sputtering by C ions with sufficient high impact energy (~ 100 eV)

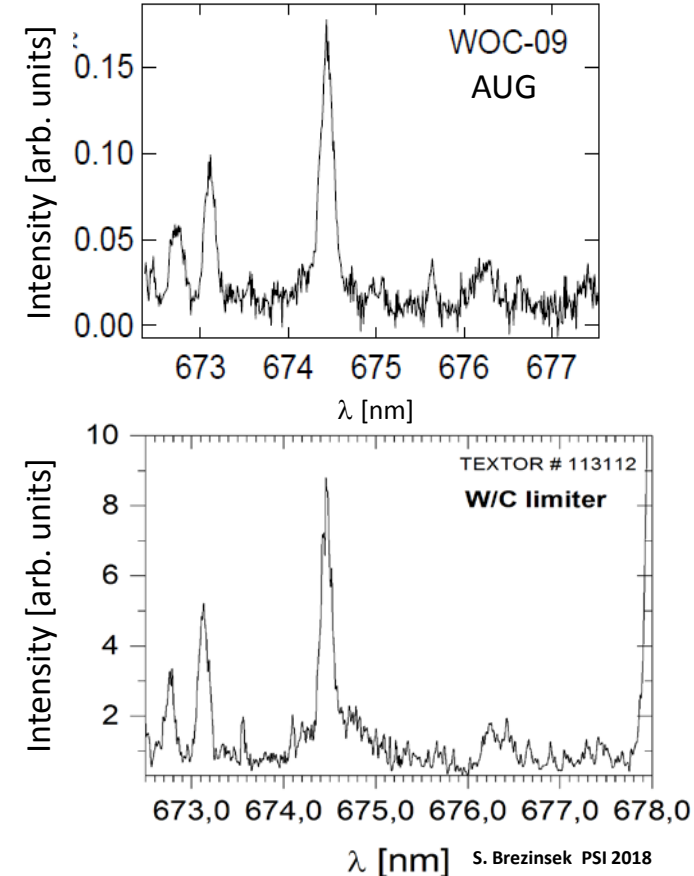
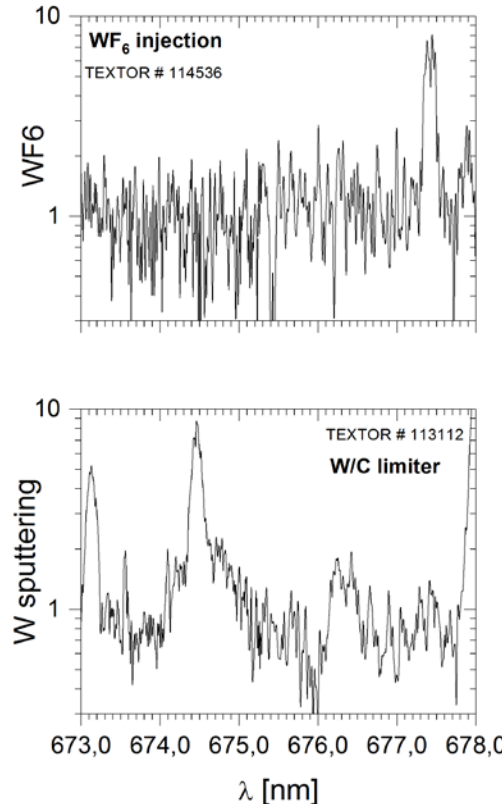


Tungsten Hydride: : ${}^6\Pi$ - ${}^6\Sigma^+$ Transition

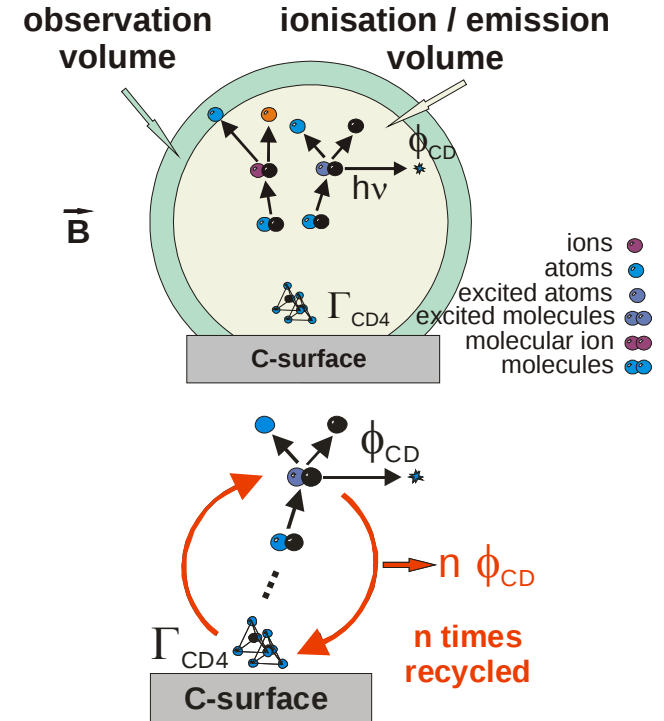
- Not produced in plasma as WF_6 injection in D plasma

- Observed in ASDEX Upgrade and produced during ELMs too (D^+ ions at high energy)

- Looking forward to see a molecular modelling....



- Introduction
- Spectroscopic techniques
- Hydrogen (and isotopes) spectroscopy
- Beryllium hydride spectroscopy
- Tungsten spectroscopy
- **Hydrocarbon and carbon spectroscopy**



Quantification of Sputtering Yields: Example C

$$\text{(hydro)carbon flux } \Gamma_C \xleftarrow{\quad} Y_{\text{chem}} = \frac{\Gamma_C}{\Gamma_D} \xrightarrow{\quad} \text{deuterium flux } \Gamma_D$$

$$\Gamma = \frac{D}{XB} \phi$$

Γ - particle flux
 ϕ - photon flux
 D - Decay rate coefficients (ionisation, dissociation etc.)
 X - excitation rate coefficient
 B - Branching ratio

- composition: CD_4 , C_2D_y
- accessible photon flux ϕ
CD: Gerö band
C₂: Swan band
- inverse photon efficiencies

- composition: D_2 , D
- accessible photon flux ϕ
D: Balmer series
D₂: Fulcher band
- inverse photon efficiencies

in-situ plasma parameter determination

- Balmer-line ratios
- Fulcher- α -band analysis

**Hydrocarbon
break-up chain**

+ other carbon lines
(C II, C III, C IV)

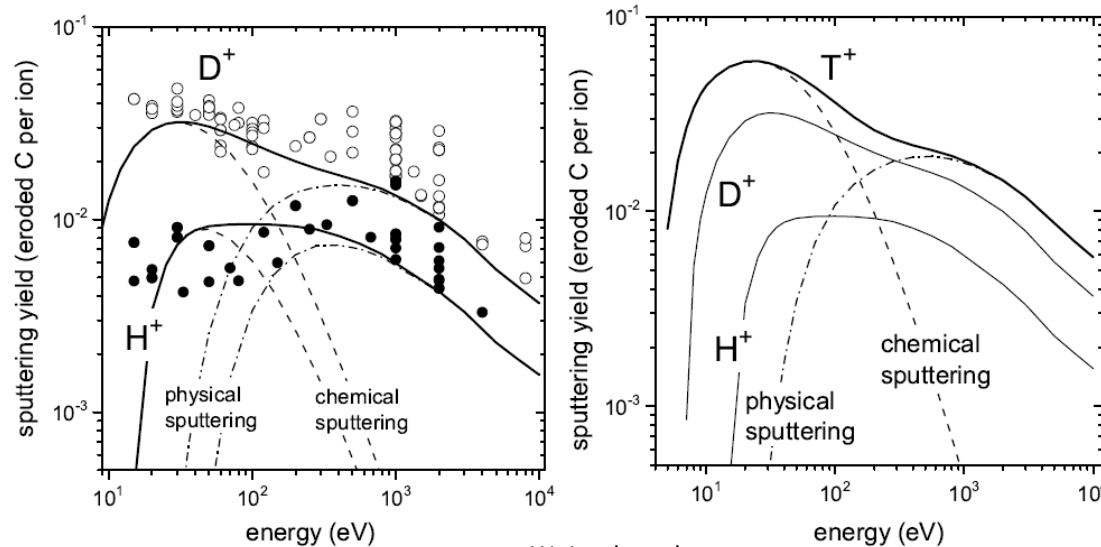
**Deuterium
recycling**

+ other molecules containing
deuterium: BD, HD ...

Identical observation volume and integration time!

Sputtering Yields for Graphite

Chemical (C_xH_y) and physical sputtering (C) of graphite by hydrogen isotopes in ion beam facilities

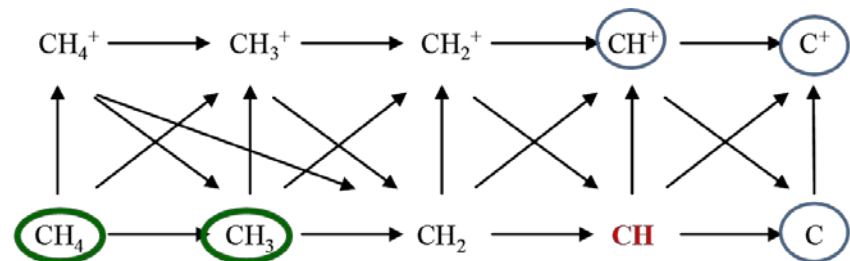
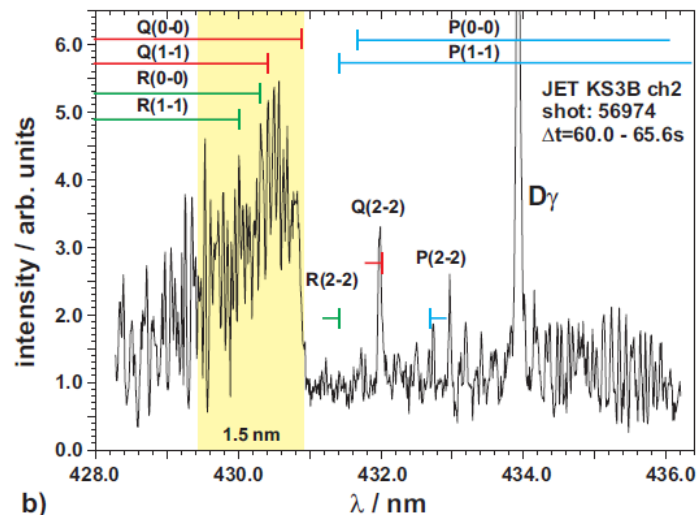
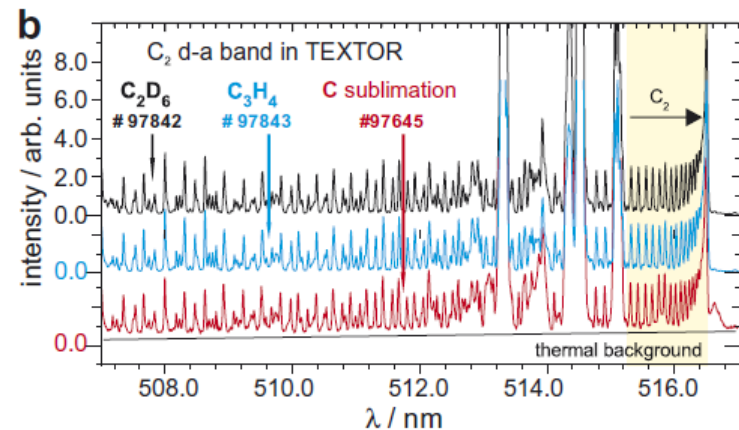
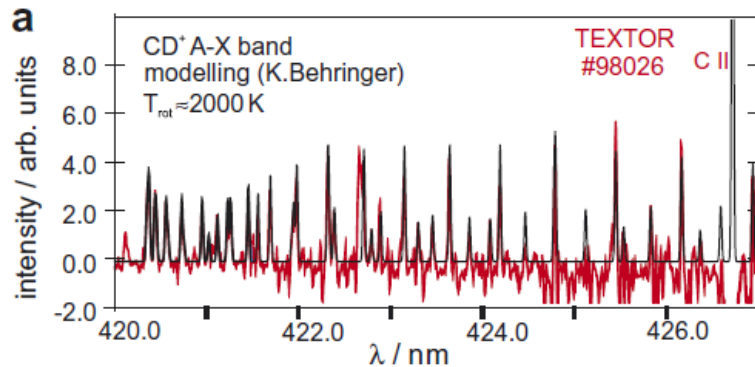


Total yield:

- Still thermal release of chemical erosion contribute below threshold for H^+
- Mass dependence in total erosion yield
- Variation if C layers present

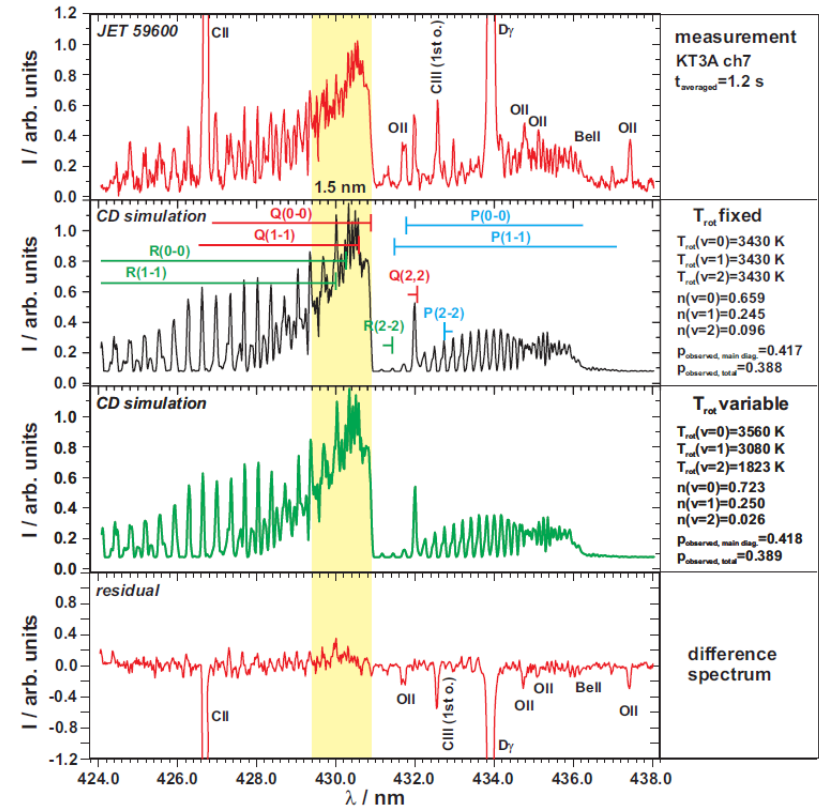
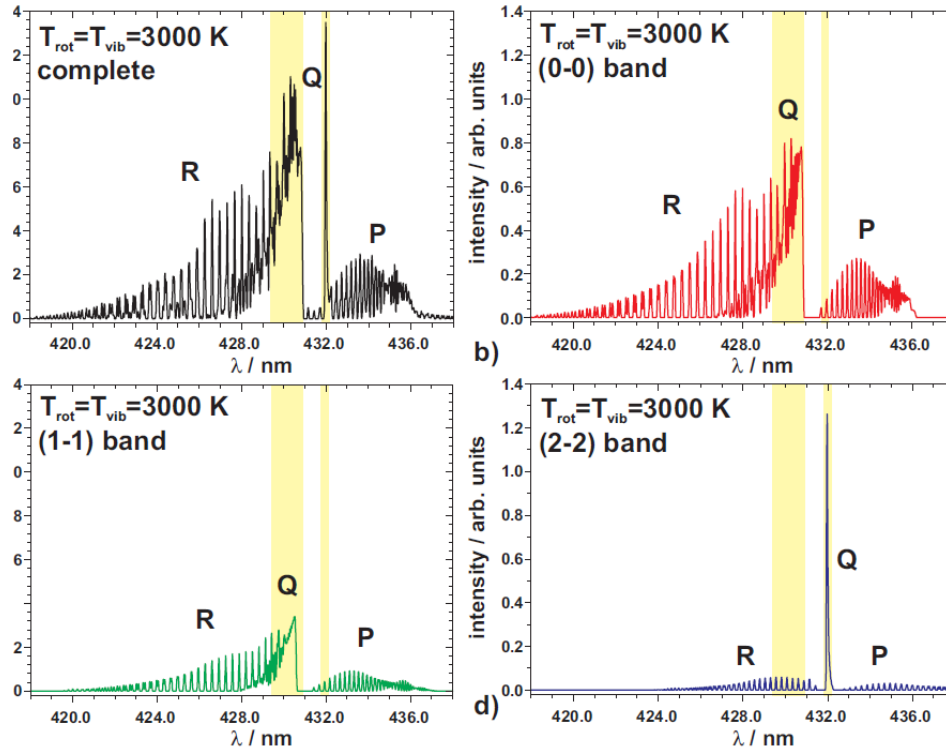
In-situ determination and origin required: chemical or physical sputtering / bulk or carbon layers?

In-situ Measurable Molecular Species: CH, CH⁺, C₂

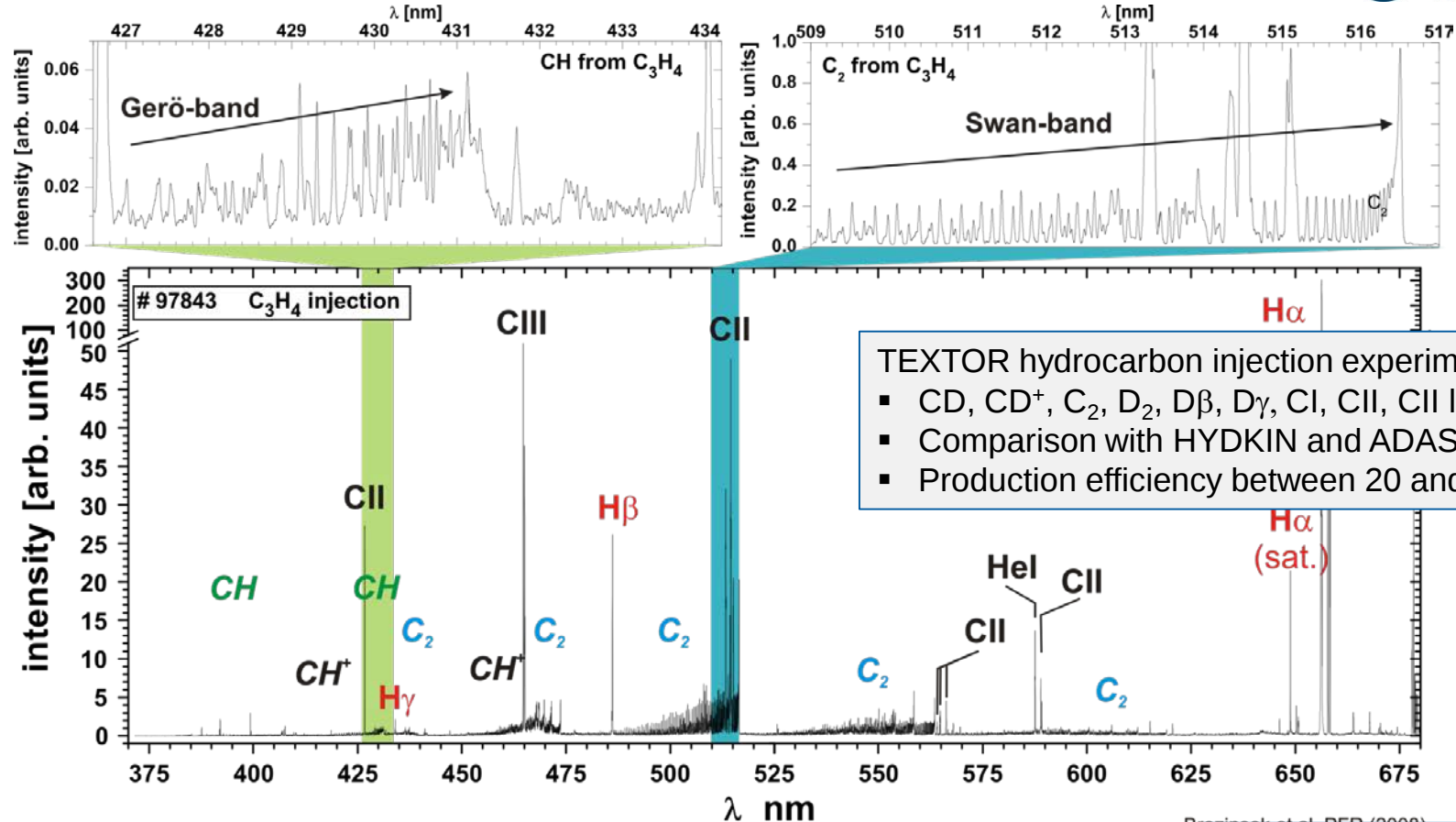


Origin not visible in emission spectroscopy –
in-situ calibration to get the footprint

Modelling of the Gerö Band



Hydrocarbon Footprint in Plasmas by C_xH_y Injection



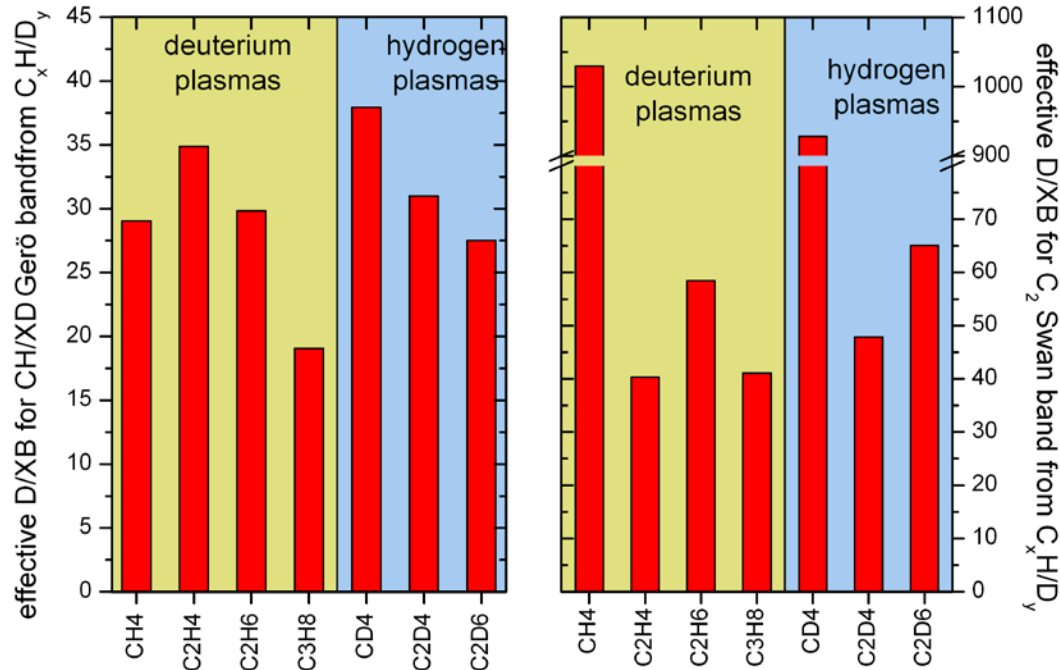
Hydrocarbon Footprint by C_xH_y Injection in Plasmas

Benchmark of HYDKIN database for hydrocarbon catabolism

JUEL-3966 Report

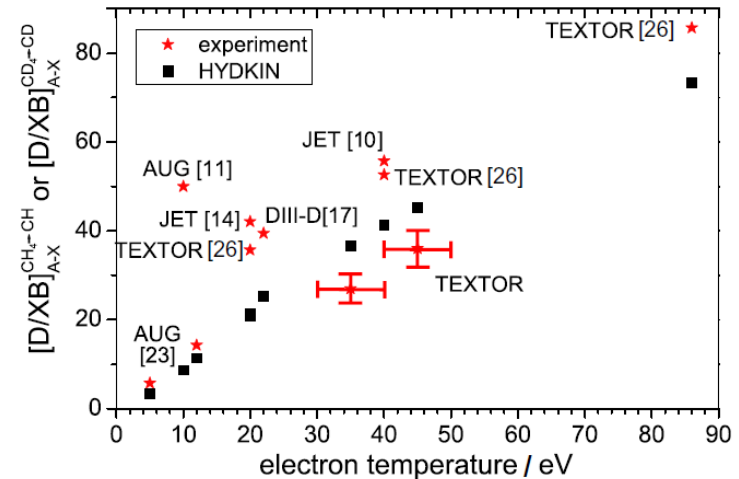
JUEL-4005 Report

www.eirene.de



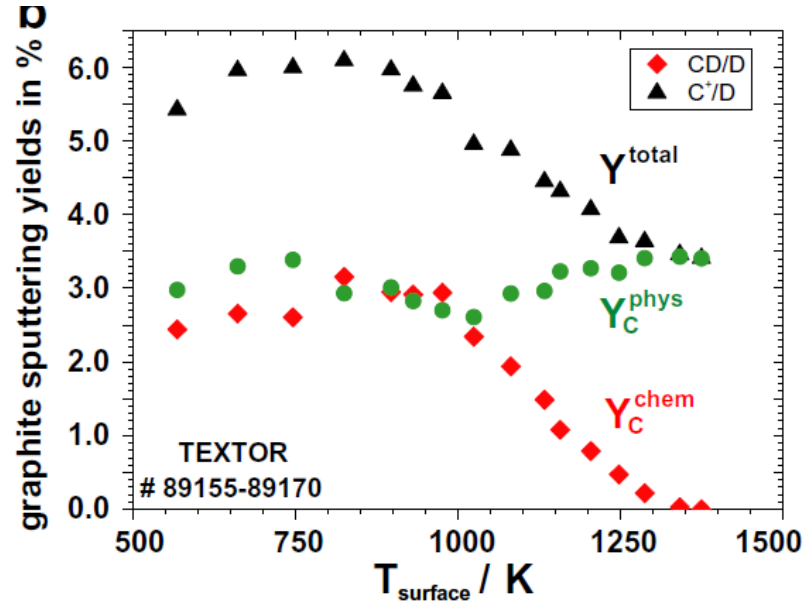
C_xH_y in D plasmas: $T_e=35$ eV, $n_e=2.2 \cdot 10^{18} \text{m}^{-3}$ at the emission location
 C_xD_y in H plasmas: $T_e=45$ eV, $n_e=1.8 \cdot 10^{18} \text{m}^{-3}$ at the emission location

Multimachine comparison of experimental tokamak data



Residual discrepancy – local C recycling and layer formation

Chemical Erosion: Temperature Dependence

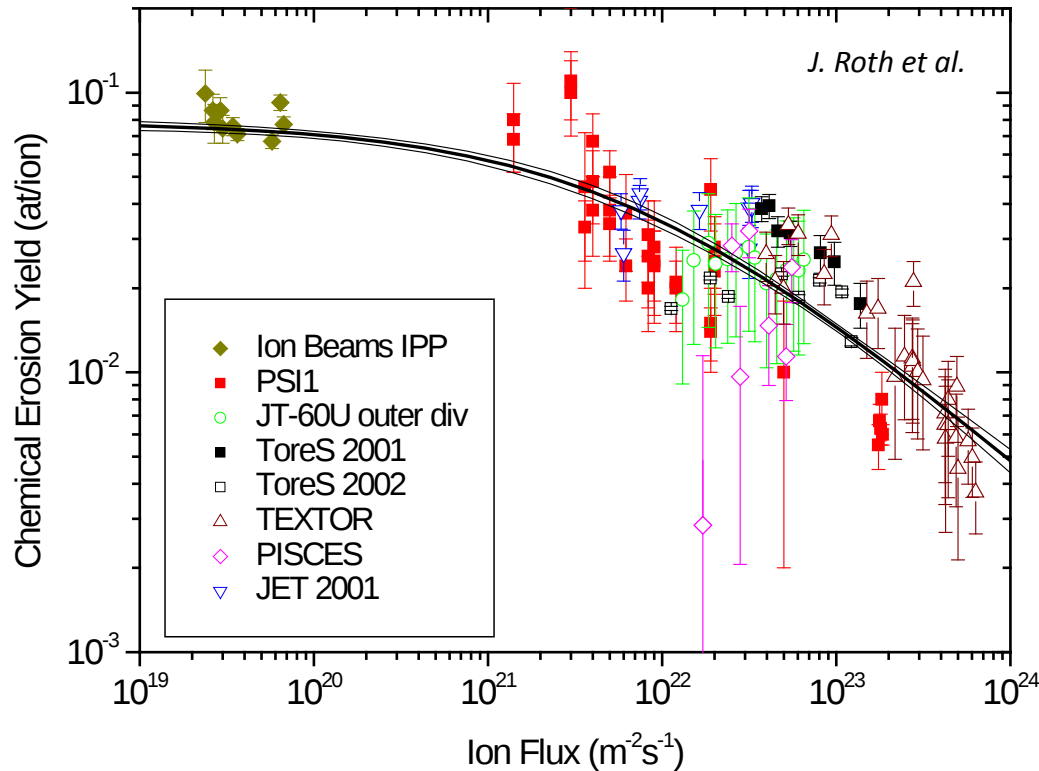


Identical plasmas at $T_e \sim 50 \text{ eV}$ with external change of surface temperature

Above 1000K chemical erosion drops and vanishes at 1300K

Flux density: $\sim 5 \times 10^{23} \text{ ions s}^{-1} \text{ m}^{-2}$

Chemical Erosion: Flux Dependence



Normalisation:
 $30 \text{ eV } T_{\text{surf}}(\text{max})$

Difficult to
decouple from E_{in}

Chemical sputtering
decreases with
increasing flux

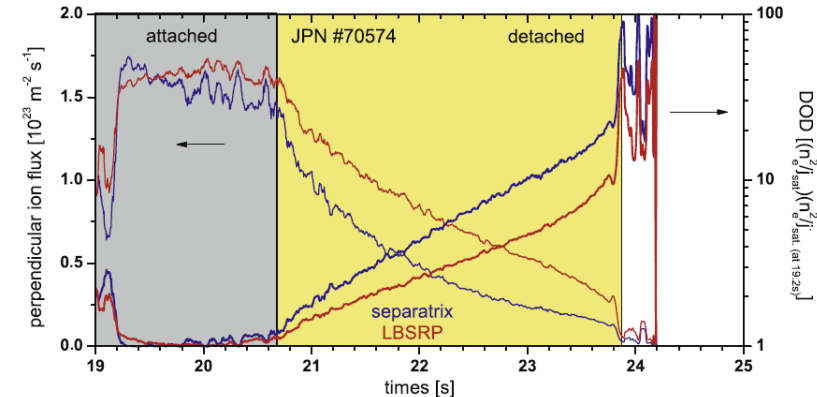
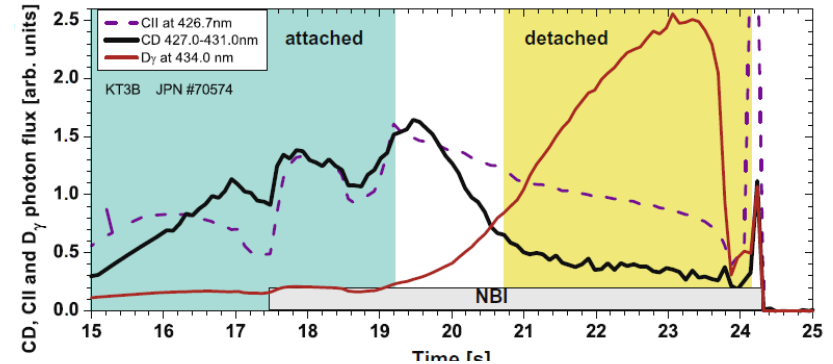
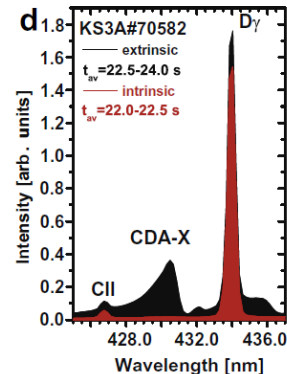
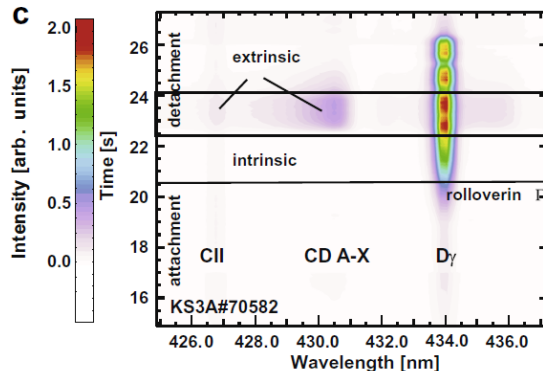
Flux dependence is predicted by model of thermal reaction cycle

Chemical Sputtering: Energy Threshold

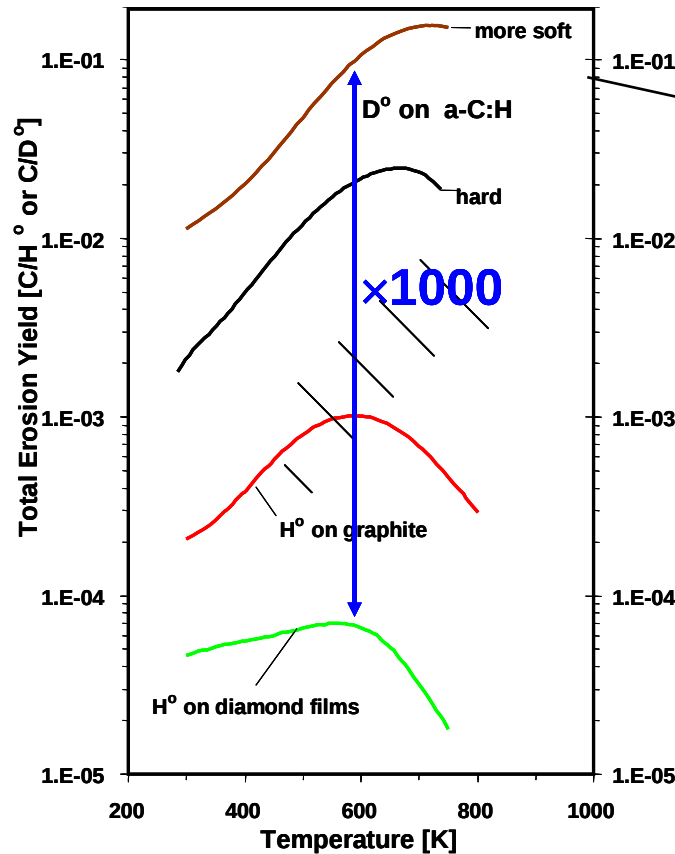
At low impact energies ($\sim 2\text{-}3\text{eV}$), the chemical sputtering part of C is almost absent

JET-C with CFC divertor

- Erosion zone on graphite
- Divertor detaches and reveals chemical sputtering threshold
- Test with local methane source injection

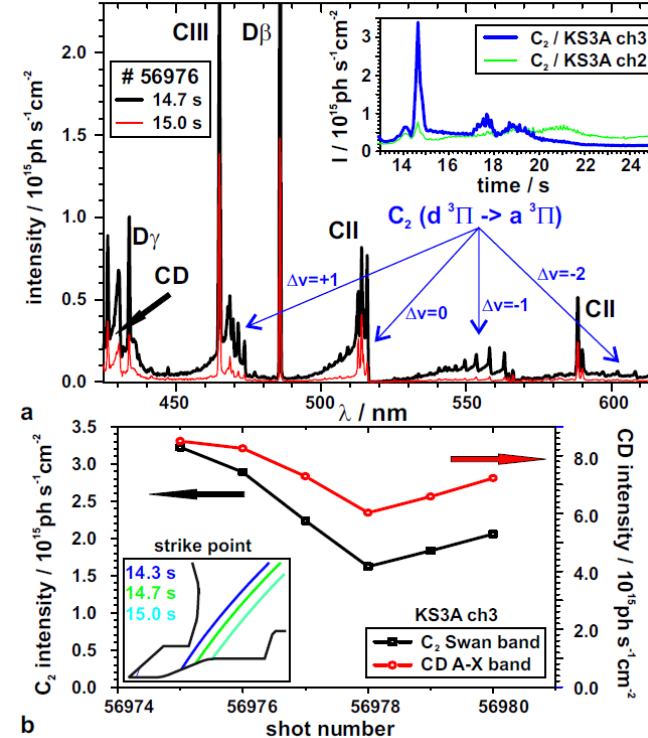


Chemical Erosion: a-C:H layers



a-C:H
amorphous
hydrocarbon layer

- soft (hydrogen-rich) carbon layers suffer from larger chemical erosion
- Lower activation energy for release with high hydrogen content
- Associated with release of higher hydrocarbons



E. Vietzke, J. Nucl. Mat.
(1987) 443