Integrated peturbative and non-perturbative collisional calculations underpinning magnetically-confined plasma diagnostics, with propagated uncertainties

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Outline

- Motivation
- Baseline and Monte-Carlo Collisional Radiative Models
- Secondary derived atomic parameters that

  are temperature and density dependent

  (Effective ionisation/recombination/excitation)

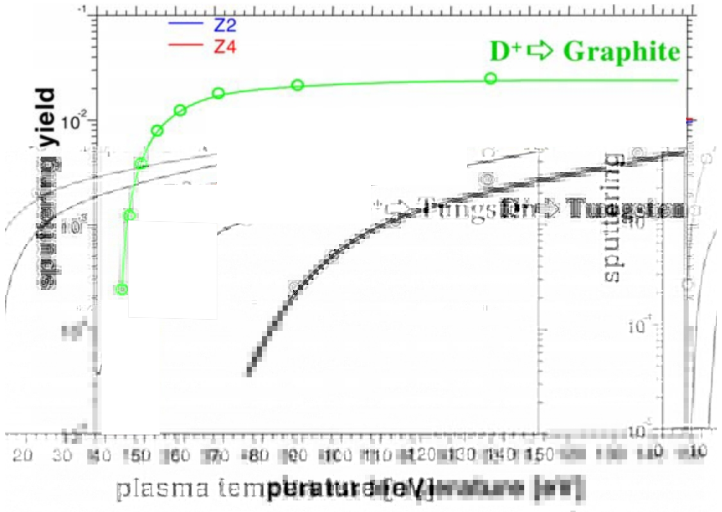
  => ionisation fraction,

  => SXB impurity influx

  => radiative power loss
- Challenges (Near Neutral W and Mo)

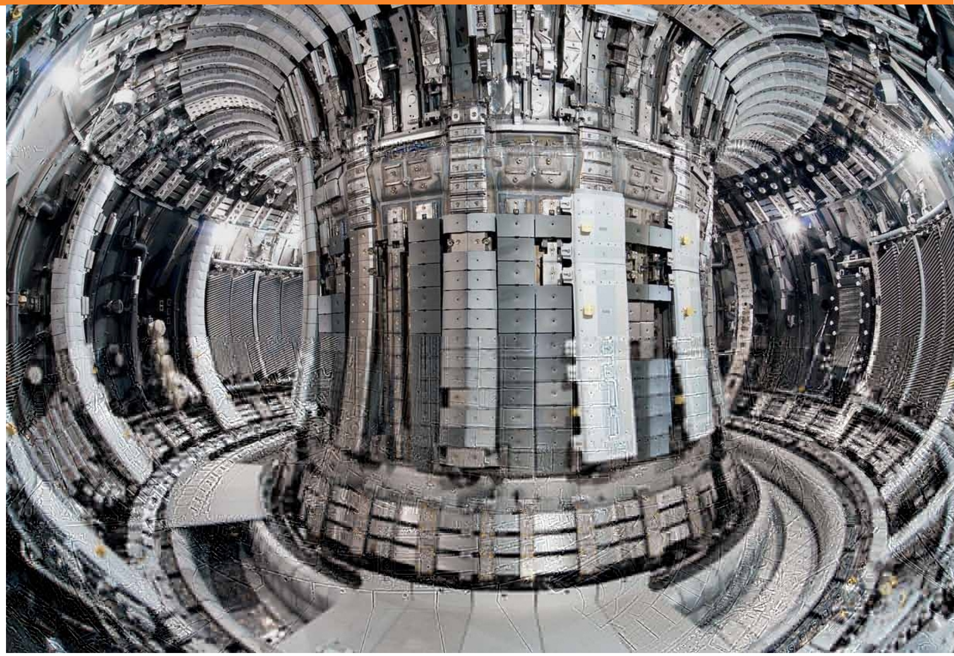
Motivation: High-Z materials are leading candidates for first wall materials in future fusion energy devices

- Reactor temperatures and heat flux will require new high-Z materials
    - High melting point and thermal conductivity
    - Reduced sputtering
    - Tritium retention is reduced
    - First wall lifetime is increased



- Tungsten (W) is a leading candidate for the divertor material for ITER

- Mo is presently being used on NSTX-U as the first wall material

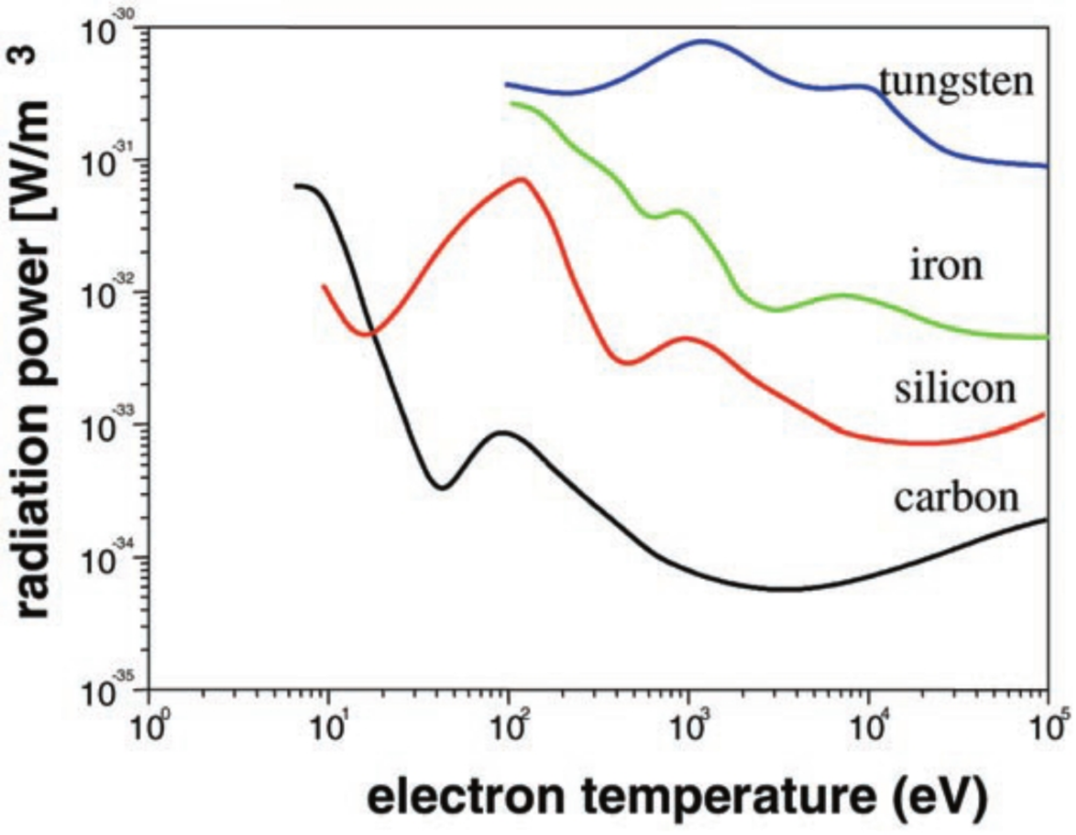


Inside of the JET tokamak W divertor, Be walls euro-fusion.org

“There is an urgent need in the fusion energy community to understand the rate of high-Z material erosion presently – DIII-D 5 year plan”

Motivation: High-Z materials are leading candidates for first wall materials in future fusion energy devices

- ***Allowable impurity concentration lower for high-Z materials***
  - High-Z materials radiate much more than previously used materials
  - Radiation significant enough to denigrate plasma performance
    - Concentration needs to be less than ~1E-4 (Putterich)
  - Need to accurately quantify and minimize erosion of wall



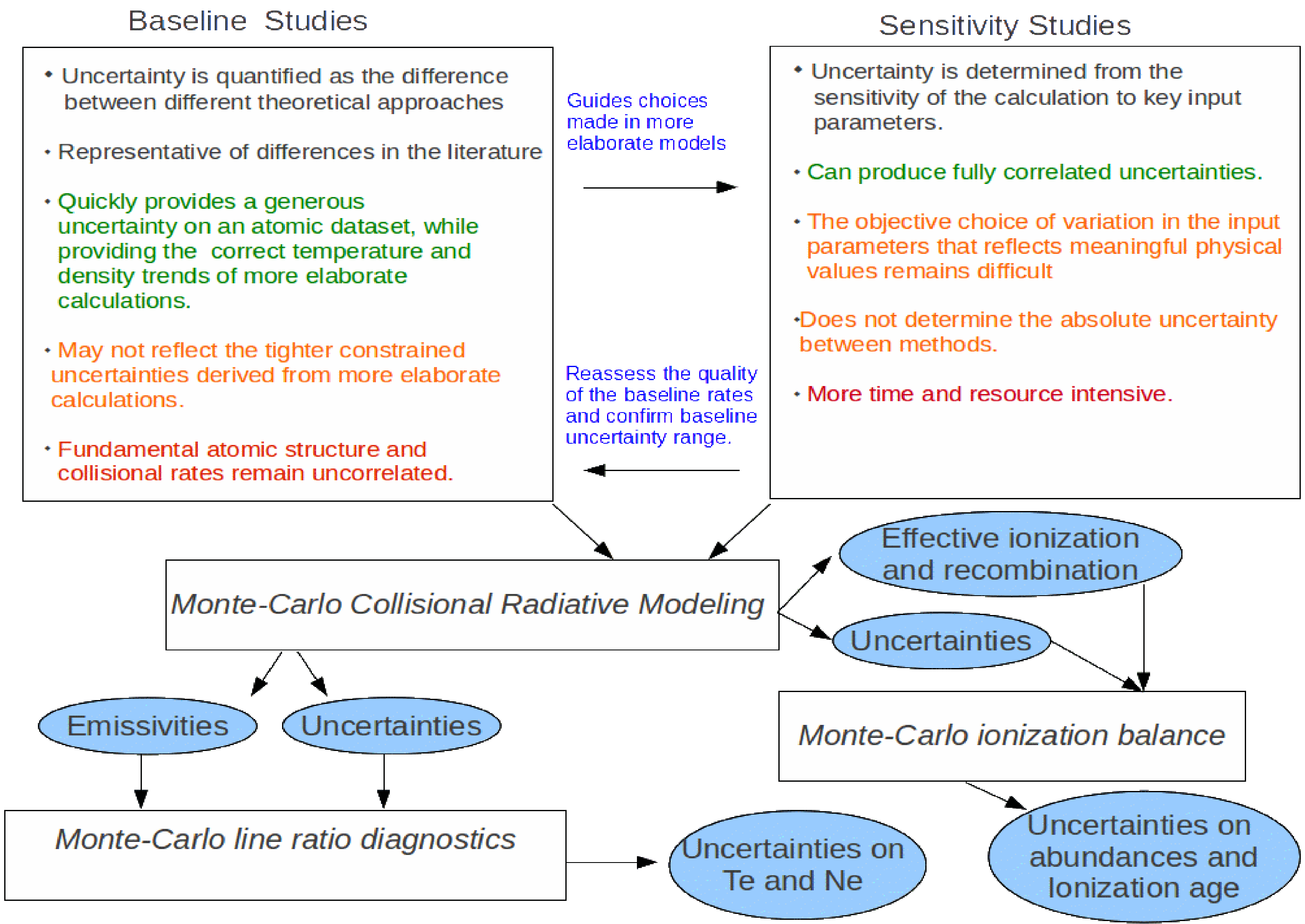
V. Philipps

Uncertainty analysis : Baseline vrs Monte-Carlo

We categorize the problem into 2 groups:

- ***Baseline*** uncertainty data to give an indication of the parameter space
- ***Method sensitivity*** uncertainty data with tighter and more realistic error bars.
- The approach is valid for both astrophysical and tokamak plasma regimes.

Baseline vrs Monte-Carlo



Monte-Carlo RMPS approach

Initially, we shall require complete data sets for the lighter fusion related elements, before moving to the heavier Tungsten-like elements.

To do list : For every ion stage

a) Electron-impact (de-)excitation between every level/term, then convoluted with a Maxwellian

b) Ground and meta-stable ionisation

c) Ground and meta-stable recombination (RR, DR, 3 body)

(This has been scripted : Structure → Collisional rate)

But although a concern, our TDCC, our many hundred term CCC and RMPS calculations do this pretty well !

However, it is not these but the secondary derived quantities , that provide diagnostics or interface with transport codes (and are density/temperature dependent)

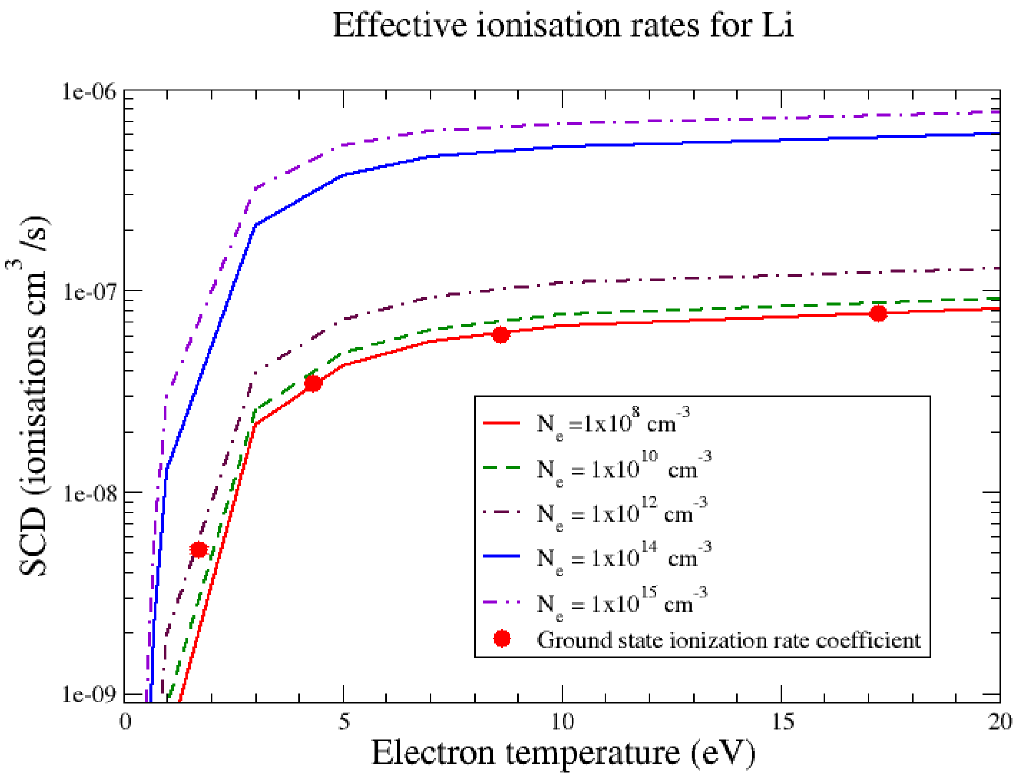
The generalized ionization rate coefficients are given by:

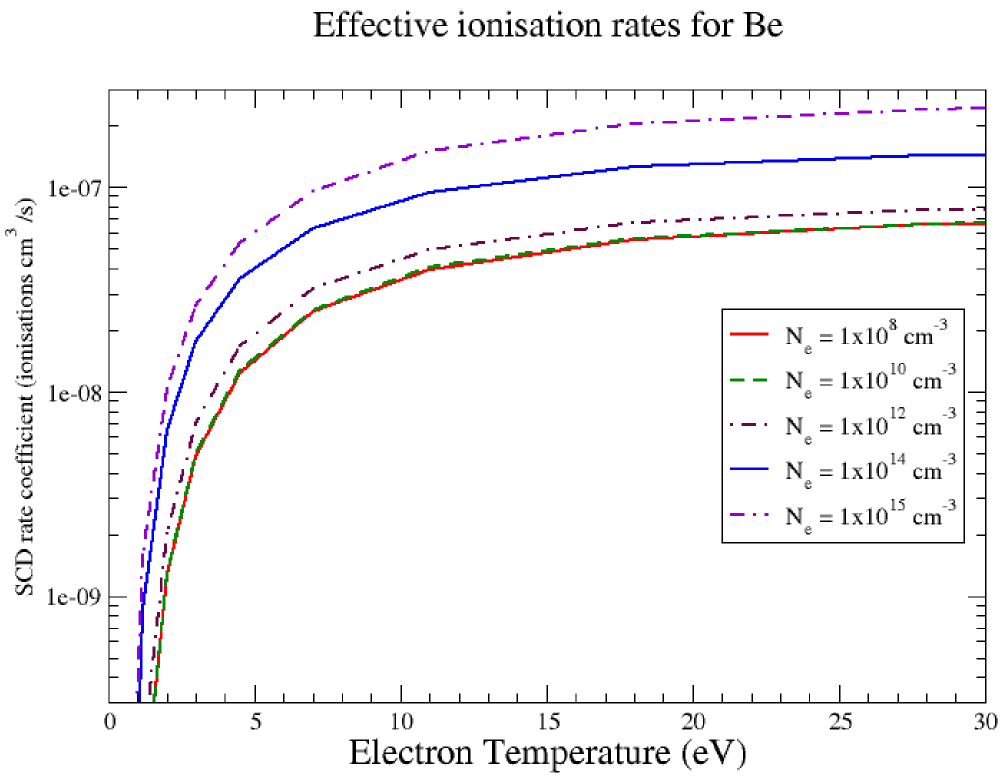
$$S_{\beta\to\gamma} = \mathscr{S}_{\beta\to\gamma} - \sum_{j} \mathscr{S}_{j\to\gamma} \sum_{j'} (\mathcal{C}^z_{jj'})^{-1} \mathcal{C}^z_{j'\beta},$$

For example, let us consider an effective ionization rate (temperature/density dependent)

It will be a function of the ground and excited state ionisation. The contribution from the excited states, requires knowledge of the excited state populations relative to the groundstate; in effect the solution to collisional radiative problem. Therefore, Our problem is now an explicit function of the atomic structure (A-values), the excitation/de-excitation rates, maybe even the ionisation/recombination of the neighbouring ion stages.

However, it is not these but the secondary derived quantities , that provide diagnostics or interface with transport codes (and are density/temperature dependent)





SXB ratio dependence on the effective ionisarion rate
Quantifying wall erosion with passive spectroscopy

- The intensity of a spectral line can be related to its influx rate [Behringer PPCF 31 2059 (1989)]
- The number of ionizations per photon (S/XB) is directly proportional to the impurity influx

$$\Gamma = \int_0^\infty N_e N^z S^{z\rightarrow z+1} dx$$

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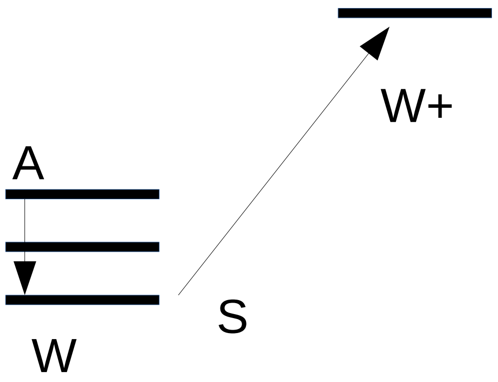

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$$= \int_0^\infty N_e SXB^z_{i\to j} \left(A_{i\to j}\frac{N_j}{N^z} \right) N^z dx$$

where $SXB^z_{i\to j} = \frac{S^{z\to z+1}(N_e, T_e)}{A_{i\to j}\frac{N_i}{N^z}(N_e, T_e)}$

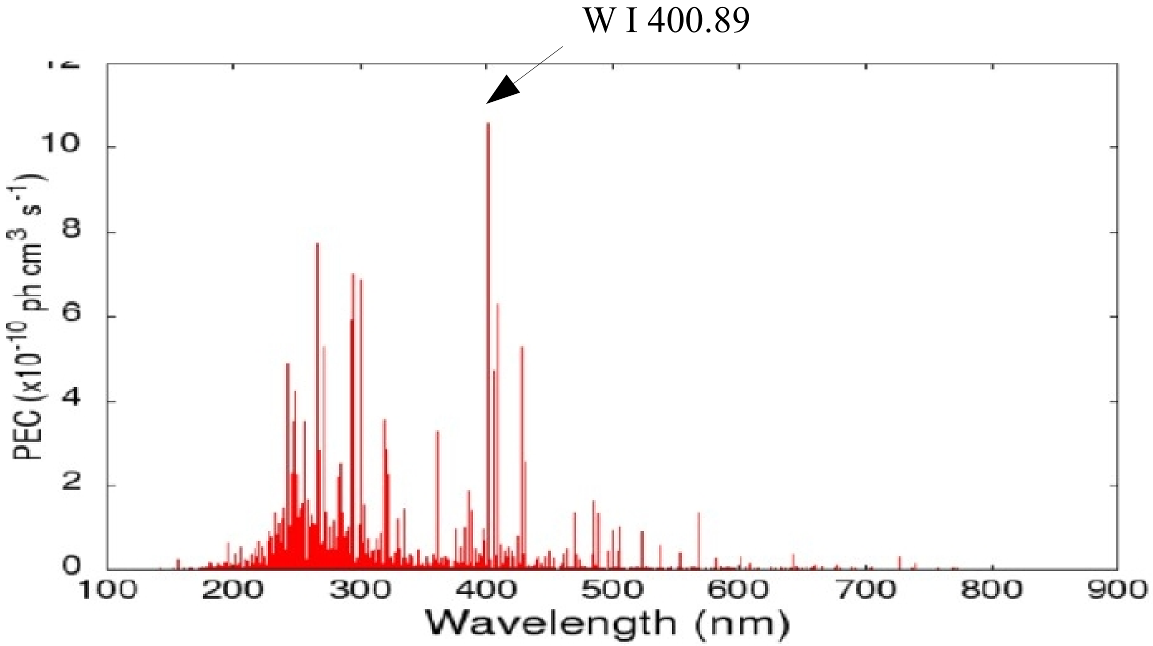
Note electron temperature and density dependence

Heavy species : Molydebnum and Tungsten

(Theory can provide a predicative capability, verified by experiment)

ADAS predicts spectral emission of W I to be predominately at UV wavelengths (it is not just the 400.9 nm line)

- Predicted lines in synthetic spectra should match real spectra
- ADAS predictions motivated installation of UV spectrometers
- Purpose was to find other strong W I lines as erosion diagnostics
- Presently the 400.89 W I lines solely used to diagnose W erosion
  - There are concerns about this line being blended with W II
  - Ideal erosion diagnostic lines would be isolated
- Other high-Z also predicted to be strong in the UV



Synthetic W I spectrum for t_e = 10 eV and N_e = 1x10 14 cm^{-3} .

Molybdenum calculations completed and benchmarked using C-Mod tokamak spectral measurements
(The need to filter Gbs of data, for good candidates)

- ADAS provides a good match with measured spectrum
- Relative line heights are not strongly density dependent
- Two lines were strongly temperature dependent
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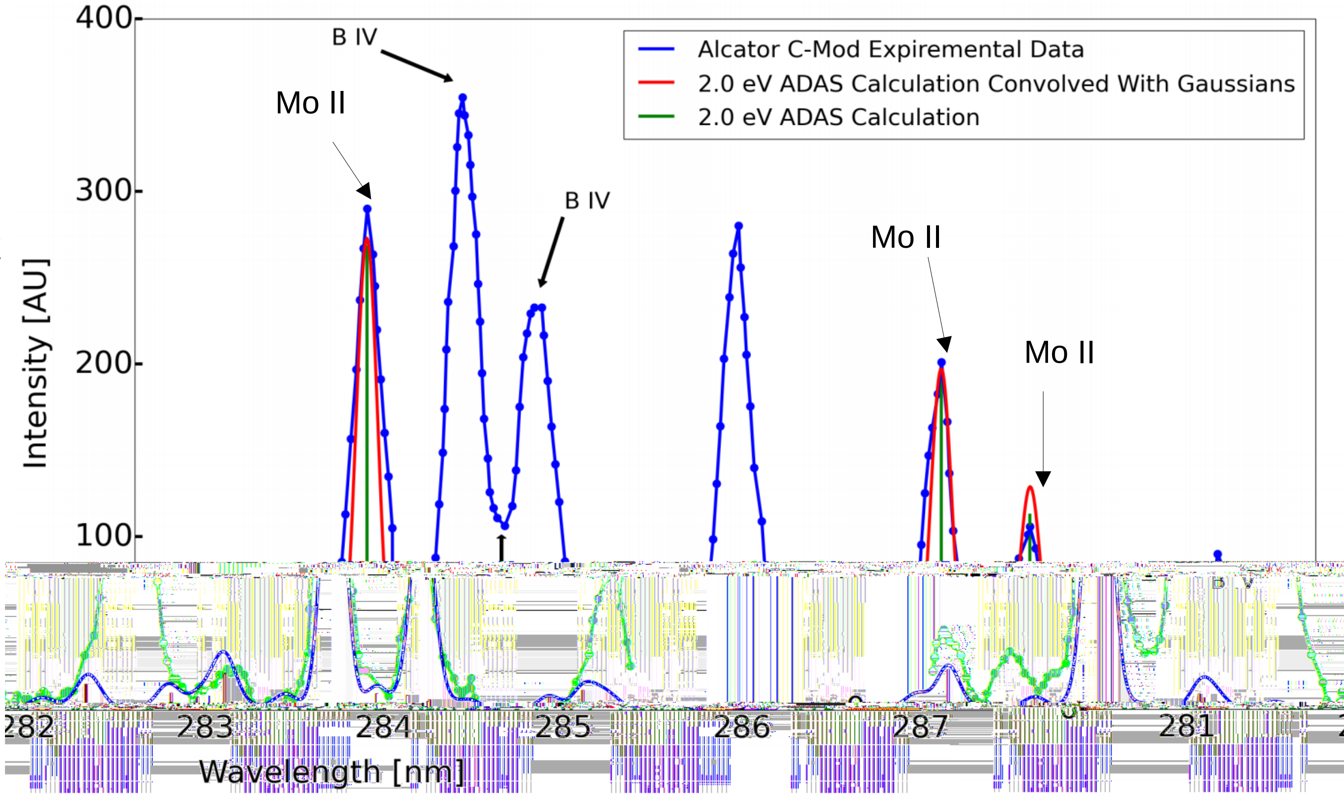
    - Ratio of the two lines can be used for electron temperature diagnostic
- S/XB dependent on temperature
    - eliminates the need for independent temperature diagnostic



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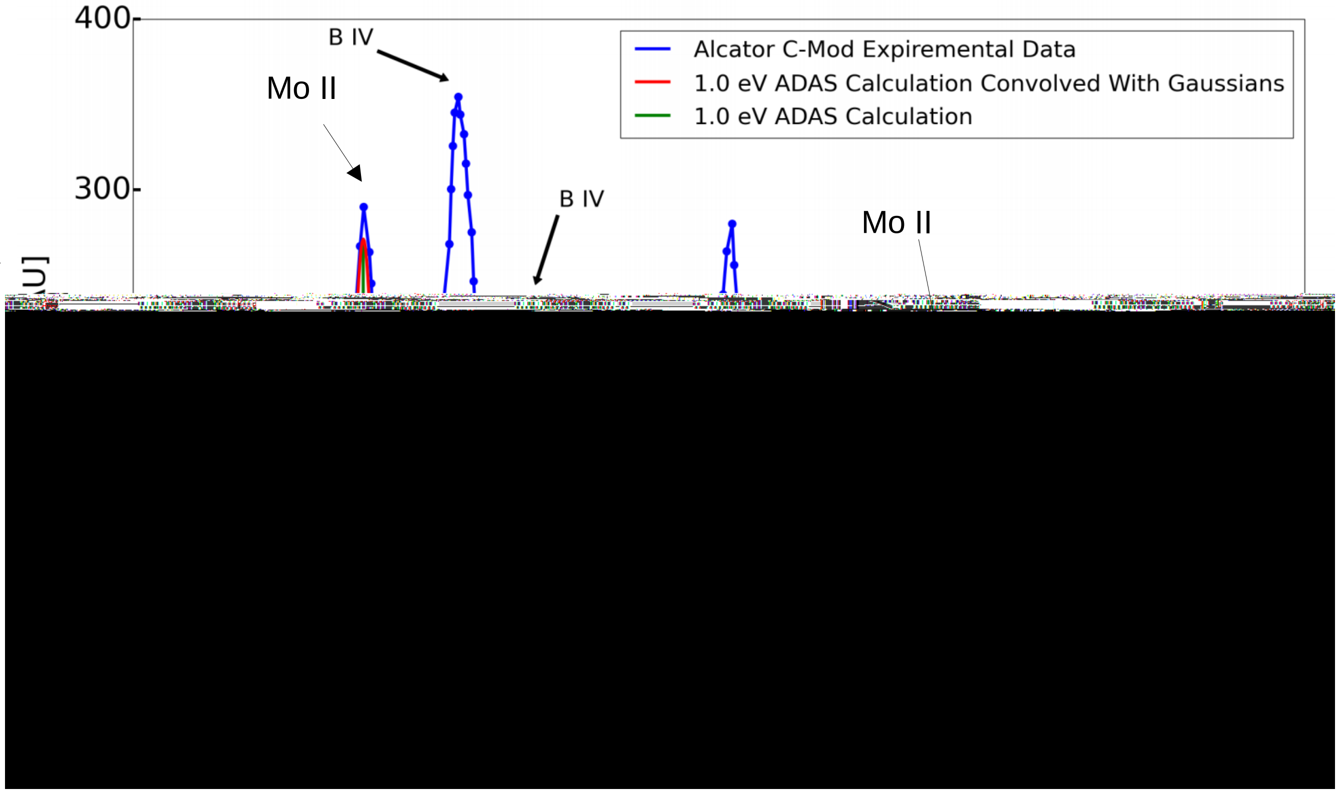
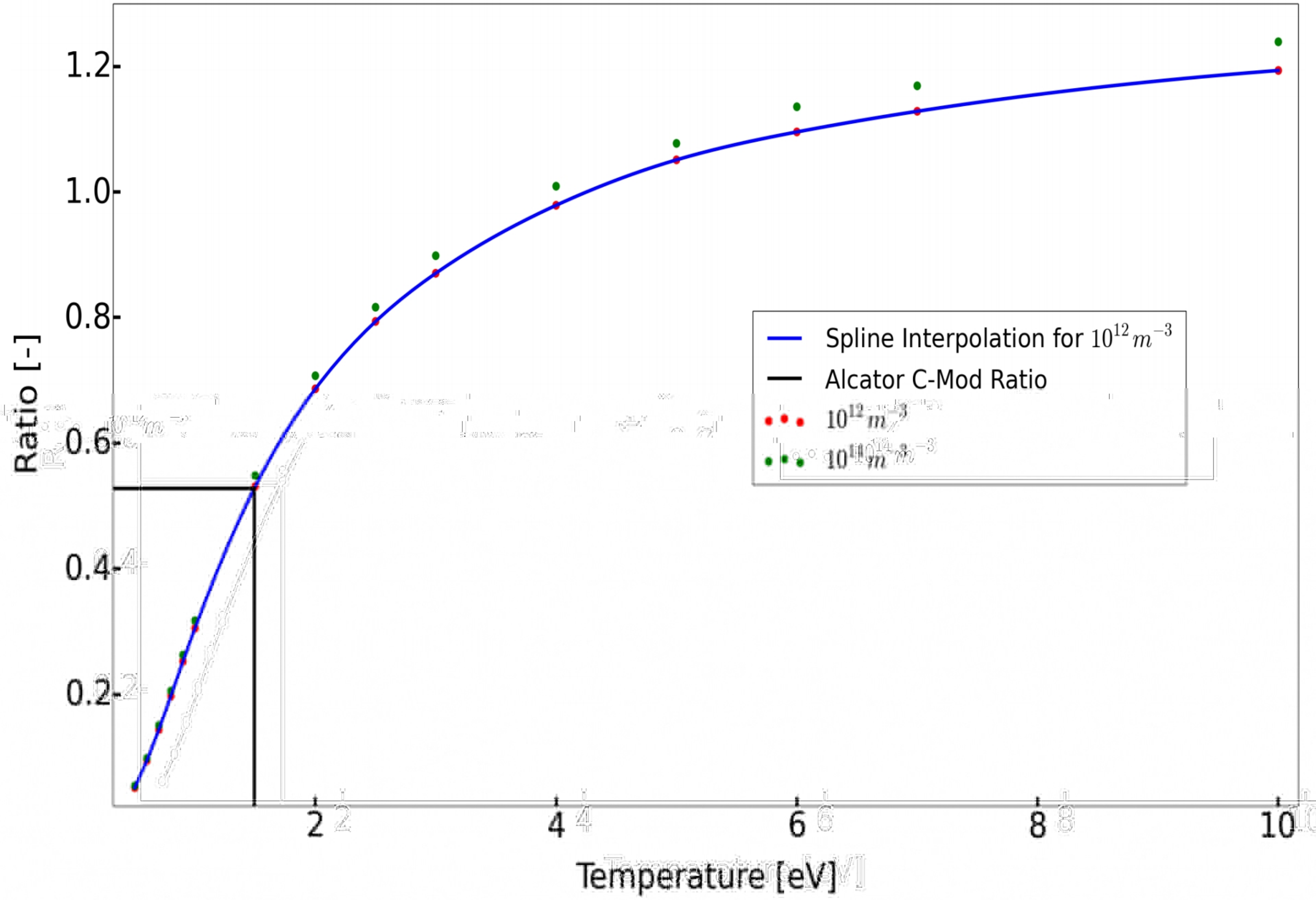


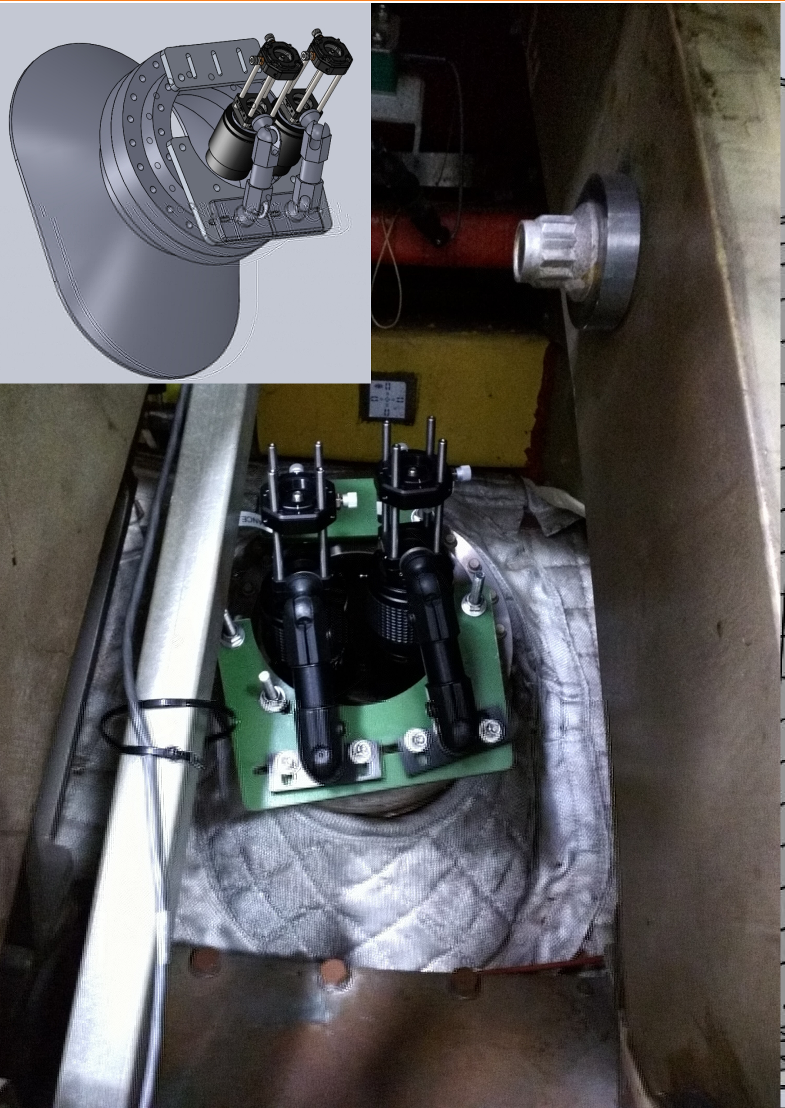
Molybdenum line ratios allow for plasma temperature in the edge to be calculated

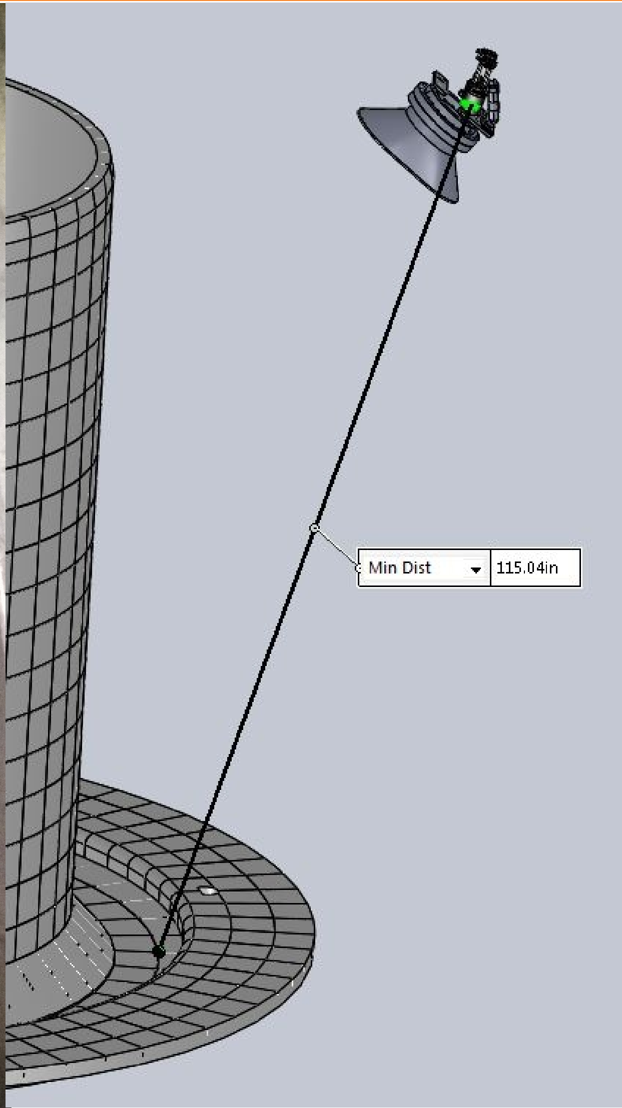
- Ratio of Mo II 284.8 nm and Mo II 286.67 nm
- Ratio of lines not density dependent but strongly temperature dependent
- Predicts a reasonable electron temperature of 1.5 eV

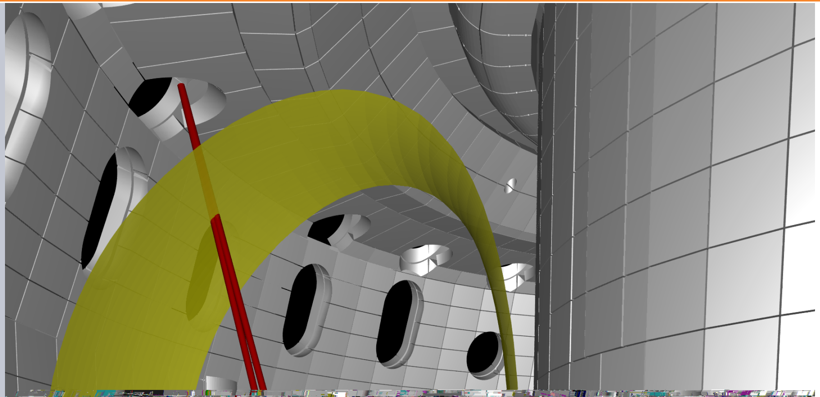


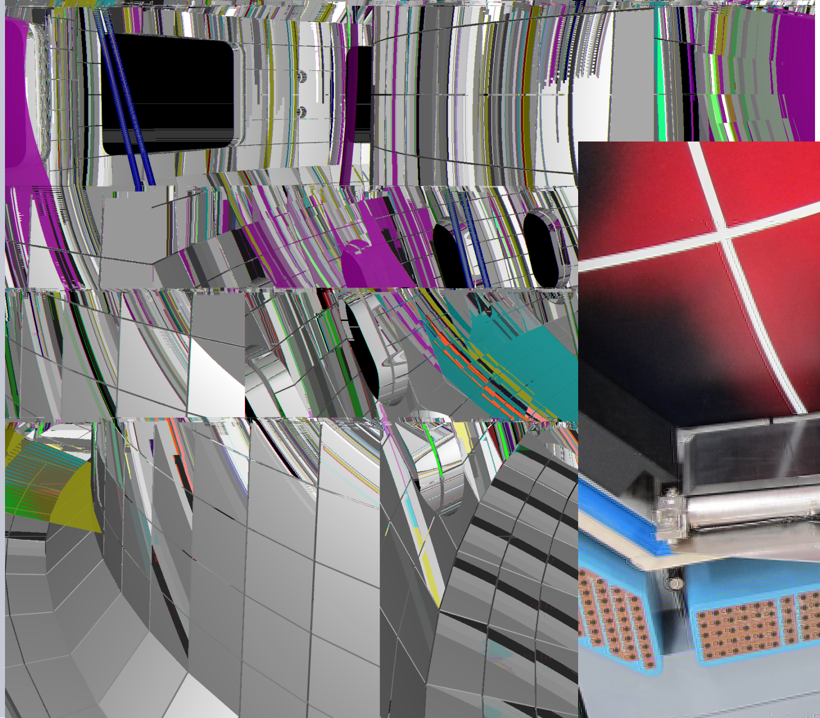
Back to Tungsten

Auburn UV survey spectrometers Installed on DIII-D: Collection optics



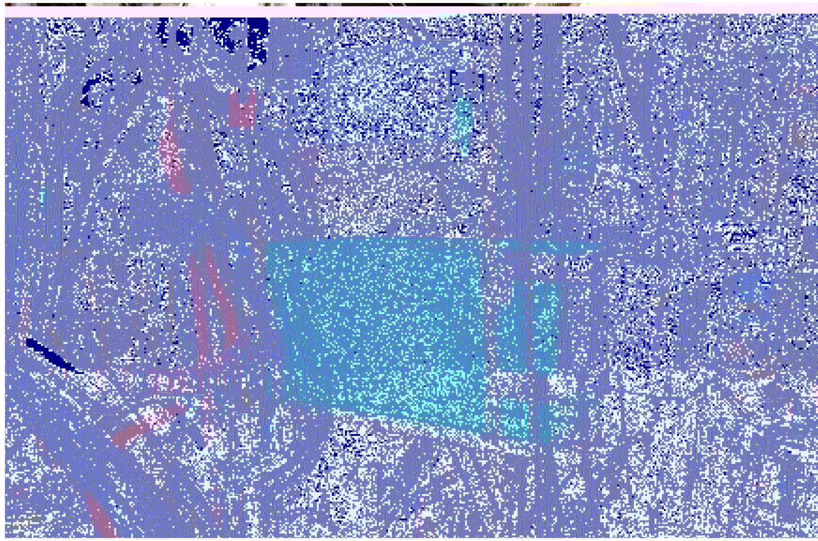






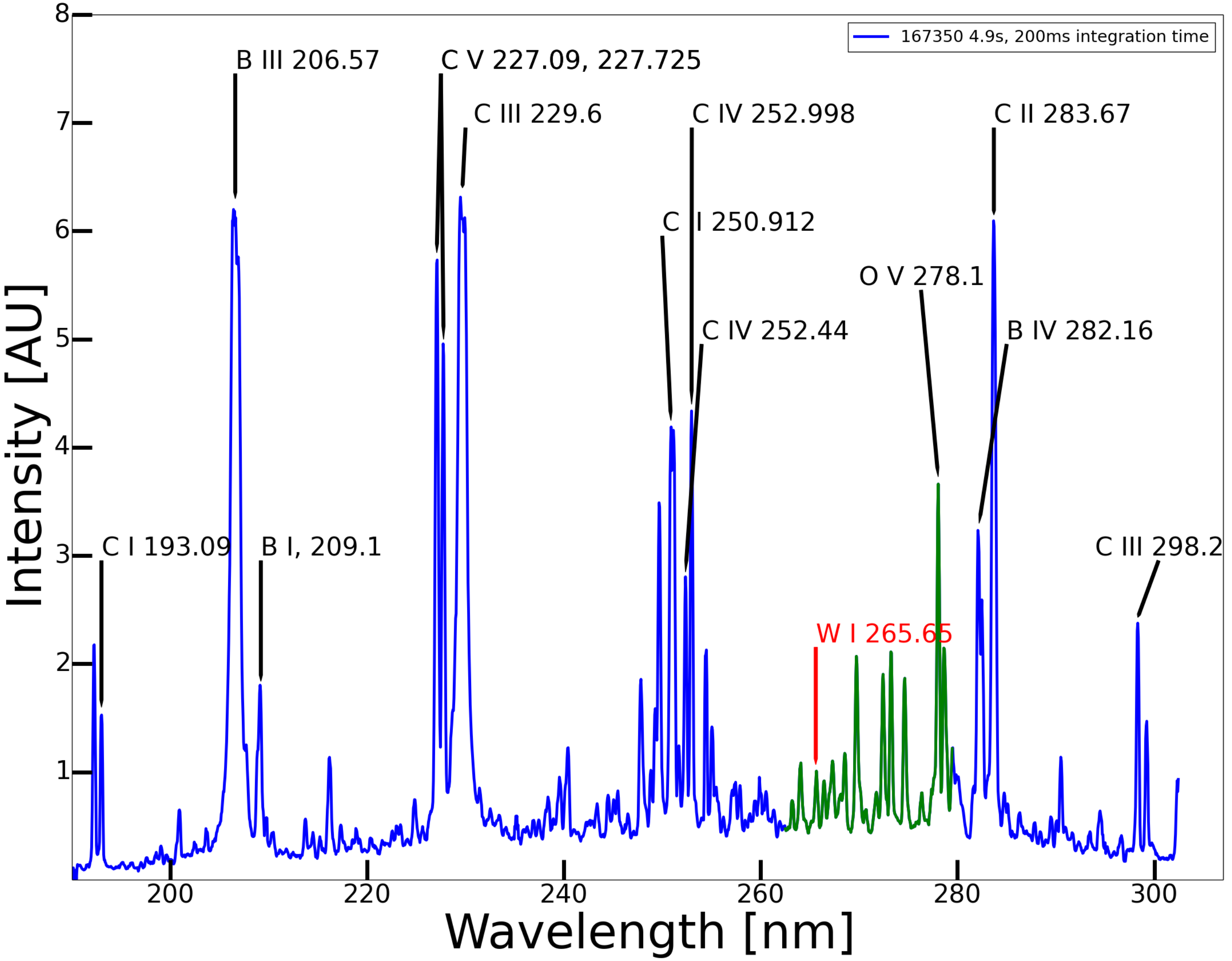
Auburn UV survey spectrometers Installed on DIII-D: Spectrometers

- Three Stellarnet USB spectrometers installed with different spectral ranges:
    - Spectrometers with 200-300 nm, 300-400 nm, and 200-400 nm ranges
    - Compact concave grating spectrometers ~20 cm length
    - Integration times of 30 to 2000 ms utilized
- Two viewing chords available simultaneously:
    - Lenses were located at a port slightly above the midplane
    - Ability to measure emission from lower divertor floor & shelf simultaneously
    - 5 m fused fibers were used to minimize UV absorption
- Spectrometers housed in radiation shield boxes
    - Neutrons and x-rays
    - Stronger magnetic and electric fields



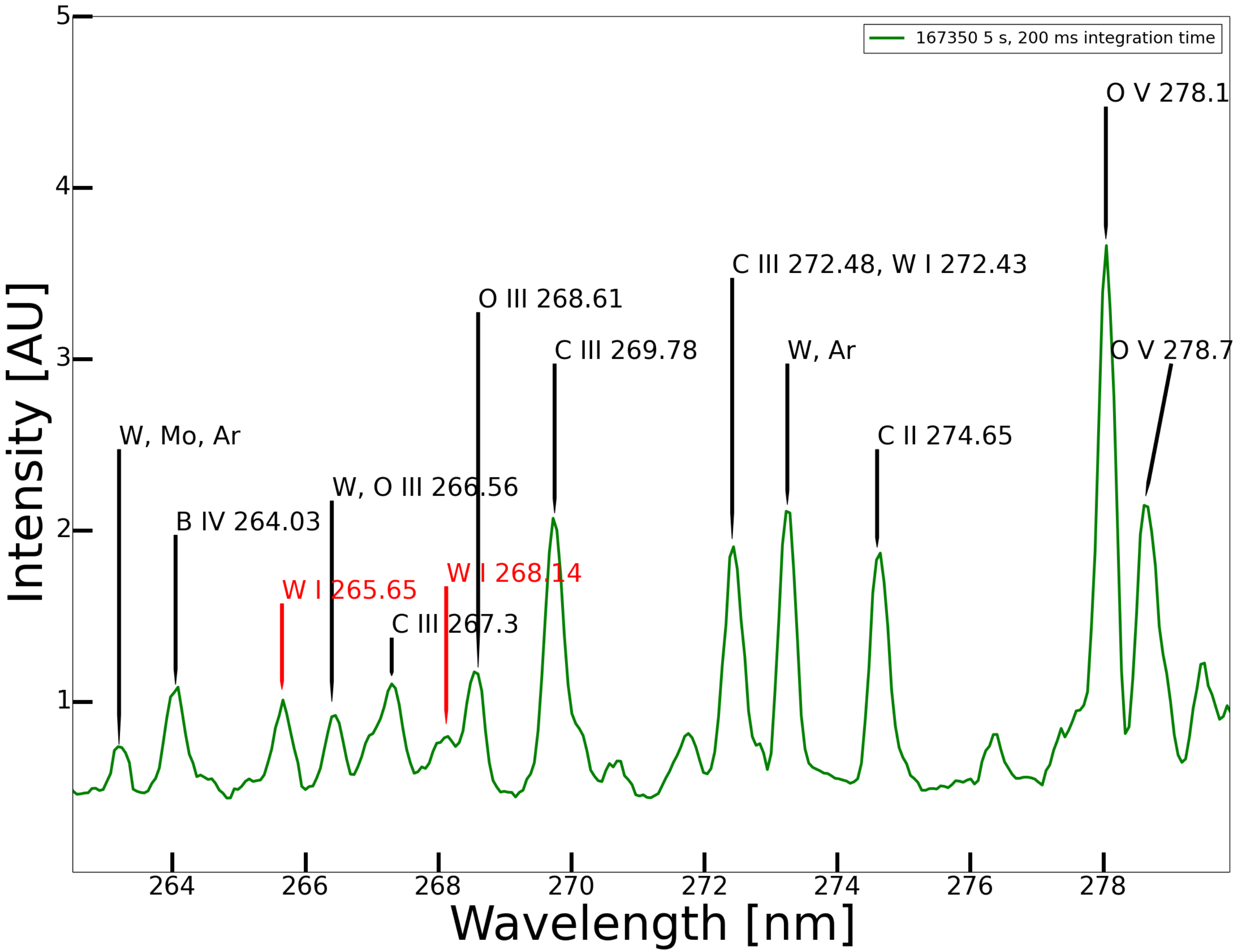
First UV survey spectral measurements in DIII-D, multiple W I lines observed

- A typical spectrum for the 200-300 nm spectrometer is shown
- 200-300 nm spectrometer viewing the lower divertor shelf
- W lines small compared to other impurities
    - Consistent with low sputtering rates
- ELMing H mode plasma 4 MW injected power (medium power shot)



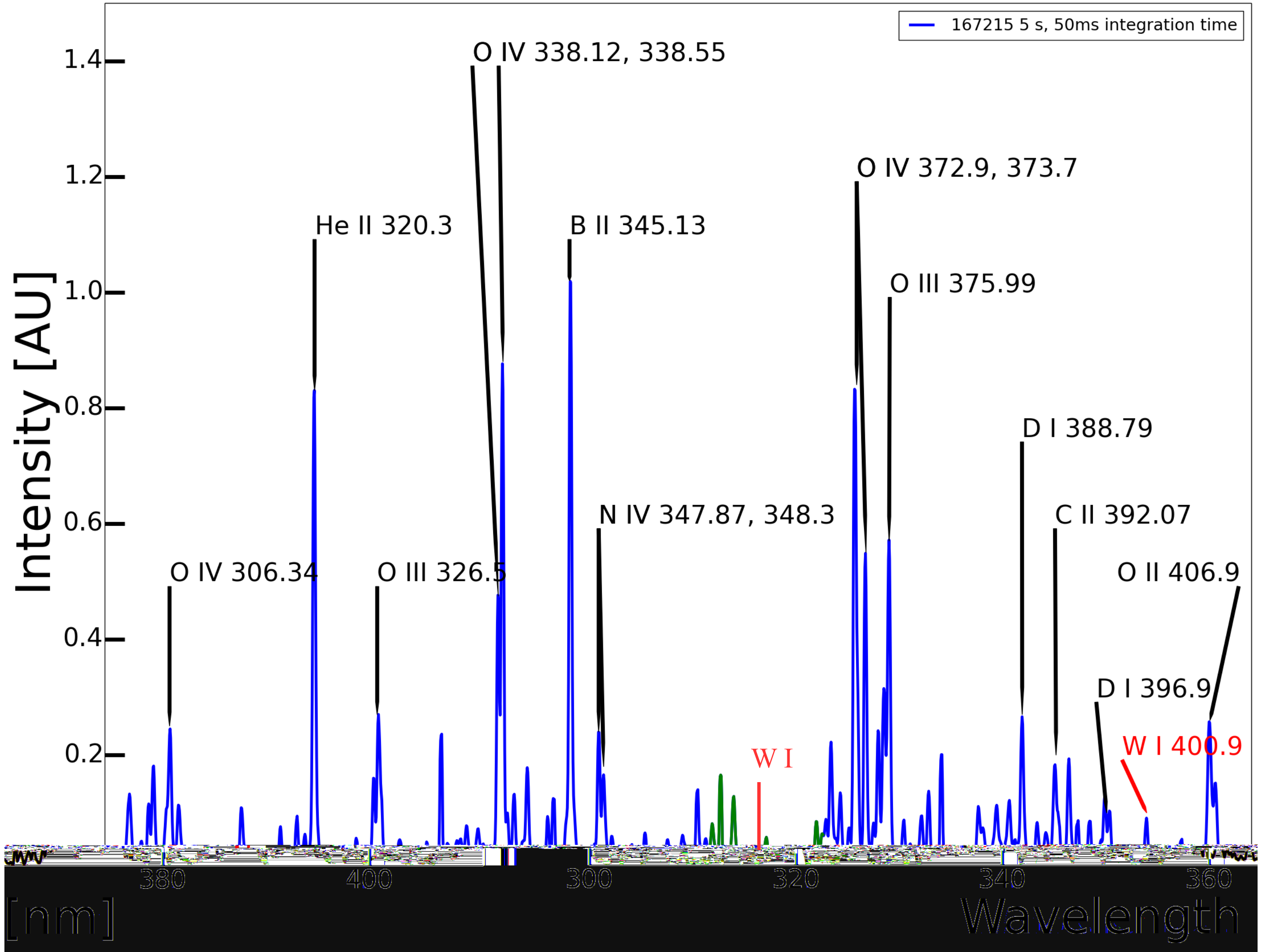
New W I candidate lines found to use for W erosion measurements

- W I 265.65 nm observed to be on the order of the widely used 400.89 line:
  - Atomic calculations using ADAS confirm that W I 265.65 nm is strong for divertor temperatures and densities ~1E19 m^3 ~ 10eV
- Multiple W I lines in the region around 265.65 region:
  - High density of lines in this region motivates higher resolution spectrometer/instrument

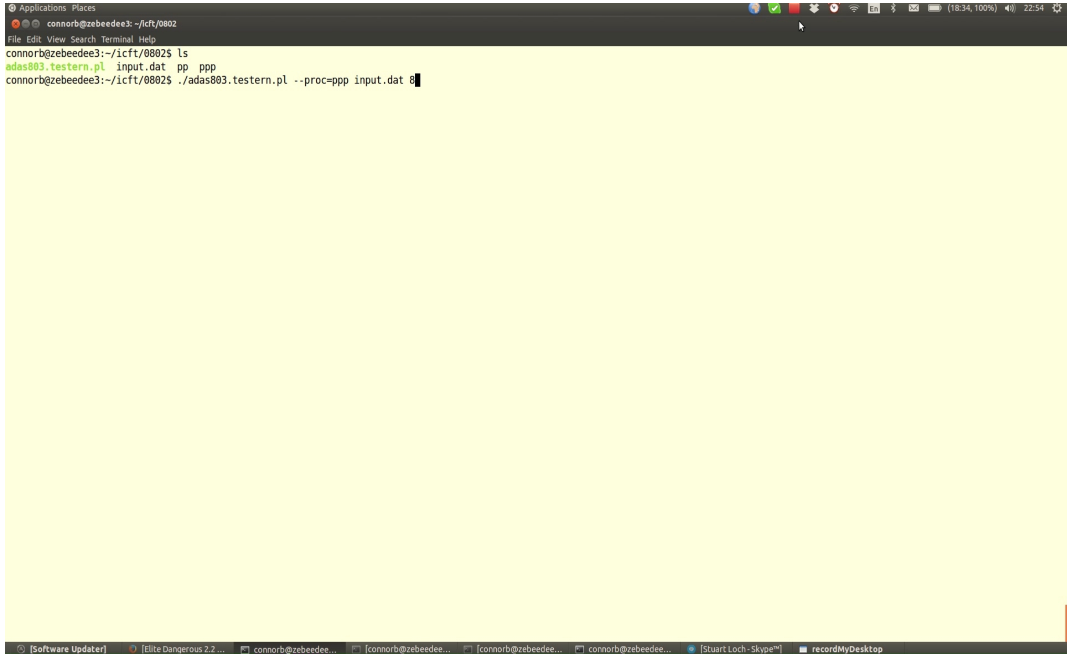


300-400 spectrometer also identified additional W I spectral lines to the 400.89 line

- 300-400 nm spectrometer view of the shelf
- L mode plasma 3.8 MW injected power (medium power)



Summary and future work



Perl/Python scripting of R-matrix calculations now feasible, but need to include RMPS ionisation / recombination aspects

- Promising new W I lines identified for erosion measurements:
  - Erosion measurements (….. mmmm) can be done after absolute calibrate to be done Nov 5th
  - Further benchmarking of W I spectra will be completed on CTH
- New R-Matrix W I (QUB) atomic calculations in the process of being calculated will compare to experiment

  New R-matrix Mo I (QUB) atomic calculations in the process of being calculated will compare to experiment