Configuration-Average Collisional-Radiative calculations, Ionization and Emission of low-density tungsten plasmas in the temperature range [800-5000] eV

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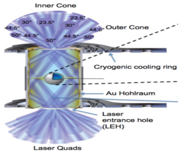
Radiative emission from more or less hot high-Z plasmas

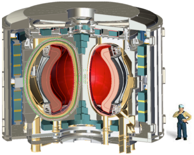
Inertial Confinement Fusion (indirect drive)

Gold ($Z = 79$) Hohlraums



Need to optimize the X-ray conversion efficiency (from laser-matter interaction)

Magnetic Confinement Fusion



Tungsten ($Z = 74$) inner-walls in tokamaks.

Sputtering $\Rightarrow$ **pollution**

Need to minimize the X-ray emission in the core, to maximize in the edge (cooling)

Atomic physics of more or less hot high-Z plasmas

Dense Plasmas

- Collisions may thermalize groups of levels ⇒ partial LTE within configs, SCs
- Excited levels significantly populated
- Highly excited levels not permitted due to Ionization Potential Depression

Diluted Plasmas

- Most of ions reside in ground levels
- Highly excited levels are permitted
- Excited levels populated by collision from the ground state and radiative cascade following resonant capture

Modeling of the radiative emission (high-Z plasmas)

⇒ **The needs :**

- Ionization Balance (or **C**harge **S**tate **D**istribution)
- Emissivity (if possible, consistent with the CSD, i.e. the same model) - Radiation Power Losses

⇒ **The difficulties :**

- Overwhelming number of levels
- Many overlapping spectral features
- *Completeness* difficult to reach for Collisional-Radiative calculations

Present work

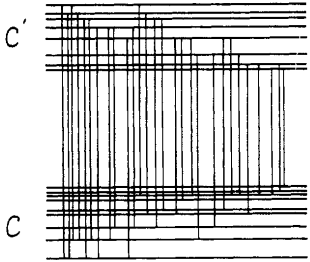
Calculations :

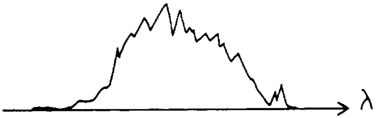
- Configuration average (CA) mode
- Unresolved Transition Arrays (UTA) and Spin-Orbit-Split Arrays (SOSA) formalism
- **No adjustment to the recombination rates**
- Full consistentcy between the CSD and the emissivity

Comparisons with some published EUV experimental spectra and some obtained on the WEST tokamak

Unresolved Transition Array : the strict definition

UTA : totality of lines between levels of 2 configurations





Defined by its

- **mean position** μ_1
- **variance** $\mu_2 - (\mu_1)^2$

$$\mu_n = \sum_{a,b} (E_b - E_a)^n \frac{W_{ab}}{W}$$

W_{ab} is the E1 strength

Compact formulae exist for μ_1 and μ_2, this is the UTA theory

When **Spin-Orbit** interaction is important, **a UTA may split into 2,3 structures : SOSA Theory**

Specificities of an Atomic model for tungsten in core tokamak conditions

For densities $N_e \sim 10^{13}$ **cm**$^{-3}$ (core)

- Populations of excited configurations are weak (majority of ions resides in the ground state)
- A superconfiguration represents too large an energy range
- No more effective SC temperatures

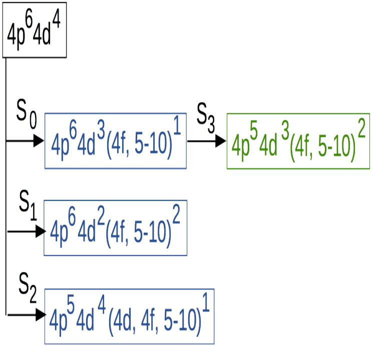
For high-Z

- Multiply-excited states above thresholds form resonances for electron capture

$\Rightarrow$ A large set of **configurations** is necessary

List : promotional strategy adopted here

Example of the ion W^{34+} (Zr-like : 40 electrons)



S$_0$: one-electron excitation from the last occupied subshell
S$_1$: excitation of a second elec. from the last occupied subshell
S$_2$: excitation of one elec. from the second last occupied subshell
S$_3$: after S_0, excitation of one elec. from the second last occupied subshell.

promotional strategy adopted here

for selecting configurations ...

4 steps ; example of the Zr-like ion (40 electrons)

S0 :

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^6\ 4d^4$

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^6\ 4d^3\ 4f$

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^6\ 4d^3\ (5\text{-}10)^1$

47 configurations

S2 :

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^5\ 4d^5$

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^5\ 4d^4\ 4f$

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^5\ 4d^4\ (5\text{-}10)^1$

47 configurations

S1 :

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^6\ 4d^2\ 4f^2$

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^6\ 4d^2\ 4f\ (5\text{-}10)^1$

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^6\ 4d^2\ (5\text{-}10)^2$

1081 configurations

S3 :

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^5\ 4d^3\ 4f^2$

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^5\ 4d^3\ 4f\ (5\text{-}10)^1$

$(1)^2\ (2)^8\ (3)^{18}\ 4s^2\ 4p^5\ 4d^3\ (5\text{-}10)^2$

1081 configurations

$\Rightarrow$ **2256 configurations in this ion stage**

$\sim$ **40 000 rate equations (all populated ion stages)**

Steady-state Collisional-Radiative Model

Configuration Average **rate equation system**

$$\sum_{z',c'} N_{c'}^{(z')} T(z',c' \rightarrow z,c) - \sum_{z',c'} N_{c}^{(z)} T(z,c \rightarrow z',c') = 0$$

$$T(z,c \rightarrow z',c') = \sum_{process} \sum_{i \in c} \sum_{j \in c'} \frac{g_i}{g_c} T^{process}(z,i \rightarrow z',j)$$

$T^{process}(z,i \rightarrow z',j)$ is a configuration average rate

Processes included

- radiative deexcitation
- collisional excitation/deexcitation
- radiative recombination
- collisional ionization
- autoionization/resonant capture

Configuration-Average rates

Properly configuration averaged rates or cross sections contain an orbital dependent part and an occupation number dependent part

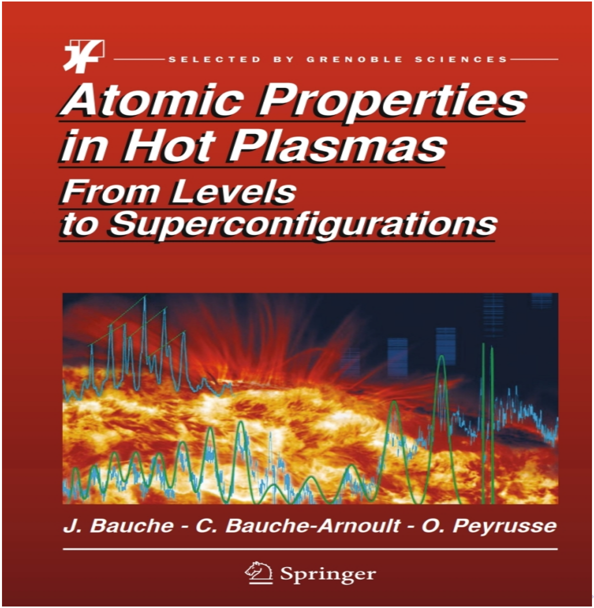
(Peyrusse, J. Phys. B (1999) ; Bauche & Peyrusse, Springer 2015)

e.g. consider the collisional strength of the jump $\alpha \rightarrow \beta$ e.g. $1s \rightarrow 2p$ between $1s^2 2s^2$ and $1s2s^2 2p$

$$\Omega^{\alpha\beta}_{C-C'} = n_\alpha (g_\beta - n_\beta) \Omega^{\alpha\beta} \text{ here } n_\alpha = 2, n_\beta = 0$$

- The part (...) is factorized out
- Methods used for calculating the radial part
  - **Distorted-Wave** for collisional excitation, ionization, autoionization
  - **Dipolar approx.** for radiative deexcitation

UTA/SOSA fomulas, CA rates, ...



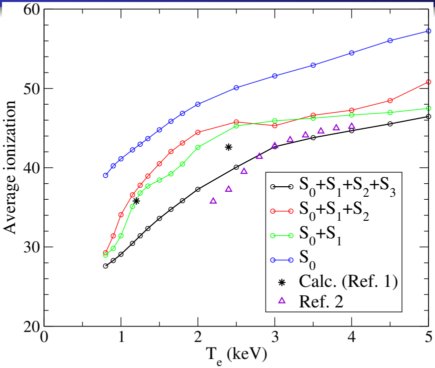
Other characteristics ...

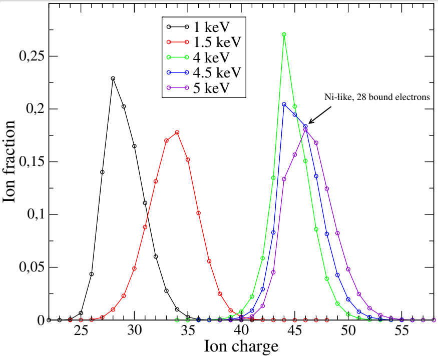
- Non-relativistic Atomic Structure, but relativistic corrections are included in the calculation of the radial orbitals (*cf* Cowan's book).
- Hartree-Fock-Slater calculations
  $v_x = -3\alpha(\frac{3}{8\pi})\ \rho^{1/3}$ with $\alpha = 0.78$
- Emissivity consistent with the full set of populations $\{N_c^{(z)}\}$
- **No adjustment to the recombination rates**

To summarize, the idea is here to

- approach *completeness*
- build a proper broadband spectrum with many UTA/SOSA structures

Results of Collisional-Radiative Modeling





→ Huge effect of Step 3

importance of configs.

$(3)^{18}$ $(4)^{10}$ $(7\text{-}10)^{2}$ (i.e. Zr-like)

same for other ions

(S0+S1+S2+S3)

Ref. 1 Colgan, *Atoms* 2015

Ref. 2 Pütterich, *PPCF* 2008

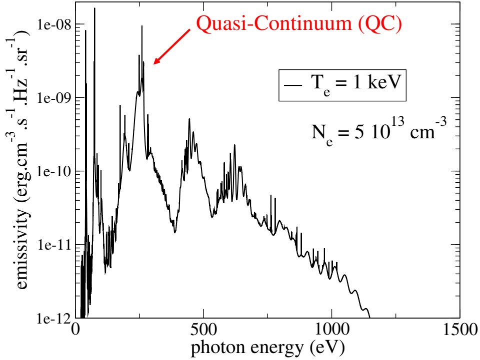
⇒ **Promotion of 2 elec. from 4p, 4d, 4f to all subshells with n=5-10 seems to play an important role**

Calculated spectra ; UTA/SOSA formalism

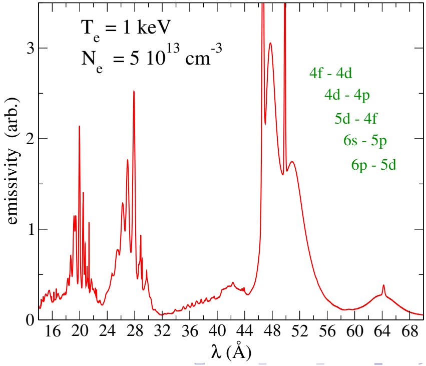
$N_e = 5\ 10^{13}\ \mathrm{cm}^{-3}$

$$j(\nu) = \sum_{c,c'} \frac{h\tilde{\nu}}{4\pi} A_{cc'} N_c^{(z)} \phi_{cc'}(\nu)$$

Total W emissivity



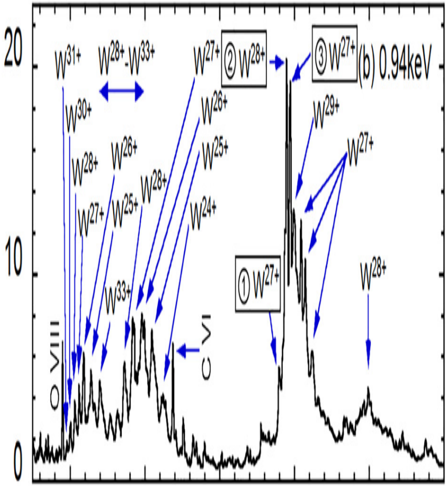
EUV emissivity



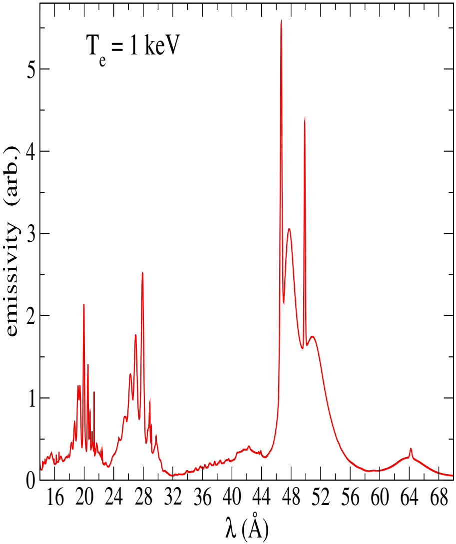
Calculated spectra ; UTA/SOSA formalism

Comparison with LHD spectra, Liu *et al* JAP **122**, 233301 (2017)

EUV emissivity (exp. LHD)

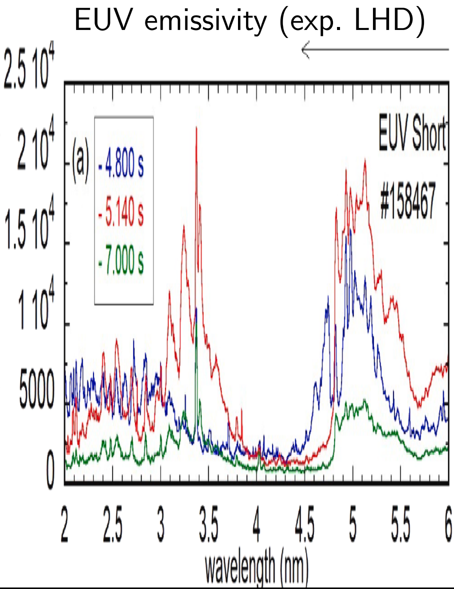


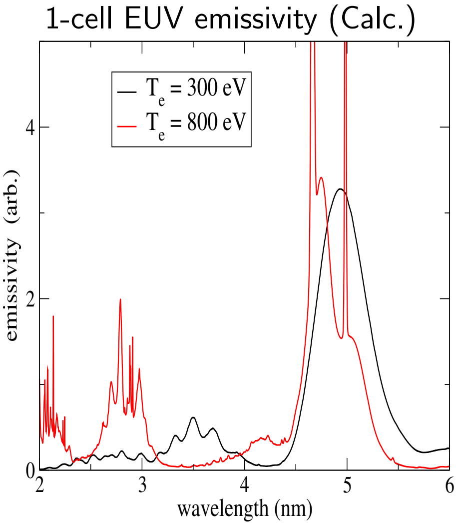
1-cell EUV emissivity (Calc.)



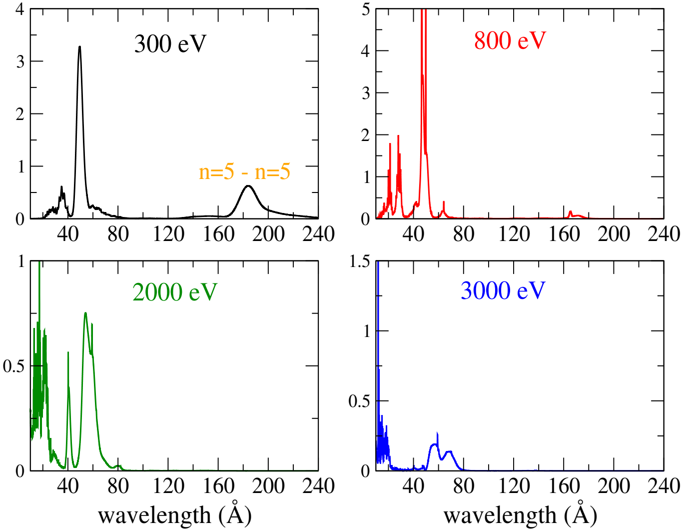
Calculated spectra ; UTA/SOSA formalism

Comparison with LHD spectra, Murakami *et al*, NME **26**, 100923, (2021)



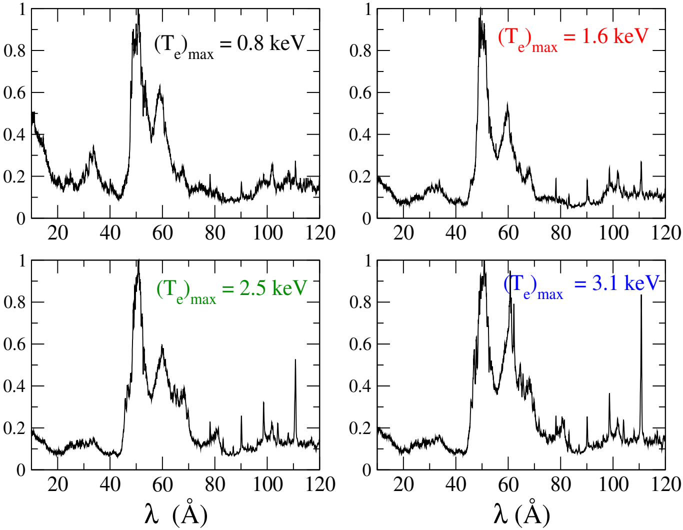


Calculations : QC ($\sim$ 50 Å) disappears above 2 keV



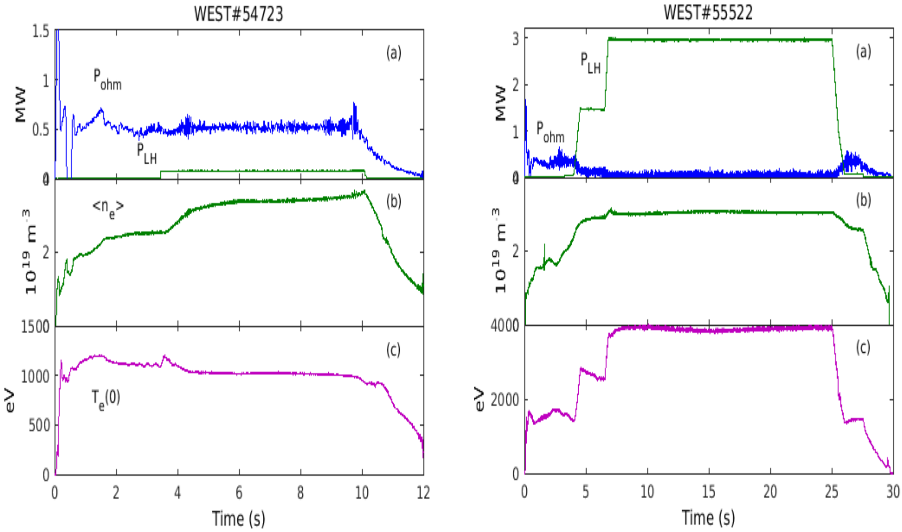
Recent WEST experimental EUV spectra

Line of Sight integration reflects lower Temperature in the QC region



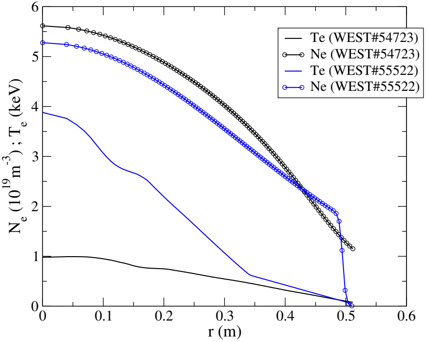
⇒ **Need to take the LOS for modeling**

WEST experiments (an older campaign)

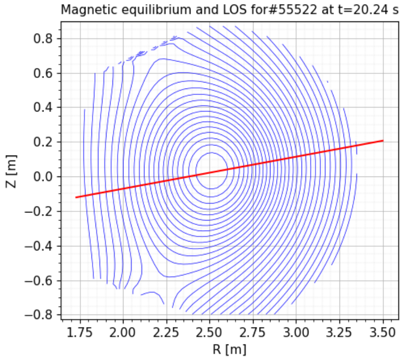


WEST experiments

Radial profiles

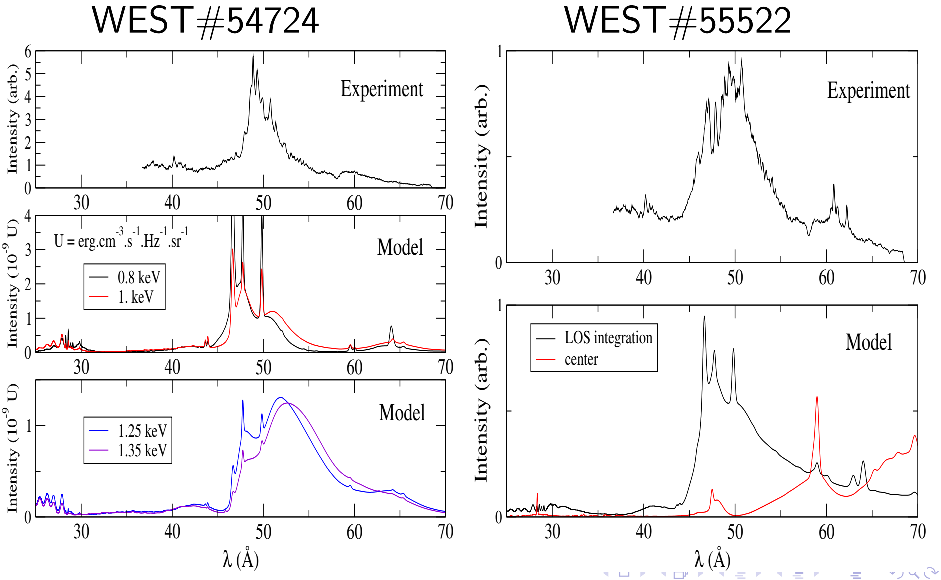


Line of Sight



Comparison modeling-experiments

Quasi-Continuum (QC) region ; Boumendjel *et al*, Phys. Plasmas **30**, (2023)



Conclusion

- Importance of the configuration list
- No need to modify the recombination rates (*cf* OPEN-ADAS project 1995-2016 ; T. Pütterich *et al*, PPCF **50**, 085016 (2008))
- UTA/SOSA formalism allows to recover most of the QC emission
- Difficulty to reproduce individual line emission between simple configurations (e.g. $4d^9$ 4f - $4d^{10}$)
- More generally, difficulty to account for $\Delta n = 0$ (n=4) transitions, strongly affected by CI
- **To be done** : an *hybrid* model mixing consistently fine-structure levels and configurations...

THANK YOU FOR YOUR ATTENTION !