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Radiation from High Energy Density Plasmas
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Reno, NV

Diagnosing HED plasmas with hybrid-structure atomic models and 3-D radiative transport

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Outline

- **Motivation:**
  Getting the most out of the extensive suite of diagnostics on Sandia's Z requires both sophisticated non-LTE spectroscopic models and a self-consistent treatment of radiative transfer.

- **Hybrid-structure spectroscopic atomic model (SCRAM):**
  - computationally tractable model that balances accuracy and completeness by combining fine structure levels with UTAs and superconfigurations
  - spectroscopic accuracy for a wide range of temperatures and densities

- **Tabular 3-D model for self-consistent radiative transfer:**
  - Modified on-the-spot method agrees with more sophisticated approaches for simple plasma geometries and two-level atoms
  - Doppler effects are included in radiative transfer and simulated spectra
  - Efficient lookup approach supports arbitrarily complex atomic models
  - Converges in a few iterations
  - Produces simulated spectra, power, and emission/ absorption images

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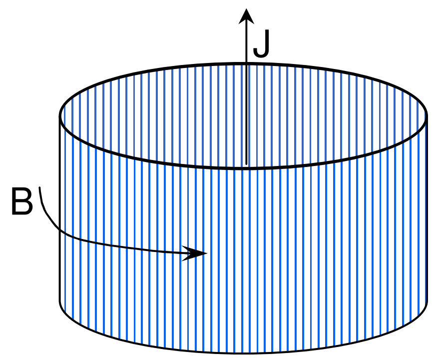
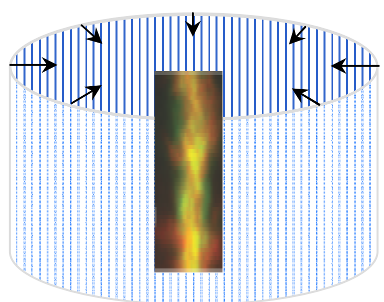
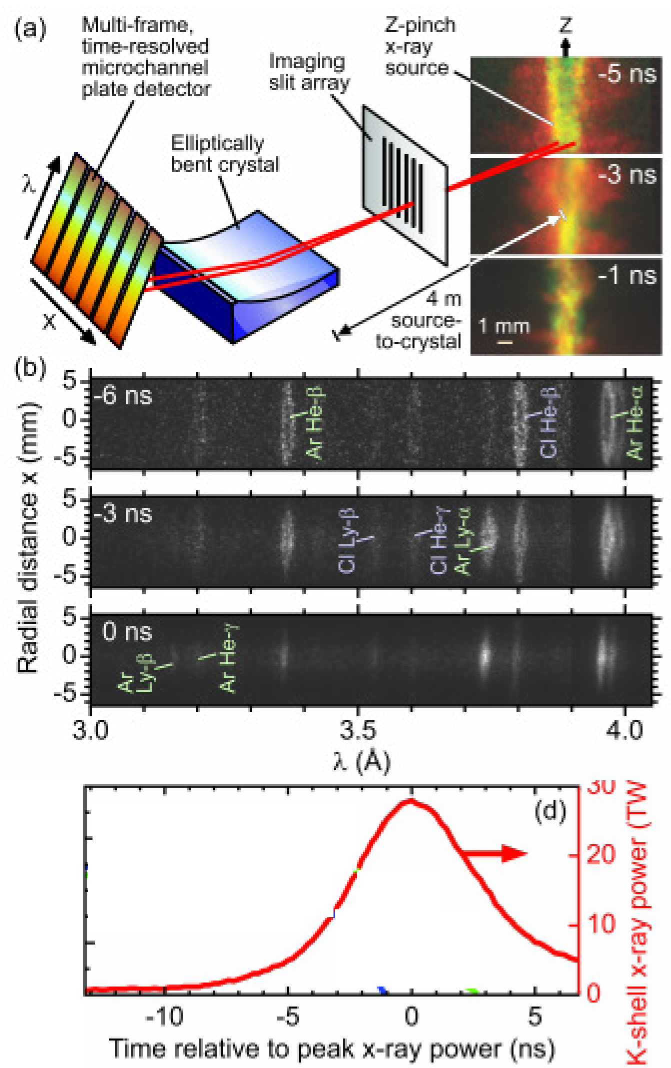
Motivation: extensive measurements of radiative plasma properties are routine on Z

~20 MA current heats and ablates thin wires



J x B force implodes wire array, forming a hot, dense plasma on axis





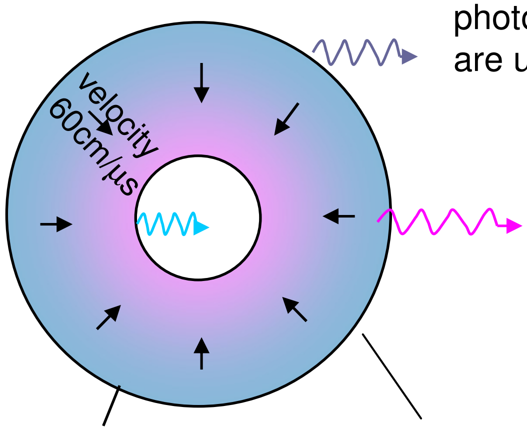
Time-gated images of different photon energies give pictures of plasma evolution

Spatially and temporally resolved spectroscopy can yield detailed information about plasma conditions

Absolutely calibrated filtered PCDs measure radiative powers and yields

Temporally and spatially resolved spectra contain a wealth of information about the emitting plasma

Imploding Cu/Ni plasma shell brightest on inner edge

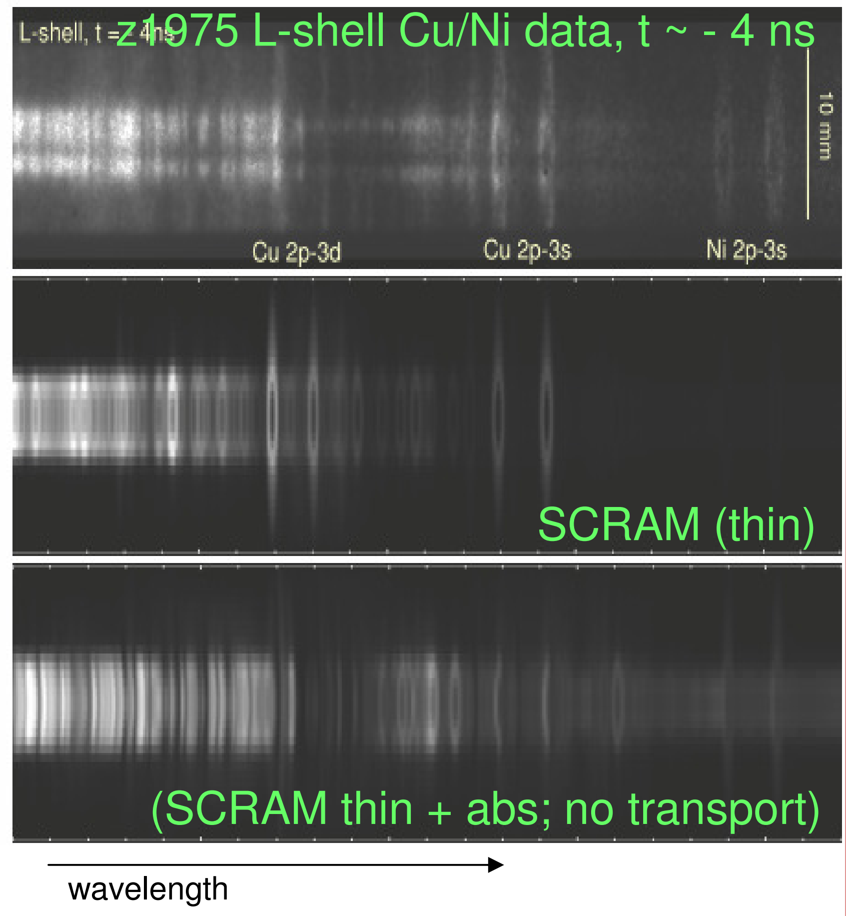


photons from shell edges are unshifted ($v_{||} = 0$)

photons from shell center are maximally shifted ($v_{||} = v$)

plasma conditions:
central Te ~ 3 keV
peak ne ~ 10^{21} cm^{-3}
peak line-center τ ~100

For optically thick lines, red-shifted photons are absorbed by co-moving plasma while blue-shifted photons are transmitted, leading to line asymmetries



Reliable atomic models and self-consistent radiative transport are <u>both</u> essential for modeling optically thick emission from complex plasmas.

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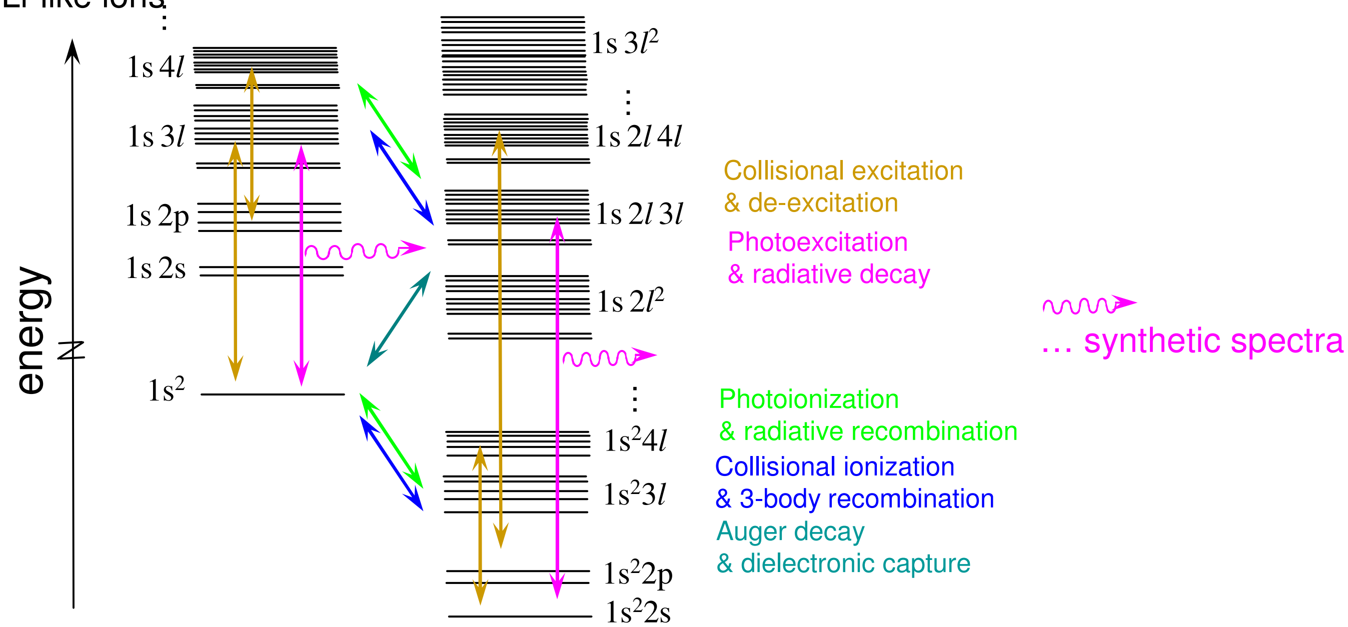
Reliable atomic models require complete level structure and accurate atomic data

Example: He- and Li-like ions



A variety of codes, (RATS, FAC, Cowan…) databases, (NIST, ATOMDB…), and approximations (screened hydrogenic, Lotz…) provide energy level structure and rate data – with various degrees of detail and accuracy.

Generally, only fine structure data includes the configuration interaction effects and detailed transition structure required for spectroscopic accuracy… but fully fine structure models are computationally intractable for complex ions.

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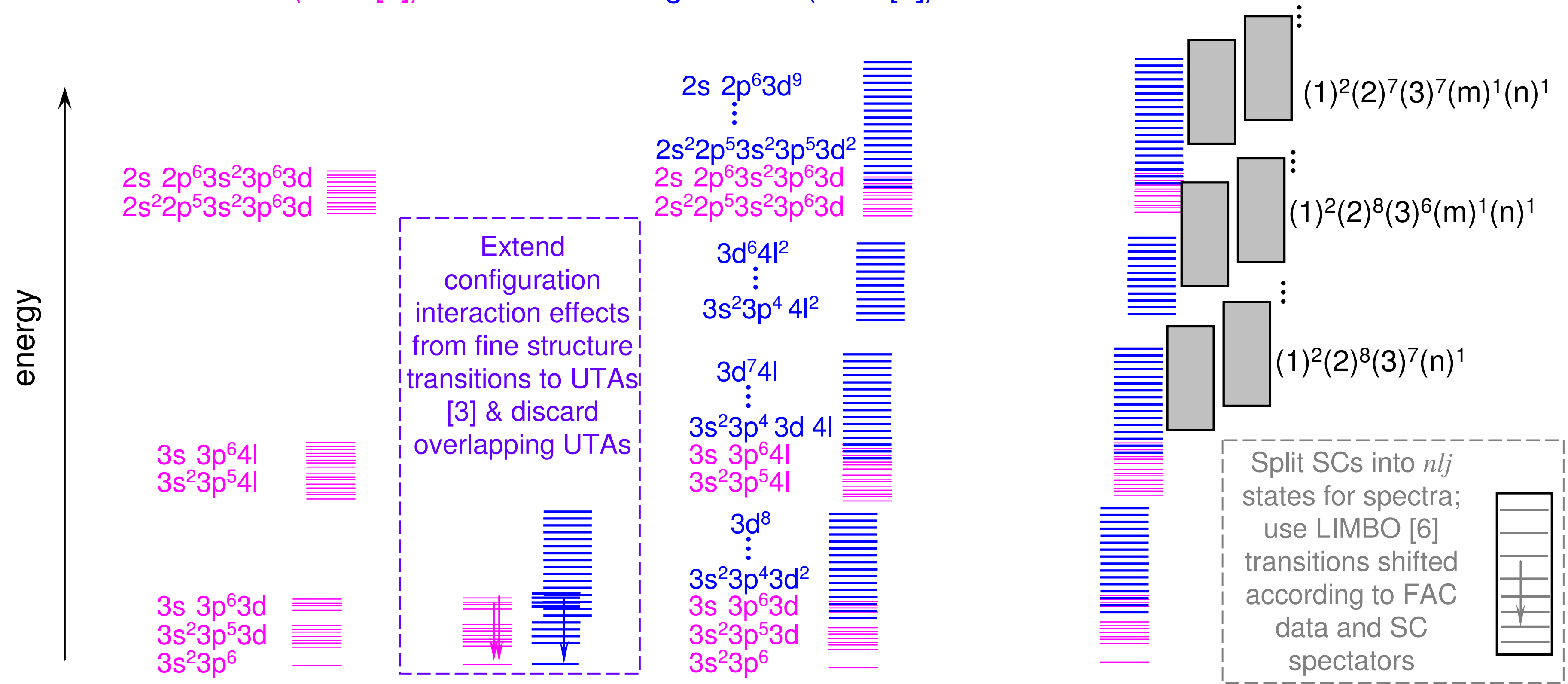
A hybrid-structure approach [1] combines the strengths of fine-structure and UTA/SC models

~200 fine structure "coronal" levels (FAC [2])

~14,000 (800) rel (non-rel) configurations (FAC [2])

~100 superconfigurations [4-5] (screened hydrogenic/LIMBO)



Coronal fine structure for singly excited states → configuration interaction and metastables.

Supplemental configurations for doubly excited states provide continuity at moderate densities.

Supplemental superconfigurations ensure statistical completeness and converged d.r. channels

[1] Hansen, Bauche, Bauche-Arnoult, and Gu, HEDP **3**, 109 (2007)
[2] Gu, Astrophys. J. **590** 1131 (2003)
[3] Hansen, Can. J. Phys. **89** (2011)
[4] Scott and Hansen, HEDP **6**, 39, (2010)
[5] Hansen, Bauche, and Bauche-Arnoult HEDP **7**, 27 (2010)
[6] Liberman, Albritton, Wilson, & Alley, Phys. Rev. A **50**, 171 (1994)

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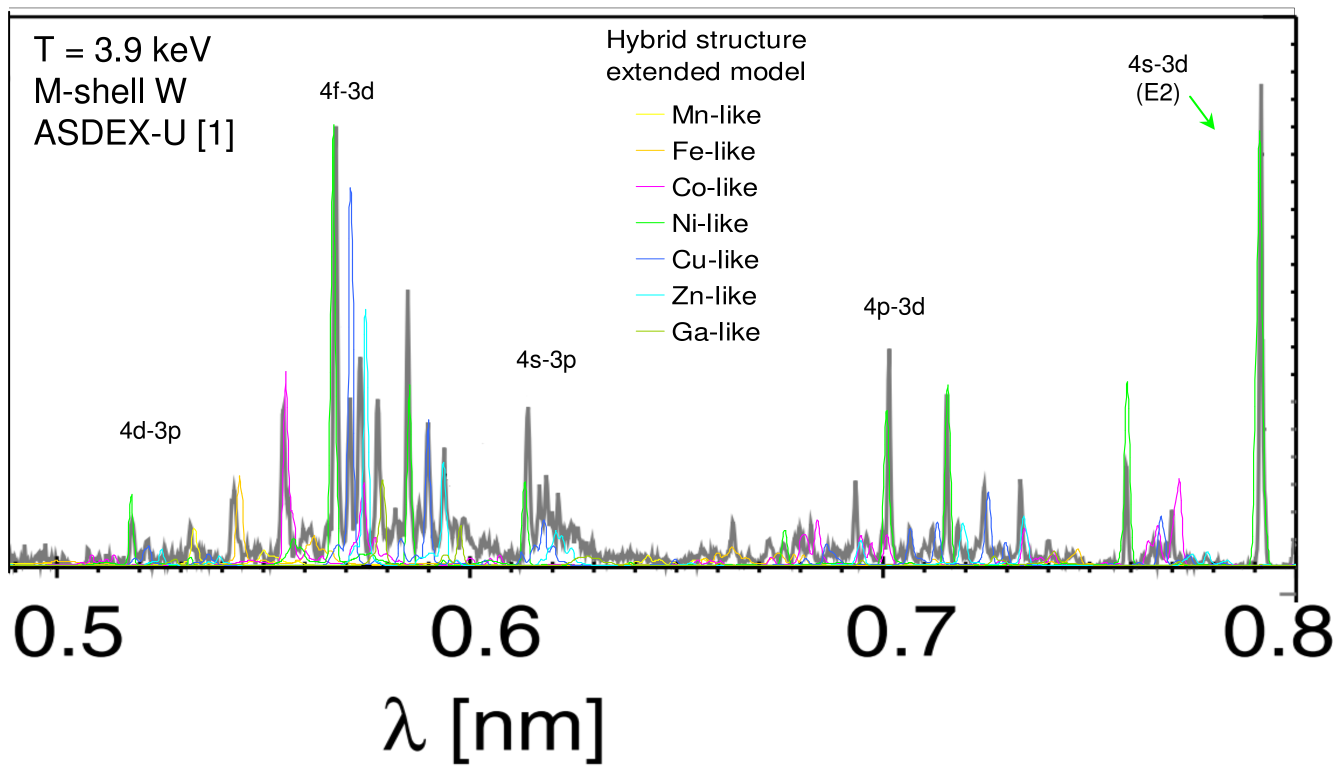
The fine-structure lines are necessary for modeling low-density plasma spectra



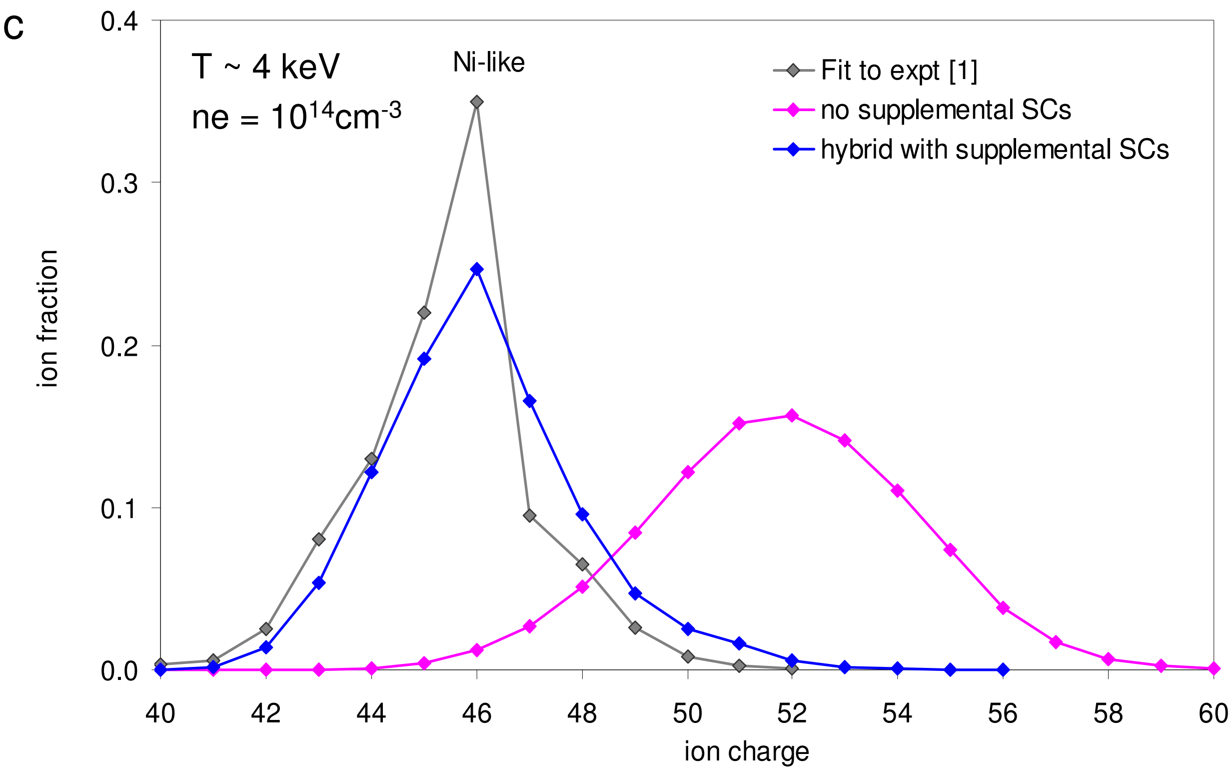
Hybrid-structure models have spectroscopically accurate wavelengths and include cascade-populated lines from metastable states.

[1] Pütterich *et al.* Plasma Phys. Control. Fusion **50**, 085016 (2008)

The supplemental superconfigurations ensure statistically complete d.r. channels

Without extensive dielectronic recombination channels, collisional-radiative models tend to predict overionized charge state distributions.

With supplemental SCs, hybrid-structure models give reliable charge state distributions *at any density*.



[1] Pütterich *et al.* Plasma Phys. Control. Fusion **50**, 085016 (2008)

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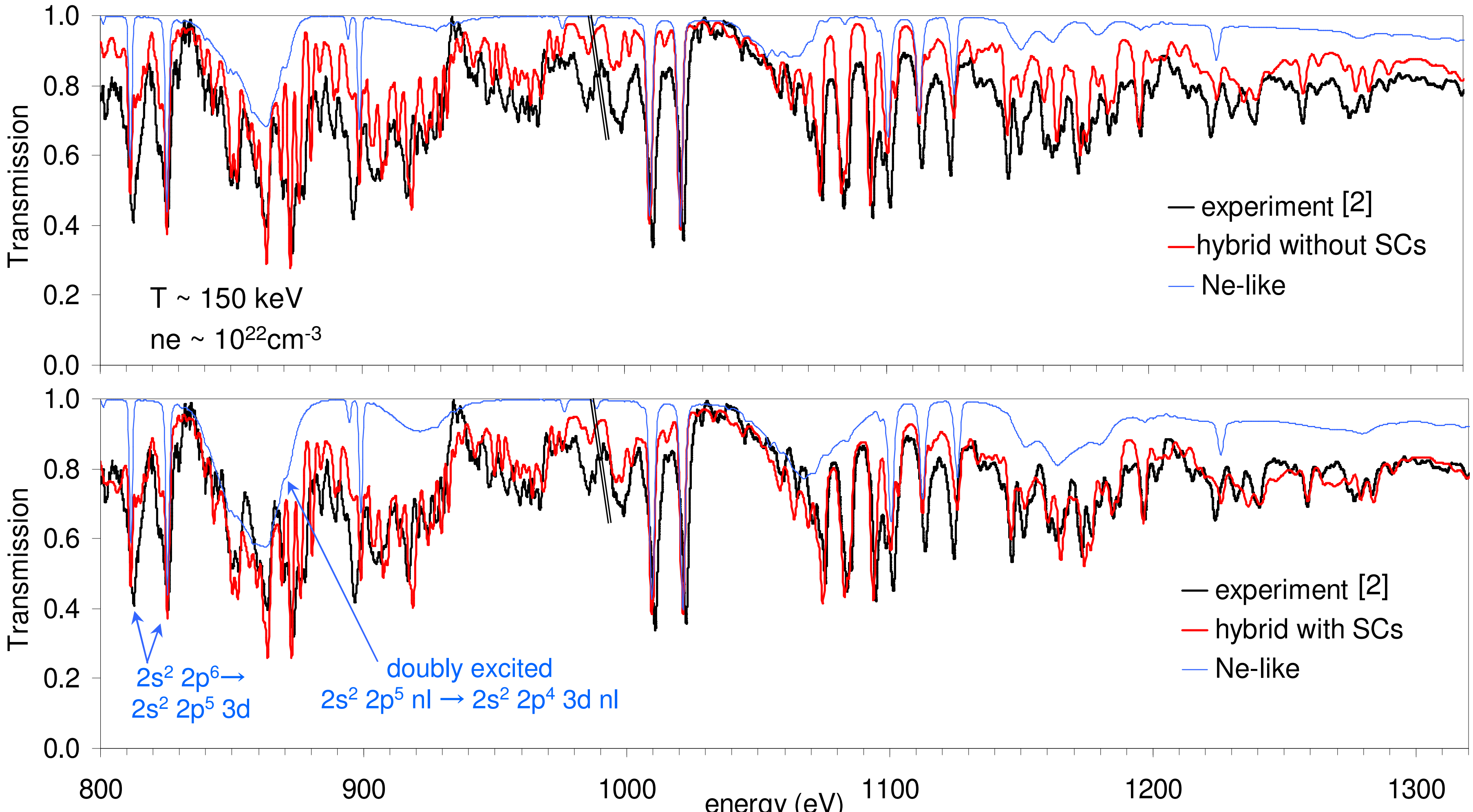
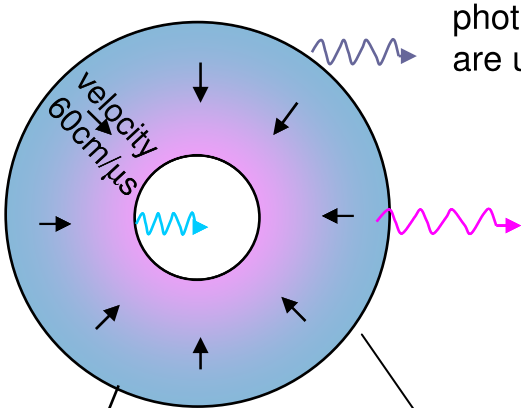
Statistical completeness and accurate wavelengths are both required for high-density absorption spectra



Fine structure, UTAs, and supplemental SCs all contribute to good data fit with only ~10^5 lines (vs. ~ 10^7 for fully fine structure model)

[2] Bailey *et al.* PRL **99**, 265002 (2007).

Accurate 0-D atomic models are not sufficient to model optically thick lines in complex plasmas



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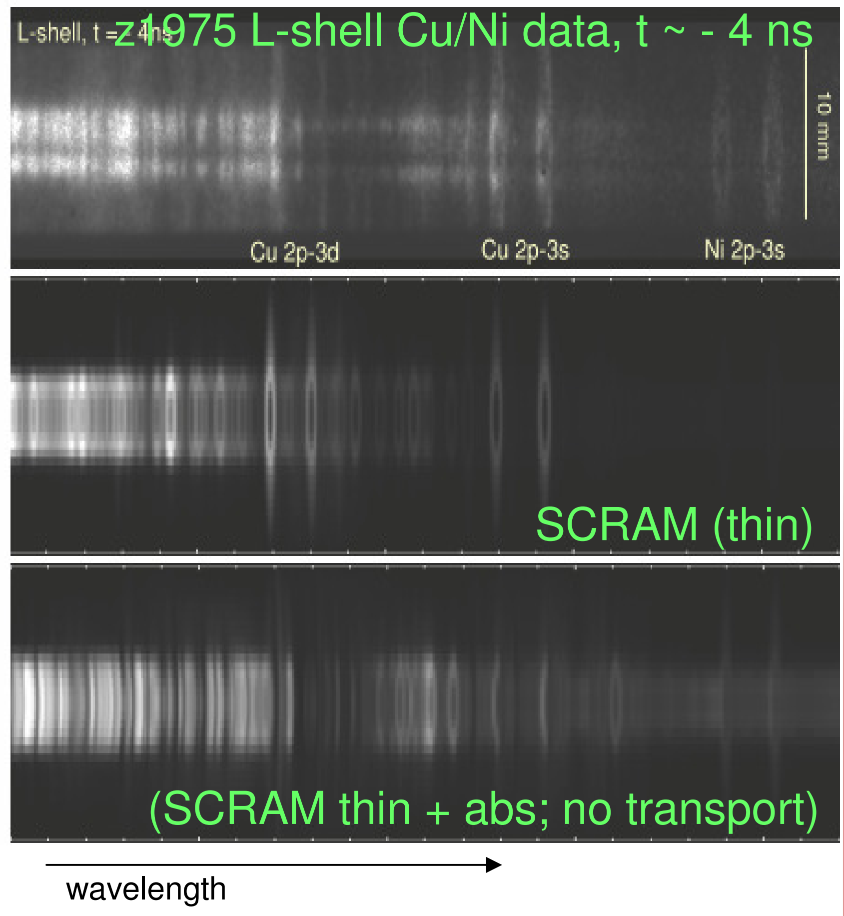


Including line absorption while neglecting transport photopumping is <u>worse</u> than treating an optically thick NLTE plasma as optically thin.

Approximate self-consistency is relatively straightforward for uniform, static plasmas

Self-consistent methods with analytical frequency-integrated escape factors P^{esc} [1,2] can be used for arbitrary geometries. They converge quickly but neglect line overlap.

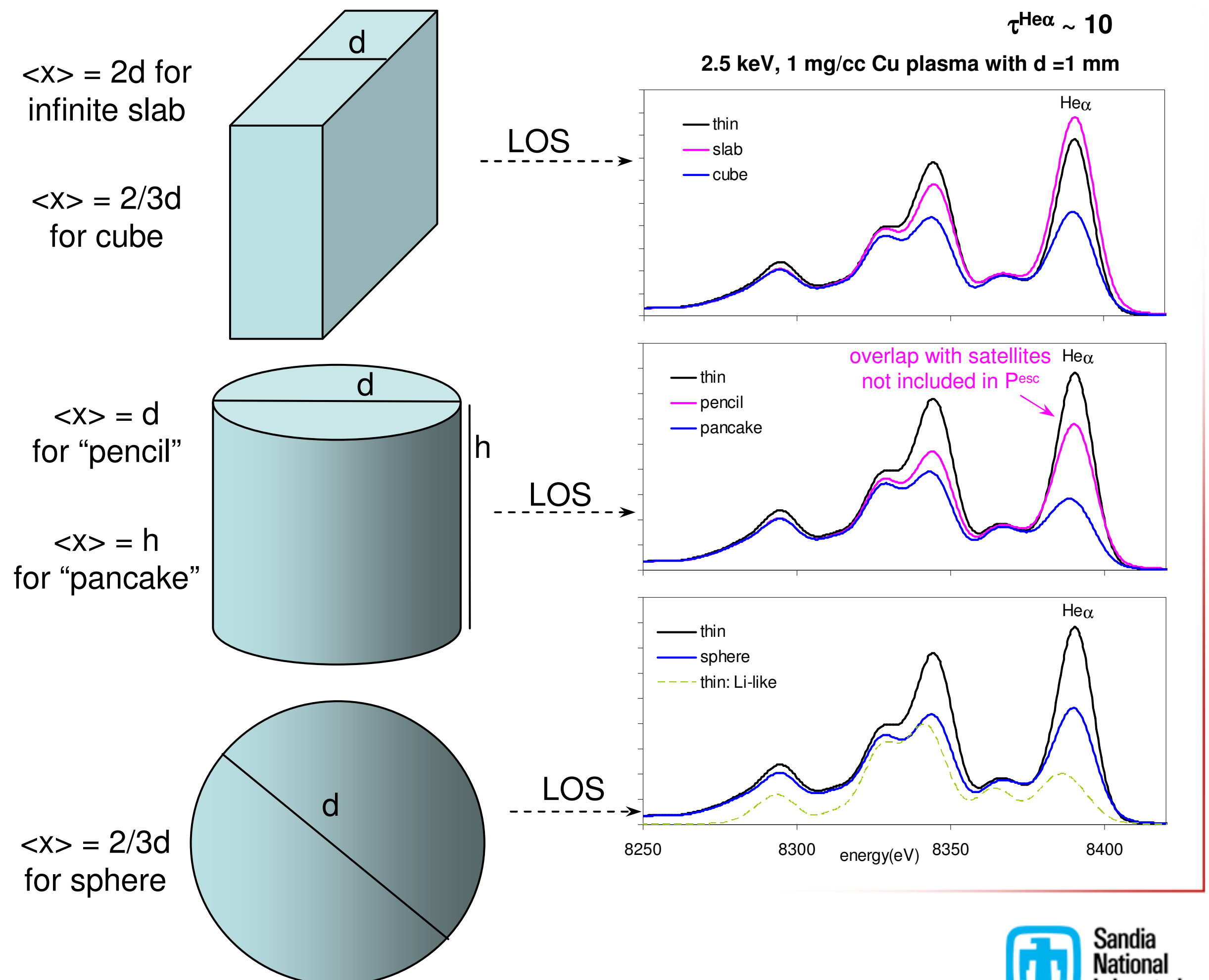
The effects of photoexcitation in a regular solid depend on the mean chord $\langle x \rangle$, while photoabsorption depends on the line of sight [3]

Self-consistent level populations: multiply A^{rad} & R^{rad} by $P^{esc}(\kappa\langle x \rangle)$

Emission profiles:
$I = j/\kappa(1 - e^{-\tau})$; $\tau = \kappa x^{LOS}$

Photoabsorbtion along x^{LOS} can be larger or smaller than photoexcitation across $\langle x \rangle$

Neglect of satellites can lead to ~ 30% error



[1] J.P. Apruzese JQSRT **23**, 479 (1980)
[2] J.P. Apruzese JQSRT **25**, 419 (1981)
[3] G.J. Phillips *et al.*, HEDP **4**, 18 (2008)

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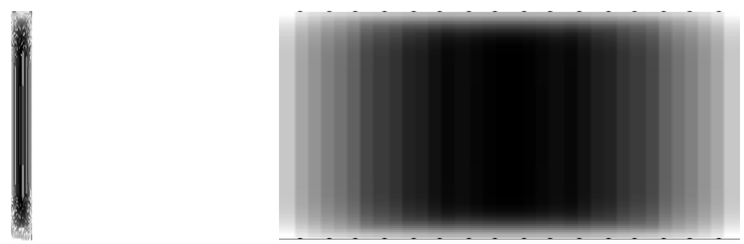
Even with uniform plasma conditions, level populations vary in space

Consider uniform cylindrical plasmas with two-level atoms; the geometry is defined by axial and radial optical depths and the source function is determined by non-local transport.

"Pinhole" images of the emission intensity from two cylindrical plasmas:

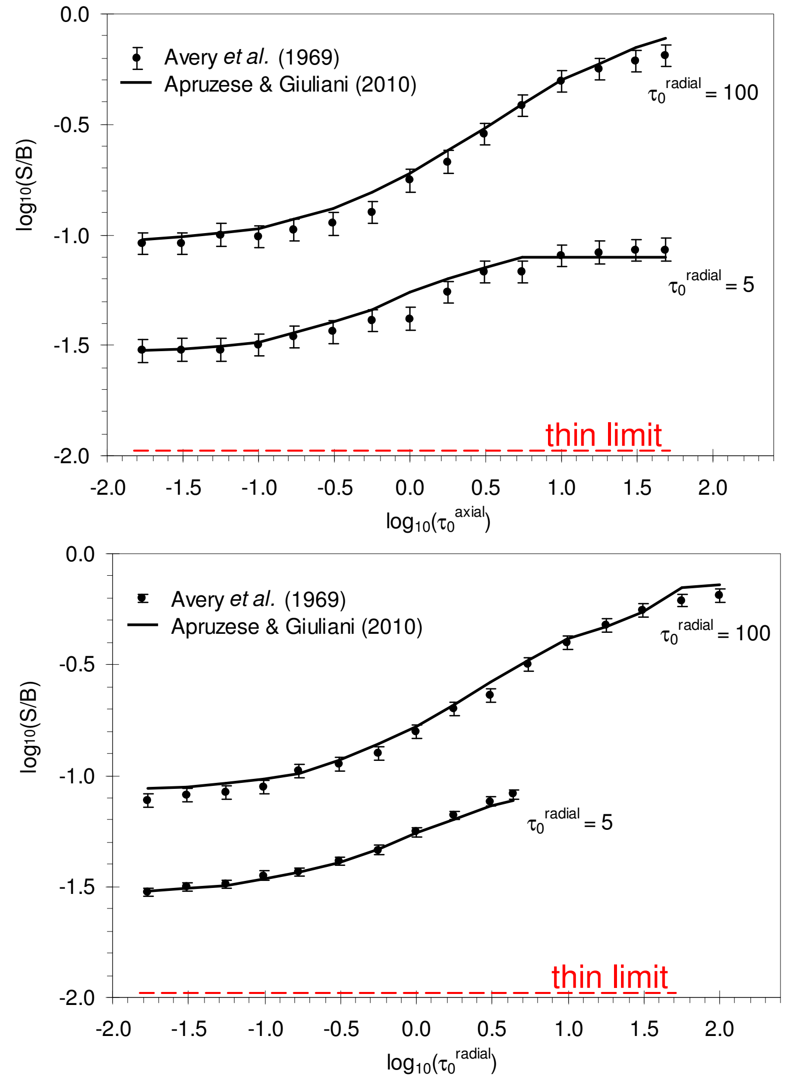


$\tau_0^{axial} = 50$
$\tau_0^{radial} = 5$

$\tau_0^{axial} = 50$
$\tau_0^{radial} = 100$

Monte Carlo [2], multi-frequency, and non-local escape factor methods [1] all predict significant global photopumping from the thin limit of $\log_{10}(S/B) = -2$, with the highest intensities at plasma center.

Axial (top) and radial (bottom) emissivities:



[1] Apruzese & Giuliani, JQSRT **111**, 134 (2010)
[2] Avery *et al.*, JQSRT 9, 519 (1969)

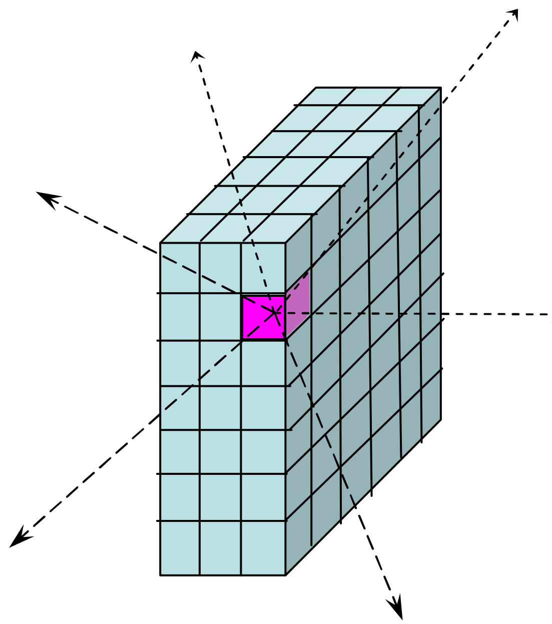
On-the-spot approximation [1] can approximately account for bulk photoexcitation

1) Tabulate emissivities and opacities from self-consistent escape factor models on grids of T_e, n_{ion}, and plasma size (τ^{eff})

2) Determine frequency-averaged escape factors $P^e = \int_\nu j(\nu)e^{-\tau}d\nu \,/ \int_\nu j(\nu)d\nu$ along various lines of sight (8 – 14 rays) and find angle average $<\tau^{eff}> \equiv -\ln(<P^e>_\Omega)$ for each plasma element

3) Set $j(\nu)$ of each plasma element to the tabulated $j(\nu)$ of the self-consistent model with $\tau^{eff} = <\tau^{eff}>$ (+ symmetry speedup)

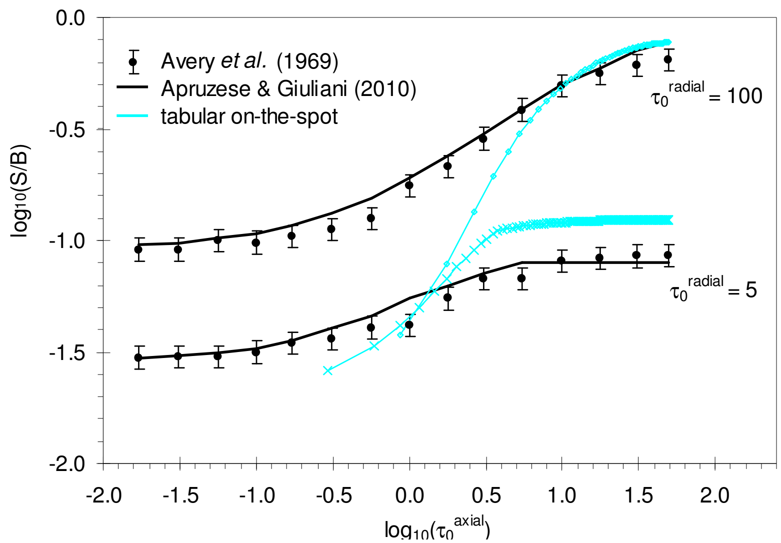
4) Transport emissivity to detector along instrumental line of sight

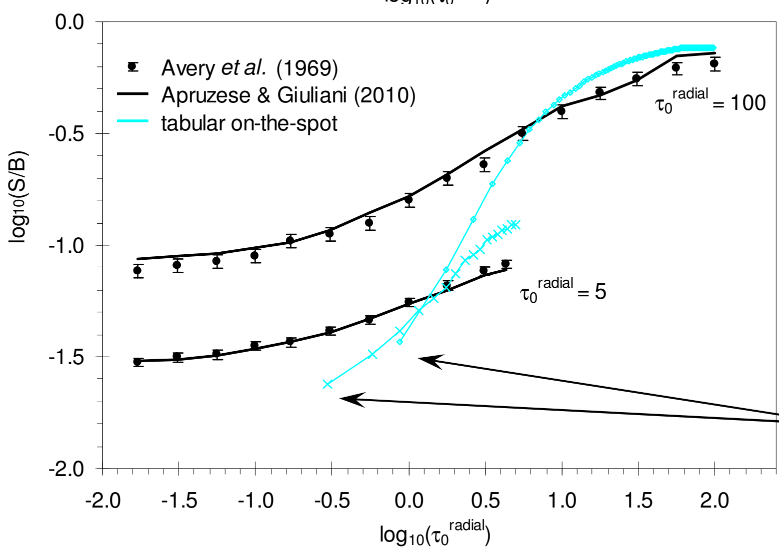


Key approximations:
- all absorbed photons are returned to originating cell (partially local transport)
- self-consistency is enforced only by table (no iteration on plasma grid)
- opacity is dependent only on T_e & n_{ion}
- escape factor method has its own inaccuracies

[1] Thornhill *et al.*, Phys. Plas. **8**, 3480 (2001)

On-the-spot method does not accurately capture non-local transport effects





+ The on-the-spot method is explicitly photon conserving and accounts for the bulk effects of photopumping on the total line intensity.

+ It also captures the trend of increasing intensities with optical depth.

+ Tabular and analytic ($S/B = (1+P^e/\varepsilon)^{-1}$) on-the-spot methods agree.

- However, because the edge cells will never have $\langle P^e \rangle_\Omega$ smaller than ~ 0.5, the method under-predicts edge intensities and over-predicts intensities at line center (photons emitted from the center are absorbed at the center, rather than transported to the plasma edge)

Minimum τ is enforced by cell size (linear grids require ~10^6 cells)

Weighting the escape probabilities and iterating significantly improves the on-the-spot method

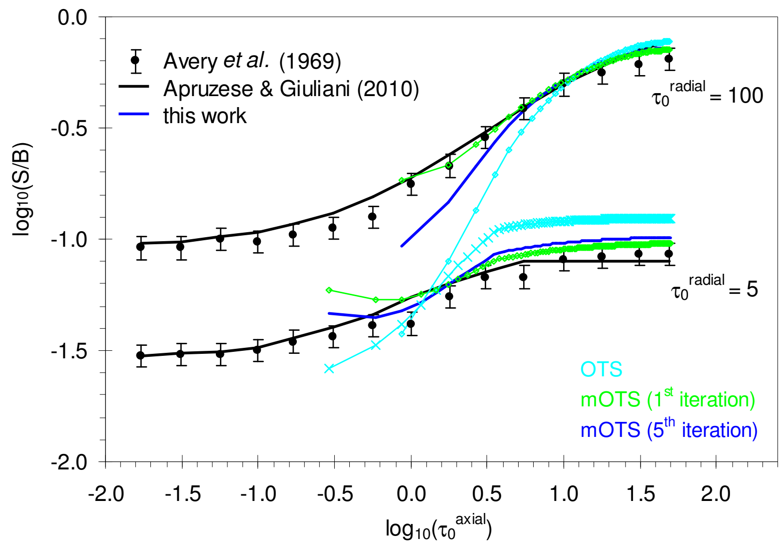
Instead of weighting angles equally, weight according to the total intensity incident on the cell along each ray:

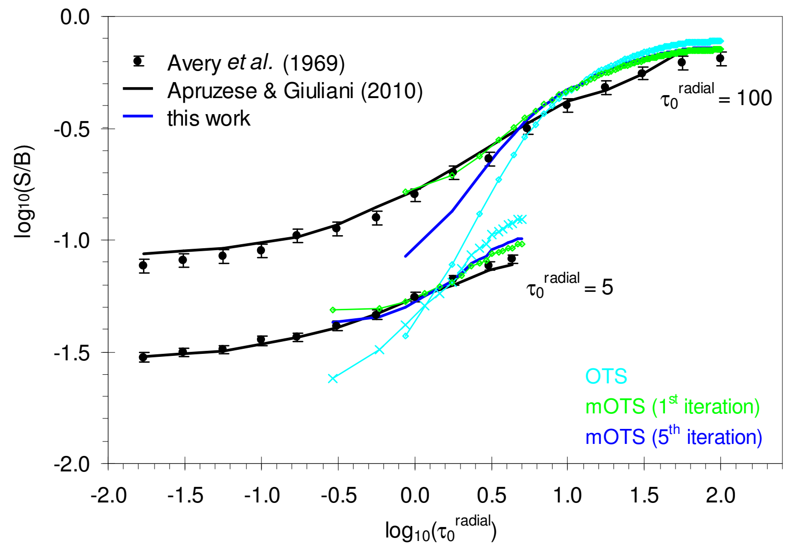
$w \sim \Sigma_k \int_\nu j_k(\nu) e^{-\Sigma\tau_k} d\nu$

Then normalize the total final intensity to that of the initial on-the-spot iteration to conserve photons.

Convergence to ~1% percent is reached in ~5 iterations.

This iterative approach captures more of the non-local transport behavior and better matches the more sophisticated models.





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The modified OTS transport model handles complex geometries, spectra, and Doppler shifts

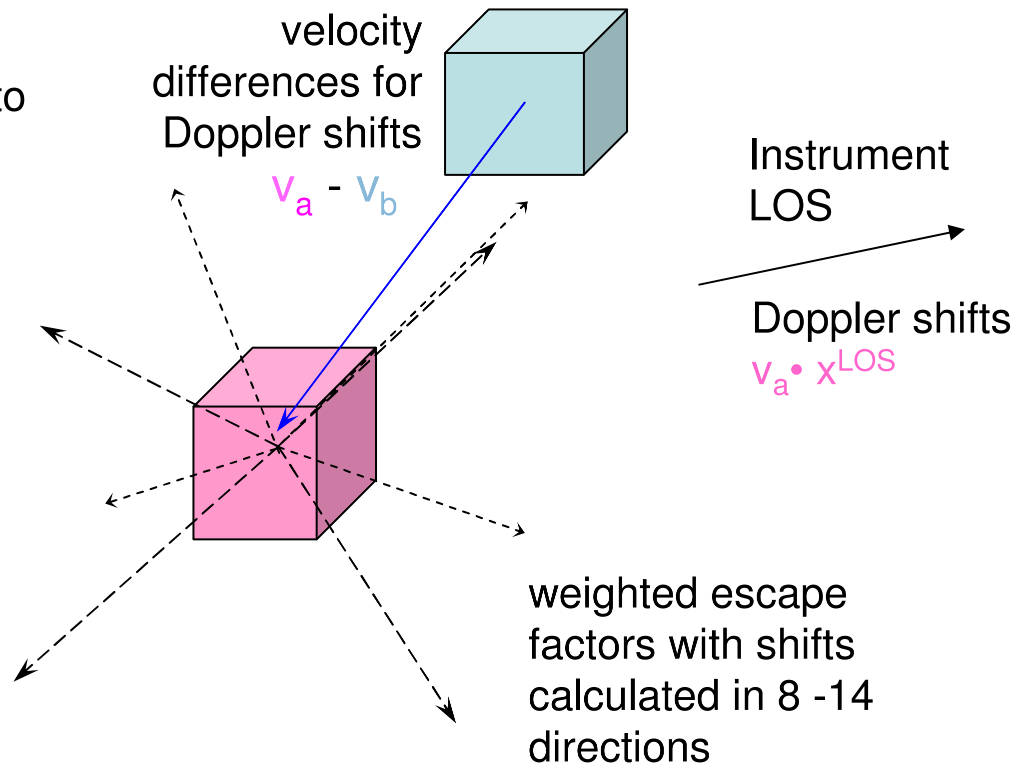
Eulerian grid & tabular approach has conceptual and computational advantages:

1) Tabulated spectra are calculated once for each element for cubes with τ_{max} ~0.3 to ~300 (for hν = 200 – 20 keV on $3x10^4$ frequency points!) then mixed & interpolated for custom materials

2) 1D and 2D plasma geometries can be spherically or cylindrically symmetrized for significant computational savings, but full 3D is possible

3) Rays for angle-averaged escape factors are taken from cube center to cube corners; velocity vectors can be mapped <u>once</u> to these rays and to instrumental line of sight

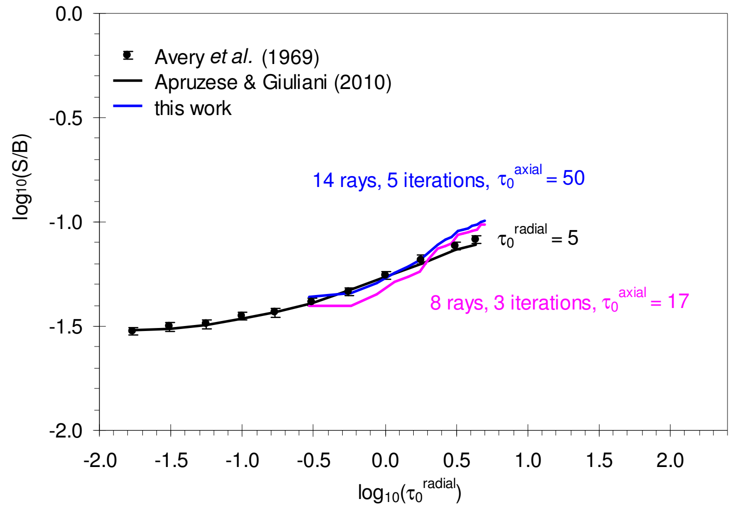
4) Fast convergence (~10 min for 10^5 cells, fully 3D)

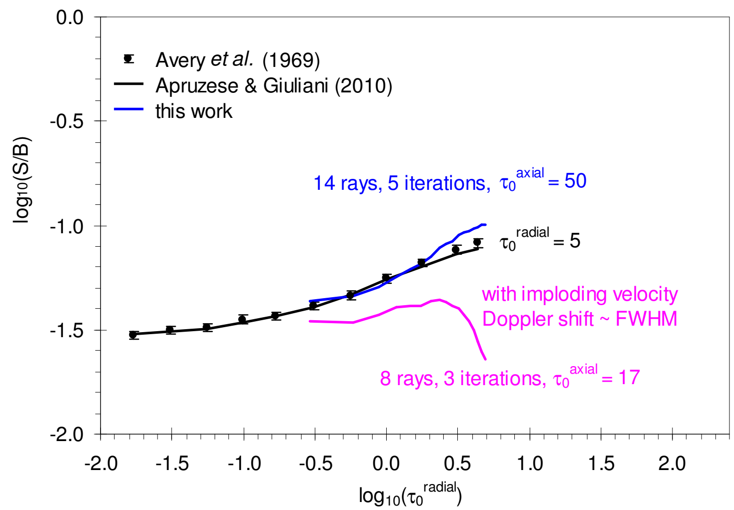


The transport model was developed with GORGON, a 3D Eulerian Cartesian code, in mind. Handshakes with this and other codes are under development.

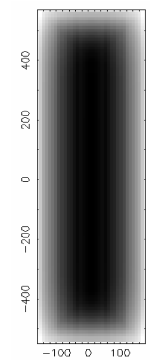
Including Doppler effects reduces photopumping and changes line profiles

Radial source functions:
no Doppler (top) & with Doppler (bottom)





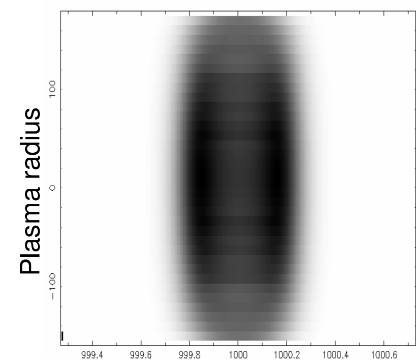
$\tau_0^{axial} = 17$
$\tau_0^{radial} = 5$



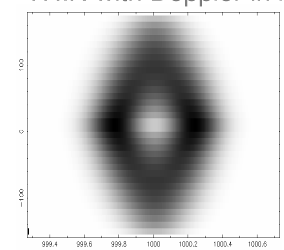
Plasma radius

Radially resolved spectra

No Doppler in transport
No Doppler in line or absorption

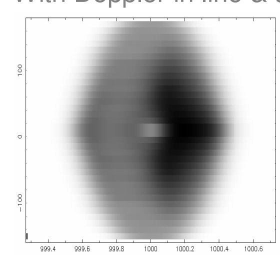


No Doppler in transport
THIN with Doppler in line



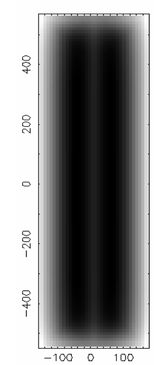
symmetric line

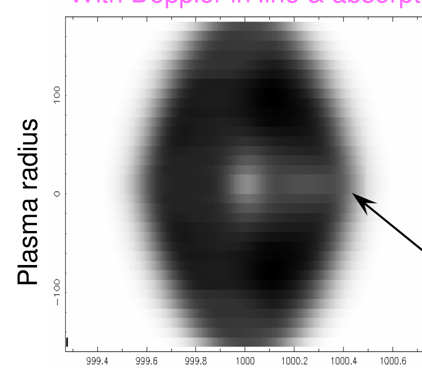
No Doppler in transport
With Doppler in line & abs.



asymmetric line

With Doppler in transport
With Doppler in line & absorption





"hollow" core
& asymmetric line

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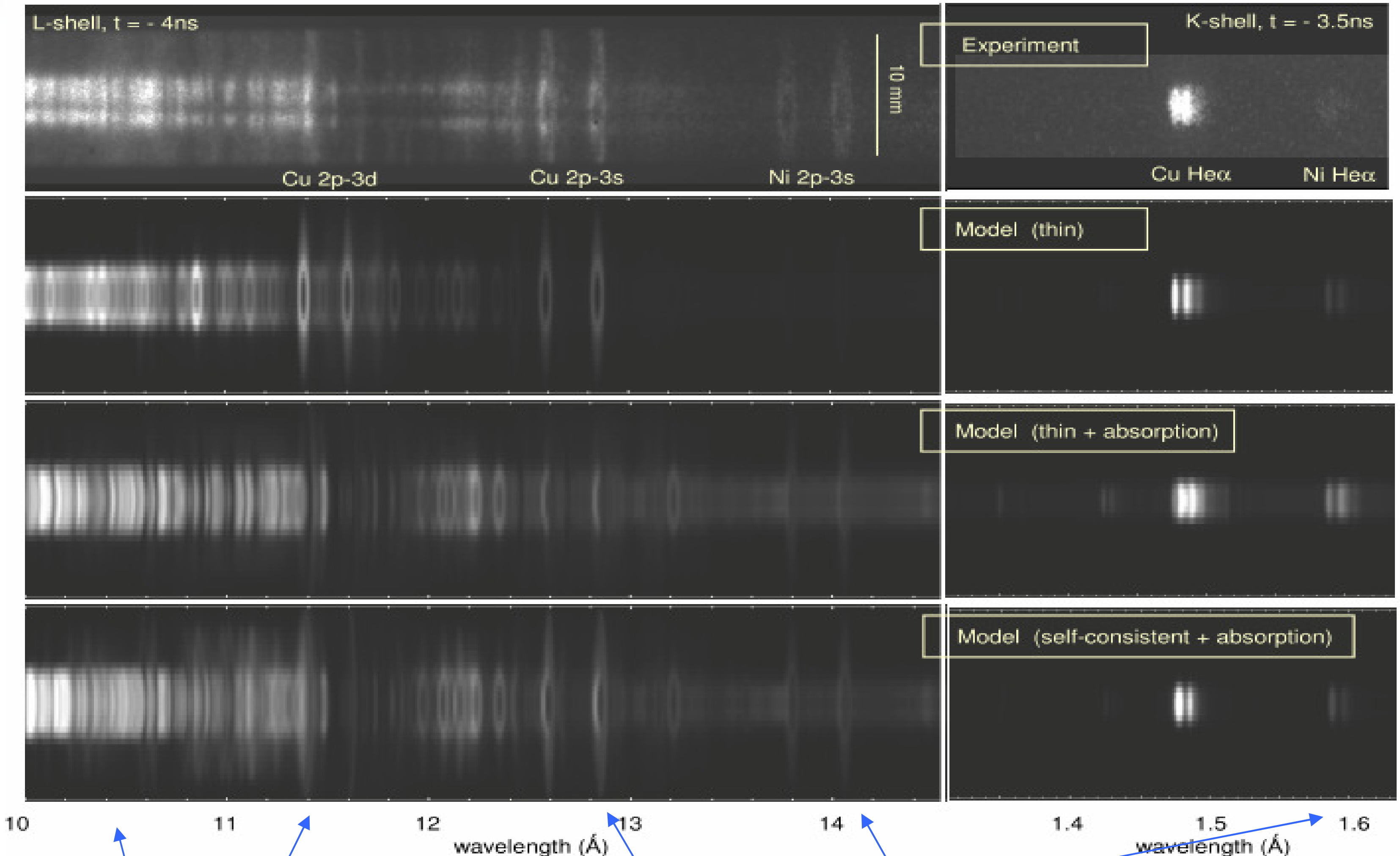
With full transport and tabulated model, we can reproduce the major features of multiply resolved data



Compact emission from highly-charged ions & extended emission from Ne-like

Line profile splitting & asymmetries

Relative intensity of ~4% Ni

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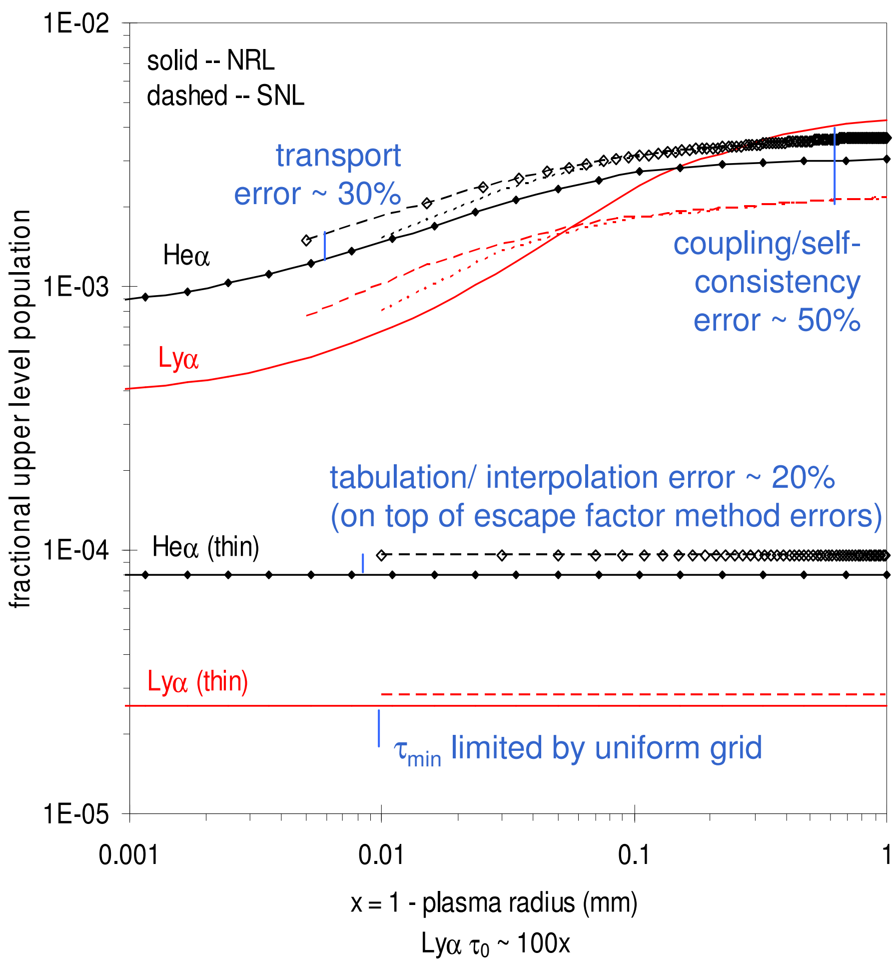
Additional comparisons that more stringently test the transport model are underway

In collaboration with NRL, we have defined an 8-level model of H- and He-like Al and performed calculations for a cylindrical plasma (T_e= 0.5 keV, n_{ion}= 10^{20}/cc, h= 20mm, r= 1mm)
see J. P. Apruzese talk this afternoon

NRL computes full multi-angle, multi-frequency transport for each line and performs fully self-consistent coupling of transported photons and level populations.

Comparisons with the modified tabular on-the-spot approach reveal consequences of various approximations: spatial gridding, spectral tabulation, transport method, and coupling consistency.

Despite these limitations, the approximate model produces reasonable results for bulk photopumping and emergent lineshapes.



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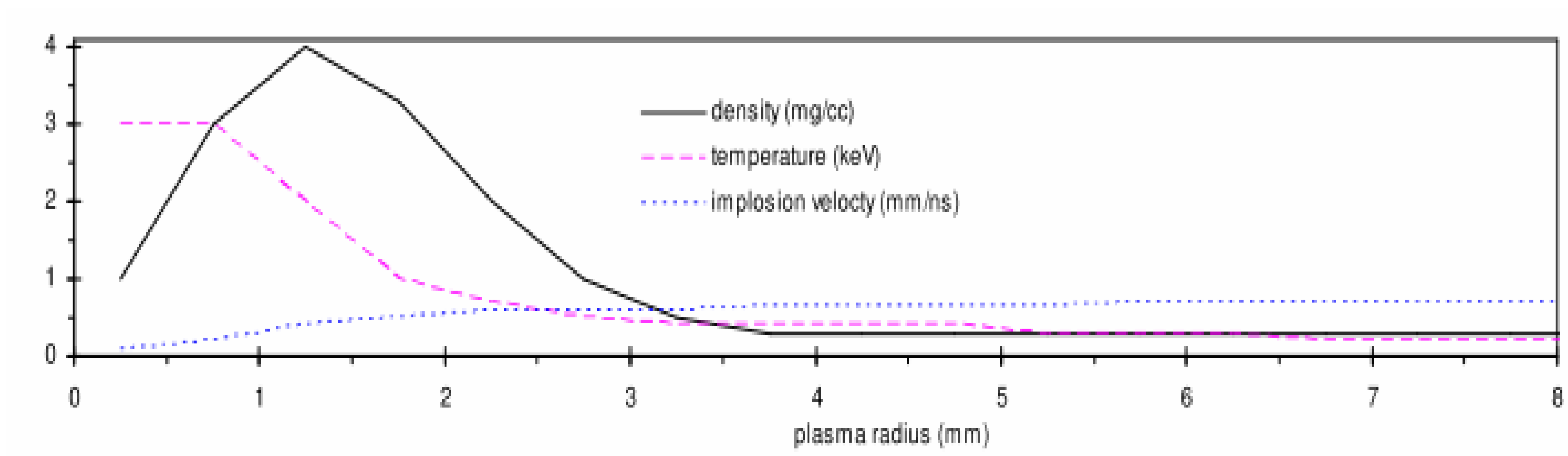
Summary/Status

- **Recent SNL progress in modeling RHEDP:**
  - Tractable hybrid-structure models designed to be spectroscopically accurate and statistically complete for all ions over wide ranges of plasma conditions
  - Magnetic field effects (Zeeman/level mixing) incorporated into atomic model
  - Approximate tabular radiation transport produces synthetic spectral & imaging data from dynamic 3D plasmas for post-processing & plasma diagnostics

- **Relevant issues:**
  - Need more extensive benchmark transport calculations & comparisons (NRL, LLNL) to help address transport model shortcomings (constant κ, fluorescence…)
  - Understand benchmarks vs. approximations vs. inline radiation in RMHD codes
  - Continued development of instrumentation & tracer methods; advocate fielding multiply-resolved instruments beyond Z (e.g. NIF)

- **Future directions:**
  - Further testing and development of transport/tabulation approach
  - Establishing handshakes and testing consistency with inline rad transport (e.g. DCA, TCRE, various radiation models in Gorgon)
  - Development of integrated diagnostic approach seeking consistency among all collected data (spectra, images, power traces (PCDs), neutronics…)

Diagnosed density, temperature, and velocity profiles



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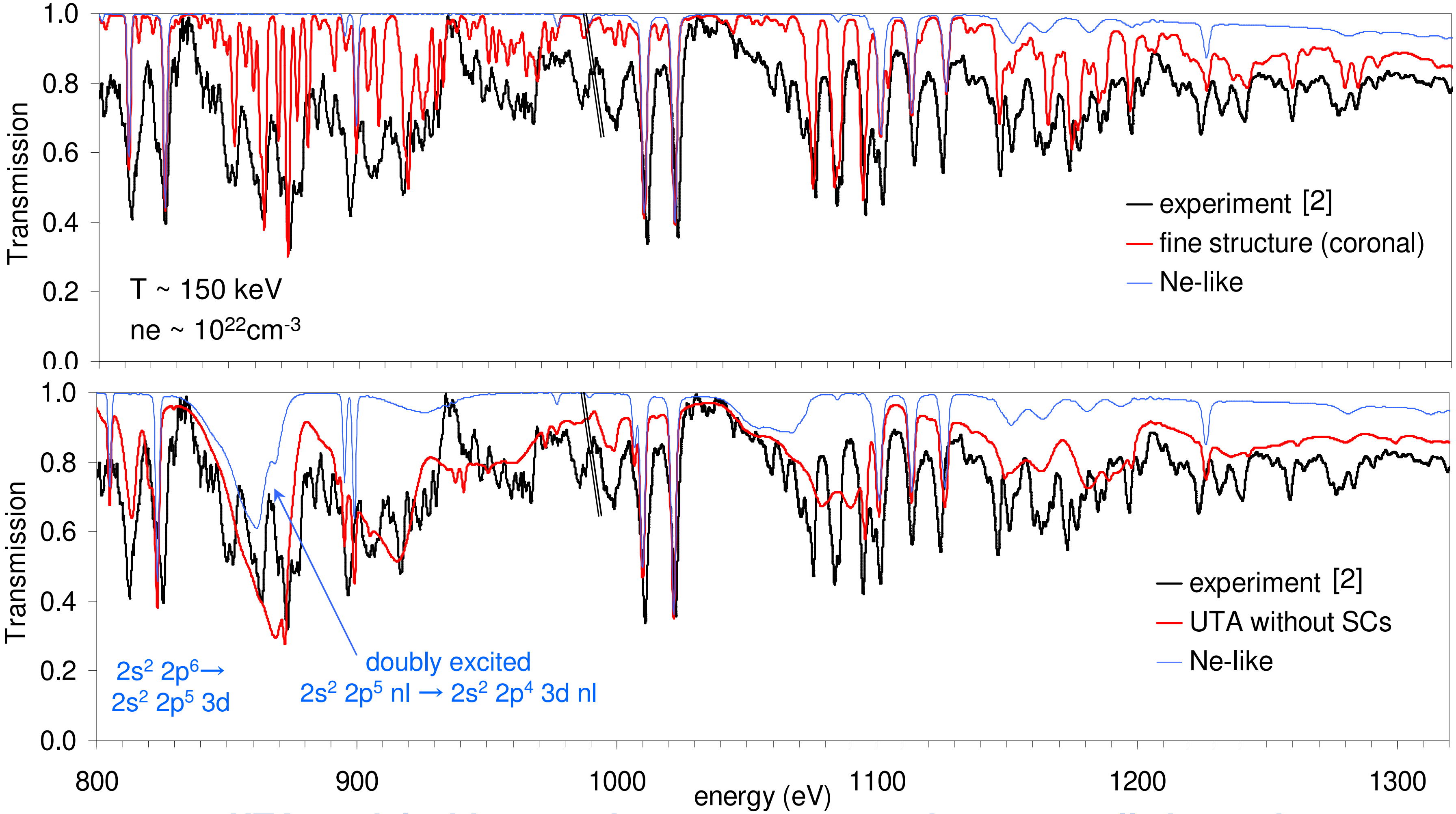
Extensive level structure is critical for high-density absorption spectra

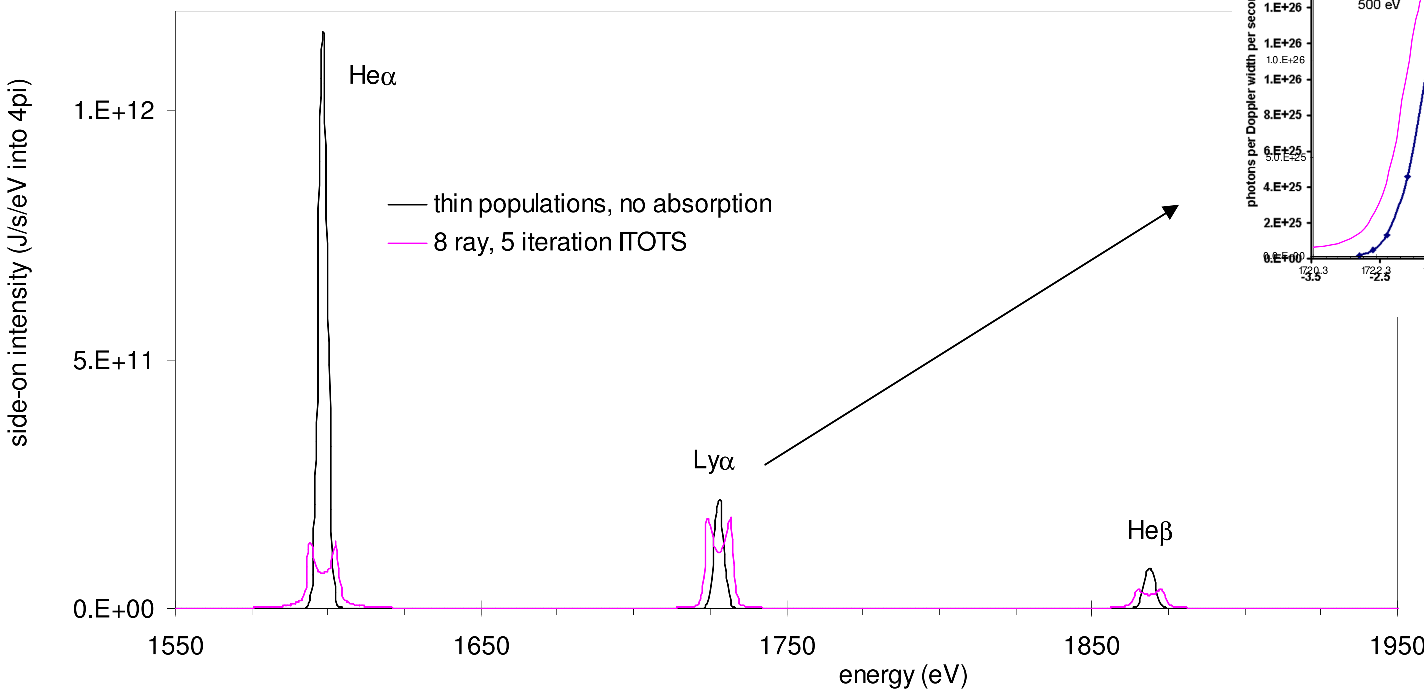


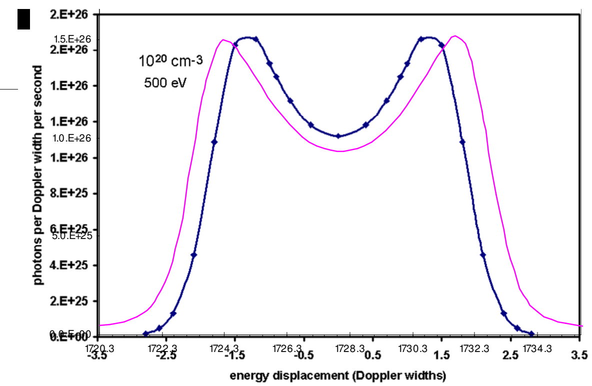
UTA model with extensive structure reproduces overall absorption but misses detailed features

[2] Bailey *et al.* PRL **99**, 265002 (2007).

Despite these weaknesses, the approximate method gives reasonable line shapes and intensities

Photopumping and opacity effects significantly alter relative intensities:





NRL and SNL Lyα line profiles show strong line-center absorption and are in reasonable agreement

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