MODELS OF LINE EMISSION FROM HIGH-PARAMETER PLASMAS

J. Limpouch

Czech Technical University in Prague,
Faculty of Nuclear Sciences and Physical Engineering,
Břehová 7, 115 19 Prague

(using contributions by A.A. Andreev, A.B. Iskakov, E.M. Ivanov, L. Kocbach, P.A. Loboda, V.V. Popova, Z. Roubíček, G.A. Vergunova)

Prepared for seminar "Pulse Plasma Systems - Modeling and Measurements" at CTU Prague, October 29, 2001

Aim of the presentation

- Introduction to line emission simulations
- Presentation of suite of codes developed
- Examples of results

Applications of line emission

- Diagnostics applications
  - Measurements of plasma density, electron temperature
  - Line ratios
  - Line forms
- Plasma as intense source of quasimonochromatic emission
  - ultrashort x-ray pulses for pulse-probe material diagnostics
  - x-ray source for biologic imaging and for lithography

Plasma dynamics simulations

- Magnetohydrodynamics codes - 1D, 2D
- Hydrodynamics codes - 1D, 2D, (3D)
- plasma density, electron and ion temperature, average ion charge
- Fokker-Planck codes (+ electron distribution)
- (PIC codes - usually only low density and details)
- Atomic physics model - mostly not with spectroscopic precision
- Average atom approximation widely used, simplified collision-radiative model and other approaches also possible
- Radiation transport - typically multigroup diffusion - continuum, groups of lines for high Z

Atomic physics post-processors

- Based on assumption - line emission does not influence energy balance significantly

Post-processor problem formulation

- Ionization and excitation states populations coupled with radiative transfer
- Rate equations for populations

$$\begin{aligned}\frac{\mathrm{d}N_k}{\mathrm{d}t} + N_k\,\mathrm{div}\vec{u} &= \sum_l \left[-N_k A_{kl} + (B_{lk}N_l - B_{kl}N_k)\,\frac{4\pi}{c}\,\overline{J}_{kl}\right] + \\ &+ \sum_m \left[N_m A_{mk} - (B_{km}N_k - B_{mk}N_m)\,\frac{4\pi}{c}\,\overline{J}_{mk}\right] - \\ &- \sum_n C_{kn}(n_e,T_e)N_k + \sum_n C_{nk}(n_e,T_e)N_n\end{aligned}$$

- Line intensity $\overline{J}_{kl}$ is spectral intensity integrated over angle $\mu = \cos\theta$ and over absorption (emission) line profile Φ_ν^{kl}

$$\overline{J}_{kl} = \frac{1}{2}\int_{-1}^{1}\mathrm{d}\mu\,\int_0^\infty I_\nu(x,\mu)\;\Phi_\nu^{kl}(x,\mu)\;\mathrm{d}\nu$$

- Rate equation for electron concentration

$$\frac{\mathrm{d}n_e}{\mathrm{d}t} + n_e\,\mathrm{div}\vec{u} = \sum_{ioniz} C_{kn}(n_e,T_e)N_k - \sum_{recom} C_{kn}(n_e,T_e)N_k$$

- Equation of radiative transfer (written in planar 1D geometry)

$$\frac{1}{c}\,\frac{\partial I_\nu}{\partial t} + \mu\,\frac{\partial I_\nu}{\partial x} = j_\nu - k_\nu I_\nu\ ,$$

- Spectral emission and absorption coefficients j_ν and k_ν are written for kl transition (frequency ν_{kl})

$$\begin{aligned}j_\nu^{kl}(x,\mu) &= \frac{h\nu_{kl}}{4\pi}A_{kl}\,N_k(x)\,\Phi_\nu^{kl}(x,\mu)\\ k_\nu^{kl}(x,\mu) &= \frac{c^2}{8\pi\nu_{kl}^2}\,\frac{g_k}{g_l}\,A_{kl}\left(N_l(x) - \frac{g_l}{g_k}\,N_k(x)\right)\;\Phi_\nu^{kl}(x,\mu)\end{aligned}$$

  g_k is degeneracy of the level k

- Spectral emission and absorption coefficients for given ν - sum of lines and of continuum

Radiative transfer simulation

- Populations may be solved without radiative transfer in 2 limiting cases
  - optical thin populations - $I_\nu = 0$
  - LTE populations - $I_\nu = S_\nu$ - blackbody radiation
- Radiative transfer - long studied in astrophysics - often diffusive transfer
- Laboratory plasmas differ from astrophysical plasmas
  - Often optically thin for continuum emission (free-free and free-bound transitions)
  - Many bound-bound are collisionally dominated (radiative transfer does not influence populations)
  - Often only several intense lines must be taken into account when radiative transfer is solved
  - density effects
  - inhomogeneity and expansion (macroscopic Doppler shift)
- Applied methods
  - ETLA (equivalent two-level atom) - *static, homogeneous plasmas, convergence problems*
  - Escape factors - *derived for large optical depths, no macroscopic Doppler shift*
  - Sobolev escape factors - macroscopic Doppler shift included, but only Doppler line profile possible
  - Linearization with respect to radiation fields - *linear system of dimension K (number of levels) $\times$ N (number of spatial points), fine for a few levels*
  - Peyrusse (1992) method - breaks iteration into two steps - iterates populations including radiative transfer only inside one cell and and then solves radiative transfer in space with given populations

Atomic physics models

- Various types of models constructed according to the purpose
- K-shell spectroscopy (detailed for H-, He- and Li- like ions)
- X-ray lasers (collisionally excited - Ne-like, Ni-like ions)
- models for high-Z ions (e.g. UTA model)
- models including excitation states of all ionization states (low Z - radiative energy transfer, diagnostics)

Code FLY - standard for K-shell spectroscopy

- developed by R.W. Lee, LLNL (R.W. Lee, J.T. Larsen, J.Q.S.R.T. **56**, 535 - 556.
- Commercially available (200 US$) - successor of RATION
- Stationary and non-stationary homogeneous plasmas ($Z = 3 - 26$)
- Finite optical thickness included
- Suite of three codes
  - FLY - populations of excitation states (only Doppler broadening - overestimates optical thickness)
  - FLYPAPER - visualization of FLY results, diagnostics (line ratios etc.)
  - FLYSPEC - spectrum synthesis (Stark broadening included for Ly-lines, Ba-lines, He-like transitions to ground state, Li-like transition to 2s and 2p states and corresponding recombination edges)

Atomic physics in K-shell postprocessor

Energetic levels

- **fully stripped**
- **H-like** – ground, excited 2 – 12
- **He-like** – ground $1s^2$, detailed excited $2\ ^3S$, $2\ ^3P$, $2\ ^1S$, $2\ ^1P$, lumped excited 3-9, autoionization 2l2l' (6 levels)
- **Li-like** – ground 2s, detailed excited 2p, 3s, 3p, 3d, lumped excited 4-9, autoionization 1s2l2l' (6 levels)

Limitation of number of excited states

- by input data
- by plasma density (ionization potential lowering)

Atomic transitions included

- Collisional ionization and three-body recombination
- Spontaneous radiative recombination
- Autoionization and dielectronic recombination
- Collisional excitation and deexcitation
- Spontaneous photo-deexcitation
- Photo-excitation and stimulated photo-deexcitation for optically thick lines

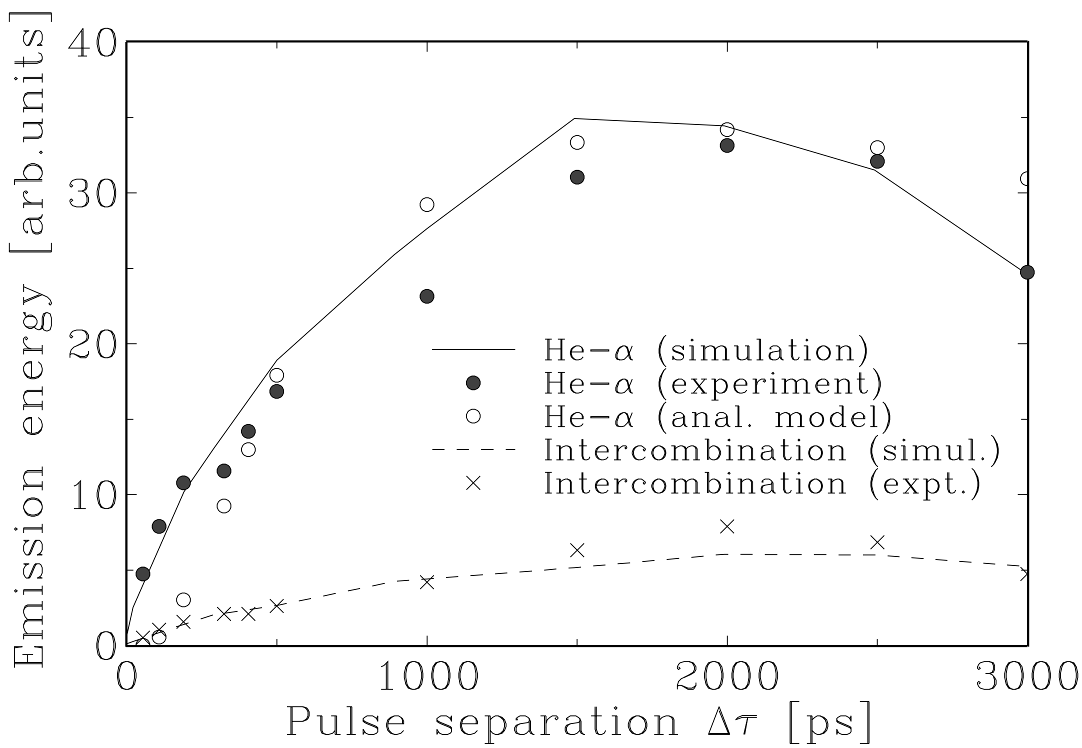
Developed atomic physics postprocessor

- Postprocessor to 1D planar Lagrangian codes
- Bulk Doppler shift makes geometry acceptable even for relatively narrow focal spots
- Atomic physics database developed for Aluminum
- Maxwellian electron distribution assumed
- Radiative transfer is solved together with populations only for potentially optically thick lines
- Fully implicit differencing is used for time discretization
- Voigt line profiles previously used, now sophisticated profiles are implemented - talk by L. Kocbach
- Core saturation method used for line transfer

Suite of 3 codes

- PLANPOP – calculates populations including impact of line transfer
- PLANSP – synthesis of spectra emitted from planar plasma
- SIDESP – synthesis of spectra emitted in lateral directions (suited for dot target experiments)

The energy emitted in He-α and intercombination lines versus pulse separation Δ



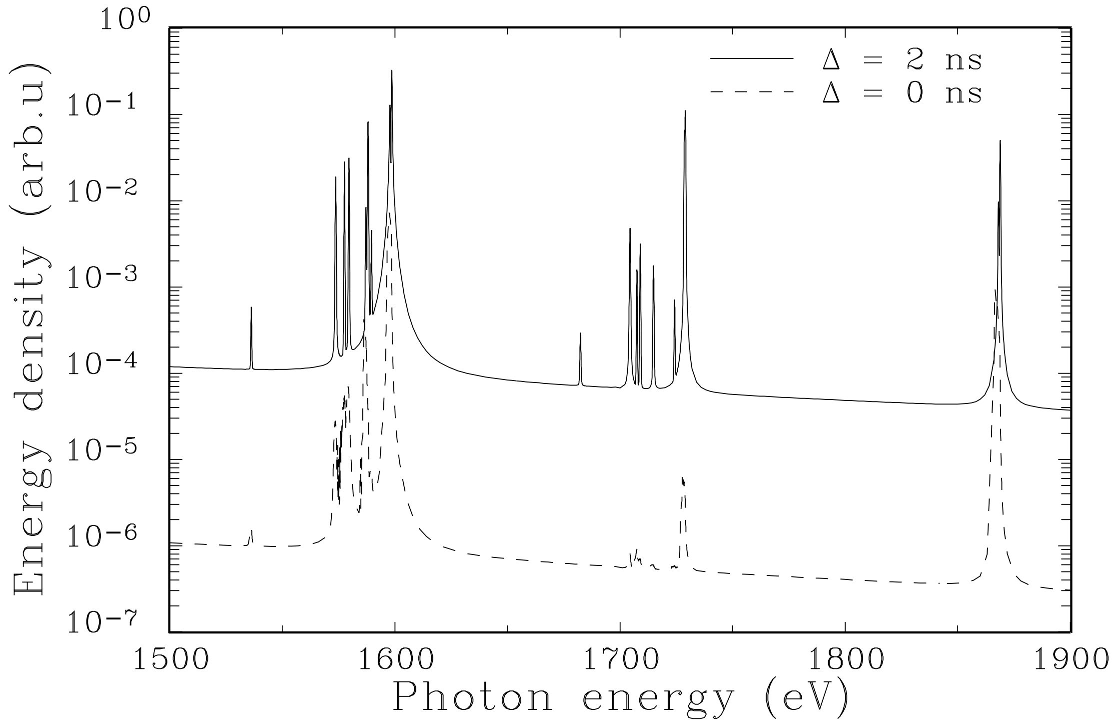
Parameters

$\lambda = 790$ nm	$\tau_{FWHM} = 100$ fs
$I_{main} = 2.3 \times 10^{16}$ W/cm^2	$I_{prepulse} = 10^{15}$ W/cm^2
Al target, normal incidence	observation angle 45°

Calculated K-shell spectra

pulse separation $\Delta = 0$ ns, $\Delta = 2$ ns

(He-α, Ly-α, He-β lines)



Simulation parameters

$\lambda = 790$ nm

$\tau_{FWHM} = 100$ fs

$I_{main} = 2.3 \times 10^{16}$ W/cm^2

$I_{prepulse} = 10^{15}$ W/cm^2

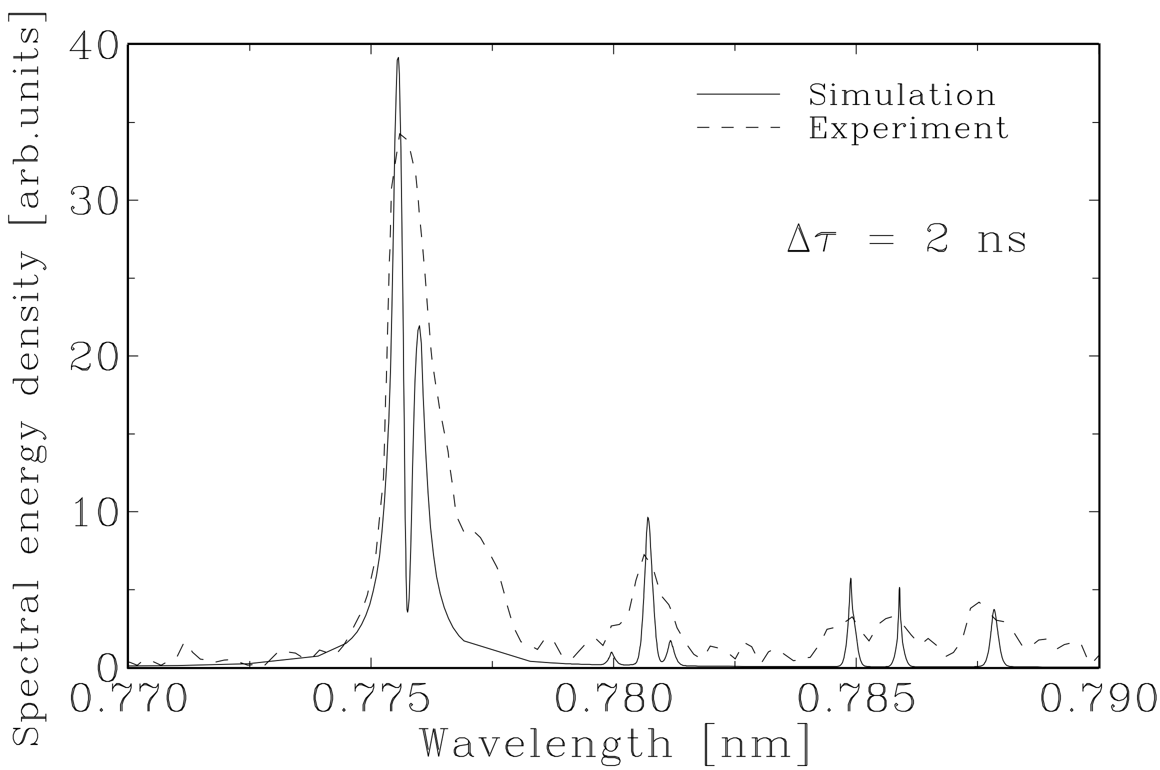
Al target

Normally incident laser

K-α lines not included in model

Experimental and simulation spectra near He-α line

(pulse separation $\Delta = 2$ ns)



Experimental parameters

$\lambda = 790$ nm

$\tau_{FWHM} = 100$ fs

$I_{main} = 2.3 \times 10^{16}$ W/cm^2

$I_{prepulse} = 10^{15}$ W/cm^2

Al target

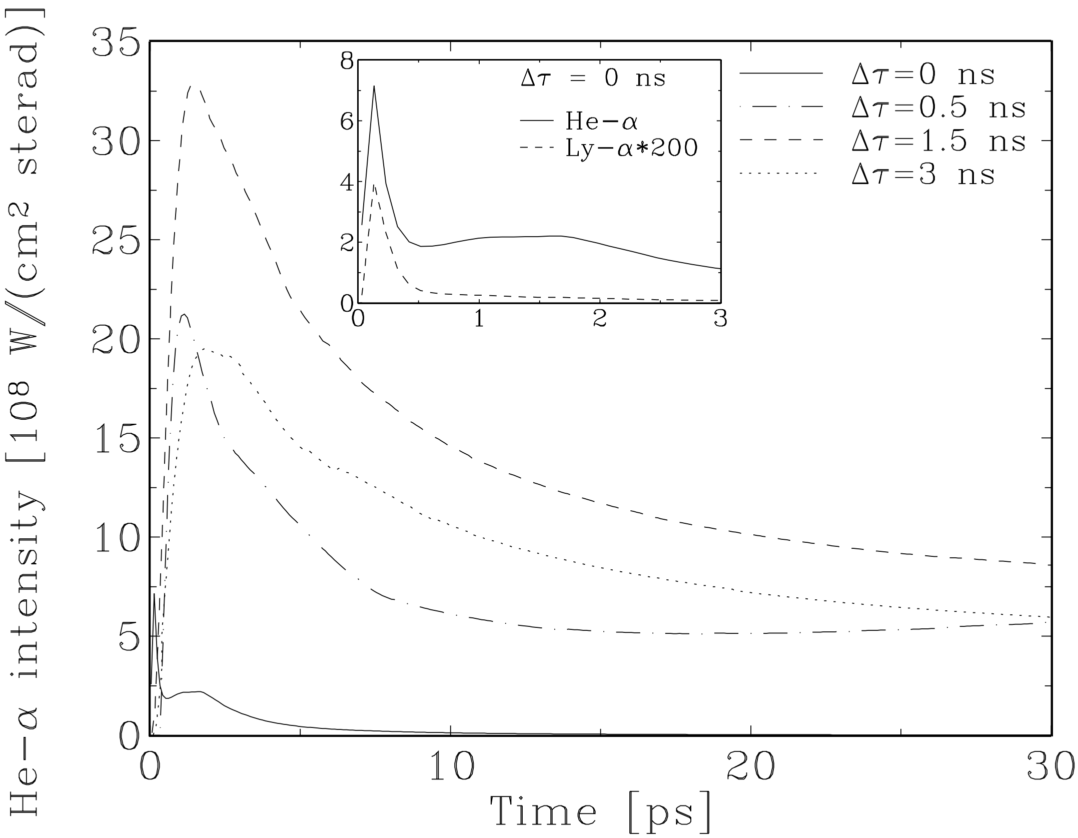
Normally incident laser

Focal diameter – 30 μm

Contrast $> 10^6$ in intensity

Temporal profiles of He-α emission

(for various pulse separations Δ)



Time measured from main pulse maximum

Simulation parameters

$\lambda = 790$ nm

$\tau_{FWHM} = 100$ fs

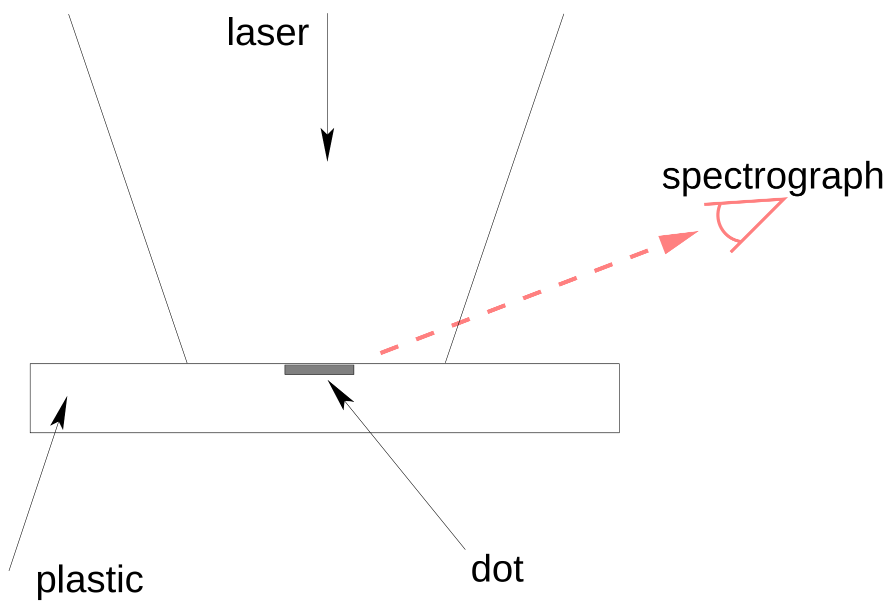
$I_{main} = 2.3 \times 10^{16}$ W/cm^2

$I_{prepulse} = 10^{15}$ W/cm^2

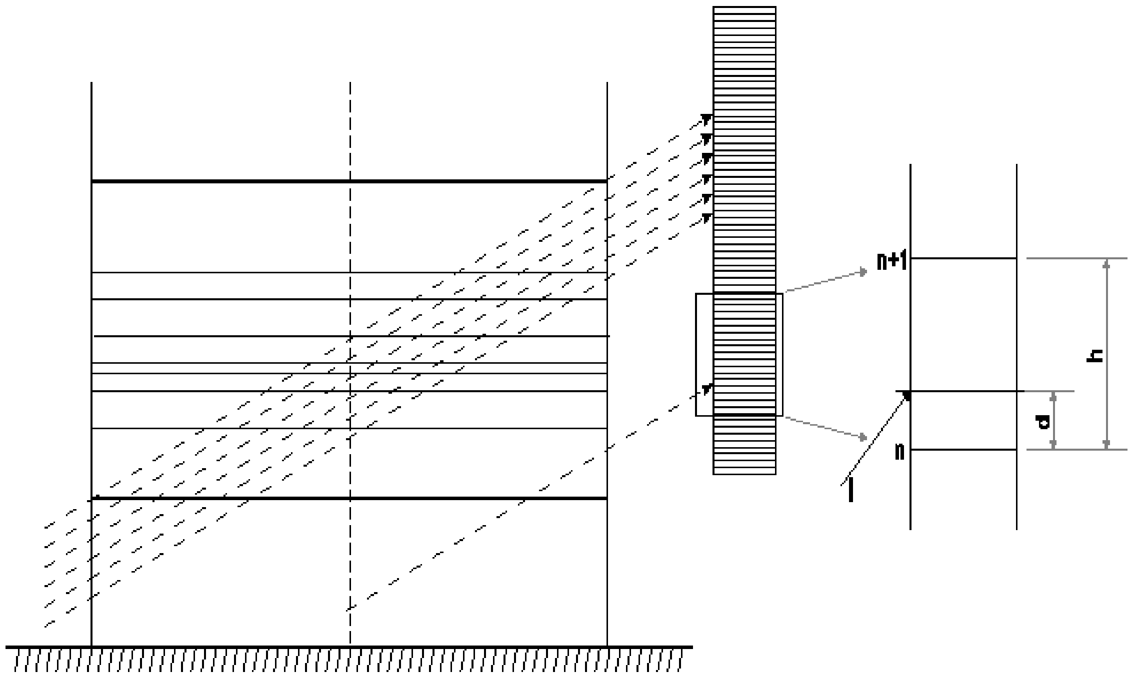
Al target

Normally incident laser

Scheme of dot target experiment



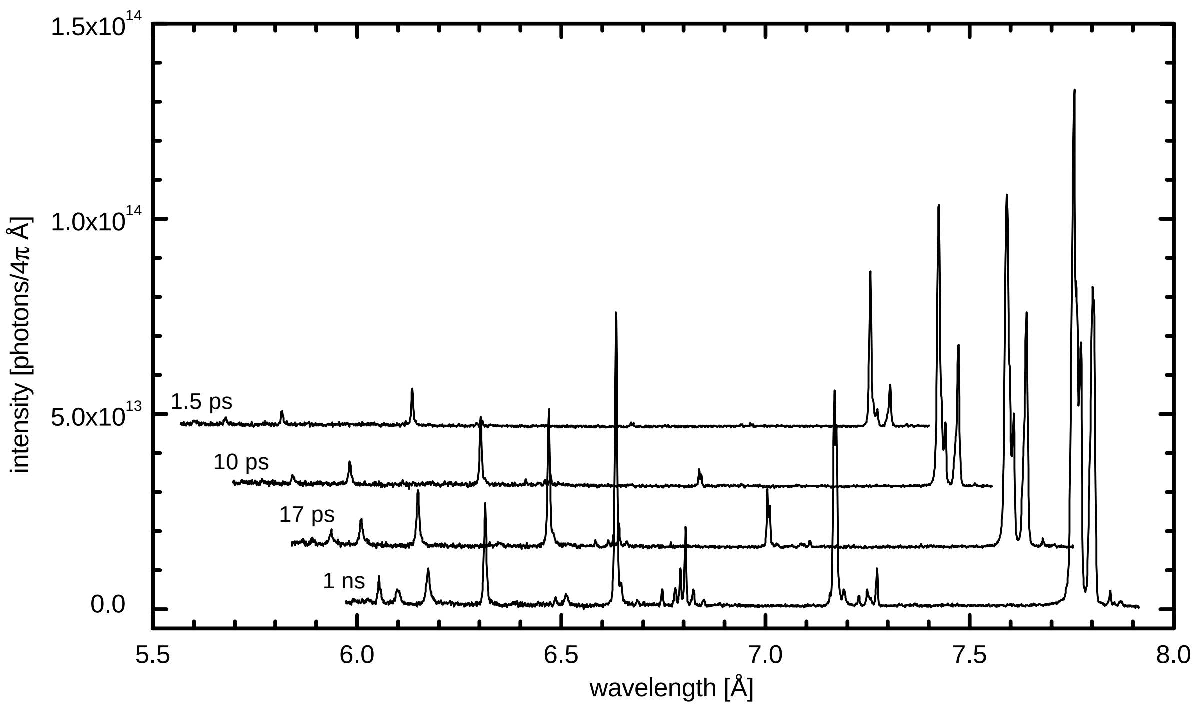
Scheme of side view spectra calculation



target

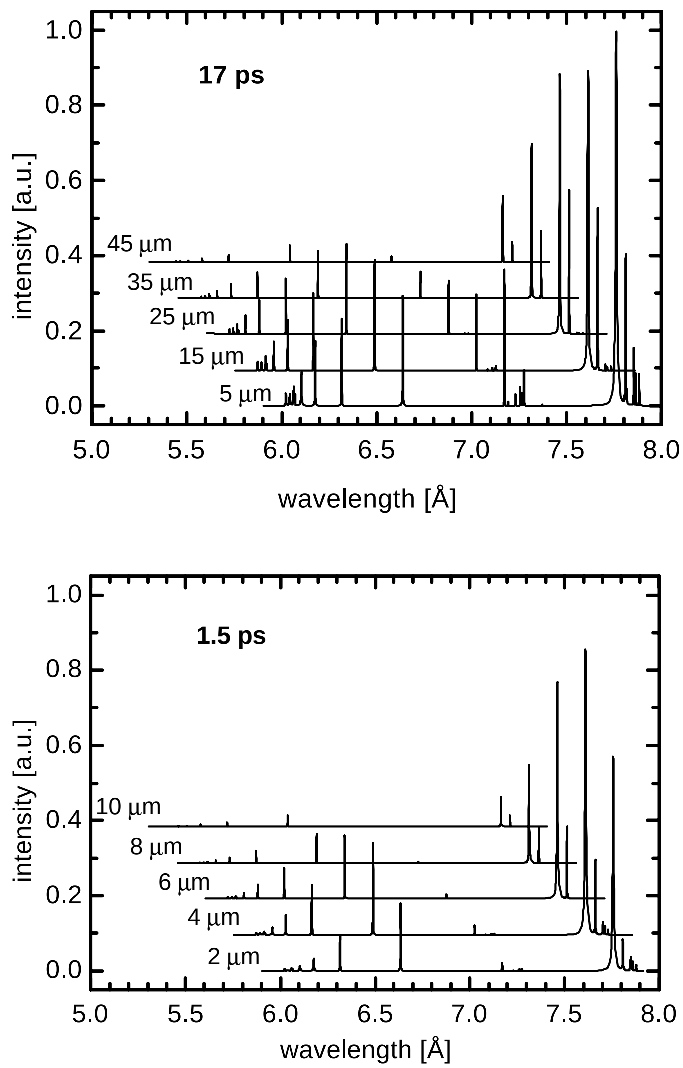
- Emission integrated along rays
- X-ray refraction assumed negligible
- Ray positions selected dynamically (associated with Lagrangian grid)
- Time integration – emission interpolated onto a static grid

Spectra measured at angle 12.5° from the target plane



Nd-laser, $E \simeq 4.5J$,
angle of incidence 45°,
focal spot diameter $< 10\mu$m

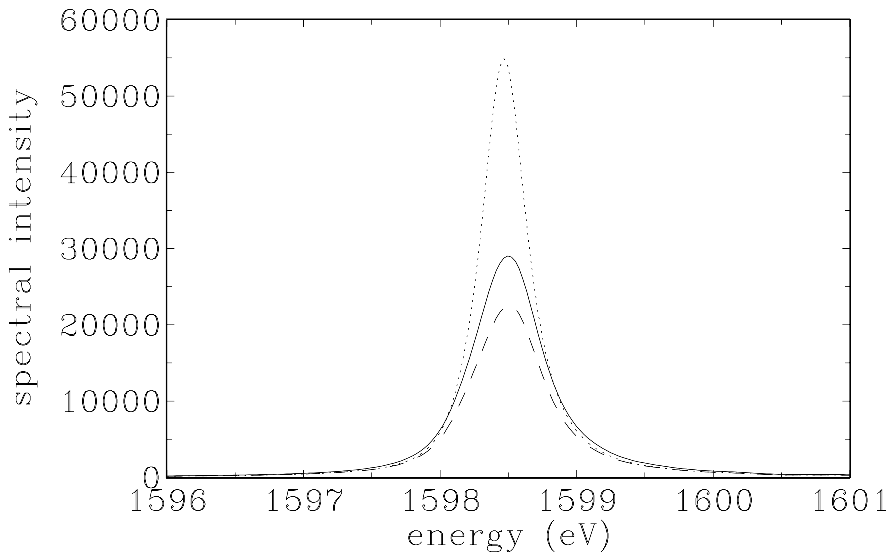
Spatially resolved time integrated synthetic spectra

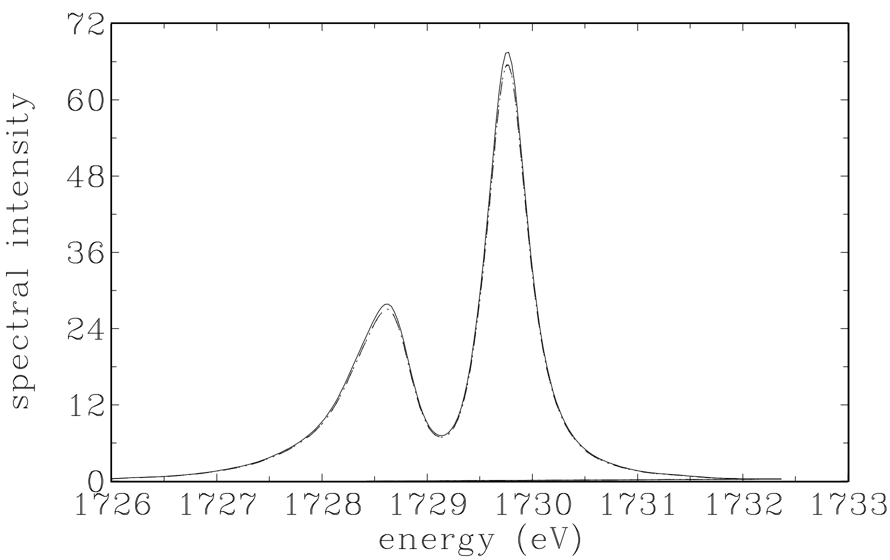


Nd-laser, $E \simeq 4.5J$,
angle of incidence 45°,
focal spot diameter $< 10\mu$m
angle of observation 12.5°

Calculations with precision line profiles

Examples of calculated emitted He-α and Ly-α lines, using precision emission line profiles (see contribution by L. Kocbach *et al.* http://www-troja.fjfi.cvut.cz/k412/en/events/pps01/docs/kocbach.pdf)





Conclusions

- Developed post-processor used for interpretation of short-pulse laser-target experiment
- Precision line shapes now being introduced - see contribution by L. Kocbach *et al.* - http://www-troja.fjfi.cvut.cz/k412/en/events/pps01/docs/kocbach.pdf
- Standard FLY code used for calculations of laser gain in capillary discharge
- Detailed kinetics code used for spectra of capillary discharge