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ATOMIC DATA AND COLLISIONAL-RADIATIVE MODELS OF TUNGSTEN IONS FOR FUSION PLASMA

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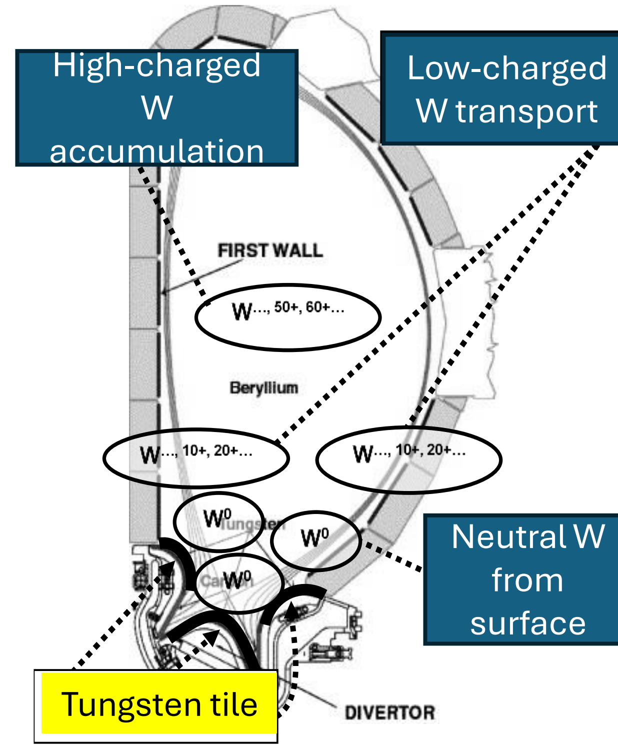
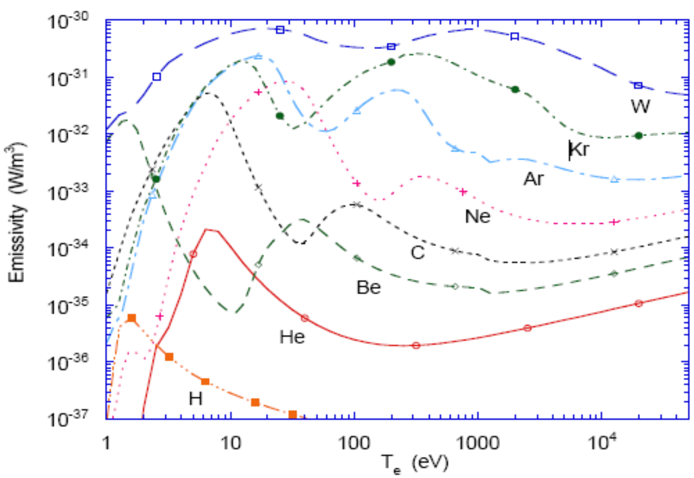
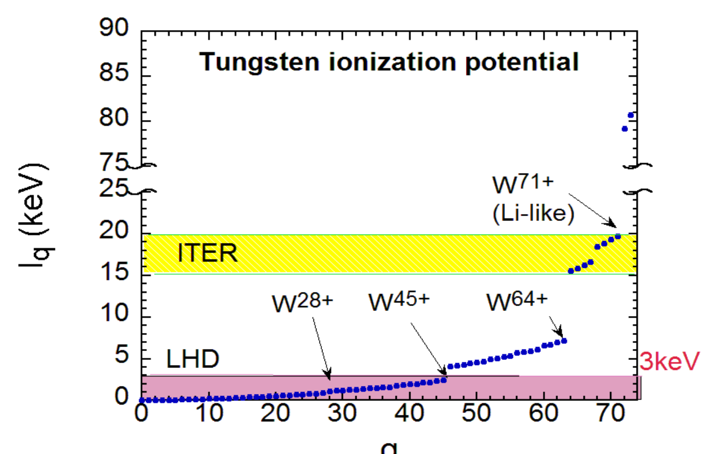
1. Introduction: tungsten in fusion plasmas (1)

- Tungsten used as plasma-facing material is sputtered by plasma particles and transported into central core plasma, causing electron temperature reduction due to large radiation power.
- Behavior of tungsten impurity in fusion plasmas is one of the important issues to be studied to achieve high-temperature plasmas for fusion reactions.

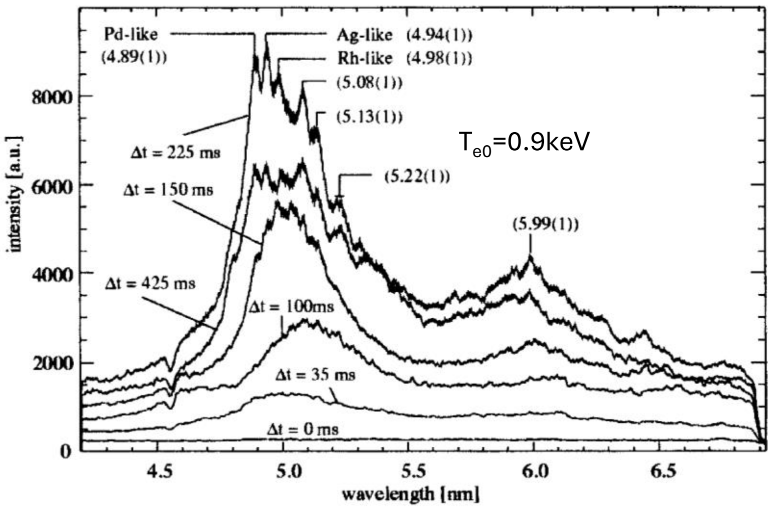




ITER Physics Expert Group on Divertor, Nucl. Fusion 39 (1999) 2391



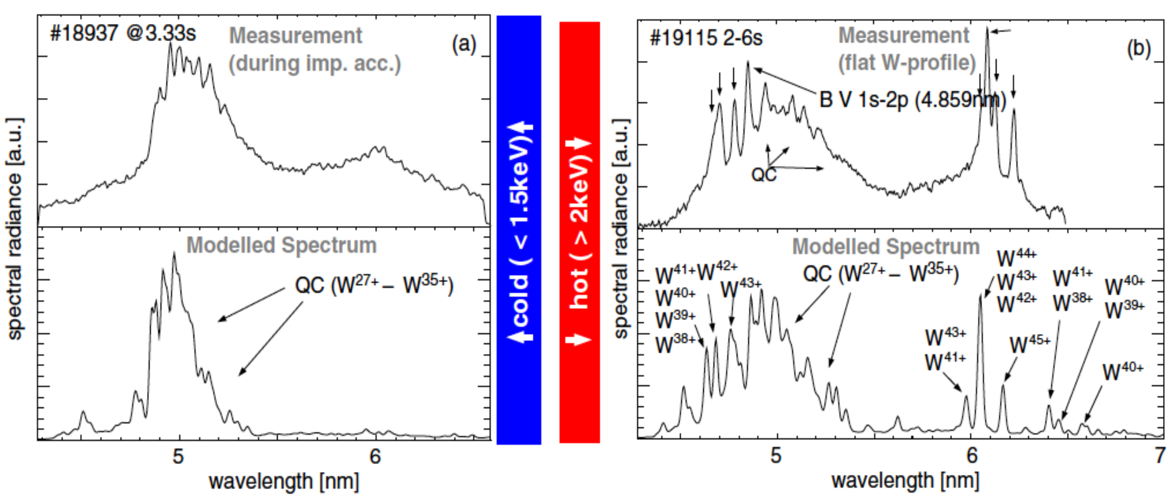
1. Introduction: Tungsten in fusion plasmas (2)



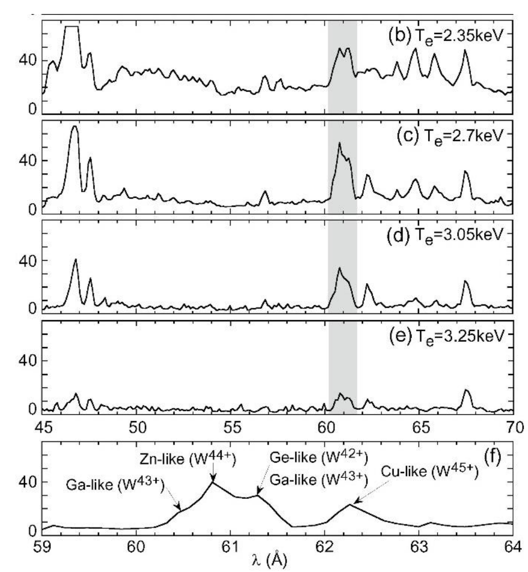
ASDEX-Upgrade; Tungsten laser ablation
Asmussen et al. (1998)

The Unresolved Transition Array (UTA) at 4.5-7nm are measured in plasmas with Te ~ 1kev, which contributed to a large part of radiation power. This feature is produced by overlapped numerous emission lines of n=4-4 transitions.

When electron temperature exceeds 2keV, the UTA changes to be discrete lines.



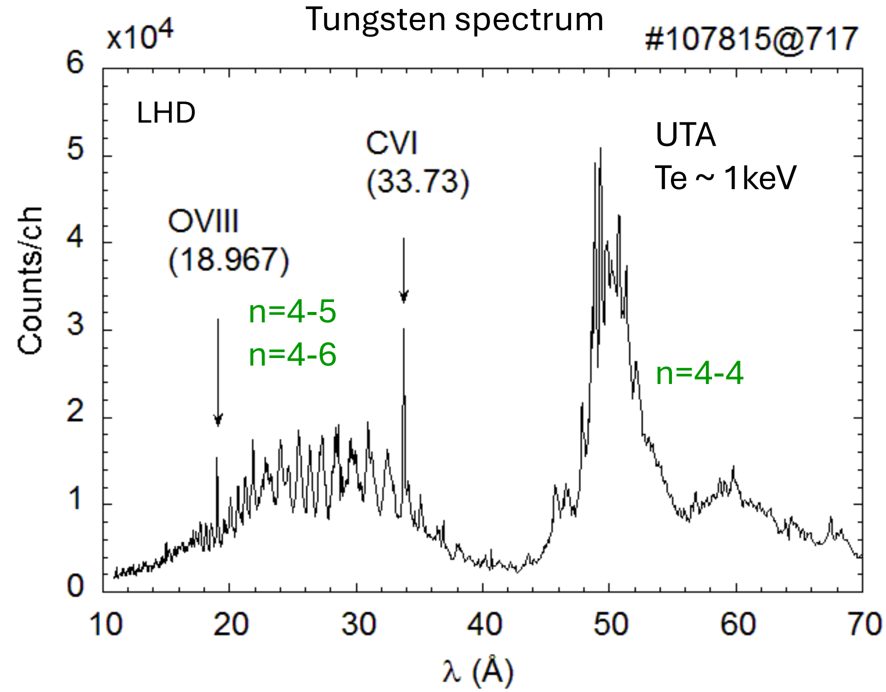
ASDEX Upgrade. Putterich et al. (2008)

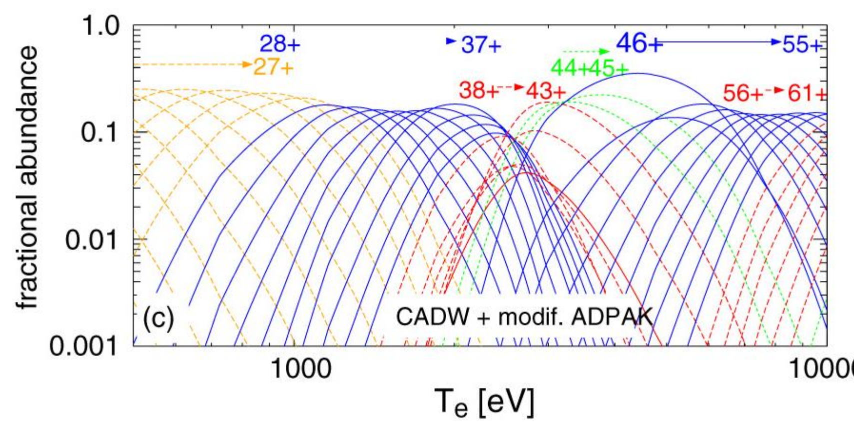


LHD. Morita et al. (2013)

1. Introduction : tungsten in fusion plasmas (3)

- In order to understand tungsten behavior in plasmas, spectroscopy is a good tool.
- So, we need to know tungsten spectra and their models to reproduce spectra with plasma parameters, such as electron temperature and density.
- But the atomic number of tungsten is 74. The charge states of tungsten ions in fusion plasma are distributed in a wide range corresponding to high to low electron temperature. Their atomic structures are complex and the spectra become complex.





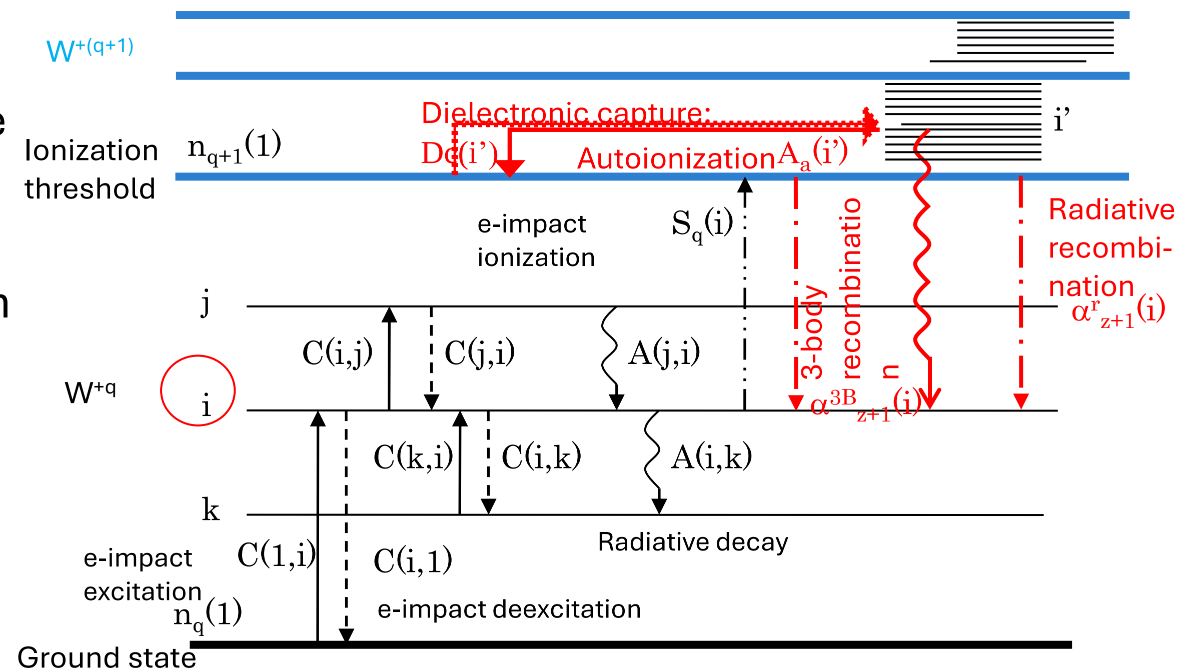
Tungsten charge state distribution (Putterich et al. 2008)

1. Introduction: Tungsten in fusion plasmas (4)

- Collisional-radiative (CR) model should be constructed for nearly whole charge states of tungsten ions for fusion plasmas for understanding tungsten behavior in fusion plasma by spectroscopy.
- Atomic data are required for CR model, i.e., energy levels, radiative transition probabilities, cross sections and rate coefficients of electron-impact excitation, ionization, and recombination, charge exchange cross sections for neutral H and W ions collision, and proton-impact excitation cross sections. However, many of them are missing.
- Calculated atomic data should be evaluated experimentally, but it is difficult in most cases. We need a method to evaluate data to have reliable data.
- Calculated spectra can be evaluated by comparing with measured spectra. Spectra measured with simpler plasma conditions is better for such evaluation.
- Here in this talk, studies on the CR model for W ions are introduced.

2. Collisional-radiative model for W spectra

- CR model is to calculate population densities of excited levels under quasi-steady-state assumption.
- Atomic processes between excited states are considered in the rate equation for the population density of level *i*, $n_q(i)$.
- Line intensity = $A(i,j) n_q(i) \Delta E(i,j)$



$$\frac{dn_q(i)}{dt} = \Gamma_{in} - \Gamma_{out} = 0$$

Solution :

$$n_q(i) = R_q^1(i) n_e n_q(1) + R_q^0(i) n_e n_{z+1}(1) + R_q^{CX}(i) n_H n_{z+1}(1)$$

Ionizing plasma component and
Recombining plasma component

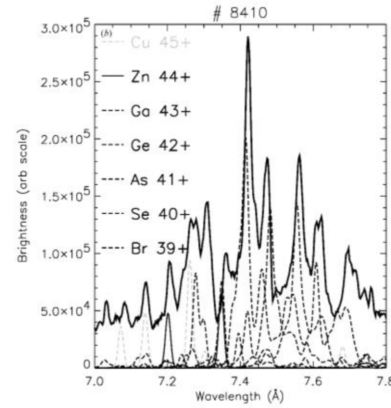
Charge exchange with H atom could be important, but often ingored

$$\Gamma_{in} = \sum_{j<i} \{C(j,i) n_e n_q(j)\} + \sum_{k>i} \{F(k,i) n_e + A(k,i)\} n_q(k) + (Dc(i) + \alpha^r(i) + \alpha^{3B}(i) n_e) n_e n_{q+1}(1)$$

$$\Gamma_{out} = [S(i) n_e + S_{ai}(i) + \sum_{k>i} \{C(i,k) n_e\} + \sum_{j<i} \{F(i,j) n_e + A(i,j)\}] n_q(i)$$

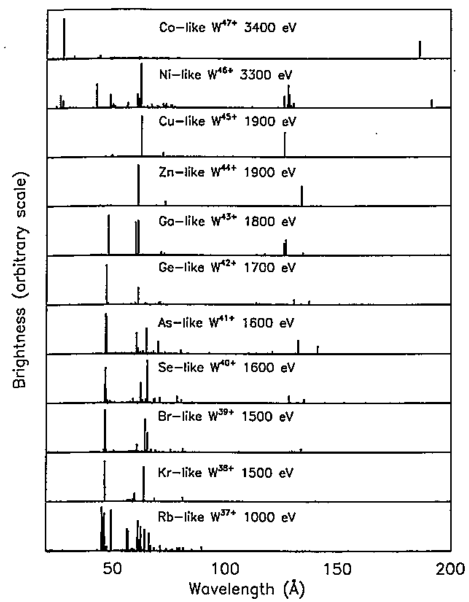
Earlier works on CR model for W ions

- Mandelbaum et al. Phys. Scr. 27, 39 (1983)
  - Co-like – Zn-like W (q=44-47) discrete lines, 3d-4p transitions, at 0.678-0.734nm
  - Laser produced plasma
  - CR model with atomic data calculated by Hullac code (Distorted wave). Energy levels up to n=4.
- Neu et al. J. Phys. B 30, 5057 (1997); Asmussen et al. Nucl. Fusion 38, 967 (1998); Fournier ADNDT 68, 1 (1998)
  - Wq+, q=37-47; 0.4-20nm, discrete lines
  - ASDEX Upgrade
  - CR model with atomic data calculated by Hullac code. Energy levels up to n=5.
- Pütterich et al. J. Phys. B 38, 3071 (2005)
  - Wq+ q=39-45; 4-14nm, 4s-4p transitions.
  - ASDEX Upgrade,
  - CR model in ADAS suite (Cowan code, plane-wave Born). Energy levels up to n=4.

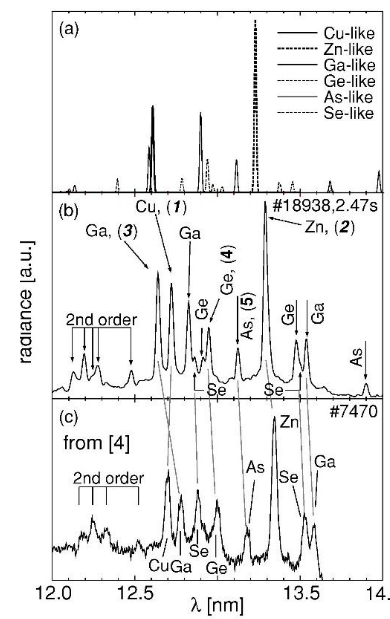


Neu (1997)

Fournier (1998)

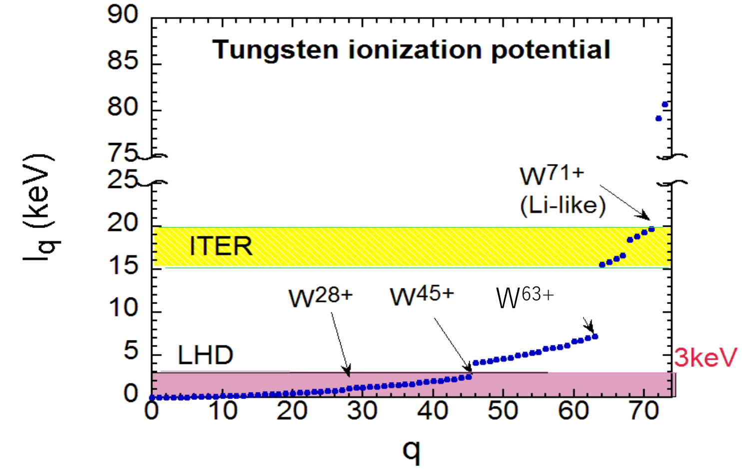


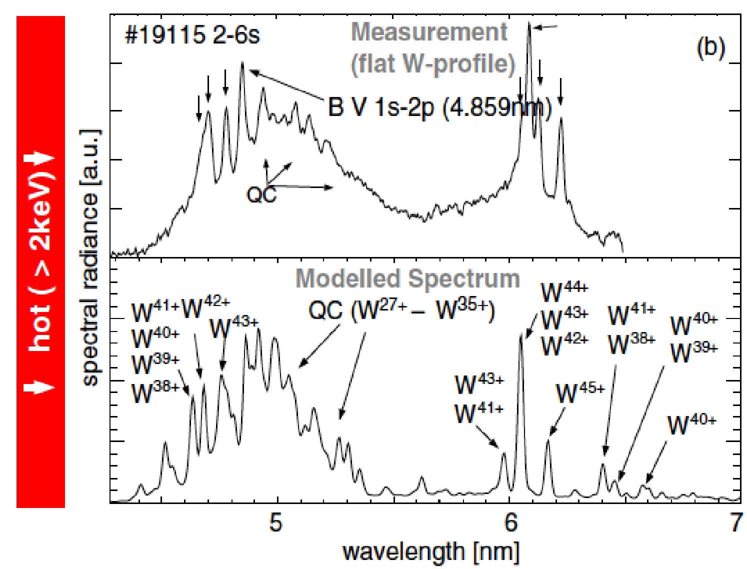
Pütterich et al. J. (2005)



3. W ions in core plasma with $T_e \gtrsim$ 2keV (1)

- W^{q+}; q≳38
  (q=38: Kr-like ($3d^{10}4s^2 4p^6$), Ip=1.829keV)
  (q=45: Cu-like ($3d^{10}4s$), Ip=2.414keV)
  (q=46: Ni-like ($3d^{10}$), Ip=4.057keV)
  (q=64: Ne-like ($2p^6$), Ip=15.566keV)
  (q=71: Li-like (2s), Ip=19.686keV)
- Spectral lines appear as discrete lines.
- M-shell ions have complex atomic structures and a large number of energy levels are to be treated. Nevertheless, conventional treatments and methods are possible for CR models and spectroscopic diagnostics.
- Line intensity ratios can be used for electron temperature or density diagnostics.





ASDEX Upgrade. Putterich et al. (2008)

3. W ions in core plasma with $T_e \gtrsim$ 2keV (2)

- Ralchenko et al. PRA 83, 032517 (2011)
  W XLVIII – W LVI (q=47-55), M1 lines at 10-20nm
  - ➢ Measurements with EBIT
  - ➢ CR model (NOMAD code) with atomic data calculated by FAC code (Distorted wave).
    Energy levels up to n=5 (open shell ion) or up to n=7 or 8 for closed-shell ions (single excitation). CX is considered.
  - ➢ Electron density diagnostics by M1 line ratios are predicted.

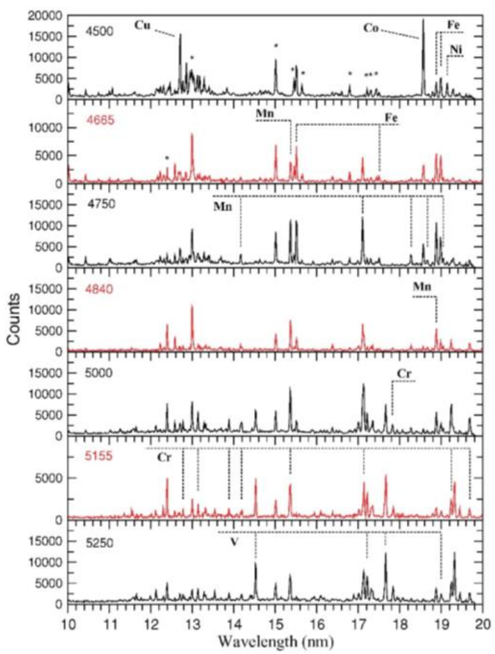


FIG. 1. (Color online) Tungsten spectra between 10 and 20 nm for beam energies between 4500 and 5250 eV. The identified transitions are indicated by vertical dashed lines. The spectra from run A are shown in black and the spectra from run B are shown in red (gray). Asterisks show the strongest impurity lines.

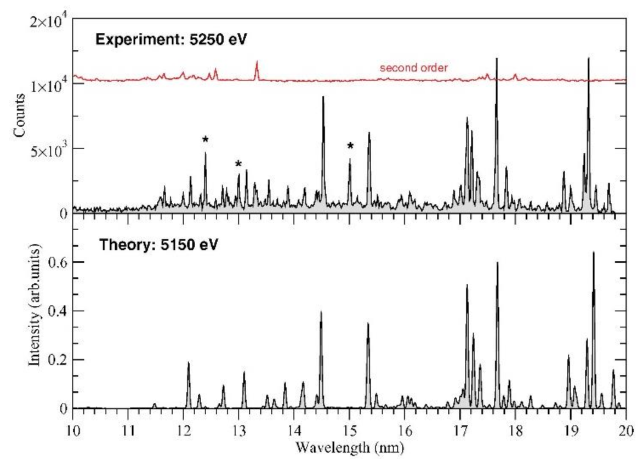


FIG. 3. (Color online) Comparison of experimental spectrum at the nominal beam energy of 5250 eV (top) and calculated spectrum at 5150 eV and $n_0 v_0 = 10^{14}$ cm^{-2}s^{-1} (bottom). The second-order spectrum is shown by the shifted line and the strongest impurity lines from Xe (12.4 and 13.0 nm) and O (15.0 nm) are indicated by asterisks.

Diagnostics with M1 liens

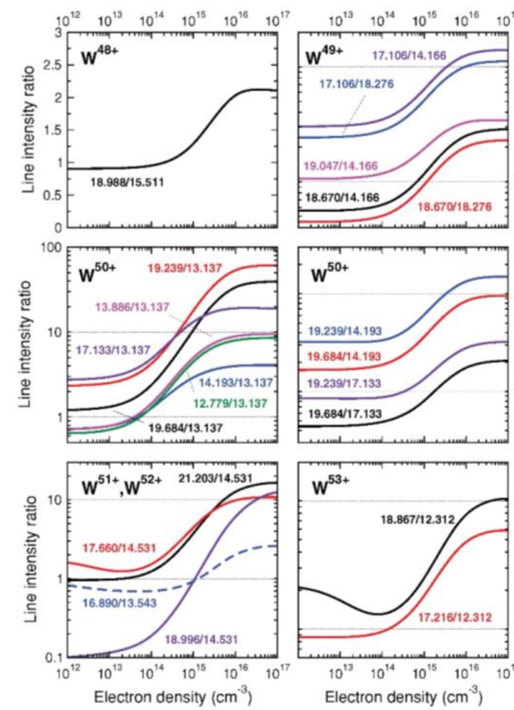
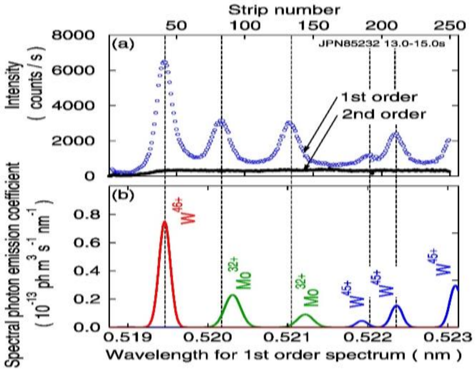


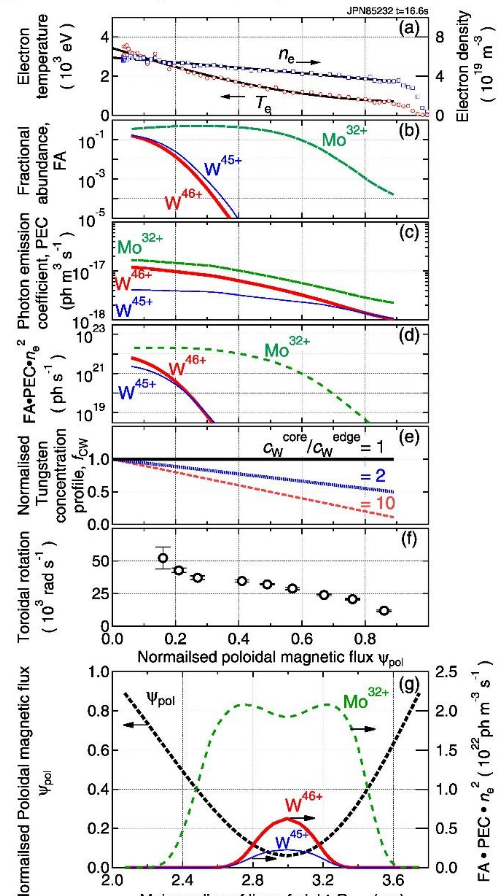
FIG. 6. (Color online) Density-sensitive line ratios for ions of tungsten from W^{48+} to W^{53+}.

3. W ions in core plasma with $T_e \gtrsim$ 2keV (3)

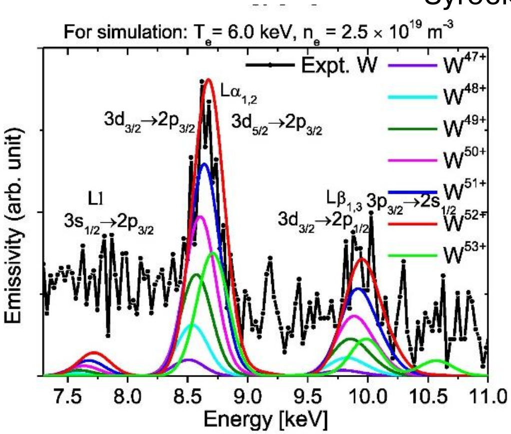
- Nakano et al. JPB 48, 144023 (2015)
  W45+, W46+ in JET-ILW, 0.51-0.53nm (~4keV)
  - ➢ CR model with atomic data calculated by FAC code
    Energy levels up to n=5 (single excitation)
  - ➢ W concentration is estimated in JET-ILW.
- Syrocki et al. Phys. Plasmas 31, 063303 (2024)
  - ➢ Wq+, q=47-53, Lα, Lβ lines (8.5-10.5keV)
    q=38-47 (1-5keV)
  - ➢ W7-X, soft x-ray pulse height analysis system
  - ➢ CR model with atomic data calculated by FAC code.

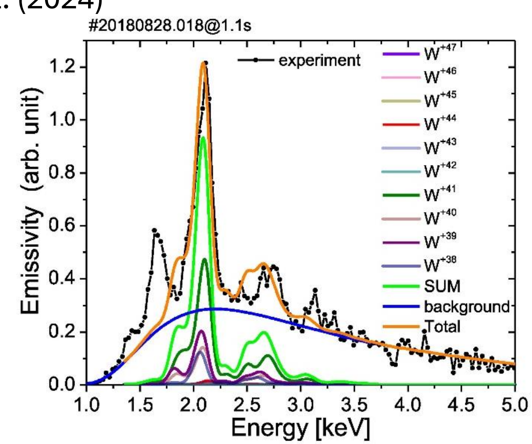


Nakano et al. (2015)



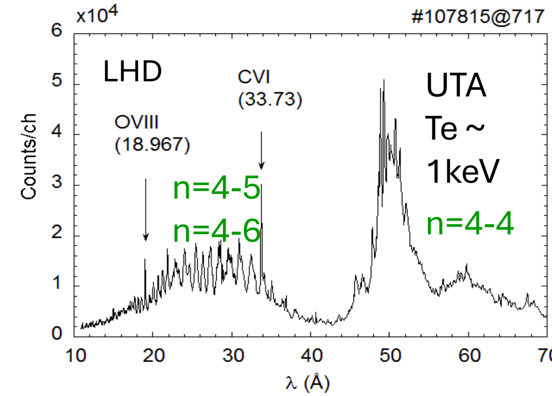
Syrock et al. (2024)



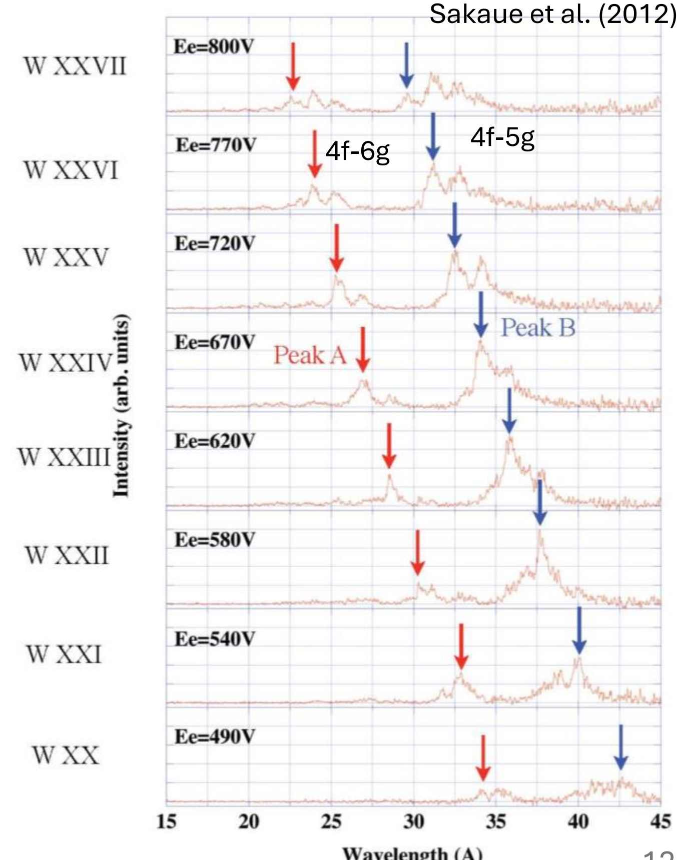


4. W ions in peripheral plasma with T_e~1- 2keV (1)

- W^{q+}; q~20-37
  (q=20: Xe-like ([Kr]$4d^{10}4f^6$, Ip=0.543keV)
  (q=28: Pd-like ([Kr]$4d^{10}$, Ip=1.132keV)
  (q=37: Rb-like ([Kr]4d, Ip=1.621keV)
- Complex atomic structures produce many transition lines.
- Open 4d and 4f shells produce UTA (n=4-4 (mainly 4d-4f) transition) which is not well reproduced by any CR model yet.
- Recombination processes need to be included.
- Prominent n=4-5 and n=4-6(4f-5g, 4f-6g transition for q<27) peaks (narrow UTAs) appear at 2-4nm. These peaks can be used for identifying charge states. Such identification is confirmed by EBIT experiments and CR model calculations (Sakaue et al. 2012).

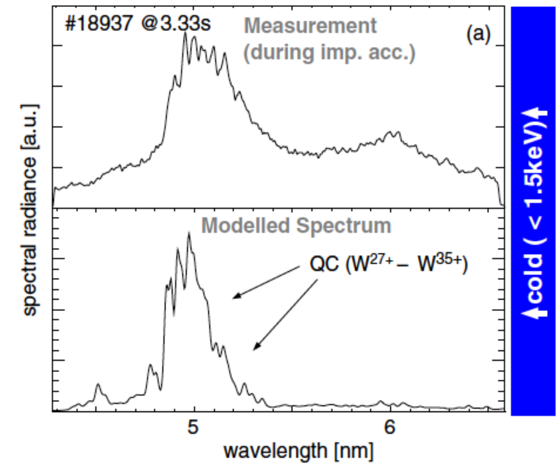


Sakaue et al. (2012)

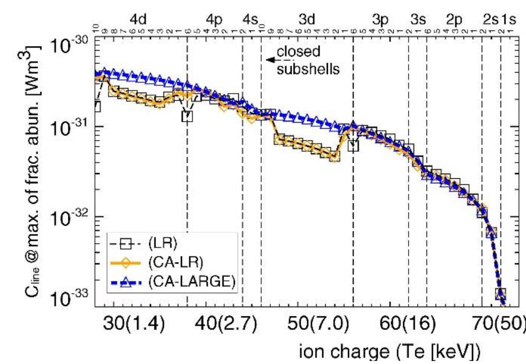


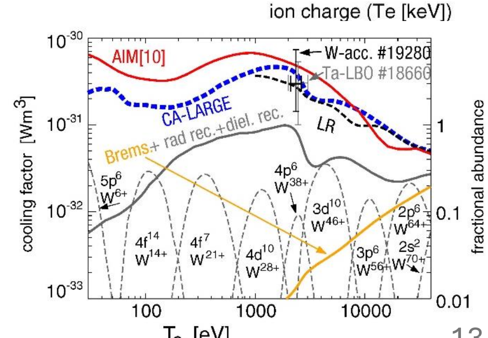
4. W ions in peripheral plasma with T_e~1- 2keV (1)

- Pütterich et al. Plasma Phys. Control Fusion 50, 085016 (2008)
  - W^{q+}: q=20-46, 0.4-0.8nm (q=39-49), 4.3-7nm, 12-14nm
  - ASDEX-Upgrade
  - CR model in ADAS suite
  - Prediction of spectrum for ITER
- Pütterich et al. Nucl. Fusion 50, 025012 (2010)
  - q=27-48, Ionization equilibrium. ADAS suites.
  - Level-resolved (LR) and configuration-averaged (CA) CR models to obtain cooling function.
- Pütterich et al. AIP Conf. Proc. 1545, 132 (2013)
  - W23+, CR model with atomic data from FAC code. Energy levels up to n=5. 10,934 levels.
  - ASDEX-Upgrade

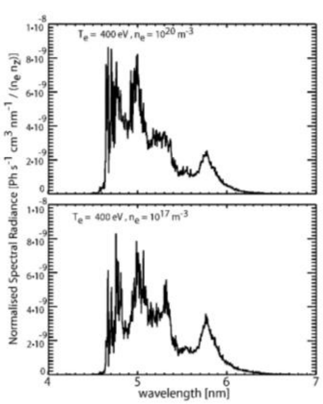


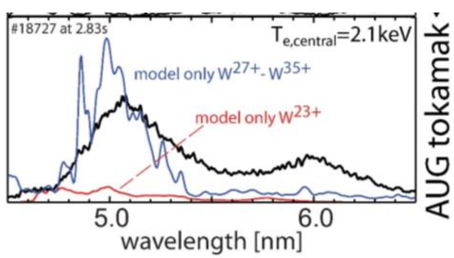
ASDEX Upgrade. Pütterich et al. (2008)



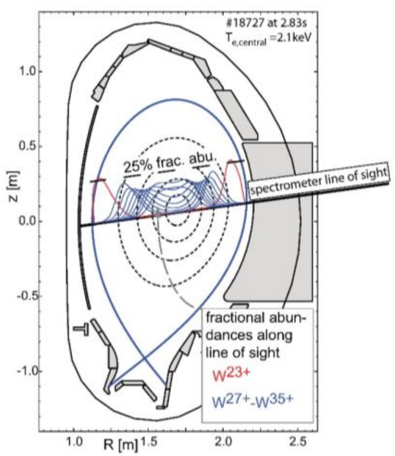


Pütterich et al. (2010)





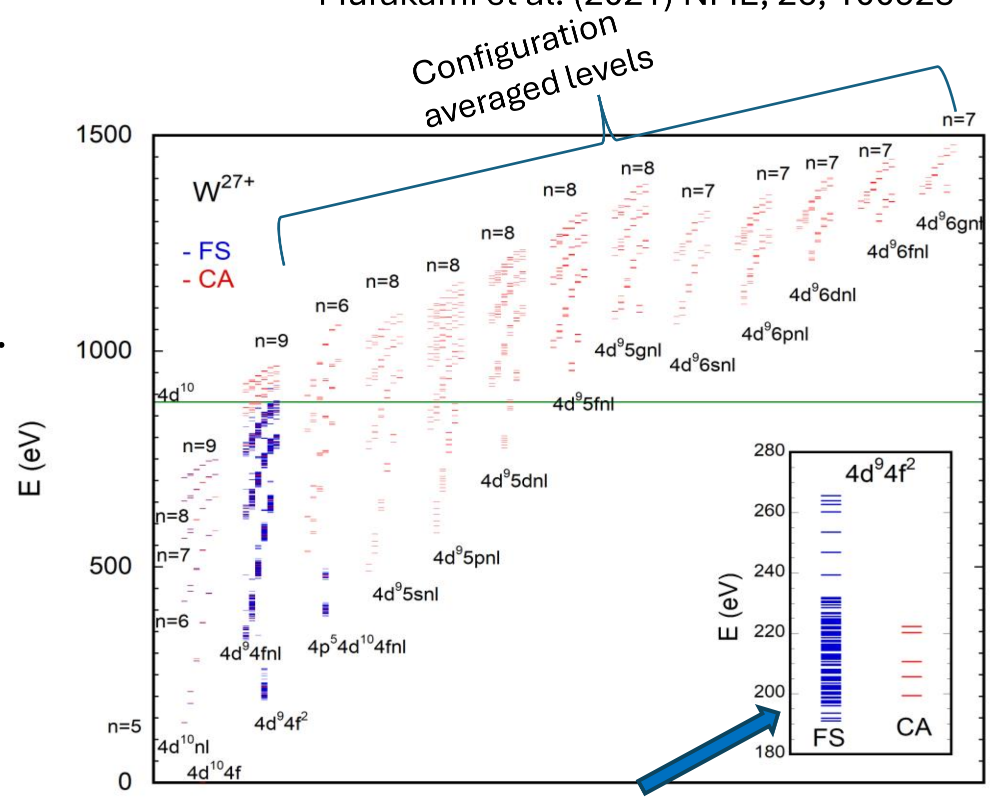
Pütterich et al. (2013)



4. W ions in peripheral plasma with T_e~1- 2keV (2)

- In order to reproduce UTA at 4.5-7nm, we need to examine the contribution from highly excited states.
- We consider **J-resolved fine-structure (FS) levels** for lower states and relativistic **configuration-averaged (CA) levels** for higher states. Total number of energy levels are largely reduced.
- Dielectronic recombination process is included implicitly as a dielectronic capture to autoionizing states and following radiative decay.
- All atomic data needed for the CR model are calculated with **HULLAC atomic code.**
- W^{25+} ~ W^{39+} ions were examined by Murakami et al. (2021) and the CR model extends to W^{24+} - W^{20+} ions (Murakami et al. IAEA TM 2023).

Murakami et al. (2021) NME, 26, 100923



3,201 levels

108 FS levels

1,359 relativistic configurations

6 relativistic CA levels

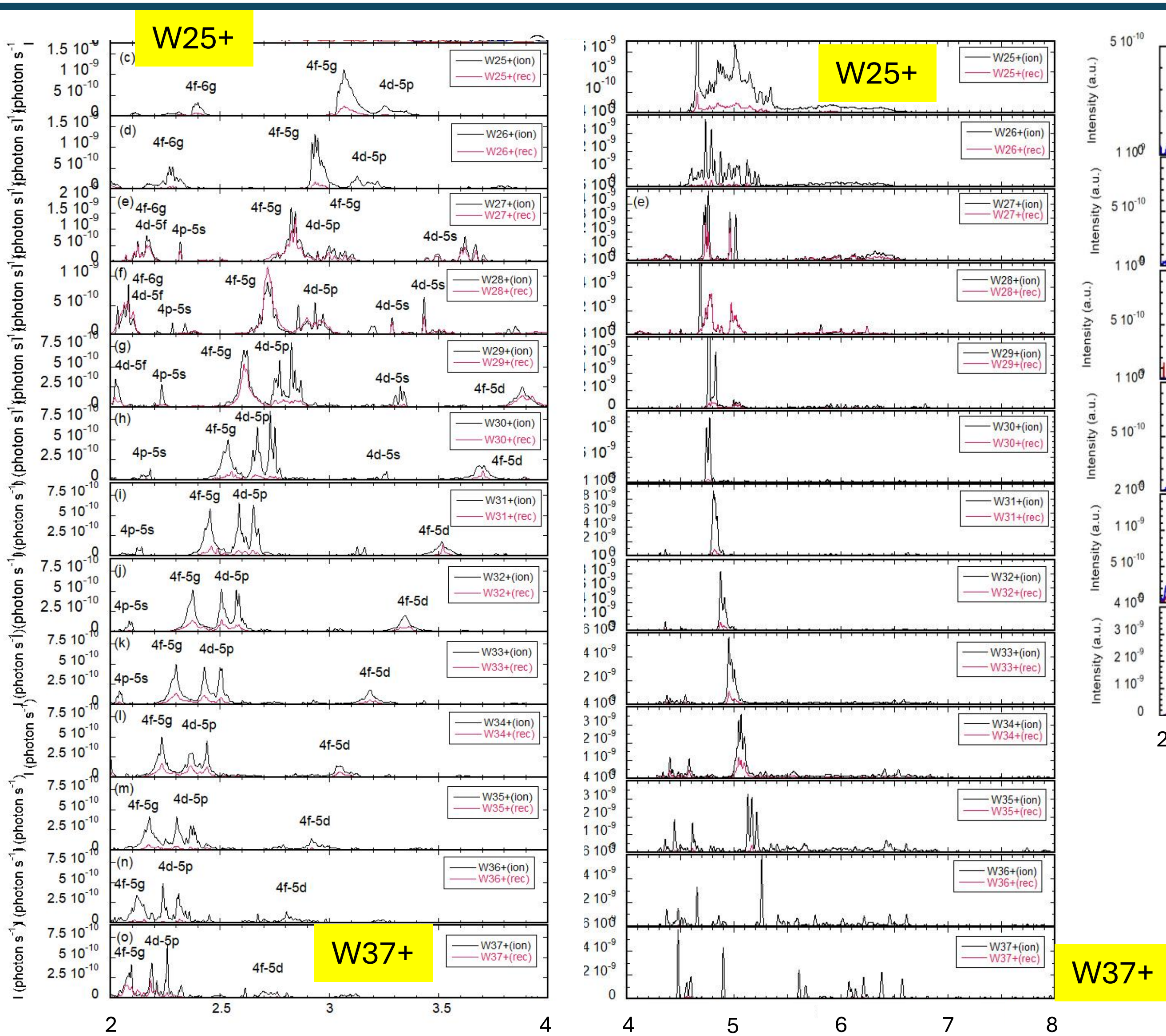
$(4d+)^5(4d-)^4(4f+)^2$
$(4d+)^5(4d-)^4(4f+)(4f-)$
$(4d+)^5(4d-)^4(4f-)^2$
$(4d+)^6(4d-)^3(4f+)^2$
$(4d+)^6(4d-)^3(4f+)(4f-)$
$(4d+)^6(4d-)^3(4f-)^2$

W^{27+} ion :

FS levels: $4d^{10}$ 4f, $4d^{10}$ *nl* (*n*=5-9, *l*=0-5), $4d^9$ $4f^2$, $4d^9$ 4f *nl* (*n*=5-7, *l*=0-5), $4p^5$ $4d^{10}$ $4f^2$,

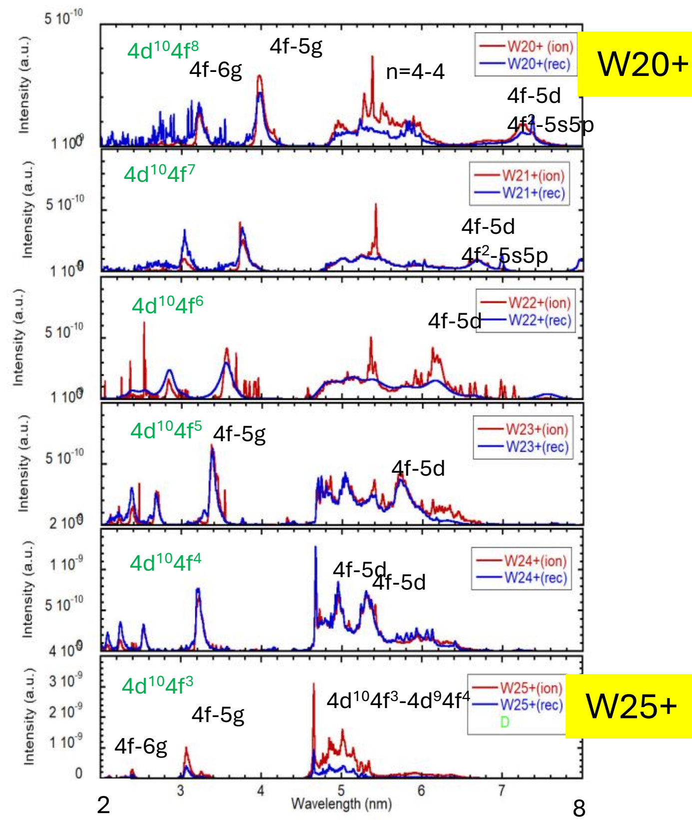
CA levels: $4d^9$ 4f *nl* (*n*=8-9, *l*=0-5), $4p^5$ $4d^{10}$ 4f *nl* (*n*=5-6, *l*=0-5), $4d^9 5l$ *nl* (*n*=5-8, *l*=0-5), $4d^9$ 6*l* *nl* (*n*=6-7, *l*=0-5)

4. W ions in peripheral plasma with T_e~1- 2keV (3)



Murakami et al. (2021)

T_e=1kev, n_e=10^{13}cm^{-3}

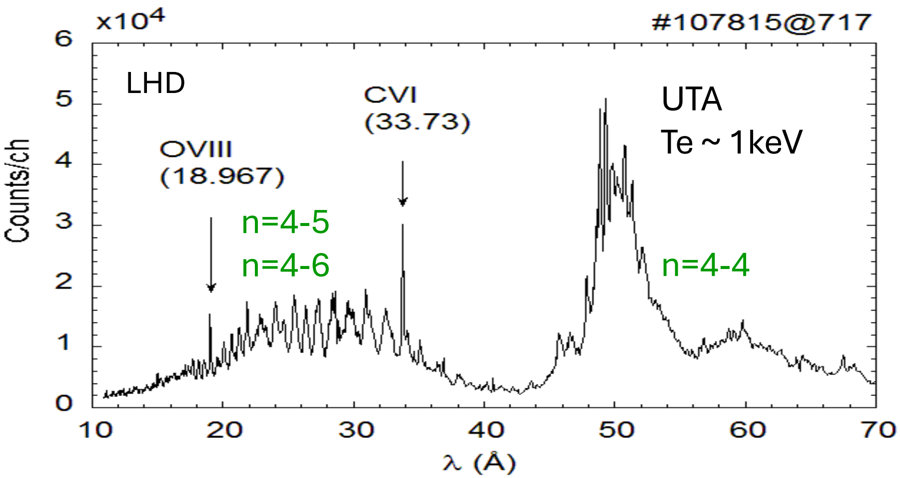


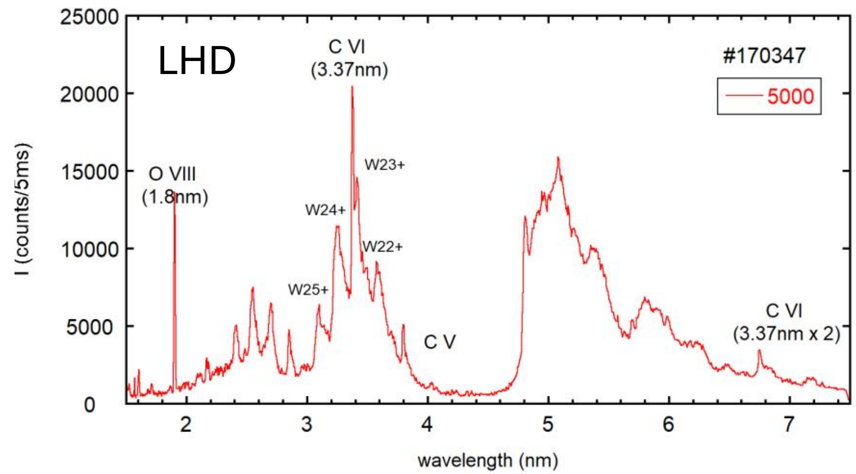
T_e=0.7kev, n_e=10^{13}cm^{-3}

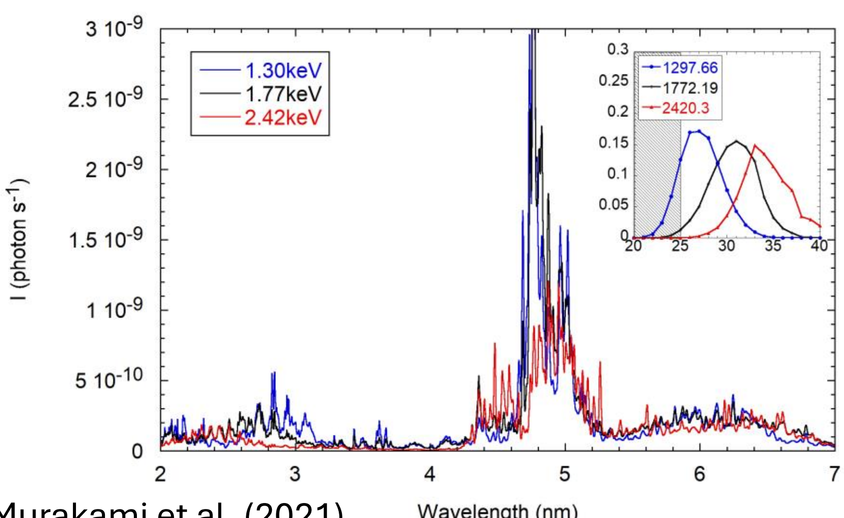
Murakami et al. (2023)

4. W ions in peripheral plasma with T_e~1- 2keV (4)

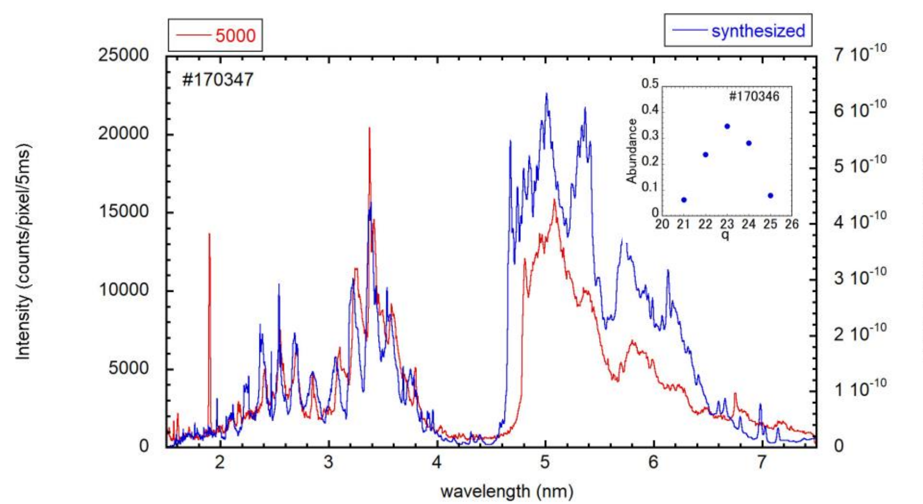
- Synthesized spectra look closer to the measured ones than before, but some discrepancies remain.







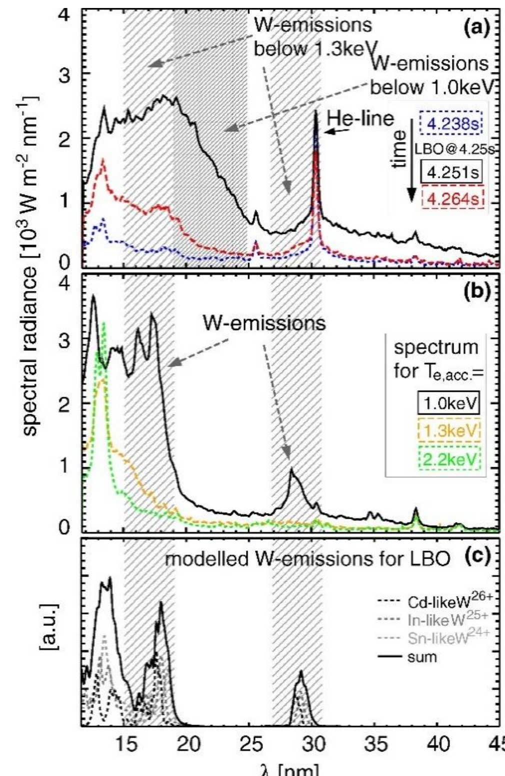
Murakami et al. (2021)



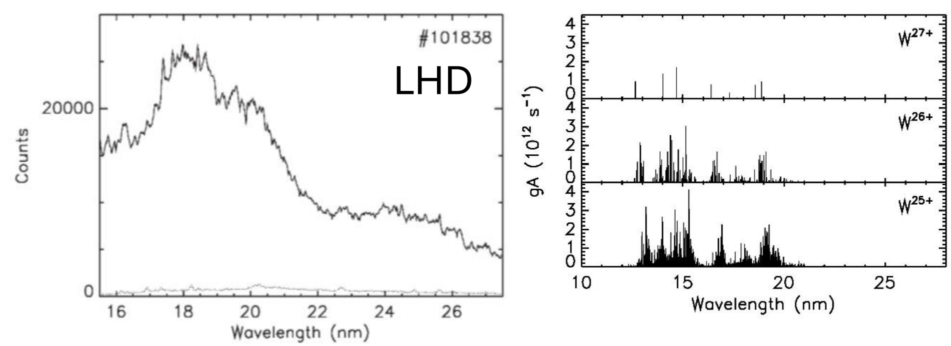
Murakami et al. (2023, IAEA TM)

5. W ions in edge plasma with T_e<1keV (1)

- W^{q+}; q~6-25
  (q=25: In-like ([Kr]$4d^{10}4f^3$, Ip=0.784keV)
  (q=17: La-like ([Kr]$4d^{10}4f^{11}$, Ip=0.421keV)
  (q=16: Ce-like ([Kr]$4d^{10}4f^{11}5s$, Ip=0.388keV)
  (q=15: Pr-like ([Cd]$4f^{11}$, Ip=0.361keV)
  (q=12: Sm-like ([Cd]$4f^{14}$, Ip=0.258keV)
  (q=8: Dy-like ([Cd]$4f^{14}5p^4$, Ip=0.160keV)
  (q=6: Er-like ([Xe]$4f^{14}$, Ip=0.122keV)
- Complex atomic structure.
- CR models are studied for a few of them.
- UTA / quasi-continuum due to n=5-5 transition appears at 15-30nm.
- Careful examination is required to identify the charge state of lines measured in EBIT due to complex ionization processes such as excitation-autoionization process.



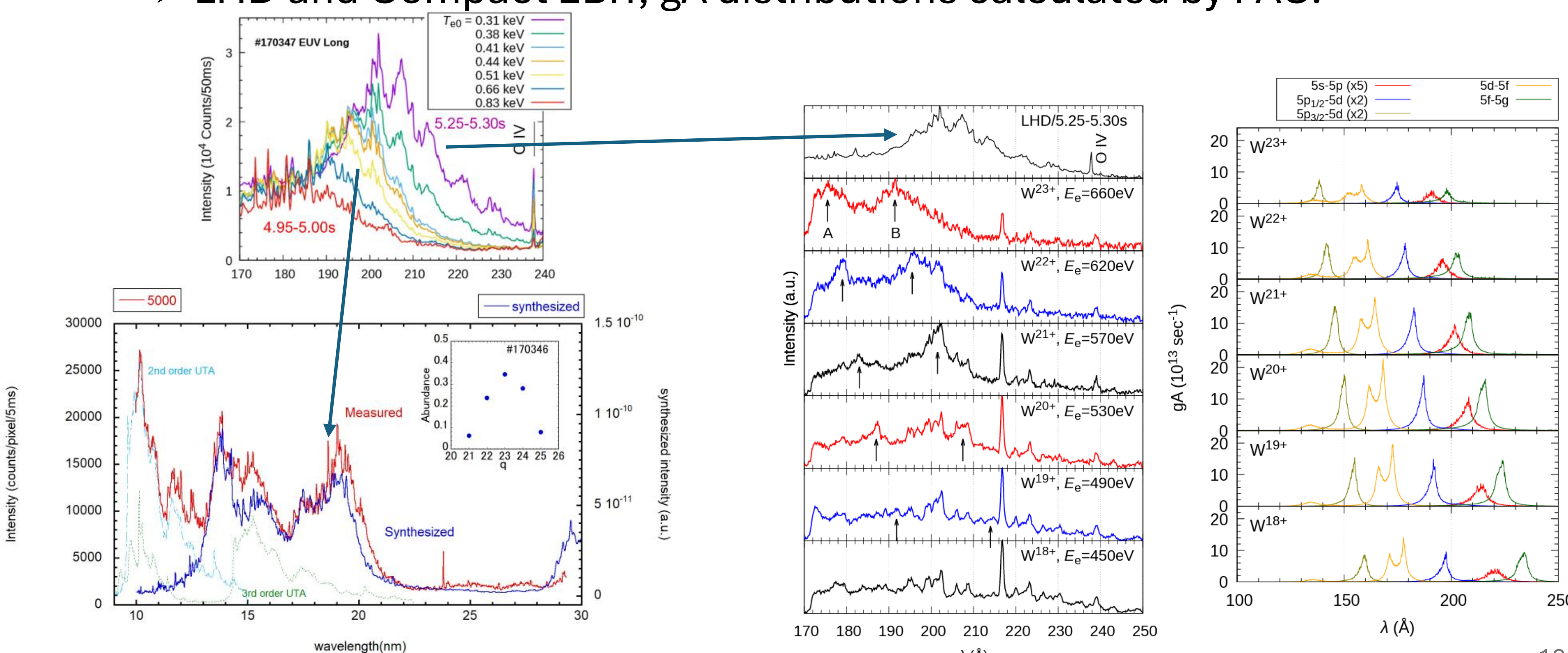
Pütterich et al. (2008)



Suzuki et al. (2011)

5. W ions in edge plasma with T_e<1keV (2)

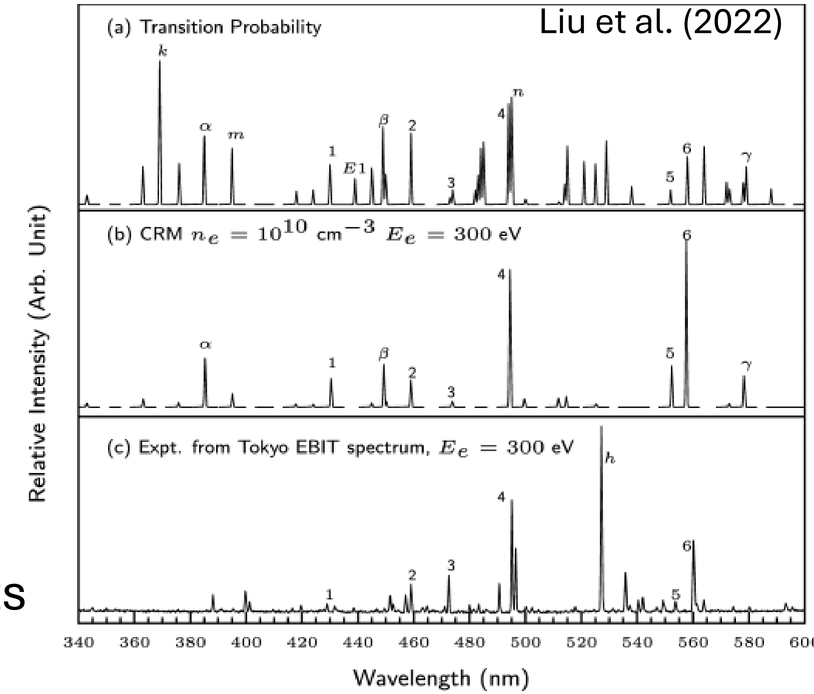
- Murakami et al. (IAEA TM 2023)
  - ➢ W^{q+} q=21-25, EUV 10-30nm measured in LHD. UTA (n=5-5)
  - ➢ CR model with atomic data calculated by HULLAC. Recombination processes are included.
- Nishimura et al. Plasma Fusion Res. 19, 1402022 (2024)
  - ➢ W^{q+}, q=18-23, EUV (~20nm)
  - ➢ LHD and Compact EBIT, gA distributions calculated by FAC.



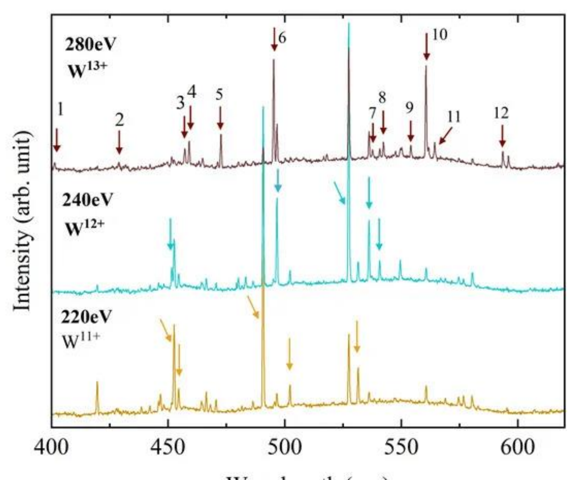
Murakami et al. (2023, IAEA TM) Nishimura et al. (2024)

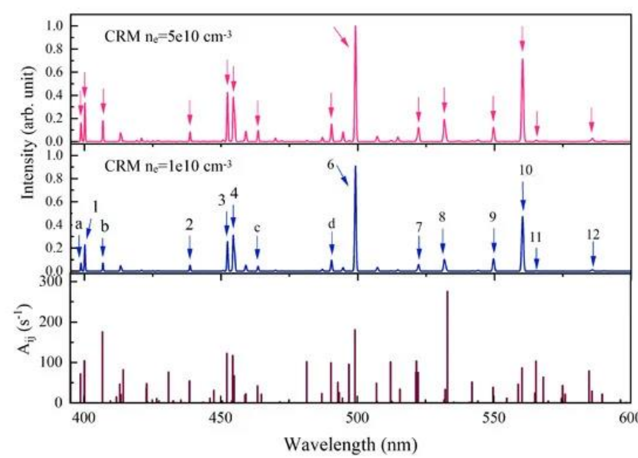
5. W ions in edge plasma with T_e<1keV (3)

- Liu et al., Physics Lett. A 454, 128500 (2022)
  - W13+, visible M1 lines, EBIT experiments
  - CR model with atomic data calculated by FAC. Energy levels up to n=7.
- Priti et al., Atoms 11, 57 (2023)
  - W13+, visible lines, EBIT experiments
  - CR model with atomic data calculated by GASP2018 and FAC. Energy levels up to n=5.



Liu et al. (2022)

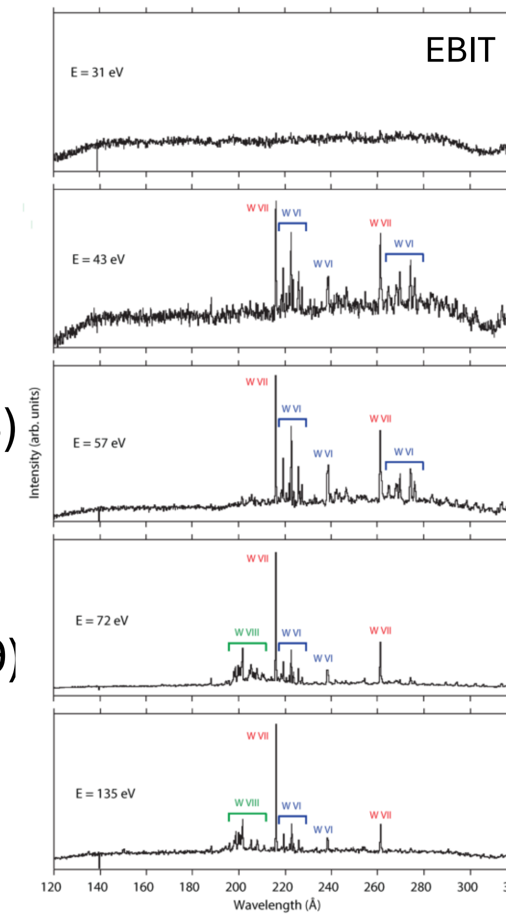


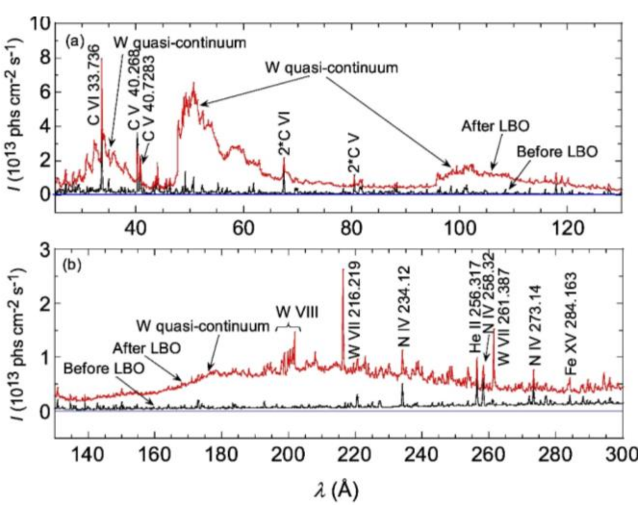


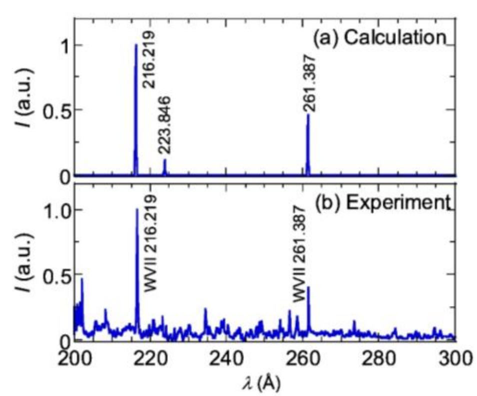
Priti et al. (2023)

6. W ions in divertor plasma with T_e<0.1keV (1)

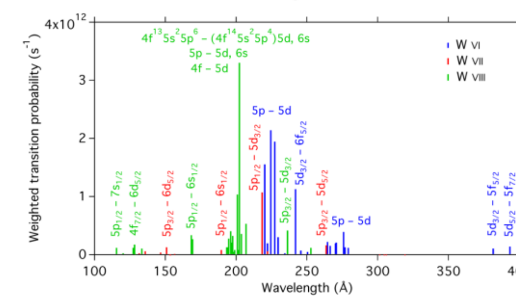
- W^{q+}; q~0-7
  (q=7: Dy-like ([Cd]$4f^{13}$, Ip=0.141keV)
  (q=6: Er-like ([Xe]$4f^{14}$, Ip=0.122keV)
  (q=0: neutral ([Xe]$4f^{14}5d^{4}6s^{2}$, Ip=0.0078keV)
- Measurements in EUV, VUV and visible region.
  q=0: 400.0875nm
  q=1: JET (van Rooij et al., J. Nucl. Mater. 438, S42 (2013)
  q=3-7: JET (Lawson et al., Phys. Scr. 97, 055605 (2022))
  q=5-7: EBIT(LLNL) (Clementson et al., Atoms 3, 407 (2015)
  q=6: HL-2A (Dong et al., Nucl. Fusion 59, 016020 (2019)
- CR model should be studied.







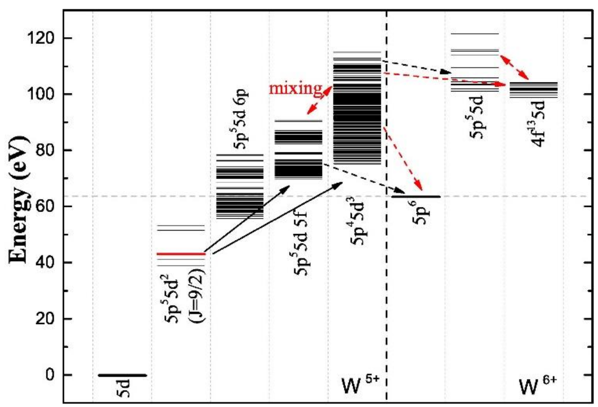
Dong et al. (2019)

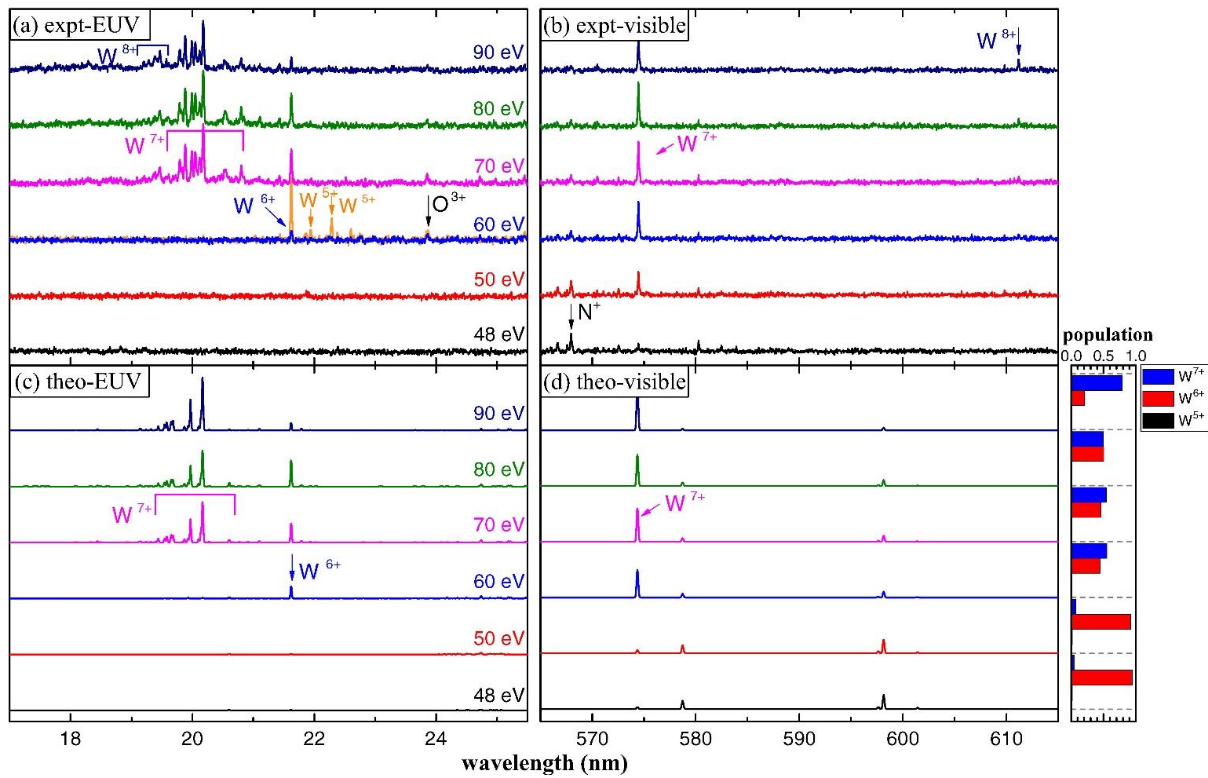


Clementson et al. (2015)

6. W ions in divertor plasma with T_e<0.1keV (2)

- Yan et al. (Phys. Rev. A 105, 032820 (2022))
  - Wq+, q=5-7
  - EBIT measurements, 18-25nm, 565-615nm
  - Multicharge-state CR model with atomic data calculated with FAC. CX and DI+EA processes are included.





7. Summary

- Atomic data and CR models for all tungsten ions are necessary to understand tungsten behavior in fusion plasma for spectroscopic diagnostics and plasma simulation. Radiation power is obtained from CR models.
- Many atomic data are missing. We need a better method to calculate low-charged W ions with complex atomic structures.
- Proton-impact excitation cross sections and charge exchange cross sections for collision of neutral H and W ions are mostly missing.
- Experimental evaluation of atomic data and CR models is important and necessary to improve CR models.