Influence of Configuration Interaction on satellite lines and on emission of EUV plasmas

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Introduction

Configuration Interaction (CI) generates a strong narrowing and shift of the 4p / 4f – 4d group of lines.

We show the same effect on doubly excited configurations of Pd- to Rb-like ions of Xenon and Tin and the subsequent satellite lines. The emissivity and opacity are strongly enhanced at 13.5 nm for Tin. We also exhibit a big contribution of 6g–4f transitions and satellites of 5p-4f to the emission at 13.5 nm of Xenon.

We present a simple spherical autosimilar hydro-radiative model to evaluate EUV Conversion Efficiency (CE) of laser-produced plasmas.

We show that the CE at 13.5nm is doubled for Tin when Configuration Interaction (CI) is taken into account. The overall radiative losses reach more than 80% of the absorbed energy and cannot be omitted. Satellite lines of ions up to Sn^{18+} strongly contribute to EUV emission. EUV Conversion Efficiency can reach 10% for low energy, long laser pulses interacting with gaseous Tin.

Atomic physics and spectroscopy

Atomic data : levels and radiative rates, are computed with the HULLAC07 suite of codes, results are similar to those of high accuracy MCDF codes.

Configuration Interaction (CI)

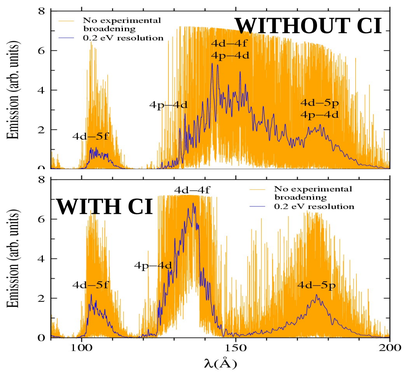
Configurations (ex : $4p^6\,4d^7\,5p$ = 5p) are composed of many levels with different J and M (ex : $|\,5p\,>_{JM}$).

Interaction between configurations close in energy generates mixing :

$$|\,A\,>_{JM} = a_1\,|\,4p\,>_{JM} + a_2\,|\,4f\,>_{JM} + a_3\,|\,5p\,>_{JM}$$

This strongly modifies transition rates (frequency redistribution) and changes emissivity and opacity

Detailed emission spectra of Sn 10+ calculated with and without Configuration Interaction. The main features come from 4p – 4d, 4f - 4d, 5p – 4d and 5f – 4d transitions. Mixing occurs mostly between 4p and 4f configurations. 5p-4d and 5f-4d transitions are less affected.



Result : Configuration Interaction in satellite lines enhances Tin emission at 13.5nm

Many groups of interacting configurations : (4p, 5p, 4f) ; (6p, 5f) ; (6d, 5g) ; (7p, 6f) ; (7d, 6g) ; (8p, 7f). Same groups for doubly excited configurations, ex : ($4p^2$, 4p 4f, $4f^2$ ...)

➡ 52 configurations interacting in each ion :

- Singly excited : ($4p^6\,4d^{N-1}$) 4f, 5s, 5p, 5d, 5f, 5g, 6s, 6p, 6d, 6f, 6g, 6h, 7s, 7p, 7d, 7f, 8s, 8p ; $4p^5\,4d^{N+1}$
- Doubly excited : $4p^4\,4d^{N+2}$; ($4p^5\,4d^N$) 4f, 5s, 5p, 5d, 5f, 6s, 6p ; ($4p^6\,4d^{N-2}\,5s$) 5s, 5p, 5d, 5f, 5g, 6s, 6p, 6d, 6f, 7s, 7p ; ($4p^6\,4d^{N-2}\,4f$) 4f, 5s, 5p, 5d, 6s, 6p ; ($4p^6\,4d^{N-2}\,5p$) 5p, 5d, 6s, 6p ; $4p^6\,4d^{N-2}\,5d^2$; ($4p^6\,4d^{N-2}\,6s$) 5f, 6p

Configuration Interaction shifts and narrows the group of satellite lines corresponding to doubly excited 4p/4f – 4d transitions. They superimpose and dominate resonant 4p/4f - 4d lines.

Synthetic emission of isolated Tin ions with and without Configuration Interaction.

Satellite lines issued from doubly excited configurations are included.

30eV, 10^{20} at/cc, 1µm long plasma

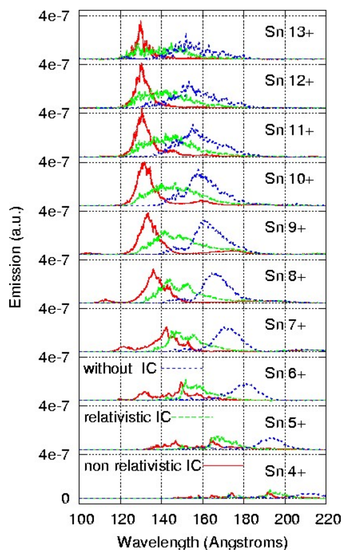
---- no Configuration Interaction

---- only relativistic CI

---- full CI (relativistic and non relativistic)

Relativistic CI, ex : 4p_1/2 + 4p_3/2

Full CI (relativistic + non relativistic), ex : 4p + 4f = 4p_1/2 + 4p_3/2 + 4f_5/2 + 4f_7/2



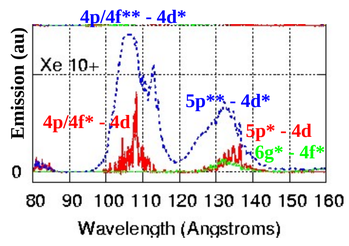
Result : 5g – 4f and doubly excited 5p – 4d transitions enhance Xe emission at 13.5 nm

At low density, EUV emission of Xenon at 13.5nm corresponds to 5p – 4d transitions of Xe^{10+}. When density increases, more excited configurations become populated.

6g – 4f transitions of Xe^{10+} also strongly contribute to the emission at 13.5nm (to a lesser extent, 6g – 4f of Xe^{9+} and 5g – 4f of Xe^{11+}).

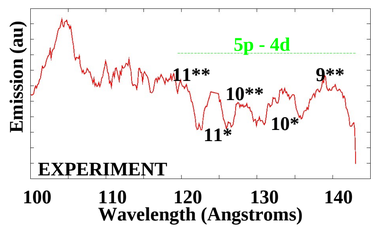
5p – 4d satellite transitions (doubly excited configurations decaying to singly excited) of Xe^{10+} (and also of Xe^{9+}) give the main contribution to the emission at 13.5nm at high density. Configuration Interaction has little influence.

Synthetic emission spectra of Xe 10+ (with CI) showing the various components of the emitting structures. 5p - 4d resonant, but also 6g* - 4f* and 5p** - 4d* satellite transitions contribute to the emission at 13.5 nm.*



At high densities, very excited N-time-ionized atoms behave like simply excited N+1/2-time-ionized atoms. This explains for misunderstood features appearing when density increases between well-known resonant 5p-4d group of lines of each ion.

*Experimental spectra : laser – droplets of Xenon interaction [Gilleron et al]. Density is approximately 10^{20} at/cc. The structures labelled ** come from doubly very excited configurations decaying through 5p – 4d transitions.*



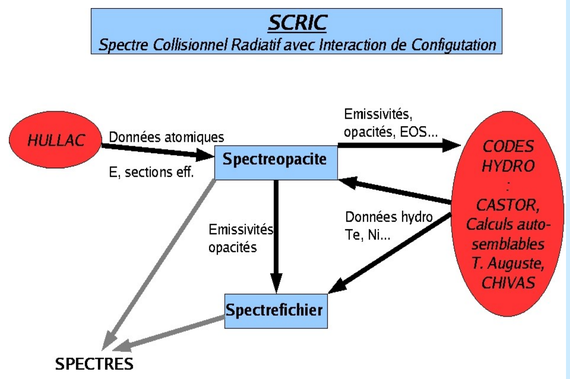
Out of equilibrium radiative modelling

We use the SCRIC code for massive detailed modelling of inhomogeneous plasmas. By example, for Tin :

- 23 ions
- 1450 non relativistic configurations
- ~ 300.000 levels
- ~ 100.000.000 lines with Voigt profile (Doppler and natural broadening)

NLTE modelling with simplified Collisional Radiative model (Colombant Tonon : semi empirical formulas for collisional ionization, 3 body- and radiative-recombination) to compute ionization and then an effective temperature for configurations populations.

Principles of the SCRIC code to determine complex spectra. The red circles are external codes for evaluating atomic and hydro data. Emissivities, opacities, EOS... can be computed in advance



Hydro-Radiative modelling and Conversion Efficiency (CE) optimisation

Result : new hydro-radiat. autosimilar model

- Spherical and homogeneous plasma ->simple emission

$$I_E(R) = \frac{j_E}{\kappa_E}\pi.R^2.\left[1 - \frac{1}{2\tau^2} + \left(\frac{1}{\tau} + \frac{1}{2\tau^2}\right)e^{-2\tau}\right]\ ;\quad \tau = N_i.\kappa_E.R \text{ : epaisseur optique radiale}$$

- Full absorption of laser : $\frac{dE_{laser}(t)}{dt} = E_{laser}.\sqrt{\frac{\ln 2}{\pi}}.\frac{2}{\Delta T}.e^{-\left[\ln 2\left(\frac{2(t-t_0)}{\Delta T}\right)^2\right]}$
- Autosimilar expansion of the sphere : $E_K(t) = \frac{3}{10}.M.V_m^2(t)$
- Impulsion balance : $\frac{3}{4}.M.\frac{dV_m(t)}{dt} + \frac{1}{c}.\frac{dE_{rad_emitted}}{dt} = (Z^* + 1).N_i.T.4\pi.R^2(t)$
- Energy balance : $\frac{dE_{internal}}{dt} + \frac{dE_K}{dt} + \frac{dE_{rad_emitted}}{dt} = \frac{dE_{laser_absorbed}}{dt}$

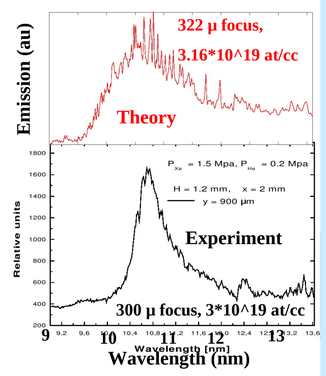
$$E_{internal} = E_{ion_internal} + \frac{3}{2}(Z^* + 1)T$$

Comparison between theoretical calculation and experiment for a laser – Xe gas puff interaction. Double puff He/Xe for less reabsorption by neutrals.

Optimum experiment for a 3.9ns, 0.5J laser : $3*10^{19}$ at/cc, 300 µm focus,

CE in 7.4% BandWidth = 2%

*Optimum theoretical CE at $3.16*10^{19}$ at/cc is obtained for 322 µm focus and reaches **3.17% in 7.4%BW** and **0.95% in 2%BW***



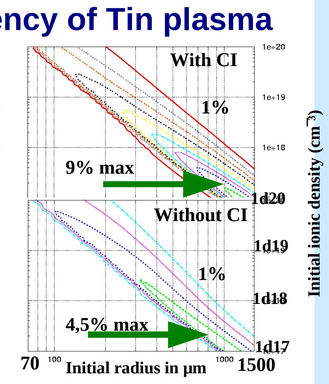
===> The model gives the good conditions to obtain the optimum Conversion Efficiency in laser – Xe gas-puff experiments. Calculated CE / Experimental CE = 1.58

Result : Configuration Interaction doubles the EUV Conversion Efficiency of Tin plasma

Conversion Efficiency in EUV of a laser-Tin sphere interaction calculated with and without Configuration Interaction. The initial ionic density and radius of the sphere is varied. Laser parameters are 3.09ns, 0.8J.

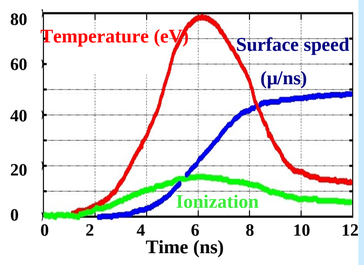
*--->**maximum Conversion Efficiency is >9% with CI and 4.5% without CI***

(lower left corner is non relevant)



Results : maximum CE occurs for high temperatures and ionization

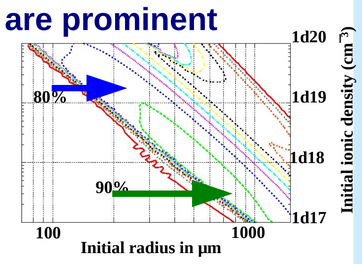
Hydro simulation of a 3.09ns, 0.8J laser – Tin sphere interaction. Initial conditions are 600µ diameter and $3.3*10^{18}$ at/cc. CE in EUV reaches 5%. Temperature reaches 80 eV and ionization 18



---> Very ionized ions (even with fully stripped 4d subshell) contribute to the emission at 13.5nm : this is satellite emission (4p / 4f** - 4d*).

Result : radiative losses are prominent

*Total radiative losses in a laser-Tin sphere interaction variating the initial ionic density and radius of the sphere. Laser is 3.09ns, 0.8J. ---> **radiative losses reach 90% where the EUV CE is maximum,** kinetic and thermal energies account for < 10%*



Results : best CE is obtained for low energy, long laser pulses in low density Tin

For short pulses (1ns), the best CE (7.6%) is obtained for low energies (0.1J) and at low density ($2*10^{17}$ at/cc). For longer pulses the CE increases and reaches 10% for 32ns. The CE is slightly better for low energies and constant on a broad range of moderate densities (10^{17} – 10^{20} at/cc).

Perspectives

- Use a more accurate Collisional Radiative treatment (needs long atomic data calculations)
- Include inverse Bremsstrahlung for laser absorption
- Use a more relevant hydro-radiative code (MULTI 1D)
- Map the resonant lines to shift the 4p/4f – 4d transitions ---> better accuracy, narrowing of the main group of lines and increase of its emissivity / opacity ---> optical length smaller ---> smaller focus

Acknowledgements

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