Mini-Workshop on Traps for Highly-exotic (highly-charged, highly-excited, rare isotope, anti-) States of Matter in POSTECH

EBIT관련 원자 데이터, 분광 모델링 연구 현황 소개

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Contents

- Atomic process in plasma
- EBIT for highly charged ions and the spectroscopic modeling
- Optical emission spectroscopy (OES) and collisional-radiative (CR) modeling for low temperature and low density plasma (Ar, He, H, atom and lowly charged ions)
- Summary and outlook

Atomic processes in plasma

- Atoms and ions in plasma are neither isolated single atom/ion nor simple approach for two, three,… levels is applicable.

- Various collision processes with electrons and ions have to be considered for the spectral line intensity.

$$I_{ji} = \frac{1}{4\pi d^2} \int G_{ji}(T_e, n_e, \cdots) dV$$

$$G_{ji}(T_e, n_e, \cdots) = \frac{n_j(A^{q+})}{n(A^{q+})} \frac{n(A^{q+})}{n(A)} A_{ji}$$

Fractional abundance for charge state distribution

- Accuracies of the collision process data are essential for the reliability of plasma spectroscopy.

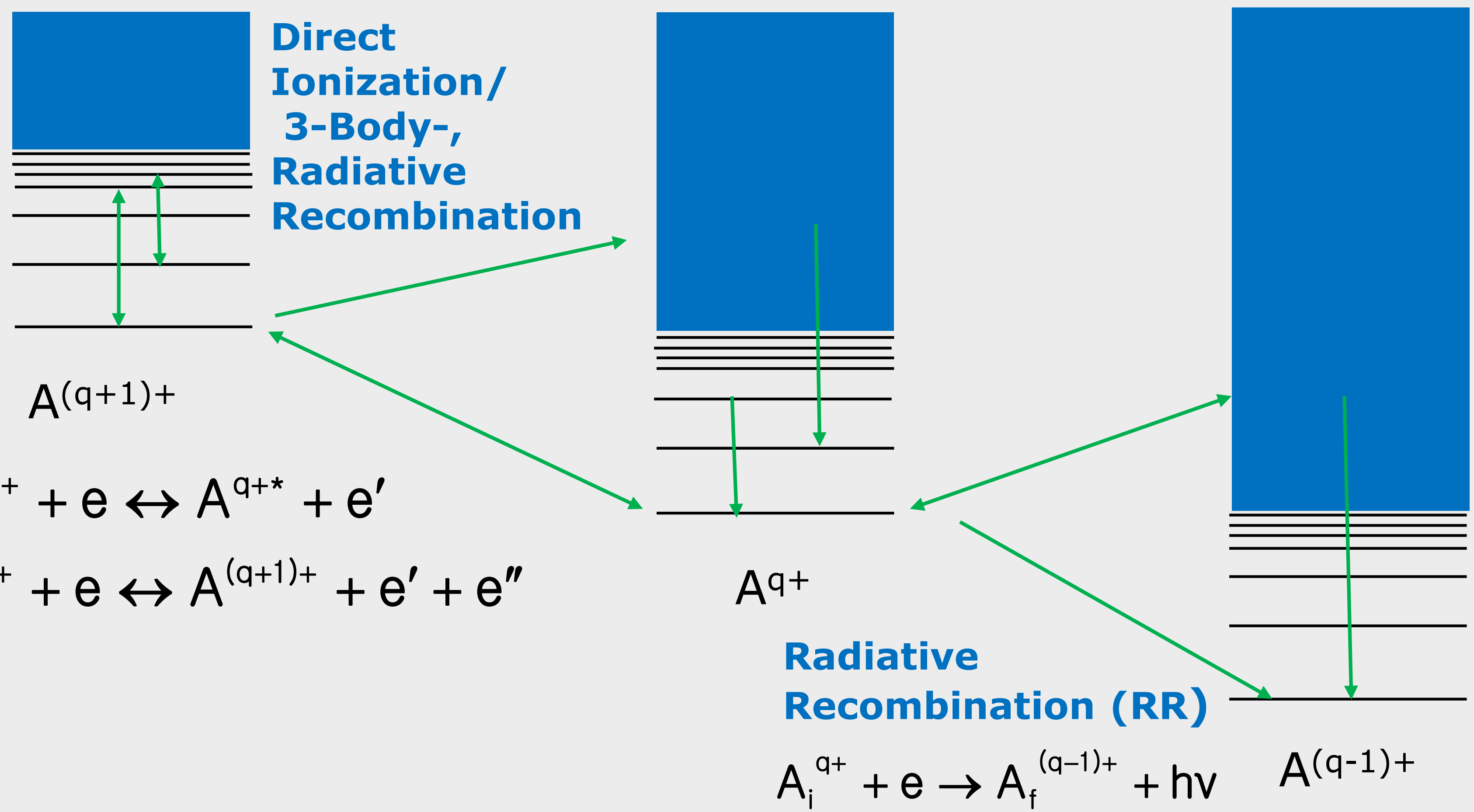
Atomic processes in plasma

Collisional (De)excitation

Radiative Decays

Autoionization/ Dielectroninc Recombination (DR)

$$A_i^{q+} + e \leftrightarrow \left[A_j^{(q-1)+}\right]^{**} \rightarrow \left[A_f^{(q-1)+}\right]^{*} + h\nu$$



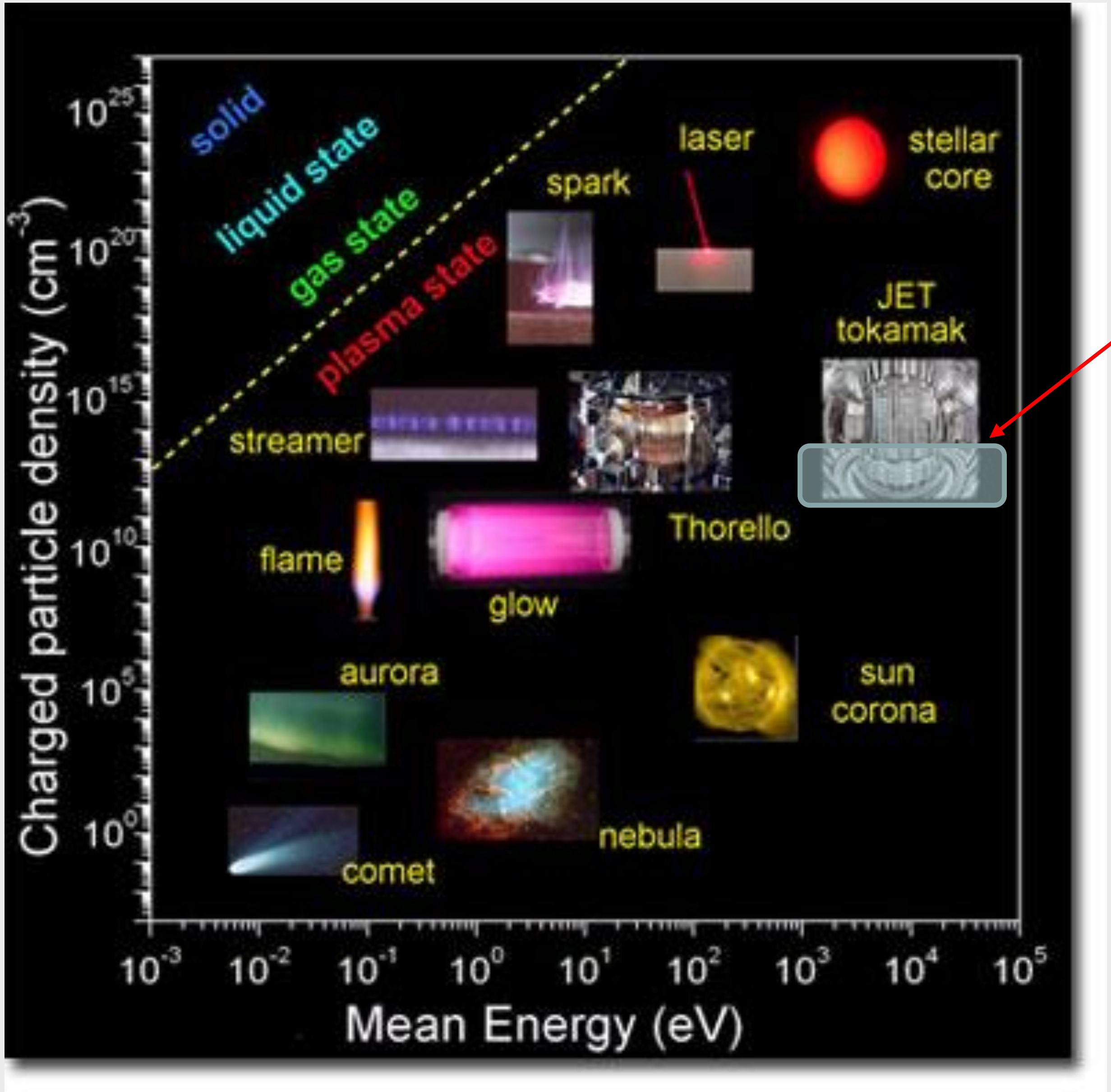
$$A^{q+} + e \leftrightarrow A^{q+*} + e'$$

$$A^{q+} + e \leftrightarrow A^{(q+1)+} + e' + e''$$

$$A_i^{q+} + e \rightarrow A_f^{(q-1)+} + h\nu$$

Heavy particle collisions such as charge exchange, penning ionization etc.

Temperatures and densities for various plasmas



EBIT
~1-~200 keV
~10^{13} cm^{-3}

Tuneable, Non-Maxwellian **Quasi-monoenergetic** electron beams enabling to selective charge state and excitation

Well-suited for studies of **electron impact excitation, ionization, radiative, dielectronic recombination, and identification of transitions from highly charged ions (HCIs)**

quora.com website

EBIT as essential spectroscopic tools

- HCIs are abundant in the visible ***universe*** such as stars, galaxies and their clusters or the intergalactic medium as well as in ***laboratory plasmas*** including ***fusion plasmas***. EBITs are used to accurately measure the ***wavelengths of spectral lines*** emitted by HCIs to ***identify and diagnose*** the charge states and behavior of impurities in fusion plasmas.
- In atomic physics, fundamental interactions due to relativistic effects, quantum electrodynamics (**QED**), and nuclear-size contributions of HCI are enhanced by several orders of magnitude compared to neutral or singly charged systems. So the *precise determination* of the ***electron mass*** *and the* ***electron magnetic moment*** as well as stringent QED tests. Moreover, several proposals contemplate HCIs as ideal laboratory probes of a possible variation of the ***fine-structure constant*** and ***as frequency references for optical clocks*** superior to state-of-the-art optical lattice or singly charged ion clocks.
- Other applications are ***tumor ion therapy*** and ***EUV nanolithography*** …
- EBIT provides HCI as the ***target for x-ray photons*** at ***synchrotron or FEL facilities.***

Models for population kinetics in plasma

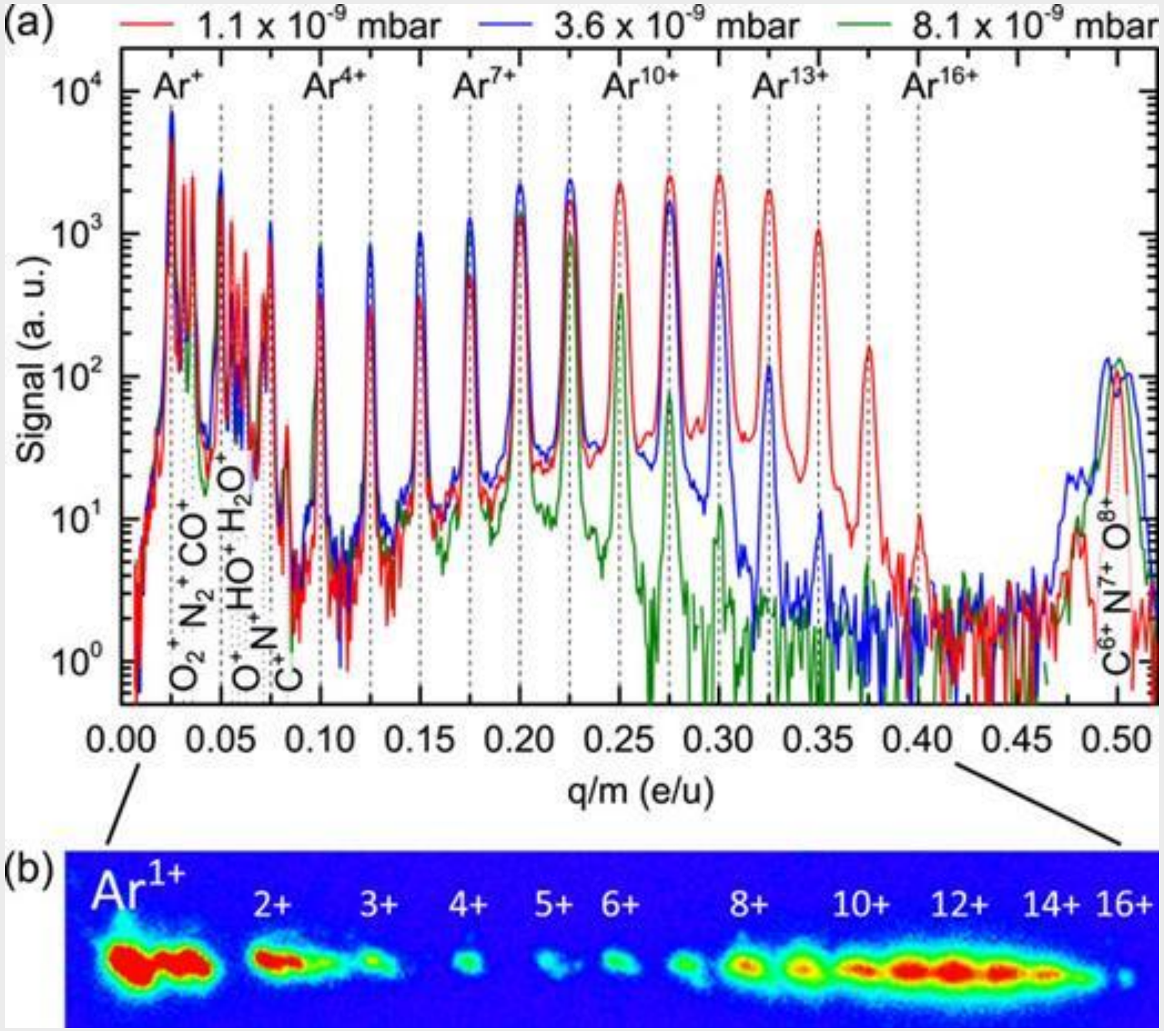
- Thermodynamic equilibrium (TE) : Ideal plasma and radiation field at constant *T* whose physical states are described as
  - ✓ Radiation field given by Plank's law
  - ✓ Particles by Maxwellian energy distribution
  - ✓ Level population densities by Boltzmann relation
  - ✓ Ion stage densities by Saha equation
  - ✓ Inverse process by detailed balance
- Local thermodynamic equilibrium (LTE) : High density plasma where collisions are so dominated that maintain steady state population densities by the Boltzmann and ionization stages by the Saha equation
- **Collisional-radiative (CR)** : All possible collisional and radiative process are considered with external terms

$$\frac{dn_z(p)}{dt} = -R_z(p \rightarrow) + R_z(\rightarrow p) + \Gamma_z(p)$$

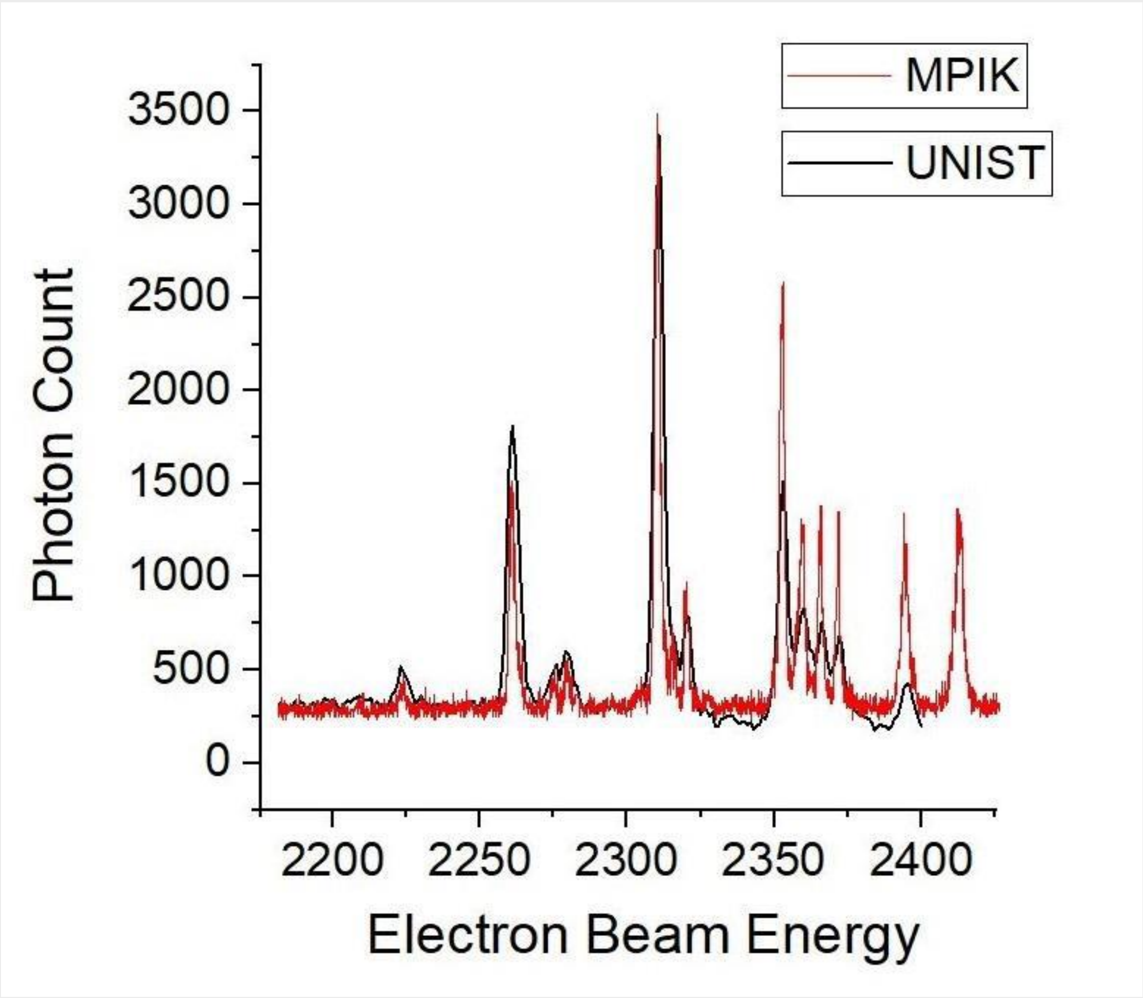
- Corona : low density plasma where

$$n_z(p)A_z(p \rightarrow) = n_e \sum_q n_z(q)\, X_z(q \rightarrow p),\ n_e n_z S_z = n_e n_{z+1} \alpha_{z+1}$$

Ar (Z=18, $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$) ions from EBITs

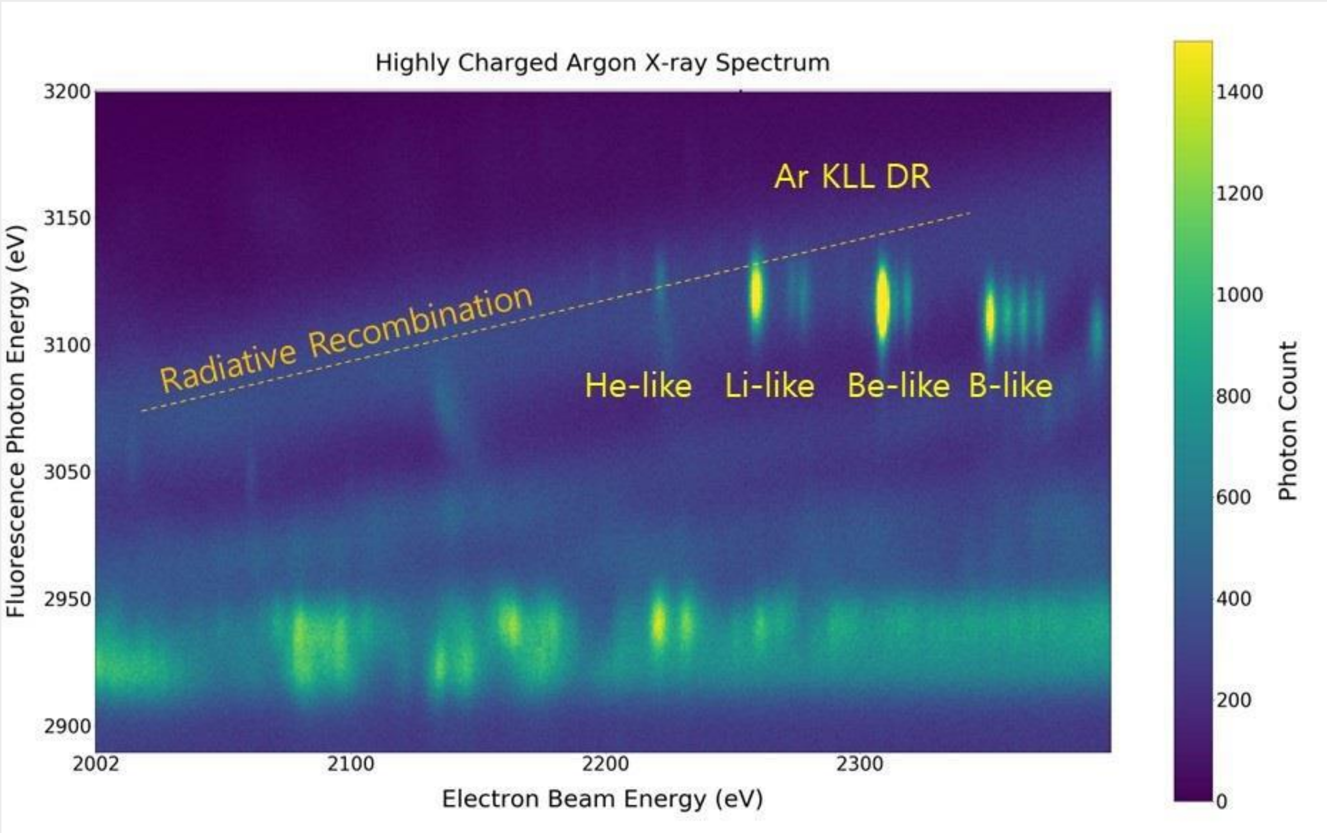


From: **The Heidelberg compact electron beam ion traps**
Rev. Sci. Instrum. 89, 063109 (2018)

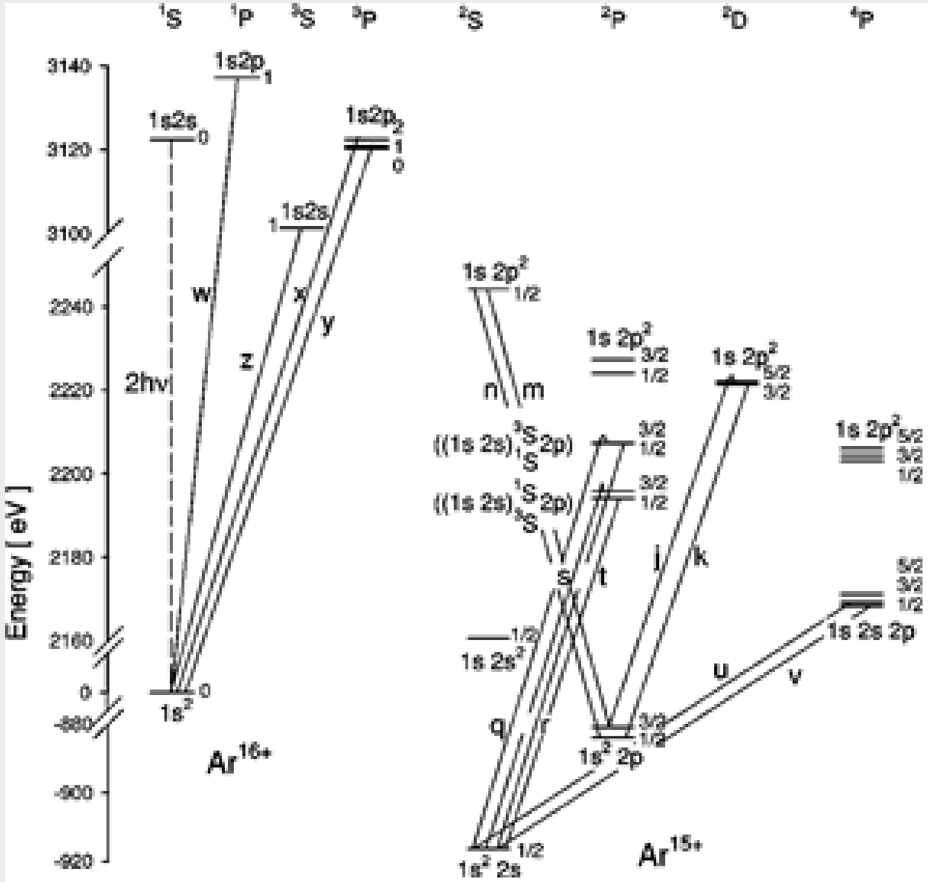


On the courtesy of Dr. S. N. Park

RR and DR spectra from EBITs

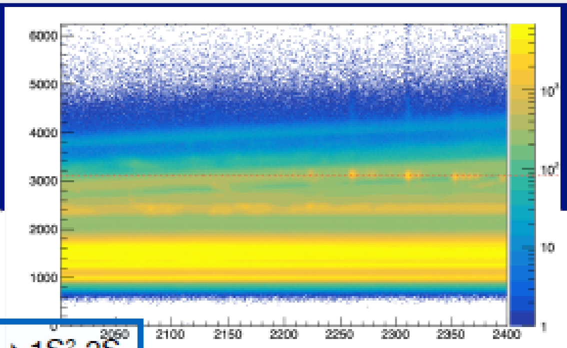


On the courtesy of Dr. S. N. Park

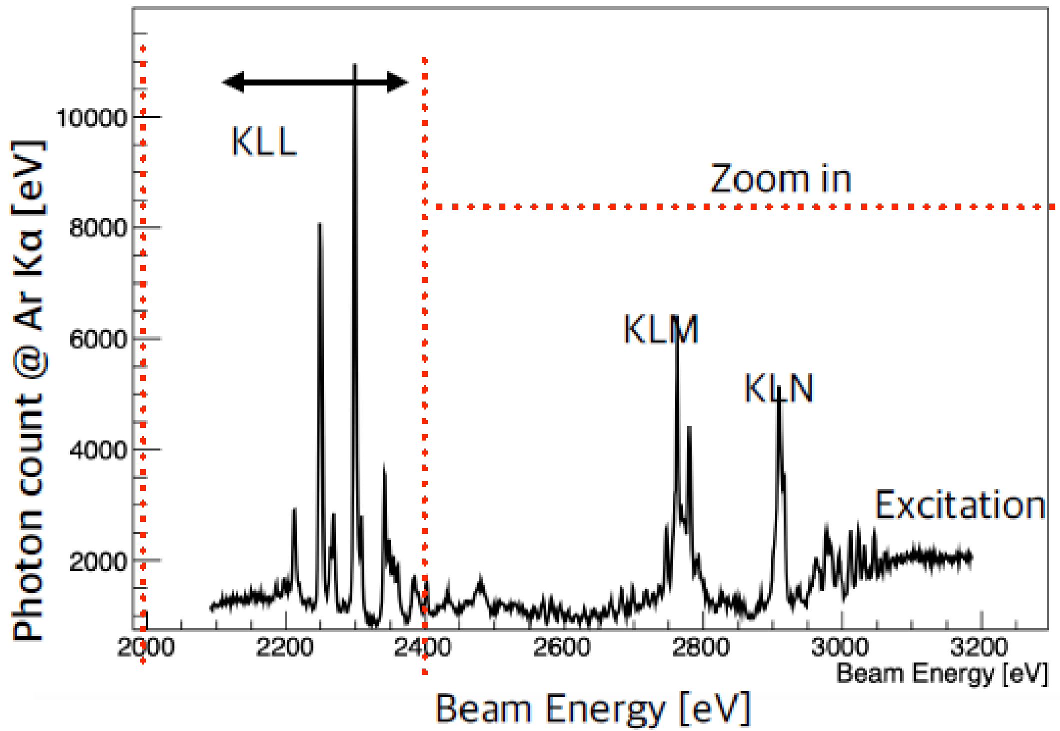


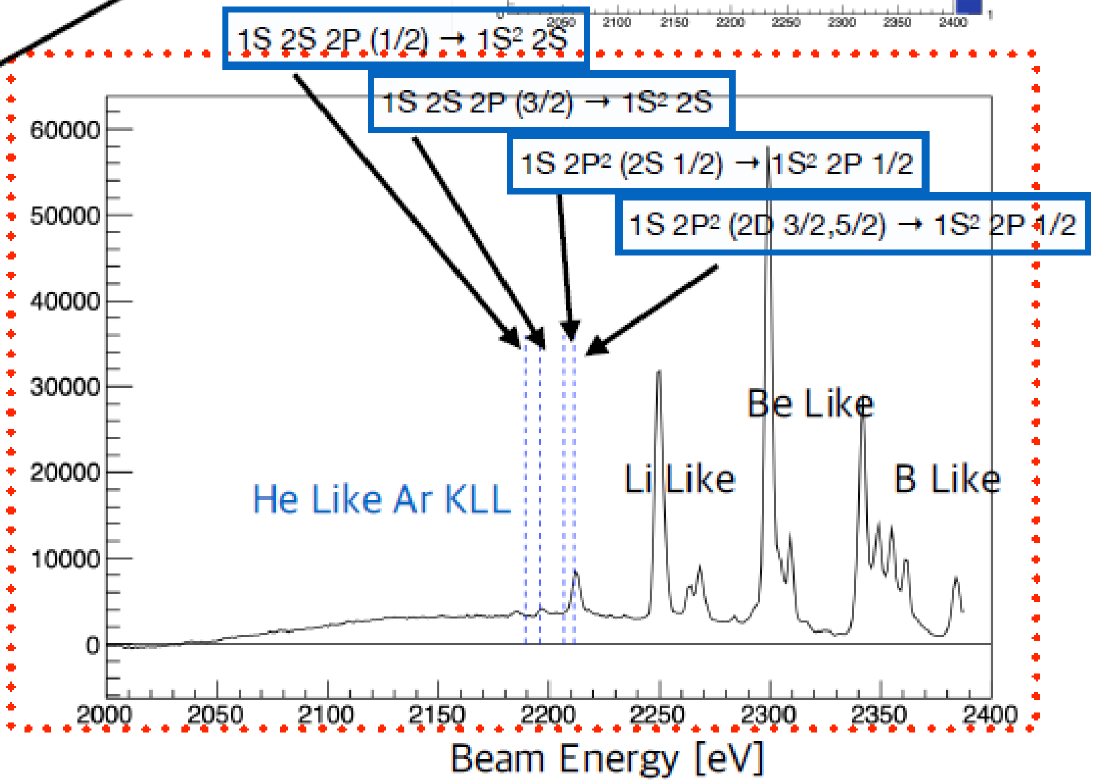
Energy levels and radiative transitions for He-like and Li-like Ar ions

Benchmark Test Using Argon(2)



On the courtesy of Dr. B. Shin



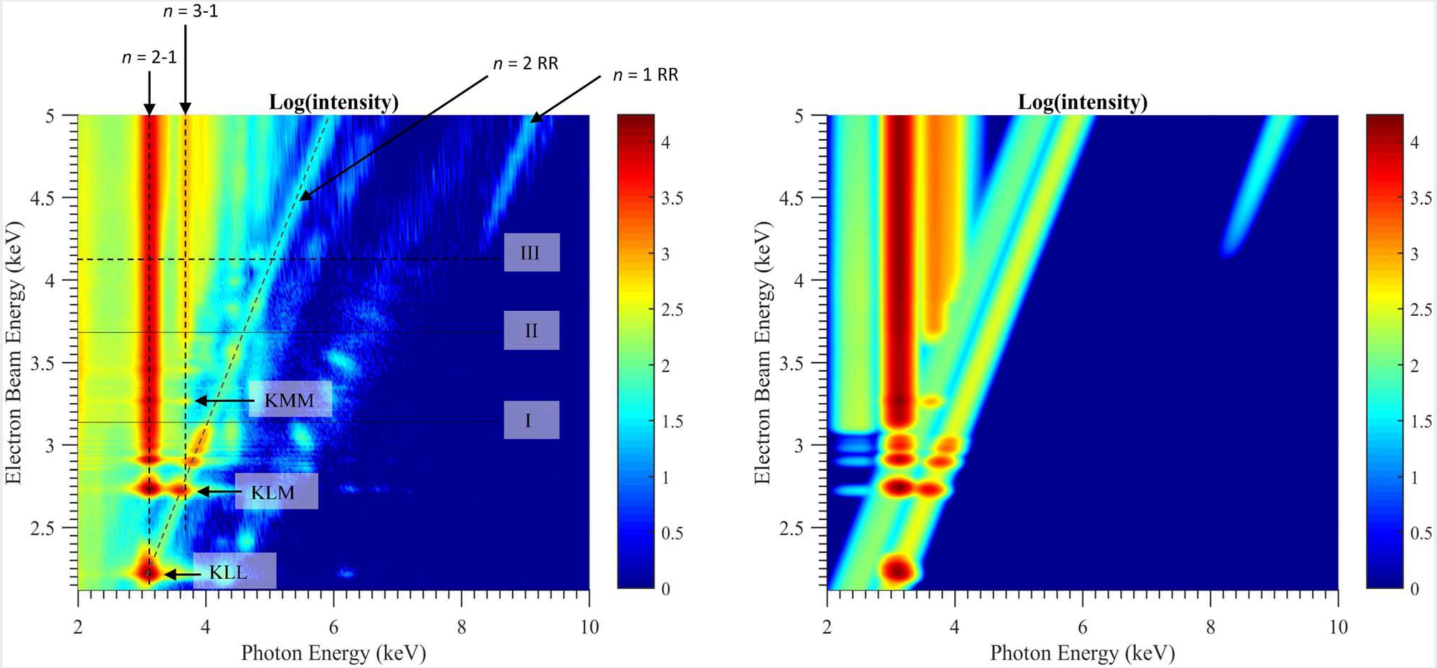


We confirmed "He Like Ar" ions were generated

To generate more He Like Ar, we will make more higher vacuum

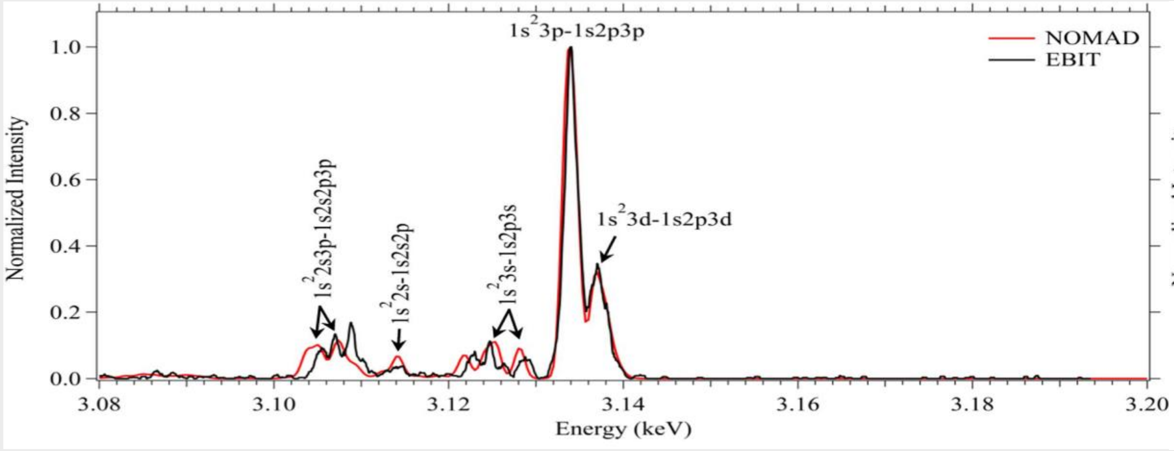
Target: **6E-9 mBar** ⇒ less than **1E-9 mbar**, Drift tube cleaning, Add up NEG pump

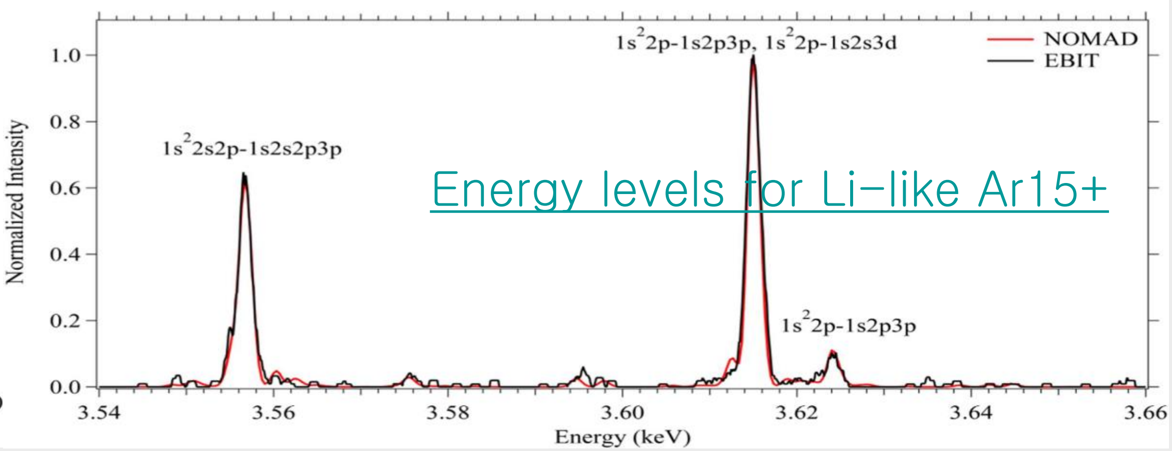
CR modeling for EBIT



EBIT (NIST) and theoretical spectra at an electron beam energy of 2.730 keV

(A. C. Gall, …, Y. Ralchenko, et al., Astrophysical Journal, **872**:194 2019)





Energy levels for Li-like Ar15+

CR modeling for EBIT

NOMAD (Non-Maxwellian, Arbitrary Distribution) CR code by Yuri Ralchenko

$$\frac{\mathrm{d}\hat{N}(t)}{\mathrm{d}t} = \hat{A}(N_\mathrm{i}, N_\mathrm{e}, f_\mathrm{e}, t)\hat{N}(t) + \hat{S}(t),$$

$$\hat{N}(t=0) = \hat{N}_0,$$

$$N_\mathrm{e}(t) = N_\mathrm{e}^0(t) + N_\mathrm{i}(t)\sum_{Z=Z_\mathrm{min}}^{Z_\mathrm{max}}(Z-1)\sum_{k=1}^{k_\mathrm{max}} N_{Z,k}(t),$$

$$\sum_{Z=Z_\mathrm{min}}^{Z_\mathrm{max}}\sum_{k=1}^{k_\mathrm{max}} N_{Z,k}(t) = 1$$

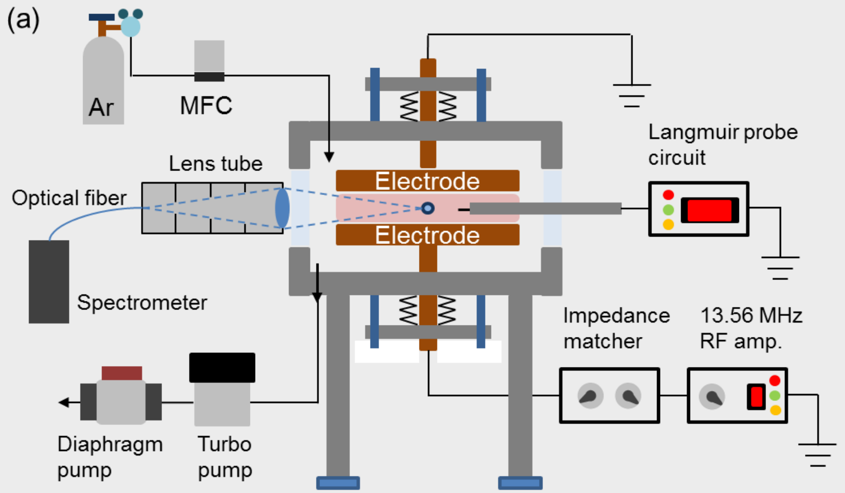
$$\sum_{j>i} N_{z,j}\cdot\left(A_{z,ij}^{rad} + n_e R_{z,ij}^{dx}\right) + \sum_{j<i} N_{z,j} n_e R_{z,ij}^{ex} + \sum_k n_e R_{z-1,ki}^{ion} + \sum_k n_e R_{z+1,ki}^{rr} + \delta_{i1} n_0 R_{z+1}^{cx}$$

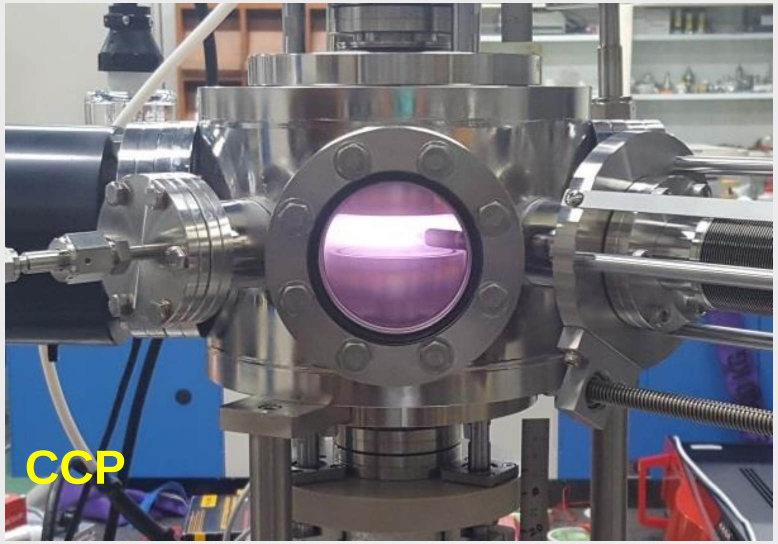
$$-N_{z,i}\left(\sum_{j<i}\left(A_{z,ji}^{rad} + n_e R_{z,ji}^{dx}\right) + \sum_{j>i} n_e R_{z,ji}^{ex} + \sum_k n_e R_{z,ki}^{ion} + \sum_m n_e R_{z,mi}^{rr} + \delta_{i1} n_0 R_z^{cx}\right) = 0$$

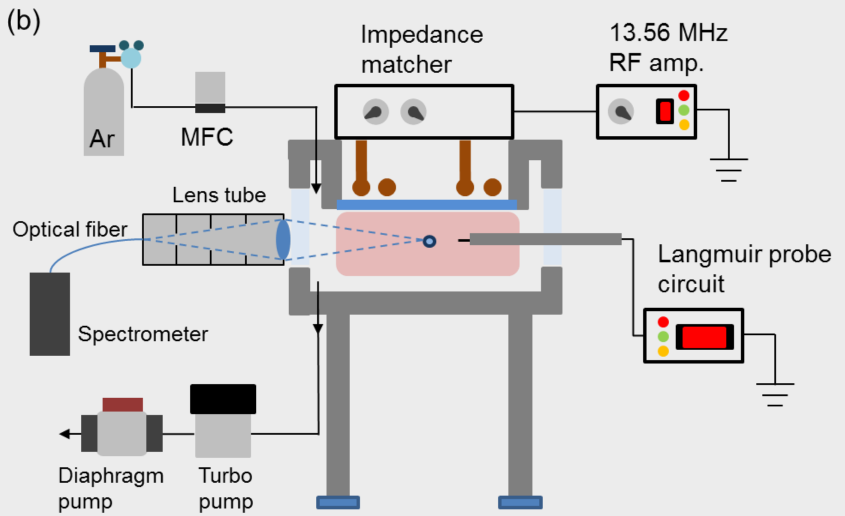
Atomic data from the flexible atomic code (FAC)

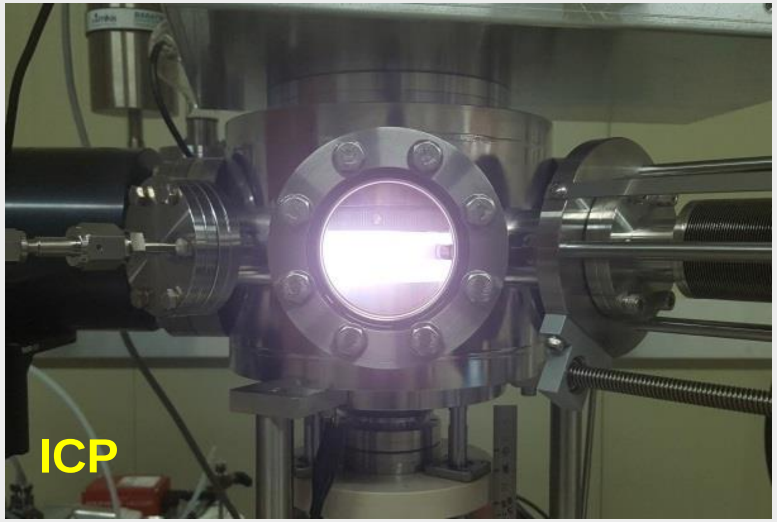
OES and CR modeling in low temperature & low density plasmas

Experimental setup

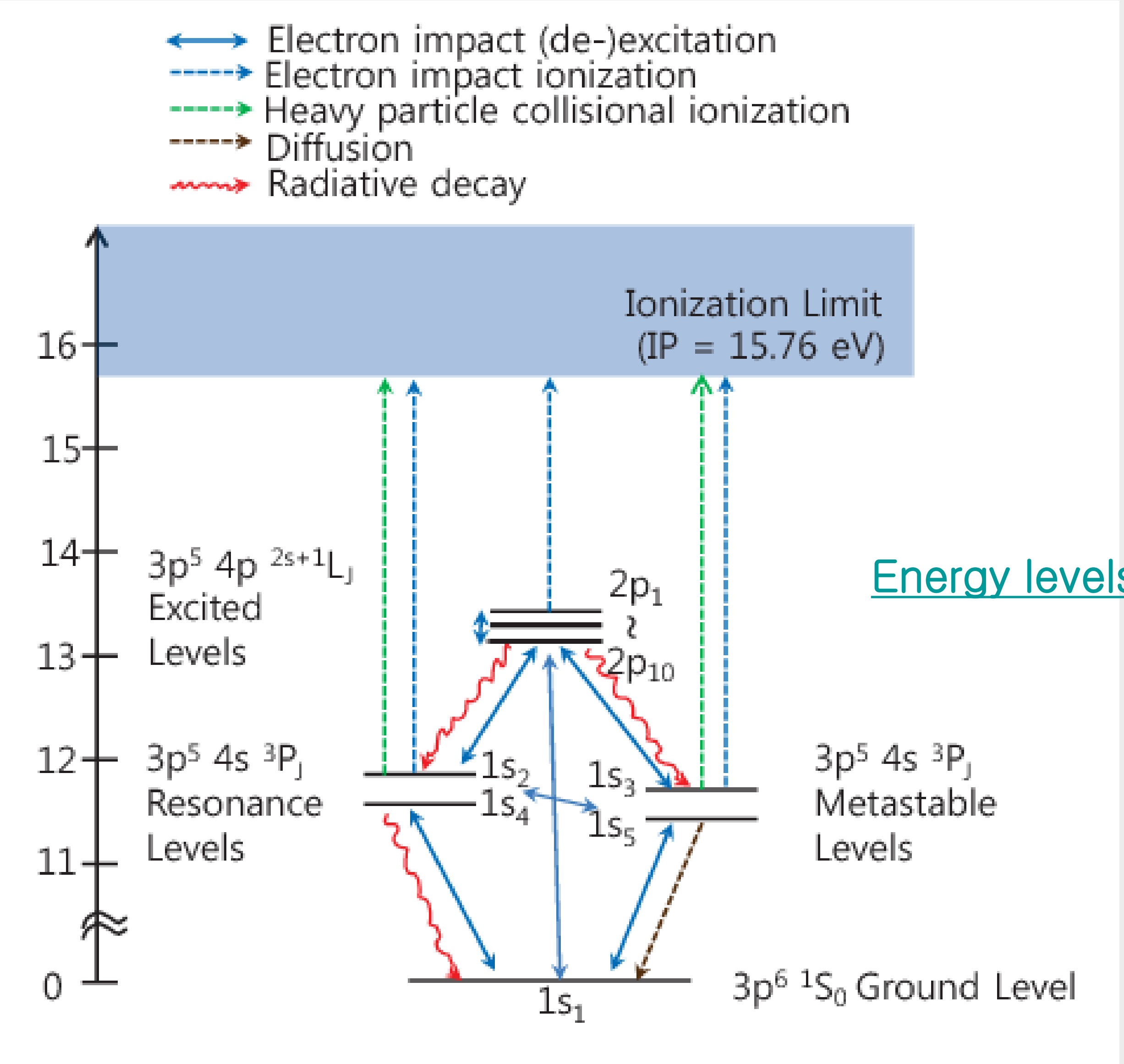








CR model for Ar I plasma



Energy levels for Ar I

Transition wavelength (nm) and probability (10^8 1/s) in parentheses

: Lines used for comparison of CRM with OES

Excited Levels	Resonance Levels		Metastable Levels	
	$1s_2$ (J=1)	$1s_4$ (J=1)	$1s_3$ (J=0)	$1s_5$ (J=2)
$2p_1$ (J=0)	750.39 (0.45)	667.73 (0.002)		
$2p_2$ (J=1)	826.45 (0.15)	727.29 (0.02)	772.42 (0.12)	696.54 (0.06)
$2p_3$ (J=2)	840.82 (0.22)	738.40 (0.08)		706.72 (0.04)
$2p_4$ (J=1)	852.14 (0.14)	747.12 (0.0003)	794.82 (0.19)	714.70 (0.006)
$2p_5$ (J=0)	858.01	751.47 (0.40)		
$2p_6$ (J=2)	922.45 (0.05)	800.62 (0.05)		763.51 (0.25)
$2p_7$ (J=1)	935.42 (0.01)	810.37 (0.25)	866.79 (0.02)	772.38 (0.05)
$2p_8$ (J=2)	978.45 (0.01)	842.46 (0.22)		801.48 (0.009)
$2p_9$ (J=3)				811.53 (0.33)
$2p_{10}$ (J=1)	1148.8 (0.002)	965.78 (0.05)	1047.0 (0.01)	912.30 (0.19)

CRM for low temperature plasma

Steady state balance equation for excited levels

From the particle balance equation $\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}) = \frac{\delta n}{\delta t}$, $n\mathbf{u} = -\nabla(D_a n)$

$$\frac{\partial N_i}{\partial t} - \nabla \cdot (\nabla D_a N_i) = \left(\frac{\delta N_i}{\delta t}\right)_{CR}, \quad \nabla \cdot (\nabla D_a N_i) \approx \nu_i^d N_i \,, \quad \frac{\partial N_i}{\partial t} = 0$$

In the weakly ionizing plasma conditions $N_0 \alpha_I \gg n_+ \alpha_R$, $n_+ \approx n_e$

Populating terms **Depopulating terms**

$$\sum_{j \neq i} n_e \alpha_{ji}^{ex} N_j + \sum_{j > i} \eta_{ji}(N_i) A_{ji} N_j = \sum_{j \neq i} n_e \alpha_{ij}^{ex} N_i + \sum_{j < i} \eta_{ij}(N_j) A_{ij} N_i + n_e \alpha_i^{\mathrm{I}} N_i + \sum_j \alpha_{ij}^{\mathrm{I}} N_i N_j + \nu_i^d N_i$$

Nonlinear terms

Ground level population

$$p_{tot} = N_0 k_B T_g + n_+ k_B T_i + n_e k_B T_e \approx N_0 k_B T_g$$

$$N_0 \cong \frac{p_{tot}}{k_B T_g} \ (constant)$$

Diagnostics for plasma parameters

Minimization of $\Delta(n_e, T_{eff}, R_{eff}, L_{eff}) = \sum \left(\frac{I_{ik}^{\mathrm{CRM}} - I_{ik}^{\mathrm{OES}}}{I_{ik}^{\mathrm{OES}}}\right)^2$, $I_{ik}^{\mathrm{CRM}} = \frac{N_i \eta_{ik} A_{ik}}{\lambda_{ik}}$

Atomic data and plasma parameters for CRM of Ar I

- **Gas temperature**

Assumed to be close to room temperature (300K) for CCP at low pressures (p) and powers (P)

- **Electron-impact excitation/deexcitation (EIE/DE)**

$Ar + e \rightarrow Ar^{*} + e$: BSR Quantum-mechanical calculation by O. Zatsariny & K. Bartschat in Lxcat DB (https://nl.lxcat.net)

- **Electron-impact ionization**

$Ar + e \rightarrow Ar^{+} + 2e$: Semi-empirical formula by L. Vriens (PRA 22, 940 (1980))

$$\alpha_i^{iz}\left(cm^3 s^{-1}\right) = \frac{9.56\times 10^{-6}(k_B T_e)^{-1.5}\exp(-\Delta E_i / k_B T_e)}{\left(\Delta E_i / k_B T\right)^{2.33} + 4.38\left(\Delta E_i / k_B T\right)^{1.72} + 1.32\left(\Delta E_i / k_B T\right)} \qquad \Delta E_i = E_{IP} - E_i$$

- **Heavy particle collisional ionization**

$$Ar^{*} + Ar^{*} \rightarrow Ar + Ar^{+} + e \;:\; \alpha_{rr}^{hiz} = 1.14\times 10^{-14}\sqrt{\frac{16 k_B T_g}{\pi M_{Ar}}},\ \alpha_{rm}^{hiz} = 2.1\times 10^{-9},\ \alpha_{mm}^{hiz} = 1.2\times 10^{-15}$$

- **Particle diffusion for metastable levels**

$$D_m = D_{sc}\frac{n_{sc}}{n_0}\sqrt{\frac{T_g}{T_{sc}}} \qquad \nu_m^d = \frac{1}{\tau_{eff}^d} = D_m\left[\left(\frac{\pi}{L}\right)^2 + \left(\frac{2.405}{R}\right)^2\right]$$

EEDF and radiation trapping for CRM of Ar I

- We consider non-Maxwellian electron energy distribution as below:

EEPF : $g_p(\varepsilon) = g_0 g_f(\varepsilon)$

EEDF : $$g_f(\varepsilon) = \begin{cases} \exp(-\dfrac{\varepsilon}{T_e^{low}}) \ (\varepsilon \le \varepsilon_k) \\ \exp(-\dfrac{\varepsilon_k}{T_e^{low}} - \dfrac{\varepsilon - \varepsilon_k}{T_e^{high}}) \ (\varepsilon > \varepsilon_k) \end{cases}$$

T_e^{low}: electron temperature in the low-energy region
T_e^{high}: electron temperature in high-energy region
ε_k: knee energy
EEPF: electron energy probability function
EEDF: electron energy distribution function

$$g_0 = \frac{n_e}{\int_0^\infty \sqrt{\varepsilon} g_f(\varepsilon) d\varepsilon}$$

- We also use an escape factor (η) for finite cylinder

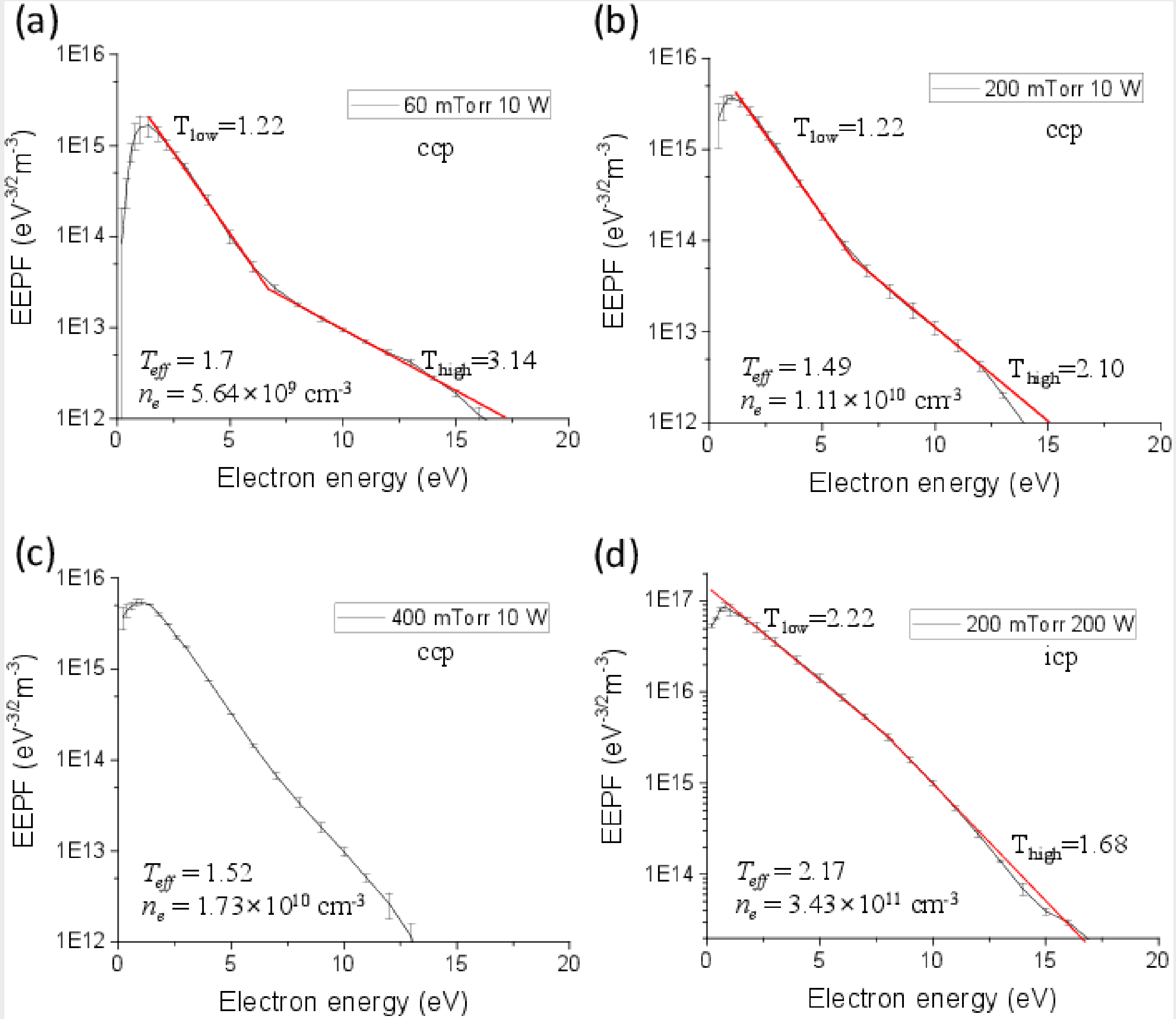
$$\eta(r,z) = \frac{1}{\sqrt{\pi \log(k_0(L-z))} k_0(L-z)} \frac{1}{2\pi} \int_0^\pi d\psi \int_{(L-z)/q_0(\psi)}^\infty \frac{\xi d\xi}{(1+\xi^2)^2}$$
$$+ \frac{1}{\sqrt{\pi} k_0} \frac{1}{2\pi} \int_0^\pi \frac{d\psi}{q_0(\psi)\sqrt{\log(k_0 q_0(\psi))}} \int_{-z/q_0(\psi)}^{(L-z)/q_0(\psi)} \frac{\xi d\xi}{(1+\xi^2)^2}$$
$$+ \frac{d\psi}{\sqrt{\pi \log(k_0 z)} k_0 z} \frac{1}{2\pi} \int_0^\pi d\psi \int_{z/q_0(\psi)}^\infty \frac{\xi d\xi}{(1+\xi^2)^2}$$

L: plasma length
R: plasma radius
k_0: absorption coefficient at the center

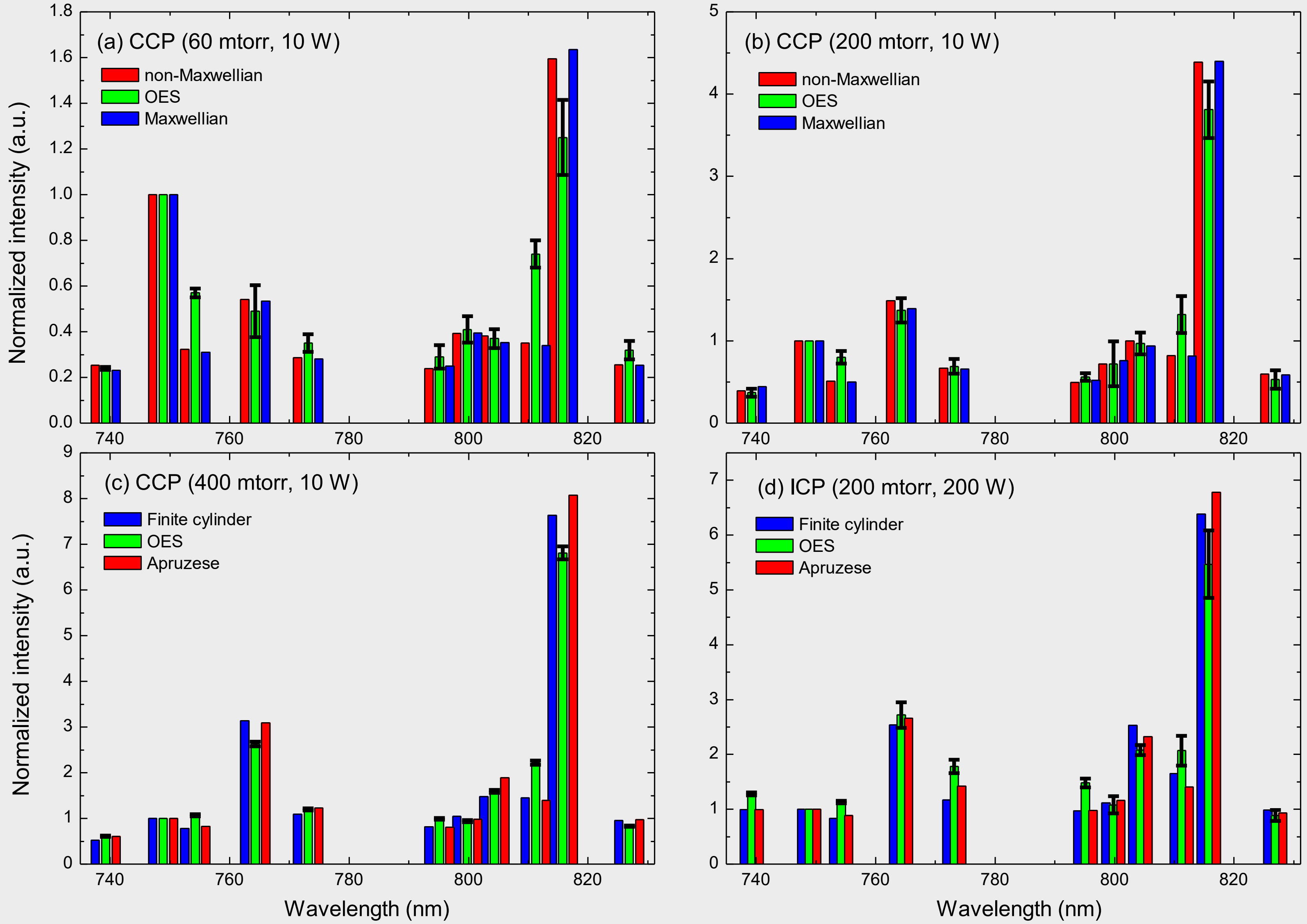
$$k_0 = \frac{\lambda^3 N_i}{8\pi} \frac{g_j}{g_i} \sqrt{\frac{A_{ji} M}{2\pi k_B T_g}}$$

K.-B. Chai and D.-H. Kwon, JQSRT **227** 136-144 (2019).

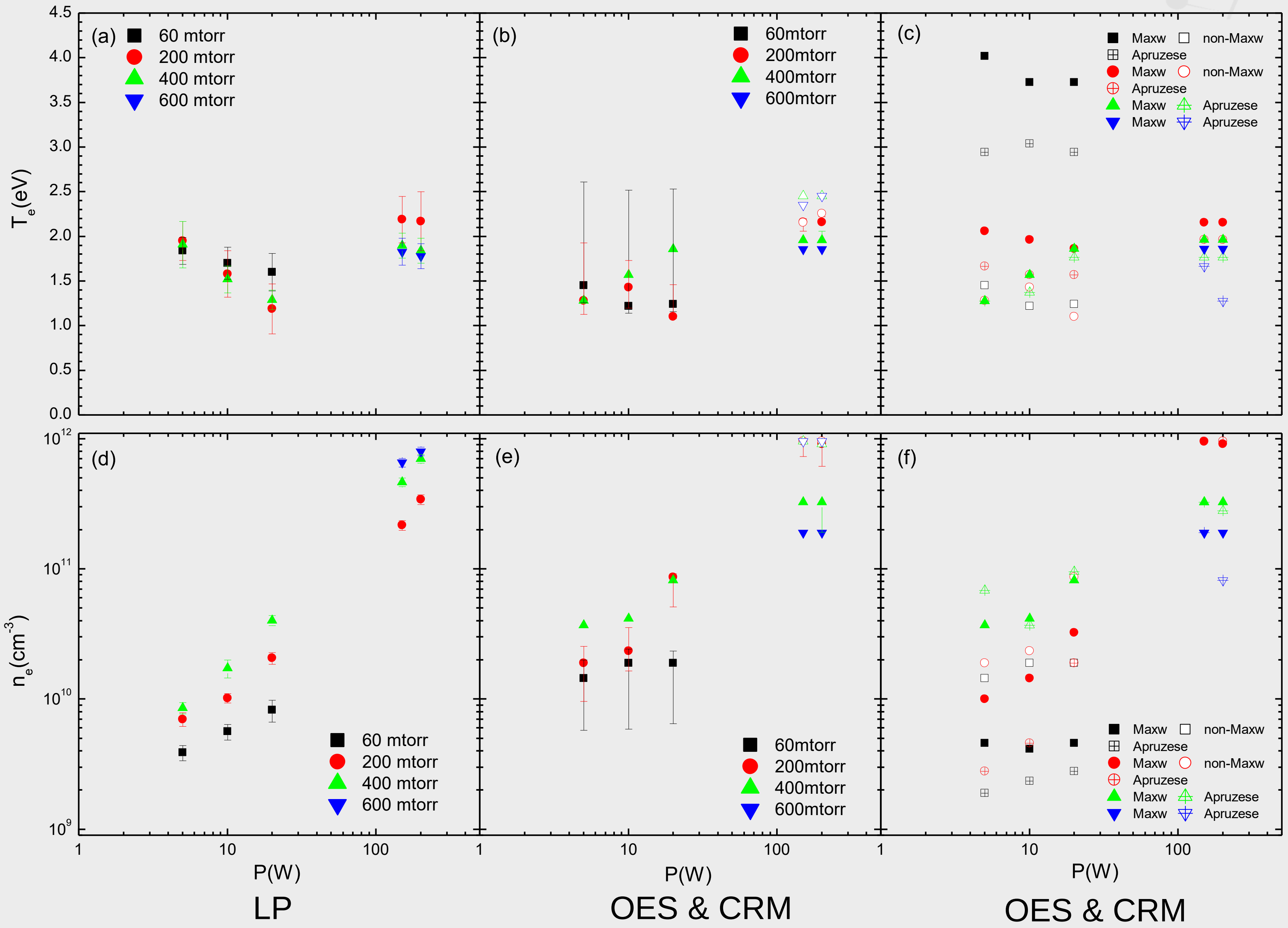
EEPF for the CCP & the ICP of Ar



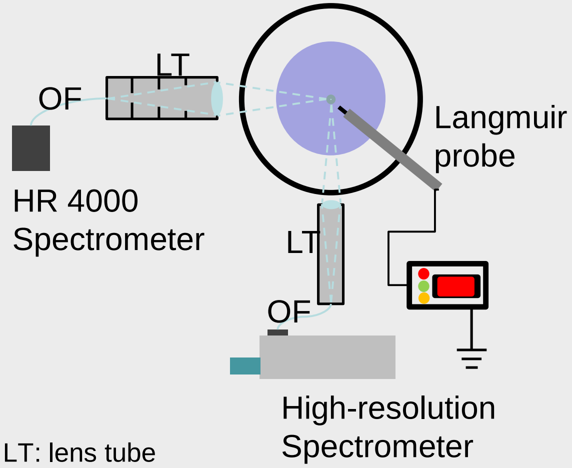
Measured and modeled spectra for Ar I



Diagnostics : OES with CRM *vs.* LP measurement

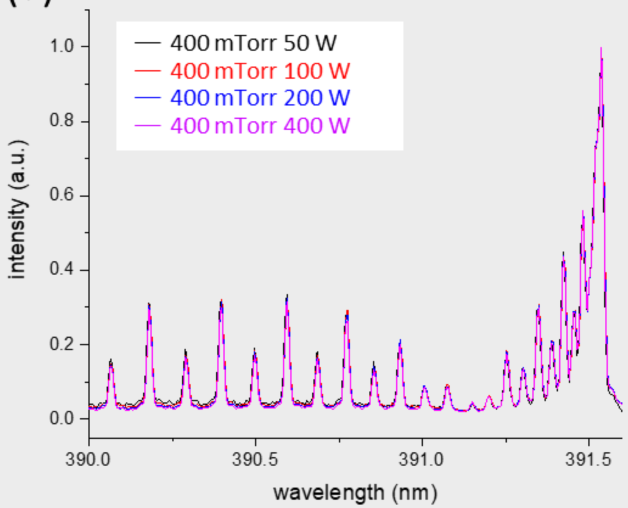


OES for low temperature He plasma

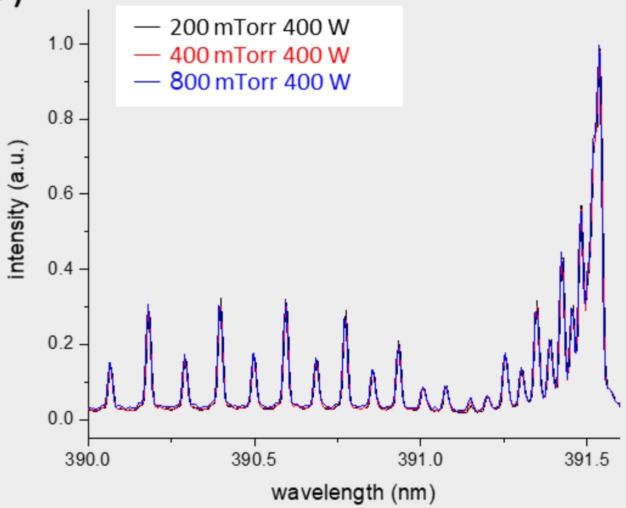


LT: lens tube
OF: optical fiber
MFC: mass flow controller

(a)



(b)



Measured spectra for N_2^+

Gas temperature

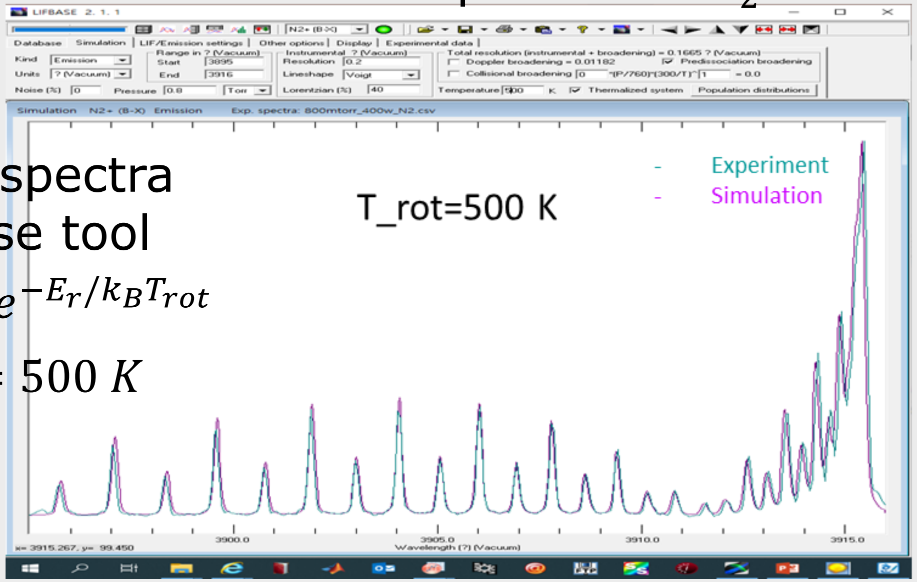
T_g can be estimated with the N_2^+ rotational temperature obtained from the emission spectra of the N_2^+ transition $B^2\Sigma_u^+, v = 0 \rightarrow X^2\Sigma_g^+, v' = 0$ by inserting small amount of N_2 gas into the He plasma.

Modeled spectra by LIFbase tool

$I = D_0 k^4 S e^{-E_r/k_B T_{rot}}$

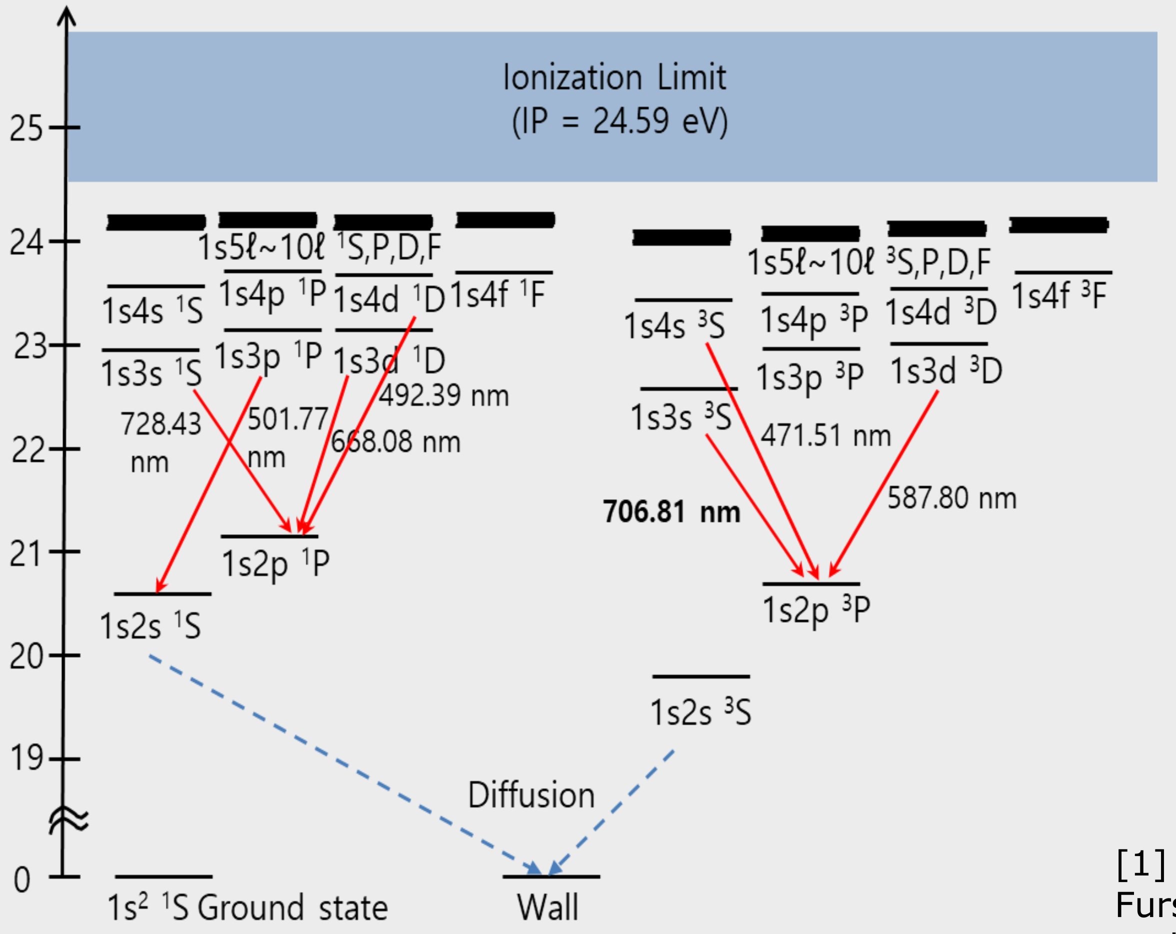
$\Rightarrow T_g \approx T_{rot} = 500\ K$

(c)



CRM for low temperature He I plasma

Energy levels



$up\ to\ 1snl\ (n = 10, \ell = 3)$

Kinetic processes

1. $\mathrm{He + e \rightarrow He^* + e}$ $\quad \alpha_{ij}^{ex}$ [1]
2. $\mathrm{He + e \rightarrow He^+ + 2e}$ $\quad \alpha_i^{\mathrm{I}}$ [1]
3. $\mathrm{He^* \rightarrow He} + h\nu$ $\quad \lambda_{ij}, A_{ij}$ [2]
4. $\mathrm{He}(1s2\ell) + \mathrm{He}(1s2\ell') \rightarrow \mathrm{He^+ + He + e}$ $\quad \alpha_{ij}^{\mathrm{I}}$

$$2.9 \times 10^{-9}(T_g/300)^{1/2}(cm^3/s)$$

5. $\mathrm{He}(1s2s) \rightarrow to\ wall$ $\quad \nu_i^d$

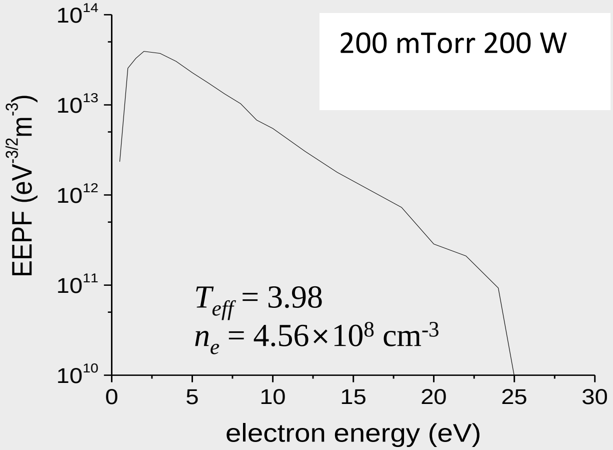
$$\nu_i^d = D_a\left(\left(\frac{2.405}{R_{eff}}\right)^2 + \left(\frac{\pi}{L_{eff}}\right)^2\right),$$

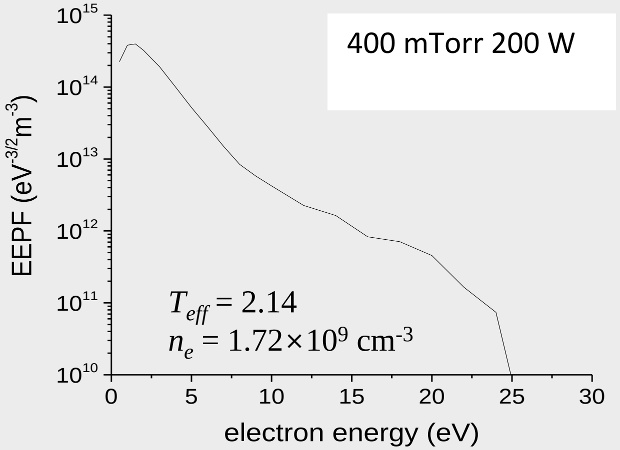
$$D_a = 8.992 \times 10^{-2}\frac{T_g^{3/2}}{p}\ (cm^3/s)$$

[1] Y. Ralchenko, R. K. Janev, T. Kato, D. V. Fursa, I. Bray, F. J. de Heer, Atomic Data and Nuclear Data Tables 94 (2008) 603.
[2] G.W.F Drake, D.C. Morton, Astrophys. J. Suppl. Series 170 (2007) 251.

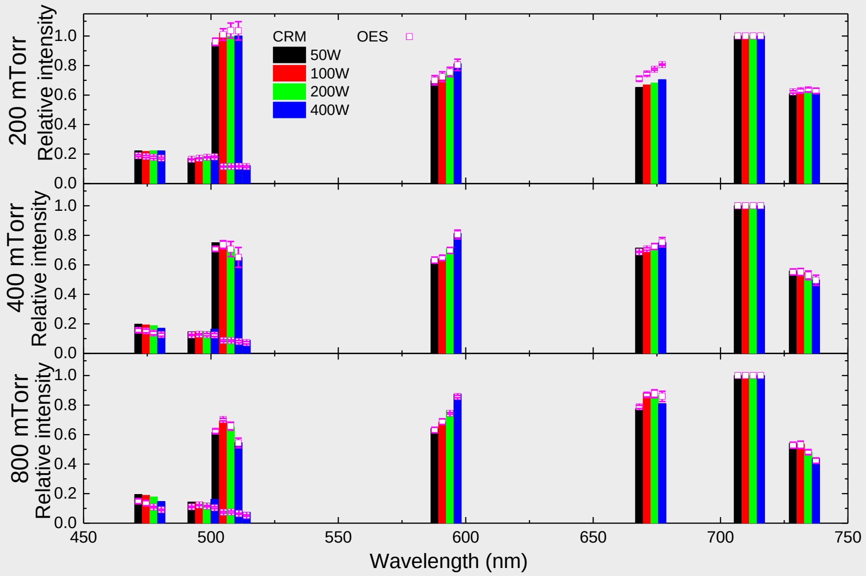
OES & CRM *vs*. LP measurement for low temperature He plasma

Non-Maxwellian electron energy distribution

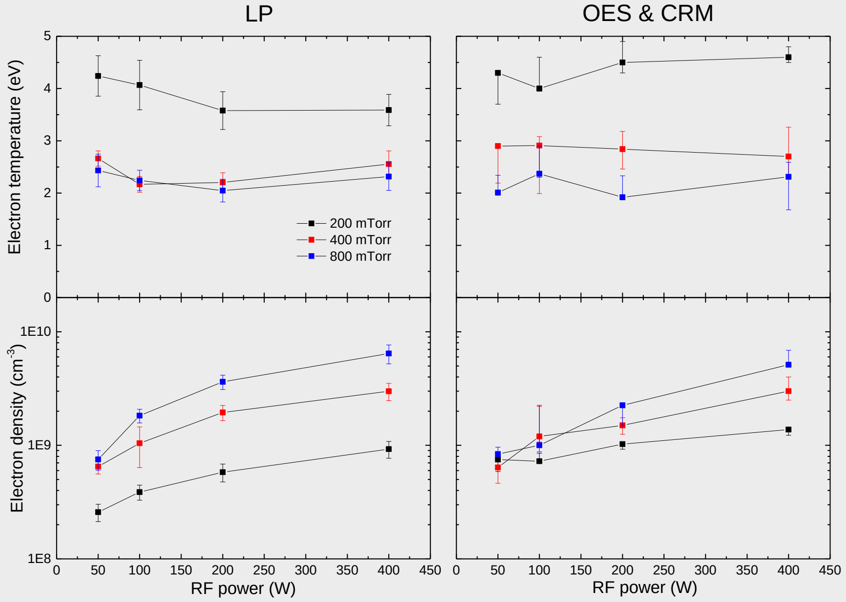




OES and CR modeling spectra



Electron temperature and density



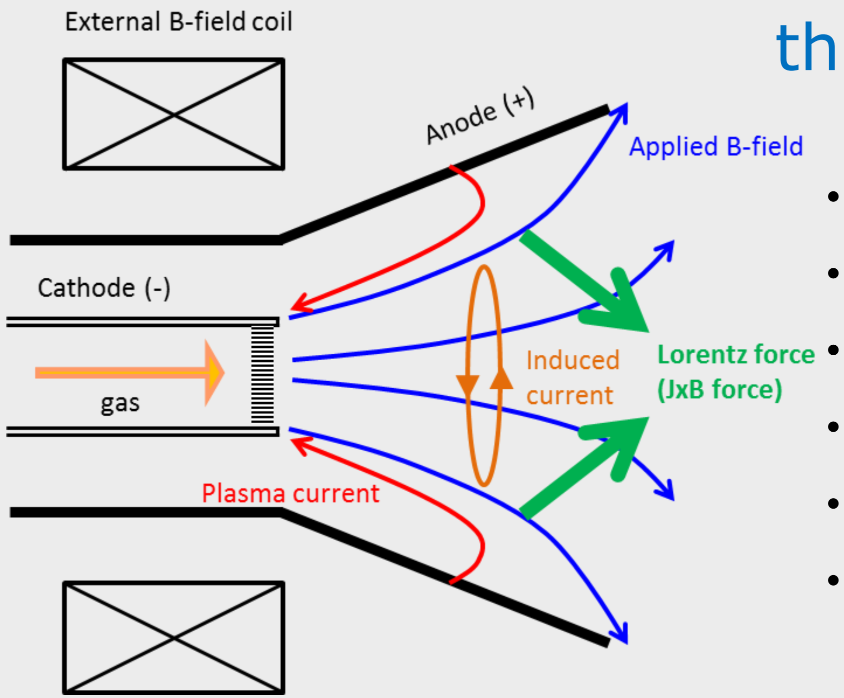
K.-B. Chai and D.-H. Kwon, Spectrochimica Acta Part B **183** 106269 (2021).

KAERI Plasma Beam Irradiation Facility (PBIF)

Motivation of the construction

In order to develop divertor materials and cooling techniques resisting **high heat** and **particle fluxes** (heat flux of 10 MW/m^2 and particle flux of 10^{24} /m^{2}s will come in ITER and much larger heat and particle fluxes will come in DEMO), we have constructed **lab-scale** divertor plasma simulator

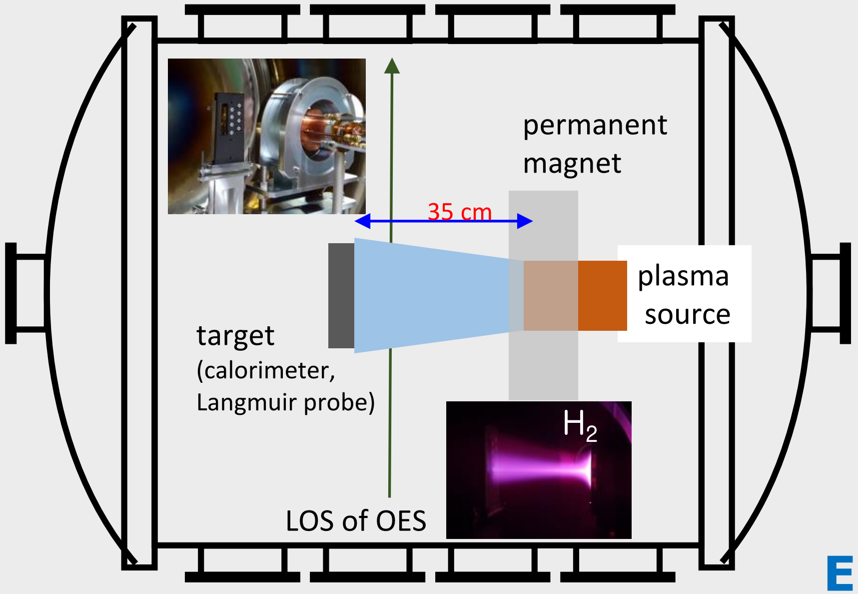
Applied field-magnetoplasmadynamic (AF-MPD) thruster concept



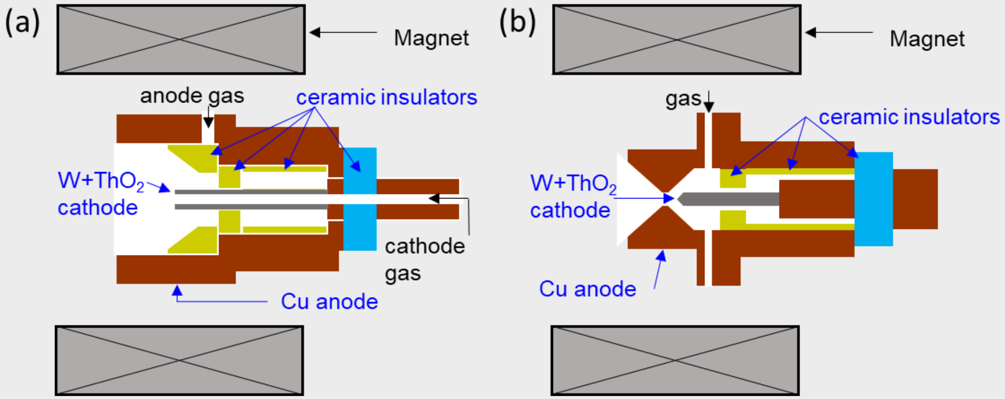
type I/ type II　　　　type I/ type II

- Anode radius = 4/2 cm, cathode radius = 0.6/0.4 cm
- Anode material: Cu, cathode material: W+ThO_2 (2%)
- Insulating material : ceramic (Al_2O_3)
- Sustain power supply : DC 10-20 kW
- External B-field: 0.17 T (NdFeB permanent magnet)
- Both anode & cathode can be water-cooled

KAERI AF-MPD PBIF



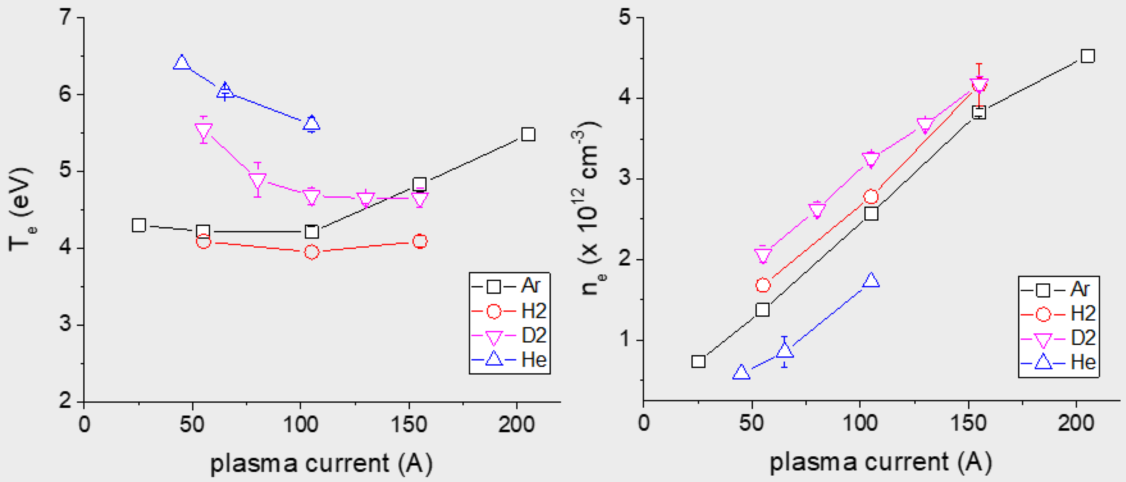
Plasma source schemes



Type I for Ar

Type II for H_2,D_2,He

Electron temperature and density by LP



K.-B. Chai, D.-H. Kwon and M. Lee, Plasma Phys. Control. Fusion **63** 125020 (2021).

CR modeling for H/D plasma

Considered processes

$\mathrm{H}(n \geq 1) + e \leftrightarrow \mathrm{H}(n' > n) + e$	(1)	[1]
$\mathrm{H}(n \geq 1) + e \leftrightarrow \mathrm{H}^+ + 2e$	(2)	[1]
$\mathrm{H}(n \leq 40) \rightarrow \mathrm{H}(n' < n) + h\nu$	(3)	[1]
$\mathrm{H}^+ + e \rightarrow \mathrm{H}(n \leq 40) + h\nu$	(4)	[1]
$\mathrm{H}_2 + e \rightarrow \mathrm{H}(n = 1) + \mathrm{H}(n' \leq 3) + e$	(5)	[2]
$\mathrm{H}_2 + e \rightarrow 2\mathrm{H}(n = 2) + \mathrm{e}$	(6)	[2]
$\mathrm{H}_2 + e \rightarrow \mathrm{H}^+ + \mathrm{H}(n = 1) + e$	(7)	[1]
$\mathrm{H}_2 + e \rightarrow \mathrm{H}_2^+ + 2e$	(8)	[1]
$\mathrm{H}_2^+ + \mathrm{e} \rightarrow \mathrm{H}(n = 1) + \mathrm{H}(n' \geq 2)$	(9)	[3]
$\mathrm{H}_2^+ + \mathrm{e} \rightarrow \mathrm{H}^+ + \mathrm{H}(n \leq 2) + e$	(10)	[3]
$\mathrm{H}_2^+ + \mathrm{e} \rightarrow 2\mathrm{H}^+ + e$	(11)	[3]
$\mathrm{H}_2^+ + \mathrm{e} \rightarrow \mathrm{H}_2^* \rightarrow \mathrm{H}(n = 1) + \mathrm{H}(n' \geq 2)$	(12)	[1]
$\mathrm{H}_3^+ + \mathrm{e} \rightarrow 3\mathrm{H}(n = 1)$	(13)	[3]
$\mathrm{H}_3^+ + \mathrm{e} \rightarrow \mathrm{H}_2 + \mathrm{H}(n = 2)$	(14)	[3]
$\mathrm{H}_3^+ + \mathrm{e} \rightarrow \mathrm{H}^+ + 2\mathrm{H}(n = 1) + e$	(15)	[3]
$\mathrm{H}_2^+ + \mathrm{H}_2 \rightarrow \mathrm{H}(n = 1) + \mathrm{H}_3^+$	(16)	[4]

[1] R. K. Janev, D. Reiter and U Samm, Collision processes in low-temperature hydrogen plasmas, Report JUEL-4105 (2003).

[2] R. K Janev et al., Elementary processes in Hydrogen-Helium plasmas, (Berlin: Springer 1987)

[3] W. L. Wiese, and J. R. Fuhr, Accurate atomic transition probabilities for H, He, Li, J. Phys.. Chem. Ref. Data **38** 565 (2009).

[4] P. del Mazo-Sevillano, ..., D.-H. Kwon, O. Roncero, Molecular physics e2183071

❖ The cross sections for electron collisions and radiative transitions of D species were used by those of H species. The heavy particle collision cross section of D species was from the ab-initio calculation for D [4]. The mass effect for rate coefficients and mobility of D were taken into account.

$$\alpha(T_{12}) = \frac{4}{\sqrt{\pi} v_{T_{12}}^3} \int_0^\infty \sigma(v_{12}) exp\left(\left(v_{12}/v_{T_{12}}\right)^2\right) v_{12}^3 dv_{12}$$

$$T_{12} = (m_2 T_1 + m_1 T_2)/(m_1 + m_2)$$

$$v_{T_{12}} = \sqrt{2(m_1 + m_2) T_{12}/m_1 m_2}$$

CRM for H/D plasma

For atomic levels n_i ($i = 1 - 40$)

$$D_{AH^+} = T_e K_1^0 \left(\frac{760}{p}\frac{T_m}{273}\right)$$

$$p = n_{H_2} T_m$$

$$K_1^0 = 15.9\ (H^+), 11.2 (D^+)$$
$$(cm^2 V^{-1} s^{-1})$$

$$D_{AH^+} : D_{AH_2^+} : D_{AH_3^+} = 1 : \frac{\sqrt{2}}{\sqrt{3}} : \frac{\sqrt{5}}{3}$$

$$\frac{dn_i}{dt} = \sum_{j>i}^{40} \eta_{ji} A_{ji} n_j - \left(\sum_{j<i} \eta_{ij} A_{ij} + \frac{Q}{V} + \frac{\gamma}{\tau}\delta_{i1}\right) n_i + n_e\left(\sum_{j\neq i} \beta_{1,ji}\, n_j - \sum_{j\neq i} \beta_{1,ij}\, n_i - \beta_{2i} n_i + \beta_{4i}\, n_{H^+}\right) + n_e(\beta_{5i} + \beta_6 \delta_{i2} + \beta_7 \delta_{i1}) n_{41} + n_e(\beta_{9i} + \beta_{10i} + \beta_{12i}) n_{42} + n_e(\beta_{13}\delta_{i1} + \beta_{14}\delta_{i2} + \beta_{15}\delta_{i1}) n_{43} + n_{41}\beta_{16}\delta_{i1} n_{42} + \left(\sum_{j=42}^{43} \varsigma_{aj} \left(\frac{\mu}{R}\right)^2 D_{Aj} n_j + \varsigma_{aD^+}\left(\frac{\mu}{R}\right)^2 D_{AH^+} n_{H^+}\right)\delta_{i1}$$

$$\tau = 2R/v_{th}$$

$$v_{th} = 2\sqrt{\frac{2T_a}{\pi M_H}}$$

$$\mu = 2.405$$

For molecule and ions n_i (i=41,42,43 for H_2, H_2^+, H_3^+)

$$\frac{dn_i}{dt} = \delta_{i41}\left(n_e \beta_{14} n_{43} + \frac{Q_{in}}{V} \times 4.48 \times 10^{17} + \frac{\gamma'}{\tau} n_1 + \sum_{j=42}^{43} \varsigma_{mj} \left(\frac{\mu}{R}\right)^2 D_{Aj} n_j + \varsigma_{mH^+}\left(\frac{\mu}{R}\right)^2 D_{AH^+} n_{H^+}\right) - \delta_{i41} n_e(\beta_5 + \beta_6 + \beta_7 + \beta_8) n_i - \delta_{i42} n_e(\beta_9 + \beta_{10} + \beta_{11} + \beta_{12}) n_i - \delta_{i43} n_e(\beta_{13} + \beta_{14} + \beta_{15}) n_i + \delta_{i42}(n_e\beta_8 - n_{41}\beta_{16}) n_i + n_{41}\beta_{16}\delta_{i43} n_{42} - \delta_{i41}\beta_{16} n_{42} n_i - \frac{Q}{V} n_i - (1 - \delta_{i41})\left(\frac{\mu}{R}\right)^2 D_{Ai} n_i$$

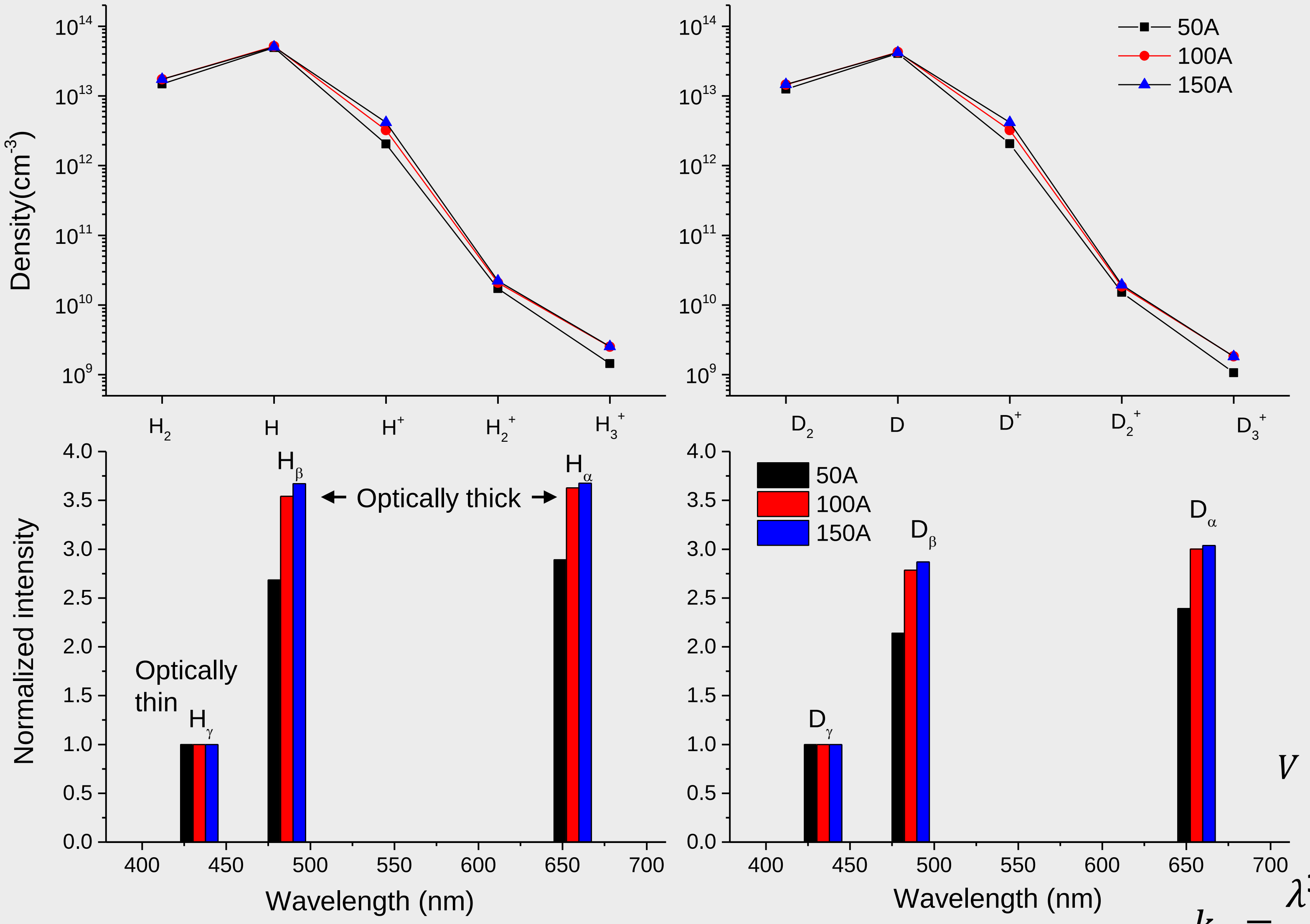
Quasi neutrality condition for H^+ ion n_{H^+} : $\boldsymbol{n_e = n_{H^+} + n_{H_2^+} + n_{H_3^+}}$

rather than **pressure balance equation** :

$$p_{tot} = n_m k_B T_m + k_B T_a\left(\sum_{j=1}^{40} n_j + n_{H^+}\right) + n_e k_B T_e + n_m k_B \left(n_{H_2^+} + n_{H_3^+}\right)$$

P. del Mazo-Sevillano, …, D.-H. Kwon, O. Roncero, "Vibrational, non-adiabatic and isotopic effects in the dynamics of the $H_2 + H_2^+ \rightarrow H_3^+ + H$ reaction: application to plasma modeling", Molecular physics e2183071 (2023)

Results for H/D CRM



$T_m = 300\text{K},$
$T_a = 600\text{K},$
$R_{eff} = 40\text{ cm},$

$T_e = 5.55\ (50\text{A}),$
$4.68\ (100\text{A}),$
$4.66\ (150\text{A})\ \text{eV}$

$n_e = 2.07\ (50A),$
$3.25\ (100\text{A}),$
$4.18\ (150\text{A}),$
$\times\ 10^{12} (\text{cm}^{-3})$

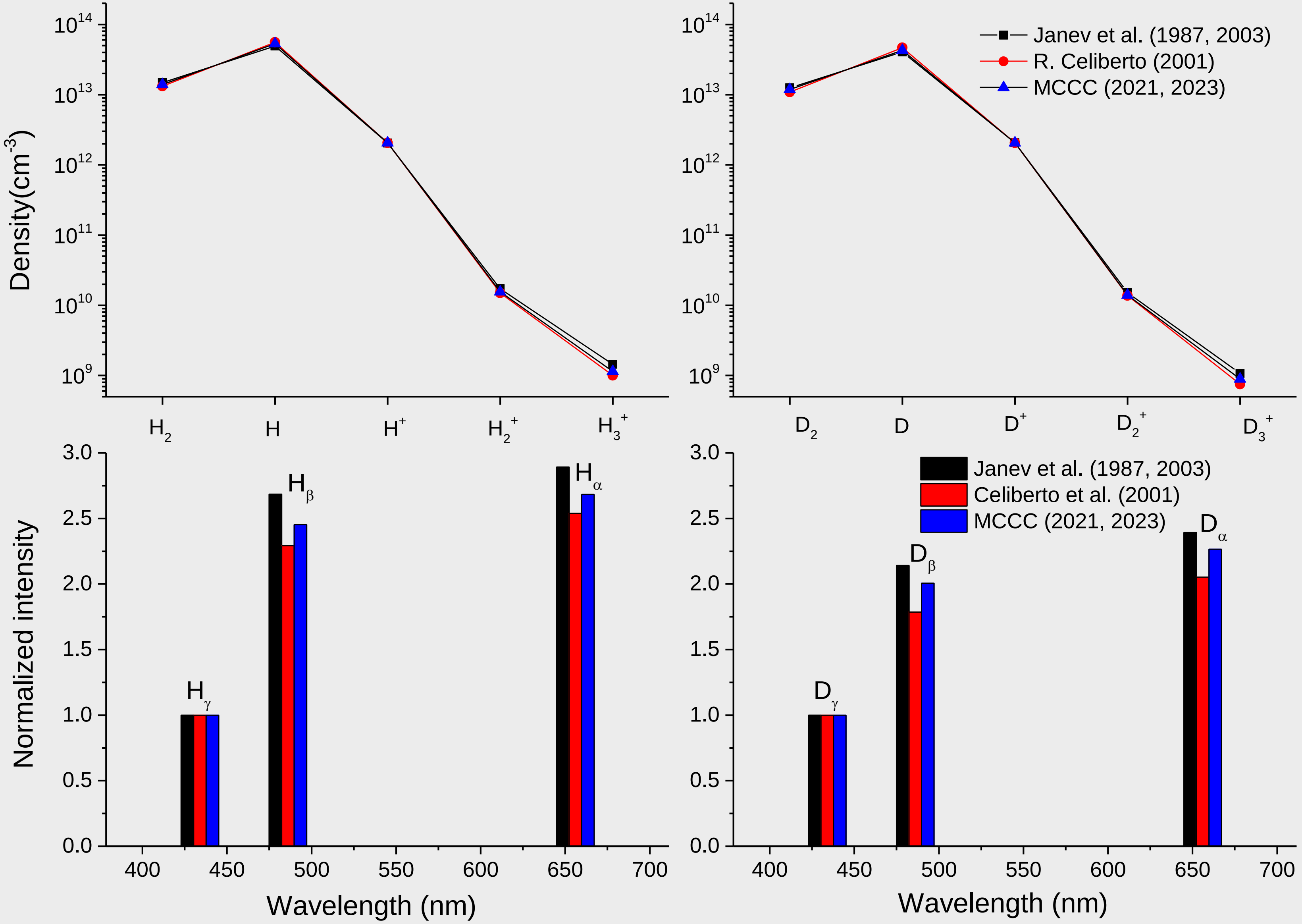
$Q_{in} = 600\text{ sccm},$
$Q = 4800\text{ lps},$

$V = 2.64 \times 10^6 \text{cm}^3,$
$R = 75\text{ cm}$

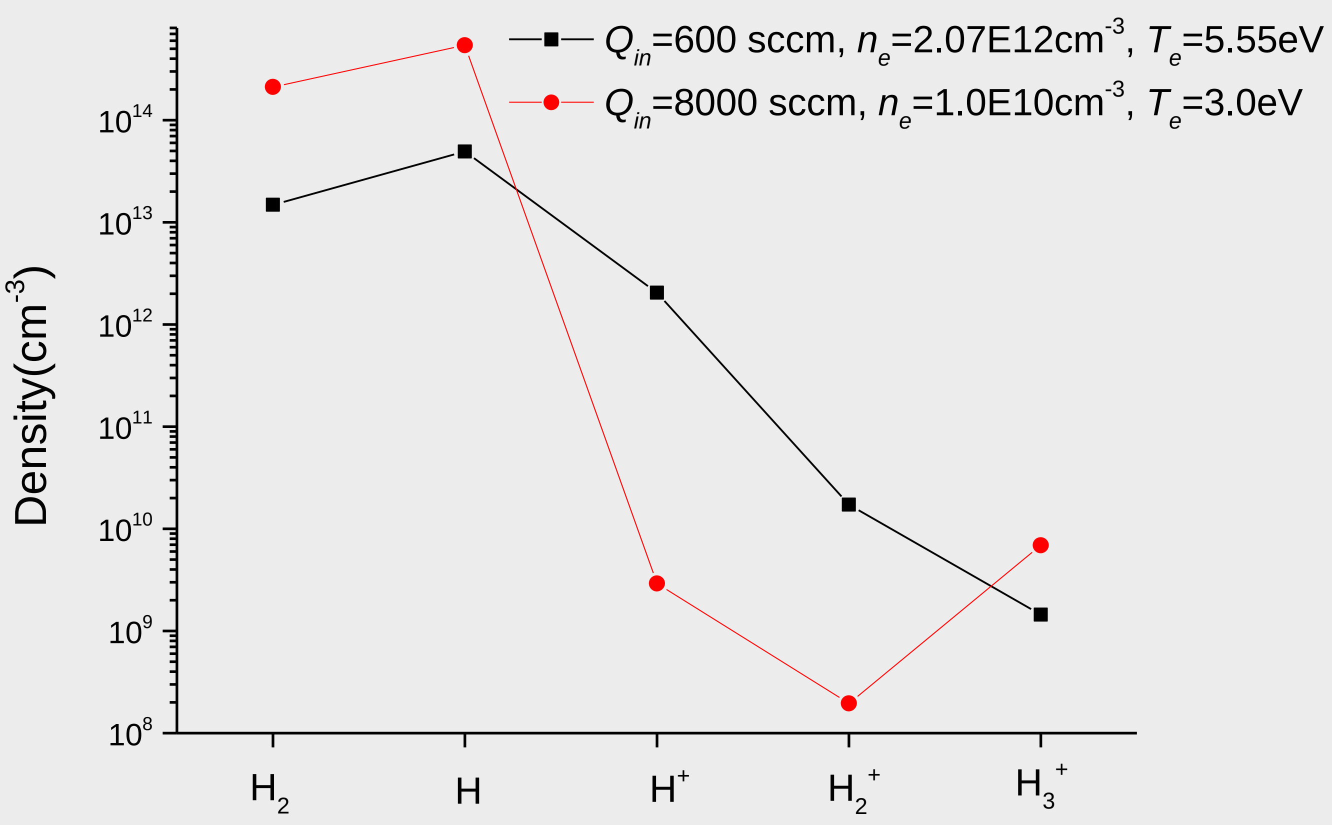
$$k_0 = \frac{\lambda^3 N_i}{8\pi} \frac{g_j}{g_i} \sqrt{\frac{A_{ji} M}{2\pi k_B T_g}}$$

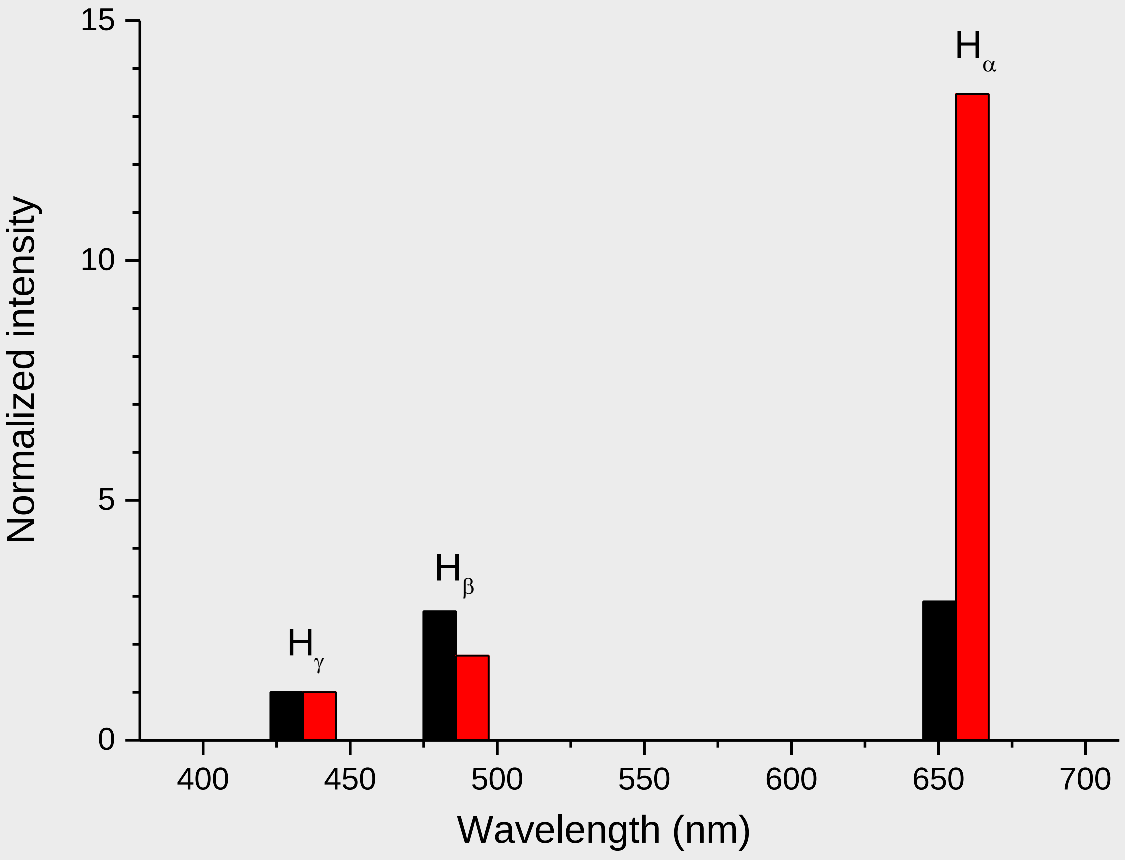
$\text{H} \rightarrow \text{D}\,, \qquad k_0 \uparrow \eta \downarrow$

Resulting populations and spectra for different atomic and molecular data sources

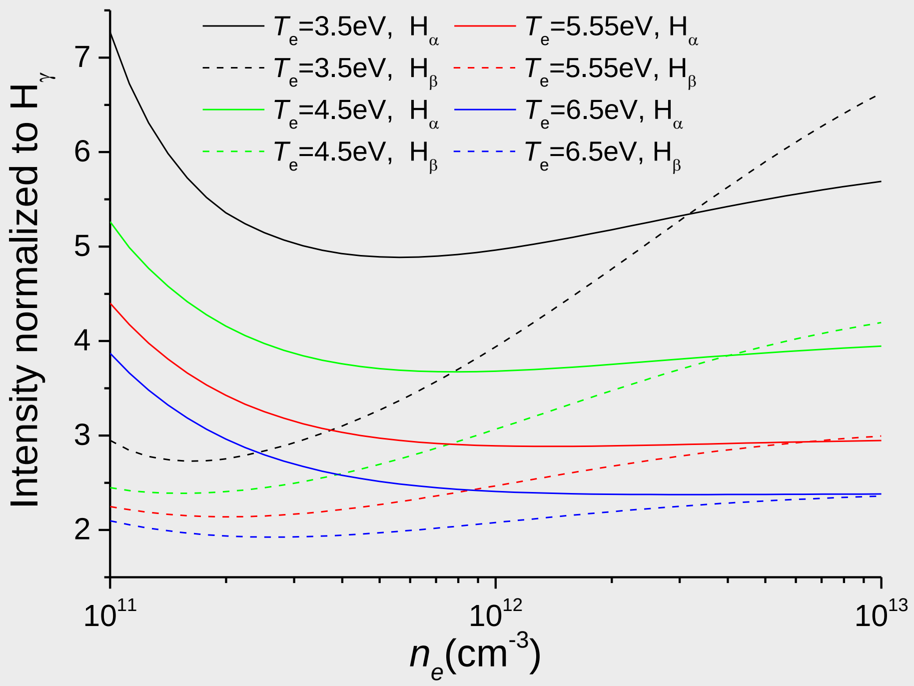


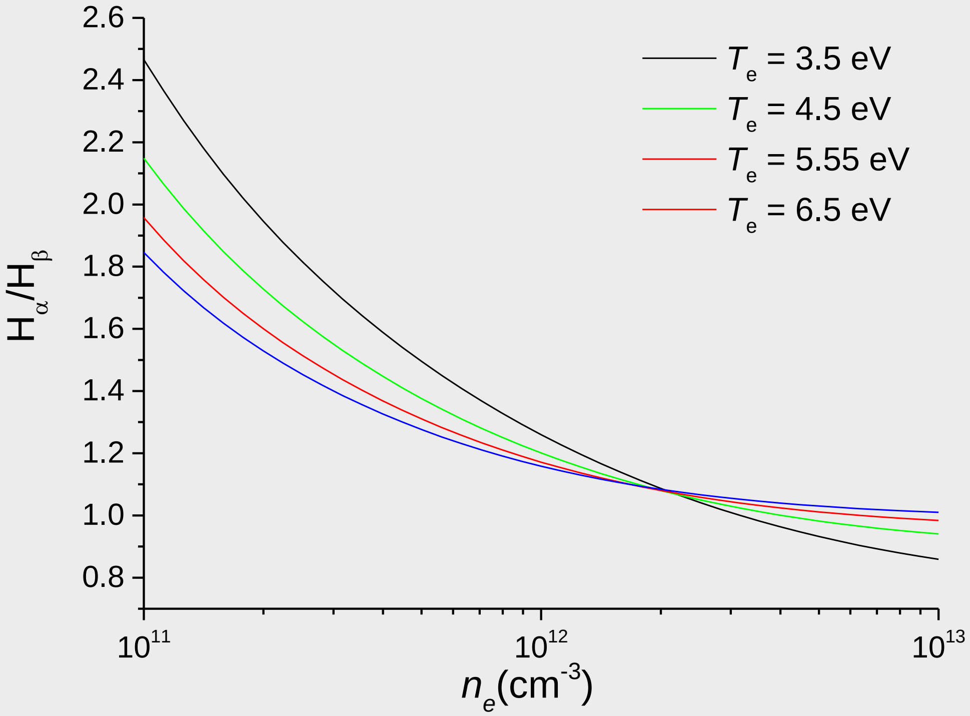
H_3^+ dominant case





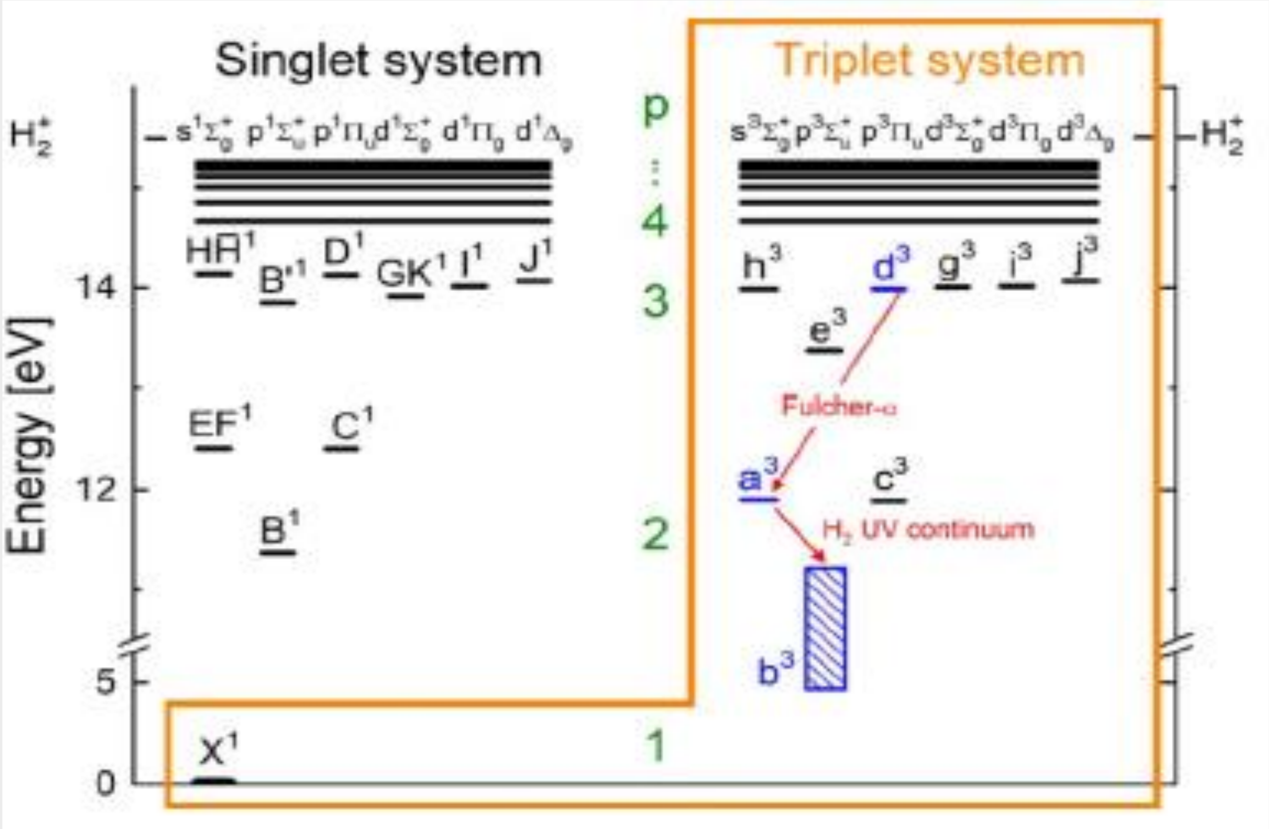
Sensitivity to plasma parameters n_e and T_e



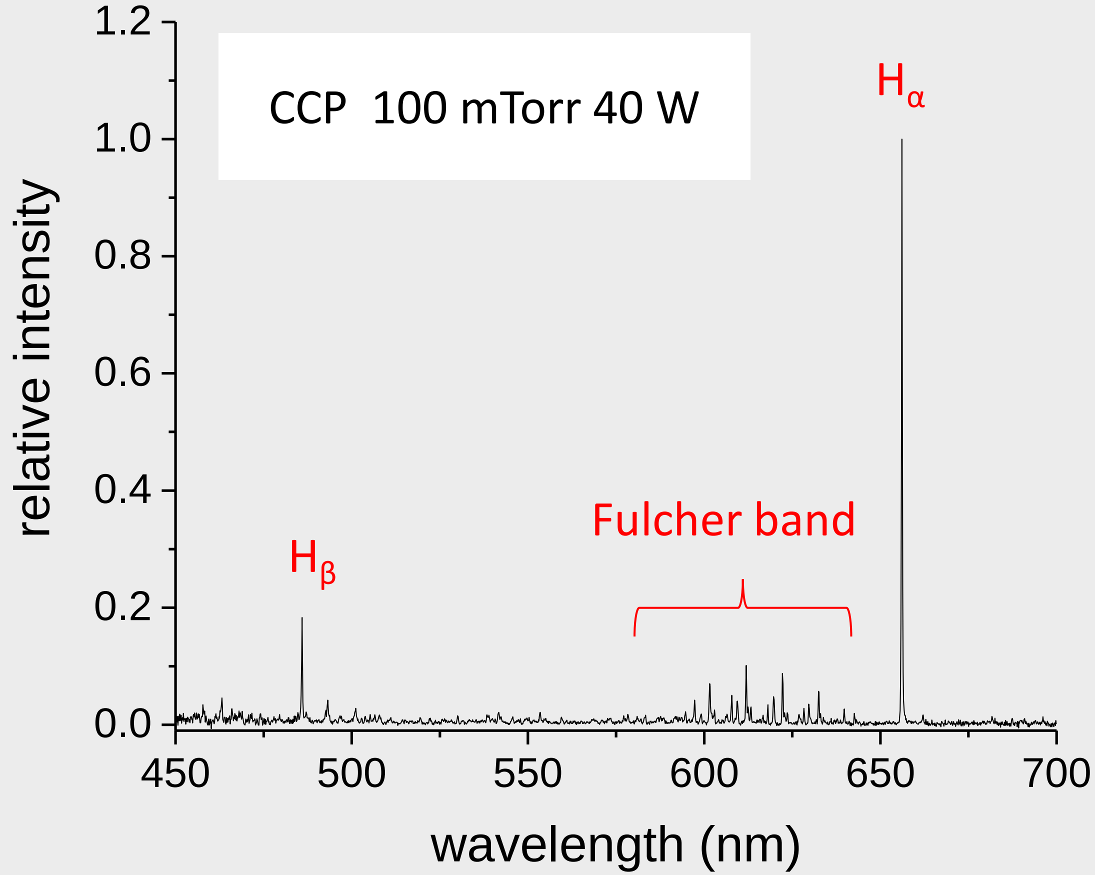


CR modeling for vibrational states of H molecules : Future works

Energy level diagram of H_2

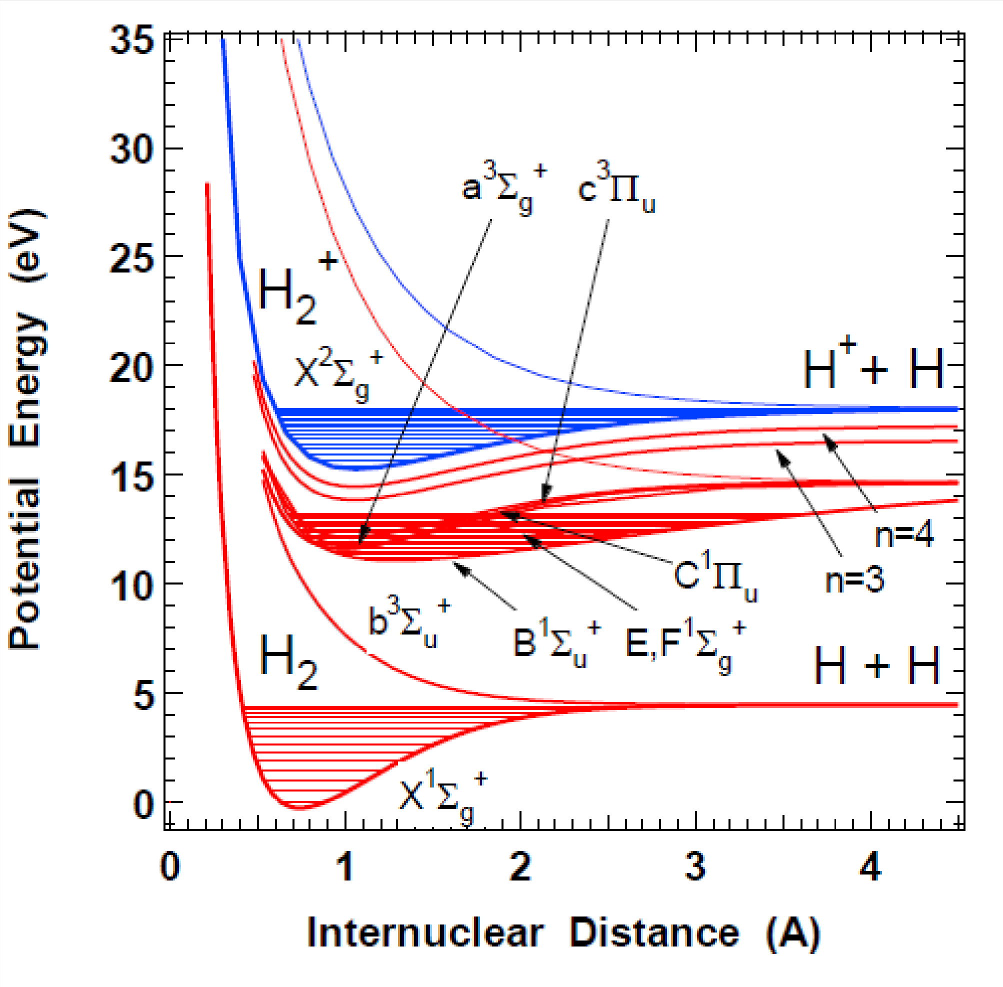


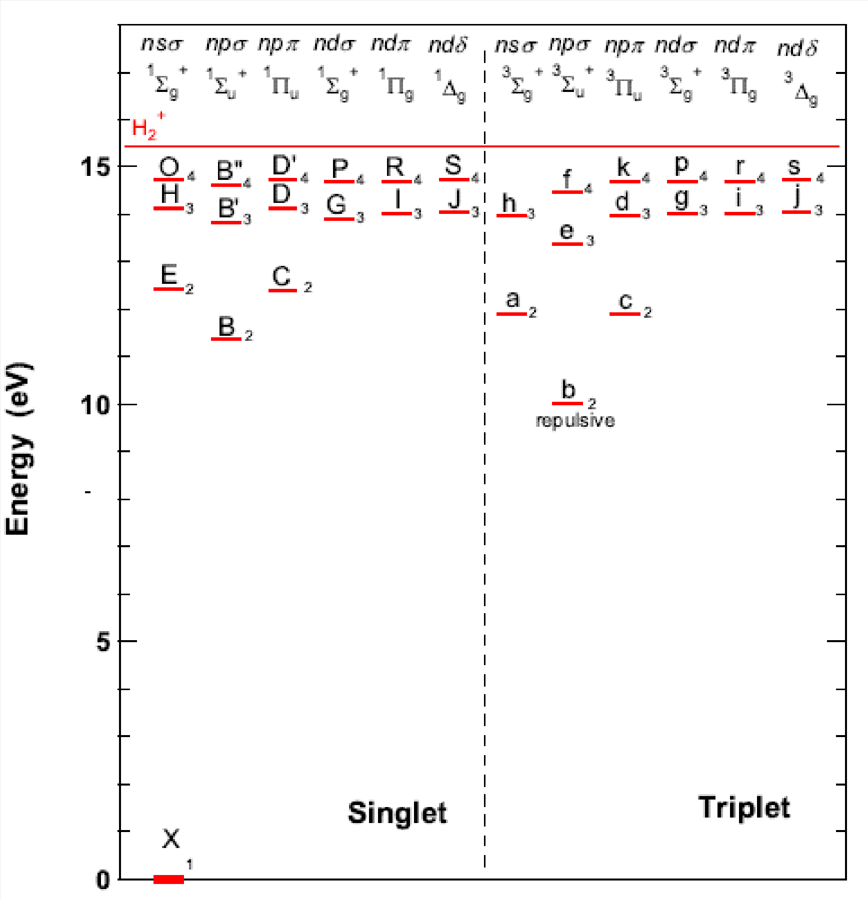
CR modeling for the measured molecular spectra



Ref. D. Wünderlich et al., J. Phys. D: Appl. Phys. **54** 115201 (2016)

H molecular energy levels

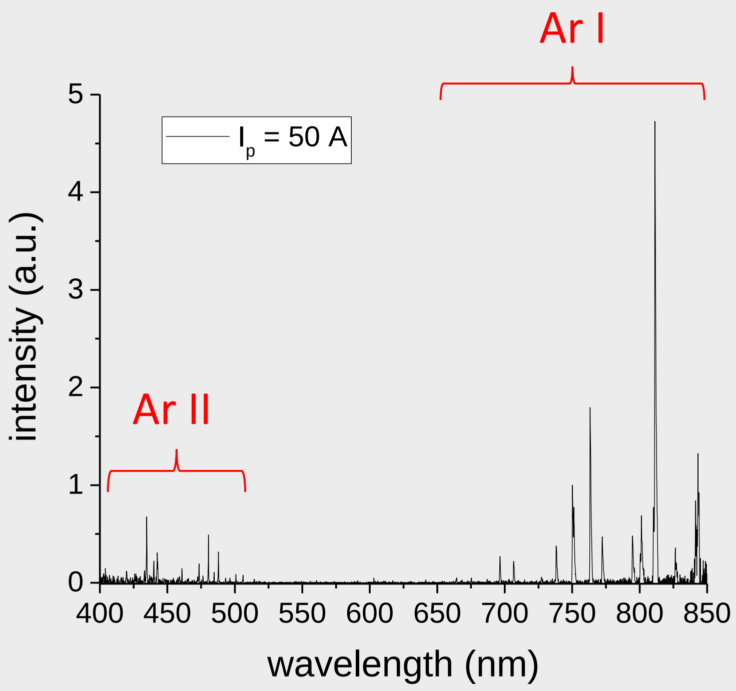




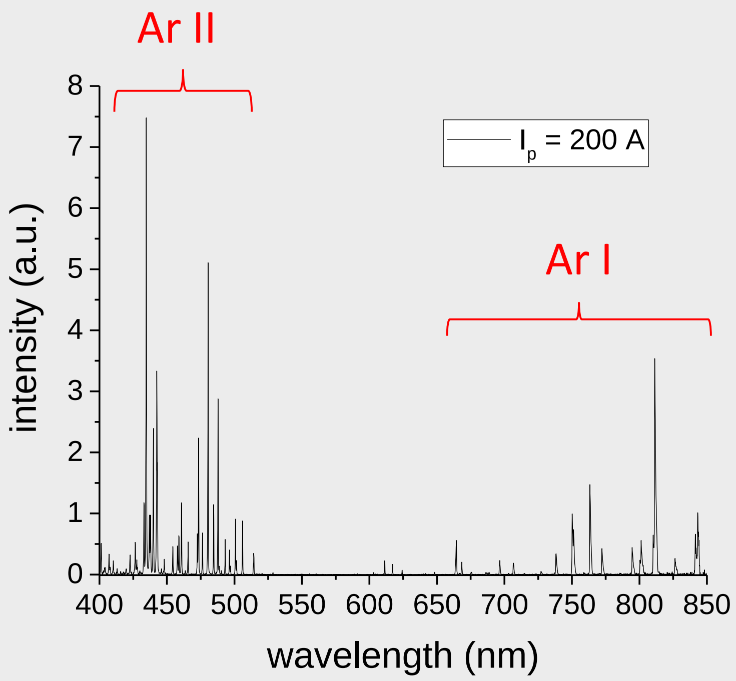
K. Sawada and M. Goto, Atoms **4** 29 (2016)

CR modeling including Ar and Ar^+ : Next works

Measured spectra in KAERI PBIF



increase I_p



As plasma current I_p increases, intensities of Ar ion lines dominate over those of Ar neutral lines

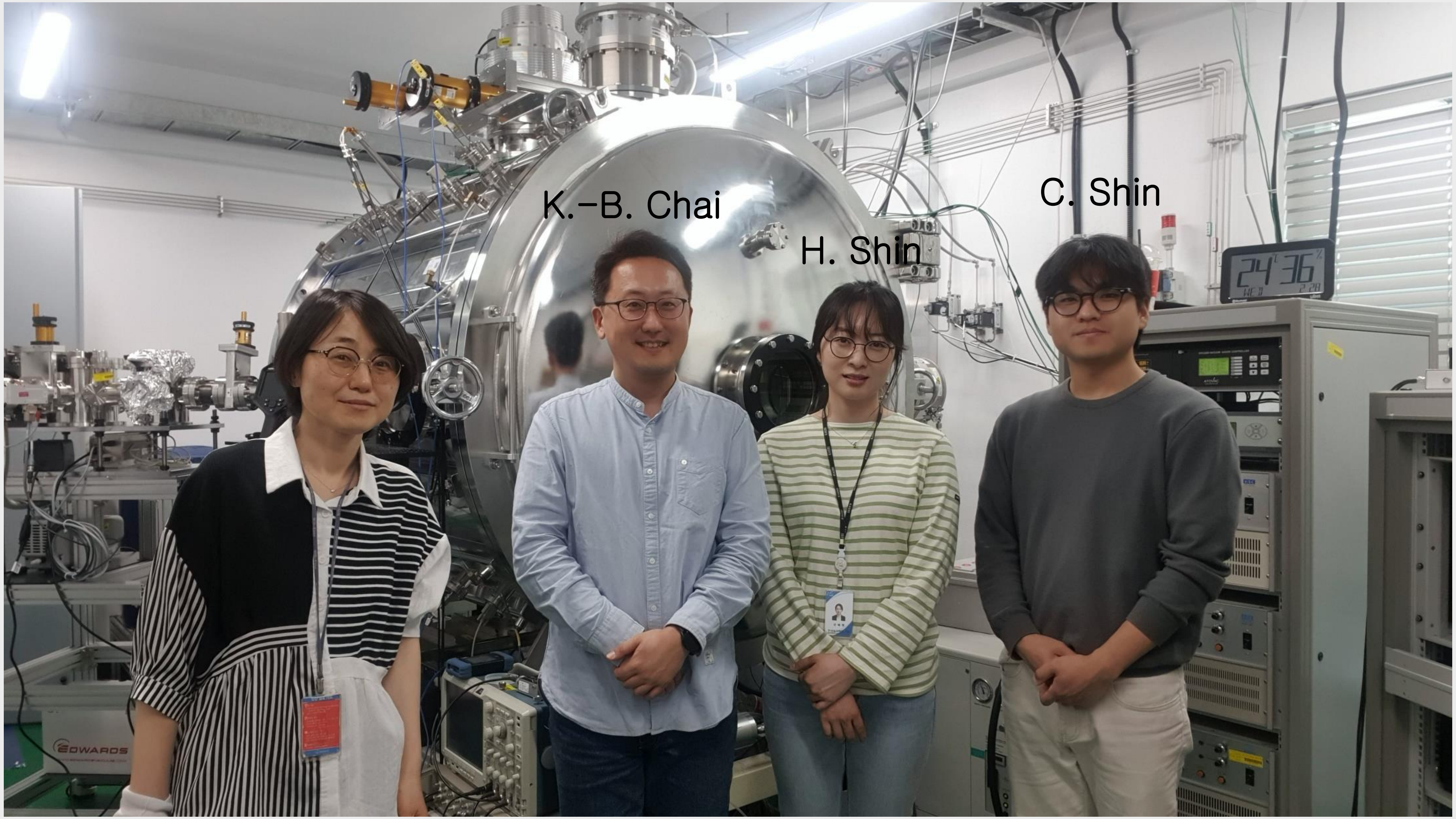
Significant change between spectra intensities of Ar I and Ar II lines are shown depending on the gas flow rate and electron density **around 487 nm** wavelengths from a plasma device in **Prof. G. Yun's team**.

→ need to **extend our CR model to include both Ar and Ar ions** for the analysis of the spectral behavior by **collaboration with Prof. Yun's team**

Summary and outlook

- CR modeling for highly charged ions from EBIT and atomic data are instructed for some selected examples. Detailed close collaboration of us with EBIT team will be desirable.
- Our developed CR model for low temperature, low density Ar, He, H/D plasma are described, which solves nonlinear steady-state balance equations including radiation trapping and heavy particle collisional ionization.
- The CR modeling for Ar will be extended to those for the both Ar and Ar^+ in highly excited states by the collaboration with Prof. G. Yun's team.

Our group members



Theoretical calculation   Experimental measurements and analysis