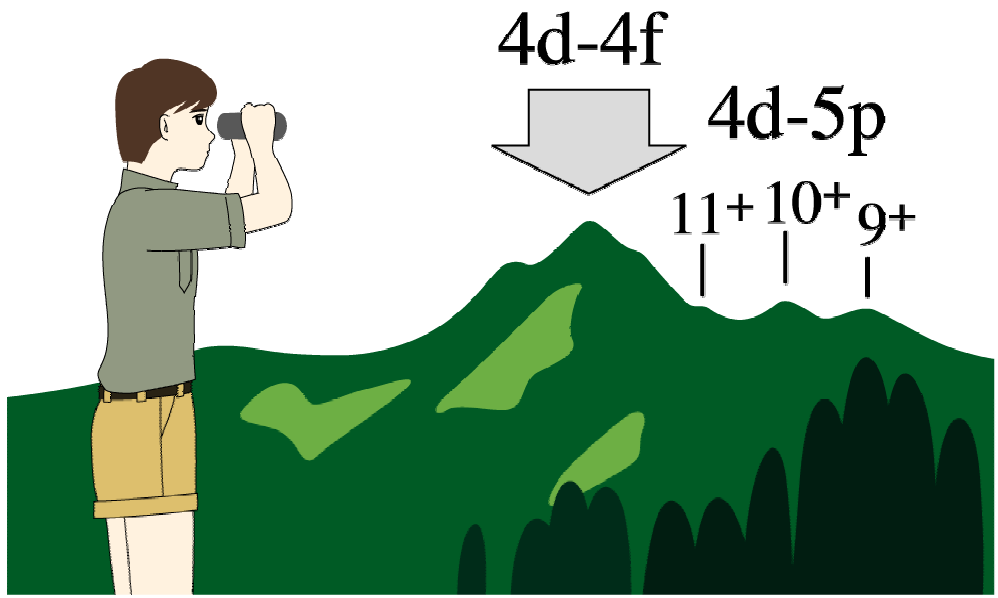
Theoretical Spectroscopy of the EUV emission of Xe and Sn



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Contents

- Assignment of emission lines of Xe and Sn is carried out by comparing observed wavelength with calculations using HULLAC and GRASP.
- Opacity and emissivity of the plasma, which will be used in radiation hydrodynamics code, is calculated using atomic data from HULLAC.
- Radiation flux and emission efficiency of the Xe plasma is estimated for a simple plasma geometry, assuming LTE.

Effect of Electron Correlations (1)

Xe 8+ Ground State Energies:

Configurations	Energy	Decriment	Total Decrement
4d(10) (minimal)	-202224.42		
4d(10)+4f(2)	-202231.75	7.33	7.33
4d(10)+4f(2)+5p(2)	-202231.87	0.12	7.45
4d(10)+5d(2)	-202225.67	1.25	1.25
4d(10)+5s(2)+5d(2)	-202225.69	0.02	1.27
4d(10)+4f(2)+5d(2)	-202232.92	8.50	8.50
4d(10)+4f(2)+5s(2)+5p(2)+5d(2)	-202233.05	0.13	8.63

Effect of Electron Correlations (2)

Ionization Potentials:

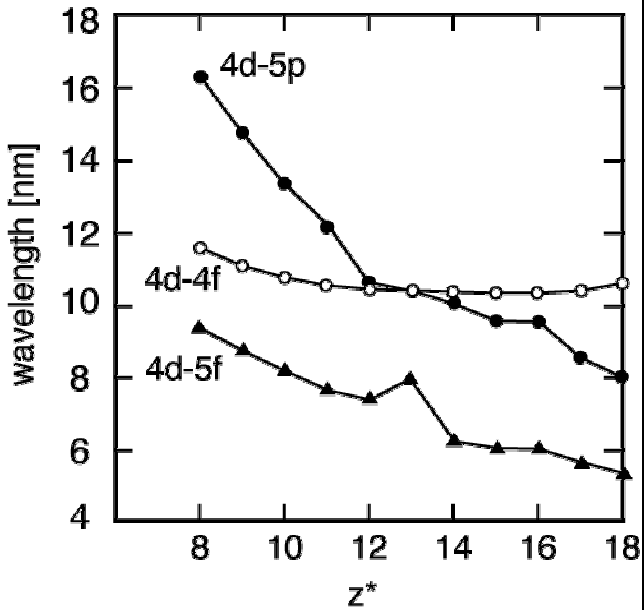
Ionicity	Symmetry	Total Energy (minimal)	I.P. (minimal)	Total Energy (with corr.)	I.P. (with corr.)	Corr. Effect
8+	0 +	-202224.42		-202233.04		
9+	5/2 +	-202046.24	178.18	-202053.3	179.74	1.56
9+	3/2 +	-202044.14	180.28	-202051.2	181.84	1.56
10+	4+	-201844.59	201.65	-201850.23	203.07	1.42
10+	2+	-201842.7	203.54	-201848.43	204.87	1.33
10+	3+	-201842.7	203.54	-201848.34	204.96	1.42
10+	2+	-201840.97	205.27	-201846.71	206.59	1.32
10+	0+	-201839.98	206.26	-201845.87	207.43	1.17
10+	1+	-201839.74	206.5	-201845.56	207.74	1.24
10+	4+	-201839	207.24	-201844.64	208.66	1.42
10+	2+			-201844.63	208.67	
10+	0+			-201838.83	214.47	

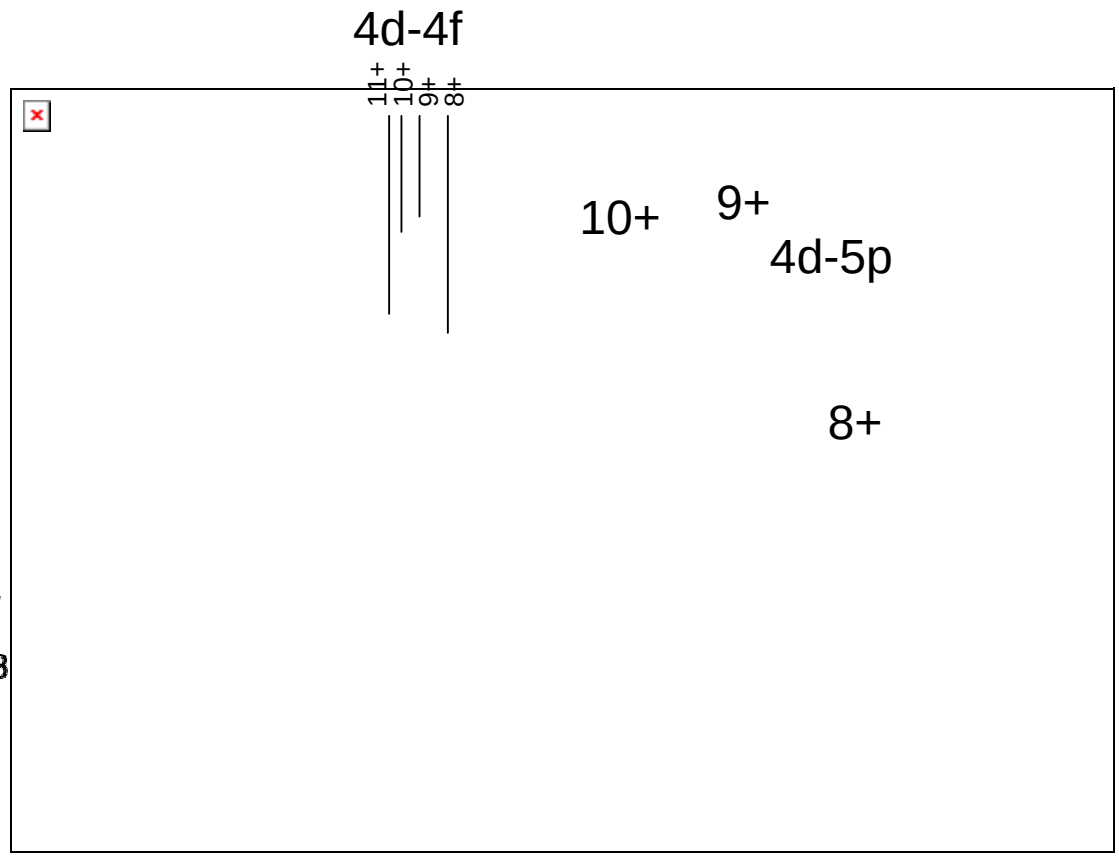
LevI-LevF	Energy (eV)	Oscillator strength GF	Decay width (eV)	
12 - 1	1.57836D+02	2.20547D-01	5.23081D-05	
11 - 1	1.57098D+02	6.28131D-01	1.47586D-04	
10 - 1	1.54070D+02	7.58588D-02	1.71434D-05	
9 - 1	1.31406D+02	1.62410D+00	2.66993D-04	5f-4d
8 - 1	1.24954D+02	5.00358D-02	7.43765D-06	
7 - 1	1.23239D+02	2.82477D-03	4.08445D-07	
6 - 1	1.04208D+02	7.34754D+00	7.59623D-04	4f-4d
5 - 1	8.69319D+01	1.77482D-02	1.27693D-06	
4 - 1	8.26920D+01	9.97598D-04	6.49435D-08	6p-4d
3 - 1	7.77258D+01	1.31231D-01	7.54778D-06	
2 - 1	7.60351D+01	8.04142D-01	4.42604D-05	5p-4d
1 - 1	7.45985D+01	3.66899D-03	1.94384D-07	

	LevI-LevF	Energy (eV)	Gauge	Oscillator strength GF	Decay width (eV)
4f-4d	6 - 1	1.04208D+02	COULOMB	7.34754D+00	7.59623D-04
	6 - 1	1.04208D+02	BABUSHKIN	7.40768D+00	7.65840D-04
6p-4d	5 - 1	8.69319D+01	COULOMB	1.77482D-02	1.27693D-06
	5 - 1	8.69319D+01	BABUSHKIN	2.54142D-02	1.82847D-06
	4 - 1	8.26920D+01	COULOMB	9.97598D-04	6.49435D-08
	4 - 1	8.26920D+01	BABUSHKIN	3.86281D-03	2.51469D-07
5p-4d	3 - 1	7.77258D+01	COULOMB	1.31231D-01	7.54778D-06
	3 - 1	7.77258D+01	BABUSHKIN	1.38446D-01	7.96279D-06
	2 - 1	7.60351D+01	COULOMB	8.04142D-01	4.42604D-05
	2 - 1	7.60351D+01	BABUSHKIN	8.76815D-01	4.82603D-05
	1 - 1	7.45985D+01	COULOMB	3.66899D-03	1.94384D-07
	1 - 1	7.45985D+01	BABUSHKIN	3.17760D-03	1.68350D-07

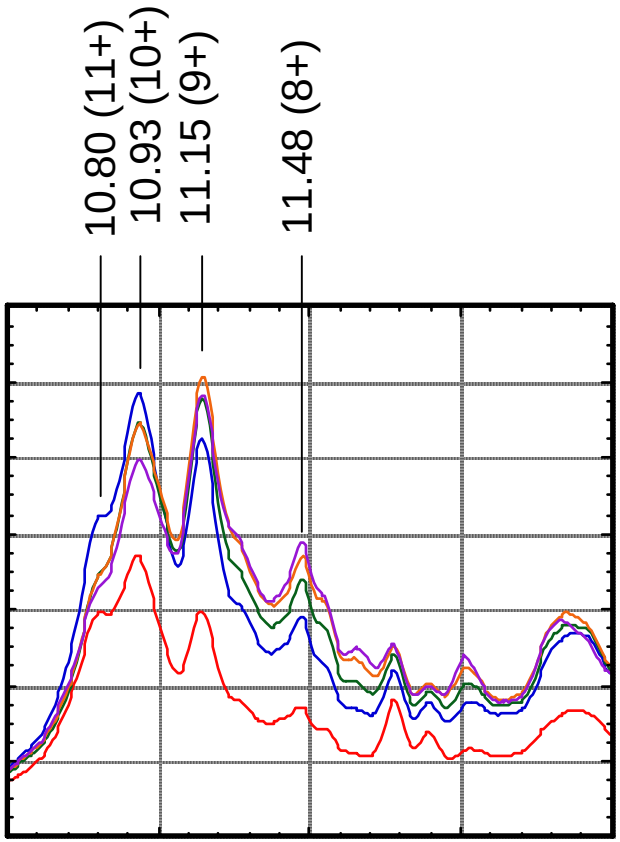
	LevI-LevF	Energy (eV)	Gauge	Oscillator strength GF	Decay width (eV)
	12 - 1	1.57836D+02	COULOMB	2.20547D-01	5.23081D-05
	12 - 1	1.57836D+02	BABUSHKIN	2.34365D-01	5.55853D-05
	11 - 1	1.57098D+02	COULOMB	6.28131D-01	1.47586D-04
	11 - 1	1.57098D+02	BABUSHKIN	6.43484D-01	1.51193D-04
	10 - 1	1.54070D+02	COULOMB	7.58588D-02	1.71434D-05
	10 - 1	1.54070D+02	BABUSHKIN	7.75528D-02	1.75262D-05
5f-4d	9 - 1	1.31406D+02	COULOMB	1.62410D+00	2.66993D-04
	9 - 1	1.31406D+02	BABUSHKIN	2.42815D+00	3.99175D-04
	8 - 1	1.24954D+02	COULOMB	5.00358D-02	7.43765D-06
	8 - 1	1.24954D+02	BABUSHKIN	8.56921D-02	1.27378D-05
	7 - 1	1.23239D+02	COULOMB	2.82477D-03	4.08445D-07
	7 - 1	1.23239D+02	BABUSHKIN	5.80348D-03	8.39149D-07

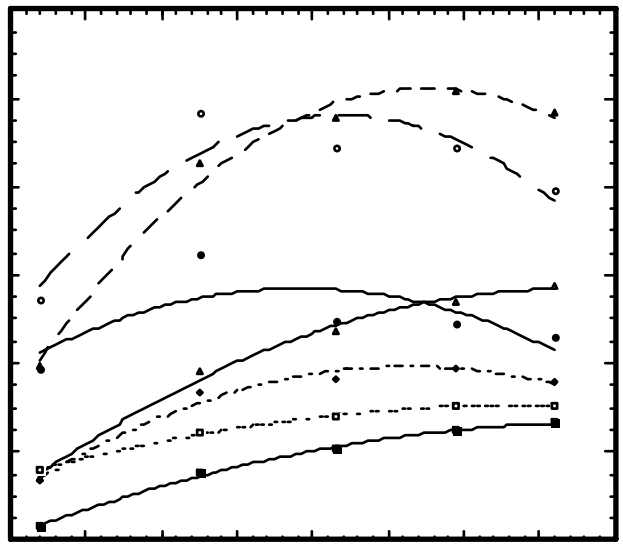
Spectrum of Xe is explained by strong 4d-4f transitions and 4d-5p transitions, which has clear dependence on Z, except for the “red-wing” structure.



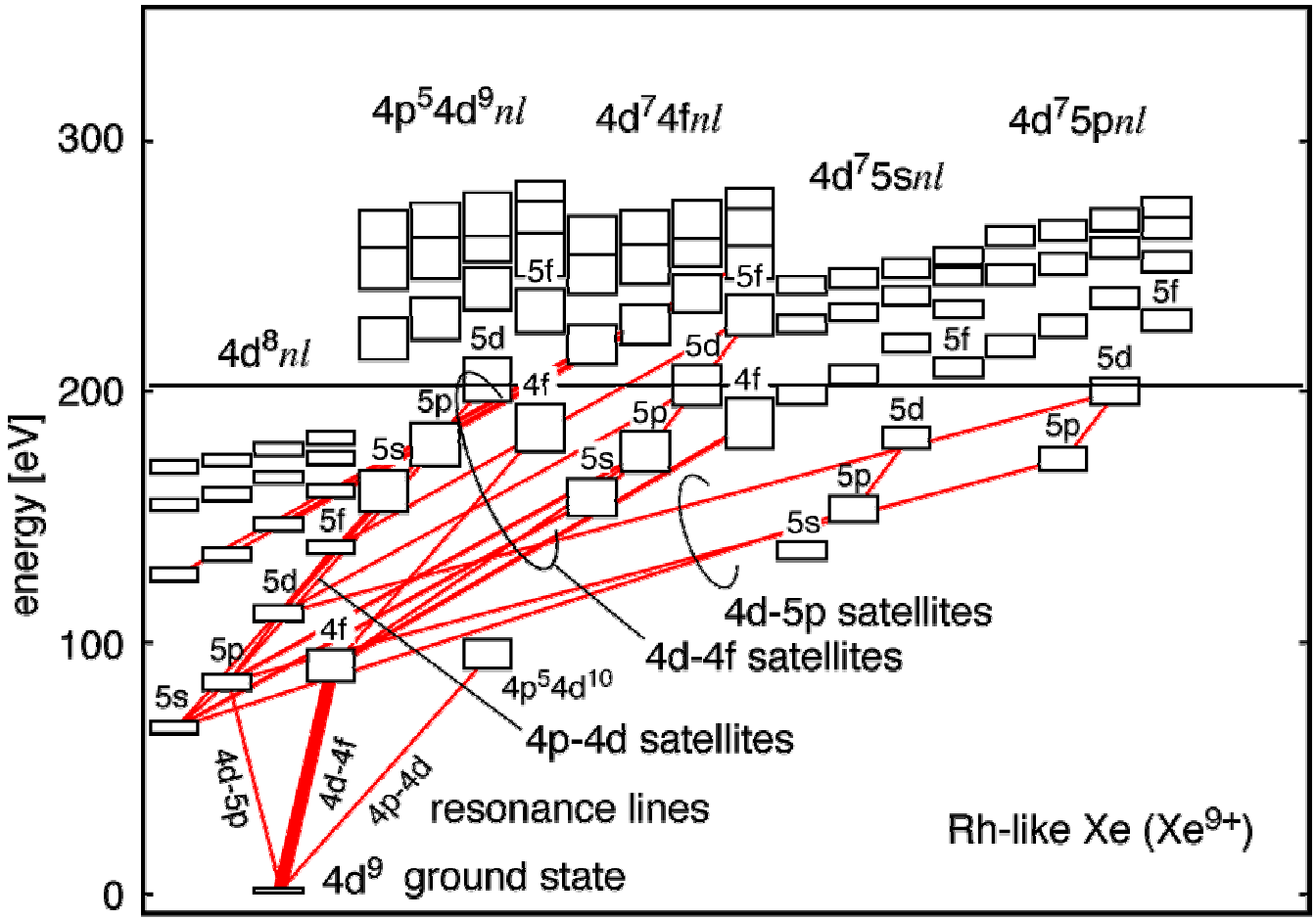


Each peak of 4d-4f transitions in the 11nm band has a maximum at different pressure, which is attributed to the different charge state.

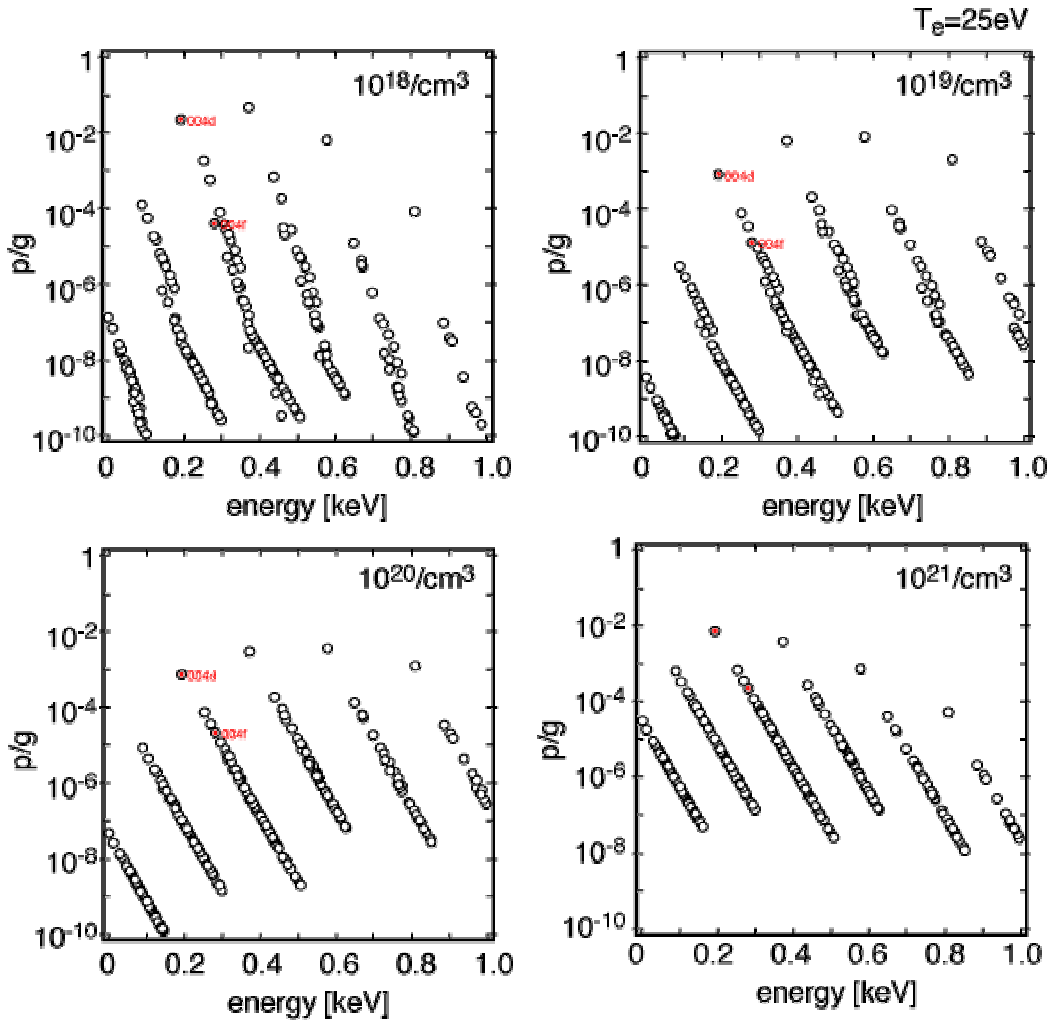




Xe ions have a large number of multiply excited states, which contribute to the satellite lines



In high density plasma (n_e>10^{20}/cm^3), population of excited states can be approximated by LTE



Satellite lines included in the model

4d-4f satellites

$4p^6 4d^{i-1} 4f\ nl \rightarrow 4p^6 4d^i\ nl$

4d-5p satellites

$4p^6 4d^{i-1} 5p\ nl \rightarrow 4p^6 4d^i 5p\ nl$

4p-4d satellites

$4p^5 4d^i nl \rightarrow 4p^6 4d^{i-1}\ nl$

charge states

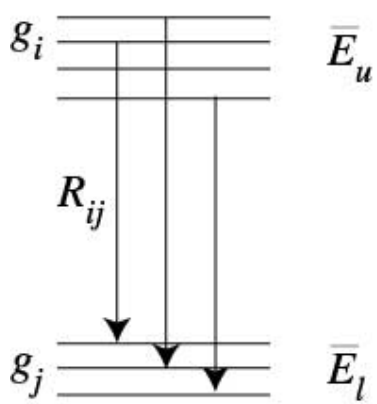
Xe^{7-11+}

location of the spectator electron

$n \leq 8$、$l \leq 3$

• Each transition consists of a large number of (>1000) fine structure transitions; separation of lines is smaller than the Doppler and Stark width.

• Width of the Unresolved Transition Array (UTA) is defined from distribution of fine structure transitions.



$$A = \frac{\sum(g_i A_{ij})}{\sum g_i}$$

Averaged transition probability

$$\bar{E} = \frac{\sum((g_i A_{ij}) E_{ij})}{\sum(g_i A_{ij})}$$

Averaged transition energy

$$\Delta E = \sqrt{\frac{\sum\left\{g_i A_{ij}\left(E_{ij} - \bar{E}\right)^2\right\}}{\sum(g_i A_{ij})}}$$

Definition of UTA line width, assuming Gaussian distribution of fine structure transitions

In the case of uniform plasma sphere in the LTE, radiation flux is determined by an analytical function of Planck radiation and radial optical depth.

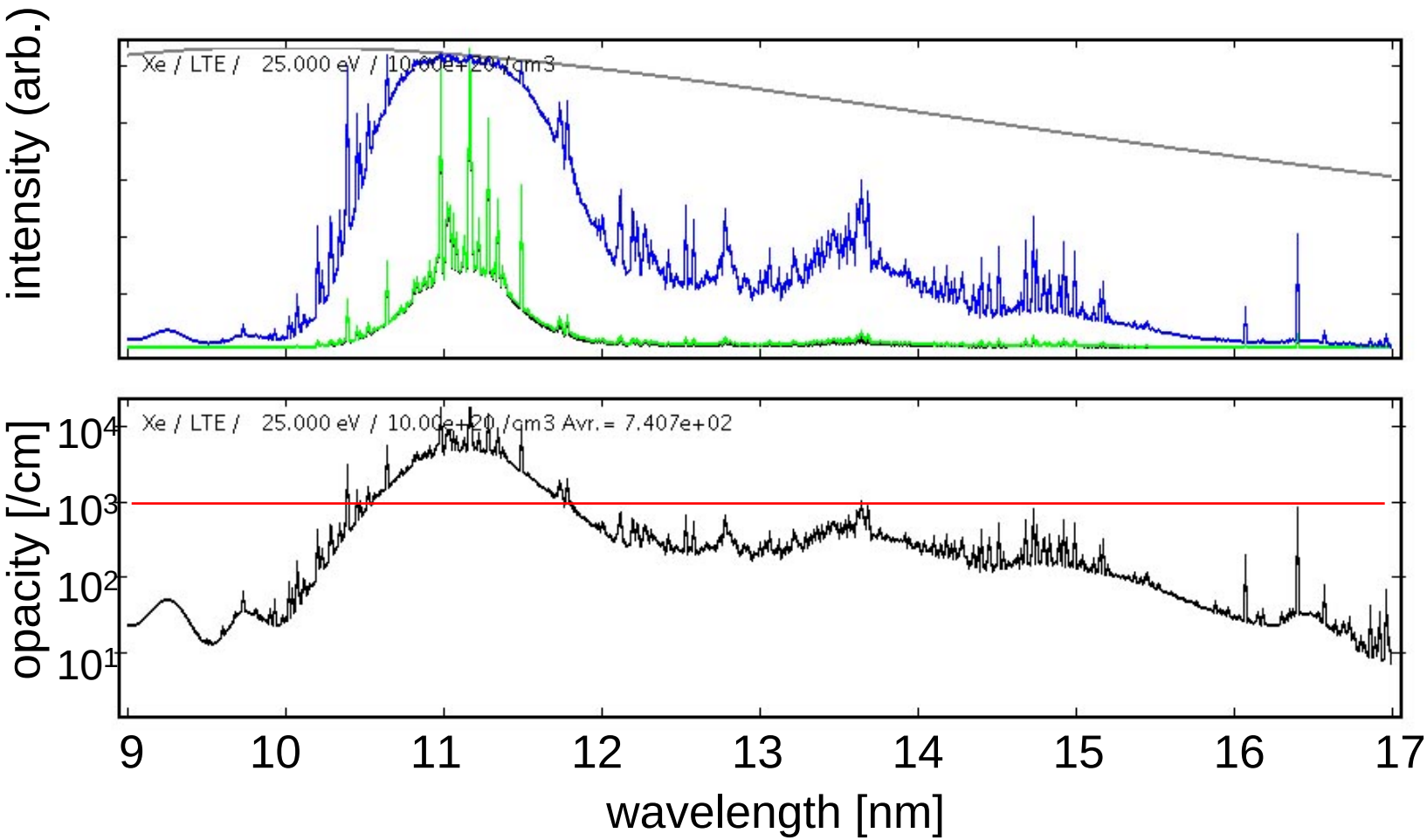
Radiative transfer equation $\Omega \cdot \nabla I_\nu = \kappa'_\nu \left(I_{\nu p} - I_\nu \right)$

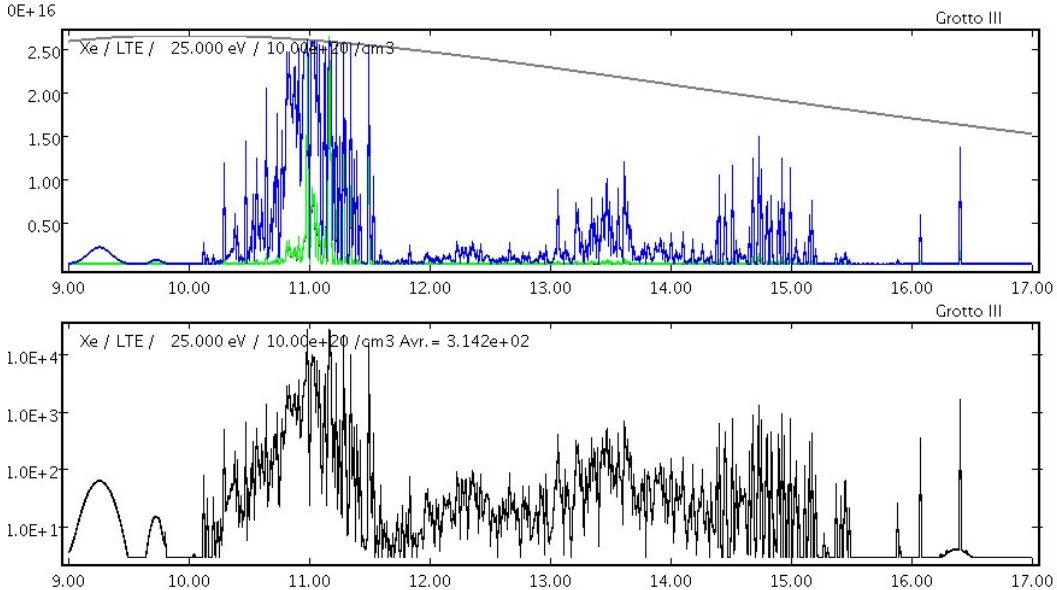
Radiation flux at the surface of the plasma

$$I_\nu = I_{\nu p} \left[1 - \frac{1}{2\tau^2} + \left(\frac{1}{\tau} + \frac{1}{2\tau^2} \right) \exp(-2\tau) \right] \quad , \qquad \tau = \kappa r_0$$

Murakami J. x-ray sci. & tech. **2**, 127(1990).

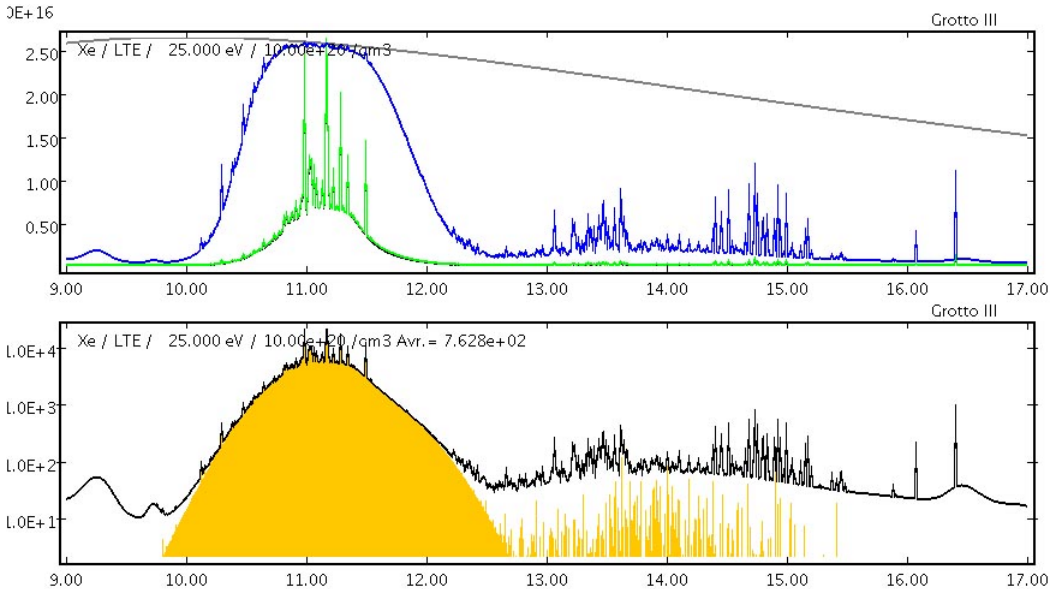
Peak opacity of the Xe plasma at 13.5nm is 10^3 at $n_e=10^{21}$/cm, with the effect of 4d-4f, 4p-4d and 4d-5p satellite lines.





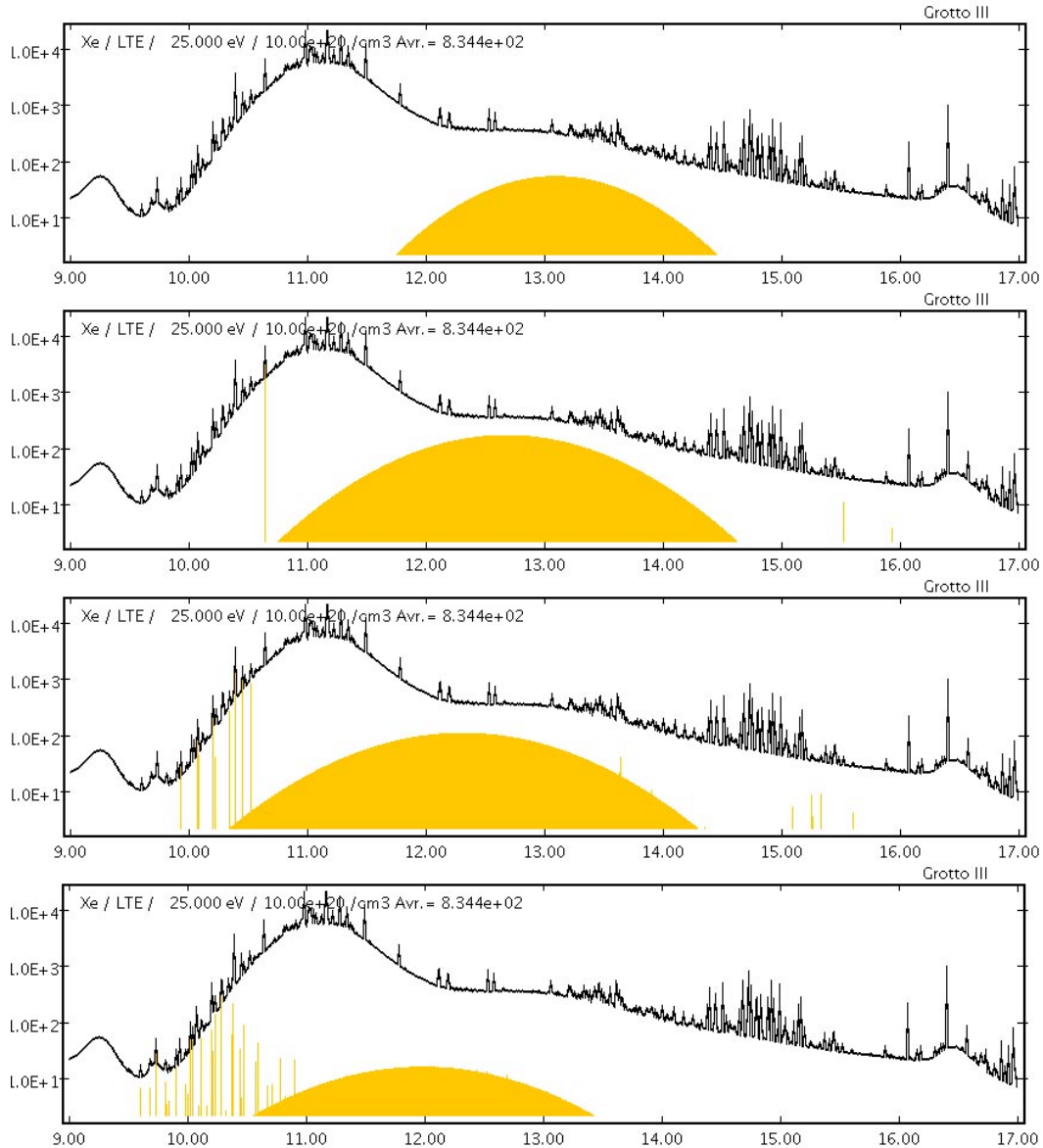
no satellites

T_e=25eV
n_e=10^{21}/cm^3
r=10µm



with satellites

effect of 4d-4f satellites (UTA)



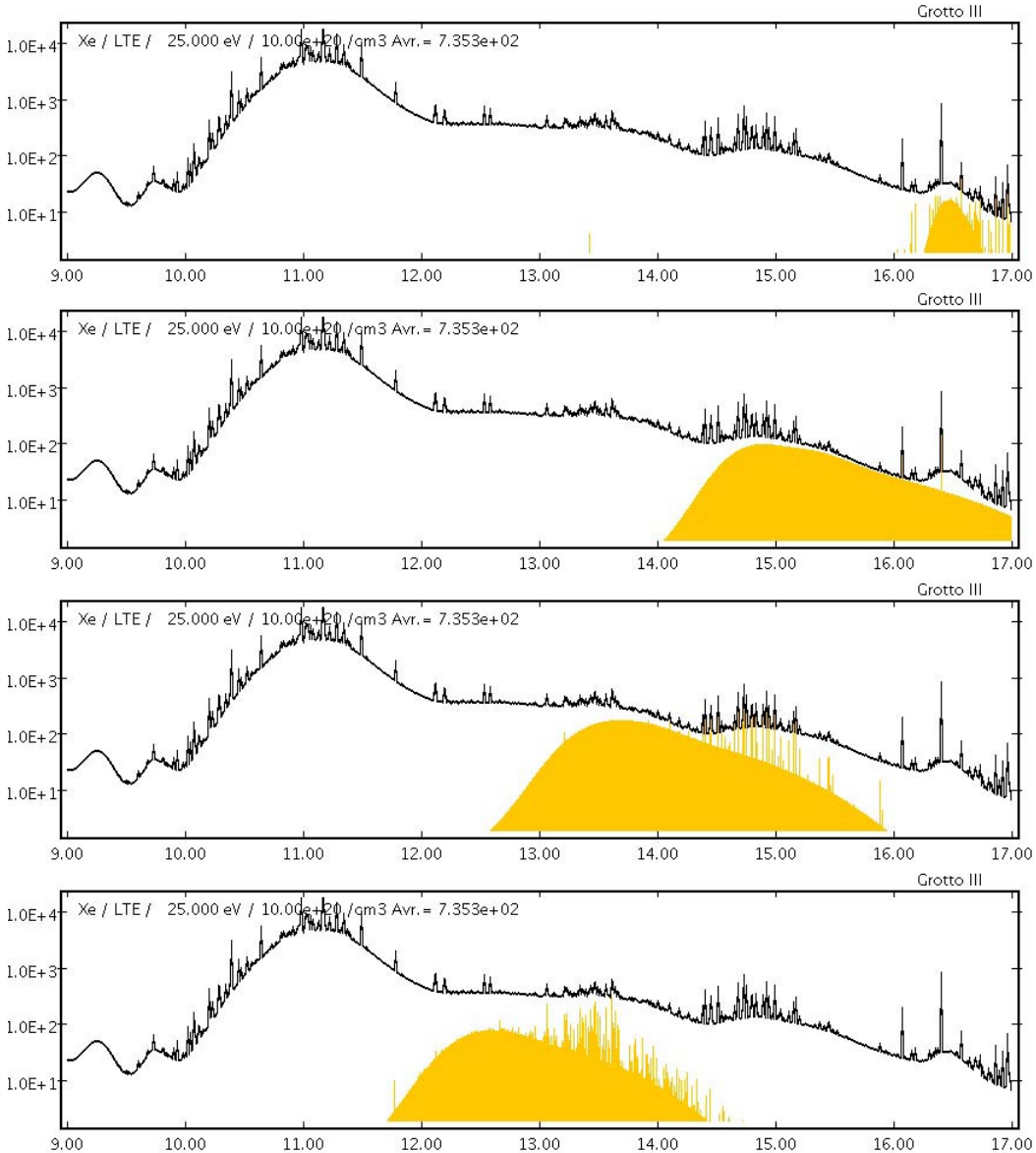
effect of 4p-4d satellites (UTA)

Pd-like

Rh-like

Ru-like

Tc-like



effect of 4d-5p satellites (UTA)

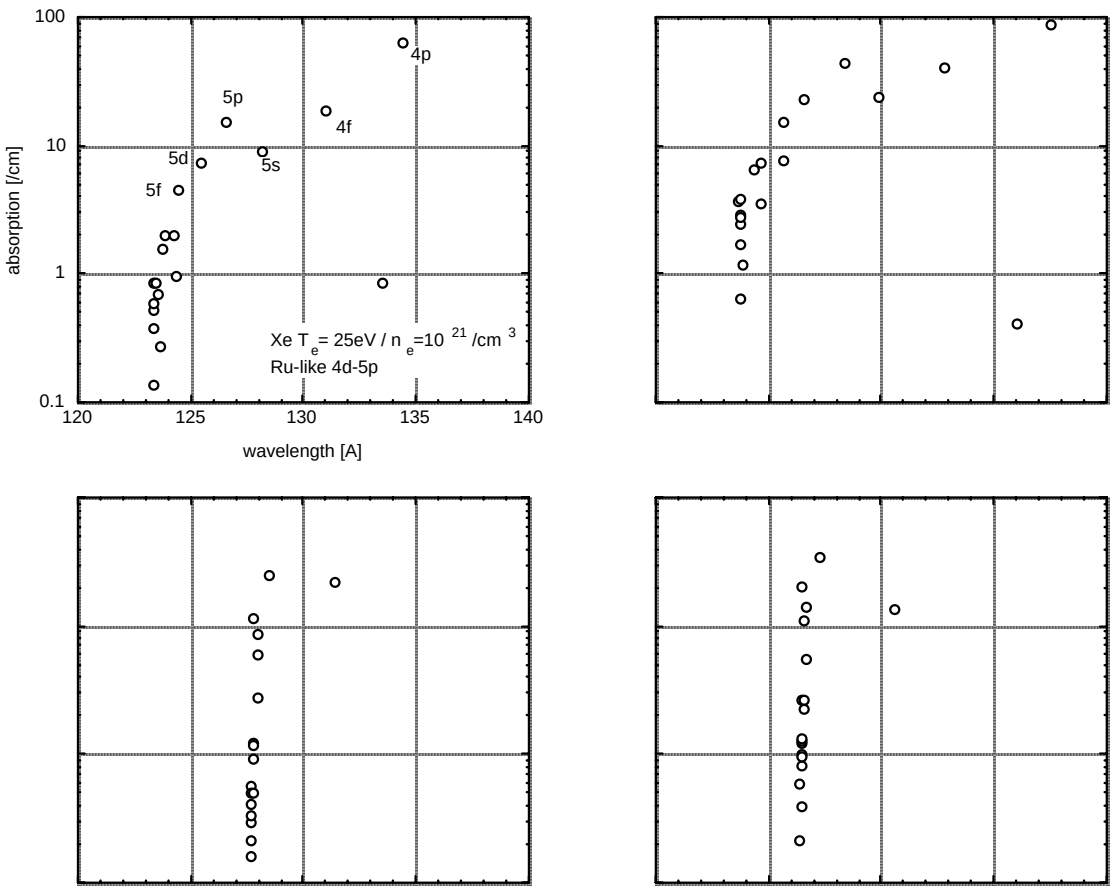
Pd-like

Rh-like

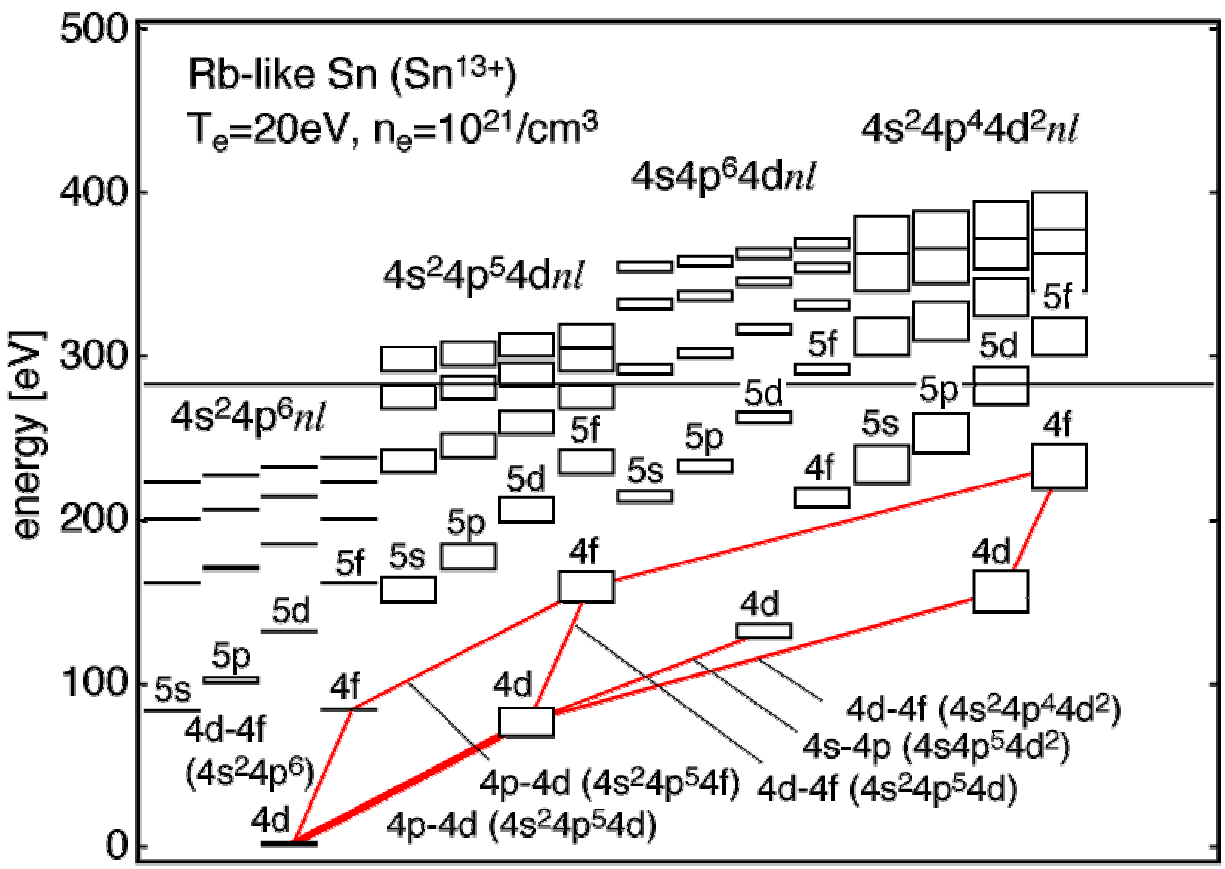
Ru-like

Tc-like

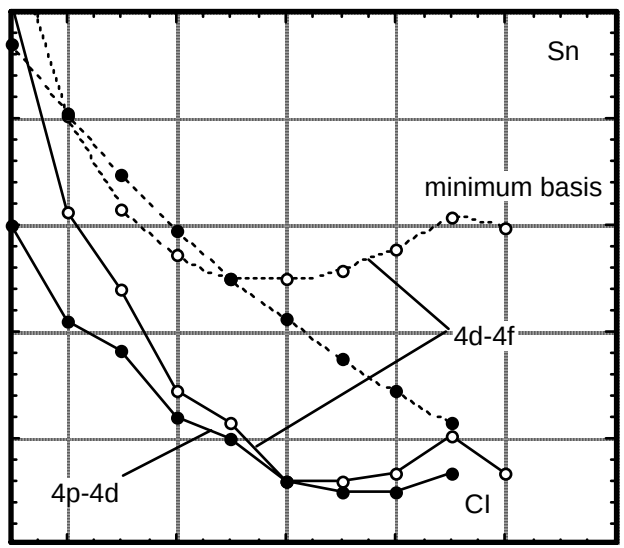
Absorption coefficient for each fine structure transition is small. Contribution from a large number of satellite lines produces the “red-wing” structure.

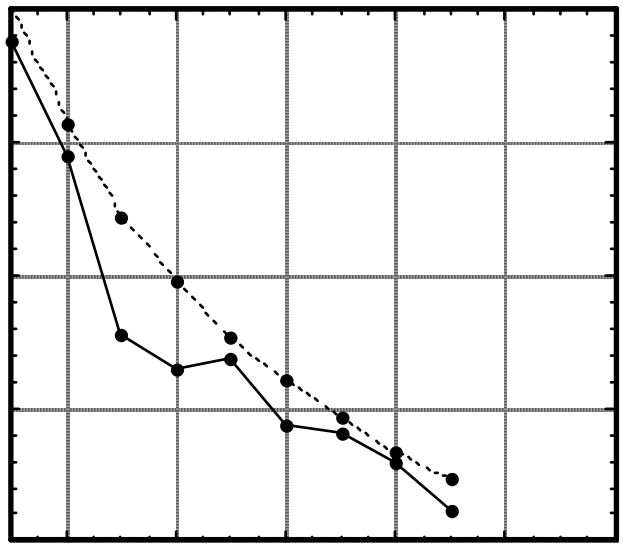


In the case of Sn of Z>10, contribution of 4d-4f, 4p-4d transitions from multiply excited states to the 13.5nm band should be considered.



Experiments suggest wavelength of 4d-4f and 4p-4d transitions from various charge states of Sn are in the 13.5nm band.
Calculation of wavelength is difficult due to the strong configuration interaction.





Summary

- Results of different atomic structure codes are compared to show the accuracy of calculated wavelength is applicable to the identification of the emission lines and calculation of opacity.
- Emission of Xe in the 13.5nm band, which is assigned to 4d-5p transition of Xe^{10+} in early calculations, is also determined by contribution from a large number of 4d-5p and 4p-4d satellite lines.

- Opacity of $10^3/cm^3$ can be obtained in the Xe plasma of $n_e=10^{21}/cm^3$. With moderate plasma thickness, the Xe plasma can become optically thick, and the maximum radiation flux determined by the Planck radiation can be obtained.