Analyzing non-LTE Kr plasmas produced in high energy density experiments: From the Z machine to the National Ignition Facility

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A. Dasgupta, R. W. Clark*, J. Giuliani, N. Ouart, and A. Velikovich

Plasma Physics Division, Naval Research Laboratory, Washington, DC USA

** Berkeley Research Associates, 6551 Mid Cities Avenue, Beltsville, MD USA*

D. J. Ampleford, S. B. Hansen, C. Jennings, , T. Flannigan, K. Bell, A. J. Harvey-Thompson, B. Jones

Sandia National Laboratories, Albuquerque, NM USA

Sandia National Laboratories

M. May, M. Barrios, H. Scott, K. Fournier, J. Colvin, G. Kemp

Lawrence Livermore National Lab, Livermore, CA USA

Lawrence Livermore National Laboratory

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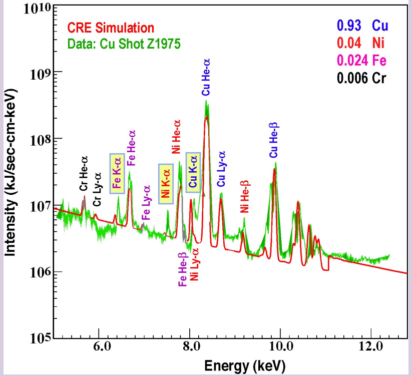
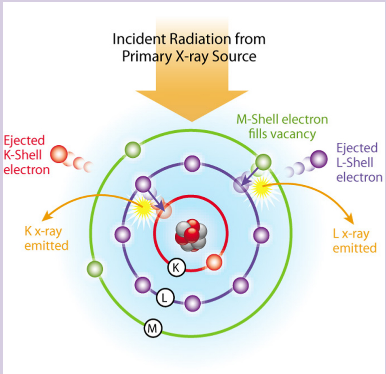
High Energy x-ray sources have many useful applications

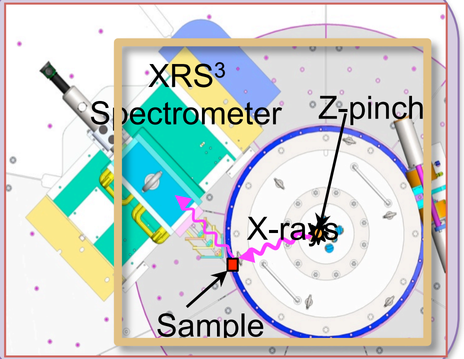
NRL PPD



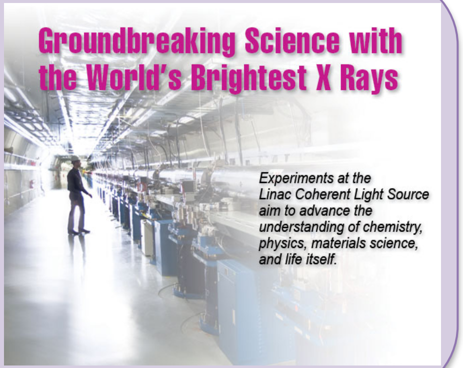
For validating atomic & plasma models



For inner-shell photoionization



For scattering experiments



For Generating world's brightest light source

Motivation: Why investigate Krypton as an X-ray source?

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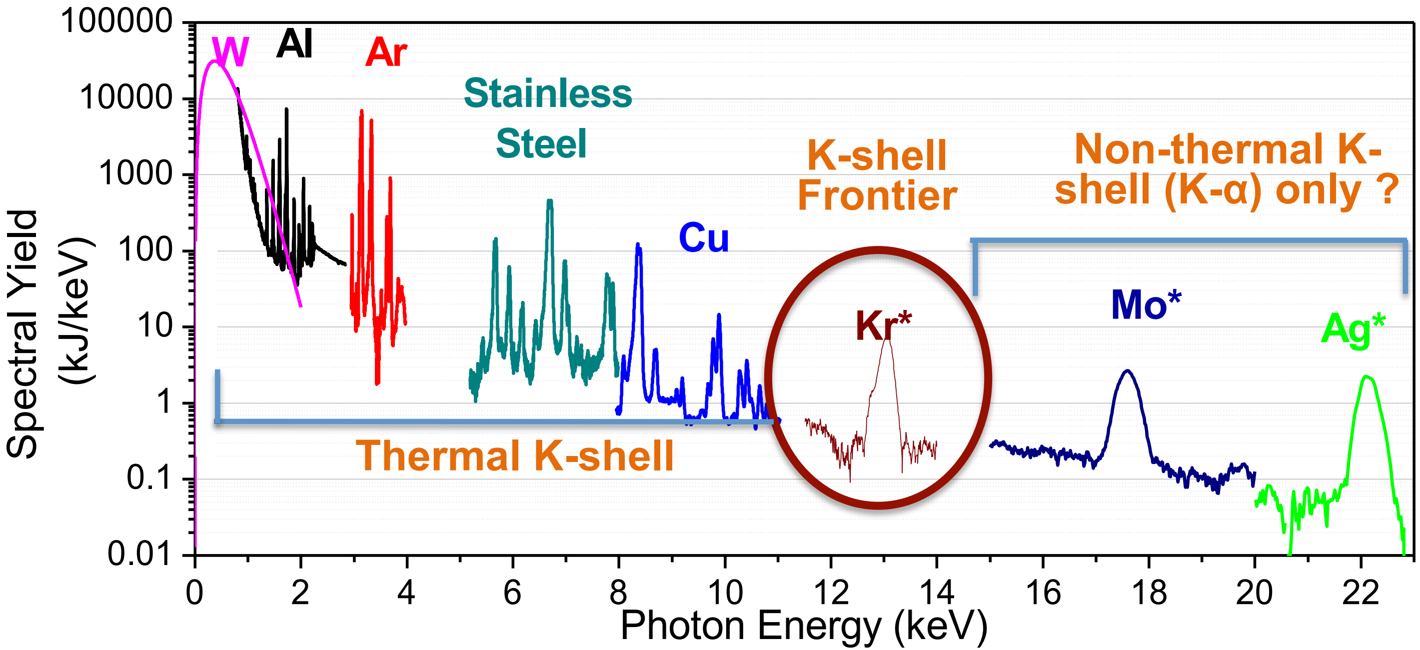
- The **refurbished Z** machine at **Sandia National Laboratories** and the **National Ignition Facility (NIF)** are energetically capable of producing **intense multi-keV** X-ray radiation sources from **High Z** materials such as **Kr**.
- Well-characterized laboratory experiments ***validate* atomic and radiation models** that are crucial for diagnosing hot dense plasmas.
- There are recent studies of **Kr** for EUV and X-ray generation in **EBIT**, pulsed-power devices, and **gas cluster** laser absorption.

Motivation: The radiation character depends upon the atomic number

As we go to higher Z, more energetic photons are produced, but the conversion efficiency falls off. Different mechanisms are responsible for emission as we go from low to high Z elements.



Courtesy: D.J. Ampleford (SNL)

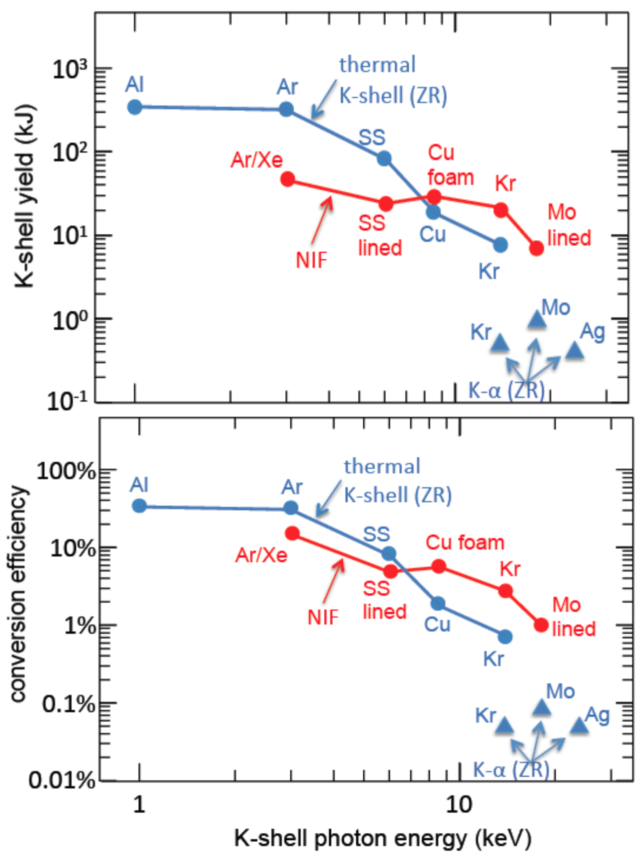
Radiative losses in L-shell inhibits K-shell ionization for high Z-materials

Motivation: X-ray sources on Z and NIF display different variations with K-shell photon energy

Z targets are wire arrays and gas puffs. Mature technology for < 5 keV sources, but K-shell yield and efficiency fall off rapidly with higher Z_A.

NIF targets are metal lined, foam, and gas filled pipes. To date, limited optimization of the target design. Note that NIF K-shell yields do not fall off with Z_A as on Z.

Why is the variation with K-shell photon energy different between Z and NIF? We know that z-pinches are effective at heating ions, whereas lasers preferentially heat electrons.



Atomic physics is the same, but the drive, energy deposition process, and target dynamics are different.

An overview of NRL atomic and radiation modeling

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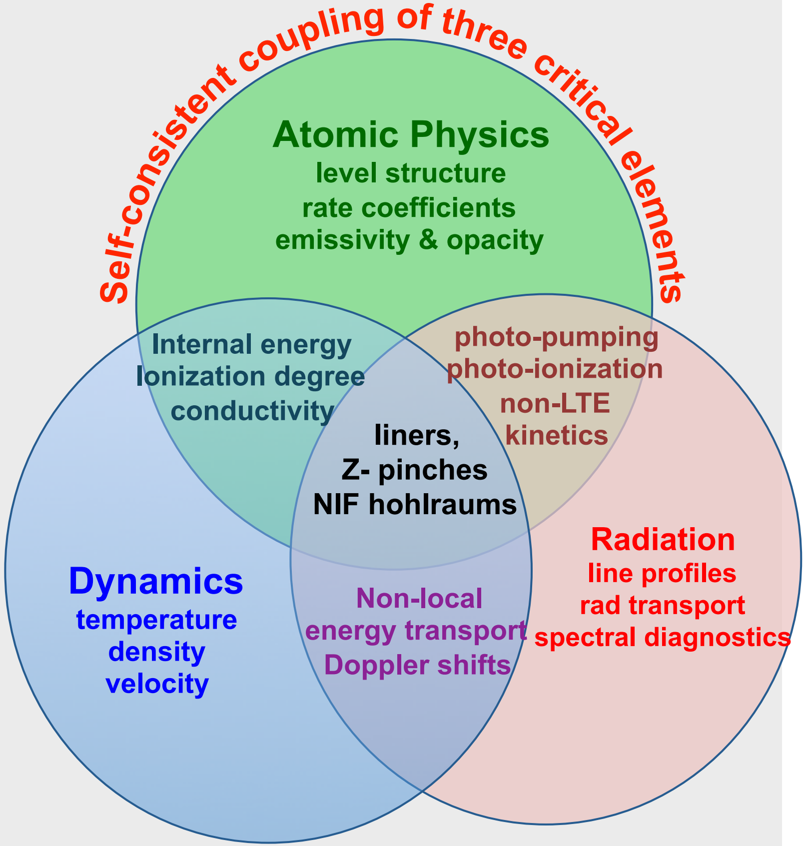
- Early atomic models had limited and configuration averaged structures; collisional-radiative data generated using simple codes or formulae.
- Radiation transport involved escape probability for emission line and recombination radiation.
- Radiation as a Z-pinch diagnostic necessitated more detailed and improved atomic and radiation modeling.
- Now atomic rates for all important processes are self-consistently generated using FAC codes at the fine-structure level.
- Detailed multi-frequency radiation transport needed for spectral accuracy at high densities, and for analysis and diagnostics.
- Self-consistent coupling of three critical physical element 1) non-LTE atomic physics, 2) radiation transport and 3) magneto-hydrodynamics form the scientific basis of our analysis and calculation of radiation in the HEDLP.



Atomic modeling: complexity and cost grow exponentially with atomic number (Z_A)

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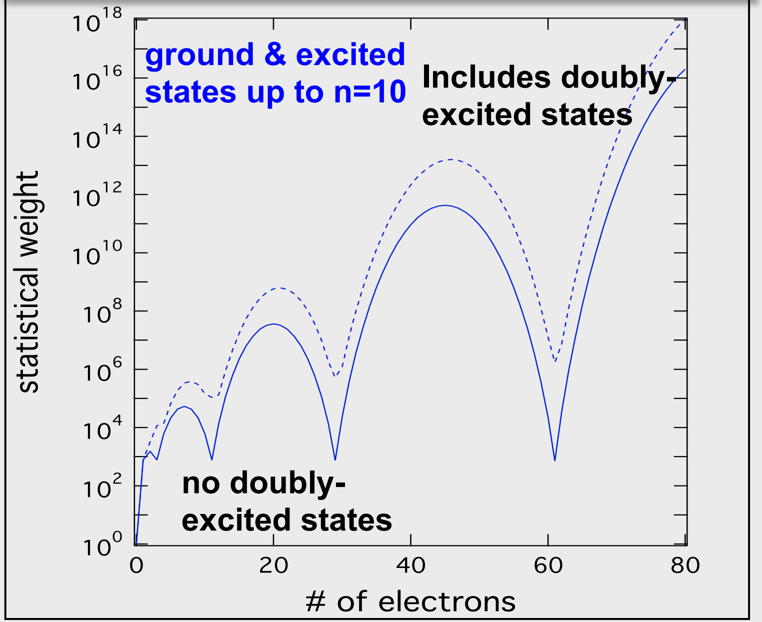
Detailed yet manageable atomic models for high Z_A elements (divertors/hohlraums and also Z-pinches) are needed for accurate ionization balance

Challenges

- Coupling enormous amount of atomic data into NLTE modeling
- Accurate <u>and</u> detailed models can be computationally intractable
- Number of levels varies by 10^5 between models ➔ runtime varies by many orders of magnitude
- Completeness is required for accuracy, but <u>some averaging is necessary</u>

Levels required for accurate NLTE ionization kinetics



Ref: HEDP 6, 2010, Scott & Hansen

The Kr atomic database includes details from H- to Ar-like ionization stages

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Ion stage	H	He	Li	Be	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar
Ionization (keV)	17.9	17.3	4.11	3.97	3.76	3.63	3.46	3.29	3.11	2.94	1.20	1.15	1.05	1.01	0.955	0.901	0.847	0.795
Levels	14	22	13	50	38	54	80	94	68	42	14	45	103	79	56	60	101	64
Lines	40	80	35	351	286	464	770	1381	776	323	51	441	1964	1213	663	1407	3020	1143

- Fully relativistic distorted-wave (RDWV) for Structure and collision calculations
- Flexible Atomic Code (FAC) used for detailed K-, L- & M-shell up to Ar-like ions
- Simple codes and formulas for lower ionization states
- Singly excited states up to n=7
- Doubly excited states up to n=10
- Full radiative and collisional coupling

All physical processes in our collisional-radiative modeling are driven by non-LTE atomic kinetics

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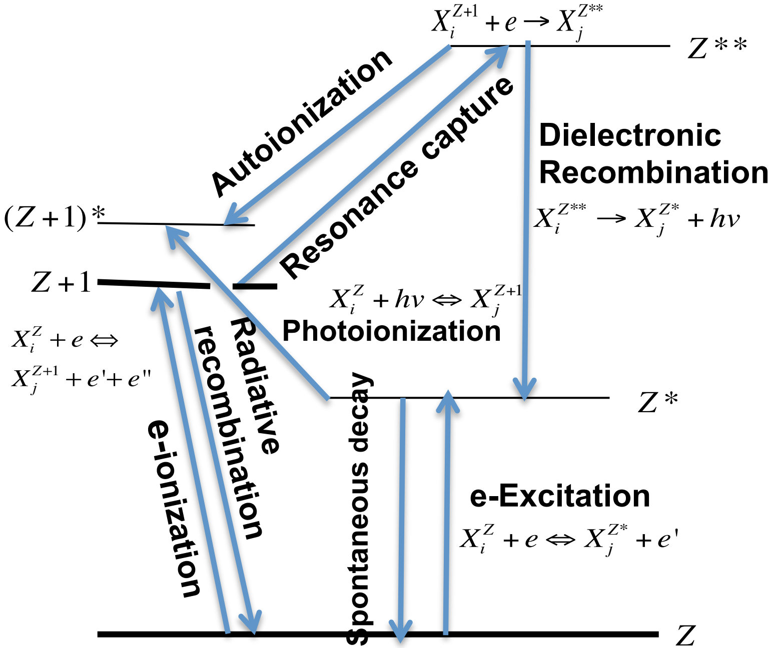
The electrons, ions, and photons interact and in doing so transfer energy from one particle to the other.



Spontaneous decay/Resonant photoabsorption : $X_j^{Z*} \Leftrightarrow X_i^Z + h\nu$

Ionization/3-body recombination : $X_i^Z + e \Leftrightarrow X_j^{Z+1} + e' + e''$

Electron impact excitation/deexcitation : $X_i^Z + e \Leftrightarrow X_j^{Z*} + e'$

Photoionization/radiative recombination : $X_i^Z + h\nu \Leftrightarrow X_j^{Z+1} + e$

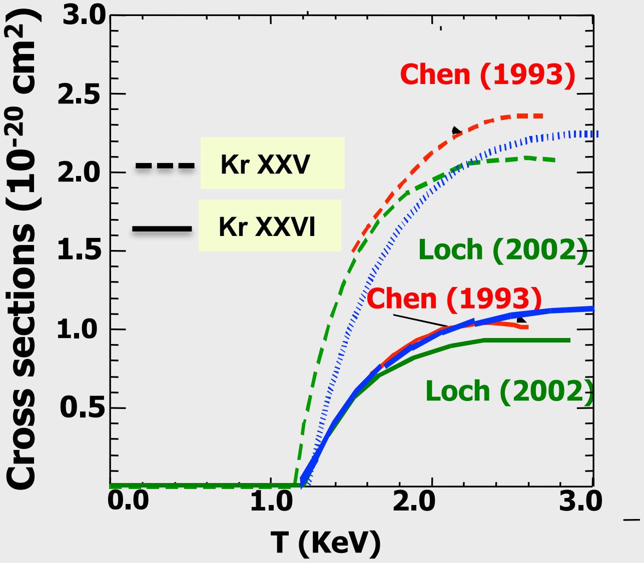
Autoionization/resonant capture : $X_i^{Z+1} + e \Leftrightarrow X_i^{Z**} \rightarrow X_i^Z + h\nu$

Bremsstrahlung/inverse bremsstrahlung: $X_i^Z + e \rightarrow X_i^Z + e + h\nu$

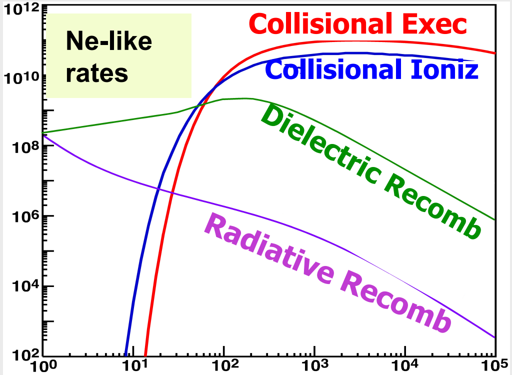
Dielectronic recombination:

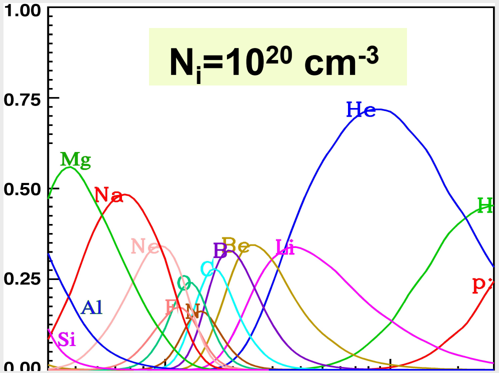
NLTE populations depend on the rates of these atomic processes and can be determined by: $\frac{dN_z^k}{dt} = \sum_{z'} \sum_{k'} (R_{zz'}^{kk'} N_{z'}^{k'} - R_{z'z}^{k'k} N_z^k) +$ **pumping by non-local radiation field**

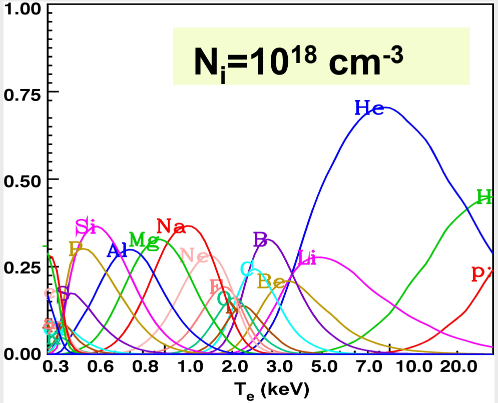
Atomic properties and effect of ion density and dielectronic recombination on Kr fractional populations

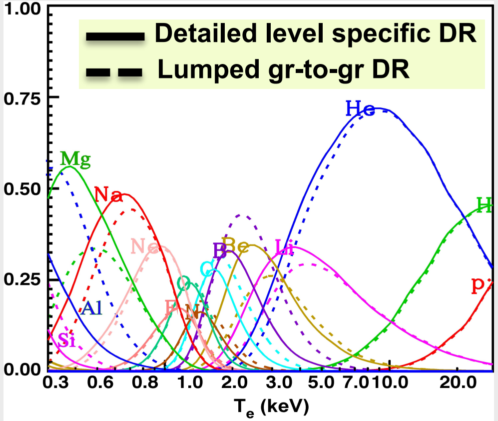


Chen & Reed (1993), PRA 47, RDW and MCDF
Loch et. al. (2002), PRA 66:
configuration-average distorted wave

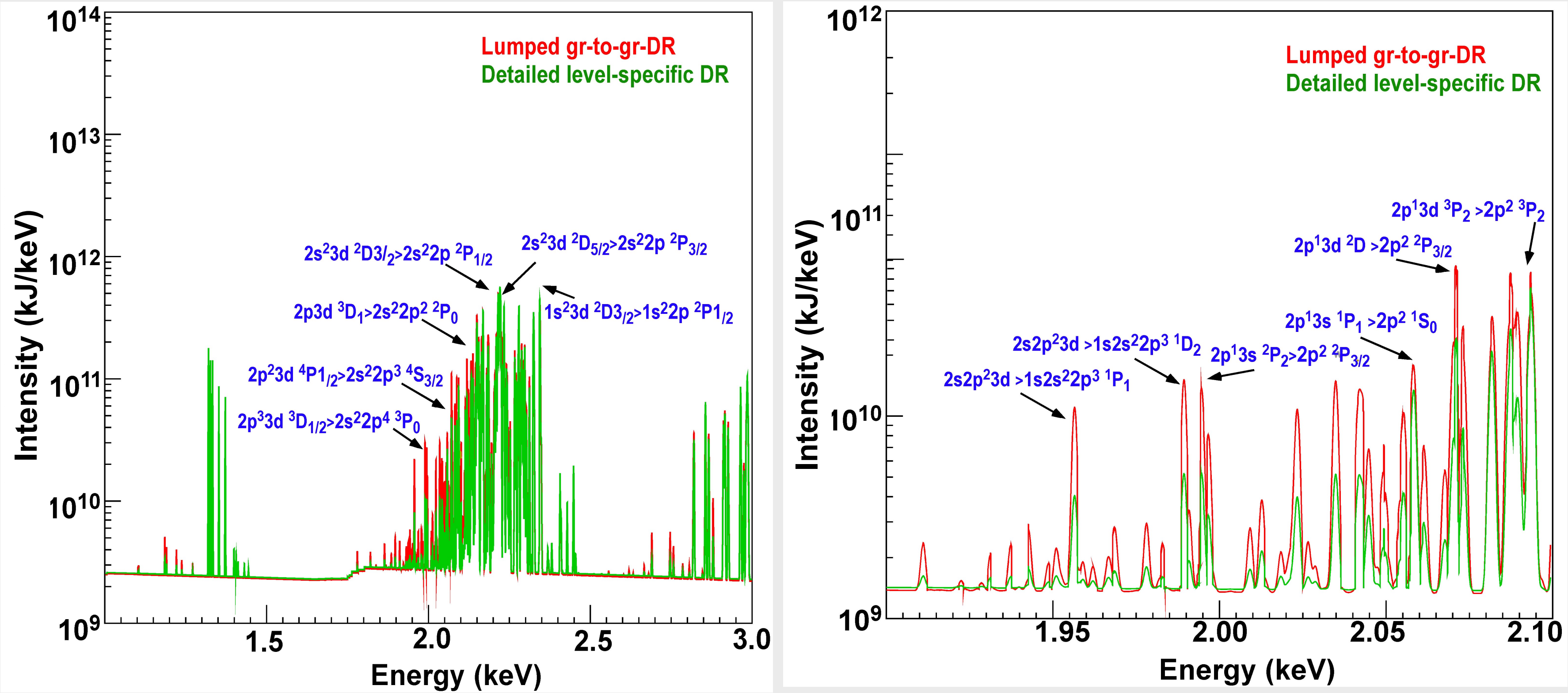








Kr L-shell spectra showing effect of detailed vs. lumped dielectronic recombination



Multi-zone Radiation transport Model: Frequency-averaged line transport

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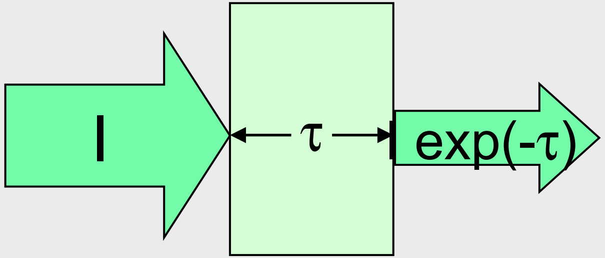
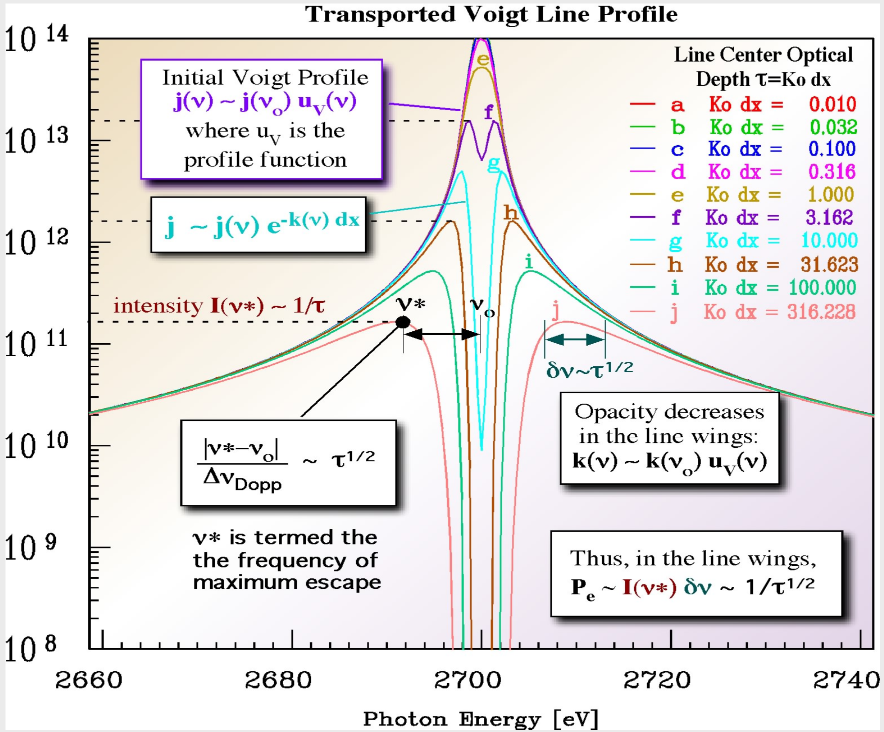
Simplest: probability that a photon of energy $h\nu$ traverses a medium of optical depth τ without any interaction is: $\exp(-\tau)$.





τ = optical depth at line center,

Doppler escape probability is given by:

$$P_e(\tau) = \pi^{-1/2} \int_{profile} e^{-x^2} \exp(-\tau e^{-x^2}) dx$$

Averaging over a spectral line profile can greatly speed computations. Escape from line wings increases P_e by orders of magnitude over the line center value.

Time integrated multi-frequency simulation shows improved agreement with data

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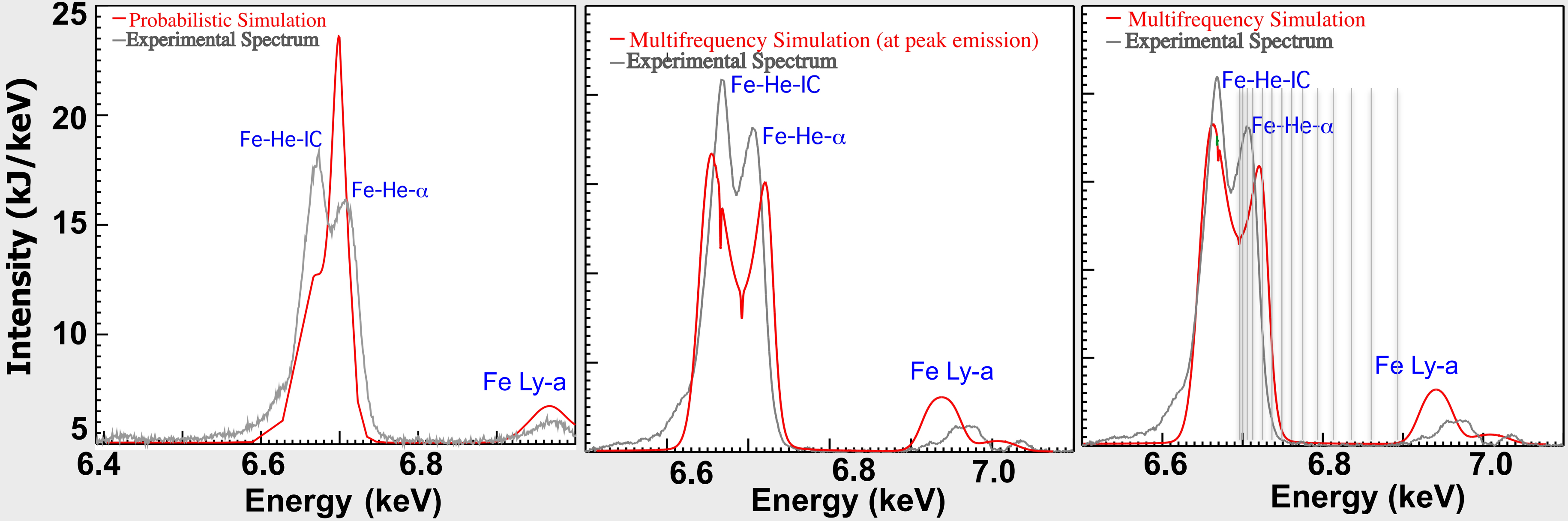
K-shell SS synthetic spectra are matched to time integrated data (SS Z578) using densities and temperatures profiles. Summation of the simulated spectra over a rad-hydro run shows better agreement.



Self-absorption of the He-α line moderated by time evolution. In Multi-frequency case, each line is resolved using a large number of frequencies (using a power law distribution) that resolve the line profile. It is important to account for the coupling of CRE to hydrodynamics when interpreting spectroscopic data.

DZAPP combines 1D MHD with detailed atomic physics and radiation transport to study the evolution of the plasma

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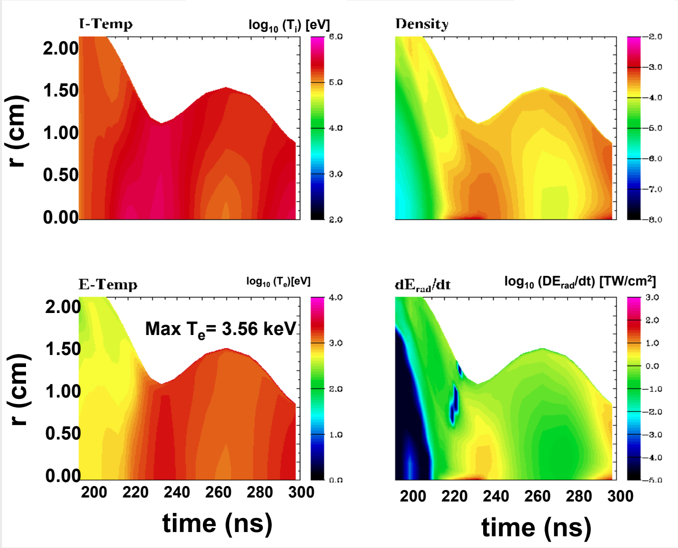
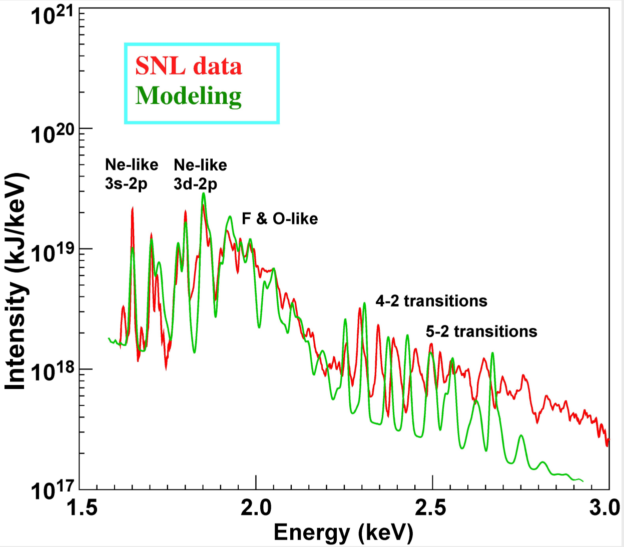
DZAPP is a **1D** simulation code, combining a transmission-line circuit model, an **MHD transport** scheme, and **detailed atomic physics** and **radiation transport**. The result is **time-dependent** plasma motion and **self-consistent radiation**.

Portion of MHD Implosion History



Time-integrated spectrum



The Z facility achieved record X-ray emission from Ar (3 keV) and Kr (13 keV) gas-puff Z-pinches

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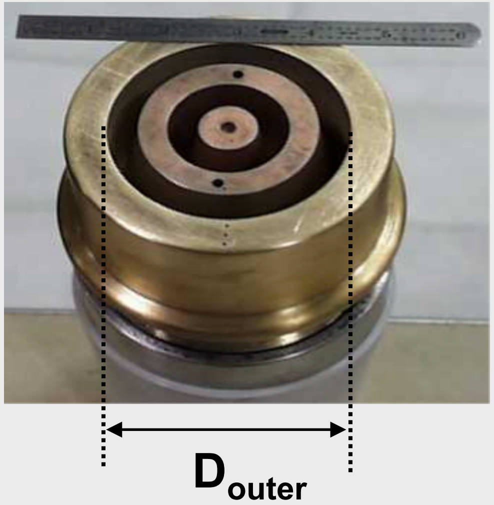
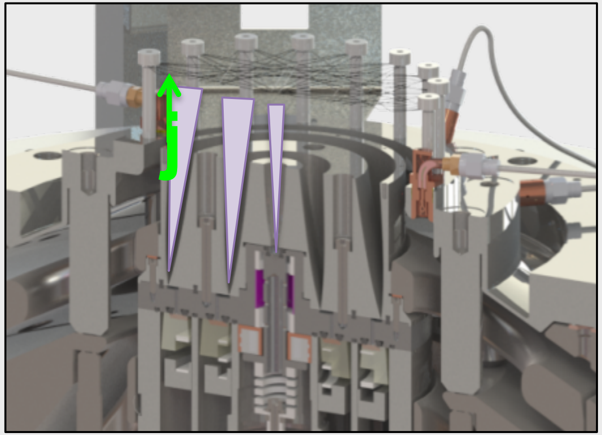


Example of a Double-puff Z-pinch Nozzle.



Initial setup is double shell gas puff

- Initial outer diameter 8cm, 12cm
- Length 20 mm

Imploded by ~20MA Z current

- Stagnates to ~0.5mm hot core
- Surrounded by ~2mm cooler 'halo'
- Azimuthally symmetric gas shells
- ~1 mg/cm
- Shell-like and ramped profile

Courtesy: D.J. Ampleford (SNL)

Kr L-shell spectra from non-LTE kinetics modeling at T_e=600 eV & N_i=8x10^{19} cm^{-3} compared to Z-2383 data

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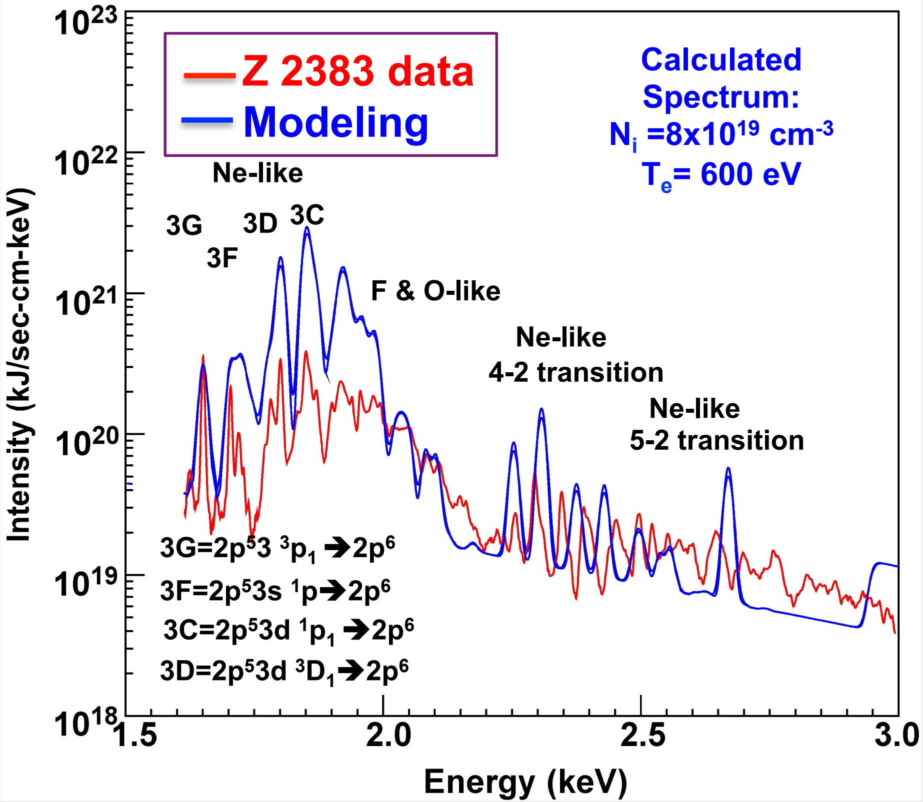

SNL Spectrum:

8cm initial diameter Kr gas puff

Calculated Snap-shot Spectrum from post-process:

- Radiation from post-process with single N_i and T_e
- Ionization using Collisional Radiative Equilibrium
- Atomic model for K- through M-shell obtained using FAC

Z data: Courtesy of S. Hansen & D.J. Ampleford (SNL)

Kr Radiation 1-D MHD simulation of 8 cm nozzle: History of plasma conditions

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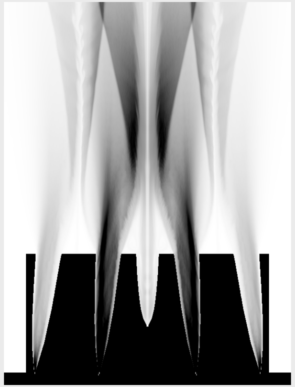
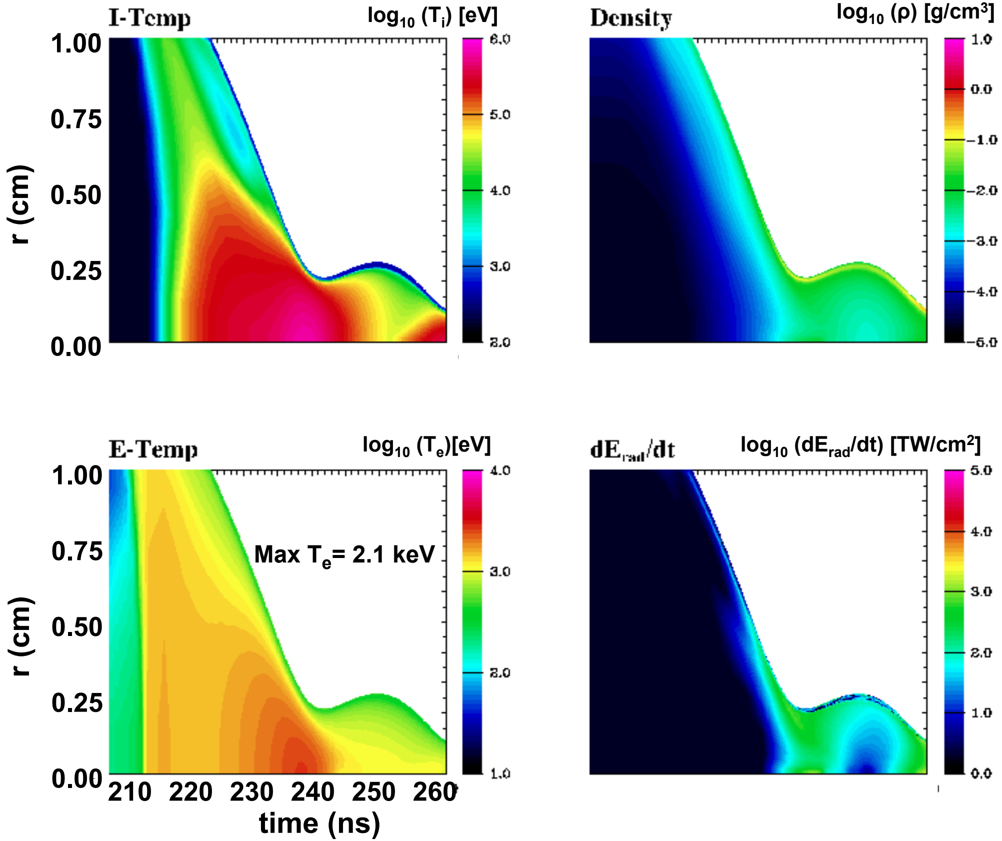
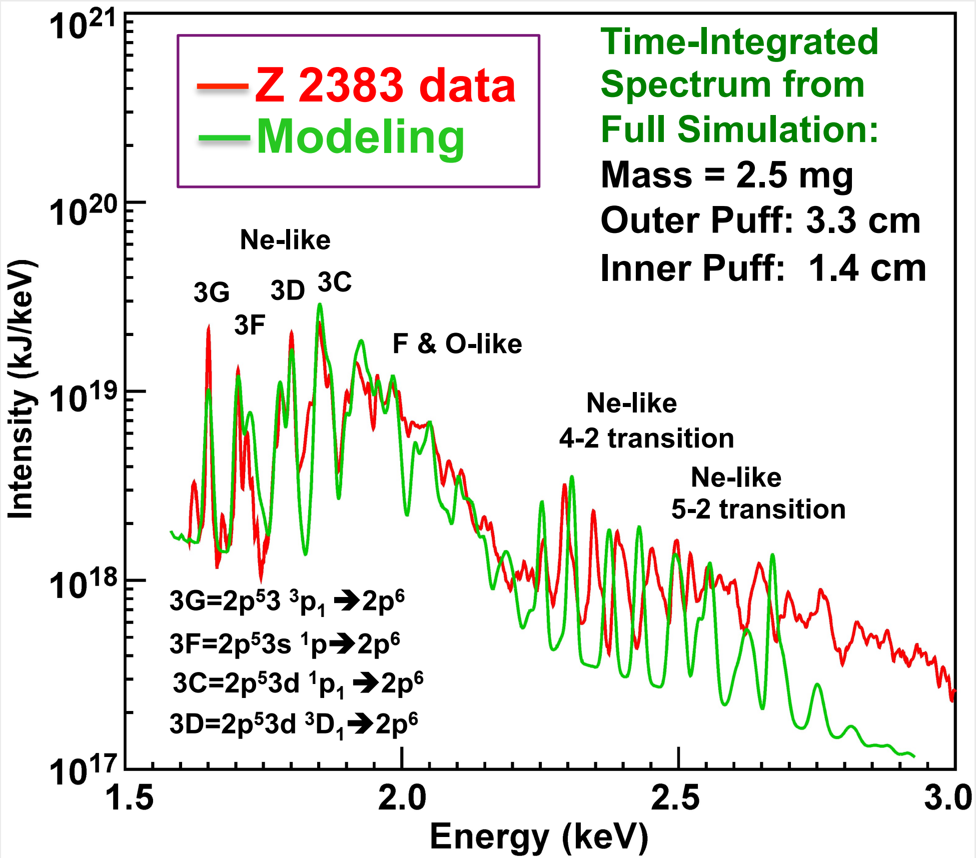
8 cm nozzle



Kr Double-Puff
Total Mass 2.50 mg
Axial Length 2.0 cm
Outer Puff: 3.3 cm;
Inner Puff: 1.4 cm



Kr L-shell spectra from full DZAPP simulation compared to 8-cm double shell Z pinch data



SNL Spectrum:
8cm initial diameter Kr gas puff

Simulated Spectrum:

- Radiation Integrated over full 1D ZR implosion simulation
- Ionization using full Non-Equilibrium integration of atomic populations in time
- Atomic model for K- through M-shell obtained using FAC

Kr Radiation 1-D MHD simulation of 12 cm nozzle: History of plasma conditions

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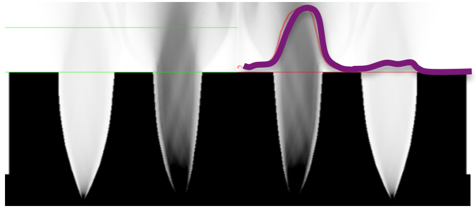
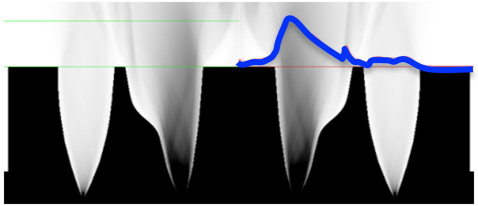
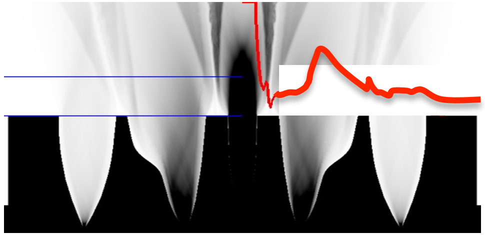
12 cm nozzle: Total Mass 1.34 mg, Axial Length 2.0 cm; Outer Puff: 5.0 cm; Inner Puff: 2.1 cm



Shell like profile

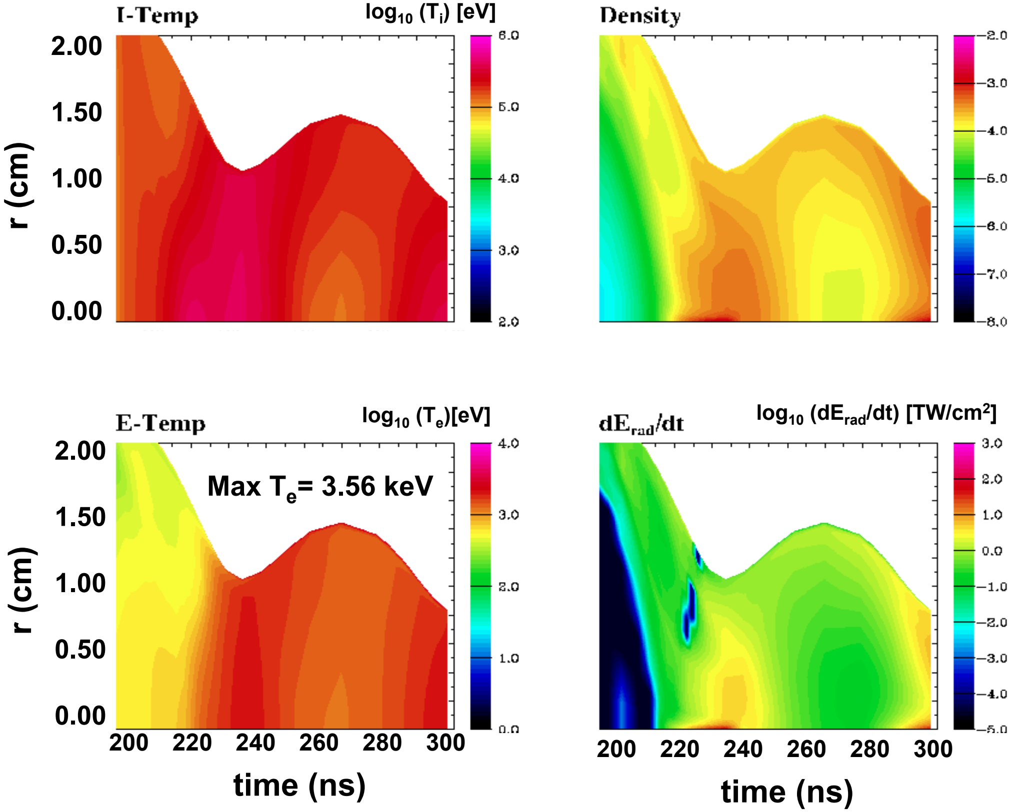


Ramped density



Ramped + jet density

Courtesy: C. A. Jennings(SNL)

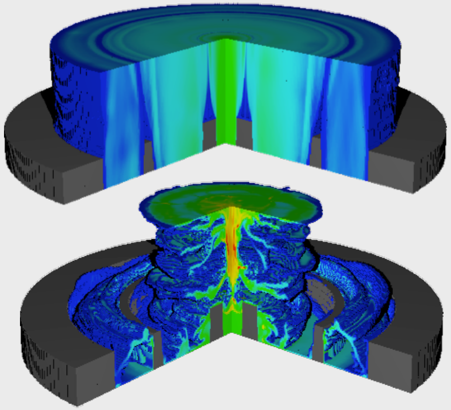


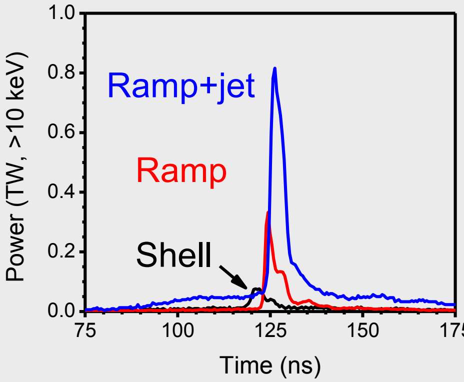
Kr gas puff implosions indicate that tailored mass distribution with dense jet on axis can significantly increase K-shell output

- Efficient emission of 13-keV Kr K-shell photons requires high velocity
  - Implode from 12cm to ~1mm in ~120 ns
  - Very susceptible to Rayleigh-Taylor instability
- MHD simulations used to design gas profiles
  - Ramped density for stable implosion
  - Jet on axis to provide high pressure target to thermalize kinetic energy
- Data demonstrates that jet can approximately double 13 keV emission
  - Initial analysis indicates ~7-9 kJ radiated at > 10 keV with jet on axis
  - Consistent with predictions

Courtesy: D.J. Ampleford (SNL)

Implosions disrupted by instabilities





C. A. Jennings(SNL) PoP 22 (2015)

Kr spectra from full 1D-DZAPP simulation for 12-cm double shell Z pinch

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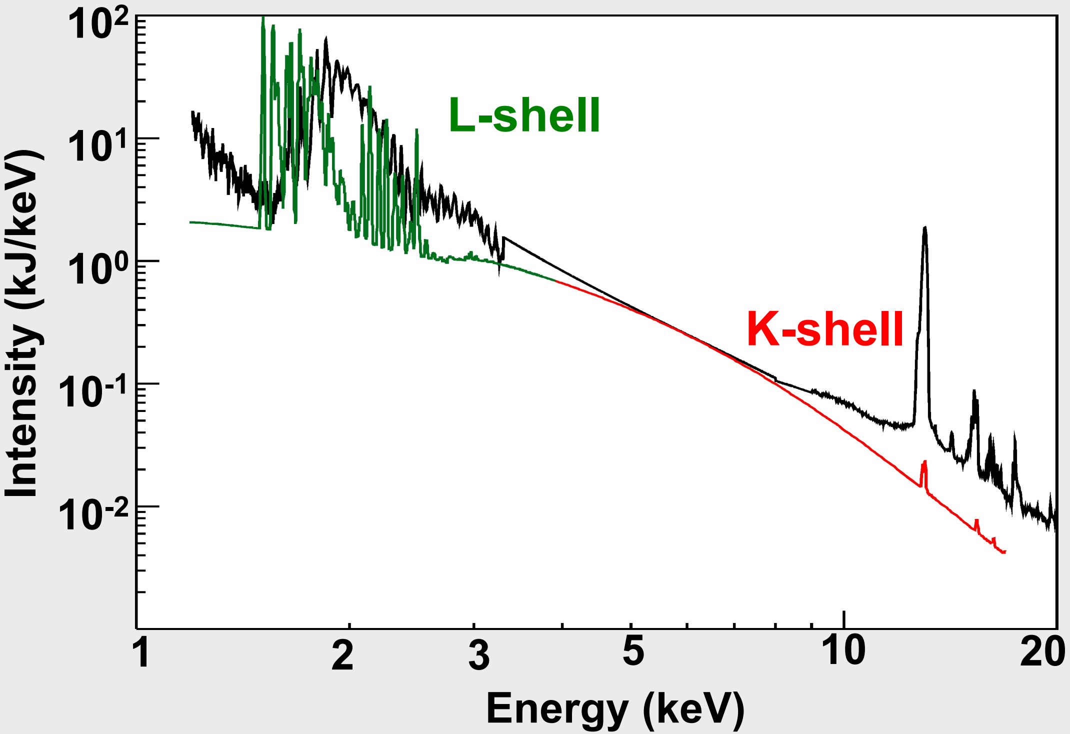

Calculated Spectrum from 12 cm initial diameter Kr gas puff

- Radiation Integrated over full 1D ZR implosion simulation
- Ionization using full Non-Equilibrium integration of atomic populations in time
- Atomic model for K- through M-shell obtained using FAC
- Z shot 2639:
  Total mass = 1.34 mg
  Outer puff = 5.0 cm
  Inner puff = 2.1 cm

Z-2639 shot with 12 cm outer nozzle (with central jet) K-shell emission indicates hot core surrounded by cooler (L-shell) region

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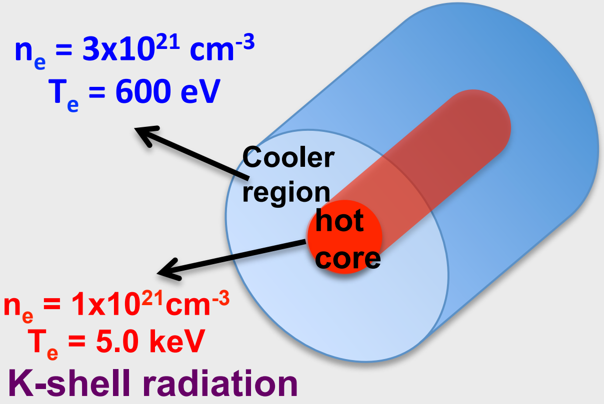
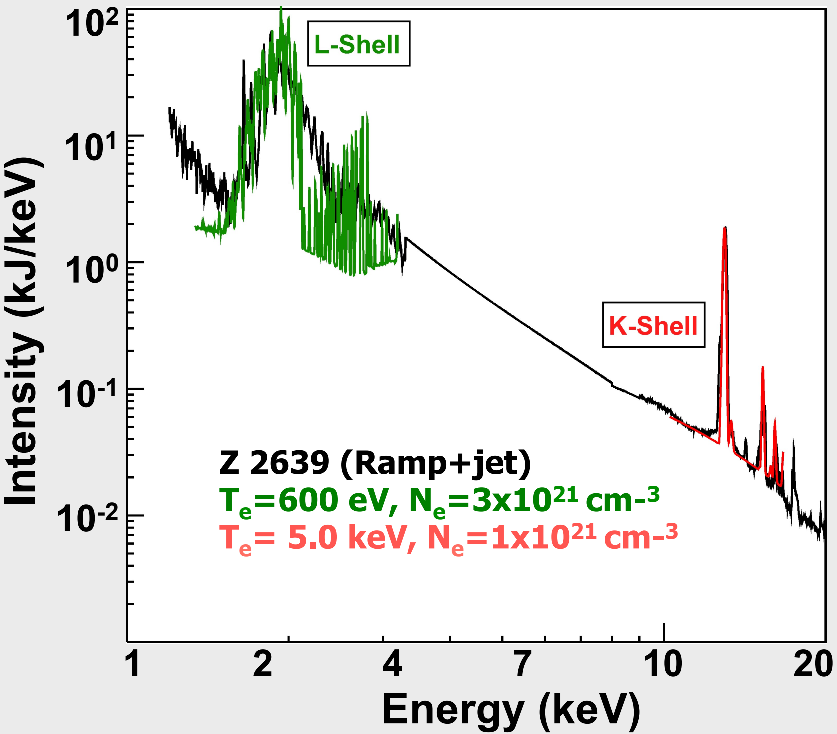
Schematic of plasma at stagnation on the axis



Calculated Spectrum



- Radiation determined from static calculations of temperature and density in the K- and L-shell producing regions of the plasma
- Ionization using collisional radiative equilibrium atomic populations and probability-of-escape radiation transport
- Z shot 2639: Total mass = 1.34 mg; outer puff = 5.0 cm; inner puff = 2.1 cm

Several 12 cm outer nozzle L-shell spectral data compared with a static NLTE simulation (n_e=3x^{21}, T_e= 600 eV

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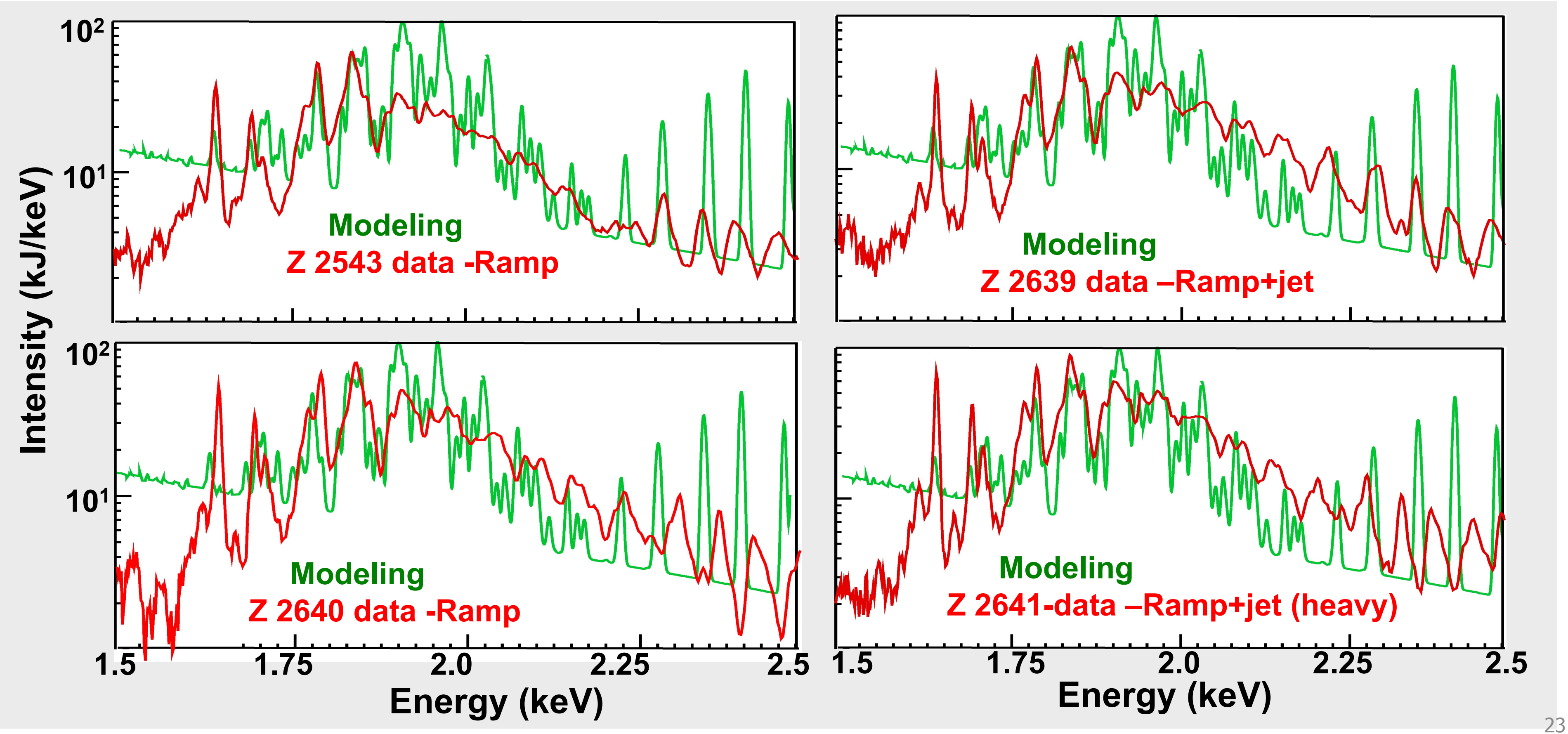
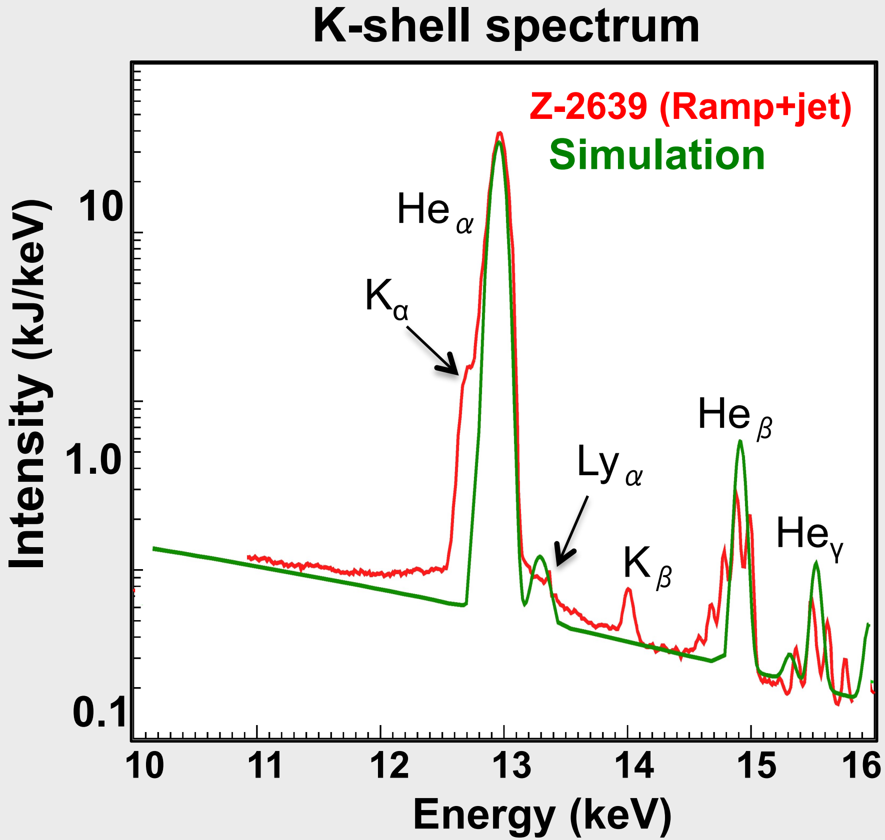
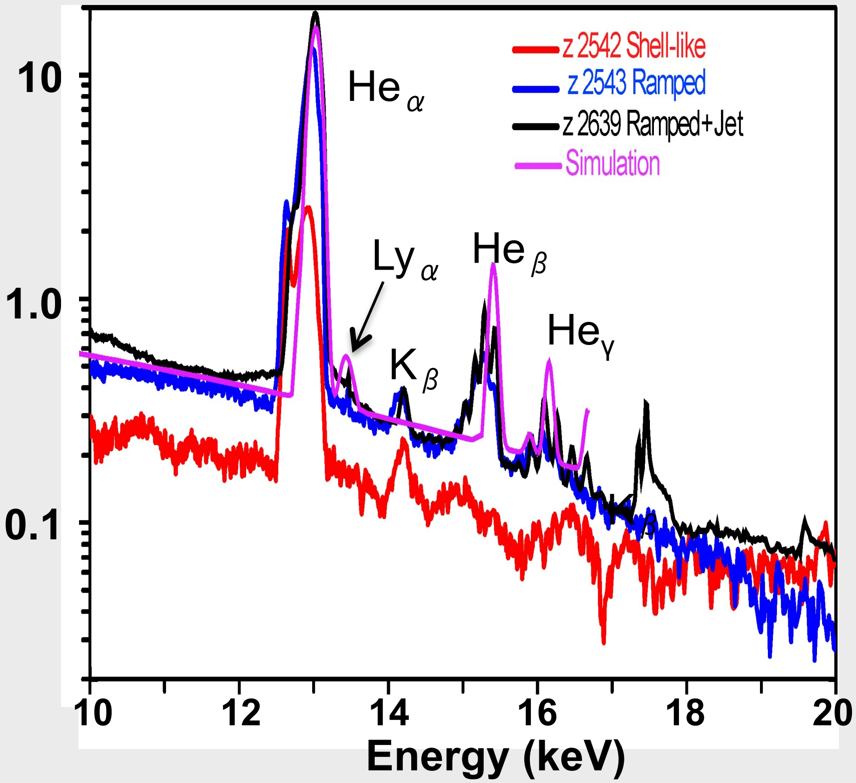


12-cm K-shell emission from several Z shots are compared with integrated spectra from a NLTE 0-D model

NRL PPD





Kr filled gas pipe target produces high X-ray K-shell yield at the National Ignition Facility (NIF)

Lawrence Livermore National Laboratory

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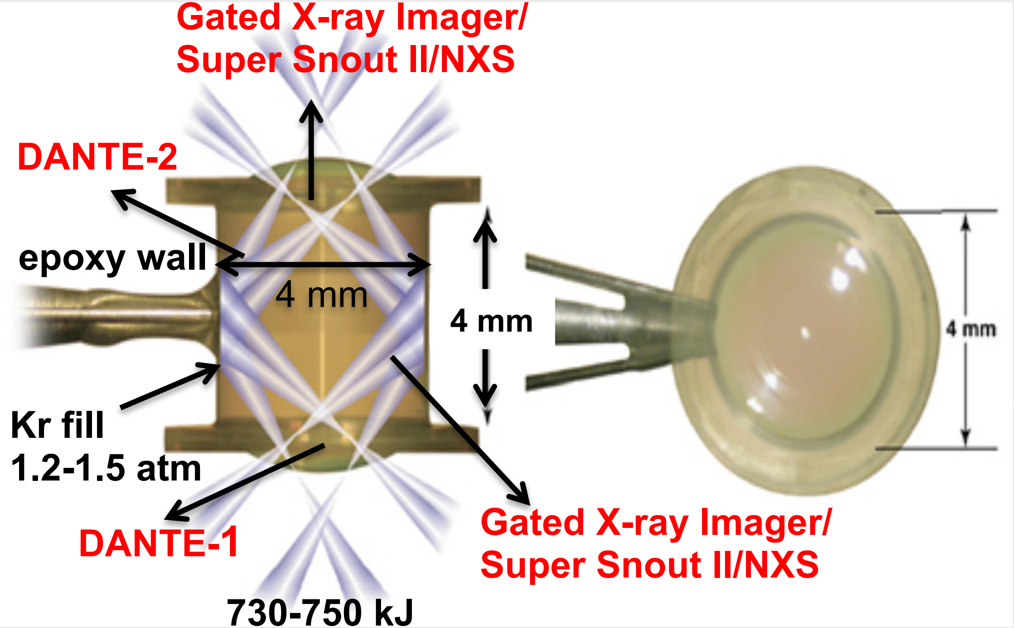
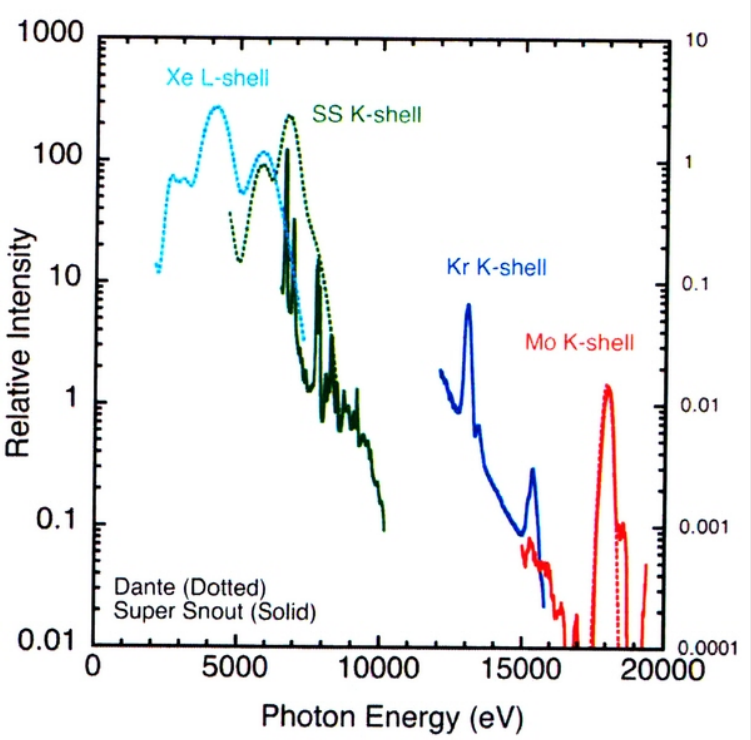


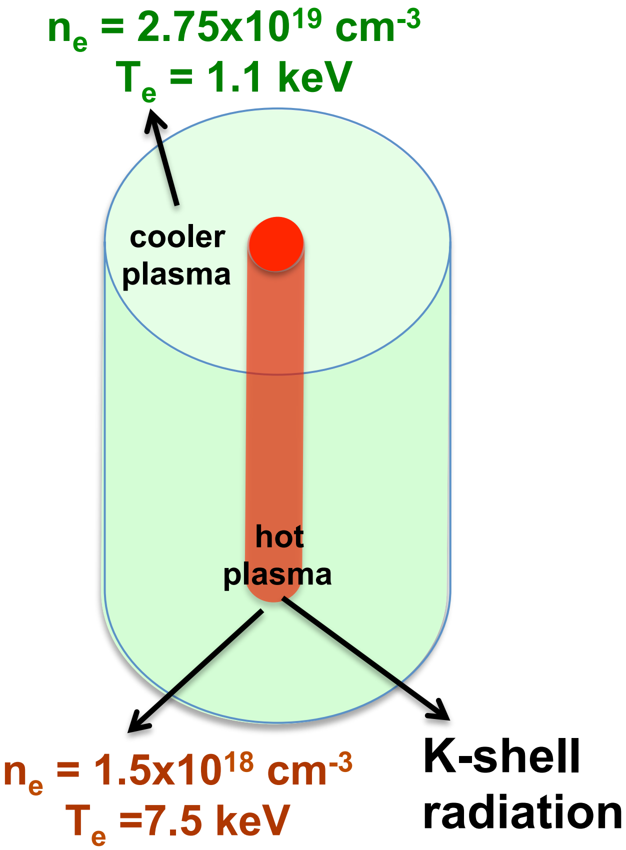
Side-on (left) and face-on (right) views of the thin-walled gas pipes used for Kr as x-ray source targets in the NIF experiments, illustrating how the laser beams were pointed with respect to the target's axis and laser entrance holes.

Production of 3 keV to 18 keV sources



Courtesy of : Mark May (LLNL)

Kr K-shell simulation on NIF using same Atomic model as on z

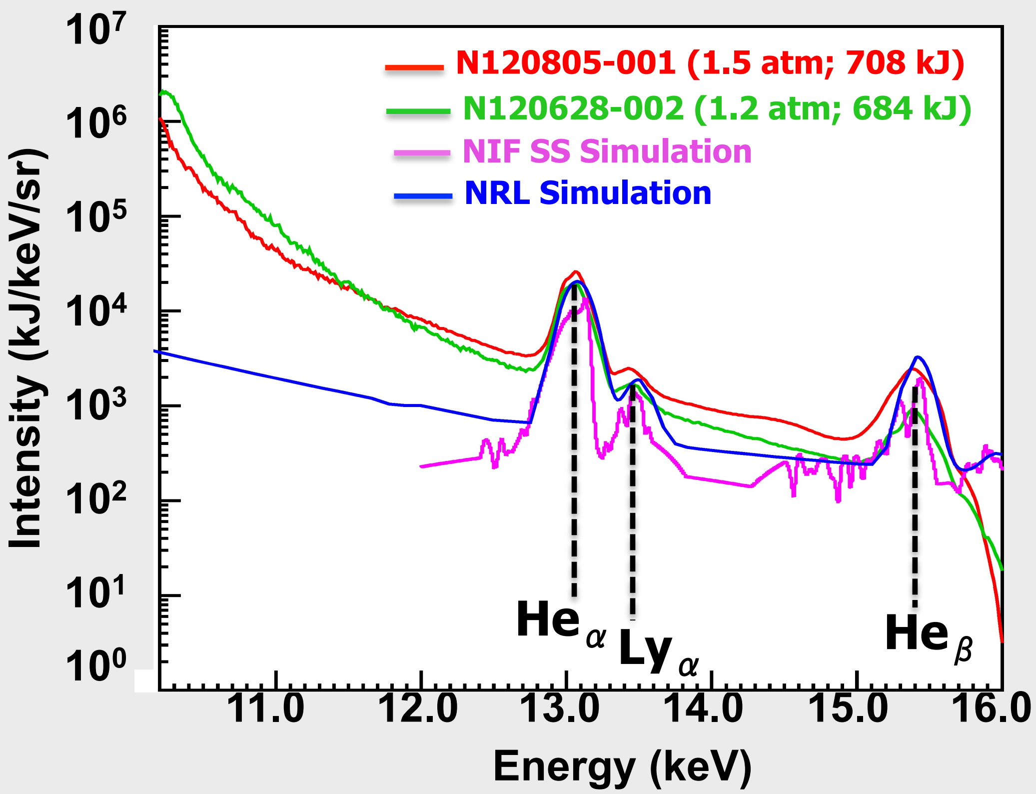


Calculated Hot-spot Spectrum from post-process:

- Radiation from post-process using 10 zones with single N_i and T_e in central zone and cooler, denser in the outer zones. This might not give accurate prediction if there are large spatial gradients in T_e.
- Non-LTE Ionization Kinetics
- Atomic model for K- through M-shell Kr obtained using FAC.
- 0-D hydrodynamics model might not predict if there is strong temporal evolution of plasma.

Kr K-shell simulation compared to NIF Super Snout (SS) spectra

NRL PPD



Calculated Spectrum

Model K-shell region with a simple density and electron temperature profile.

Hot core (T_e=7.5 keV and n_e=1.5x10^{18} cm^{-3}), surrounded by cooler, denser plasma (T_e=1.1keV, n_e=2.75x10^{19} cm^{-3}).

SS data : Courtesy of M. May, M. Barrios, T. Flannigan, K. Bell

Big Picture

NRL PPD

- Detailed and accurate Atomic and Radiation models enable us to link material properties on the atomic scale to the radiation that drives HED plasmas. Diagnostic applications of intense plasma x-ray sources are enabled by such models.
- Our understanding of energy coupling into Z-pinch and laser produced plasmas is still limited.
- We are still unable to harness this energy source for increasing X-ray radiation yields and peak powers in relevant spectral ranges.
- In order to improve our understanding of the plasma structure and the dynamics of high-Z radiation source materials, the development of dedicated platforms using proper diagnostics is absolutely crucial.
- It is important that research into the physics of radiation production in these novel plasmas be supported.

Back-up Slide

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