

# **The Role of Interference and Correlations in 13.5 nm Radiations of Sn and Xe Atomic Ions**

**--- For Precise and Accurate Determination of Spectral Lines ---**

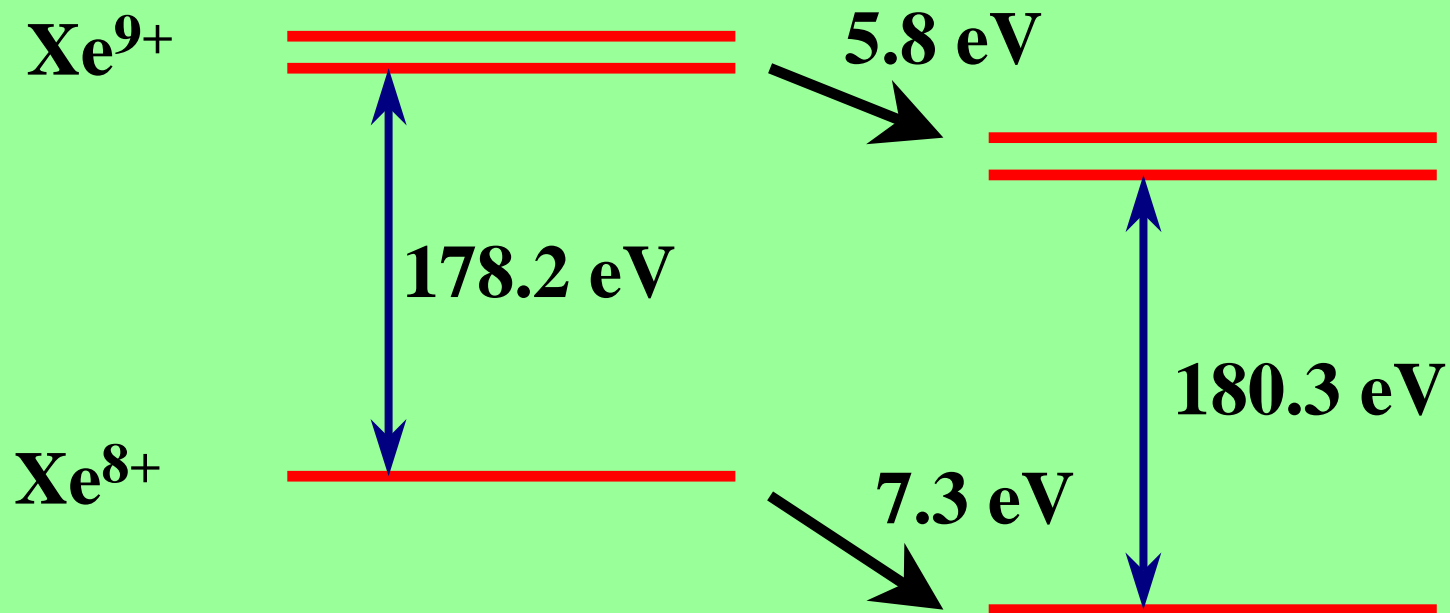
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# Scope of the research

- Recently, the 13 nm range extreme ultra-violet emissions of many electron atomic ions are of interest in relation to the semiconductor technologies. We theoretically studied the intra N shell ( $n=4$  shell) transitions of Sn and Xe atomic ions. In this type of the ions, especially of the Sn ions, a peculiar behavior in the emission spectra has been pointed out by O'Sullivan and Faulkner[1]; they discussed the narrowing of 4f-4d spectra as due to the configuration interactions. To gain a further insight of the effects, we carried out a sophisticated calculation using GRASP92[2] and its earlier versions. We found in Sn  $12+$  ions, for example, that the positions of main peaks of all the  $n=4$  orbitals fall in almost the same radial distances, which enhances the configuration interactions in the N shell. And these configuration interactions considerably modify the geometry of the excited electronic states and induce the so called spectral narrowing. This work is supported by the Leading Project for advanced semiconductor technology of MEXT.
- References
- [1]G. O'Sullivan, and R. Faulkner, Opt. Eng. 33, 3978 (1994)  
[2] F. A. Parpia, C. F. Fischer, and I. P. Grant, Compt. Phys. Commun. 94, 249(1996).

# Ground State Energy of Xe<sup>8+</sup> and Xe<sup>9+</sup> Ions

$$\Phi_1(4d^{10}) \quad C_1\Phi_1(4d^{10}) + C_2\Phi_2(4d^8 4f^2)$$



# Configurations Included

## Excited State Configurations

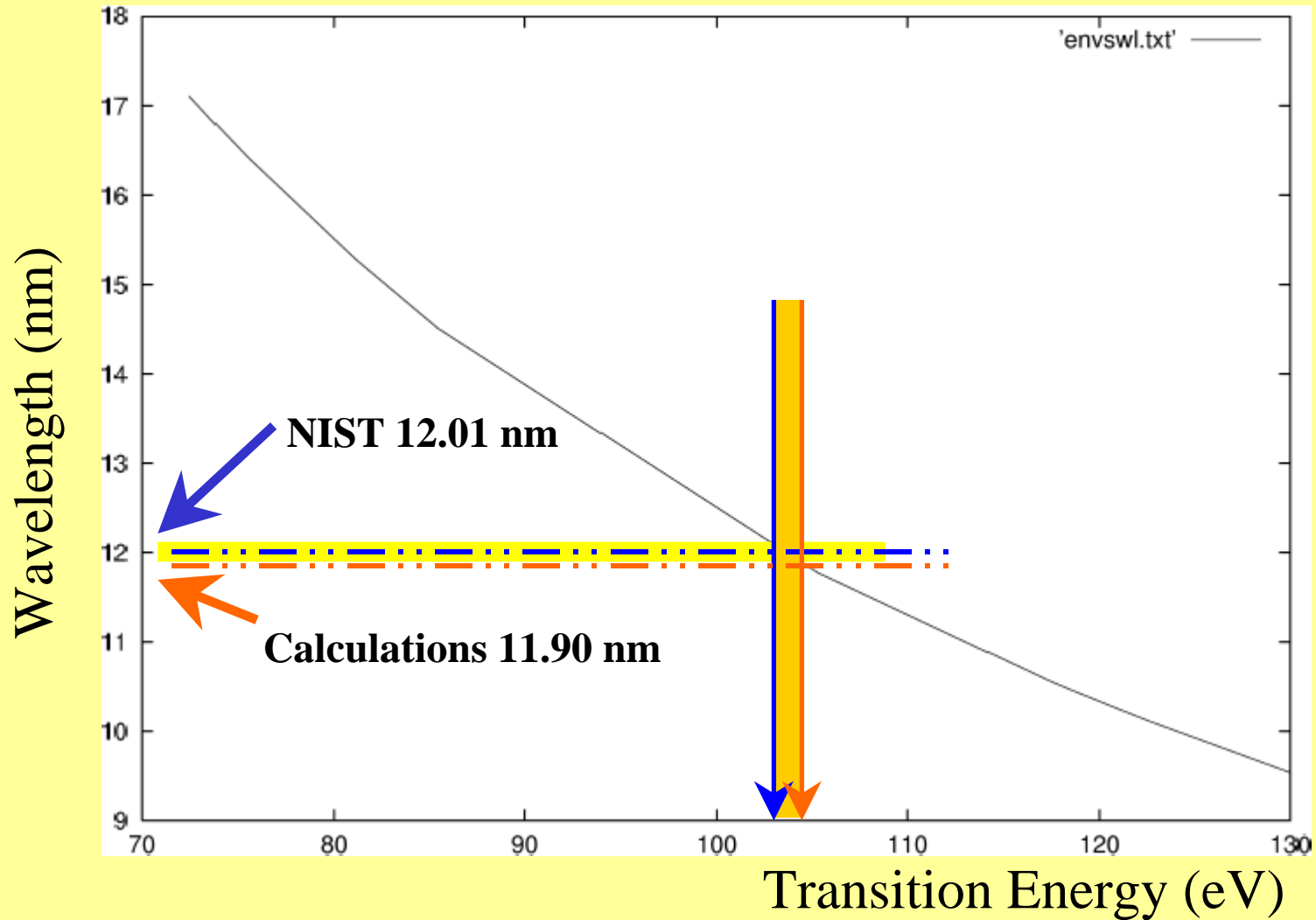
- $4d(9)4f(1)$  ,  $4d(7)4f(3)$ ,  $4d(7)4f(1)5p(2)$
- $4d(9)5p(1)$ ,  $4d(7)5p(3)$ ,  $4d(7)4f(2)5p(1)$
- $4d(9)5f(1)$ ,  $4d(7)4f(2)5f(1)$
- $4d(9)6p(1)$ ,  $4d(7)4f(2)6p(1)$

## Ground State Configurations

$4d(10)$ ,  $4d(8)4f(2)$ ,  $4d(8)5p(2)$

$4d(8)5f(2)$ ,  $4d(8)6p(2)$

# Energy of Xe<sup>8+</sup> 4d-4f Transitions



# Configurations for more Sophisticated Calculation

## Excited State Configurations

- $4d(9)4f(1)$ ,  $4d(7)4f(3)$ ,  $4d(7)4f(1)5p(2)$
- $4d(9)5p(1)$ ,  $4d(7)5p(3)$ ,  $4d(7)4f(2)5p(1)$
- $4d(9)5f(1)$ ,  $4d(7)4f(2)5f(1)$
- $4d(9)6p(1)$ ,  $4d(7)4f(2)6p(1)$
- $4d(9)6f(1)$ ,  $4d(9)7p(1)$ ,  $4d(9)7f(1)$ ,
- $4d(9)8p(1)$ ,  $4d(9)8f(1)$ ,  $4d(9)9p(1)$

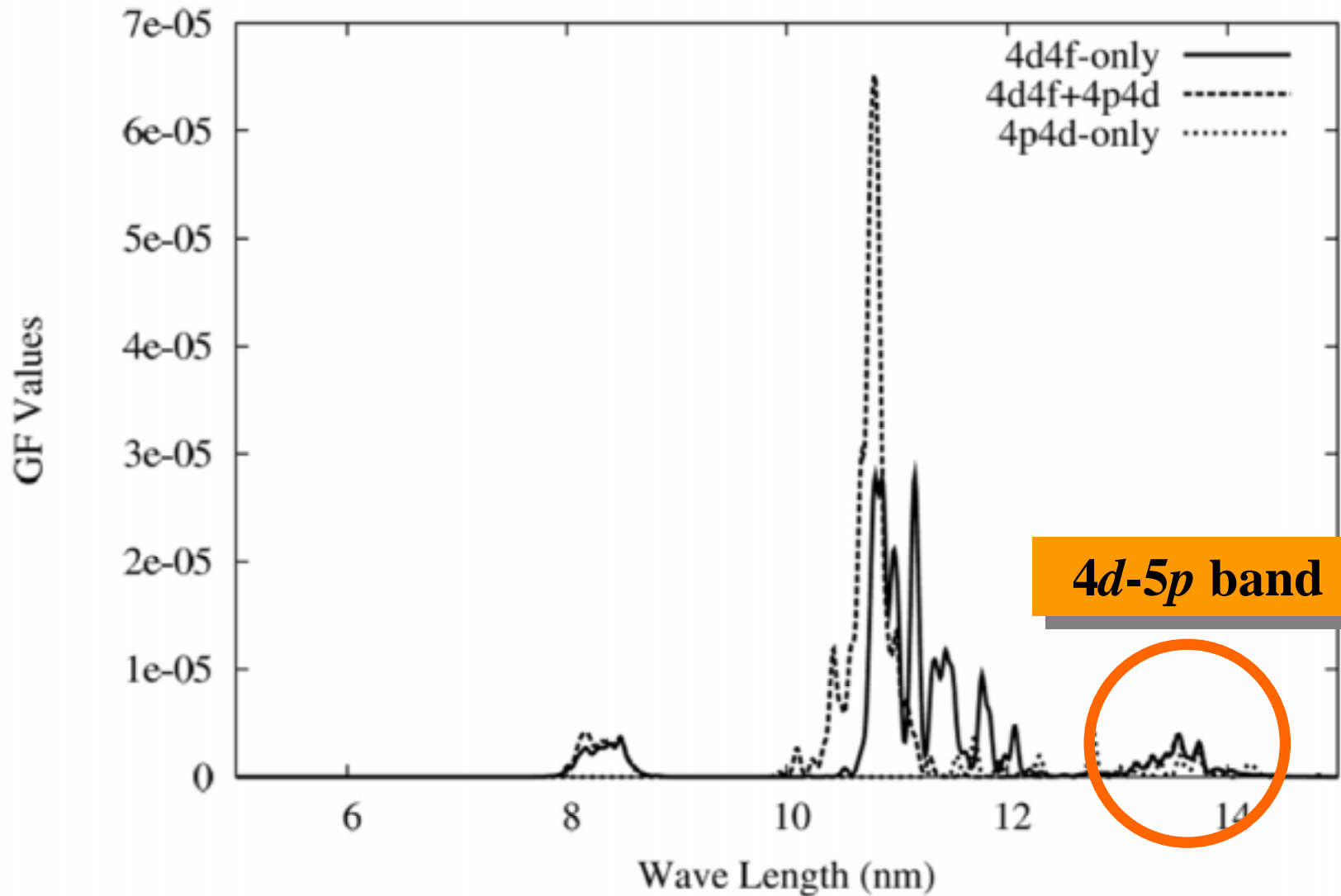
## Ground State Configurations

$4d(10)$ ,  $4d(8)4f(2)$ ,  $4d(8)5p(2)$

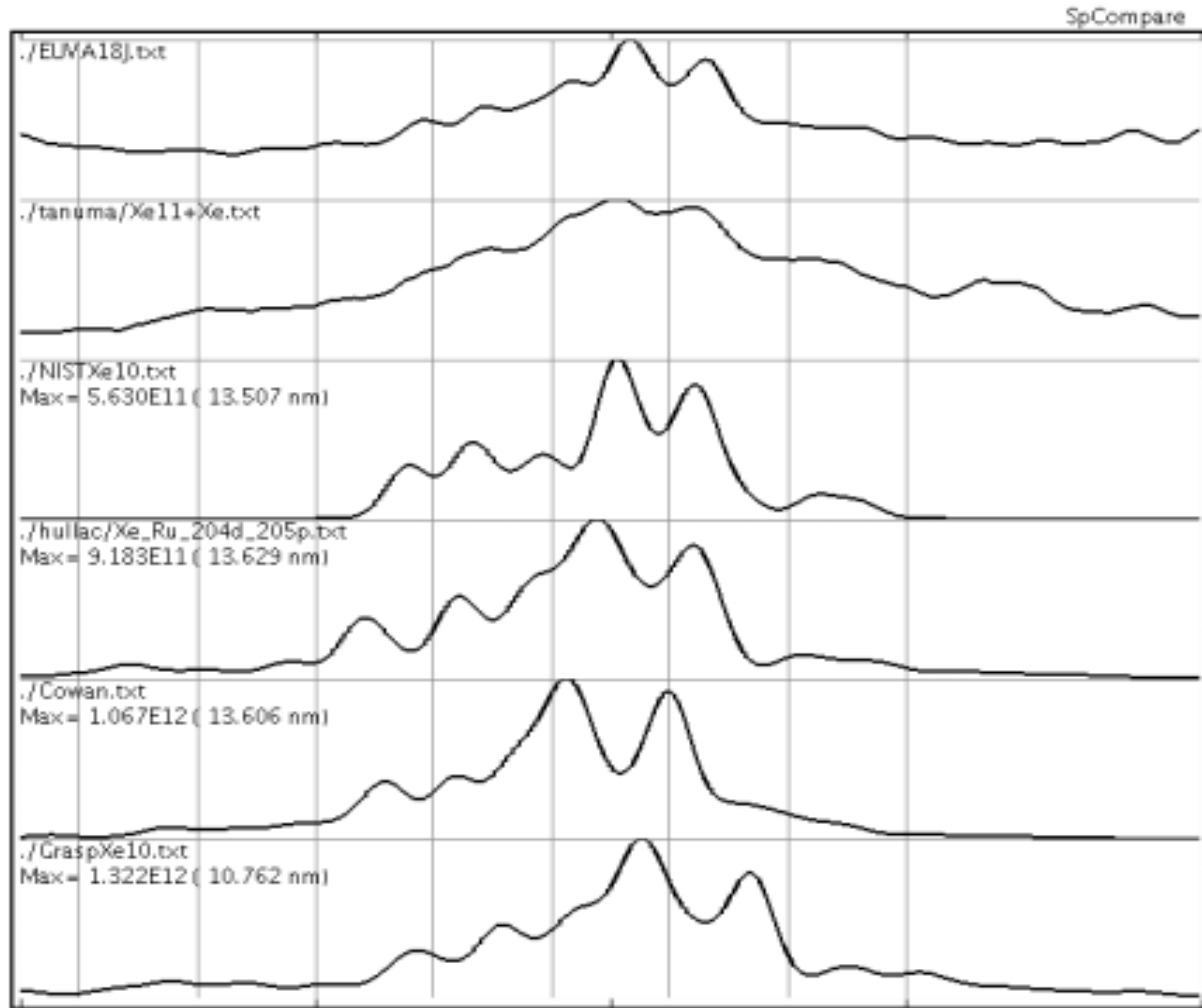
$4d(8)5f(2)$ ,  $4d(8)6p(2)$

**No Change!**

GF Value Distributions for Xe<sup>10+</sup>



# Theoretical and Experimental Xe<sup>10+</sup> 4d-5p Transitions



EUVA/DPP

TMU

NIST(Part)

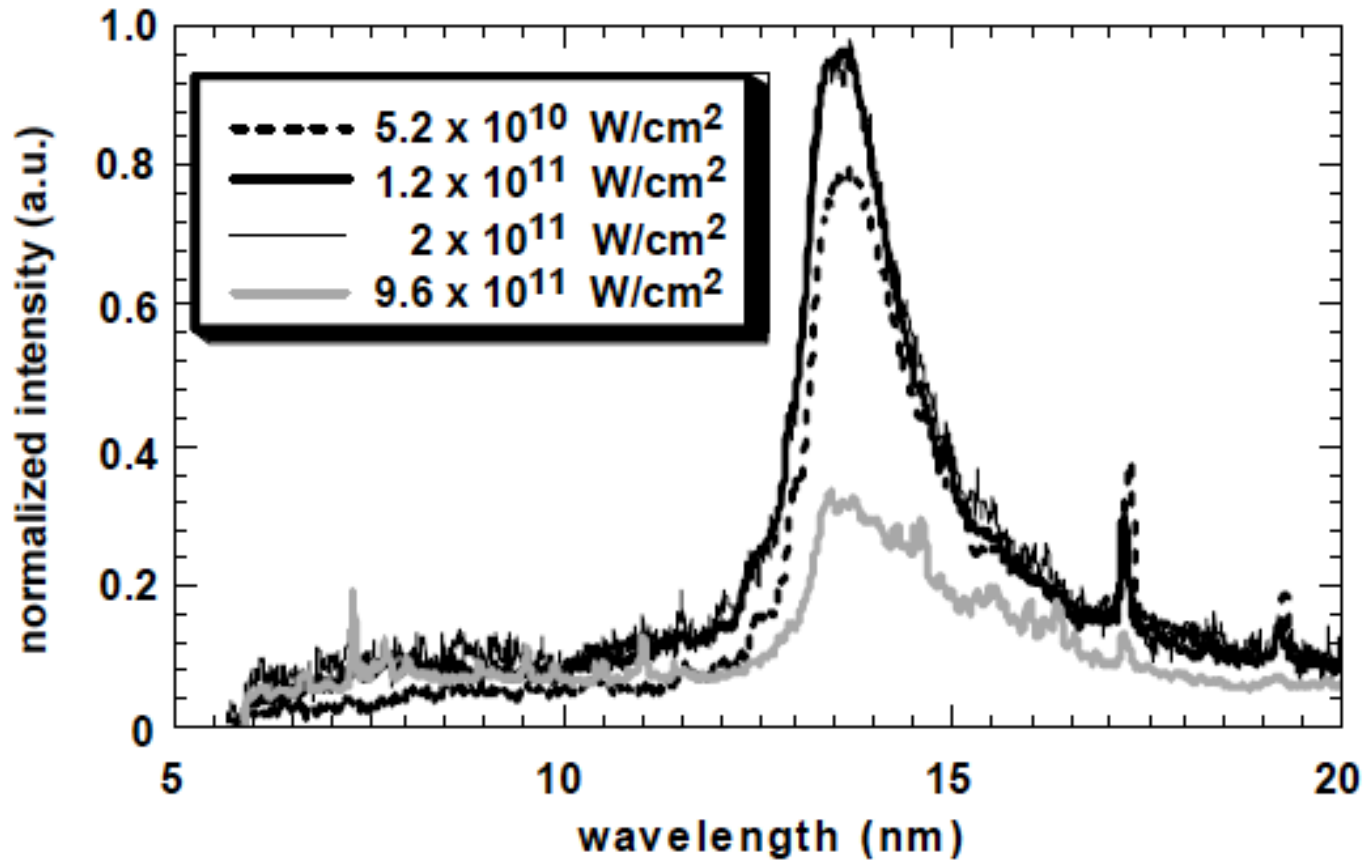
Hullac

Cowan

Grasp(Present Work)

12.5 13.0 13.5 14.0 14.5

$\lambda(\text{nm})$



Time integrated Sn EUV spectra  
for various laser power

# O'Sullivan and Faulkner's Pioneer Work

## Tunable narrowband soft x-ray source for projection lithography

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**Abstract.** EUV emission from laser plasmas produced on low  $Z$ -target material such as plastics and araldites that contain 1 to 10% concentrations of the elements  $50 < Z < 70$  emit narrow regions of intense quasi-continua in the 6 to 13-nm wavelength range. The typical bandwidth of the emission is 0.5 to 1.5 nm and the features are brighter than any individual lines emitted from the host substrate materials. Similar spectra can be obtained from hydrated salts of these elements, so suitable targets can be prepared as compressed pellets of crystalline or hydrated salts or alternatively from oxides mixed into an araldite matrix. Spectra of tin salts prepared in this way provide an excellent narrowband source for 13.5-nm radiation for use with Mo/Si multilayers. Since the peak shifts toward shorter wavelengths with increasing  $Z$ , plasmas of these elements provide "tunable" narrowband EUV radiation sources.

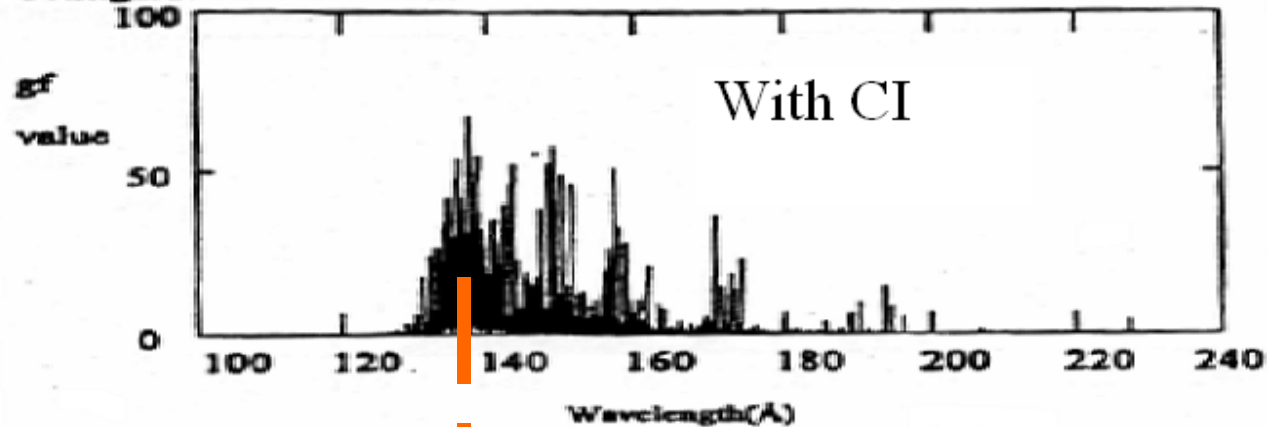
*Subject terms:* laser-produced plasmas; XUV emission; XUV sources; lithography; spectra.

*Optical Engineering* 33(12), 3978-3983 (December 1994)

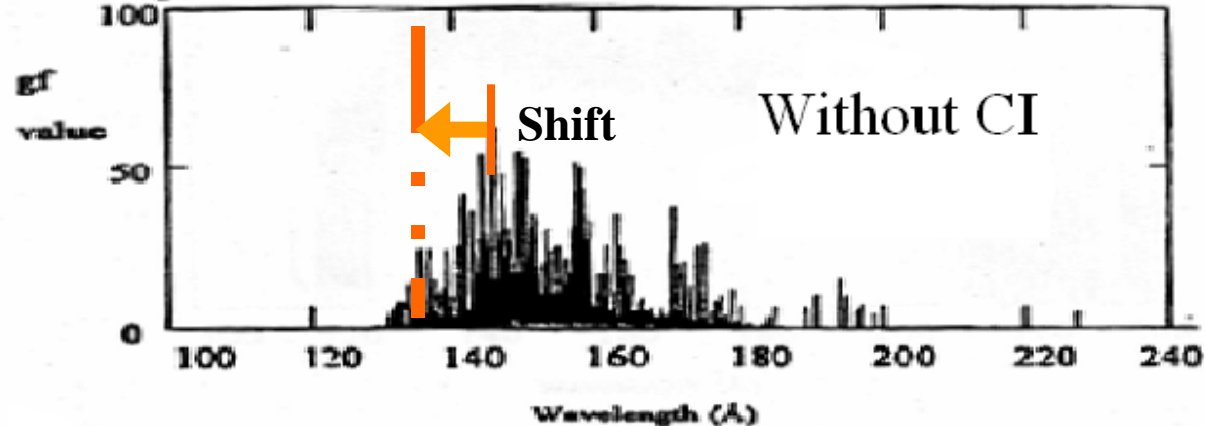
G. O'Sullivan, and R. Faulkner, *Opt. Eng.* **33**, 3978 (1994)

# Spectral Shift due to the Configuration Interaction

Configuration interaction:



No configuration interaction:



Configuration interaction effects and their effect on the profile of the  $4p^64d^{N-4}p^24d^{N+1} + 4p^64d^{N-1}4f$  UTA in ionized tin.

# Z-Dependence of Single Electron Orbitals in Neutral Atoms

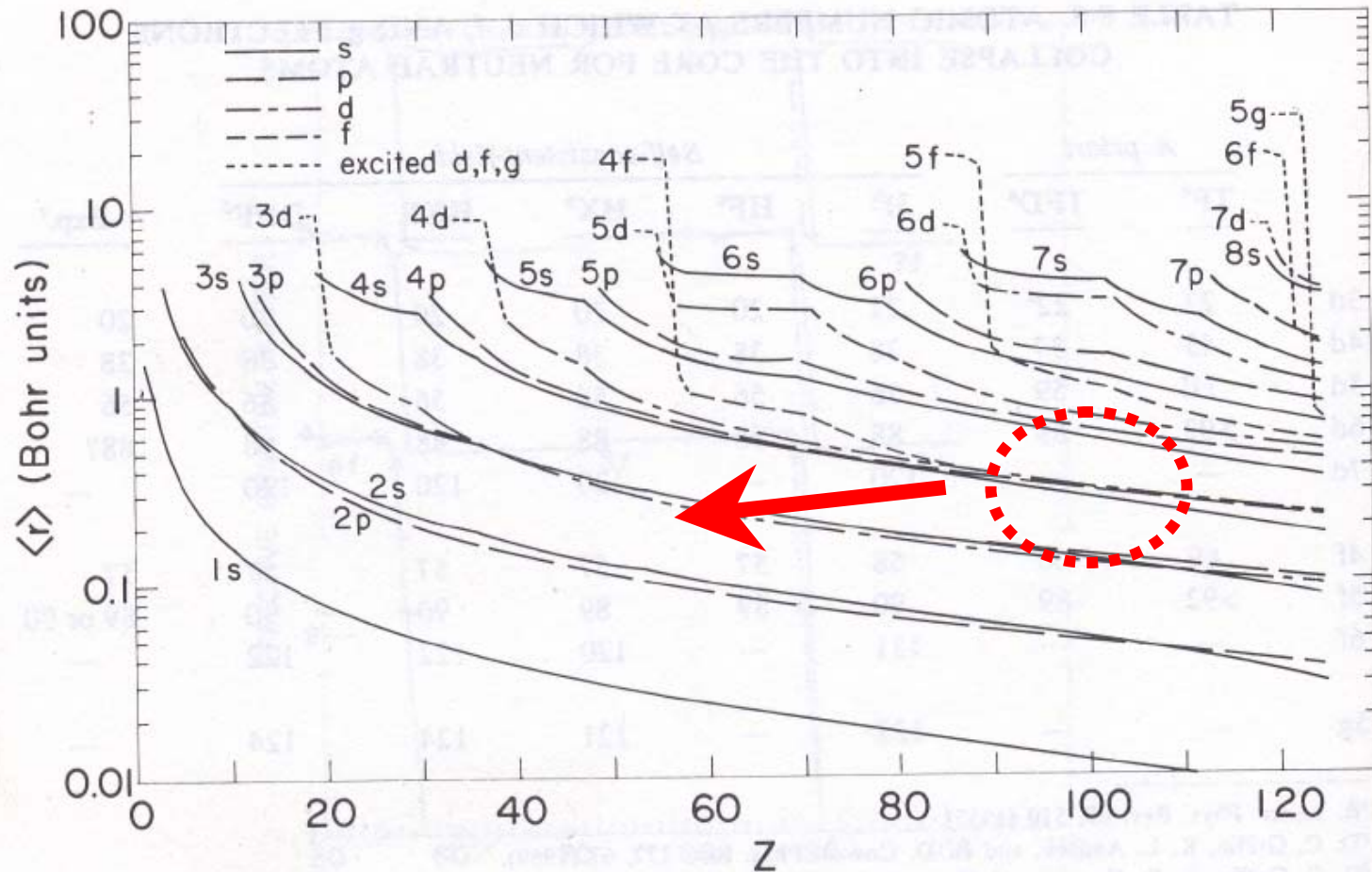


Fig. 8-10. Expectation values of  $r$  for the various orbitals of neutral atoms, computed by the HXR method. (The 3s and 3p curves are indistinguishable for  $36 \leq Z \leq 80$ .)

R.D.Cowan, *The Theory of Atomic Structure and Spectra* (Berkeley, 1981)

# Z-Dependence of Single Electron Orbital Energies in Neutral Atoms

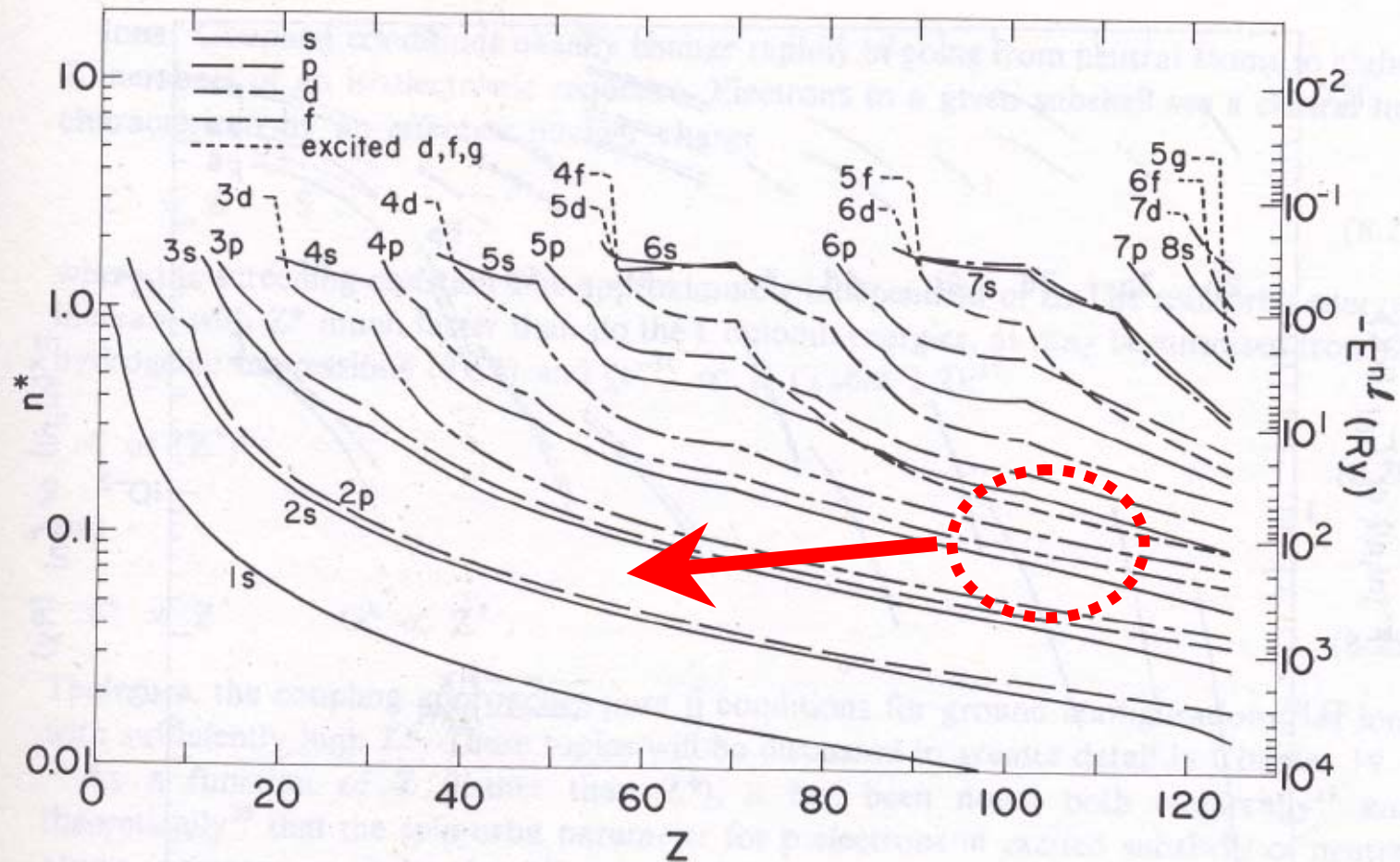
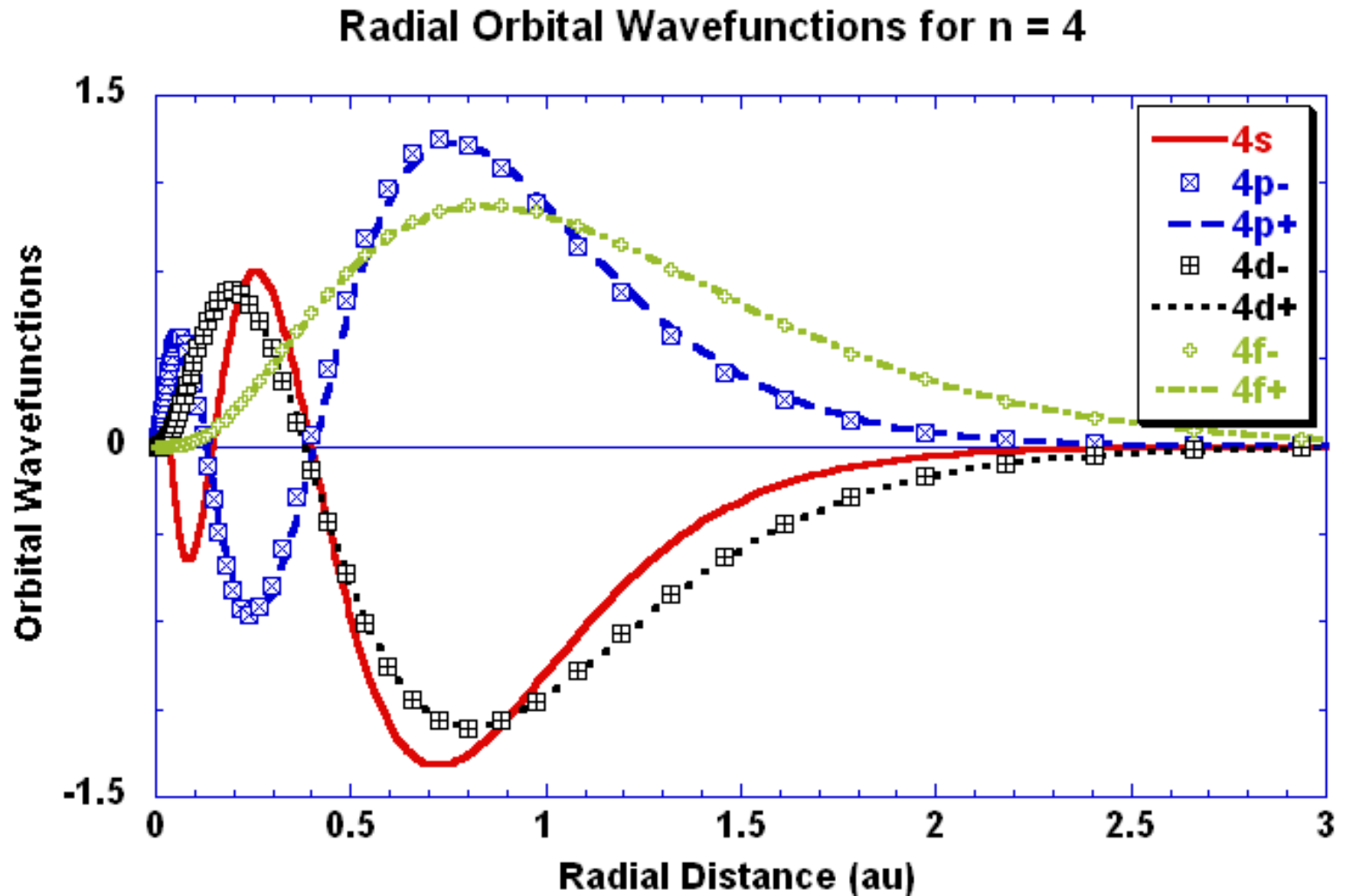


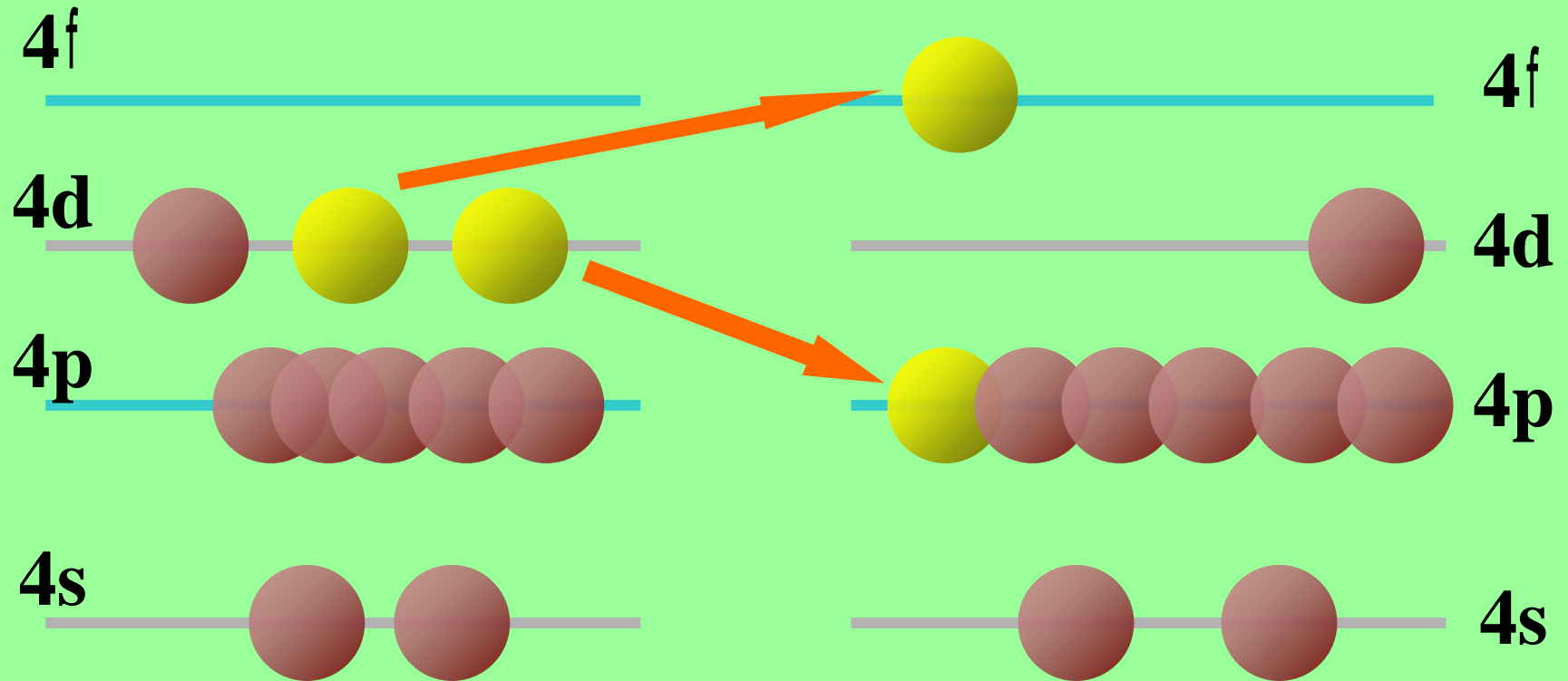
Fig. 8-11. One-electron binding energies  $|E^{nl}| \cong |\epsilon_{nl} + E_c^{nl}|$  and effective quantum numbers  $n_{nl}^* = |E^{nl}|^{-1/2}$  for the various orbitals of neutral atoms, computed by the HXR method.

R.D.Cowan, *The Theory of Atomic Structure and Spectra* (Berkeley, 1981)

# Radial Wavefunction of Sn<sup>12+</sup>



# Configuration Mixing



# Orbital Hybridization

$$\begin{aligned} & (4d + 4p)(1) \cdot (4d + 4f)(2) \\ & + (4d - 4p)(1) \cdot (4d - 4f)(2) \\ & = 4d(1)4d(2) - 4p(1)4f(2) \\ & = C_1 (dd) + C_2 (pf) \end{aligned}$$

# Electron Densities and Transition Probabilities

$$\text{Case:} \quad = \quad (dd) + (pf)$$

Electron Density: Grows up at Outside

State Energy: Goes up Higher

Transition Amplitude: Constructive Interference

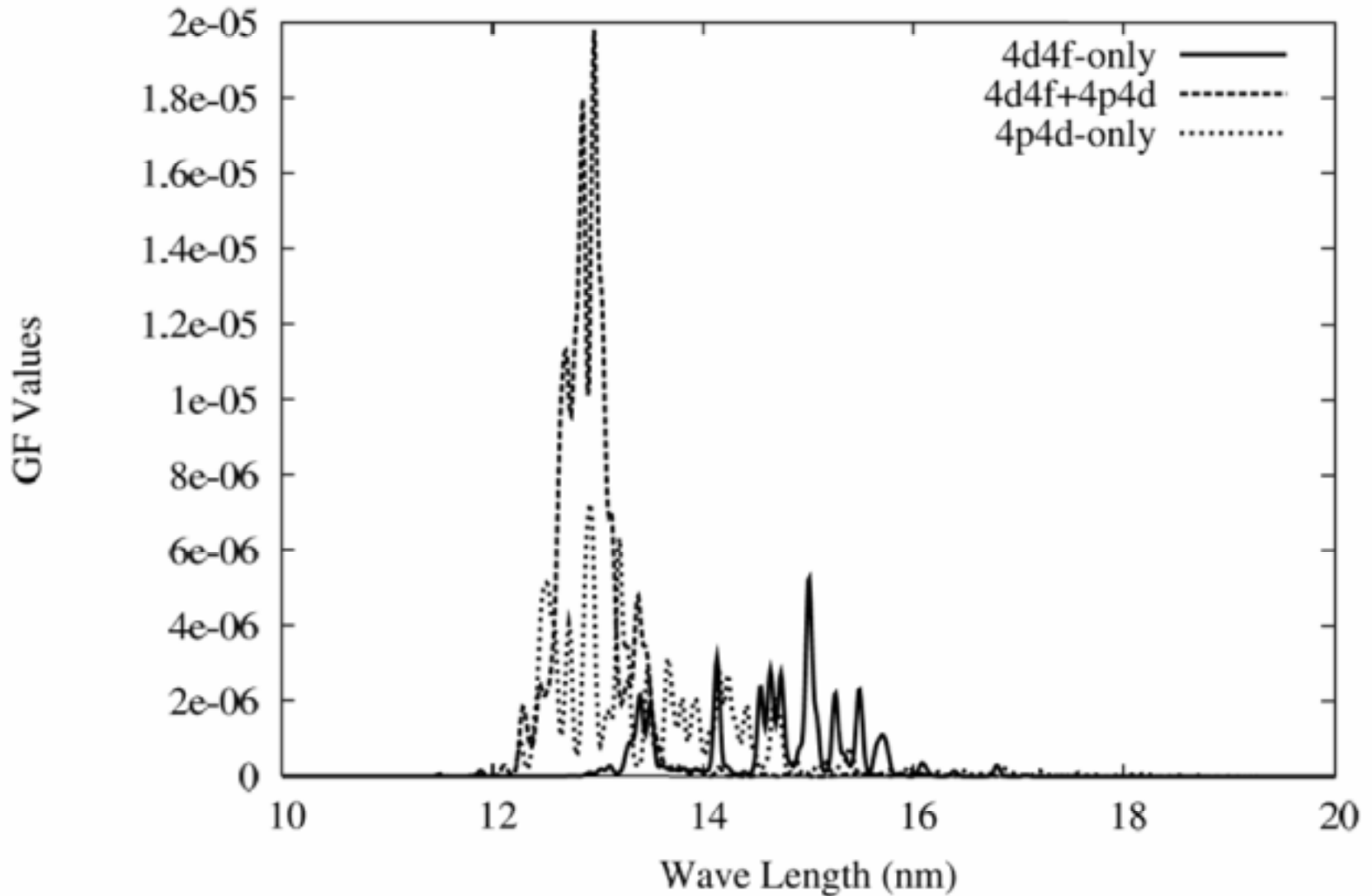
$$\text{Case:} \quad = \quad (dd) - (pf)$$

Electron Density: Grows up at Inside

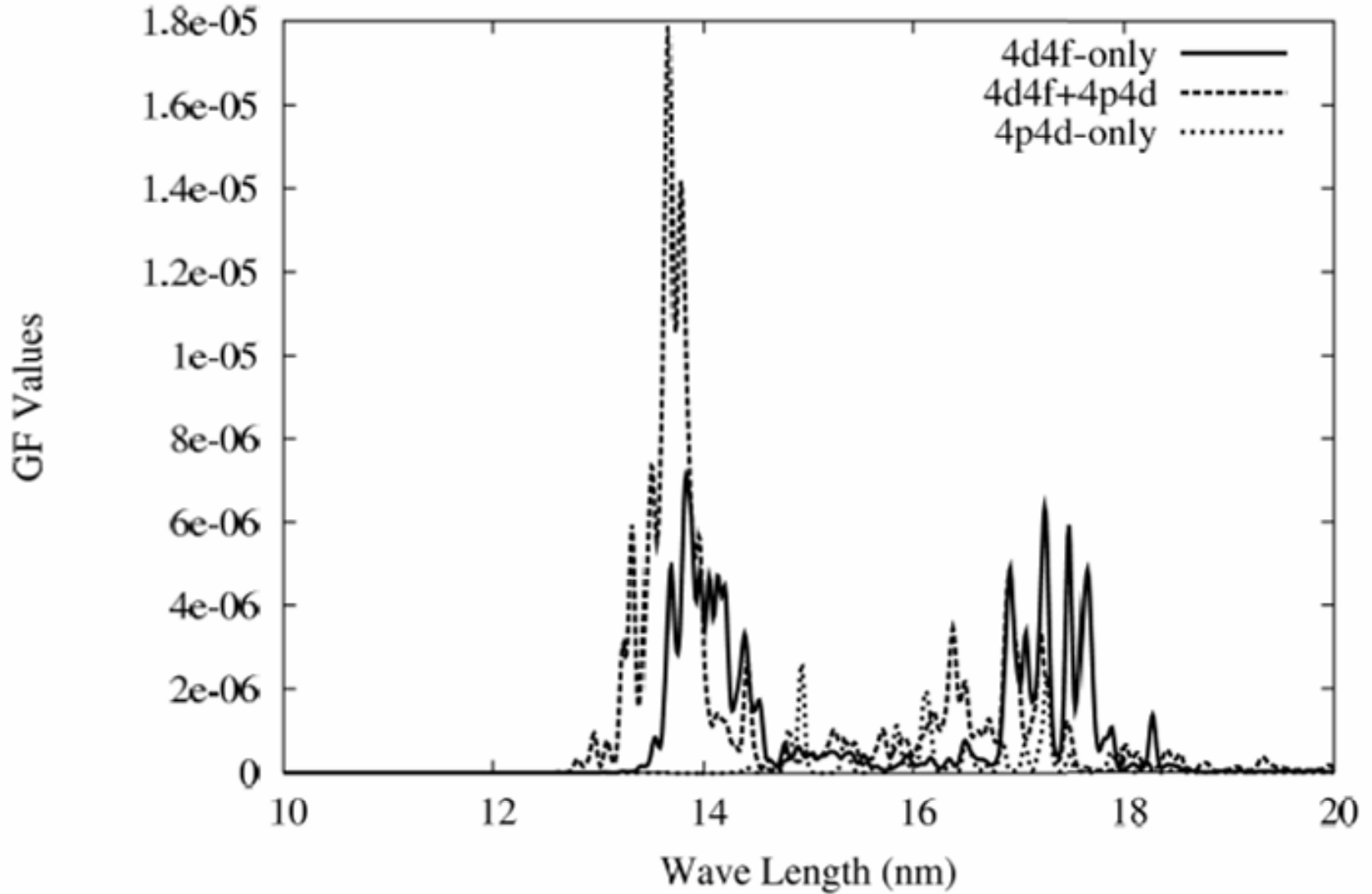
State Energy: Goes down Lower

Transition Amplitude: Destructive Interference

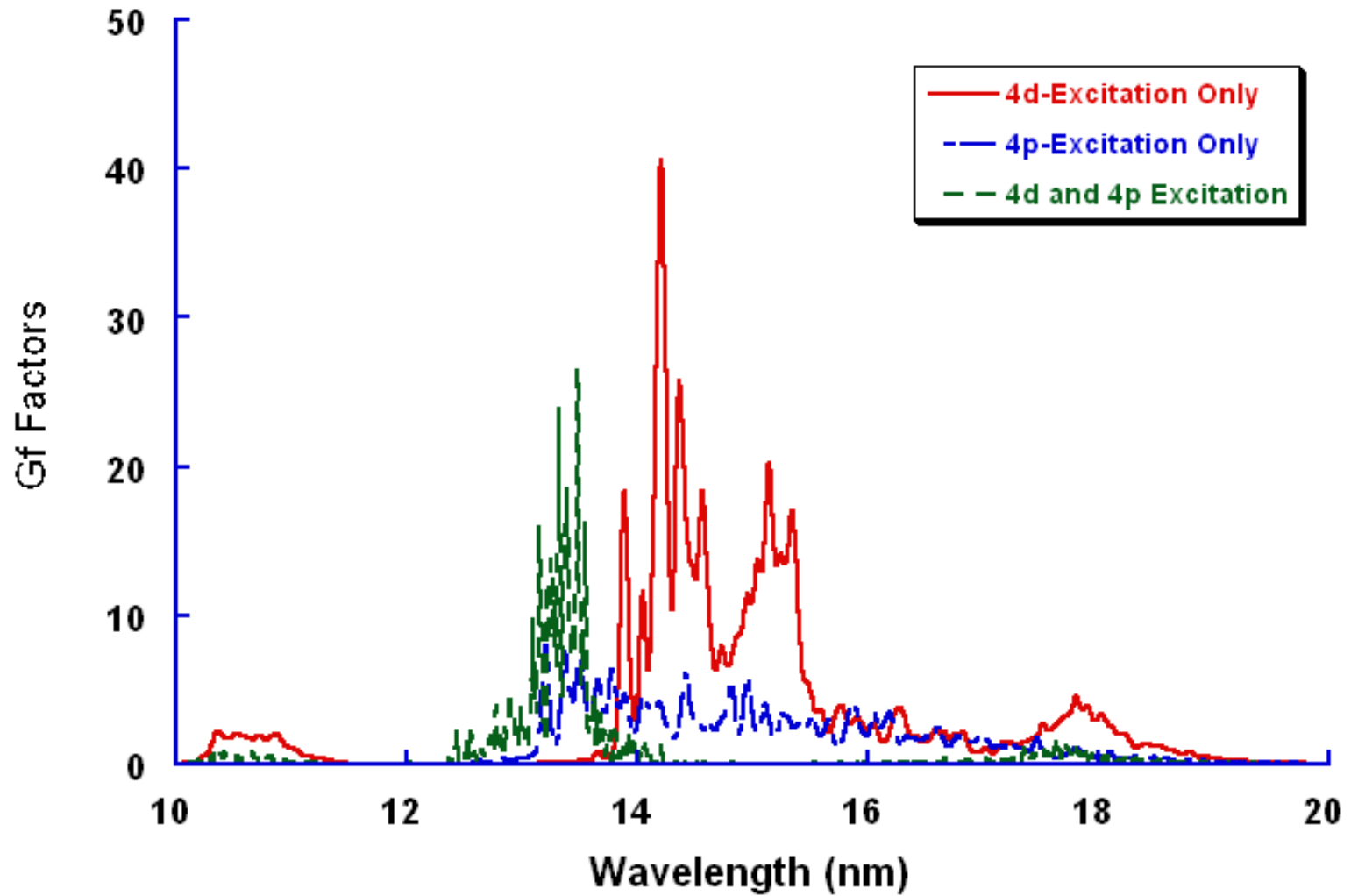
GF Value Distributions for Sn<sup>12+</sup>



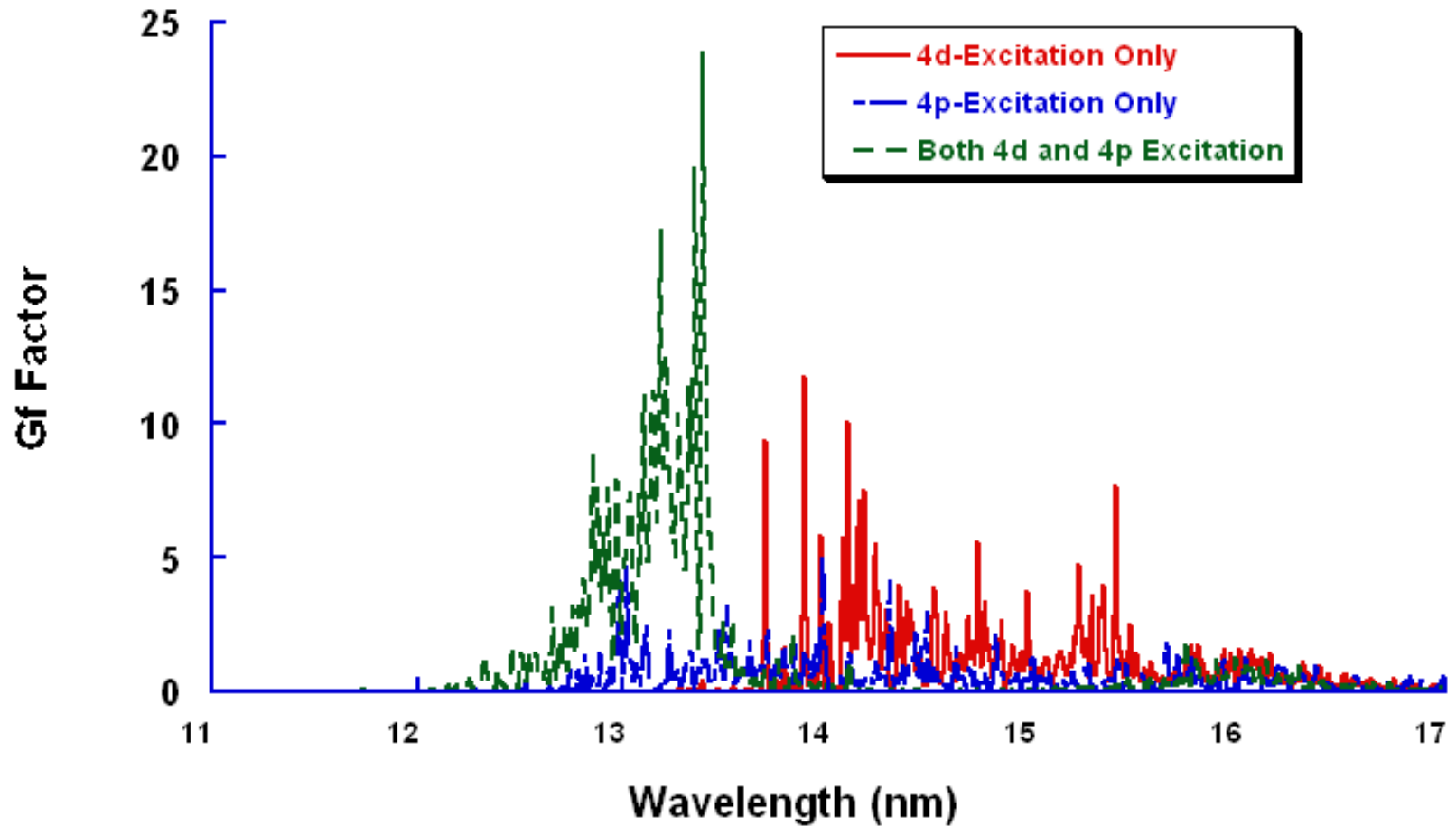
GF Value Distributions for Sn<sup>06+</sup>



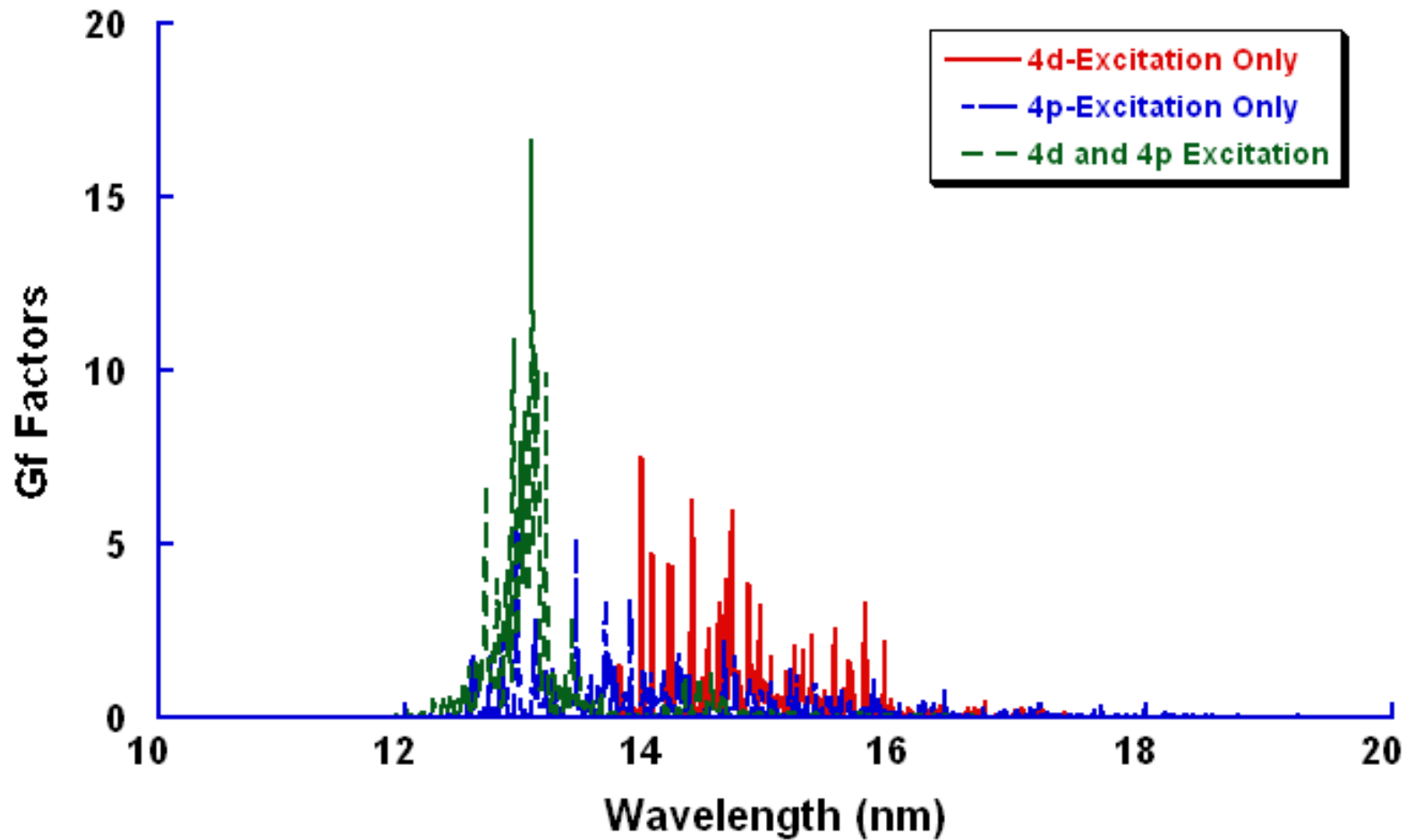
### Gf Factor Distribution of Sn09+ Ions



## Gf Factor Distributions in Sn 10+ Ions



## Gf Factor Distribution in Sn11+ Ions



# Summary

- *dd – pf* type configuration mixing has been considered for 13.5 nm band optical radiation of Sn ions
- Strong configuration interactions have been observed in Sn<sup>8+</sup> to Sn<sup>12+</sup> ions
- The spectral narrowing is the effect of interference between the *4d – 4p* and *4f – 4d* transition amplitudes.
- The use of the ions in the range  $q=9$  to 11 might be plausible to obtain efficient narrow band radiation around 13.5 nm.