X-ray plasma spectroscopy

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Plasma Physics course, TU Dresden

HZDR
HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

Outline

- Collisional – radiative (CR) model:

  yet another view on plasma
- Spectra synthesis
- Measuring spectra
- **Experiments**

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CR model: Atomic states

- Detailed view: each ion in plasma has a specific ionization and excitation state.
- Such state can be described in terms of electron occupancy of shells or subshells
- Neutral Al ion, ground state (13 electrons):

  $K2\ L8\ M3$, $1s^2\ 2p^6\ 2s^2\ 3s^2\ 3p^1$

  Al 11+ (ionized so there are only 2 bound el. left):

  ground state: $1s^2$, most common excited state: $1s^1\ 2p^1$
- Copper (29 el.): $K2\ L8\ M18\ N1$, $1s^2\ 2p^6\ 2s^2\ 3p^6\ 3s^2\ 3d^{10}\ 4s^1$
- We label all relevant states by number i and define their fractional population as n_i.

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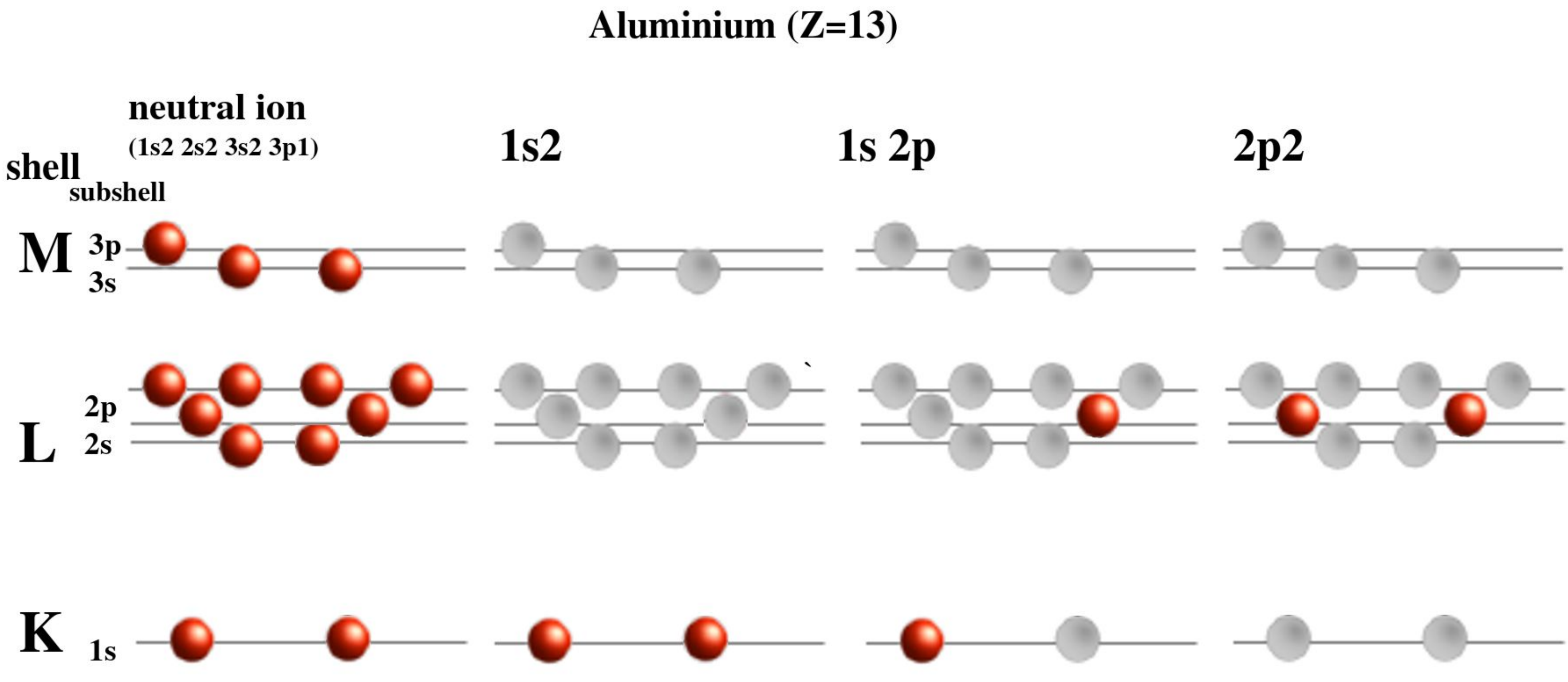
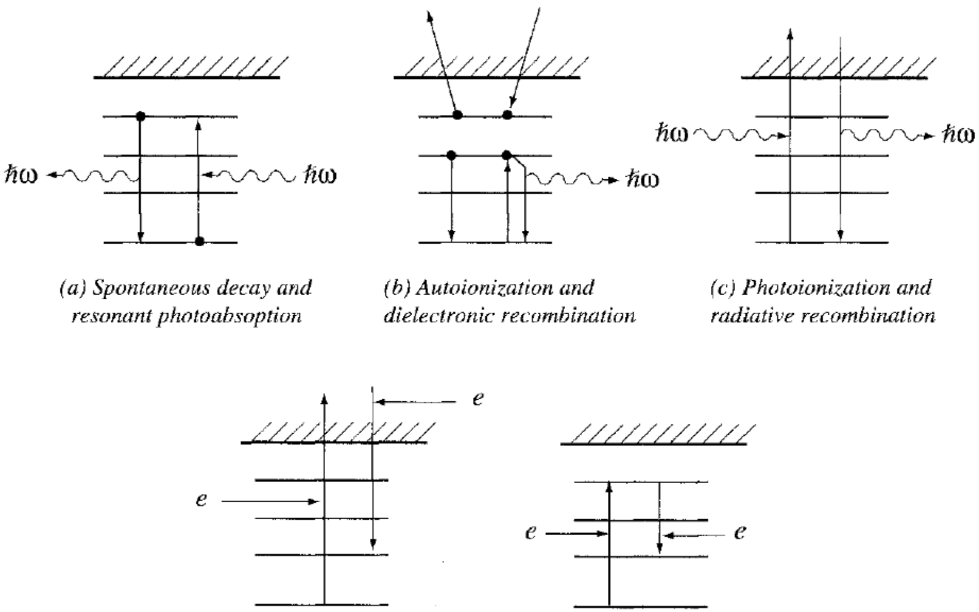
CR model: Atomic states (Al)



CR model: atomic processes

Direct process	Inverse process
Spontaneous decay	Photoexcitation
Electron collisional excitation	El.coll. deexcitation
Autoionization	Dielectronic capture
Electron collisional ionization	3–body recombination
Photoionization	Radiative recombination



(a) Spontaneous decay and resonant photoabsoption

(b) Autoionization and dielectronic recombination

(c) Photoionization and radiative recombination

(d) Electron impact ionization and 3-body recombination

(e) electron impact excitation and de-exitation

- Processes are described by **rate coefficients**, i.e. *how often they happen in given plasma conditions.*

- If plasma is in equilibrium, then by definition the rate of direct process is proportional to the inverse one.
- Calculating only one of them is enough! **Detailed balance**

- CR codes need a huge amount of atomic data, which are calculated by atomic codes.

- The accuracy and reliability of CR codes is dominantly given by the quality of its atomic data

Atomic data

- Still not complete model of single ***Cu ion***:
- Thousands levels
- Tens of thousands transitions
- could be tens MB per ionization state

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CR solver

- Solving population dynamics & radiation transport
- populations n_i are dependent on radiation (through photoabsorption)
- Radiation intensity is dependent on populations (radiative deexcitation)
- 1 equation for each atomic state, equations are connected to each other by atomic processes.
- Very numerically unstable.

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = -n_i \sum_{j,j\neq i} W_{ij} + \sum_{j,j\neq i} n_j W_{ji}$$

$$\frac{\mathrm{d}I(\omega)}{\mathrm{d}x} = \epsilon(\omega) - \kappa(\omega) I$$

n_i . . . density of ions in state i
W . . . transition matrix
I . . . spectral intensity
ϵ . . . emissivity
κ . . . absorptivity

Equilibria

- LTE Local Thermodynamic Equilibrium: particles in TE, photons not - they can escape. i.e. like TE, but limited volume.

  Population given by Saha eq., independent on atomic processes:

$$\frac{N_\zeta n_e}{N_{\zeta-1}} = 2\left(\frac{mc^2 T_e}{2\pi(\hbar c)^2}\right)^{3/2} \frac{z_\zeta(T_e)}{z_{\zeta-1}(T_e)} \exp\left(-\frac{E_{\zeta-1} - \Delta E_{\zeta-1}}{T_e}\right) \qquad (5.2.7)$$

- CE Corona Equilibrium: good for diluted plasmas (e.g. sun's corona). Dominated by electron-impact ionization and recombination

- CR Steady state: *assuming the population do not evolve* $\frac{dn_i}{dt} = 0.$

- Time-dependent CR: *we have the 'full model', we do not have to assume anything.*
  - Obviously very sensitive to quality of the model
  - Boundary conditions: usually either LTE or CRSS

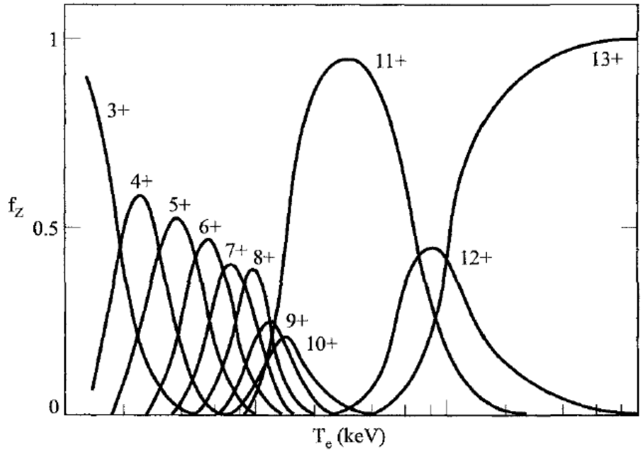


Figure 5.1 Charge state distributions for an aluminum plasma of ion density of $n_i = 1 \times 10^{22}$ cm^{-3} as a function of temperature, calculated assuming LTE.

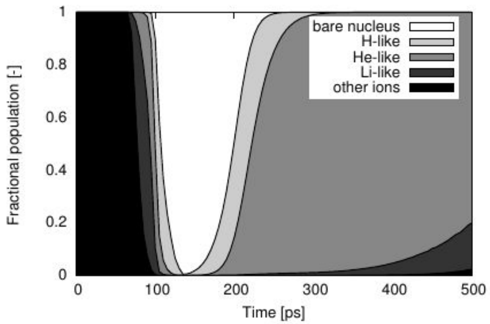


Figure 4.7.: Ionization evolution in steady–state regime.

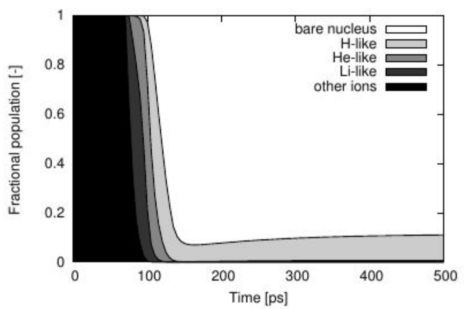
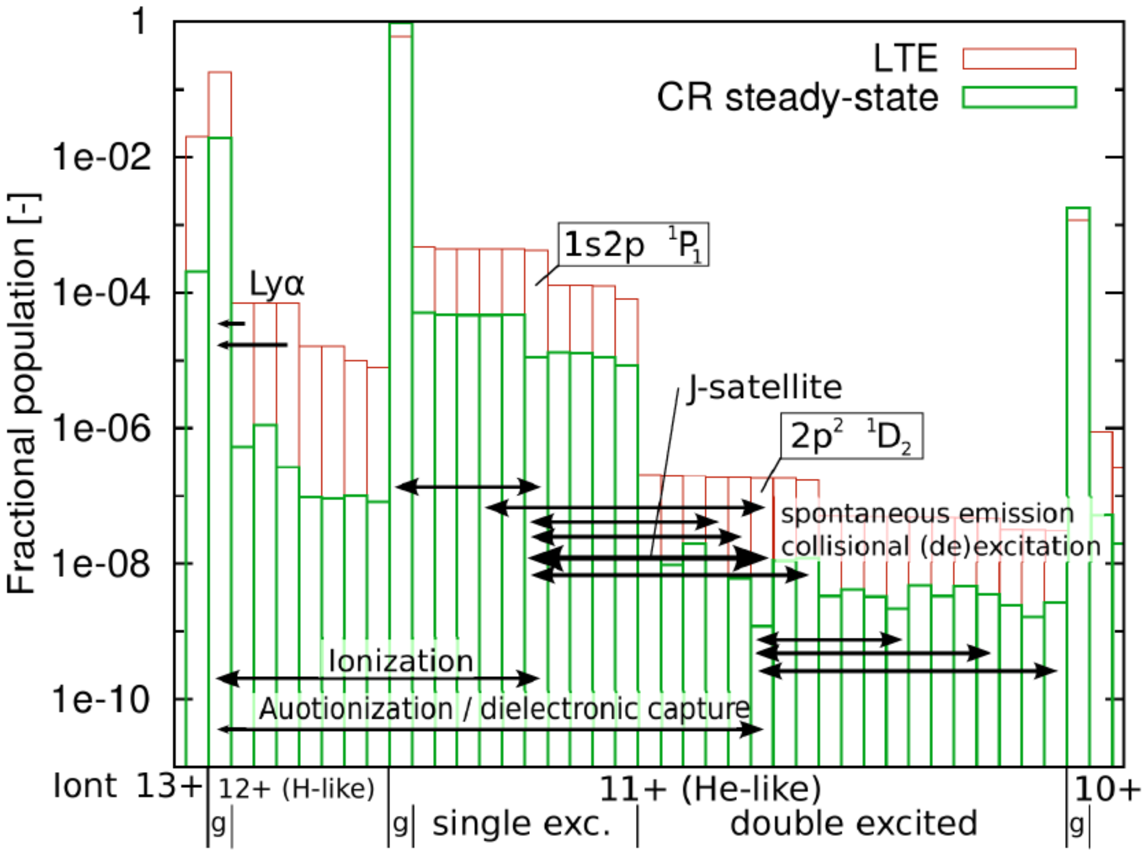


Figure 4.8.: Ionization evolution in time–dependent regime.

e

Very simple CR model



Synthetic spectra

- Making synthetic spectra is relatively ‚easy’:

1) You have the populations
2) You see the radiative deexcitation rates = Oscillator strengths of each transition.
3) Multiply these two. You have the intensity of each spectroscopic line.
4) Find the correct lineshape!

Line broadening:

- Natural - given by finite lifetime of upper level, usually very narrow
- Doppler: each ion has thermal velocity-> Doppler shift. Resulting line has a Gaussian shape corresponding to Maxwellian distribution of temperatures. Reflects ionic temperature.
- Stark: dependent on density: surrounding ions influence the ion’s potential. If there is a lot of ions, potential is influenced and the transition is shifted. Fluctuation of surrounding ions causes fluctuation of transition energy -> broadening.
- Opacity: see radiation transport.
- Mixing of different lines. All these effects should be ‚convoluted together’ to produce the resulting line shape


24th ICSLS
June 17 – 22, 2018
Dublin, Ireland
24th
International Conference on Spectral Line Shapes
SCOPE
Atomic and molecular transitions in gaseous mixtures
Cold atoms and molecules, collision-induced spectra
Fundamentals of narrow optical resonances
Quantum gases, BEC and optical clocks
Spectroscopy of stellar atmospheres and interstellar media
Spectroscopy of planetary atmospheres and exoplanets
Processes in intense laser fields
Single and multi-photon ionization processes
High and low temperature (including fusion) plasmas
Innovative techniques of line shape applications for diagnostic purposes
Clusters and helium droplets
Nanophotonic processes
Applications in industrial, environmental, medical, etc. sectors
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Spectroscopic radiation transport

Optical depth of a material, denoted τ, is given by:[2]

$$\tau = \ln\left(\frac{\Phi_e^i}{\Phi_e^t}\right) = -\ln T,$$

where

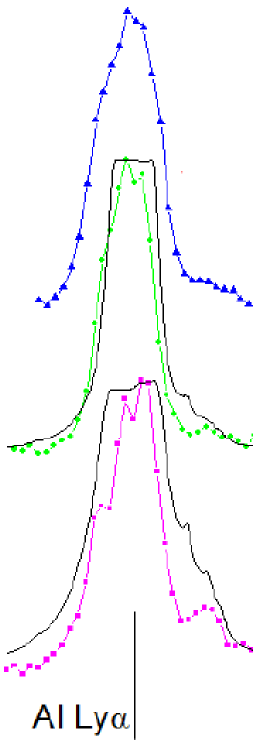
- $\Phi_e{}^i$ is the radiant flux received by that material;
- $\Phi_e{}^t$ is the radiant flux *transmitted* by that material;
- T is the transmittance of that material.

Opacity broadening:

Center of line has higher optical depth -> higher reabsorption -> decrease

Wings of line - lower opt. depth - lower reabsorption -weaker decrease

-> broadening



form for stationary homogeneous 1D plasma as [8]

$$\frac{\mathrm{d}I}{\mathrm{d}\tau} = \frac{\varepsilon}{\kappa} - I, \tag{2.1}$$

where $\varepsilon(\nu)$ and $\kappa(\nu)$ are the plasma emissivity and absorption coefficient and $I(\nu, z(\tau))$ is the radiation intensity. Optical depth $\tau(z,\nu)$ substitutes the spatial coordinate z and is defined as $\tau(z,\nu) = \int_0^z \kappa(z',\nu)dz'$.

Its solution for homogeneous plasma with thickness L is

$$I = \frac{\varepsilon}{\kappa}(1 - e^{-\tau}) = \frac{\varepsilon}{\kappa}(1 - e^{-\kappa L}). \tag{2.2}$$

From this equation, two regimes of radiation transport can be derived. For radiation with low optical depth,$\tau = \kappa L \ll 1$, the exponential factor can be expanded into the lowest orders of its Taylor series and the equation is simplified as

$$I = \varepsilon L, \tag{2.3}$$

thus the emission is proportional to emissivity and plasma size and the absorption can be neglected. For optically thick lines, $\tau = \kappa L \gg 1$, the exponential function goes to zero and the equation (2.2) approaches its limit

$$I = \frac{\varepsilon}{\kappa}, \tag{2.4}$$

where the right–hand side is called the *source function*, which is, in the case of LTE plasmas, equal to the black-body radiation, thus not having the significant spectral dependence as emissivity or absorption coefficient.

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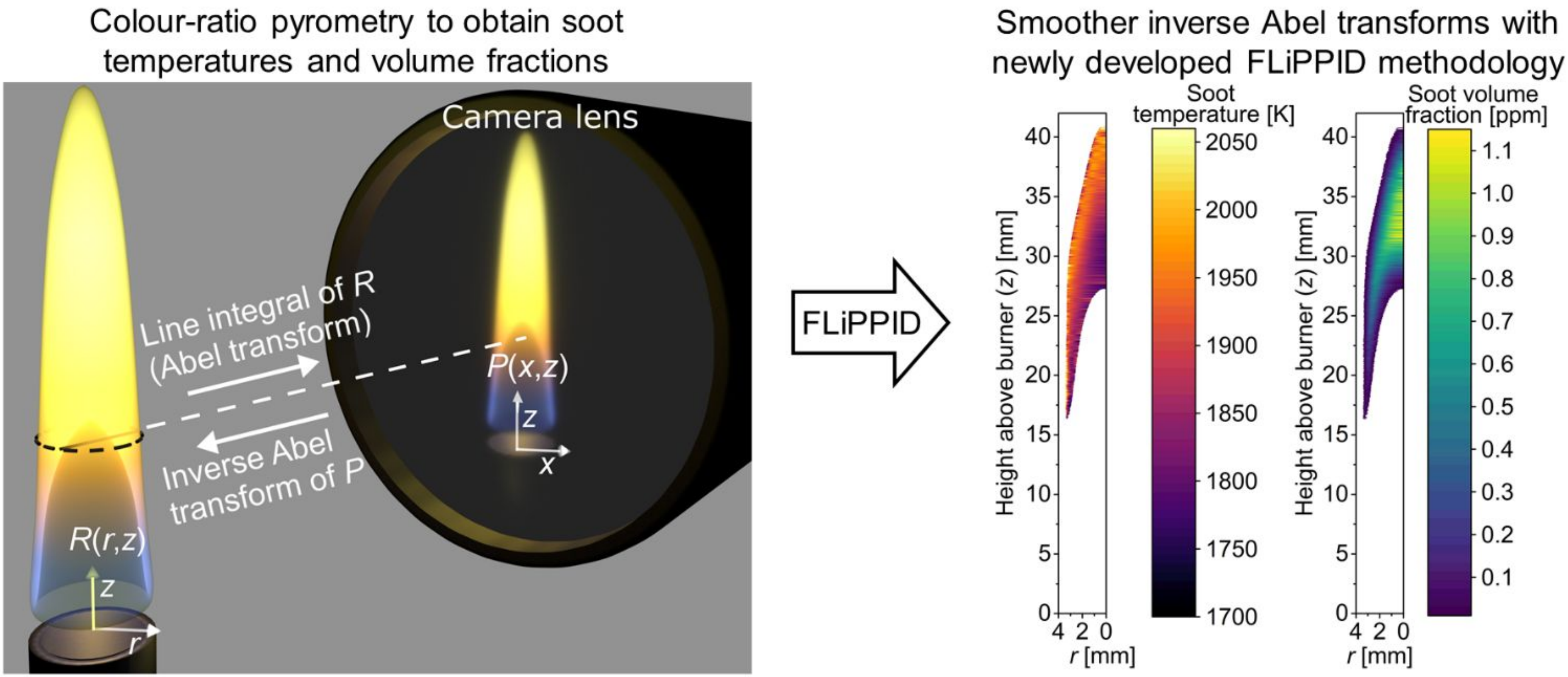
Line-of-sight integration

- Spectra is ‚always' integrated over various plasma condition
- Abel inversion can help to find which emission goes from where.




RPHDM 2014
The 16th International Workshop on
Radiative Properties of Hot Dense Matter
29 September through 3 October 2014

Timeline

November 10 -- submission deadline
November 24 -- online database accessible (password protected)
November 28 -- Workshop opens
December 1 -- Workshop adjourns

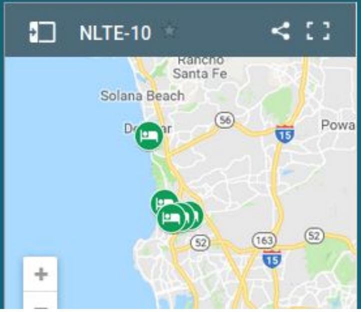
Local Organizing Committee

S.B. Hansen (SNL, USA)
F. Beg (UCSD, USA)
H.A. Scott (LLNL, USA)
C.J. Fontes (LANL, USA)
Yu. Ralchenko (NIST, USA)

Documents

Call for Submissions: PDF | HTML5
Supplemental file: Old | New
PRL paper on Si photoionization: PDF
PRL paper on Al: HTML
Nature paper on Ne: HTML

Area map



The 10th NLTE Code Comparison Workshop

November 28 - December 1 2017, San Diego, CA, USA

Supported by:
UCSD, SNL

Advanced collisional-radiative (CR) models are extensively used in plasma spectroscopy to analyze plasma kinetics and spectra produced far from local thermodynamic equilibrium (LTE). Non-LTE atomic models also play a critical role in radiation-hydrodynamic simulations used to help design plasma experiments. It is therefore not surprising that verification and validation (V&V) of these complex CR models are of significant interest. Since experimental benchmarks for validation are extremely challenging, computational experiments and comparisons are one of the primary tools for V&V of CR codes. The NLTE Workshops aim at development of such tools and techniques.

Meeting	Year	Location	Results
NLTE-1	1996	Gaithersburg, USA	Lee et al, JQSRT **58**, 737 (1997)
NLTE-2	2001	Virtual Workshop	Bowen et al, JQSRT **81**, 71 (2003)
NLTE-3	2003	Gaithersburg, USA	Bowen et al, JQSRT **99**, 102 (2005)
NLTE-4	2005	Las Palmas de Gran Canaria, Spain	Rubiano et al, HEDP **3**, 225 (2007)
NLTE-5	2007	Santa Fe, USA	Fontes et al, HEDP **5**, 15 (2009)
NLTE-6	2009	Athens, Greece	
NLTE-7	2011	Vienna, Austria	Chung et al, HEDP, **9**, 645 (2013)
NLTE-8	2013	Santa Fe, USA	
NLTE-9	2015	Paris, France	Piron et al, HEDP **23**, 38 (2017)

Important!

Similar to the previous workshops, **a necessary and sufficient condition** for participation would be to submit at least one calculated case. A detailed description of the cases and format requirements can be found in the Call for Submissions.

It would also be very helpful if you inform the organizers on your intention to participate in this Workshop.

Summary of cases

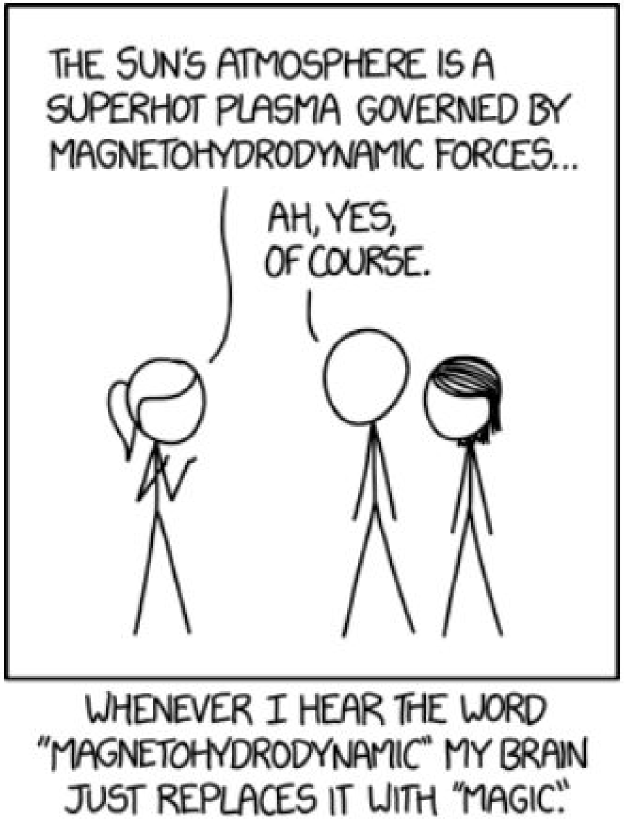
Element	Case ID	No. of cases	T_e (eV)	N_e (cm^{-3})	T_{rad} (eV), dilution factor	Plasma radius (cm)	Spectral ranges
Ne	Ne	12	50, 100, 200, 500	10^{19}, 10^{20}, 10^{21}			800-1400 eV, $\delta\varepsilon$=0.3 eV (2001 points)
Ne	NeTD	3	T_e(t) for 3 cases in supplemental file	$N_e(t) = Z^*(t)\times N_i$ with $N_i=10^{18}$	E_{rad}: 800, 1050, 2000		800-1400 eV, $\delta\varepsilon$=0.3 eV (2001 points)
Al	Al	8	10, 30, 100, 300	2×10^{23}, 5×10^{23}			
Al	AlTD	2	T_e(t) for 2 cases in supplemental file	$N_e(t) = Z^*(t)\times N_i$ with $N_i=6\times10^{22}$	E_{rad}: 1580, 1650		1400-2400 eV, $\delta\varepsilon$=0.5 eV (2001 points)
Si	Si	12	30	10^{19}, 3×10^{19}	T_{rad}: 63 (1.0), [48 (0.28) + 92 (0.081) + 170 (0.0067)]	Corrected values: 0.1, 0.3, 1.2	1700-2500 eV, $\delta\varepsilon$=0.25 eV (3201 points)
Cl	Cl	9	400, 500, 600	10^{21}, 10^{22}, 10^{23}			2600-3800 eV, $\delta\varepsilon$=0.15 eV (8001 points)

Comparison with other models

Sorted by amount of details:

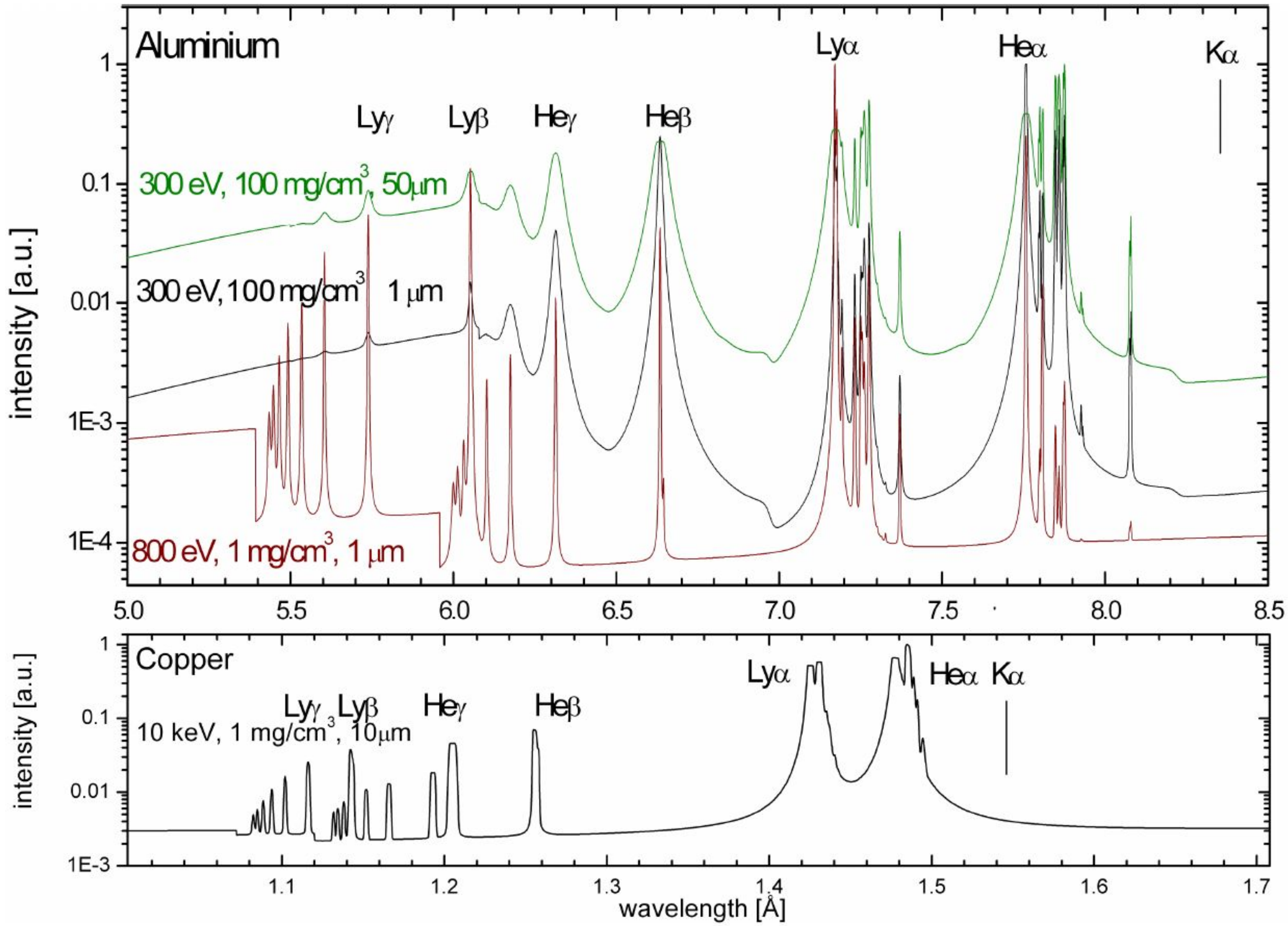
- **Atomic** (quantum) simulations - *tells me the atomic properties of single ion (calculates levels, energies, transition rates..). Single particle, single process*
- DFT-MD (Density Fluctuation Theory - Molecular dynamics, quantum) - *solves the exact motion of few ions by using Quantum theory. Few ions, some fs*
- **CR:** n_i - *takes into account atomic structure of ions, but doesn't solve for density or temperature (need to assume those). Discrete amount of cells, most often single cell (0D)*
- Particle In Cell (**PIC**) - *uses (macro)particles and EM field. Typically 2D, 100 µm, 100 fs, can be used in 3D as well*
- **Kinetic** - *f*(r,v) - d*on't assume Maxwell's distribution of velocities. Rather for analytical approach.*
- **MHD** - *you add charge to the hydrodynamics game. Honestly, I've never used that, similar as HD*
- Hydrodynamics (HD) - T + rho. S*ay that plasma is like hot gas, you just need good Equation Of State (EOS). Assumes Maxwellian distribution. Can simulate 10 mm, several ns.*

xkcd: Magnetohydrodynamics

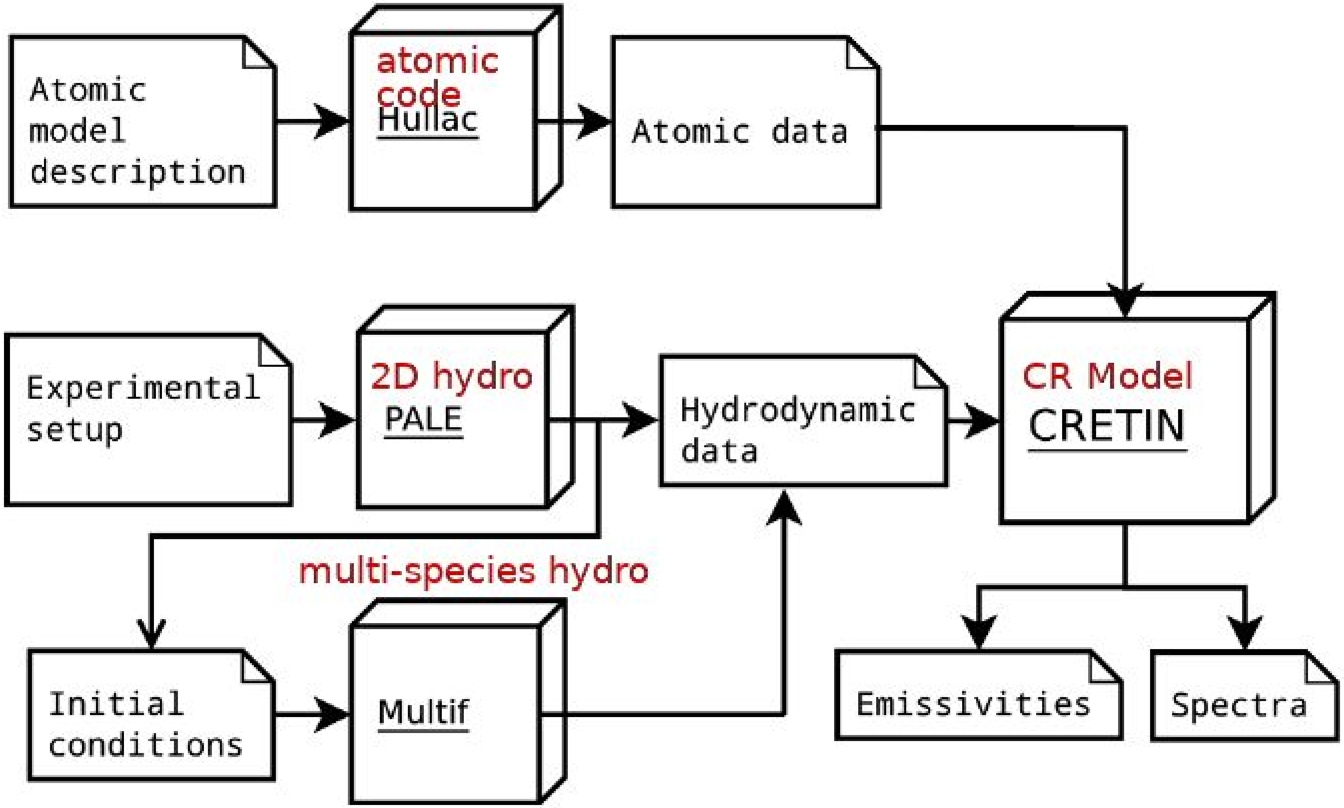


Magnetohydrodynamics combines the intuitive nature of Maxwell's equations with the easy solvability of the Navier-Stokes equations. It's so straightforward physicists add "relativistic" or "quantum" just to keep it from getting boring.

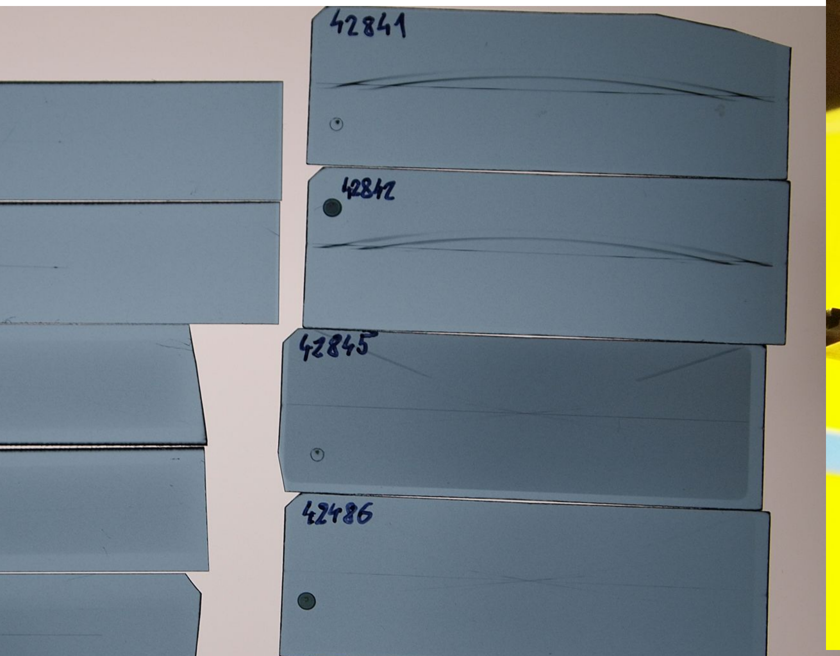
Correspondance between elements

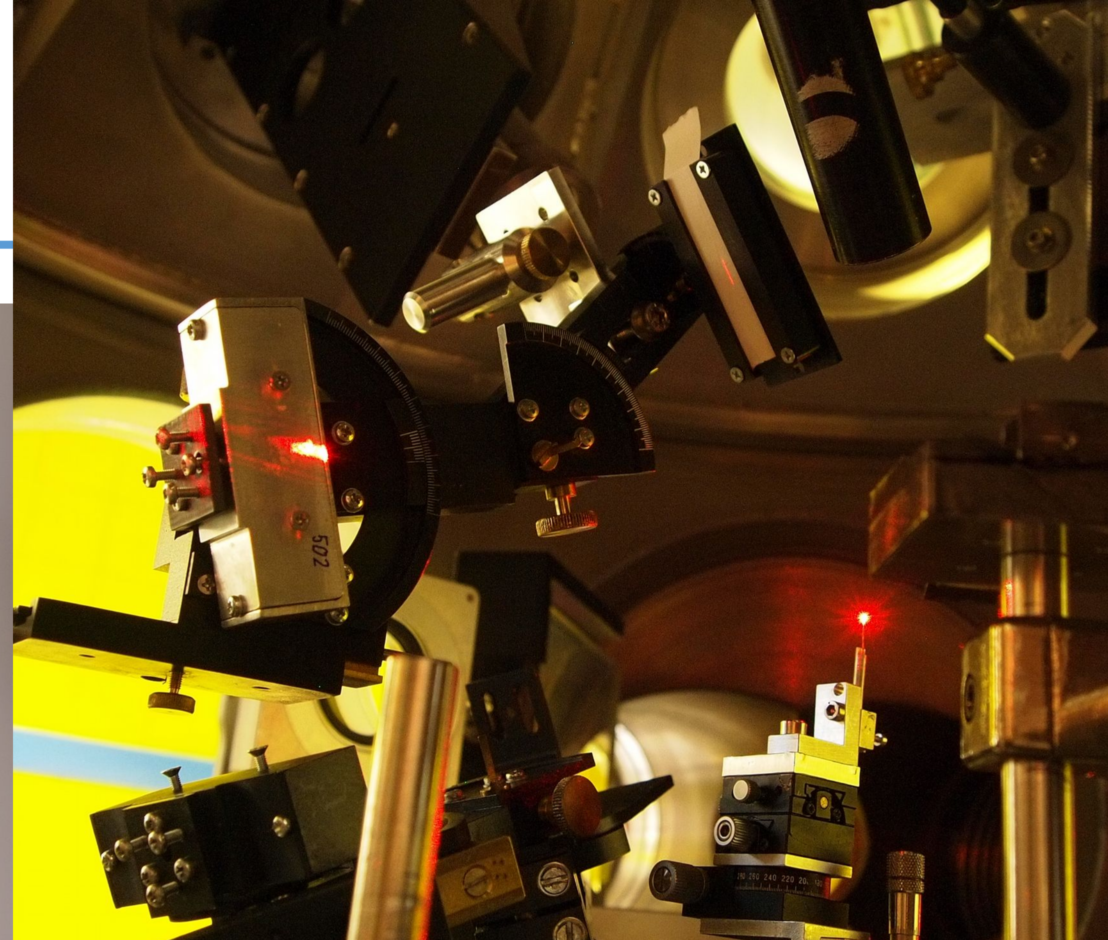


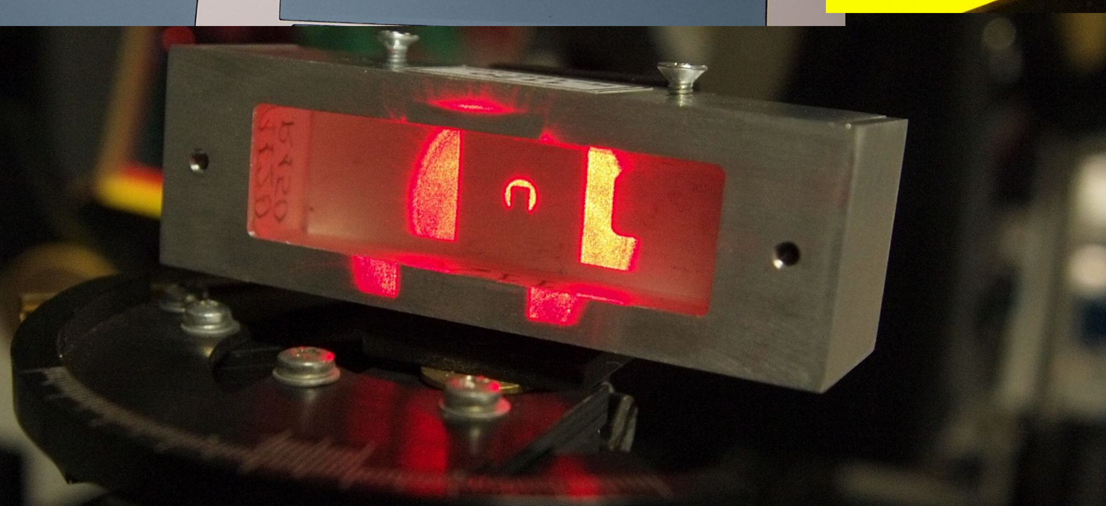
Complex modeling



Detection

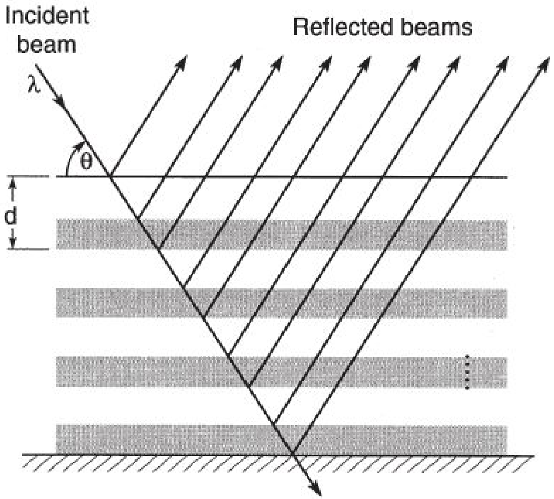


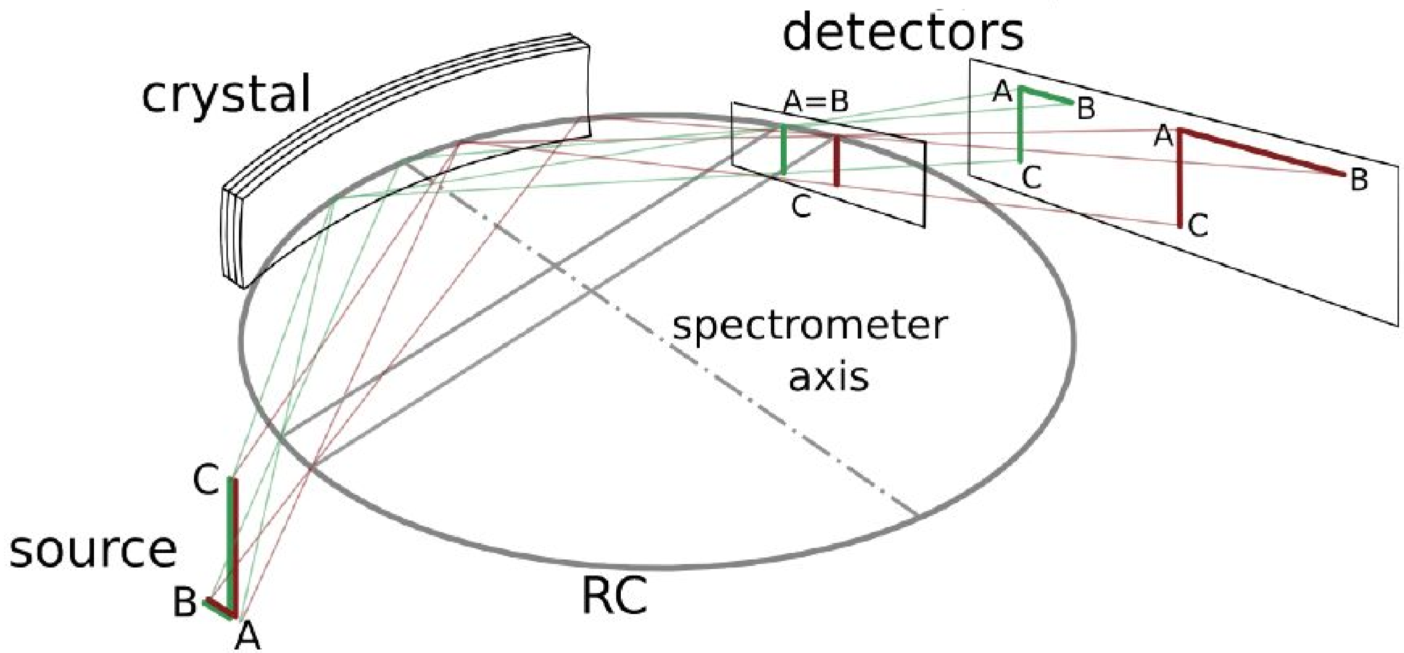




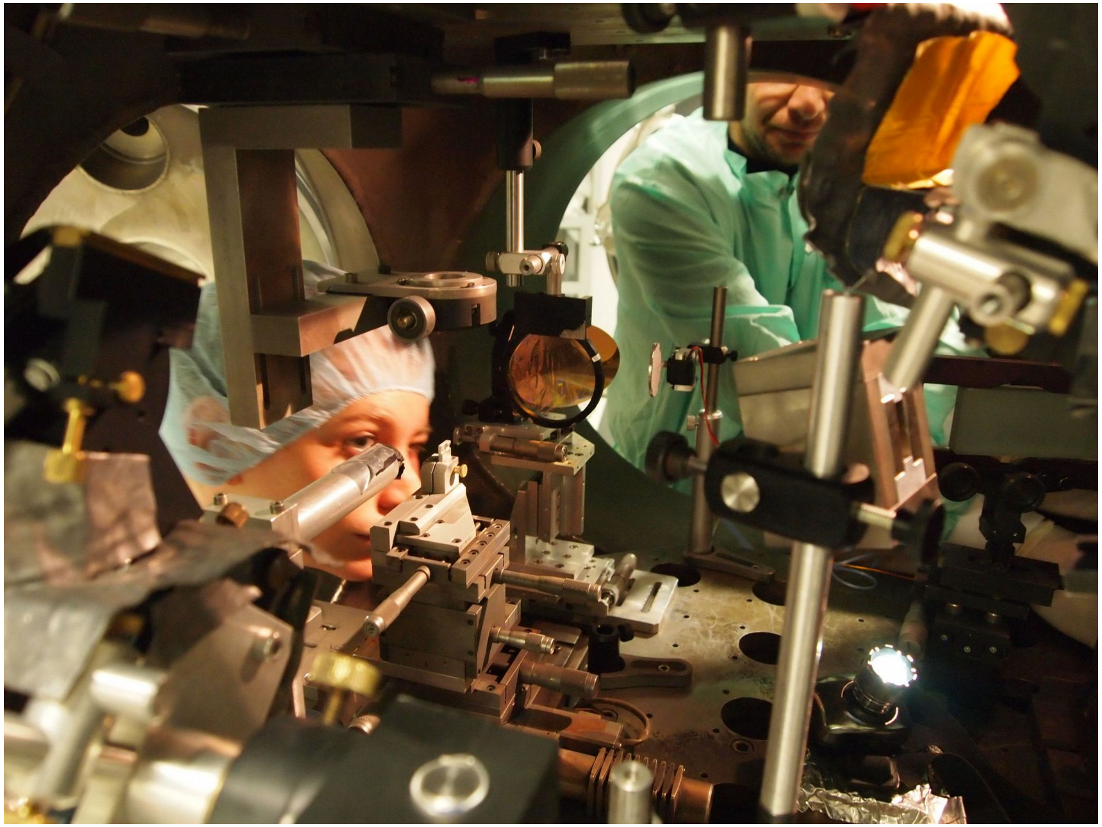
Crystal Spectrometers

- Bragg law: **$n\lambda = 2d\sin(\theta)$**
  λ - wavelength of radiation
  d - spacing of crystal lattice
  θ - incidence angle
  n - spectroscopic order





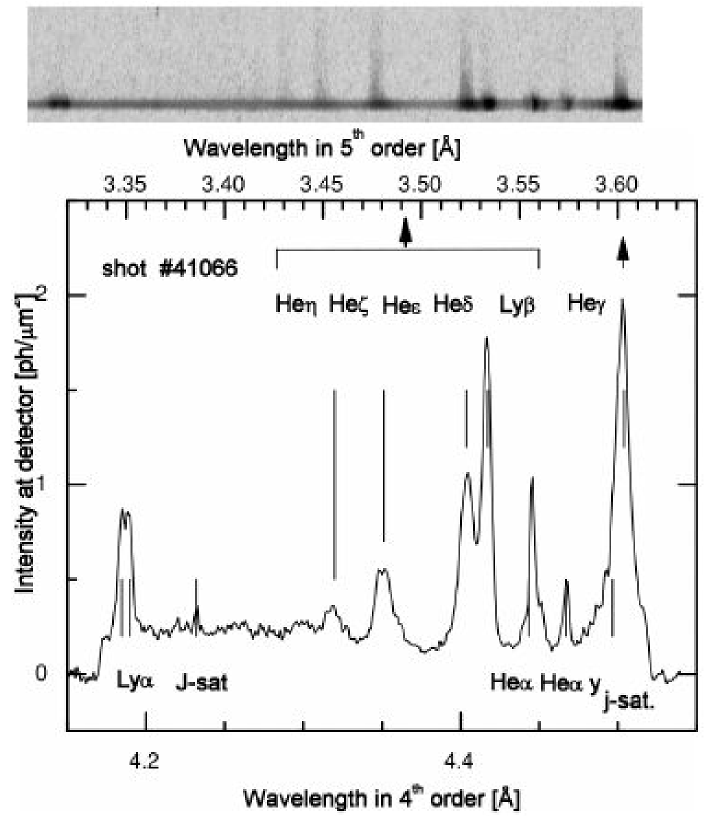
Experiments



1. Basic parameter evaluation

SMS X–ray spectrometer

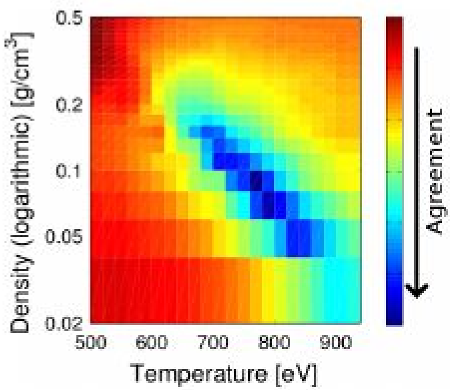
- **Crystal**: spherically bent mica
- **Detector**: X–ray film
- **Covered**:
  4^{th} order: Cl Ly_α , He_α
  5^{th} order: Cl $He_\gamma \div He_\eta$
- **Resolution**:
  Spatial: 10 μm
- Data split into spectroscopic orders, recalculated using known crystal reflectivity and filter transmission.
- Ly_β and He_δ used for evaluation.



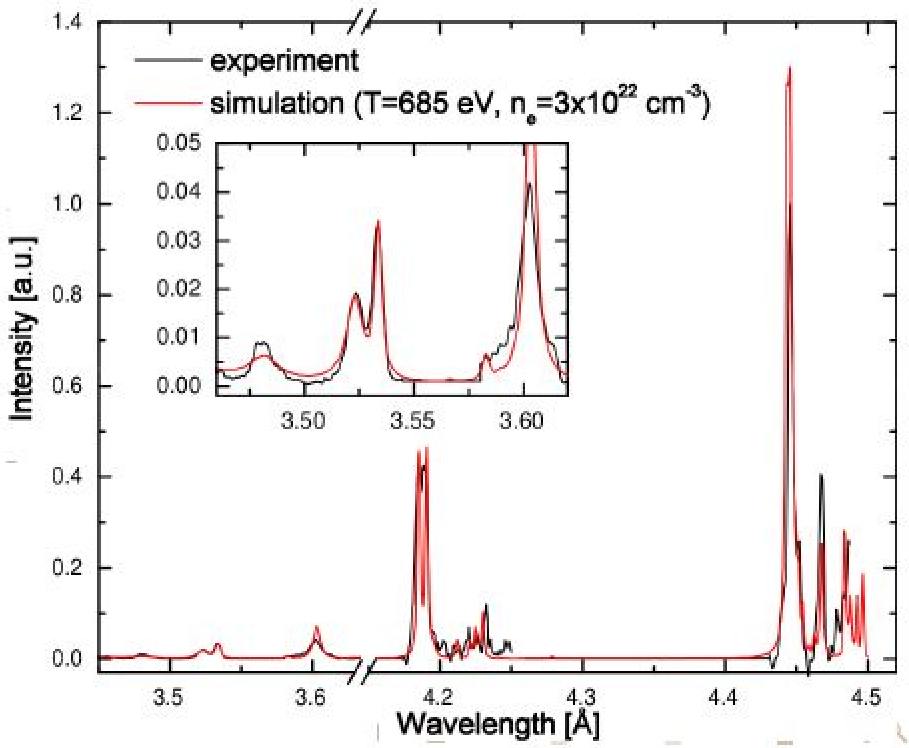
1. Basic parameter evaluation

Spectra evaluation

- To estimate plasma temperature and density.
- Comparison of an experimental spectrum with a set of theoretical ones.
- Theoretical spectra generated by the PrismSpect[?] code.
- Automatic calculation and minimization of a merit function (least squares of differences between spectra)
- Improvement of fit:
  separate density estimation using the width of the the Ly_β line.



Agreement between the experimental and theoretical spectra for various parameters.



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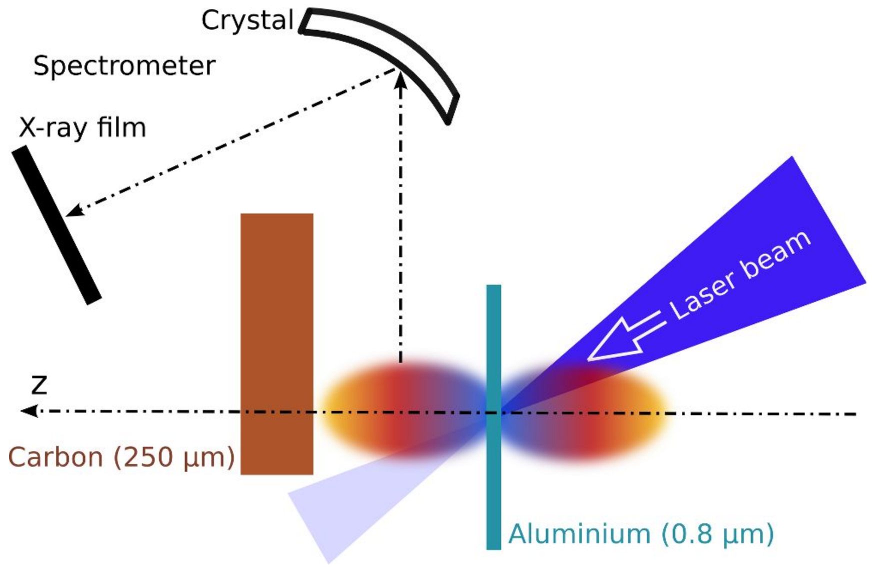
2. Doppler shift & splitting

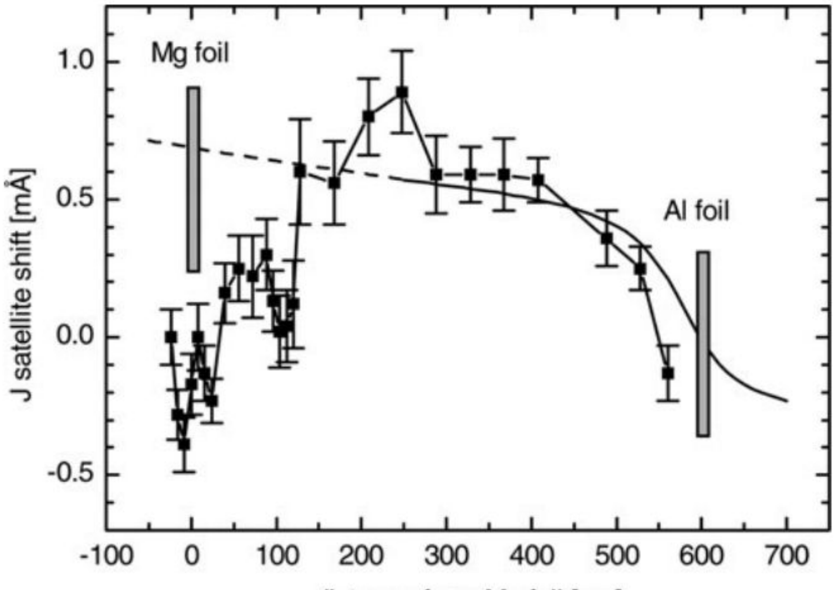
- Laser creates an expanding Al plasma
- Rear plasma plume hits a secondary (Carbon) target
- Spectrometer observes in perpendicular direction:

  -> Resolution along axis

  -> Observation of Doppler shifts

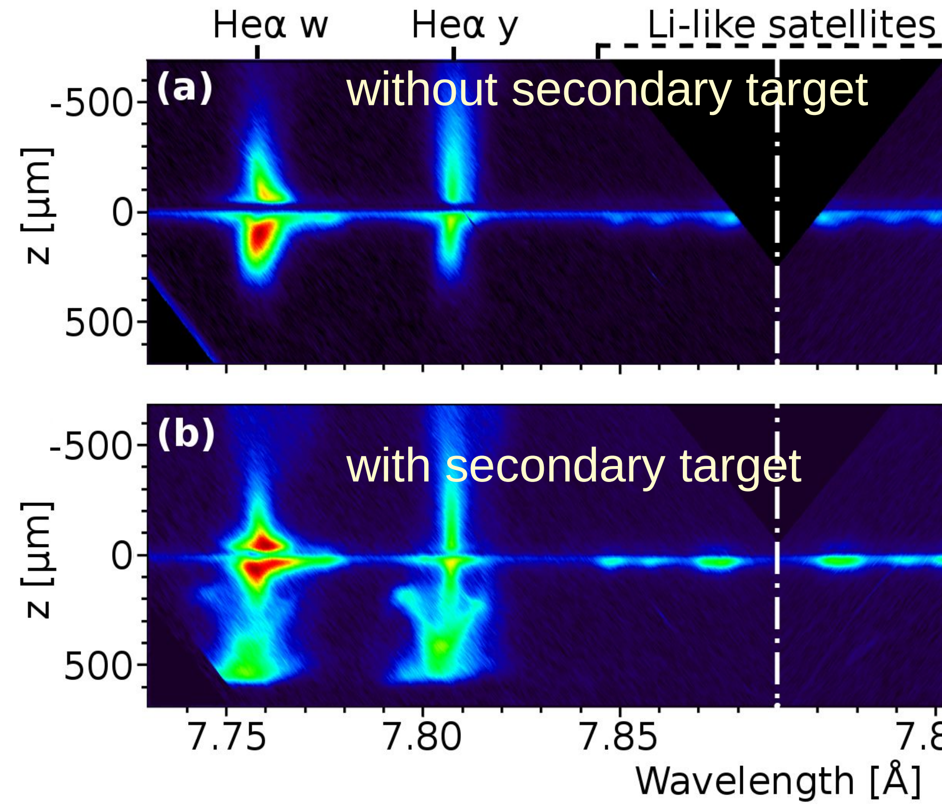


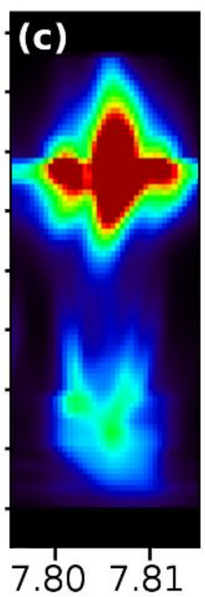
When spectrometer is not exactly perpendicular:

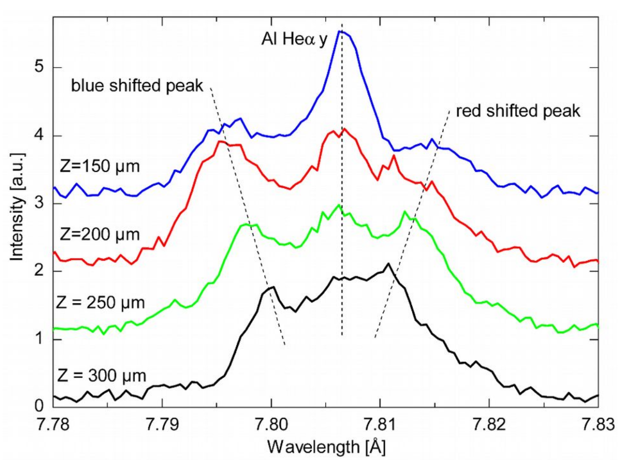


2. Doppler splitting

- We can see ‘strange’ behavior of the line while hitting the secondary target
- Explained as reflection and radial expansion of the plasma
- Modeled by complex simulations







3. Cu Kα satellites

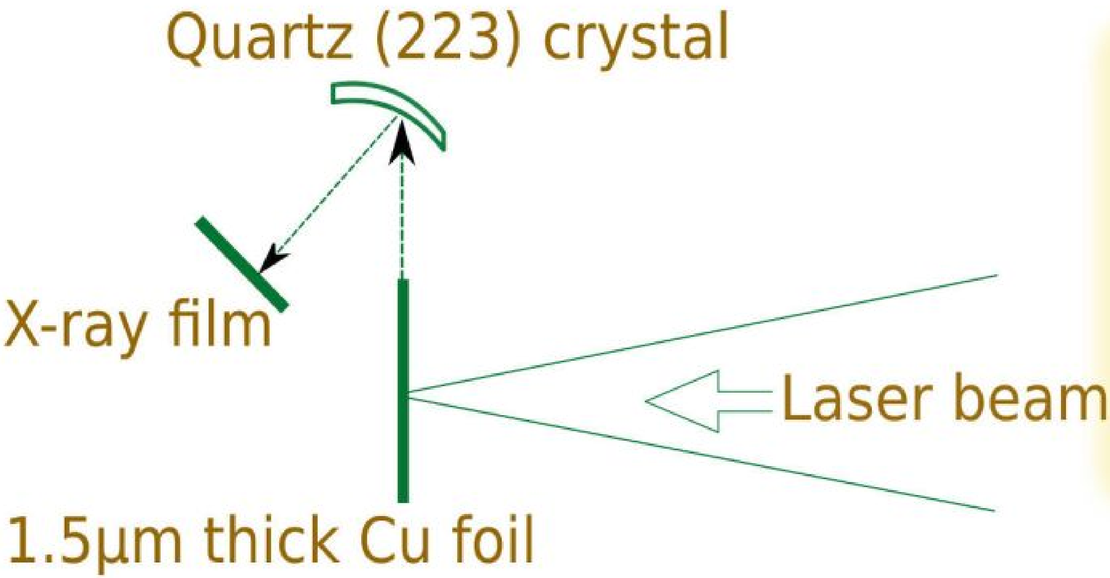
-

without secondary target

with secondary target

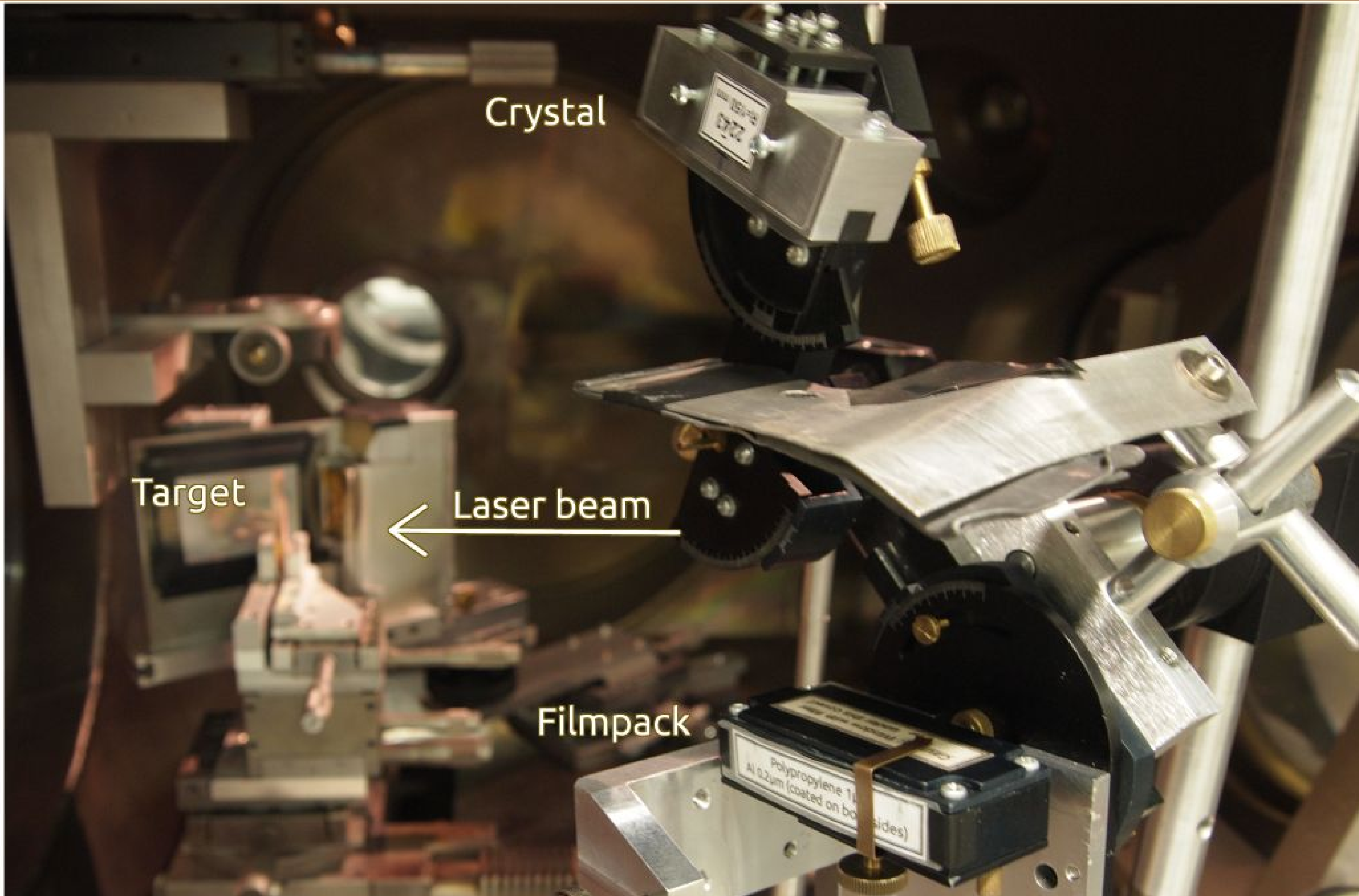
Experimental scheme

- Irradiation of thin Cu foil with high-power laser.
- Principal diagnostics: high-resolution x-ray spectroscopy.

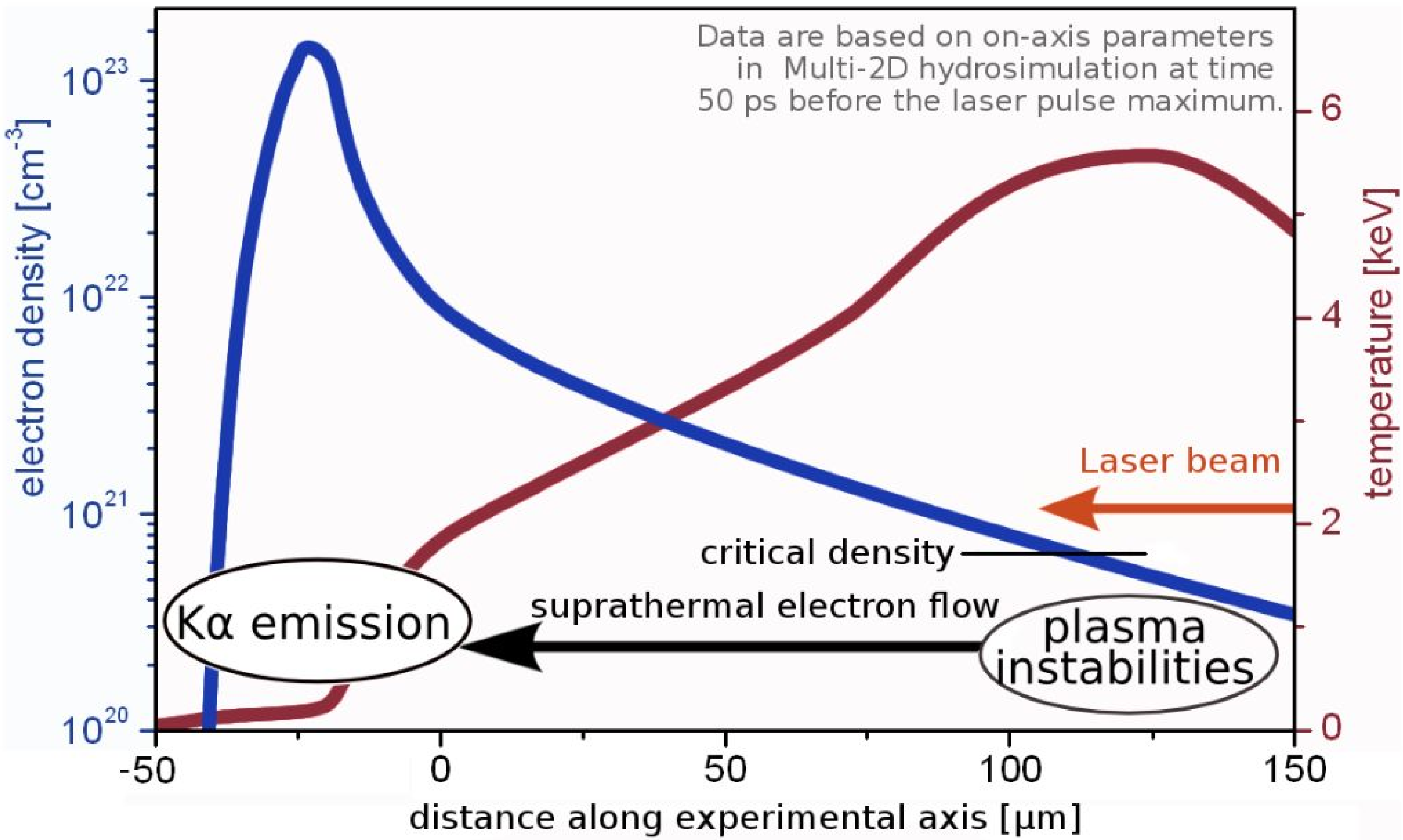


PALS laser[1]
Wavelength:
438 or 1315 nm
Energy: 400 J
Focus: ∅ 70 µm
Intensitity:
4×10^{16} W/cm^2

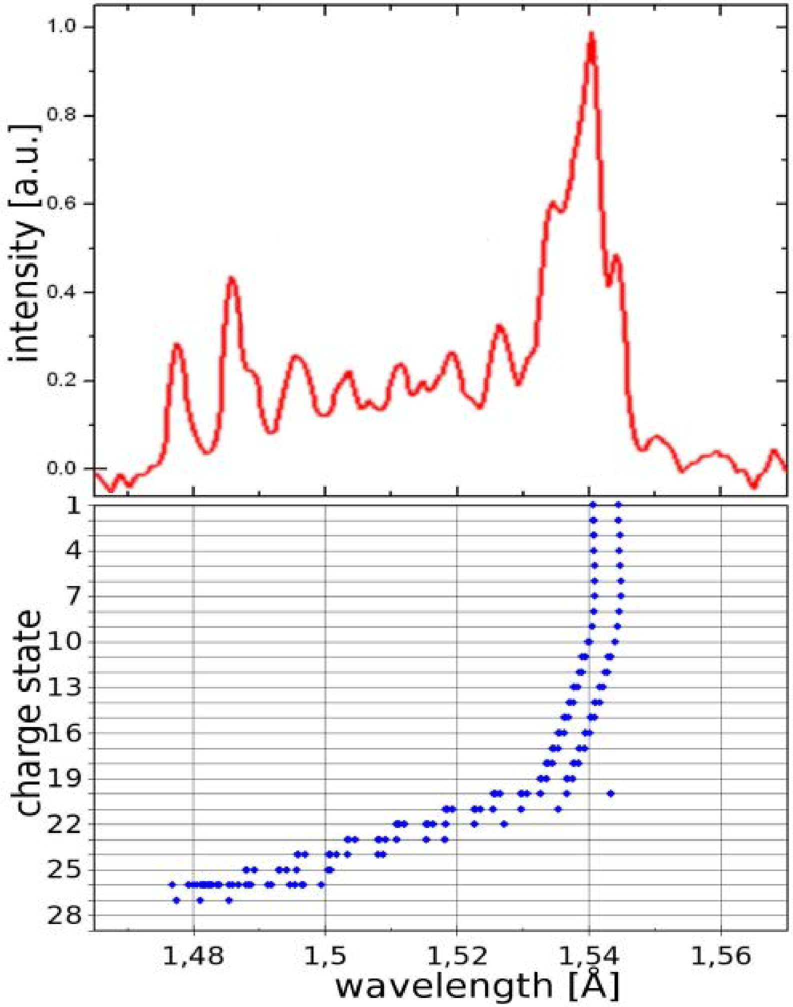
X-ray spectrometer



Experimental scenario



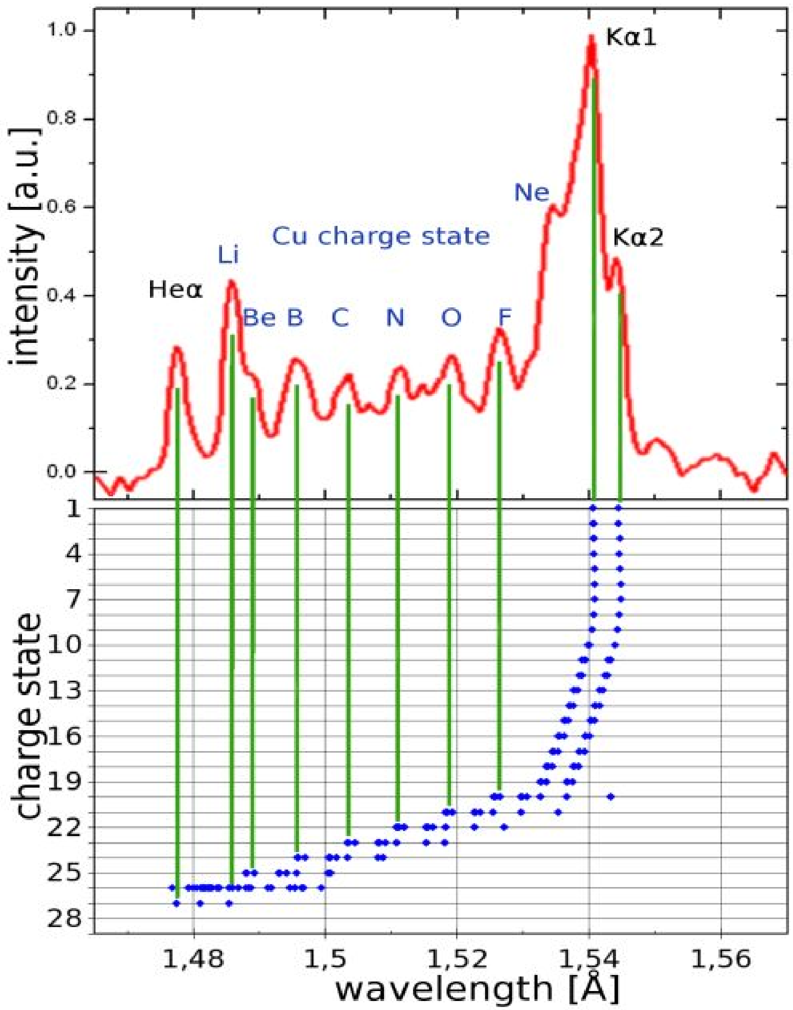
Theoretical spectral lines



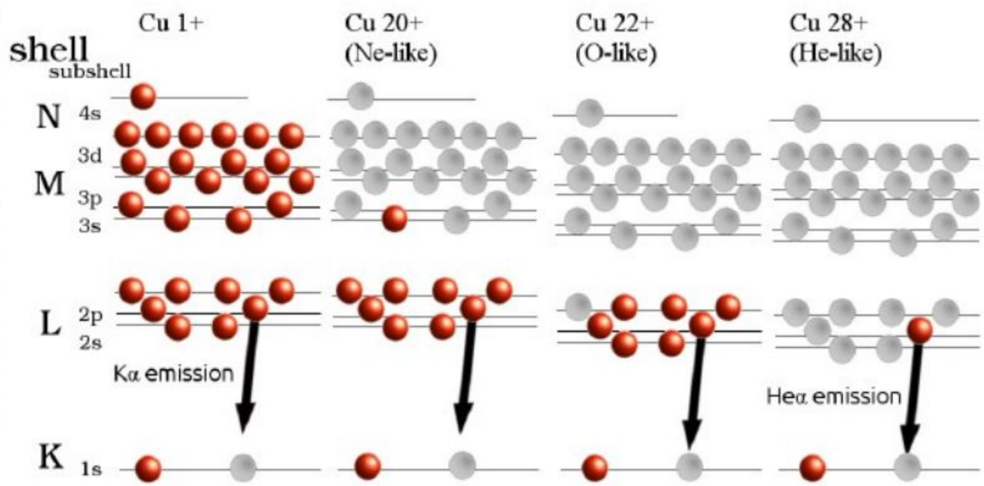
Experimental (1ω) spectra, averaged over 6 shots to reduce noise.

Spectral lines included in the Flychk Collisional-radiative model according to their wavelength and the charge state they originate in. All lines represents the **1s – 2p** transition!

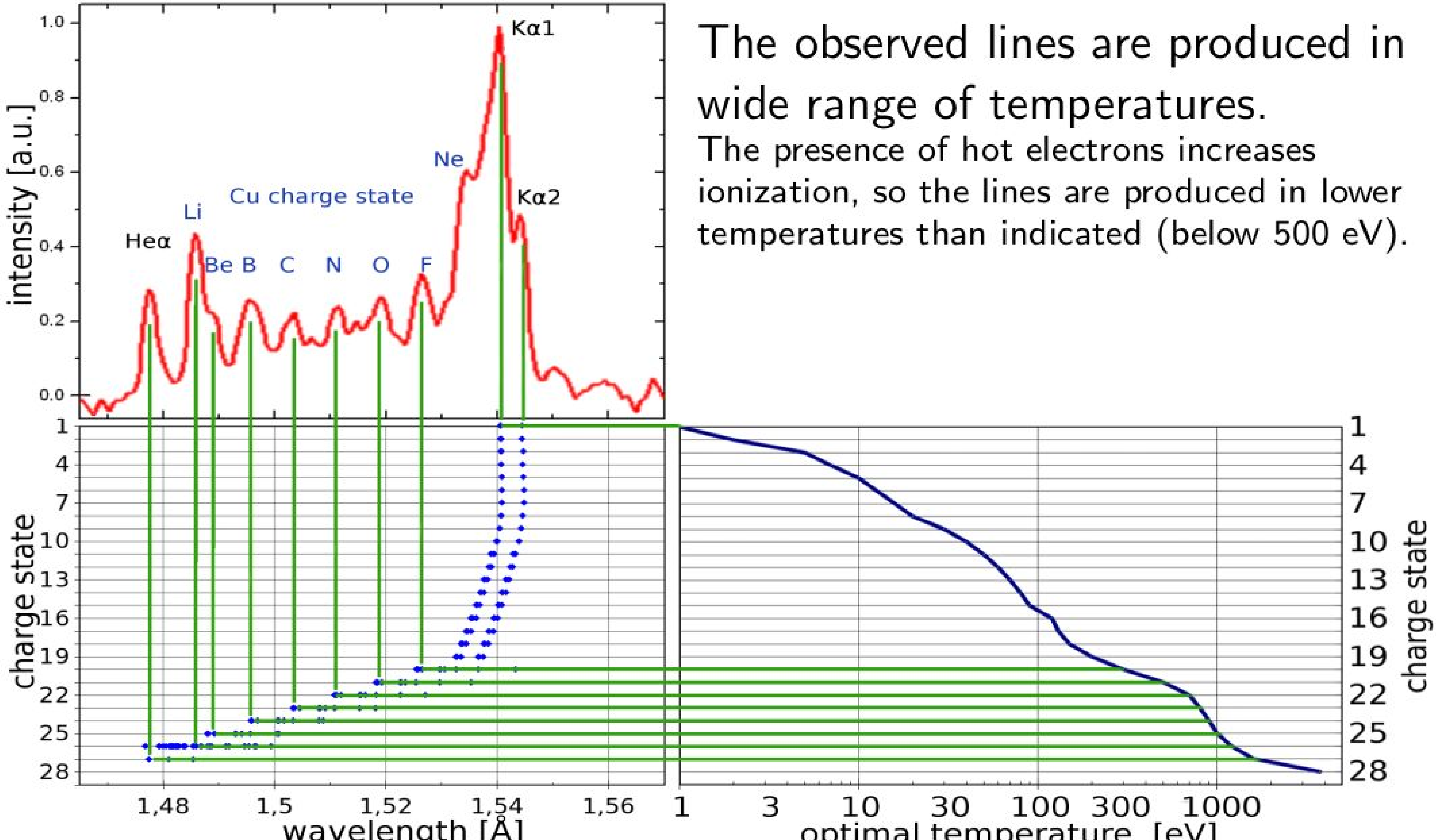
Theoretical spectral lines



Experimental (1ω) spectra, averaged over 6 shots to reduce noise.



Theoretical spectral lines



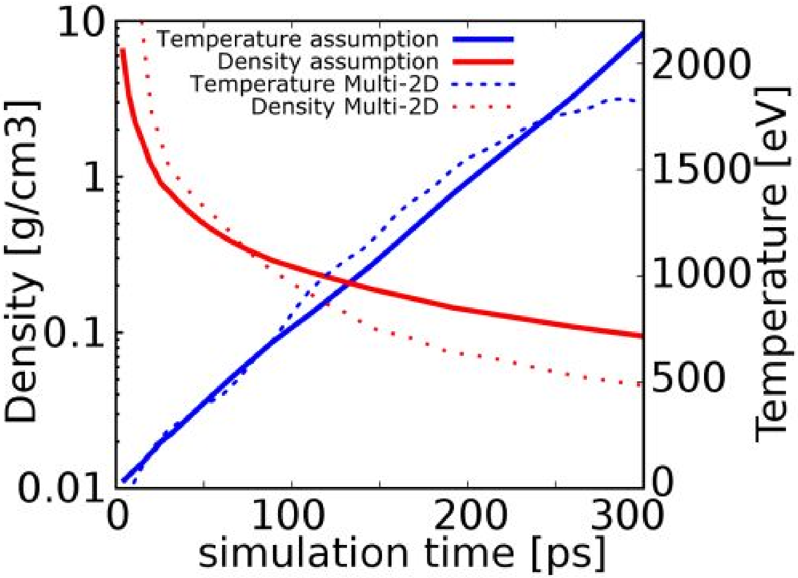
The observed lines are produced in wide range of temperatures.

The presence of hot electrons increases ionization, so the lines are produced in lower temperatures than indicated (below 500 eV).

Model assumptions

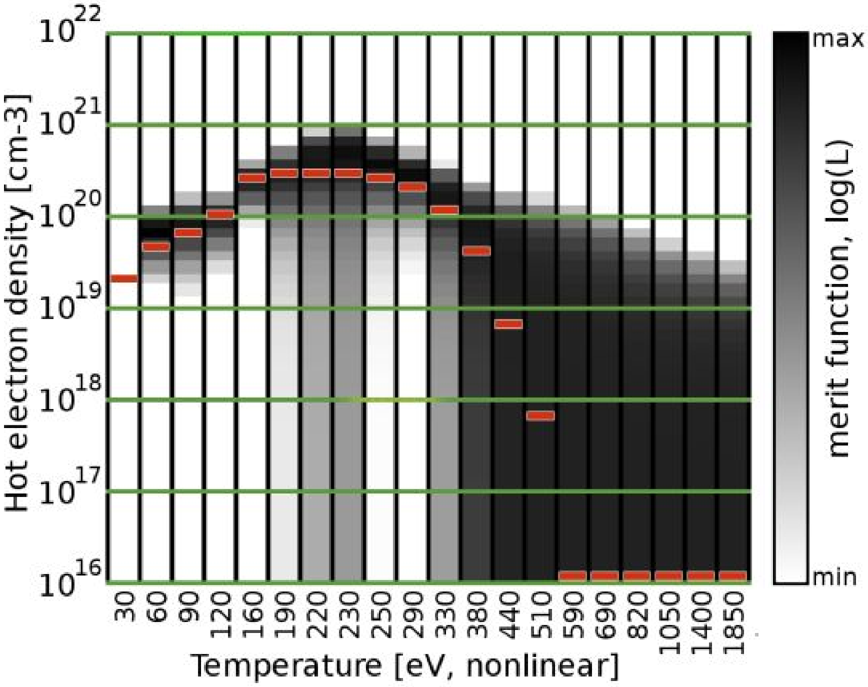
- Usual evaluation - comparing with single–parameter synthetic spectrum - is not possible.
- Attempt to make the most simple suitable model:

- Single-cell with **temporal** evolution.
- Temperature **linearly** increasing
- Density decrease according to an **isobaric expansion**.
- good agreement with Multi-2D hydrodynamics.
- $T_{he} = 100\text{keV}, p = 100\text{Mbar}$



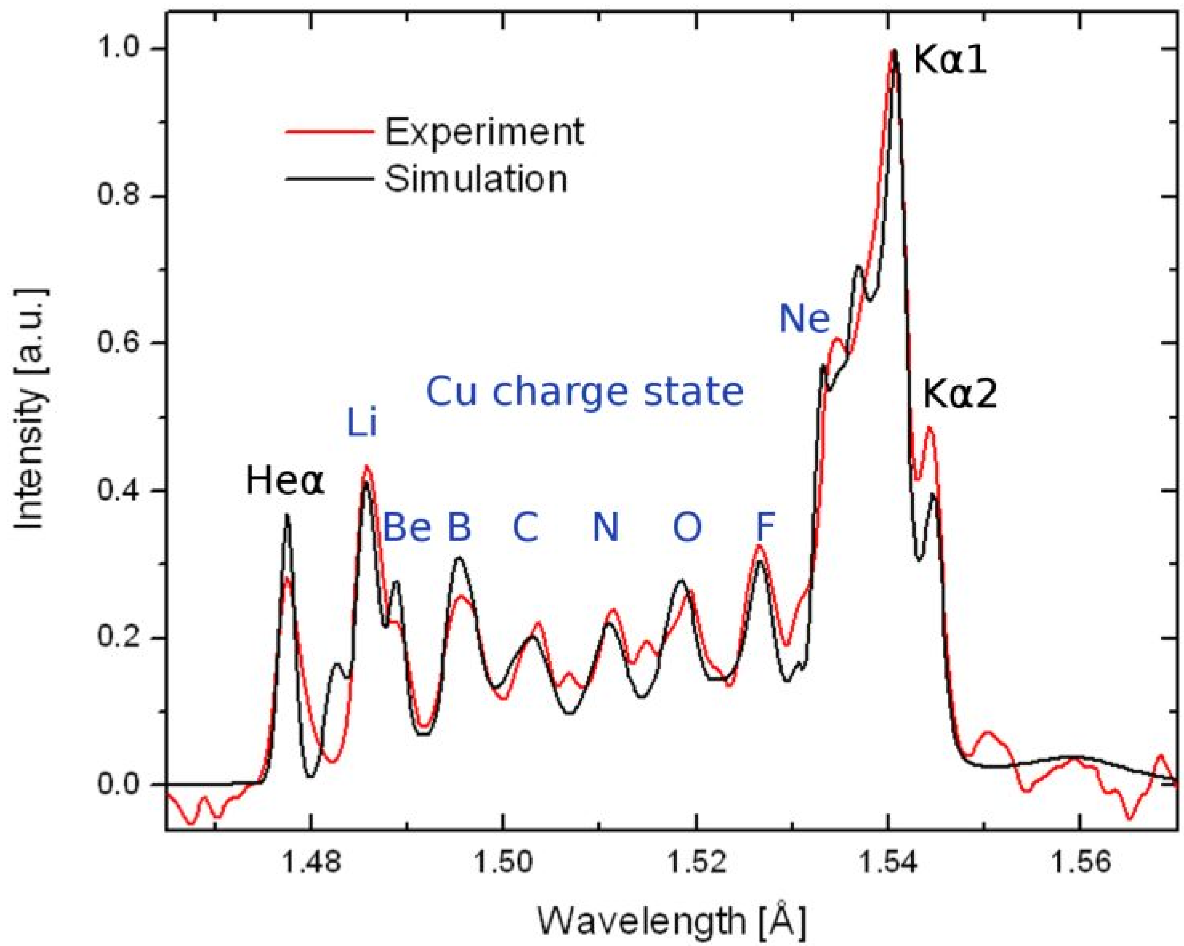
Fitting

- Time–evolution split into ≈ 20 *points*.
- For each point, set of spectra were calculated by *Flychk* for T and ρ given by the model, and $n_{\rm he}$ varied $10^{16} \div 10^{22}$ cm^{-3}.

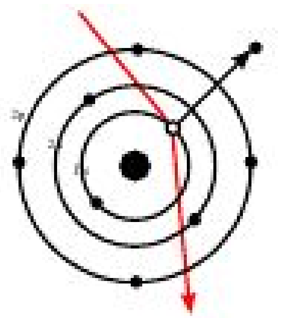


- Iterative fitting algorithm varies the $n_{\rm he}$ evolution and searches the best agreement between the experimental and theoretical spectra.

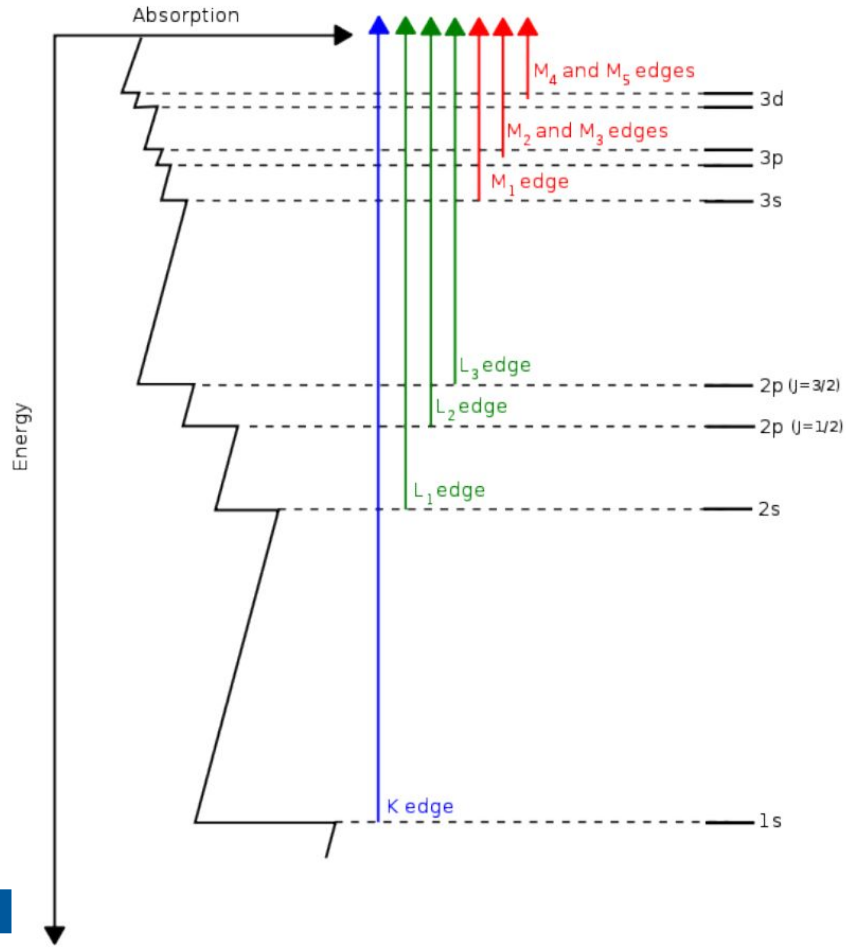
Fitted spectra (7900 ÷ 8460 eV)

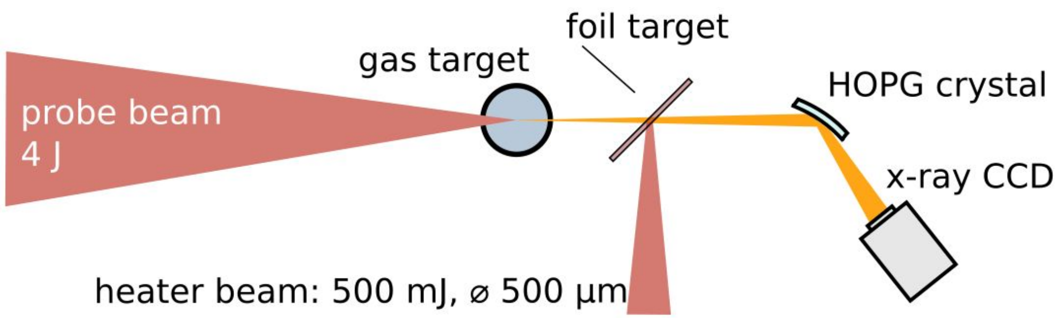


4. Absorption spectroscopy

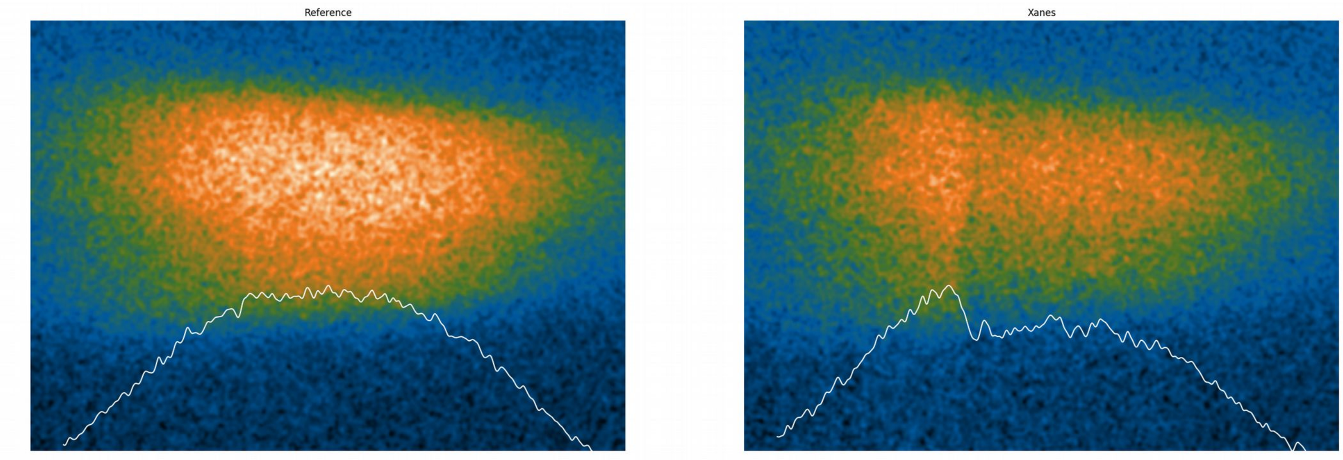


- All experiment above were based on *spontaneous radiative deexcitation*.
- If plasma is not that hot (<1 mil °C), this self-emission is not strong (plasma emits in softer x-rays which might not escape its volume.
- Absorption spectroscopy: We use a backlighter and probe *photo ionization* or *photo excitation*
- More complicated in experiment, but better control.
- Possible temporal resolution: *pump probe* setup

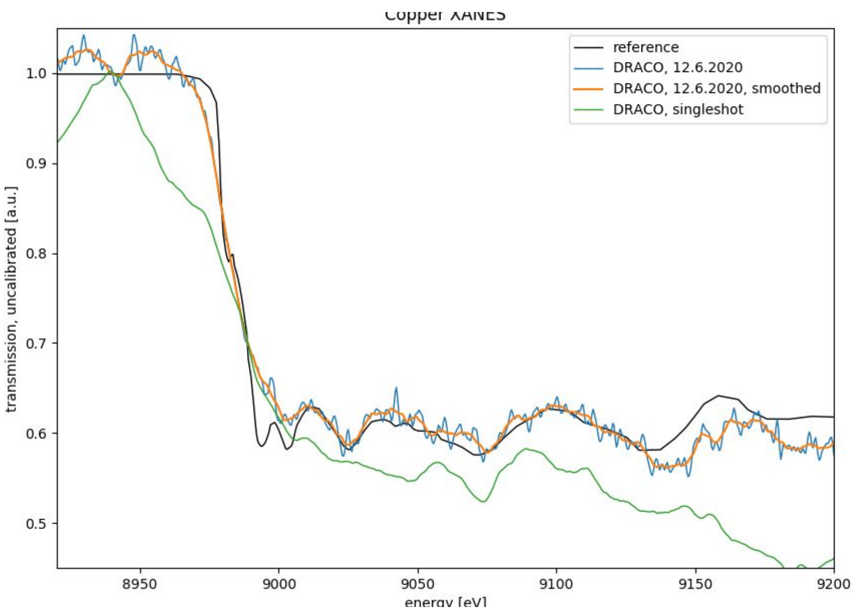




4. Absorption spectroscopy



- The raw measured spectra without (left) and with (right) the copper target.
- Dispersion direction is horizontal, energy increasing towards right.
- Right figure shows the appearance of the edge.



- XANES spectra measured in the laser experiment (orange) are agreeing to the theoretical reference.
- The waves between 9000 and 9200 eV are corresponding to the ionic structure of the matter.

Summary

- Collisional Radiative model provides view of what happens in plasmas on atomic level.
- Spectroscopy provides deep view into atomic physics of plasmas, but also shows the basic plasma properties.
- Due to high temperatures of plasmas, most interesting spectroscopy is in soft x-ray regime.
- X-ray spectroscopy is relatively ‚easy’ to measure, but pretty difficult do correctly evaluate

Most used references:

- M.Šmíd, PhD thesis (not really online, available upon request) and master thesis (https://physics.fjfi.cvut.cz/publications/FTTF/DP_Michal_Smid.pdf)
- D.Salzmann: Atomic Physics in Hot Plasmas, ISBN: 0195355156
- some pictures from Wikipediea...

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