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Computational modeling of K-shell argon spectra from Z-pinch dynamic hohlraum experiments

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Abstract

Computational modeling of K-shell argon spectra from Z-pinch dynamic hohlraum experiments

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Z-pinch dynamic hohlraum experiments on the Z-Machine at Sandia National Laboratories measured K-shell argon spectra using a focusing spectrometer with spatial resolution. [1] The spectra are modeled using Hullac [2] atomic data input, Cretin [3] nonlocal thermodynamic equilibrium (nlte) atomic kinetics and radiative transfer calculations, and Dakota [4] optimization capabilities. Hullac provides atomic structure and cross section data for Ar XIX, Ar XXVIII (n = 1 ¡ 5), Ar XXVII (n = 1 ¡ 10), and Ar XXVI (n = 1 ¡ 5), where n is the principal quantum number. Cretin calculates the area-integrated spectral intensity escaping an argon doped D_2 capsule as a function of electron density, electron temperature, and capsule radius. Dakota optimizes the plasma properties for the best t to the measured spectrum by minimizing an objective function comprised of argon spectral line ratios and full-width at half-maximums (fwhms). We highlight the framework of this general spectroscopic capability and discuss the extension to magnetized plasmas using Totalb [5] spectral line shapes.

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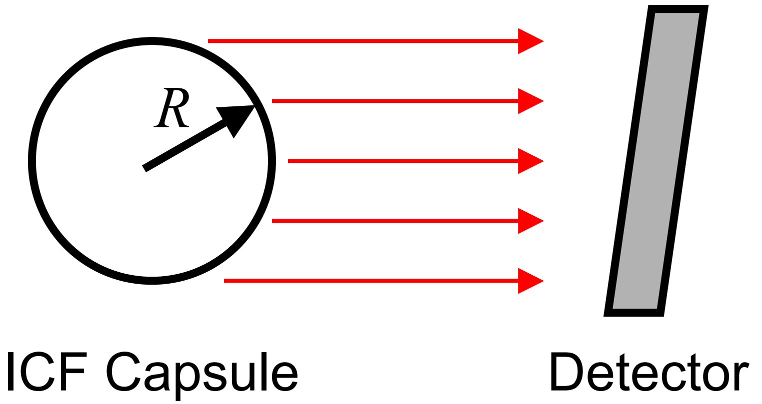
1. Sinars DB, et al. These proceedings.
2. Bar-Shalom A, Klapisch M, Oreg J. JQSRT 2001;71:169.
3. Scott HA. JQSRT 2001;71:689.
4. Elred MS, et al. Technical report, SNL, 2002. SAND2001-3796.
5. Adams ML, Lee RW, Scott HA, et al. Phys Rev E 2002;66:066413.

Z-pinch dynamic hohlraum spectroscopic computational geometry

- What are the system properties as a function of time?



- ICF Capsule:
  - Time independent sphere
  - Mixture of D_2 and Ar
  - Uniform $f(R, n_e, T_e)$
- Detector:
  - Area-integrated intensity
  - No instrumental broadening
  - Spectral range [2.95,3.75] Å

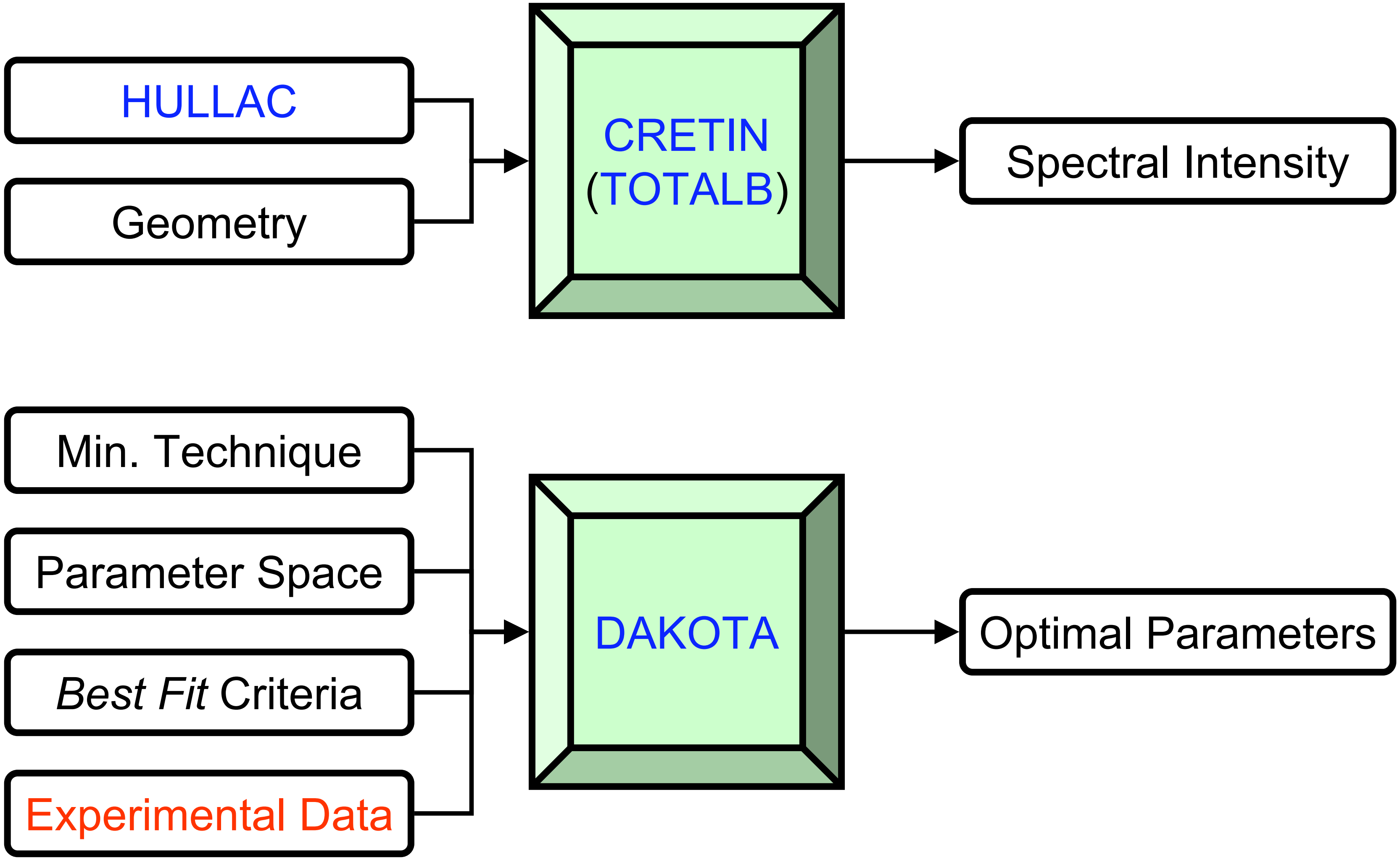
- What are the best values of (R, n_e, T_e) for a given experiment?

Computational tools for plasma spectroscopy

- Computational tools to model ICF capsule spectra:
  - HULLAC:
    - Relativistic atomic structure and cross section data
  - TOTALB:
    - Many electron atom spectral line shapes
    - Includes the effects of an applied magnetic field
  - CRETIN:
    - Nonlocal thermodynamic equilibrium (NLTE) atomic kinetics and radiative transfer
    - Multi-dimensional geometries and many electron atoms

- Computational tool to determine the best plasma properties:
  - DAKOTA:
    - *D*esign *A*nalysis *K*it for *O*ptimization and *T*erascale *A*pplications

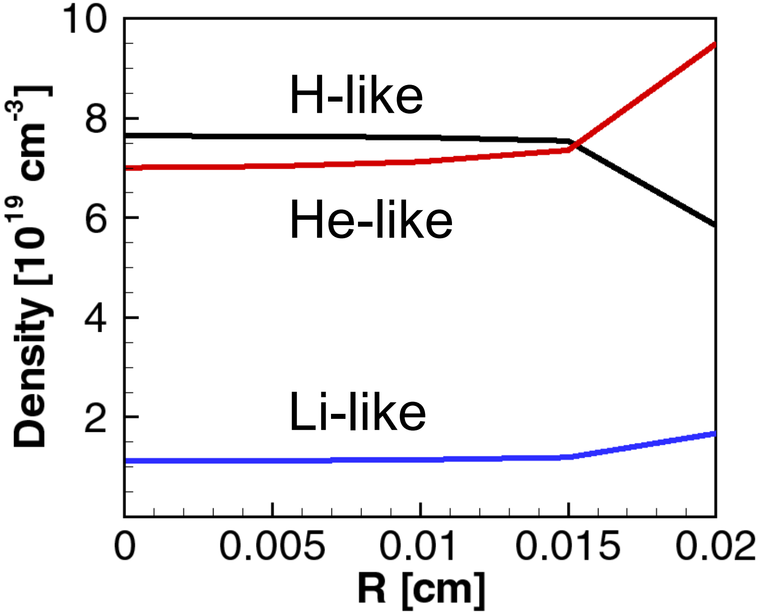
Using new computational tools to implement established spectroscopic techniques



Example: CRETIN model of an ICF capsule with R= 200 μm, $n_e = 10^{23}$ cm^{-3}, T_e = 1 keV

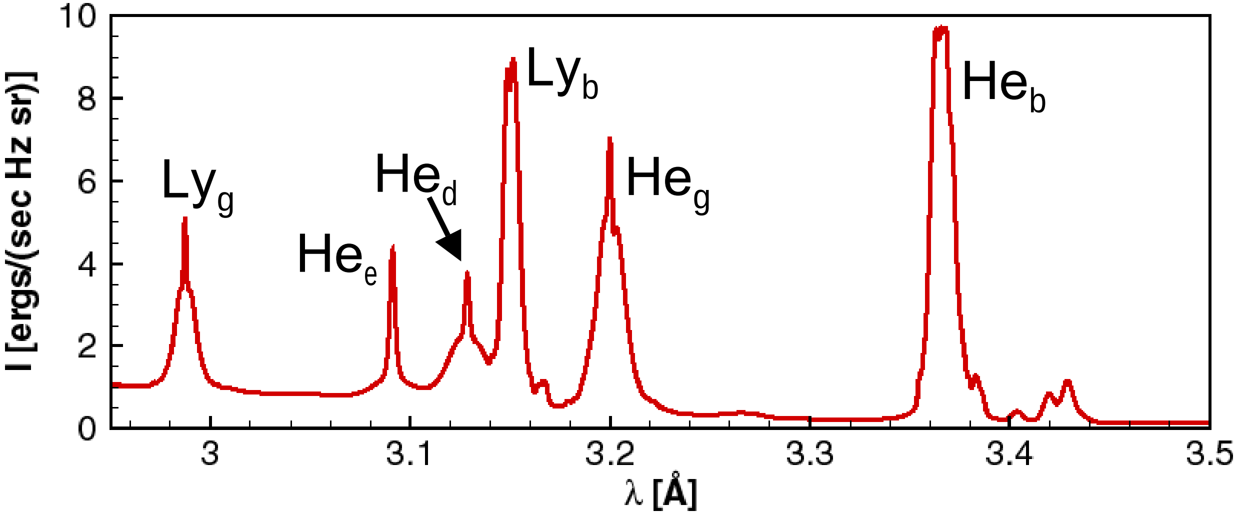
- HULLAC *Ar* atomic model
  - H-like: 58 levels; n=1-8
  - He-like: 952 levels; n=1-8; Satellites through n=5
  - Li-like: 1676 levels; n=1-8; Satellites through n=5
- TOTALB spectral line shapes are in use for:
  - Ly_a, Ly_b, Ly_g
  - He_a, He_b, He_g, He_d, He_e
- Continuum lowering

Ar isoelectronic densities

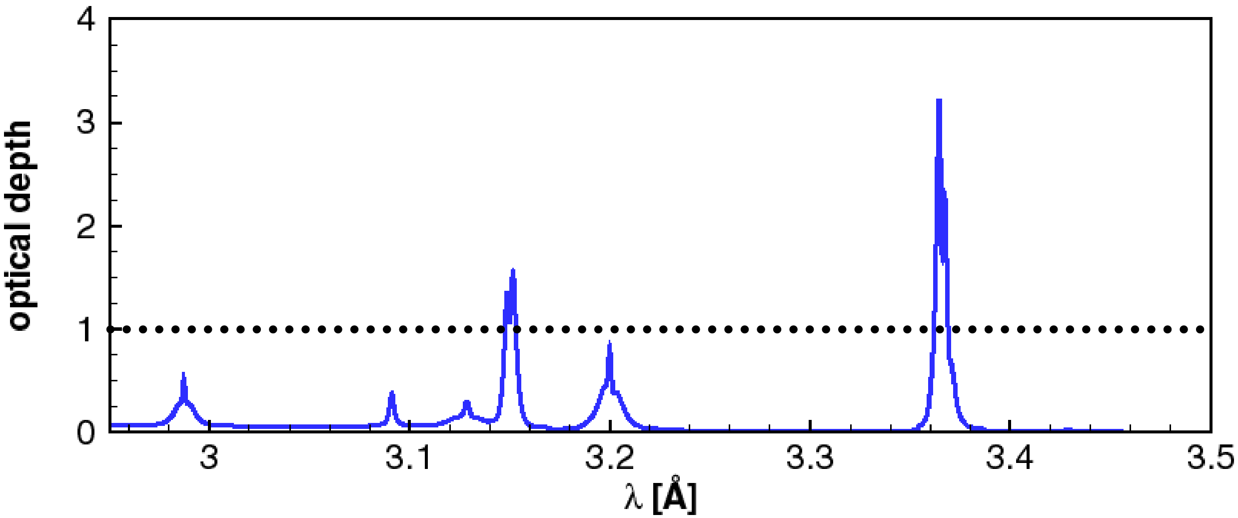


Since CRETIN accounts for optical depth effects, the isoelectronic sequence varies with position.

CRETIN K-shell *Ar* spectra from a capsule with R= 200 μm, n_e = 10^{23} cm^{-3}, T_e = 1 keV



Central features of spectral line shapes are not seen in experiments.



Both the alpha and beta lines are optically thick.

DAKOTA determines best plasma properties using established spectroscopic techniques

- Minimization Technique:
  - Parameter study on a fine mesh

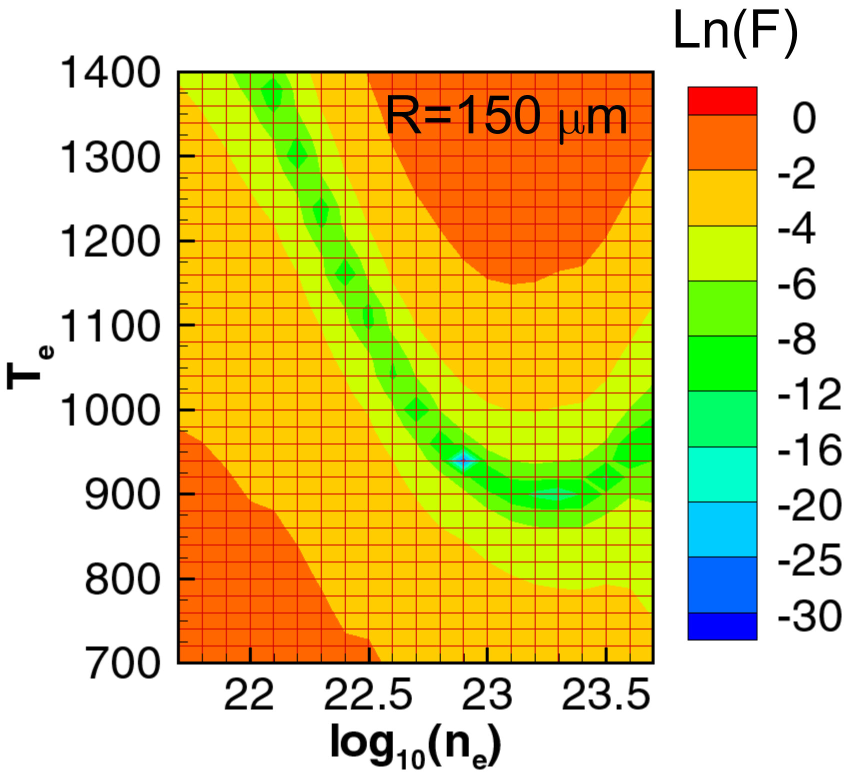
- Parameter Space: (8x21x36=6048)
  - R: 50-400 μm, 8 points linear spacing
  - n_e: 10^{21}-10^{24} cm^{-3}, 21 points log spacing
  - T_e: 700-1400 eV, 36 points linear spacing

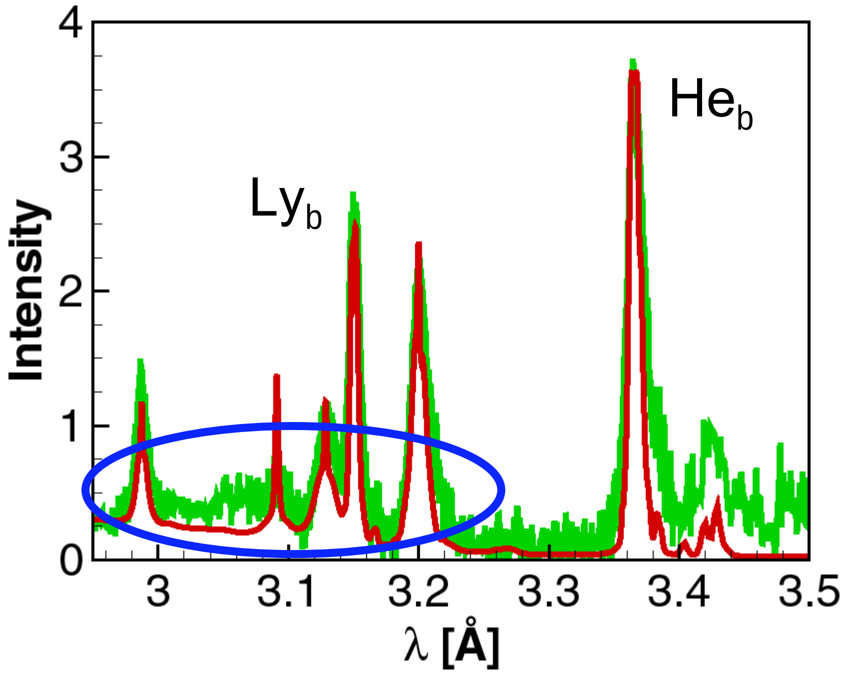
- *Best Fit* Criterion:
  - Line ratios between: Ly_a, Ly_b, Ly_g, He_b, He_g
  - Full-width at half-maximum (FWHM) of He_b
  - Chi-square comparison of simulated line ratios and FWHM with experimental data

- CRETIN simulations are performed once and comparisons with experimental data are performed in a postprocessing fashion.

Analysis of z1294 FSSR data using *Ar* Ly_b and *Ar* He_b line ratios reveals valley of candidates

- Optimal properties: R = 150 μm, n_e = 7.9•10^{22} cm^{-3}, T_e = 940 eV

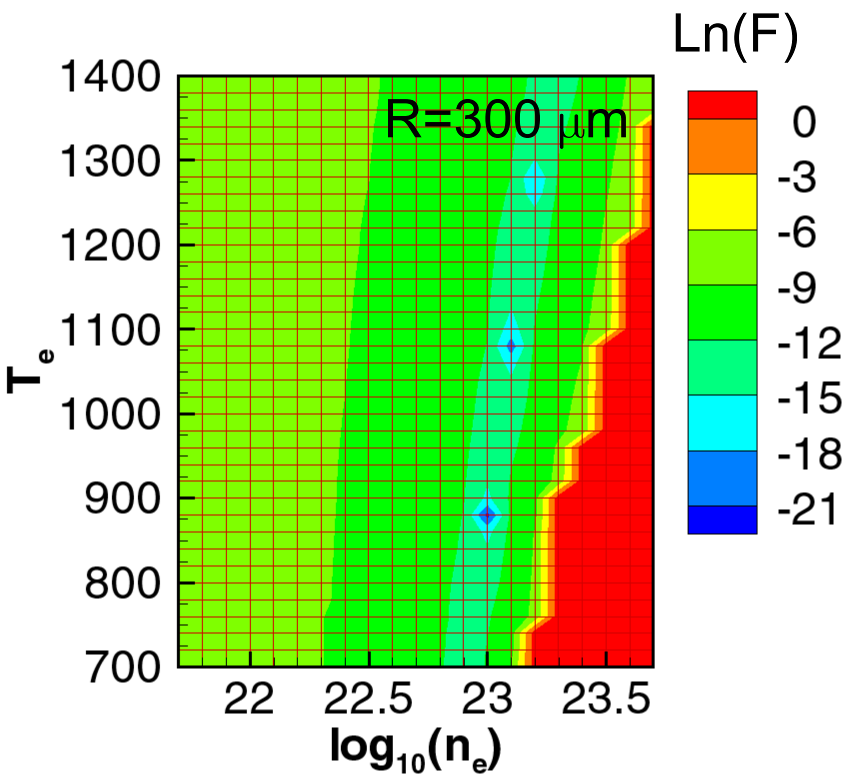


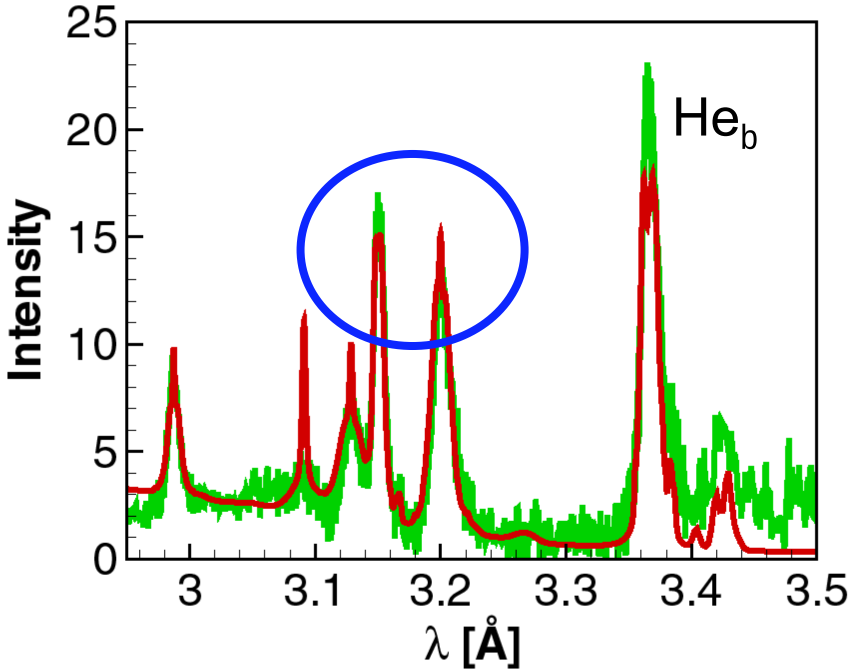


Continuum and high-n lines are different

Analysis of z1294 FSSR data using the FWHM of *Ar* He_b shows a strong density dependence

- Optimal properties: R= 300 μm, n_e =10^{23} cm^{-3}, T_e = 880 eV

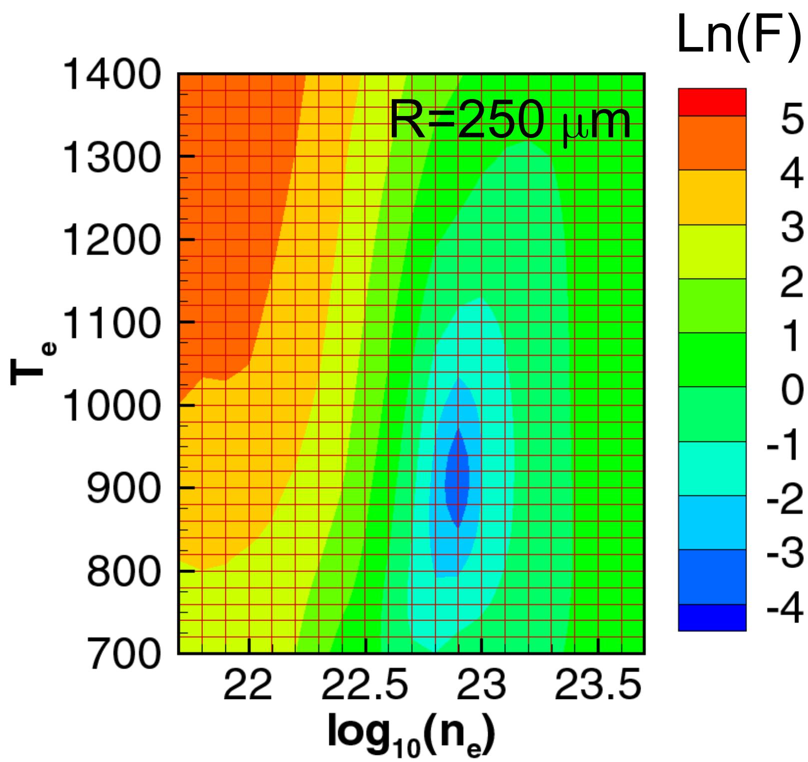


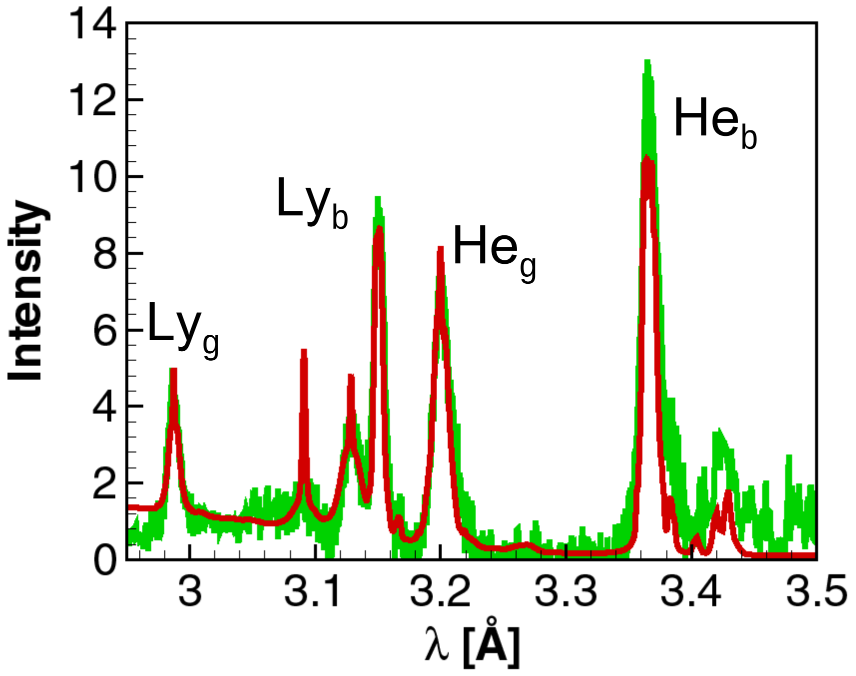


Line ratios are different

Analysis of z1294 FSSR data using the FWHM of *Ar* He_b shows a strong density dependence

- Optimal properties: R= 250 μm, n_e = 7.9•10^{22} cm^{-3}, T_e = 920 eV





Framework of this general spectroscopic capability is now established

- Self-consistent modeling of argon doped ICF capsule:
  - Relies on relativistic atomic data (HULLAC)
  - Implements detailed spectral line shapes (TOTALB)
  - Performs full NLTE atomic kinetics and radiative transfer calculations in multi-dimensional geometries (CRETIN)

- Due to the spatial resolution of the ICF capsule, opacity effects are more accurately represented in the spectral intensity. (*Ar* Ly_a and He_a lines significantly affect the level populations.)

- Automated spectroscopic analysis of experimental data:
  - Computationally expensive simulations are performed once for a given gas fill (typically not altered between experiments)
  - Optimization analysis of experimental data takes minutes

More details are needed to obtain better agreement between experiment and theory

- Spectral line shapes (SLSs):
  - Central features of SLSs are not observed in experiment.
  - Continuum lowering is affected by the broadening of large upper principal quantum number lines
  - Satellites are not included in the SLS due to computational cost

- Larger questions for spectroscopy:
  - How is the spectral intensity affected by spatial averages?
  - How can time integrated experimental spectra be dissected to yield information about peak implosion conditions?

TOTALB enables extension of the framework to magnetized plasmas

- Ar H-like lines with plasma conditions: $n_e = 10^{21}$ cm^{-3}, $T_e = 1$ keV