EUV emission from tin plasmas

James Colgan, A. J. Neukirch, D. P. Kilcrease,
J. Abdallah, Jr., M. E. Sherrill, C. J. Fontes, P. Hakel

Los Alamos National Laboratory

Francesco Torretti, Ruben Schupp, Joris Scheers,
John Sheil, Oscar Versolato
ARCNL, Amsterdam, The Netherlands

jcolgan@lanl.gov

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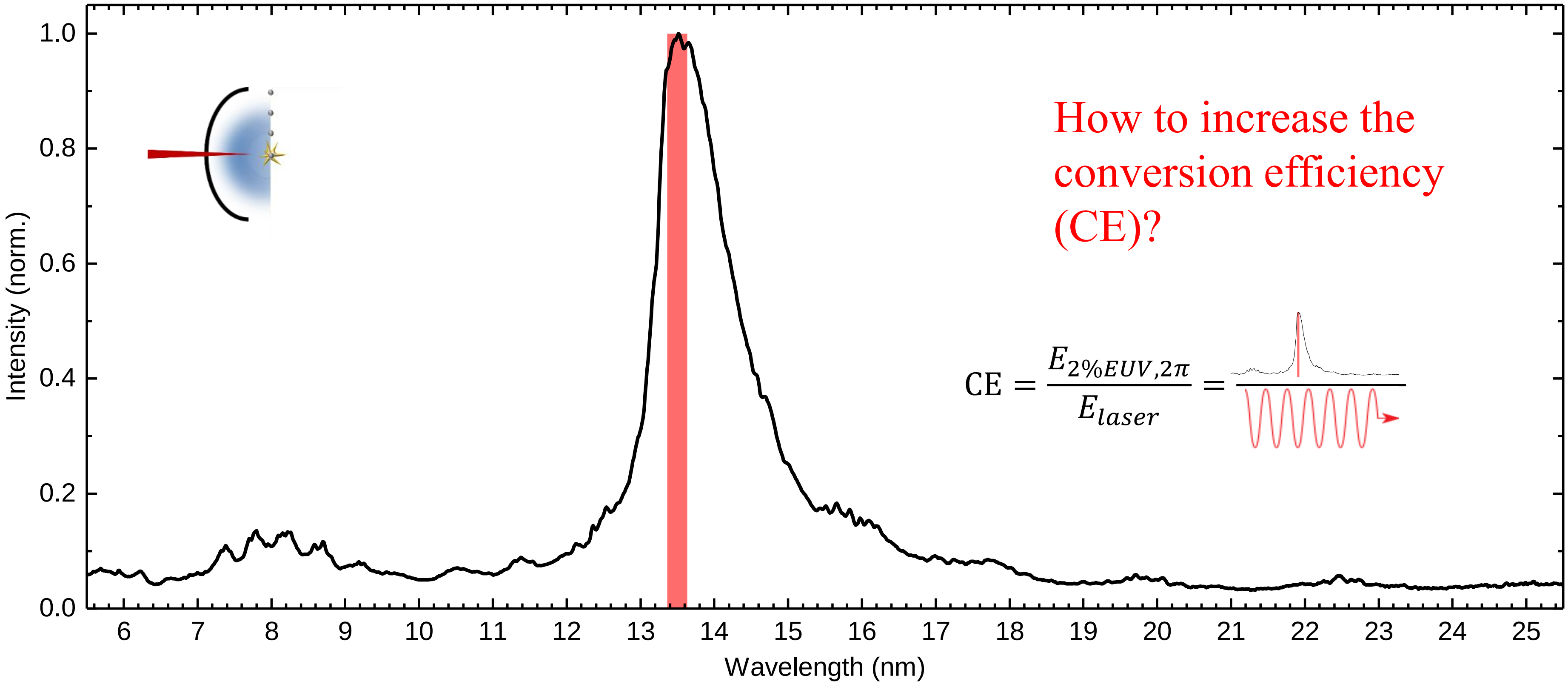
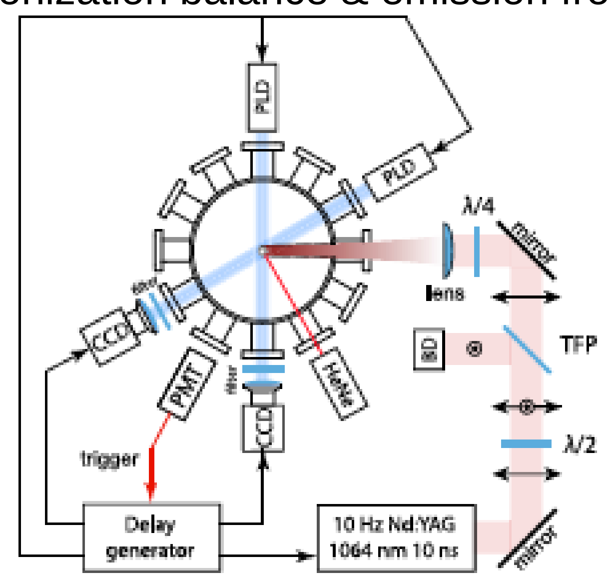
Why do we care about emission from tin? - lithography

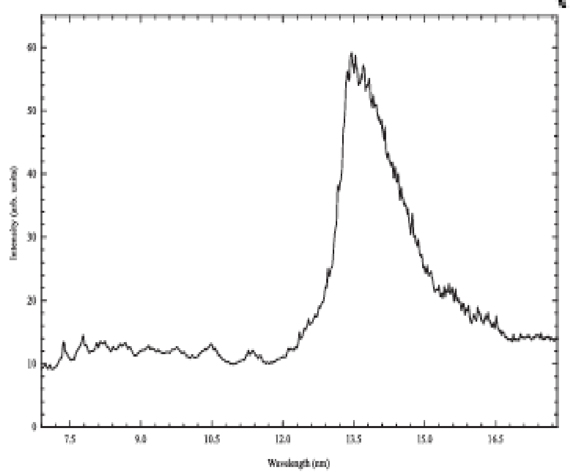


- A laser-produced Sn plasma emits strong radiation in a narrow band centered around **13.5 nm**. This has high potential as an efficient EUV radiation source for use in the micro-electronics industry. The challenge is to make this efficient!

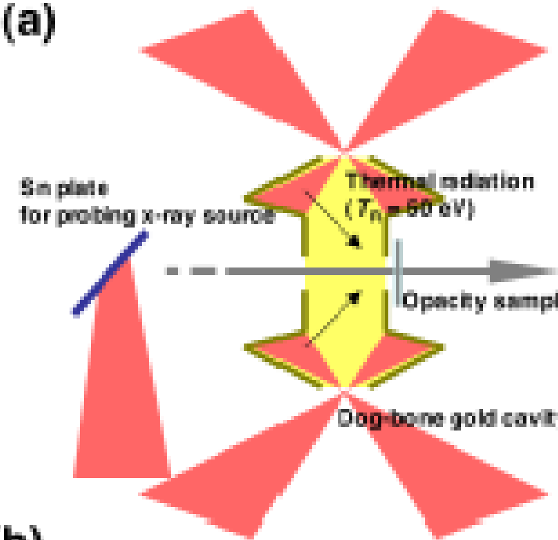
Why do we care about emission from tin? – atomic physics

- We are always interested in measurements that will help us validate our atomic physics models
- The plasma conditions (around 30 eV, 0.1% or less of solid density) lead to emission from Sn ions that have between 7-14 electrons removed
- The challenge for theory is to accurately describe these due to strong configuration-interaction effects in the atomic structure involving 4p-4d and 4d-4f transitions
- AND construct a plasma model that can efficiently predict the ionization balance & emission from such a plasma

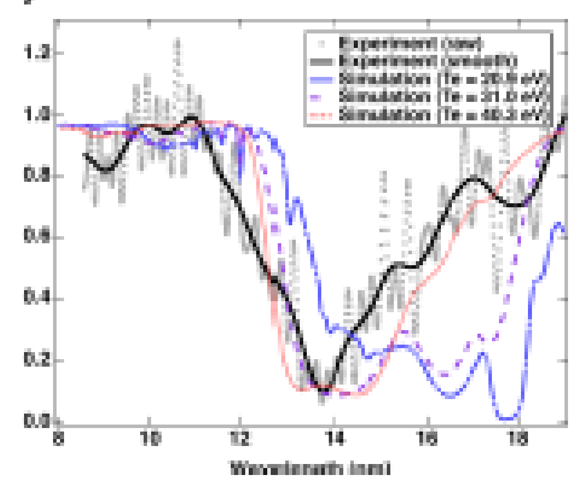




(a)



(b)



The LANL suite of atomic modeling codes

Atomic Physics Codes → Atomic Models → ATOMIC

CATS: Cowan Code

RATS: relativistic

ACE: e^- excitation

GIPPER: ionization

http://aphysics2.lanl.gov/tempweb

fine-structure
config-average
UTAs
MUTAs
energy levels
gf-values
e^- excitation
e^- ionization
photoionization
autoionization

LTE or NLTE populations

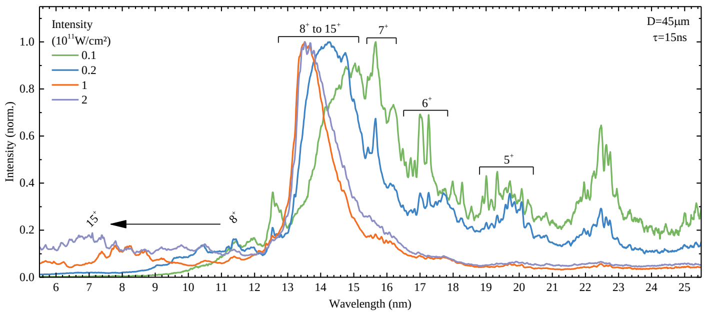
spectral modeling
emission
absorption
transmission
power loss

Atomic structure calculations - additions

- Our version of **Cowan's code** (**CATS**) has been extensively re-written into Fortran90 and parallelized so that each Jpi symmetry is on a separate processor of a parallel machine. This speeds up runtime considerably
  - Also, when computing dipole matrix elements (for gf values), each J/J' combination is also placed on a separate processor.
  - The memory requirements and runtime requirements are still considerable – sometimes 100s GB RAM memory and runtimes approaching one week per ion stage
  - We have a dedicated workstation to perform atomic structure calculations, with a large hard drive
- We also include a **2-mode** option. This modification allows a user-specified number of configurations to be treated with full configuration-interaction (CI), while any other configurations are treated through intermediate-coupling (IC).
  - IC is much cheaper, computationally, and many (up to 10^4 configurations or more) may be treated this way. This provides enough excited configurations to ensure a well-converged partition function when computing an opacity.
- The **scale factors** used in CATS are defaulted to an option that was designed to scale with Z and ion stage. We have used these for the ground state to excited state calculations, but modified the scale factors for the excited-state to excited state calculations.

Scale factors? According to Cowan, these are necessary to improve agreement with experimentally measured transition wavelengths – and are used to account for the "***infinity of small perturbations***" that are necessarily omitted in practical calculations

Defining the atomic physics problem – accuracy and quantity of data both issues

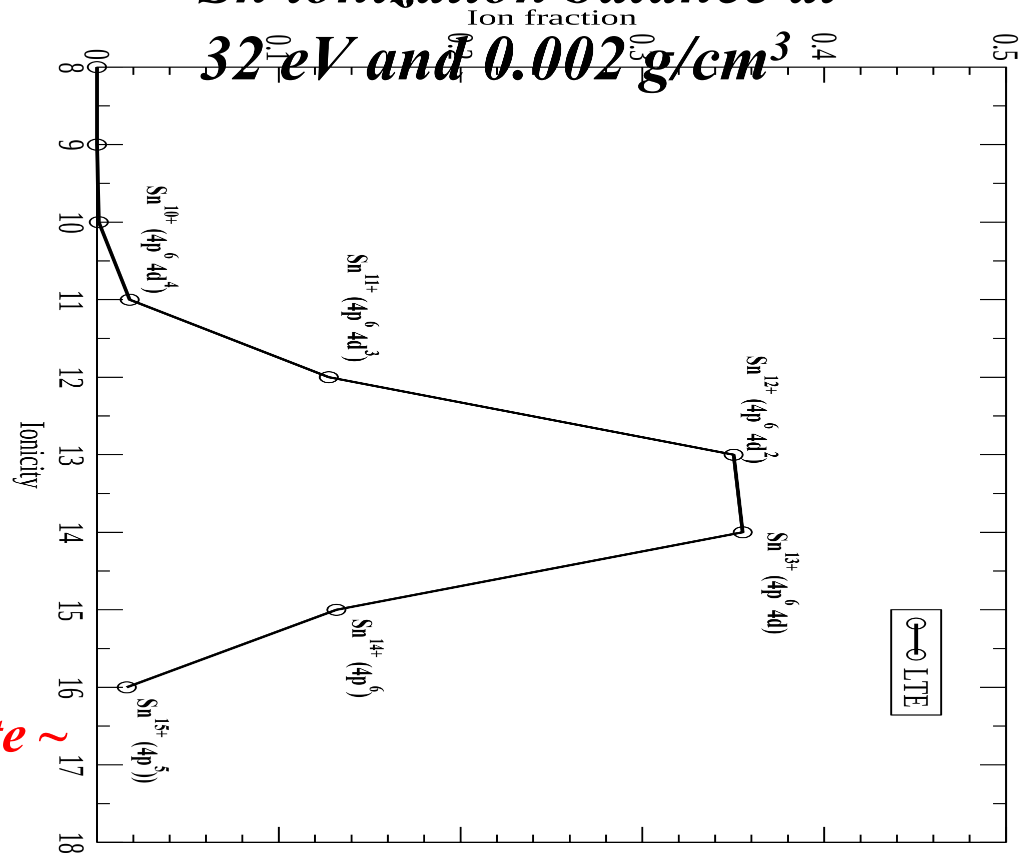


Our FS model contains all the configurations we expect to be important for CI effects:

- ***Sn 14+: 114 cfgs; 94115 levels***
- ***Sn 13+: 135 cfgs; 273330 levels***
- ***Sn 12+: 94 cfgs; 355742 levels***
- ***Sn 11+: 81 cfgs; 259181 levels***

Just these 4 ionization stages generate ~ 30 billion dipole-allowed transitions!

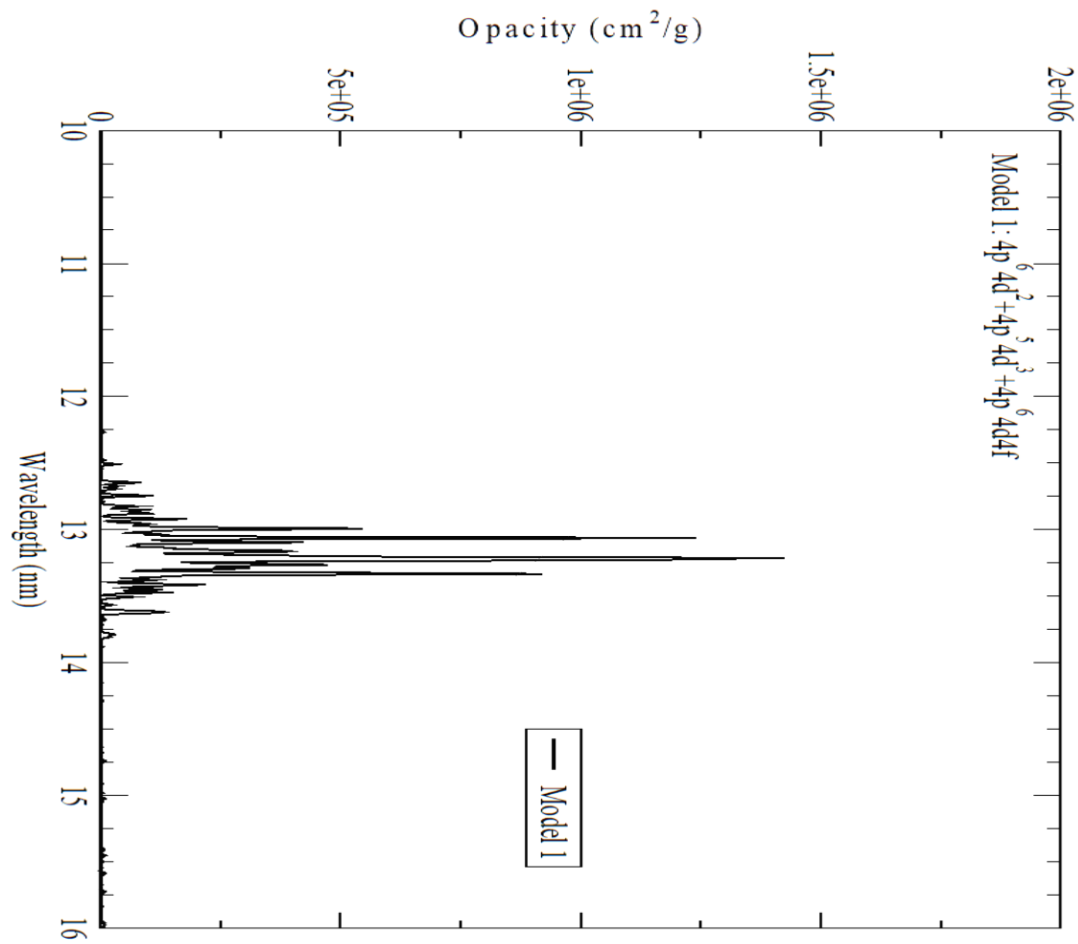
Sn ionization balance at 32 eV and 0.002 g/cm³



Sn opacity convergence study: Sn^{12+}

- ***How does the position and magnitude of the absorption features change as more configurations are added?***

Model 1: 3 cfgs; 141 levels; 547 transitions



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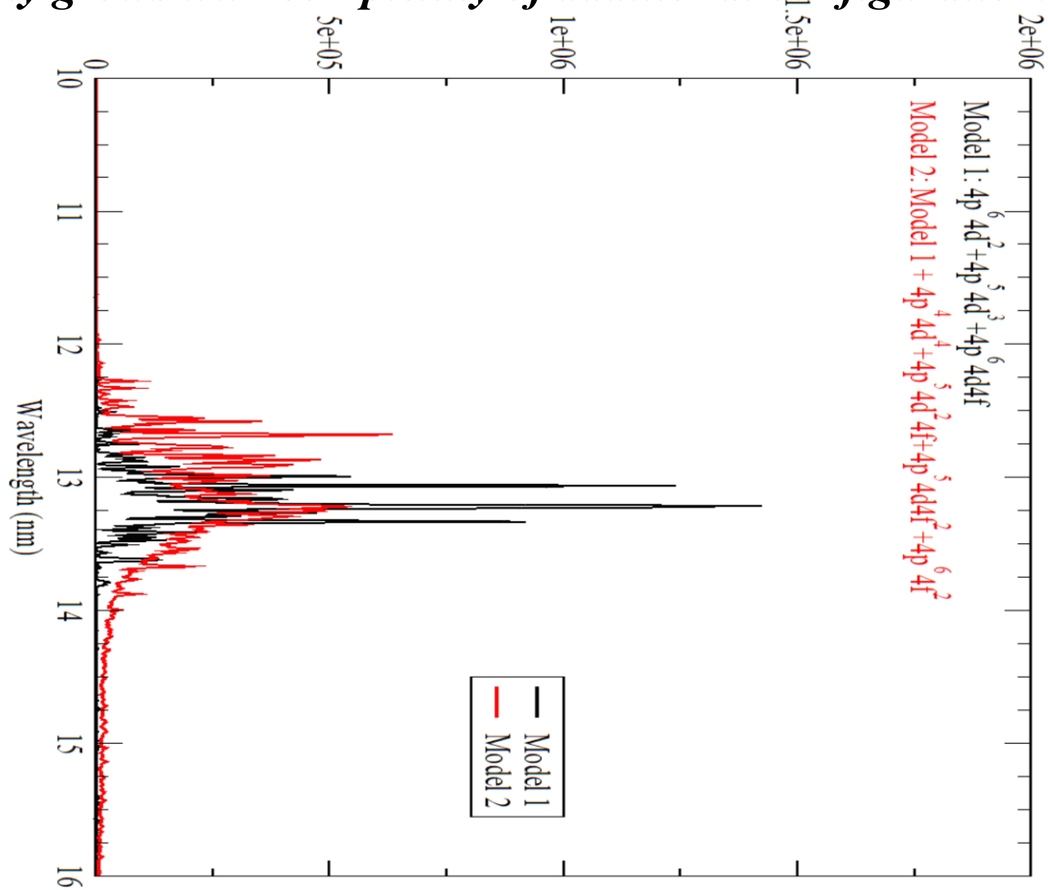
Number of levels & transitions quickly grows with complexity of additional configurations

Model 1: 3 cfgs; 141 levels; 547 transitions
Model 2: 7 cfgs; 1696 levels; 282216 transitions



Significant difference is caused by addition of just a few configurations

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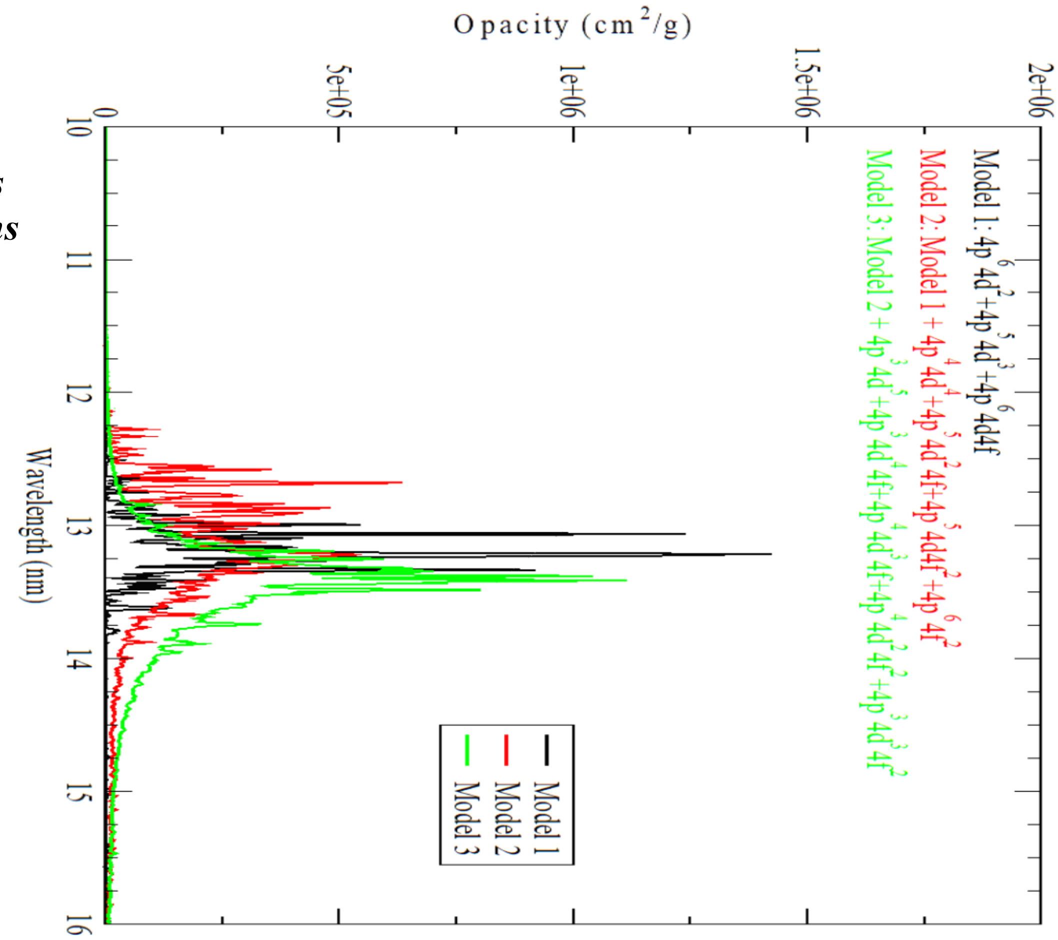

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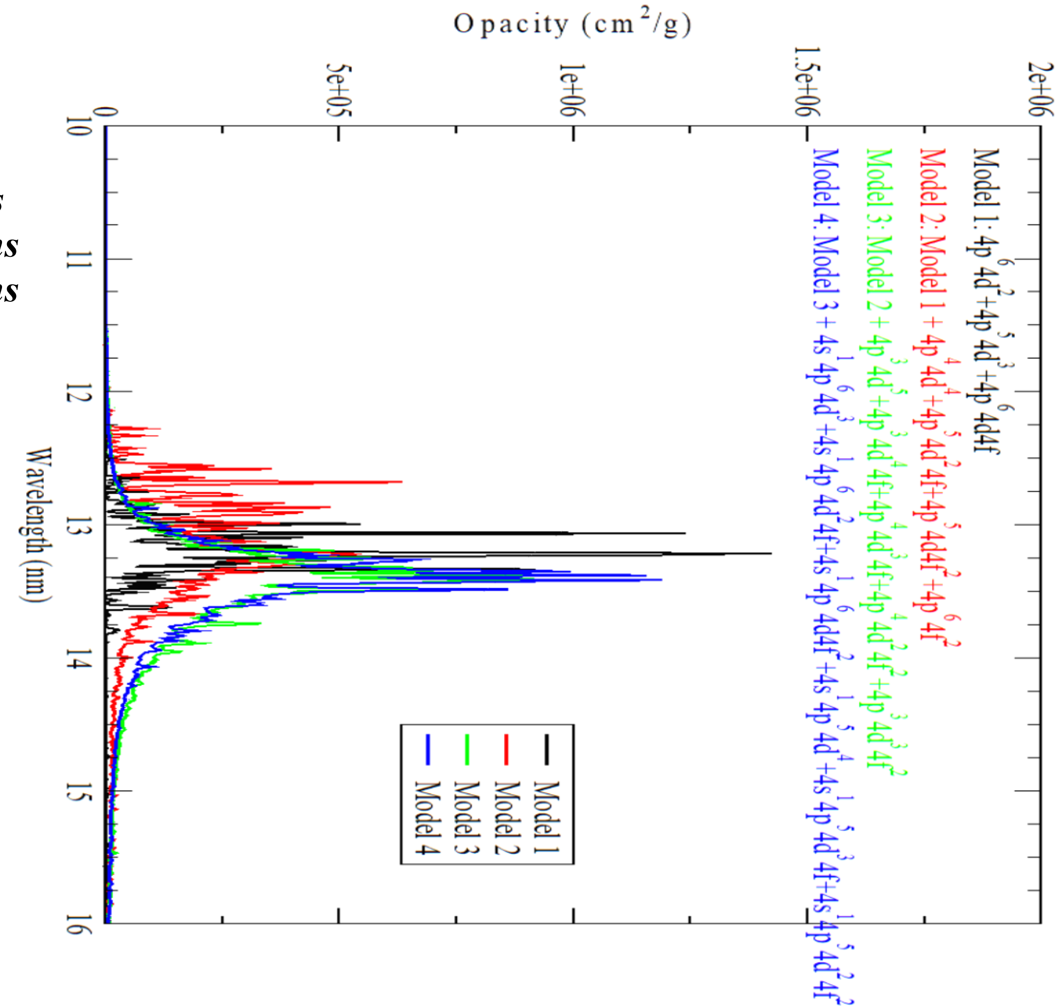

Main feature around 13.5 nm starts to show signs of convergence

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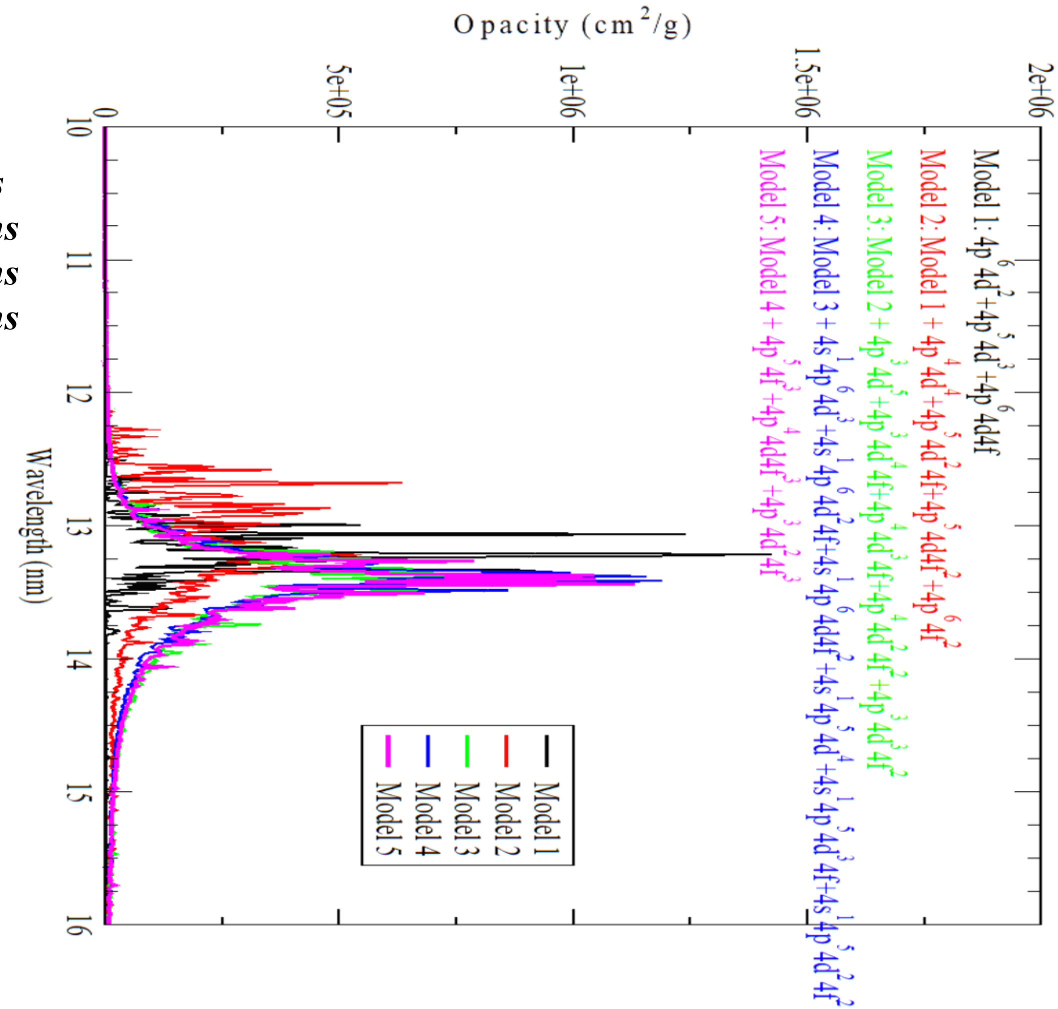

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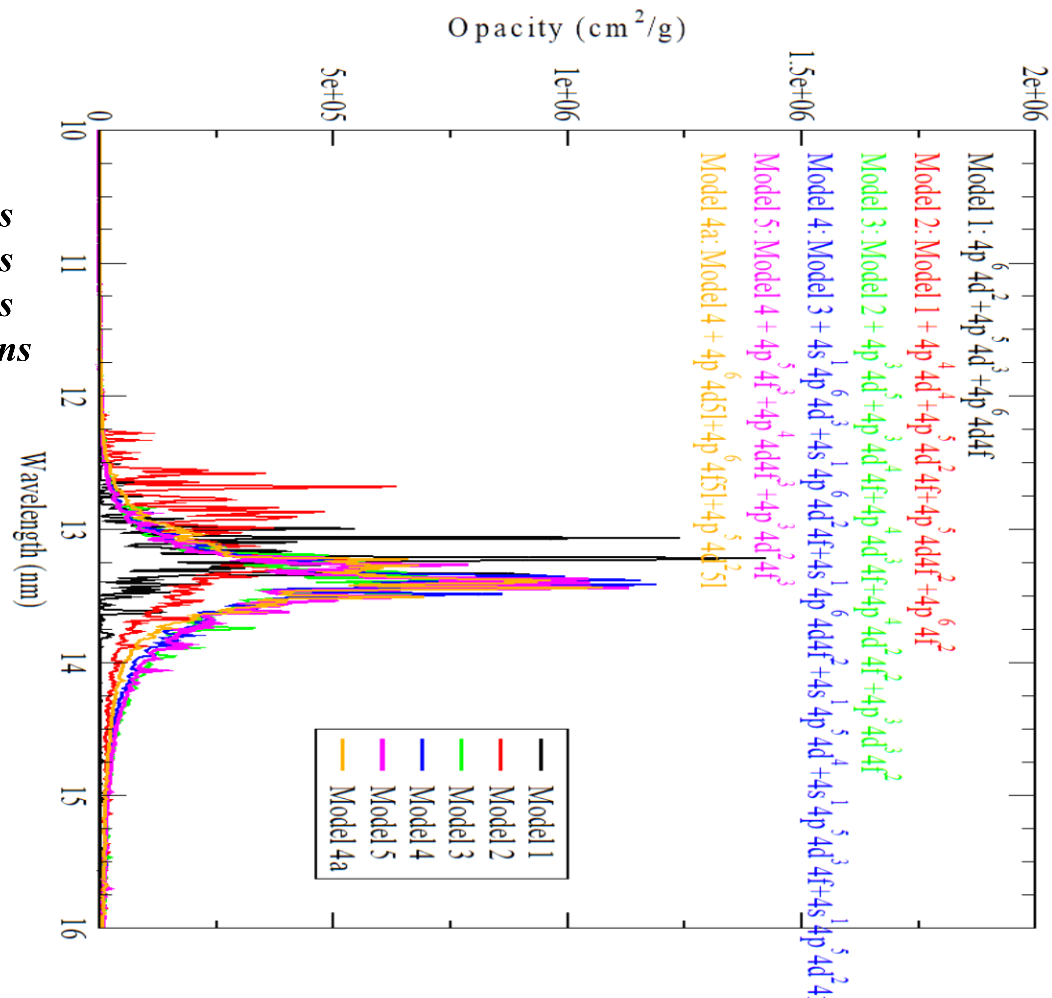
Model 4a: 33 cfgs; 50561 levels; 200M transitions



Addition of excitations to n=5 also modify the main feature

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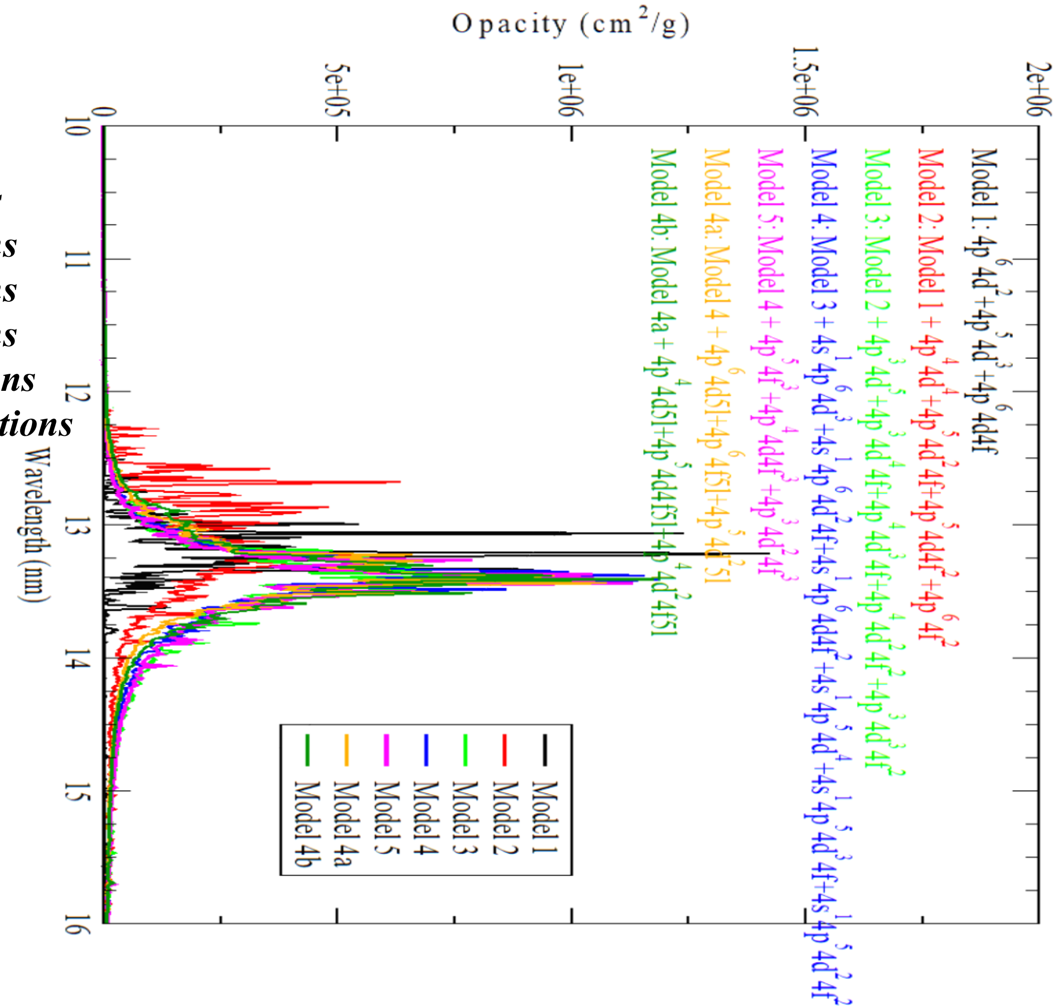

Addition of excitations to n=5 also modify the main prominent feature

Sn opacity convergence study: Sn^{12+}

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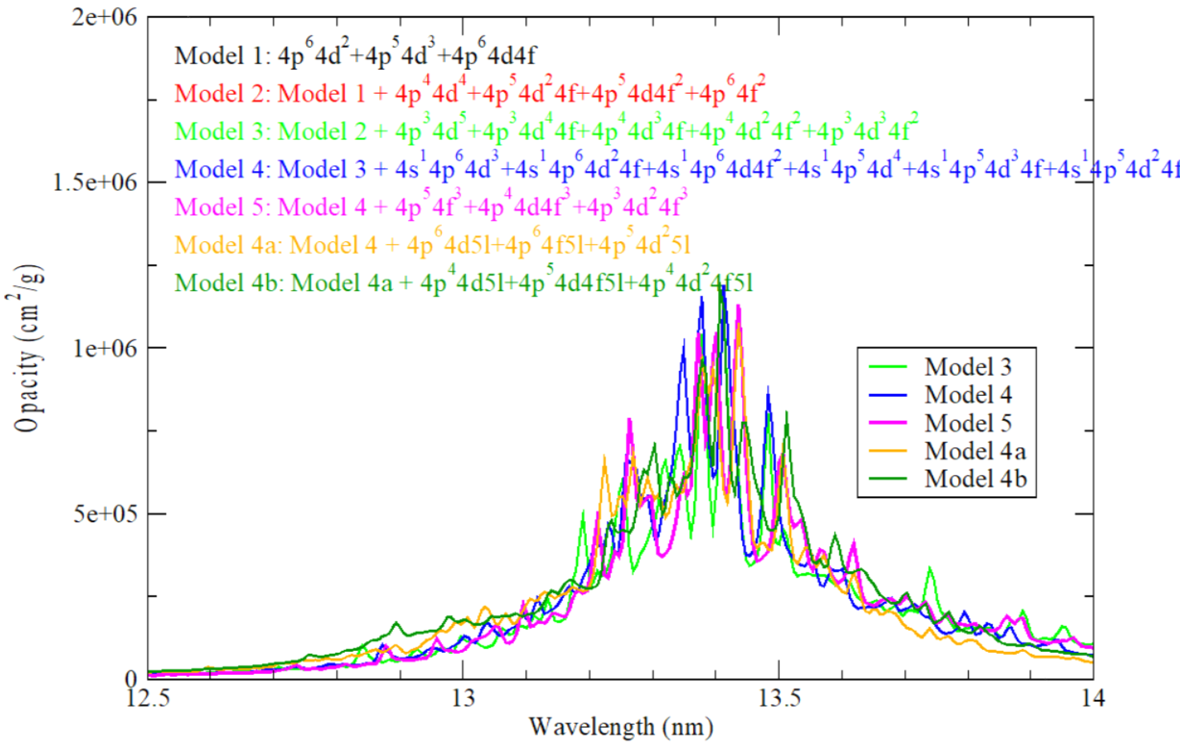
However: closer examination of the individual features shows that absolute convergence is difficult to obtain!



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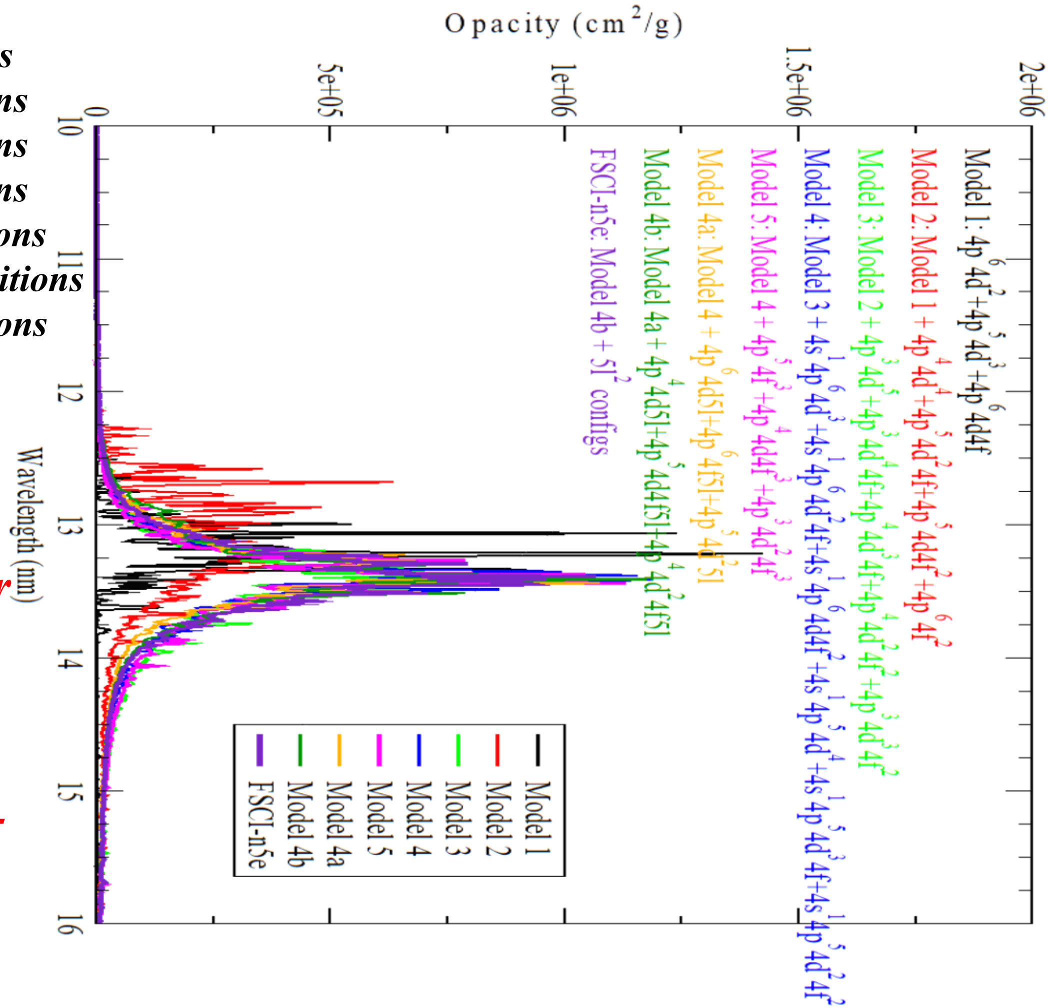
FSCI-n5e: 94 cfgs; 355742 levels; 10B transitions



- *FSCI model appears reasonably well converged with respect to main absorption feature*
- *This is then repeated for all other relevant ion stages*
- *Calculations are extended using our "2-mode" method to include contributions from other, higher-lying, transitions*

Conclusions & Future Work

- Emission spectra of Sn plasma at moderate temperatures is very demanding to compute
- Configuration-interaction is very important in such species, making the structure calculations complex and demanding
- Multiply excited states are found to make significant contributions to the plasma, even at moderate densities
- Agreement with laser-produced plasma measurements is very encouraging
  - Comparisons also show that taking into account radiation transport effects is important
- We continue towards our ultimate goal of a predictive set of opacity and emissivity calculations for such systems