Flexible Non-LTE atomic-kinetics and detailed Stark-broadened lines profiles for spectroscopic characterization of high-energy-density plasmas

Ricardo Florido

iUNAT - Departamento de Física, Universidad de Las Palmas de Gran Canaria (Spain)

GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA E INNOVACIÓN

EUROfusion

FAIR

Workshop on
High Energy Density Physics Opportunities at FAIR
November 18, Madrid

Outline

1 **Who are we?**

2 **Computational platform for spectroscopic characterization of HED plasmas**

3 **BCoilCompress: magnetized cylindrical implosions in OMEGA**

4 **Modeling K-α emission in shock-ignition relevant experiments**

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2 Computational platform for spectroscopic characterization of HED plasmas

3 BCoilCompress: magnetized cylindrical implosions in OMEGA

4 Modeling K-α emission in shock-ignition relevant experiments

Who are we?

Team

- Ricardo Florido
  Universidad de Las Palmas de Gran Canaria (Spain)
- Marco A. Gigosos, Gabriel Pérez Callejo
  Universidad de Valladolid (Spain)

ULPGC
Universidad de Las Palmas de Gran Canaria
Departamento de Física

UVa
Universidad de Valladolid

Collaborators

- Roberto C. Mancini, Enac Gallardo-Díaz
  University of Nevada, Reno (USA)
- Mathieu Bailly-Gradvaux, Farhat Beg
  University of California San Diego (USA)
- Chris Walsh
  Lawrence Livermore National Laboratory (USA)
- Taisuke Nagayama, Marc Schaeuble
  Sandia National Laboratories, (USA)
- Patrick Adrian, Johan Frenje
  MIT (USA)
- Joao J. Santos, C. Vlachos, P. Bradford
  CELIA, Université de Bordeaux (France)
- Francisco Suzuki-Vidal
  Imperial College London
- Anette Calisti, Sandrine Ferri
  PIIM, Aix-Marseille Université (France)
- Javier Honrubia, Luca Volpe
  Universidad Politécnica de Madrid (Spain)

UC San Diego

Sandia National Laboratories

University of Nevada, Reno

Lawrence Livermore National Laboratory

Massachusetts Institute of Technology

CELIA

université de BORDEAUX

PIIM

Aix*Marseille université

Imperial College London

POLITÉCNICA

UNIVERSIDAD POLITÉCNICA DE MADRID

Granted Research Projects

- Plan Nacional I+D+i "Retos de la Sociedad". Spectroscopic diagnosis of plasmas based on atomic-kinetics and Stark-broadened line profiles: an application to the shock-ignition scheme for ICF.
  PI: R. Florido (ULPGC). Duration: 01/01/2016-31/12/2018.
- Plan Nacional I+D+i "Retos de la Sociedad". Spectroscopic characterization of HED laboratory plasmas by means of collisional-radiative atomic-kinetics and molecular dynamics.
  PI: R. Florido (ULPGC), M.A. Gigosos (UVa). Duration: 01/06/2020-31/05/2023.

- H2020 - FP8, EUROfusion Consortium. Towards a universal Stark-Zeeman code for spectroscopic diagnostics and for integration in transport codes. PI: J.J. Santos (CELIA, U. Bordeaux, France). Duration: 01/01/2017-31/12/2018.
- H2020 - FP8, EUROfusion Consortium. Preparation and realization of European shock-ignition experiments.
  PI: D. Batani (CELIA, U. Bordeaux, France). Duration: 01/01/2017-31/12/2018.
- H2020 - FP8, EUROfusion Consortium. Study of direct-drive and shock ignition for IFE: theory, simulations, experiments, diagnostics development. PI: D. Batani (CELIA, U. Bordeaux, France). Duration: 01/01/2019-31/12/2020.
- FP9, EUROfusion Consortium. Advancing shock ignition for direct-drive inertial fusion.
  PI: D. Batani (CELIA, U. Bordeaux, France). Duration: 01/04/2021-31/03/2024.
- Academic Access LMJ-PETAL Experiment, CEA (France). Driving extreme magnetizations in compressed high-energy-density plasmas. PI: J. J. Santos (CELIA, U. Bordeaux, France). Experiments scheduled for 2024-2026.

- NLUF Program, Department of Energy (USA). Driving compressed magnetic field to exceed 10 kT in cylindrical implosions on OMEGA. IP: M. Bailly-Grandvaux (UCSD, USA). Duration: 01/01/2020-31/12/2021.
- NNSA-Department of Energy (USA). Driving plasmas to extreme magnetizations using strong laser compression and high initial magnetic field. IP: M. Bailly-Grandvaux (UCSD, USA). Duration: 06/01/2021-31/05/2023.
- LBS Program, NNSA-Department of Energy (USA). Using isoelectronic ratios to measure density in nLTE plasmas. PI: M.B. Schneider, G. Pérez-Callejo. Duration: 01/09/2021-30/08/2022.
- NLUF Program, Department of Energy (USA). Phase contrast imaging of inner shell release through Talbot-Lau X-ray interferometry. PI: M.P. Valdivia. Duration: 01/09/2021-01/09/2023
- NIF Discovery Science Program. Study of extended-MHD effects and confinement properties of strongly magnetized cylindrical implosions. PI: M. Bailly-Grandvaux. Pre-selected (fingers crossed).

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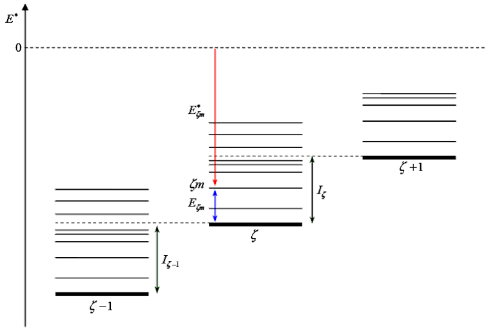
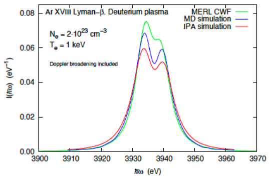
Computational platform for spectroscopic modeling of HED experiments

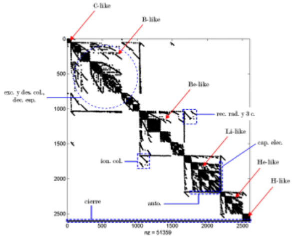
Flexible Atomic Code (FAC)[1]
fundamental atomic data



[1] M. F. Gu, Can. J. Phys. 86, 675 (2008)

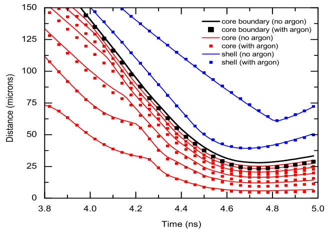
ABAKO[2], **MERL**[3], **MODELA**[4], **SIMULA**[5], **DinMol**[6]
CR modelling, population distributions, line shapes, radiative properties





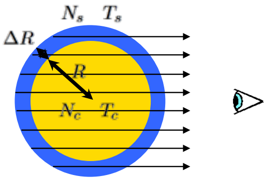
[2] R. Florido et al., Phys. Rev. E 80, 056402 (2009)
[3] R. C. Mancini *et al.* Comput. Phys. Commun. **63**, 314 (1991)
[4] M. A. Gigosos, private communication
[5] M. A. Gigosos et al., J. Phys. B: At. Mol. Opt. Phys. 29, 4795 (1996)
[6] M. A. Gigosos et al., Phys. Rev. E 98, 033307 (2018)

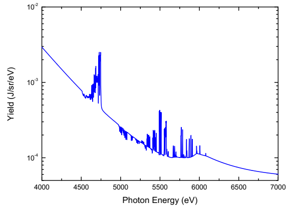
Gorgon[7], **FLASH**[8]
time-resolved spatial profiles of plasma conditions



[7] C. A. Walsh et al., Phys. Plasmas 27, 022103 (2020)
[8] FLASH Center, https://flash.rochester.edu/site/index.shtml

FESTR[9], **RadTrans**[10]
radiation transport, synthetic spectra





[9] P. Hakel. Comput. Phys. Commun. 207, 415 (2016)
[10] R. Florido, private communication

- Cluster ULPGC: 7 workstations: 2 Intel Xeon Silver (10 cores), 128 Gb RAM, 1 SSD 240 Gb, 3 HD 2 Tb
- Cluster UVa: 100 PCs (Intel i3 or higher), 64 Gb RAM, 20 GPUs (Cuda), 2 workstations

ABAKO: a code for flexible NLTE atomic-kinetics

Versatility

- Low- to high-Z elements can be studied.
- Wide range of temperatures and densities.
- EDFs for thermal and hot-electrons.
- Optically thin and optically thick cases can be considered.
- Ready for steady-state and time-dependent calculations:

(TD) $$\frac{d\mathbf{f}}{dt} = \left(\sum \mathbb{R}^{+} - \sum \mathbb{R}^{-}\right)\mathbf{f} = \mathbb{A}\mathbf{f}$$

(SS) $$\frac{d\mathbf{f}}{dt} = 0 = \left(\sum \mathbb{R}^{+} - \sum \mathbb{R}^{-}\right)\mathbf{f} = \mathbb{A}\mathbf{f}$$

Balance between accuracy & computational cost

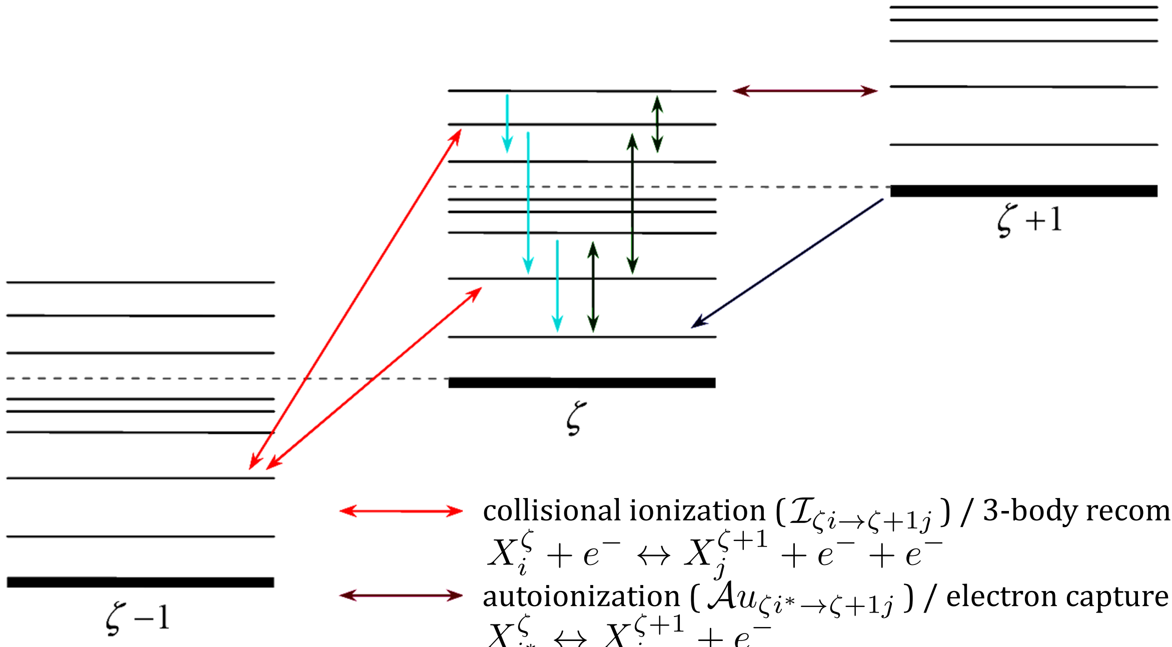
- ABAKO assembles a set of simple analytical models which yield substantial savings of computer resources.
- It provides good comparisons with more elaborated codes and models.

[2] R. Florido *et al.* Phys. Rev. E **80**, 056402 (2009)

ABAKO: a code for flexible NLTE atomic-kinetics

- It accounts for the most-relevant collisional and radiative atomic processes.
- Autoionization states are explicitly included.
- Effort in having a tractable and consistent set of levels and transitions to represent the physical reality.

Atomic processes rate coefficients



⟷ collisional ionization ($\mathcal{I}_{\zeta i\to\zeta+1 j}$) / 3-body recombination ($\mathcal{R}^{3b}_{\zeta+1 j\to\zeta i}$)

$$X_i^{\zeta} + e^- \leftrightarrow X_j^{\zeta+1} + e^- + e^-$$

⟷ autoionization ($\mathcal{A}u_{\zeta i^*\to\zeta+1 j}$) / electron capture ($\mathcal{C}_{\zeta+1 j\to\zeta i^*}$)

$$X_{i^*}^{\zeta} \leftrightarrow X_j^{\zeta+1} + e^-$$

→ radiative recombination ($\mathcal{R}_{\zeta+1 j\to\zeta i}$)

$$X_j^{\zeta+1} + e^- \to X_i^{\zeta} + h\nu$$

⟷ collisional excitation ($\mathcal{E}_{\zeta i\to\zeta j}$) / deexcitation ($\mathcal{D}_{\zeta j\to\zeta i}$)

$$X_i^{\zeta} + e^- \leftrightarrow X_j^{\zeta} + e^-$$

→ spontaneous decay ($\mathcal{A}_{\zeta j\to\zeta i}$)

$$X_j^{\zeta} \to X_i^{\zeta} + h\nu$$

[2] R. Florido *et al.* Phys. Rev. E **80**, 056402 (2009)

Stark-broadened line shapes

Line shapes in plasmas are important since:

- They are needed for a detailed model/calculation of line intensity distribution.
- Line widths can be either temperature (Doppler broadening) or density (Stark broadening) sensitive: spectroscopic diagnostic of temperature or density.
- In the ICF context (hot and dense plasmas), Stark-broadening becomes the dominant broadening mechanism. Detailed and accurate Stark-broadened line shapes are required for analysis of experimental data.
- In our team, we have **different codes** for the calculation of Stark-broadened line shapes:

Analytical

MERL: Developed within the framework of the standard Stark-broadening theory and extended for highly charged ions. Ion dynamics is included via BID model. [3] R. C. Mancini *et al.* Comput. Phys. Commun. **63**, 314 (1991)

MODELA: Standard Stark-broadening theory. Ion dynamics is included either using computer simulations or FFM. [4] M. A. Gigosos, private communication
[11] B. Talin *et al.* Phys. Rev. A **51**, 1918 (1995)

$$I(\omega) = \int P(E) J(\omega, E) dE$$

Computer simulations

(testbed for improvement of theoretical models)

SIMULA: It generates multiple time-histories of the perturbing electric field by means of an independent particle simulation. In a second step, the electric dipole autocorrelation function of the emitter is computed to finally obtain the spectrum. [5] M. A. Gigosos, V. Cardeñoso. J. Phys. B: At. Mol. Opt. Phys. **29**, 4795 (1996).

DinMol : Computer simulation model. It's a *true* classical molecular dynamics code, so the electric field sequences comes from a system of interacting particles. [6] M. A. Gigosos et al. Phys. Rev. E **98**, 033307 (2018).

$$\vec{E}(t) \Rightarrow D(t) \Rightarrow C(t) \Rightarrow I(\omega)$$

$$I(\omega) = \frac{1}{\pi} \mathbb{R}\mathrm{e} \int_0^\infty e^{i\omega t} \{C(t)\} dt$$

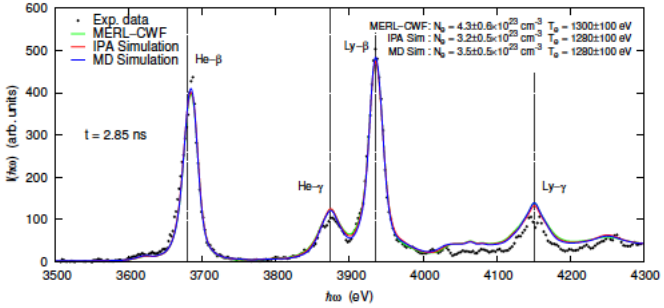
$$C(t) = \mathrm{tr}\left[\mathbf{D}(t) \cdot \mathbf{D}(0)\right]$$

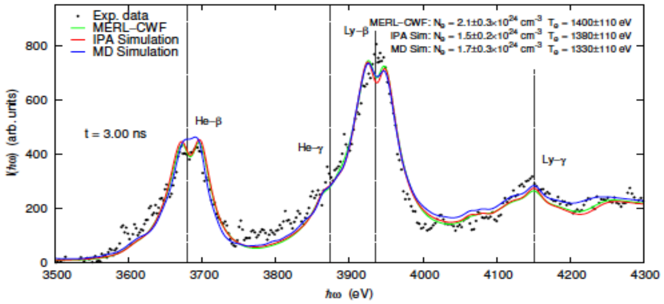
$$\mathbf{D}(t) = U^{+}(t)\mathbf{D}(0)U(t)$$

$$i\hbar \frac{d}{dt} U(t) = \left[H_0 + q\mathbf{E}(t) \cdot \mathbf{R}\right] U(t)$$

Stark-broadened line shapes

Comparison MERL / SIMULA / DinMol



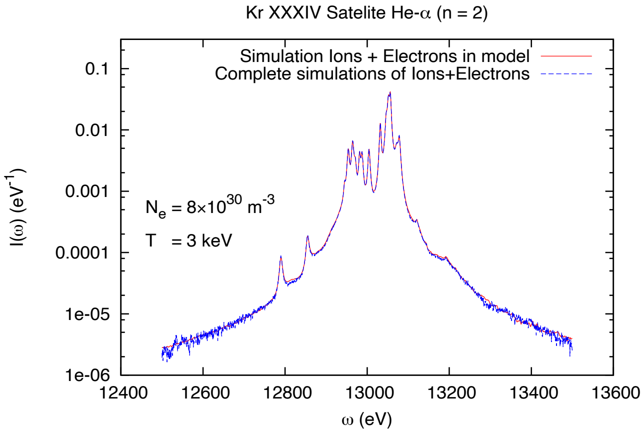


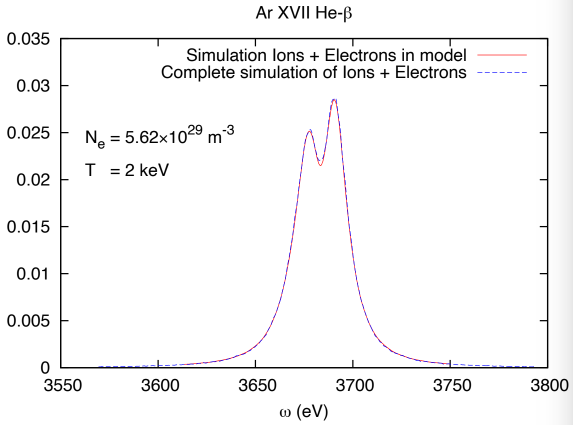
[12] M. A. Gigosos *et al.* Atoms **9**, 9 (2021)

- Ar K-shell spectra from spherical implosions experiments at OMEGA.
- Results of diagnosis (based on *n=3, 4* → *n=1* transitions) are likewise indistinguishable considering the data analysis uncertainty.
- However, noticeable differences were found in *n=2* → *n=1* transitions, as shown later.

Comparison MODELA / SIMULA

- **Electron broadening** computed **using this model agrees within 99% with** that obtain from **computer simulations** (for selected and affordable cases of interest) .
- Computational time drastically reduced in MODELA (particularly important for satellite transitions).





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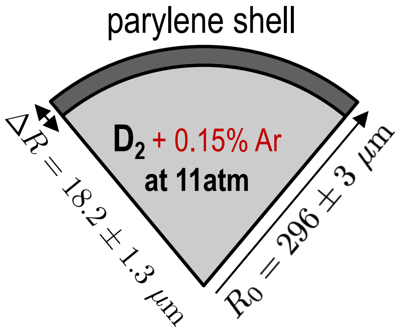
BCoilCompress: a platform for magnetized HEDP

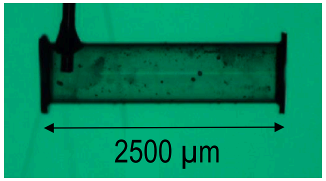
- **OMEGA-60** experimental campaign (DoE-NLUF). **PI:** M. Bailly-Grandvaux (UCSD).

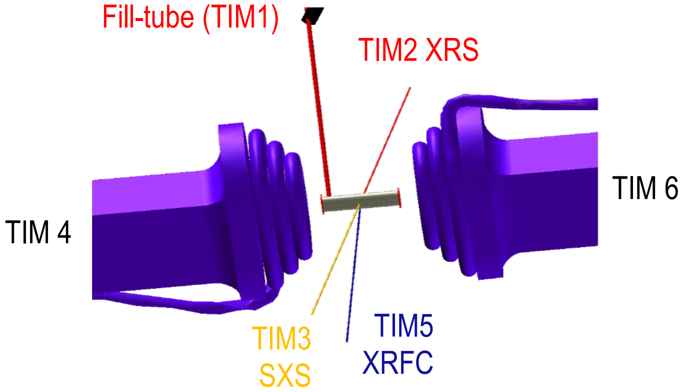
Setup

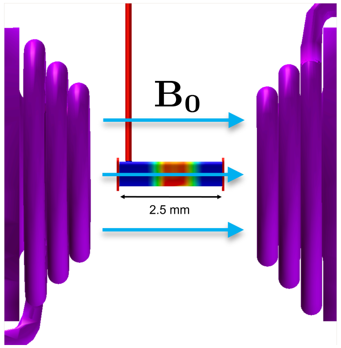
- Targets were cylindrical tubes filled with 11 atm of D_2 gas and a tracer amount (0.15%) of Ar.
- Seed B-field ~ 30 T driven externally using dual MIFEDS[13] (capacitor bank discharge).

[13] Gotchev et al. Rev. Sci. Instrum. **80**, 043504 (2009)





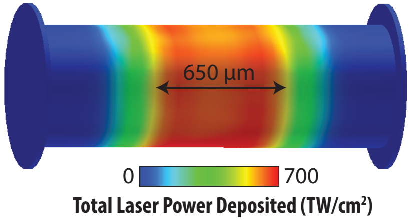




- Laser drive[14]: 40 UV beams, 1.5 ns, total energy ~ 14.5 kJ

[14] Hansen et al., Phys. Plasmas 27, 062703 (2020)

> 5×10^{14} W/cm^2 fairly uniform across 650 µm



Motivation

- 2D MHD simulations (Gorgon code[7]) of magnetized cylindrical implosions using a seed B-field of 10-50 T predict a compressed B-field of 8 to 30 kT, which is strong enough to alter the implosion hydrodynamics and the characteristic conditions of the compressed core[15].

[7] C. A. Walsh et al., Phys. Plasmas **27**, 022103 (2020) [15] C. A. Walsh et al., Plasma Phys. Control. Fusion **64**, 025007 (2022)

- **Measure the imploded plasma conditions** (density, temperature) throughout the implosion collapse in magnetized conditions via **spectroscopic changes in Ar K-shell emission.**

Modelling the experiment: 2D MHD simulations

Extended-MHD 2D Gorgon simulations

laser heating

- Ray-tracing
- Inverse bremsstrahlung

thermal transport

- Anisotropic conduction
- Righi-Leduc

radiation transport

- Non-diffusive multi-group approx.

magnetic transport

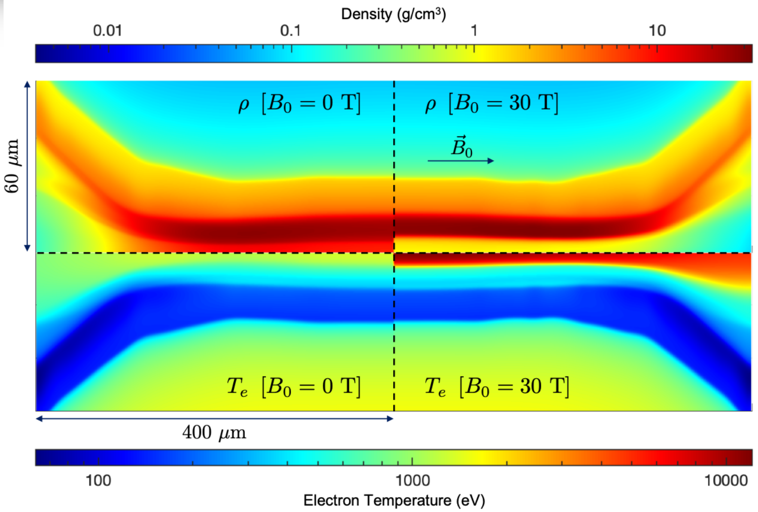
- **Advection:**
  - Bulk plasma
  - Nernst + cross-gradient Nernst
- **Source terms:**
  - Bierman Battery
  - Sadler
- **Resistive diffusion**

others

- Lorentz force
- Updated transport coefficients[16].

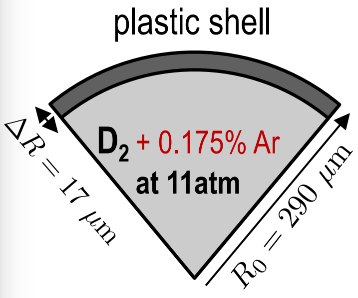
[15] C. A. Walsh et al., Plasma Phys. Control. Fusion **64**, 025007 (2022)
[16] J. D. Sadler et al., Phys. Rev. Lett. **126**, 075001 (2021)

2D map of target conditions at stagnation (t=1.5 ns)

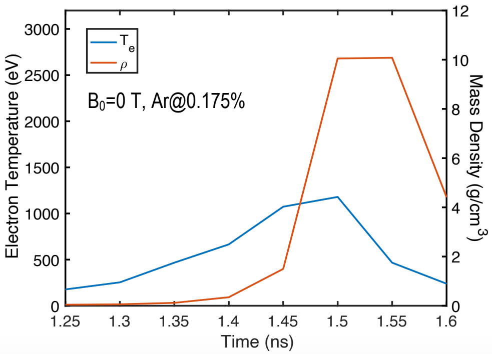


- At stagnation[15], owing to the high compressed B-field (>10 kT):
  - **Temperature increases** from 1 keV to 3 keV
  - **Density decreases** from ~ 10 g/cc to ~ 5 g/cc

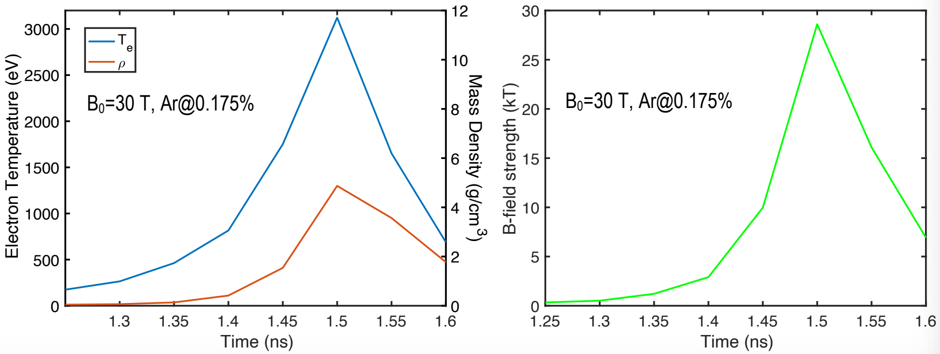
Time-histories of average core conditions



unmagnetized



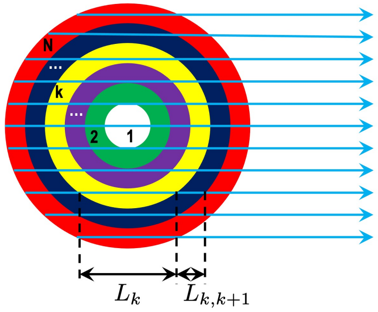
magnetized



Modelling the experiment: Ar synthetic spectra

Post-processing of Gorgon simulation, non-uniform radiation transport model

Radiation transport

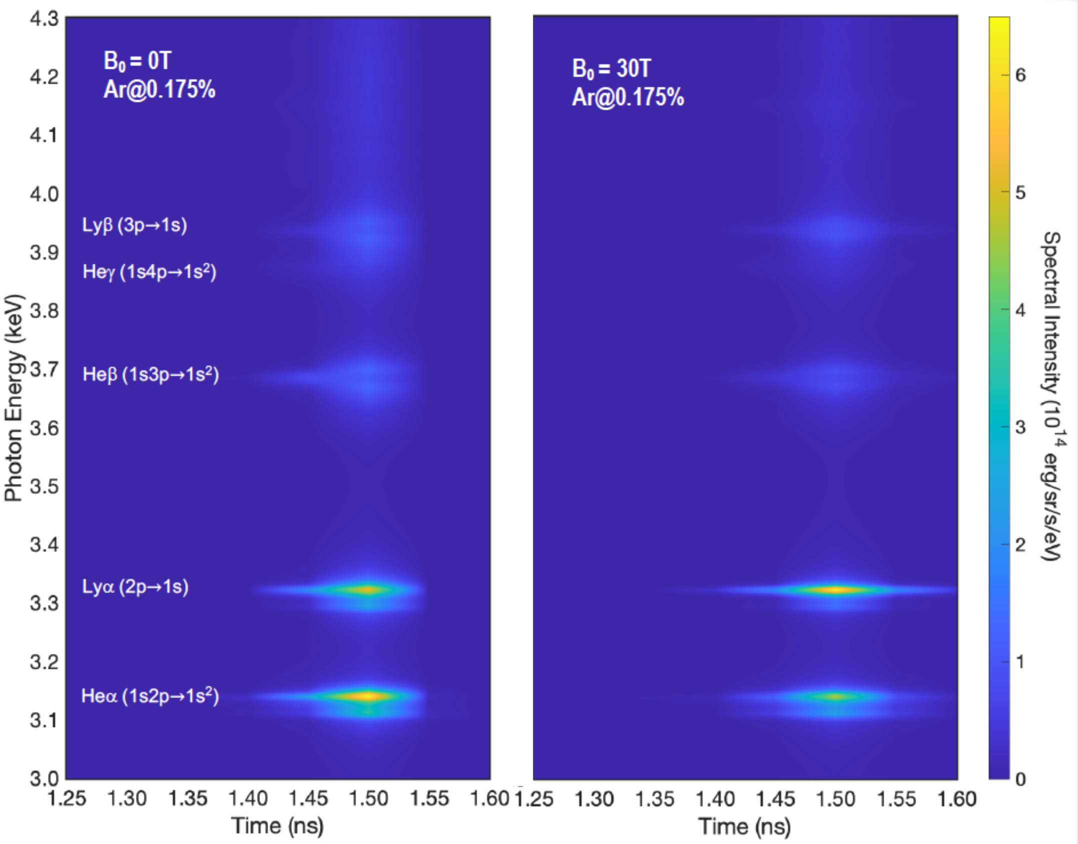


- It accounts for spatial gradients.
- Collection of slabs with appropriate chord lengths.
- Emissivities and opacities computed at plasma conditions given by Gorgon spatial profiles. No averaging or interpolation was done.

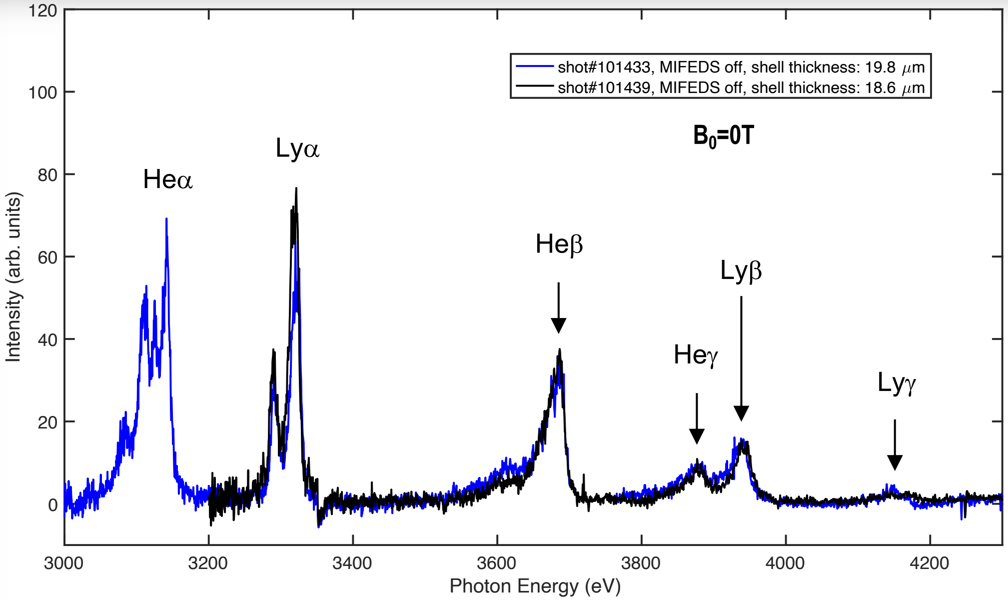
- Differences are observed between the magnetized and non-magnetized case.
- Variations in plasma conditions to be inferred from Ar K-shell spectroscopy.
- Potential use of Kr K-shell spectroscopy.

Synthetic X-ray streaked images

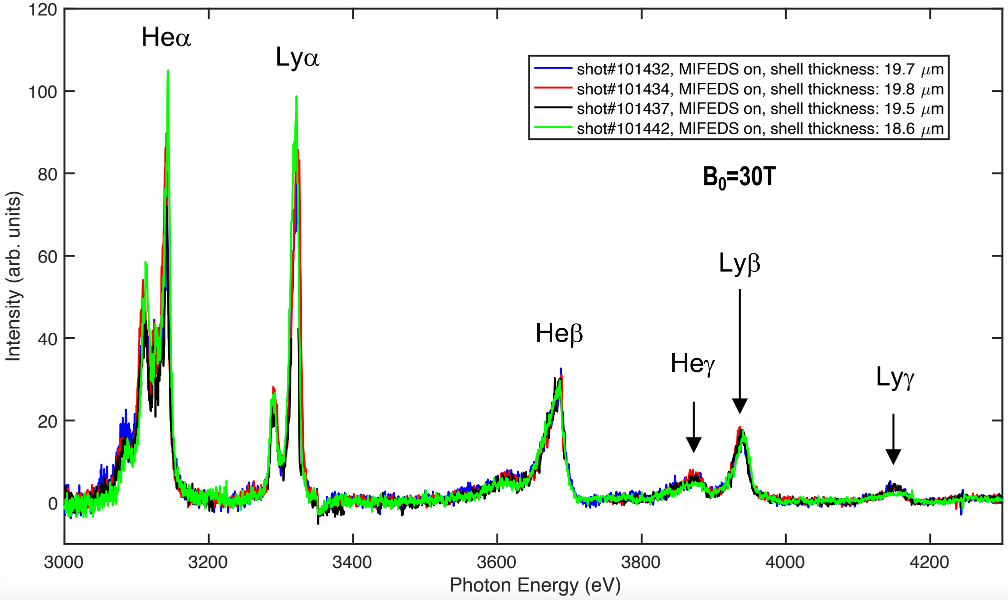
unmagnetized **magnetized**



Experimental data: time integrated spectra



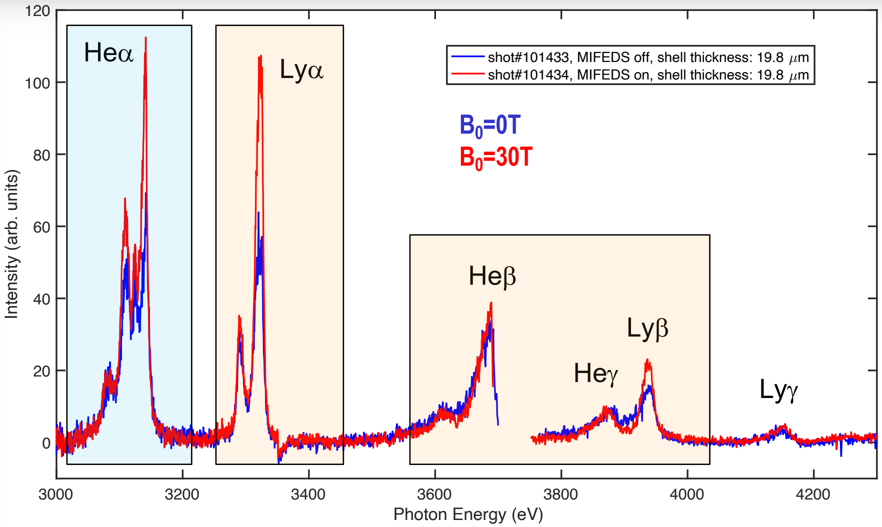
unmagnetized implosion



magnetized implosion

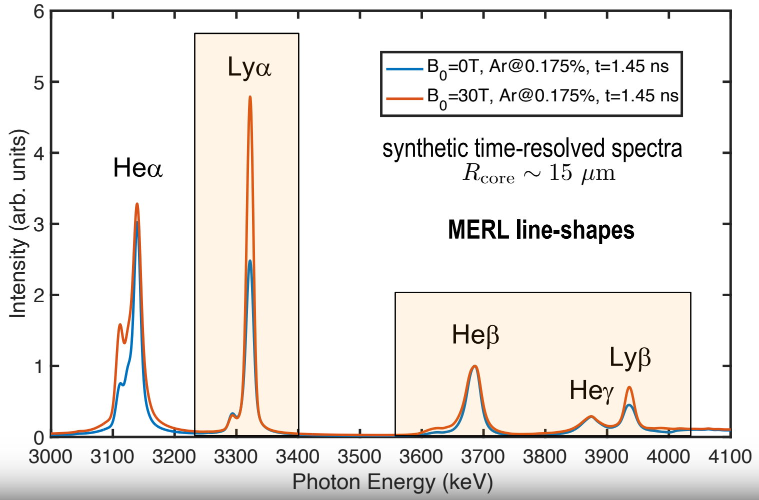
- We sucessfully recorded the time-integrated spectra for six shots in our campaign of Ar-doped cylindrical implosions in OMEGA.
- **High reproducibility** for both shots with and without imposed B-field.
- The observed time integrated spectrum does not show differences due to small changes in target shell thickness.
- For the non-magnetized case, Heα region was recorded in only one shot. Poor statistics. Ratio Heα/Li-like sat. suspiciously low.

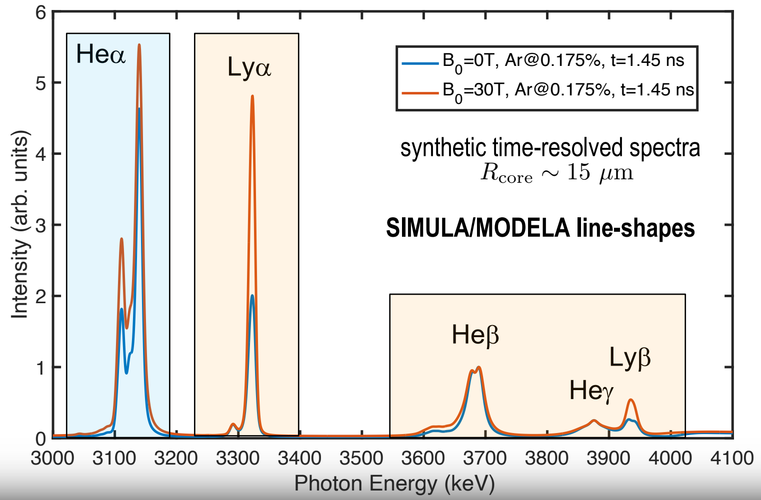
Experimental vs. synthetic spectra



- Several **systematic observations** are noticed.
- Heβ shows the same *shape* for the both cases.
- For the magnetized case, the Lyβ/Heβ line intensity ratio is higher.
- For the case of the strong α emission, in the magnetized case, the Lyα/He-like satellite intensity ratio is clearly higher than in the non-magnetized implosion.
- The last two observations suggest a hotter core for the magnetized implosion.

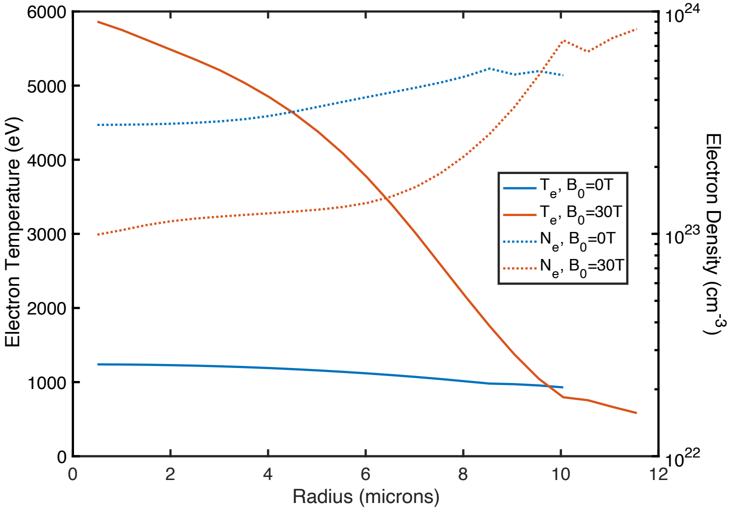
- **Qualitatively, all these observations are predicted by our synthetic spectra simulations.**
- Analysis of XRFC data shows a similar compression for both scenarios (R_{min}~15 microns). MHD simulations predict higher compression (~ 5 and 8 microns without and with B-field respectively). **Comparison is better when looking at 50 ps earlier (when the core radius agrees with that measured at stagnation).** [17] G. Pérez-Callejo et al., RSI 27, 062703 (2020)

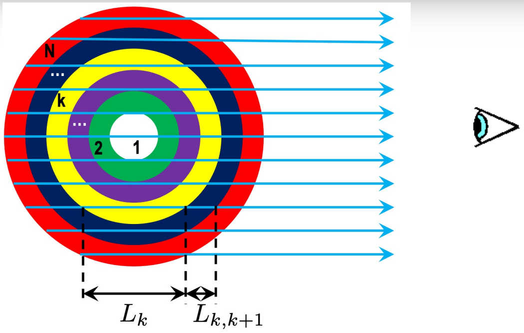




Spatial gradients and formation of the spectrum

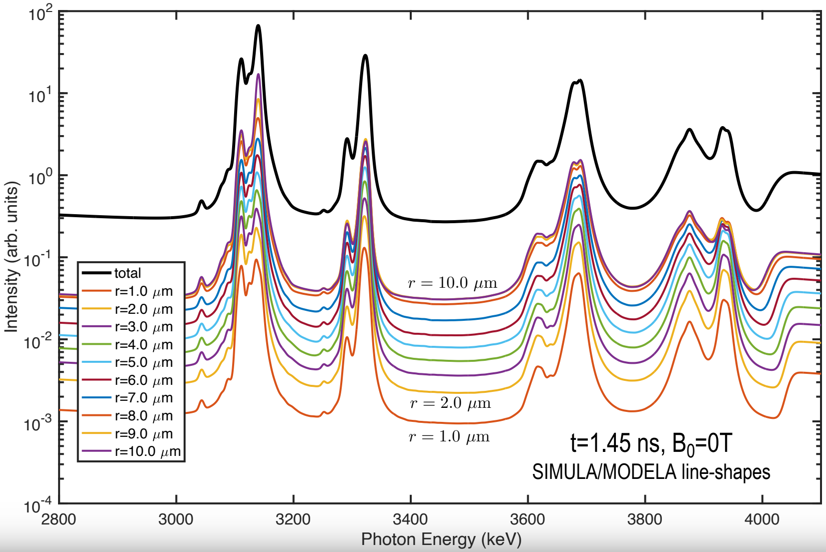
spatial profiles at t=1.45 ns



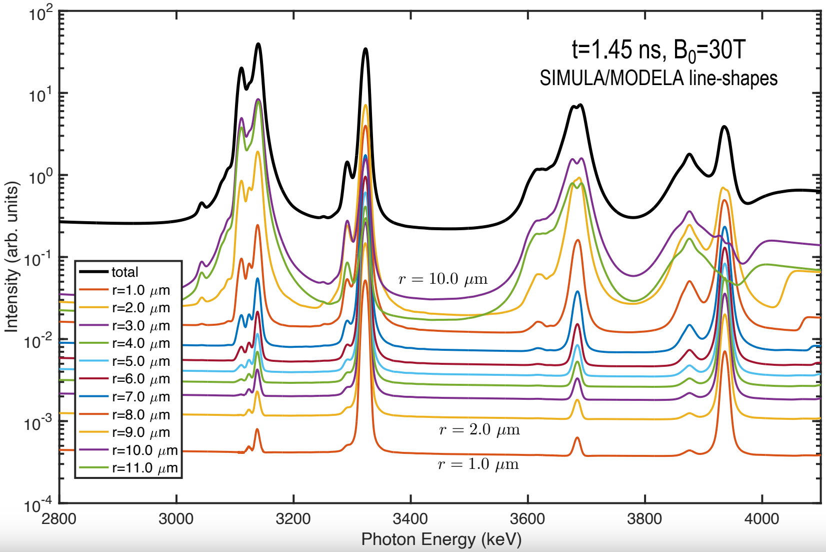


- Splitting the emergent spectrum in the corresponding radial contributions helps to understand the spectrum formation.
- Clearly, in the magnetized case, emission mostly comes from the core periphery.

unmagnetized implosion

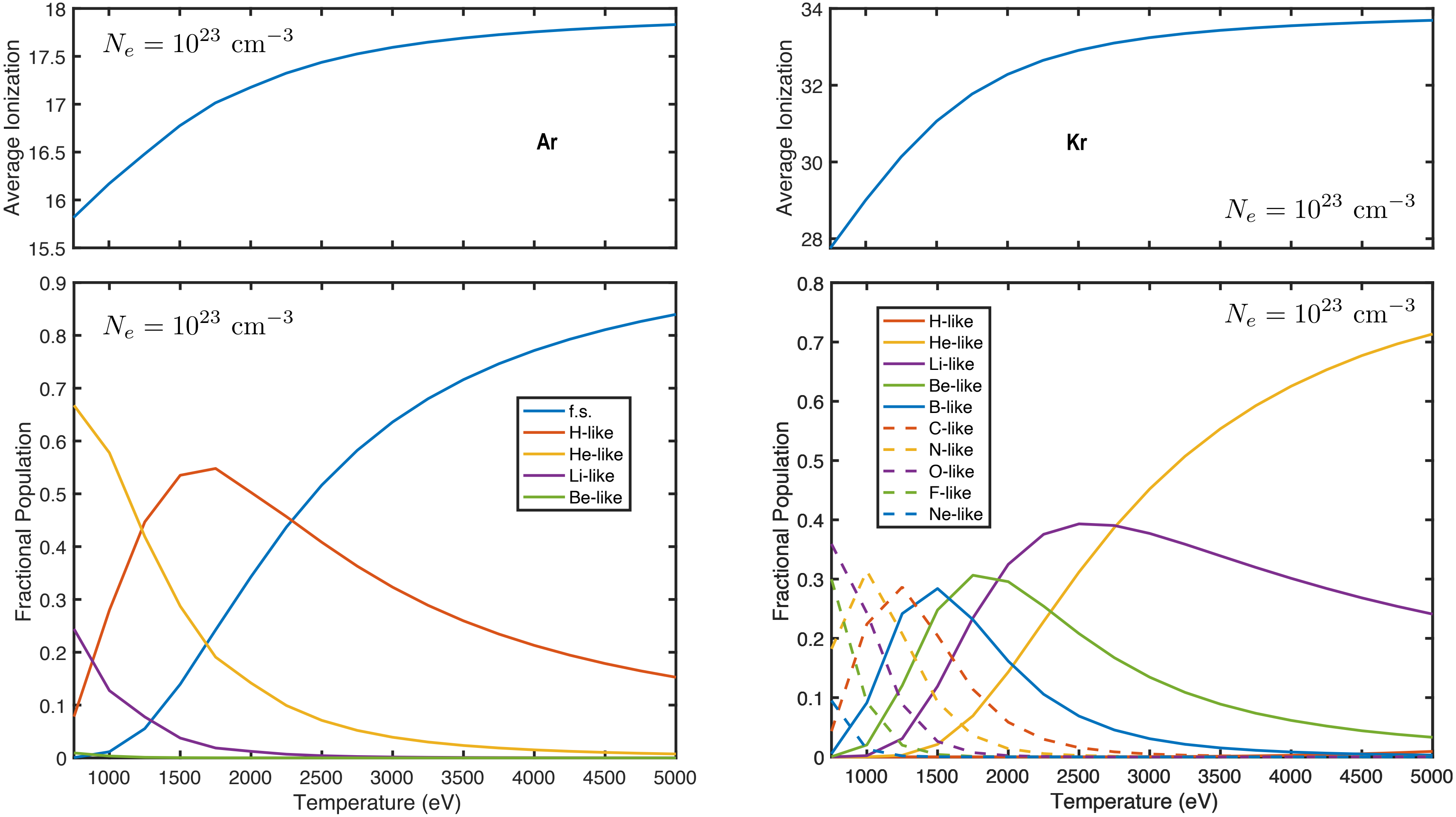


magnetized implosion



Improving the experiment: Ar & Kr doping

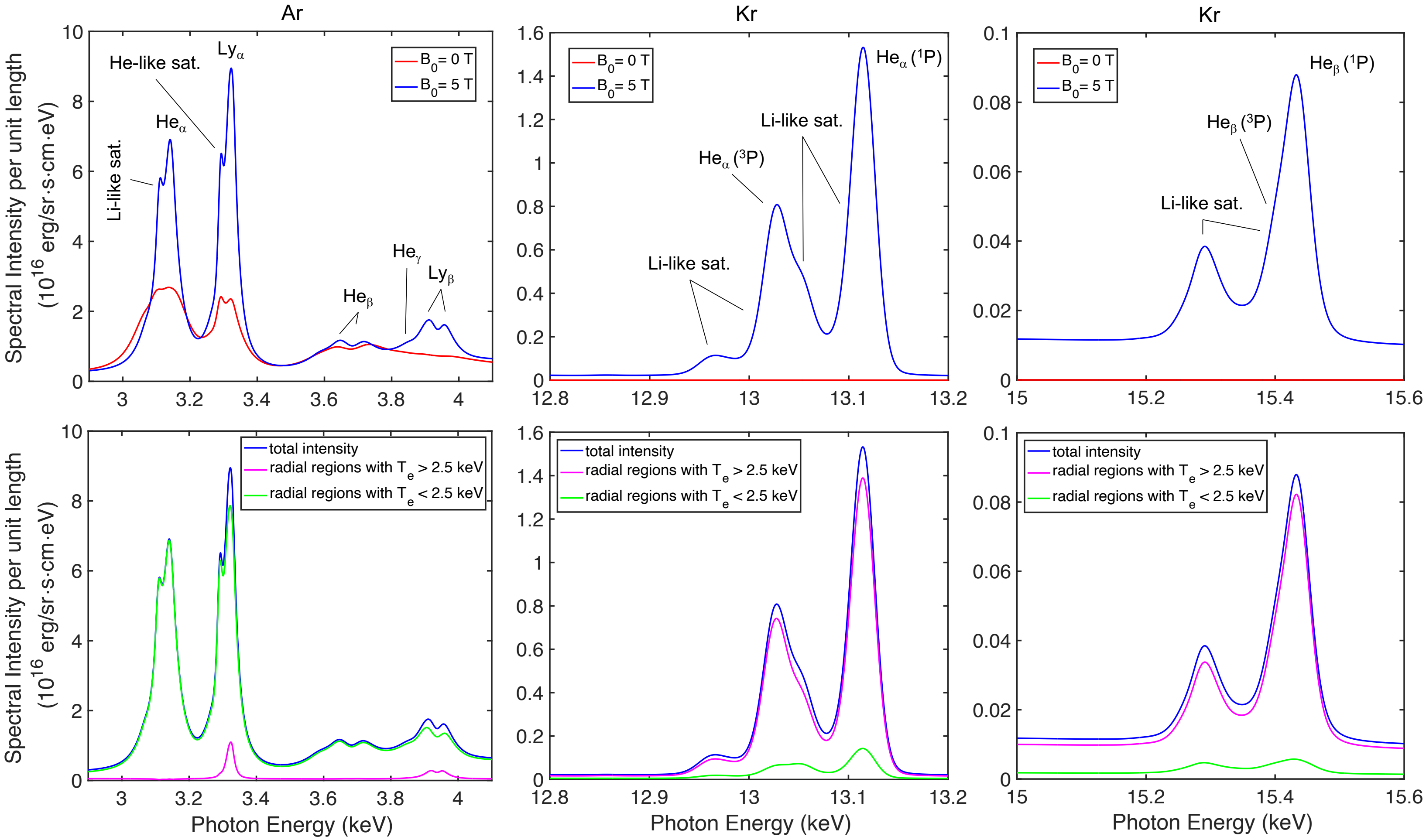
Study of temperature sensitivity



- Basic atomic-kinetics calculations provide information about dopant suitability depending on temperature.
- Ar K-shell spectroscopy (He-like and H-like) works for ~750-2500 eV.
- Kr K-shell spectroscopy (Li-like and H-like) seems appropriate for > 2500 eV.

LMJ cylindrical implosions: Ar & Kr doping

Modelling the Ar and Kr spectra



- Simultaneous use of Ar and Kr dopants has been proposed to study core conditions of magnetized cylindrical implosions at LMJ. Experiments are scheduled for 2024-2026. [18] G. Pérez-Callejo et al., Phys. Rev. E **106**, 035206 (2022)
- Kr acts like a temperature gauge. Simulteneous use of Ar and Kr results in an *effective spatial resolution*.

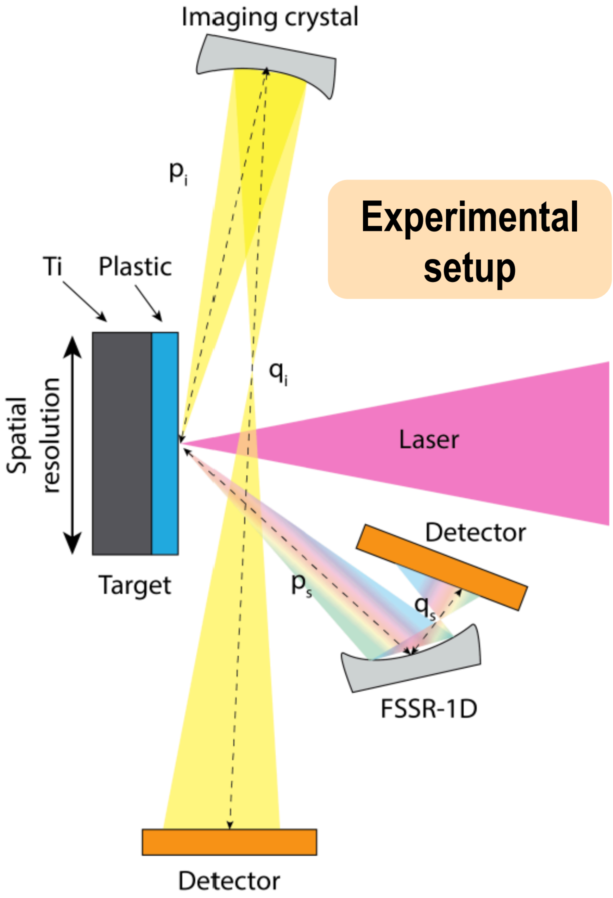
Outline

- 1 Who are we?
- 2 Computational platform for spectroscopic characterization of HED plasmas
- 3 BCoilCompress: magnetized cylindrical implosions in OMEGA
- 4 Modeling K-α emission in shock-ignition relevant experiments

Modeling K-α emission in SI-relevant experiments

- Experiments performed in PALS for investigation of parametric instabilities were performed on PALS at intensities relevant to SI[19].

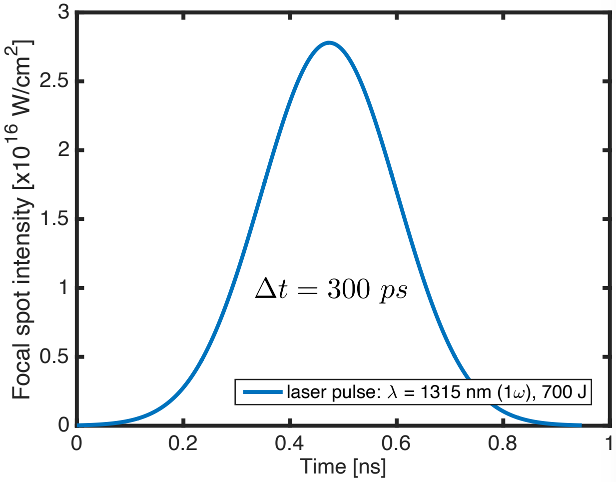
[19] G. Cristoforetti *et al. Phys. Plasmas* **25**, 012702 (2018)



Experimental setup

Laser pulse

$$\lambda = 1315\ /\ 438\ nm \quad (1\omega/3\omega)$$
$$E = 600 - 730\ /\ 100 - 250\ J$$
$$I = 3\times 10^{16}\ /1\ \times 10^{16}\ W/cm^2$$



Targets

- Ti foil (5 mm)
- plastic coating (different thickness)

Instruments

- FSSR-1D spectrometer

  Spectral range: 4.4 - 4.8 keV

  $E/\Delta E$ = 5000, Δx = 11 μm
- Imaging spectrometer

Modeling K-α emission in SI-relevant experiments

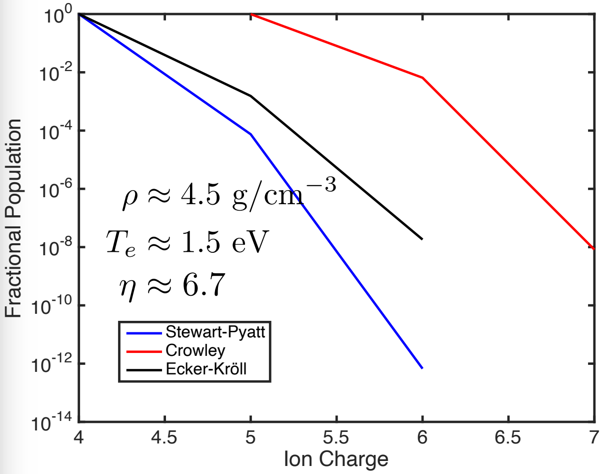
ABAKO improvements for this applications

- Appropriate selection of ions to be include in the CR calculation is done in an automatic fashion. Atomic data obtained from FAC.
- Spectrum formation is studied by post-processing of hydrodynamic simulations and performing the corresponding radiation transport. NLTE atomic-kinetics for both Ti and CH mixture has been explicitly solved. Calculations span over a wide range of plasma conditions.
- Continuum-lowering takes into account atomic mixture when appropriate.
- Special care to have a **consistent set of electronic configurations**, including those with **K-shell vacancies for proper K-α spectrum modeling** .
- **Hot-electron temperature and density spatial distributions are taken into account**. A two-maxwellian distribution is assumed to account for hot (SRS and TPD) electrons.
- Possibility of chossing between **three different CL models (EK, SP, Crowley[20])** and introduced free (thermal) **electron degeneracy effects** on NLTE rate equations.

[20] B. J. B. Crowley, HEDP 13, 84 (2014)

Modeling K-α emission in SI-relevant experiments

Basic atomic kinetics: impact of CL model



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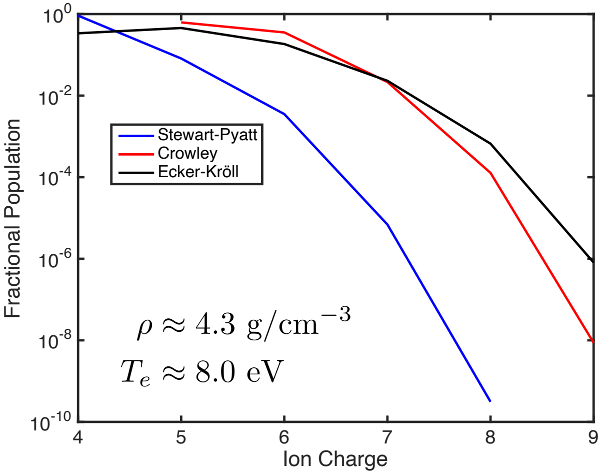

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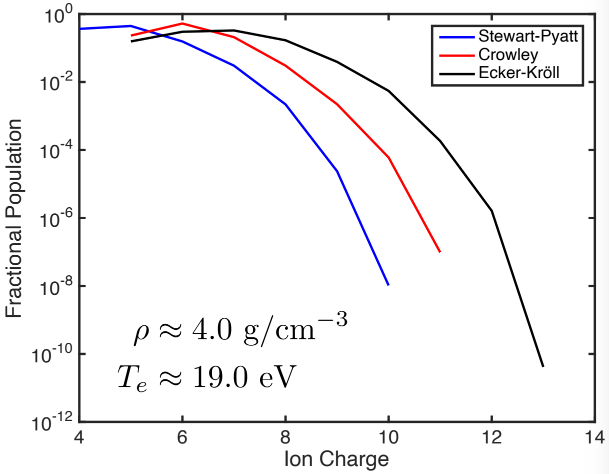

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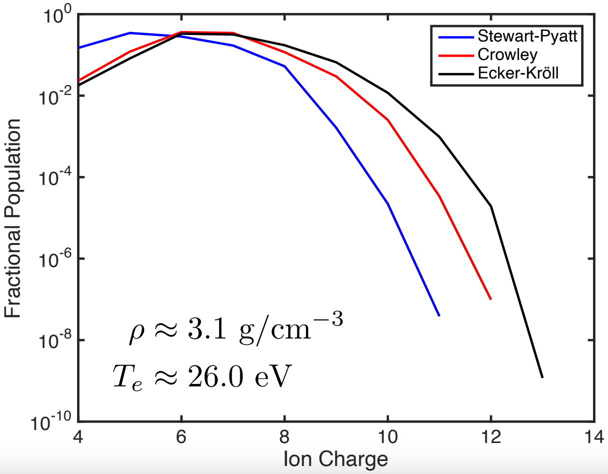

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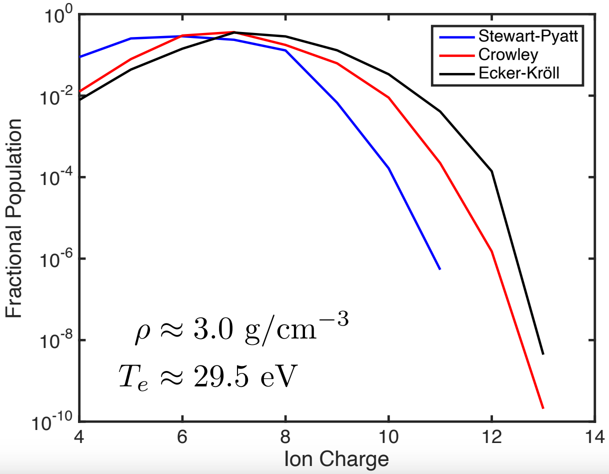
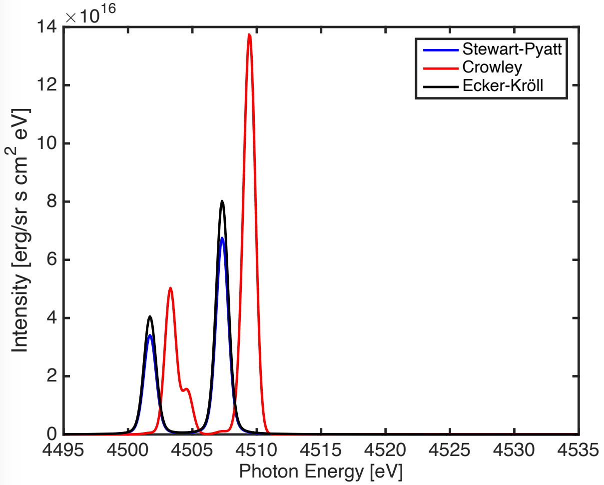


t=650 ps

Modeling K-α emission in SI-relevant experiments

K-α emission spectrum: impact of CL model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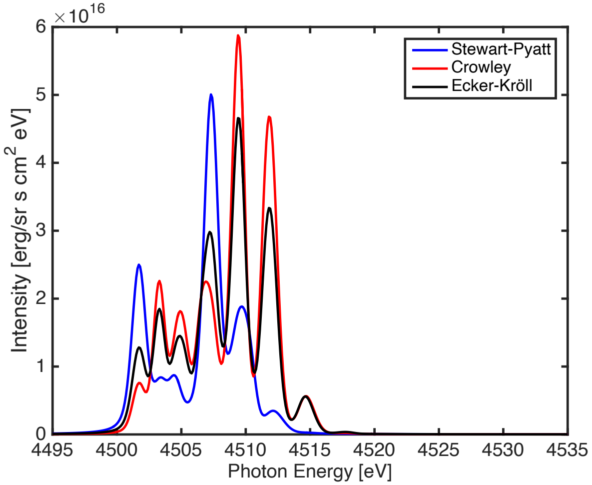
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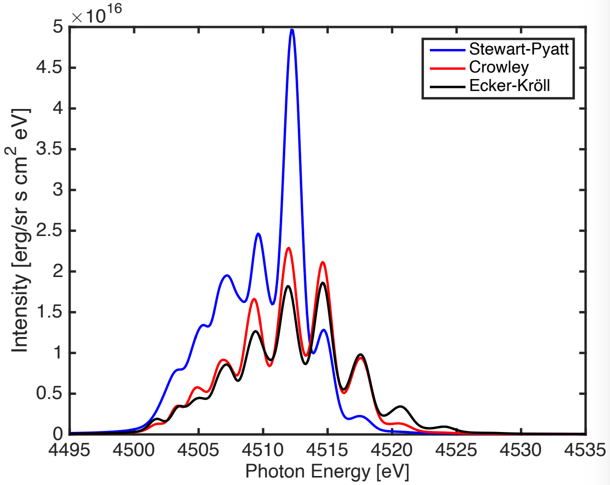
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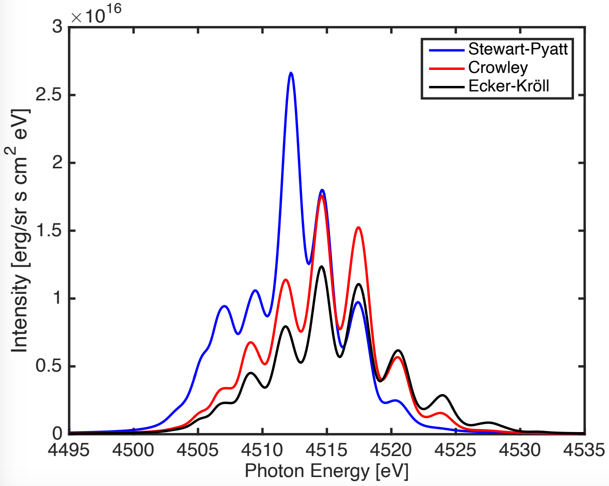
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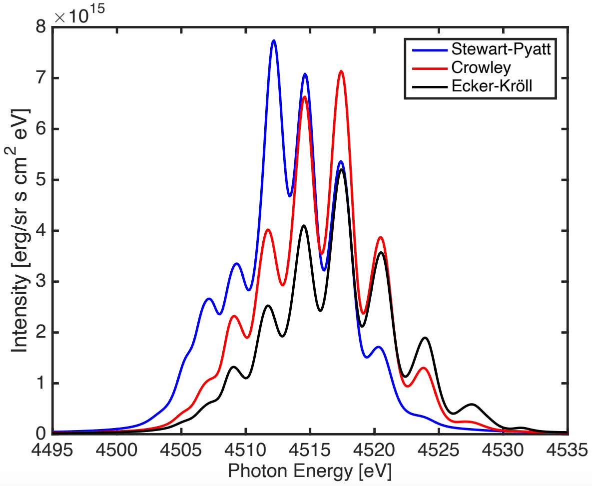
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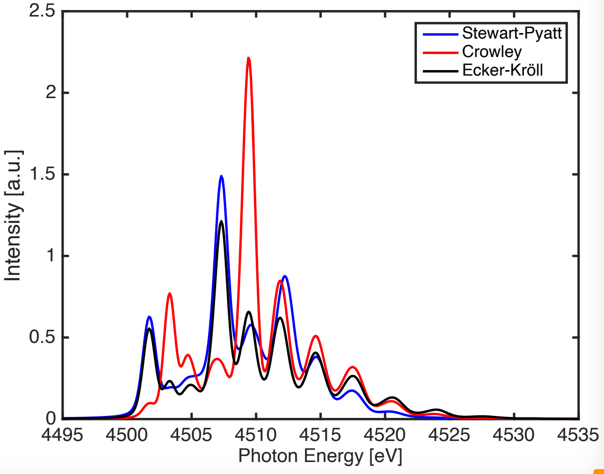
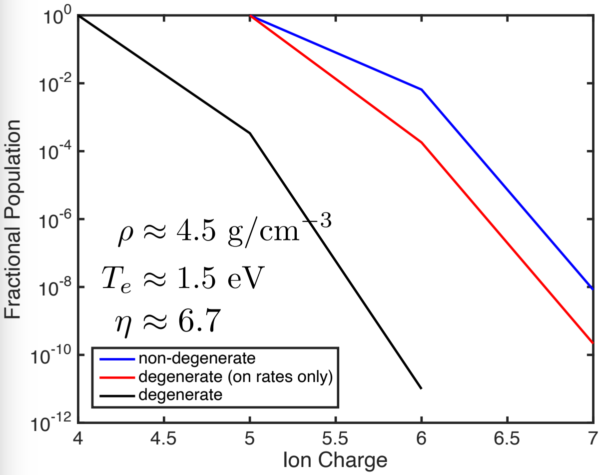

time integrated

Application to PALS conditions: electron degeneracy

Basic atomic kinetics

t=250 ps

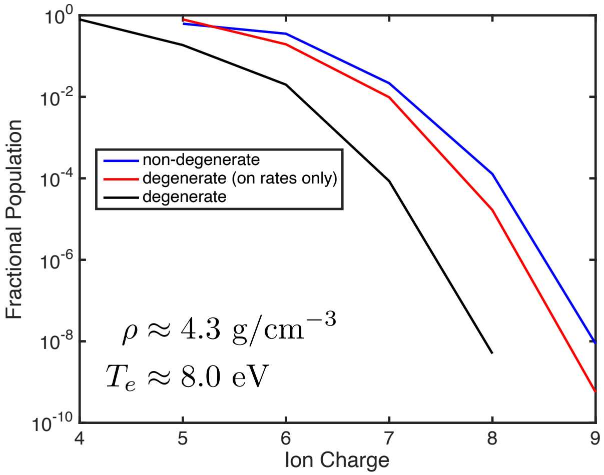


$\rho \approx 4.5\ \mathrm{g/cm^{-3}}$

$T_e \approx 1.5\ \mathrm{eV}$

$\eta \approx 6.7$

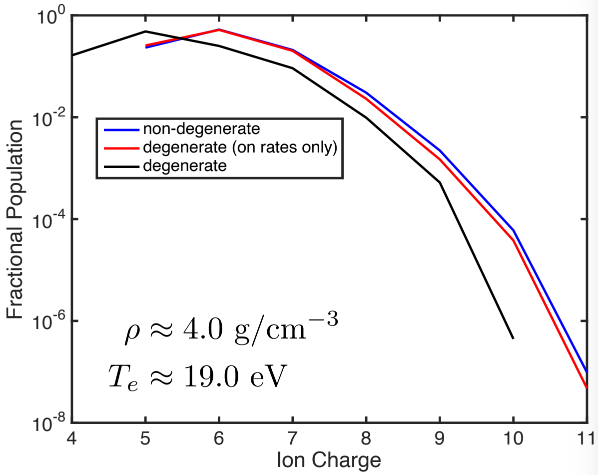
t=350 ps



$\rho \approx 4.3\ \mathrm{g/cm^{-3}}$

$T_e \approx 8.0\ \mathrm{eV}$

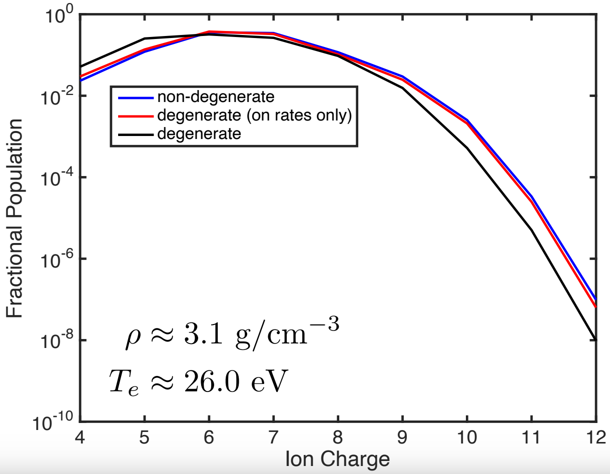
t=450 ps



$\rho \approx 4.0\ \mathrm{g/cm^{-3}}$

$T_e \approx 19.0\ \mathrm{eV}$

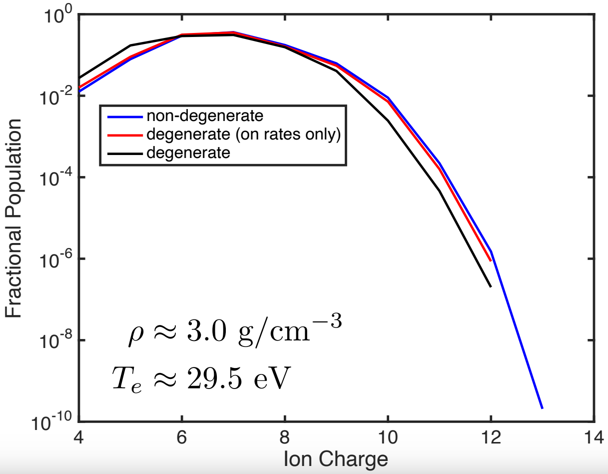
t=550 ps



$\rho \approx 3.1\ \mathrm{g/cm^{-3}}$

$T_e \approx 26.0\ \mathrm{eV}$

t=650 ps



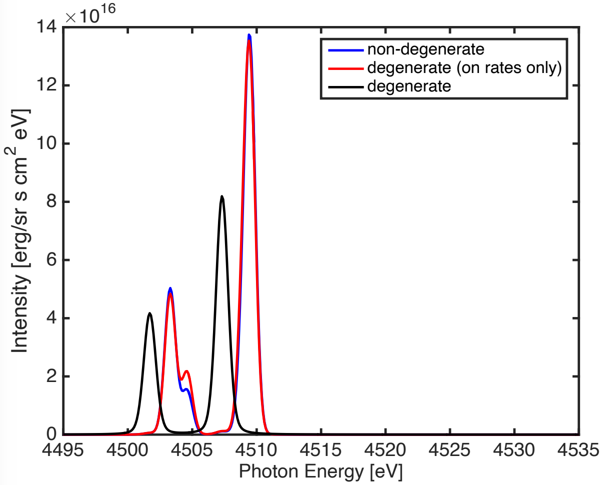
$\rho \approx 3.0\ \mathrm{g/cm^{-3}}$

$T_e \approx 29.5\ \mathrm{eV}$

Application to PALS conditions: electron degeneracy

K-α emission spectrum

t=250 ps



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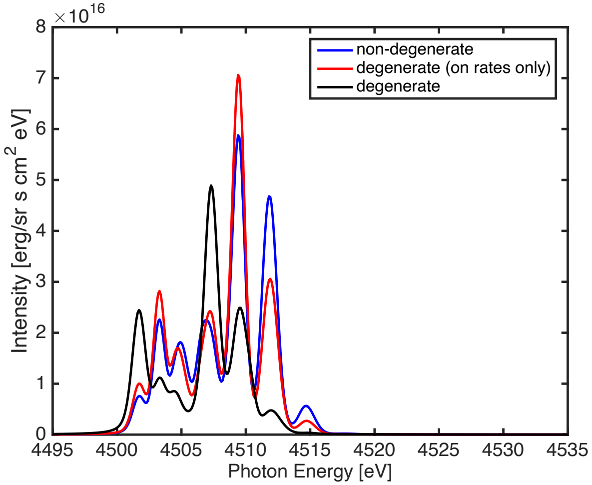

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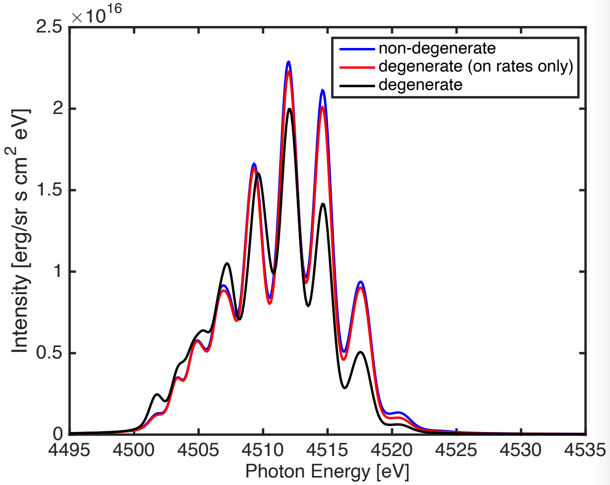

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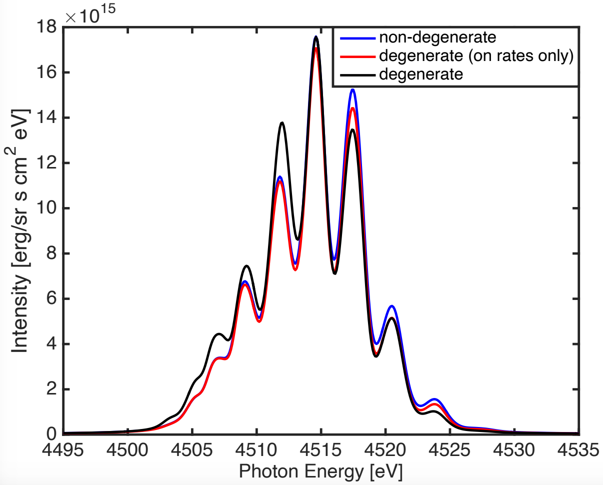

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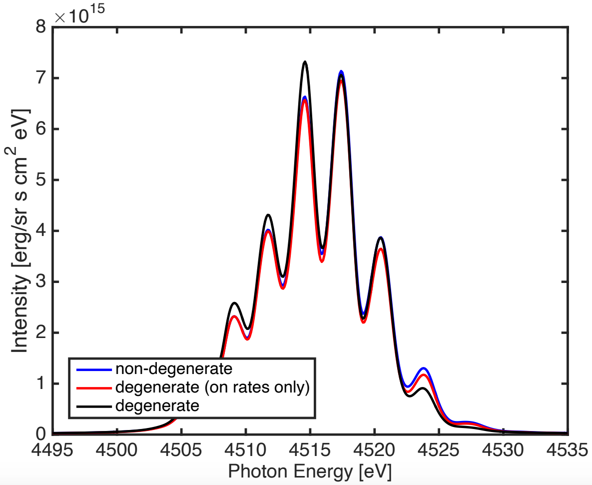

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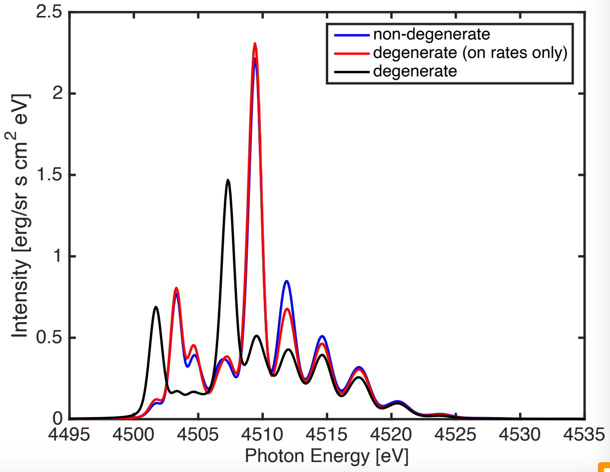

Flexible Non-LTE atomic-kinetics and detailed Stark-broadened lines profiles for spectroscopic characterization of high-energy-density plasmas

Ricardo Florido

iUNAT - Departamento de Física, Universidad de Las Palmas de Gran Canaria (Spain)

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