Introduction to FLYCHK

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Joint ICTP-IAEA School on Atomic and Molecular Spectroscopy in Plasmas
Trieste, Italy

FLYCHK COLLISIONAL-RADIATIVE MODEL

Population Kinetics Modeling

Rate equations are solved for level population distributions for given plasma conditions

$$\frac{dn_i}{dt} = -n_i \sum_{j \neq i}^{N\max} W_{ij} + \sum_{j \neq i}^{N\max} n_j W_{ji}$$

$$W_{ij} = B_{ij}\overline{J_{ij}} + n_e C_{ij} + \beta_{ij} + n_e \gamma_{ij}$$

$$W_{ji} = A_{ij} + B_{ji}\overline{J_{ji}} + n_e D_{ji} + n_e(\alpha_{ji}^{RR} + \alpha_{ji}^{DR}) + n_e^2 \delta_{ij}$$

B_{ij} Stimulated absorption

C_{ij} Collisional excitation

γ_{ij} Collisional ionization

B_{ij} Photoionization (+st. recom)

A_{ij} Spontaneous emission

B_{ij} Stimulated emission

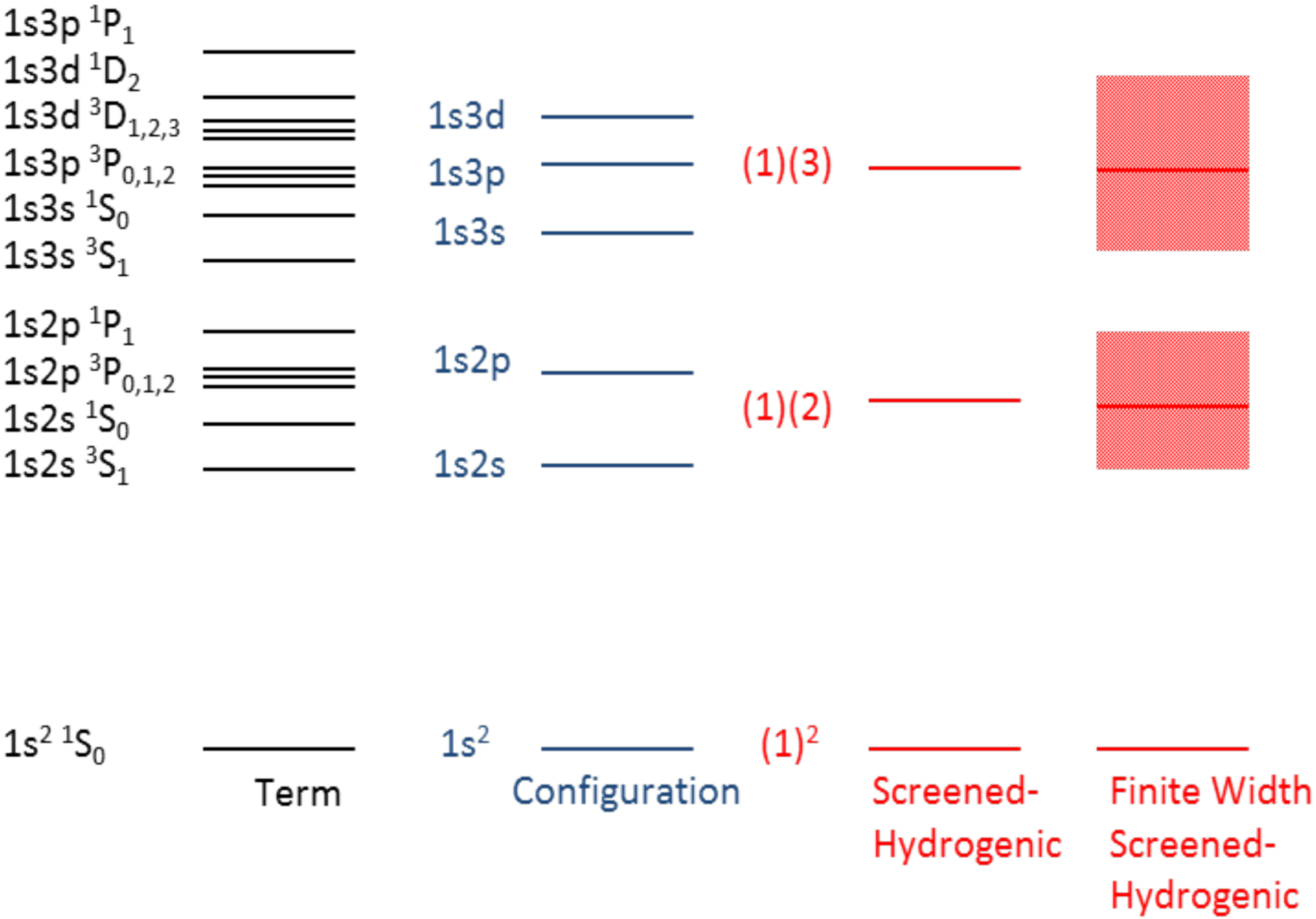
D_{ij} Collisional deexcitation

a_{ij}^{DR} Dielectronic recombination

a_{ij}^{RR} Radiative recombination

δ_{ij} Collisional recombination

FLYCHK uses screened hydrogenic levels (super configurations)



$1s3p\ ^1P_1$

$1s3d\ ^1D_2$

$1s3d\ ^3D_{1,2,3}$

$1s3p\ ^3P_{0,1,2}$

$1s3s\ ^1S_0$

$1s3s\ ^3S_1$

$1s2p\ ^1P_1$

$1s2p\ ^3P_{0,1,2}$

$1s2s\ ^1S_0$

$1s2s\ ^3S_1$

$1s^2\ ^1S_0$

Term

1s3d

1s3p

1s3s

1s2p

1s2s

$1s^2$

Configuration

(1)(3)

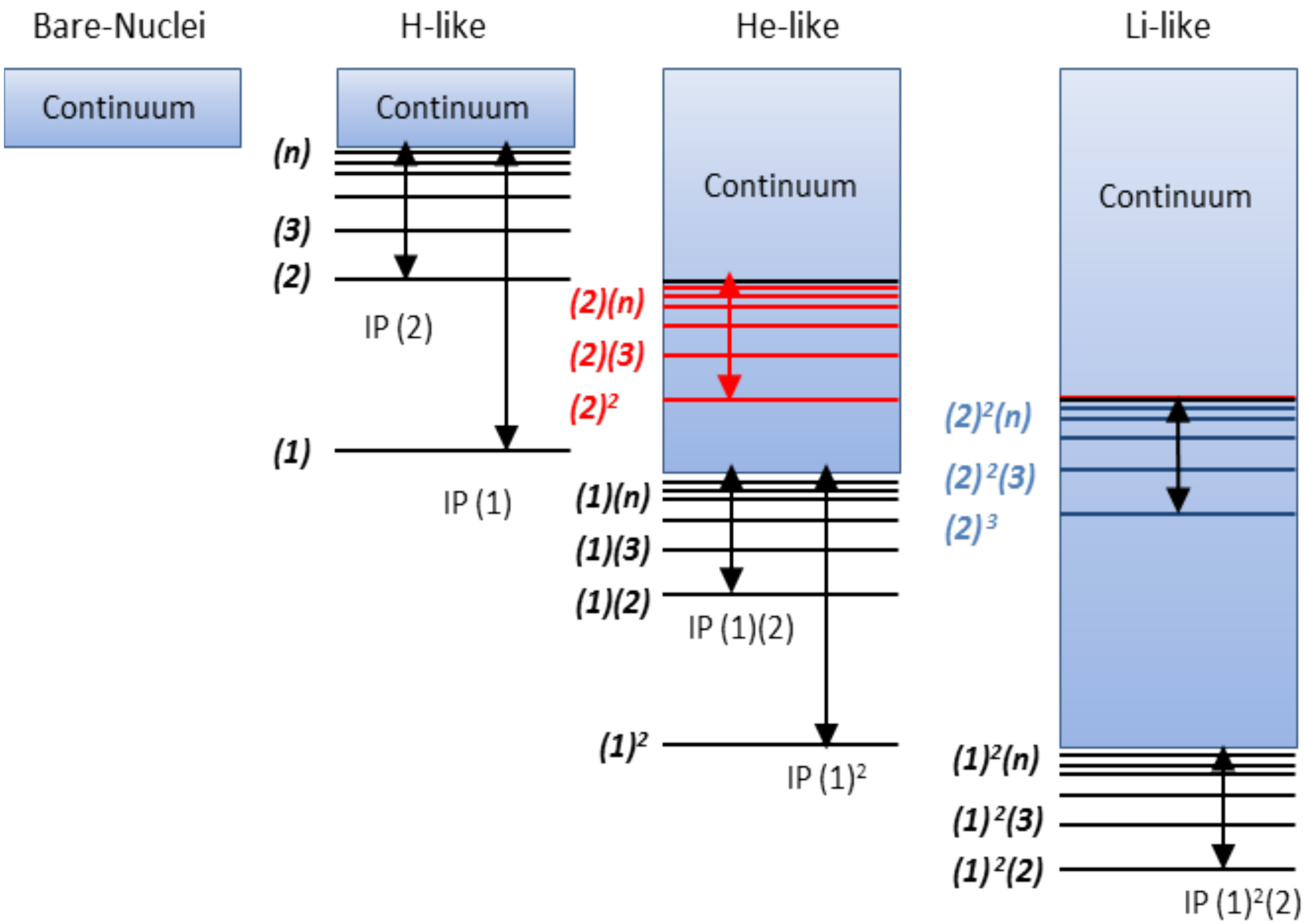
(1)(2)

$(1)^2$

Screened-Hydrogenic

Finite Width Screened-Hydrogenic

Level energy obtained with ionization potential from its 1st continuum level



Atomic processes included in FLYCHK

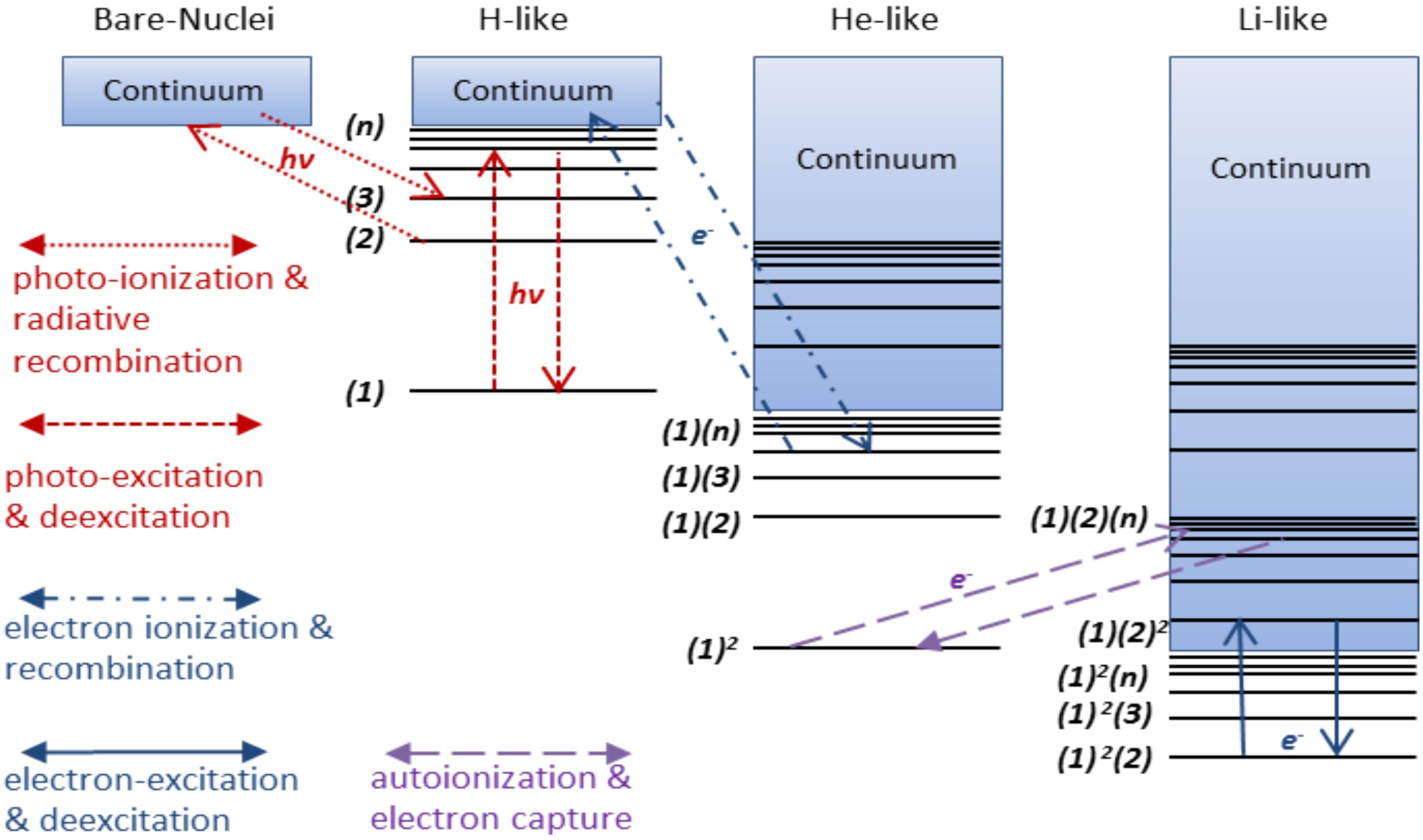


photo-ionization & radiative recombination

photo-excitation & deexcitation

electron ionization & recombination

electron-excitation & deexcitation

autoionization & electron capture

FLYCHK Model : *simple, but complete*

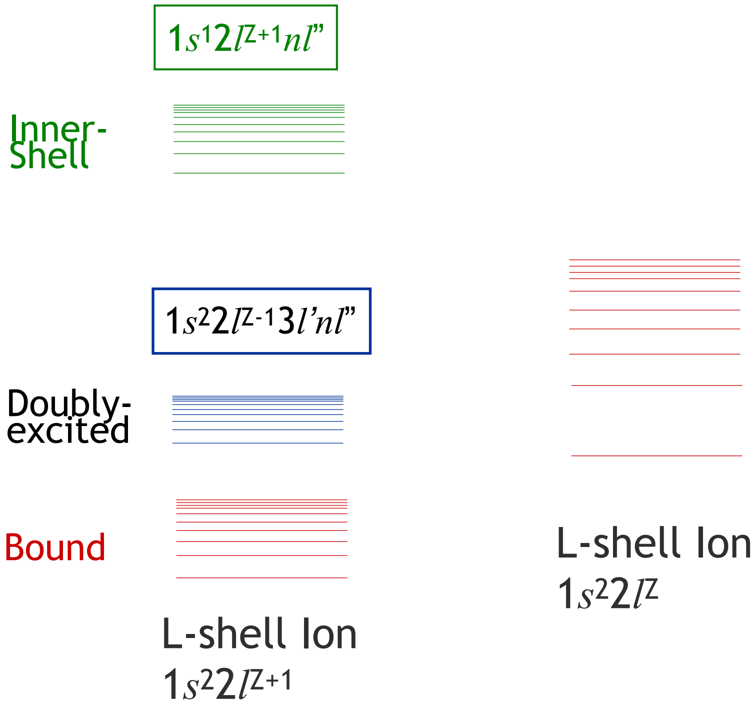
- Screened hydrogenic energy levels with relativistic corrections
- Relativistic Hartree-Slater oscillator strengths (M. Chen) and photoionization cross-sections (J. Scofield,+ Kramer)
- Fitted collisional cross-section to PWB approximation (M. Chen)
- Semi-empirical cross-sections for collisional ionization (A. Burgess)
- Detailed counting of autoionization and electron capture (M. Chen)
- Continuum lowering (Stewart-Pyatt, Ecker-Kroll)

Application to a wide range of Z & experiments:

Excitation autoionization (EA) /Dielectronic recombinationa (DR) processes are modeled with extensive inner-shell (IS) states

Low Z atom

Promotion of IS electrons leads to states far from continuum limit and *rarely matters in CSD* (charge state distribution)



$1s^{1}2l^{Z+1}nl''$

Inner-Shell

$1s^{2}2l^{Z-1}3l'nl''$

Doubly-excited

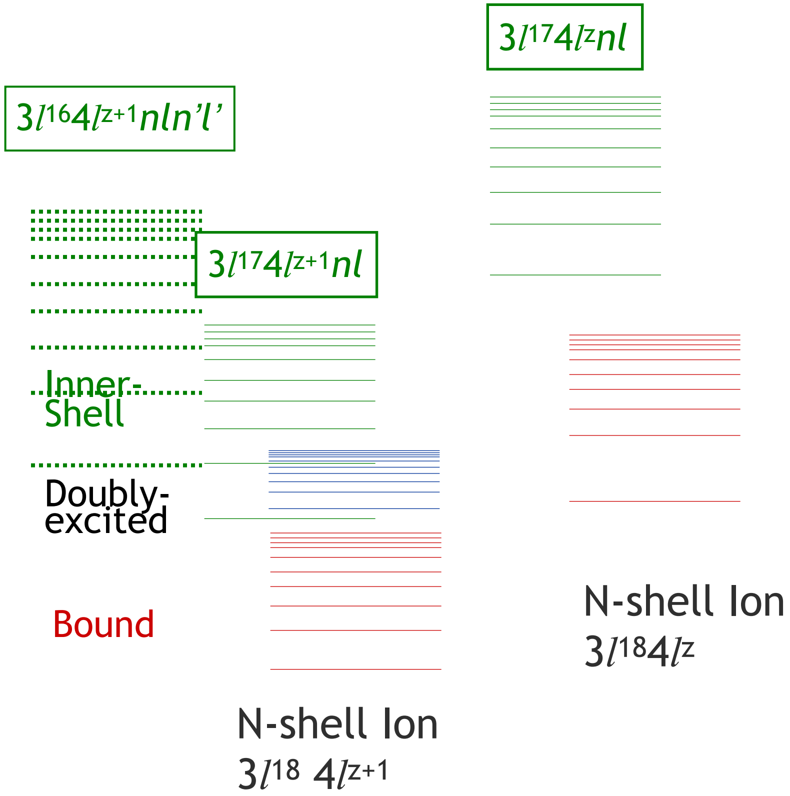
Bound

L-shell Ion
$1s^{2}2l^{Z+1}$

L-shell Ion
$1s^{2}2l^{Z}$

High Z atom

Promotion of IS electrons can lead to states near the continuum limit and hence EA/DR process is ***critical in CSD***



$3l^{17}4l^{z}nl$

$3l^{16}4l^{z+1}nln'l'$

$3l^{17}4l^{z+1}nl$

Inner-Shell

Doubly-excited

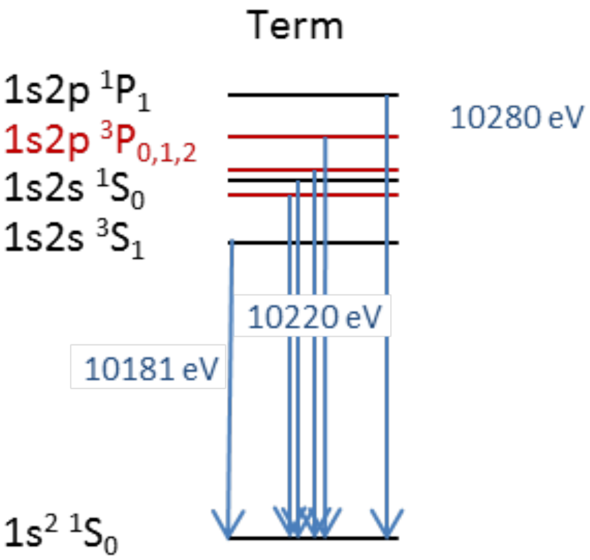
Bound

N-shell Ion
$3l^{18}\,4l^{z+1}$

N-shell Ion
$3l^{18}4l^{z}$

FLYSPEC SPECTROSCOPIC MODULE

FLYSPEC uses detailed (H, He, Li-like) and Super Transition Array for spectra


Term

$1s2p\ ^1P_1$

$1s2p\ ^3P_{0,1,2}$

$1s2s\ ^1S_0$

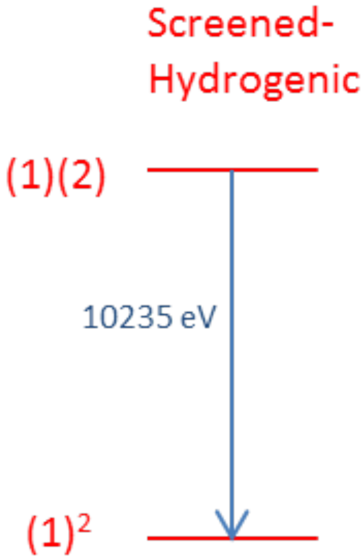
$1s2s\ ^3S_1$

$1s^2\ ^1S_0$

10280 eV

10220 eV

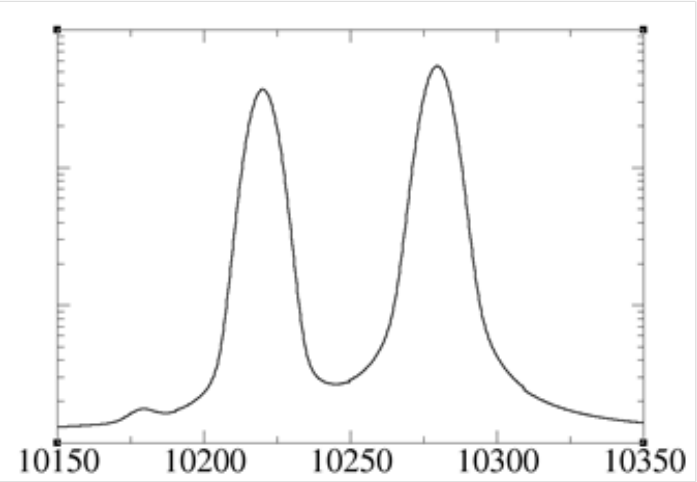
10181 eV

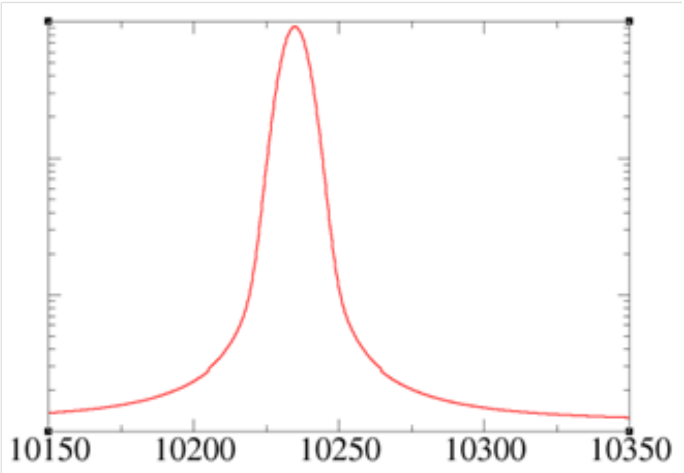

Screened-Hydrogenic

$(1)(2)$

$(1)^2$

10235 eV





Data Types for Spectroscopic Model

Z < 27 H, He and Li	FLY model
Z > 27 H, He and Li	HULLAC data (term levels up to n=4)
Be-like and lower charge states	Super Transition Array (STA) made with Configurations (jj) 1s, 2s, $2p^-$, $2p^+$, 3s, $3p^-$, $3p^+$, $3d^-$, $3d^+$, Up to n=6

Energy-dependent spectral intensity in the STA formalism

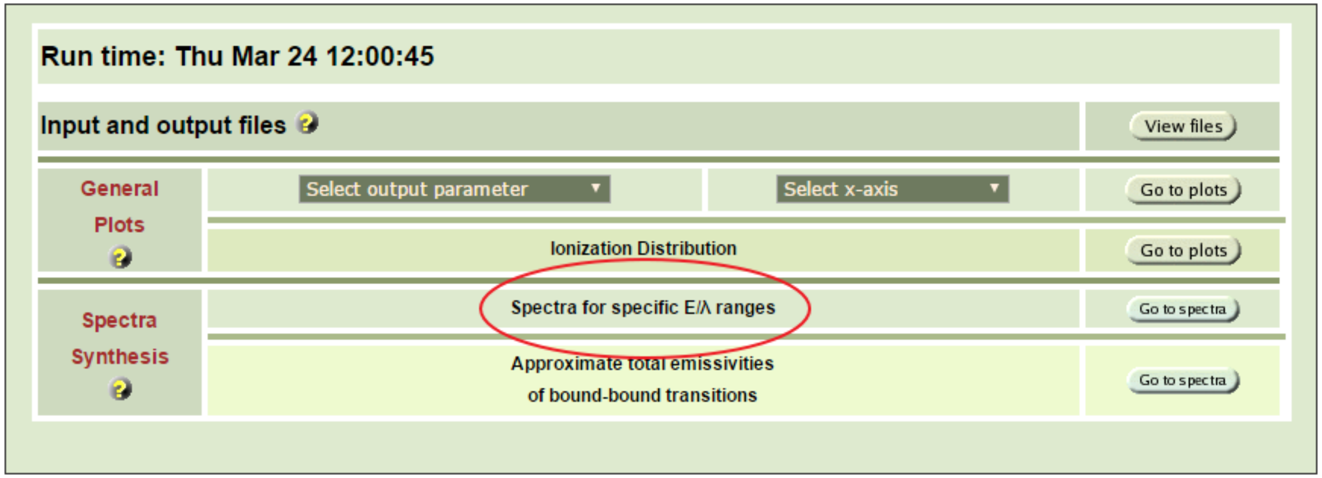
Spectra for specific E/ ranges: STA formalism

Spectra using configuration-average atomic data generated by the DHS (Dirac-Hartree-Slater) code (M.Chen)

$$\eta(\nu) = n_A A_{AB} E_{AB} \phi(\nu) = \frac{n_A \sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij} E_{ij} \phi(\nu)}{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e)}$$

[ergs/s/Hz/cm^3/ster]

$$A_{AB} = \frac{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij}}{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e)} \qquad E_{AB} = \frac{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij} E_{ij}}{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij}} \qquad \mu^2_{AB} = \left[\frac{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij} E^2_{ij}}{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij}} \right]^2 - E^2_{AB}$$



Run time: Thu Mar 24 12:00:45

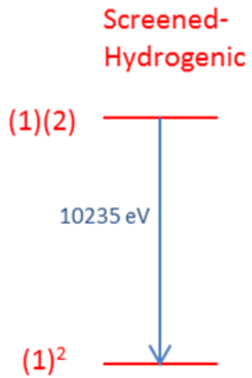
Input and output files

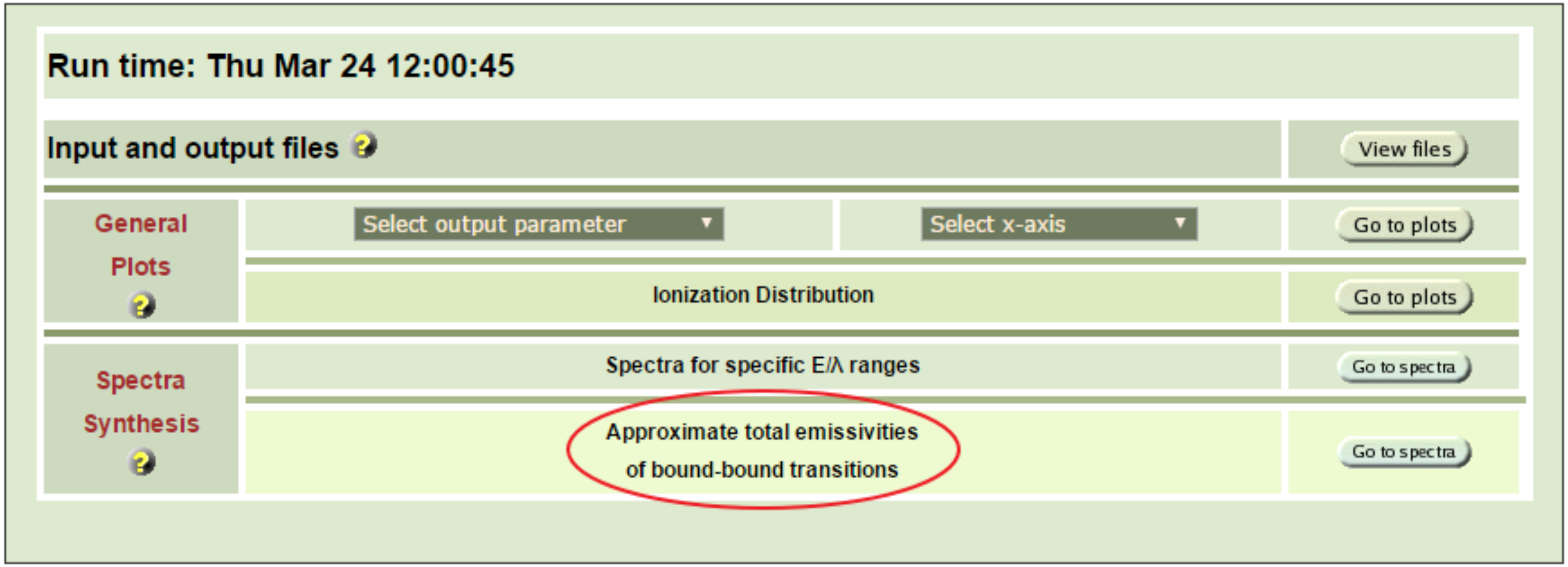
Total line emissivity in the STA formalism

Approximate total line emissivity:

A plot show approximate line emission spectra and provides information on energy range of dominant emission

$$S = n_u A_{ul} E_{ul} / N_e$$





Run time: Thu Mar 24 12:00:45

Input and output files

General Plots

Ionization Distribution

Spectra Synthesis

Spectra for specific E/Λ ranges

Approximate total emissivities of bound-bound transitions

FLYCHK APPLICATIONS

FLYCHK Help Pages

- http://nlte.nist.gov/FLY/Doc/Manual_FLYCHK_Nov08.pdf
- http://nlte.nist.gov/FLY/README.html
- http://nlte.nist.gov/FLY/EXAMPLE.html
- Click on the Question Marks
  - http://nlte.nist.gov/FLY/Help/runfile.html
  - http://nlte.nist.gov/FLY/Help/opacity.html

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Available to the community at password-protected NIST website: http://nlte.nist.gov/FLY

Advantages: simplicity and versatility→ applicability

- <Z> for fixed any densities: electron, ion or mass
- Mixture-supplied electrons (eg: Argon-doped hydrogen plasmas)
- External ionizing sources : a radiation field or an electron beam.
- Multiple electron temperatures or arbitrary electron energy distributions
- Optical depth effects

Outputs: population kinetics code and spectral synthesis

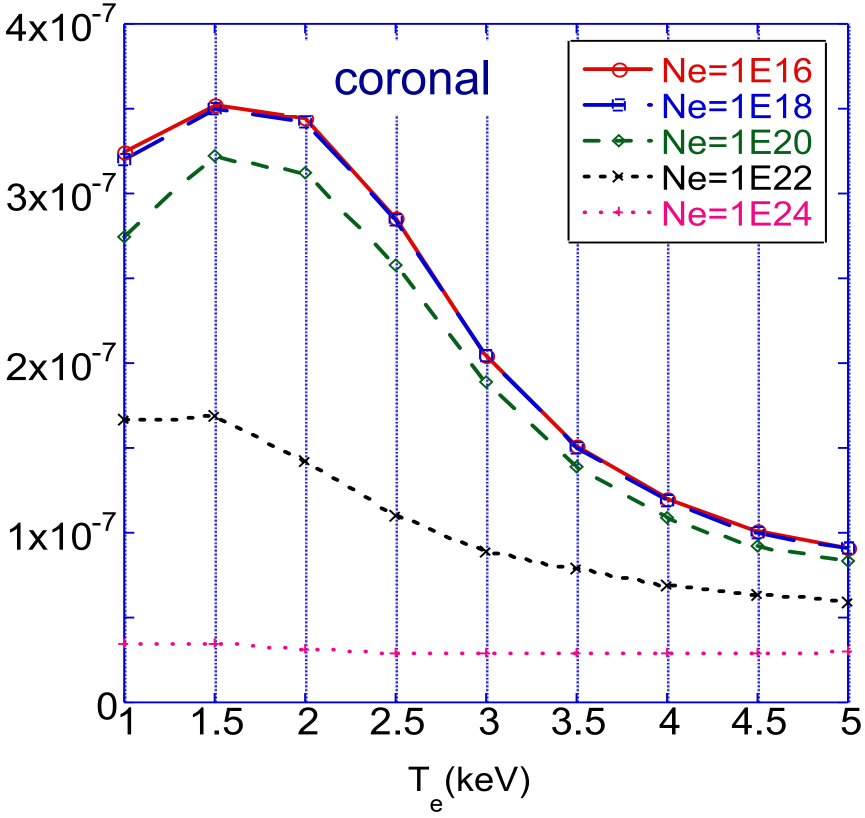
- <Z> and charge state distribution
- Radiative Power Loss rates under optically thin assumption
- Energy-dependent spectral intensity of uniform plasma with a size

Caveats: simple atomic structures and uniform plasma approximation

- Less accurate spectral intensities for non-K-shell lines
- Less accurate for low electron densities and for LTE plasmas
- When spatial gradients and the radiation transport affect population significantly

Example: Radiative loss rates are important as an energy loss mechanism of high-Z plasmas

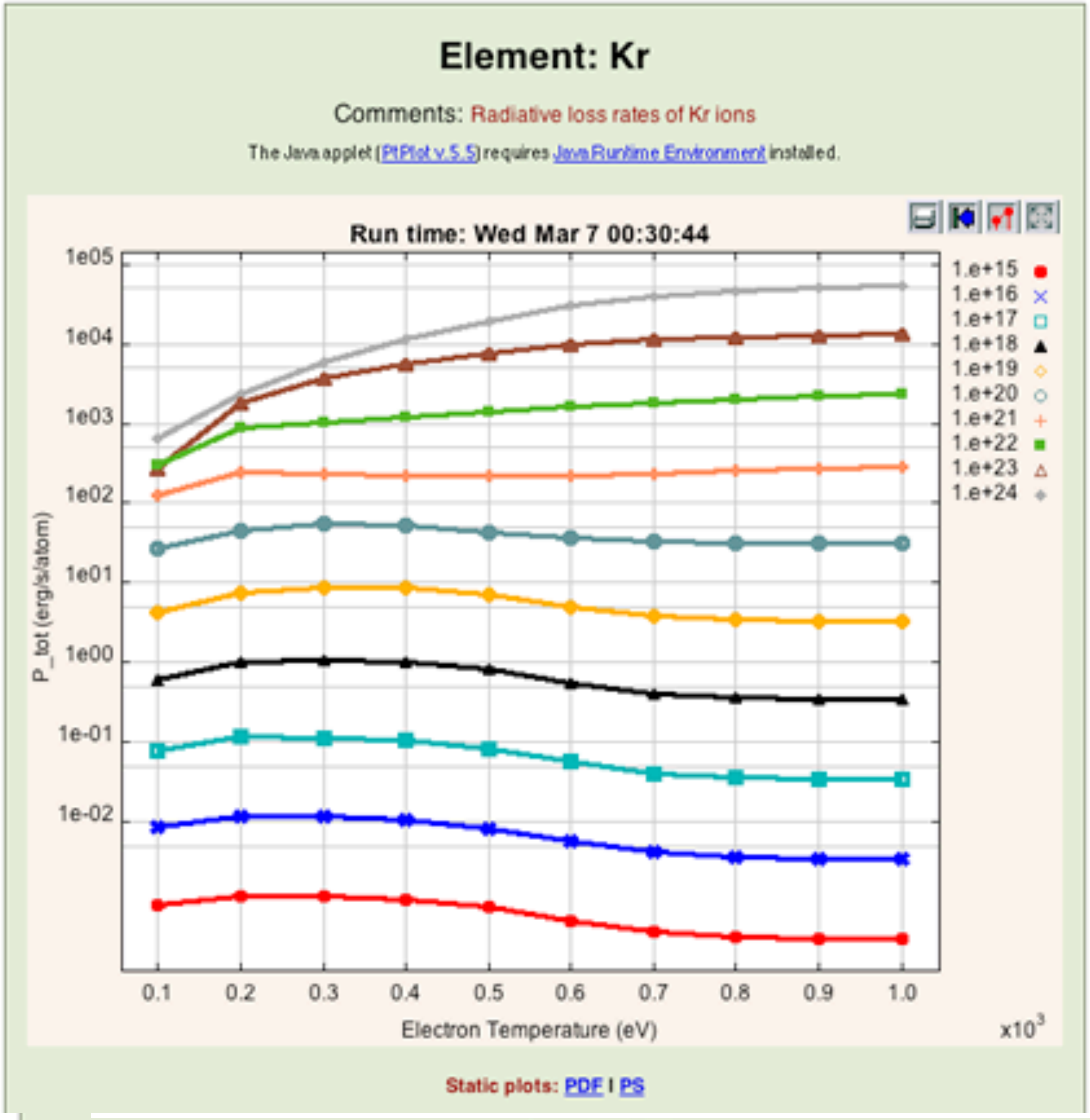
Calculated Kr radiative cooling rates per N_e [eV/s/atom/cm^{-3}]



# of radiative transitions using HULK code

Ion	HULLAC+DHS
1	3049
2	27095
3	30078
4	404328
5	3058002
6	5882192
7	7808014
8	6202123
9	5544814
10	1050919
11	841094
Sum	30,851,708

Data for Radiation Hydrodynamics: Kr Radiative loss rates over (Ne, Te)



Element: Kr

Comments: Radiative loss rates of Kr ions

The Java applet (PtPlot v.5.5) requires Java Runtime Environment installed.

Run time: Wed Mar 7 00:30:44

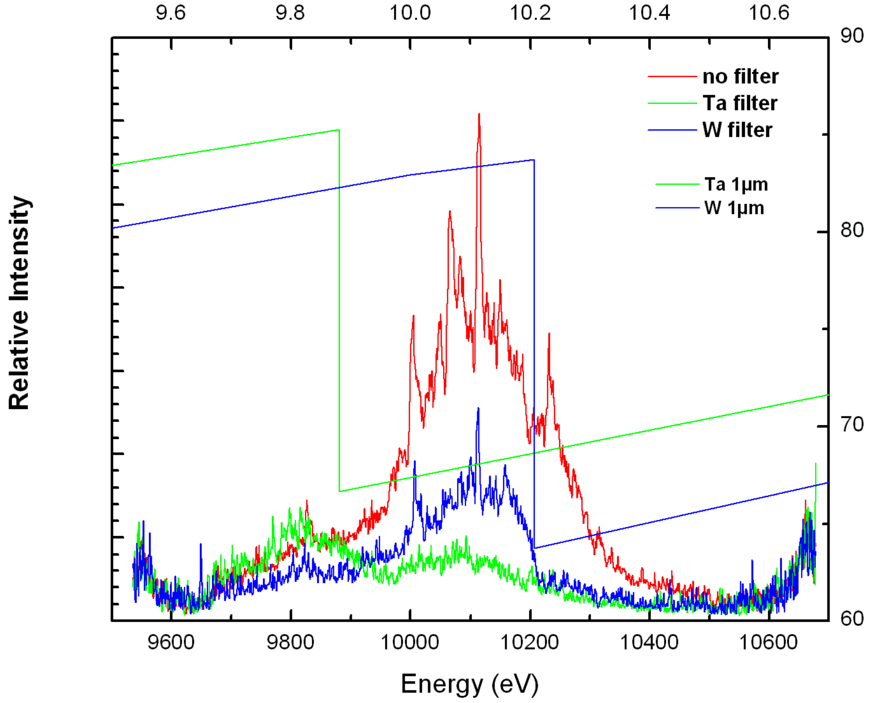
Static plots: PDF | PS

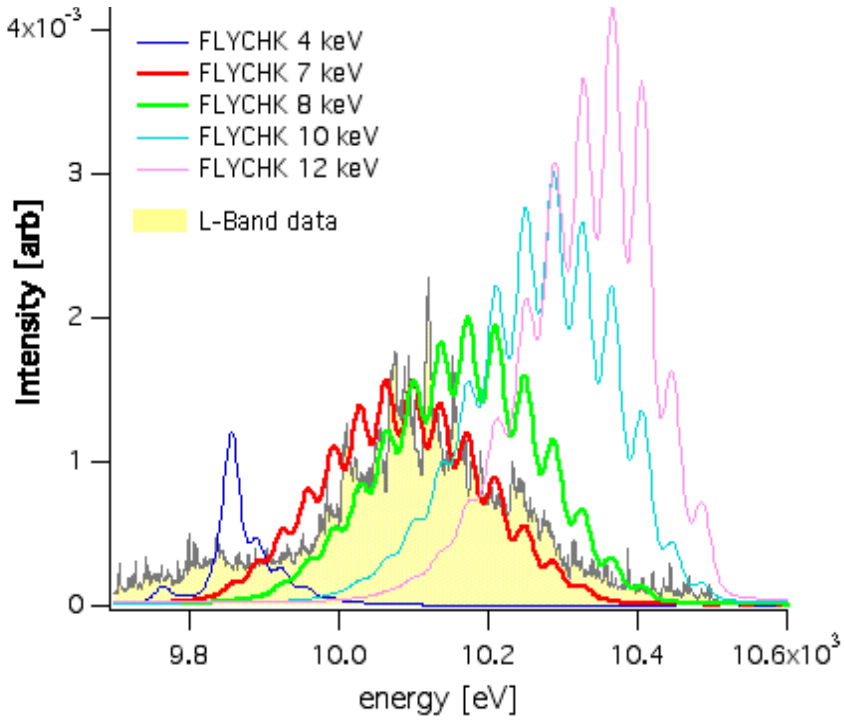
List of Selected Cases	
Dens	**Data**
1.e+15	file
1.e+16	file
1.e+17	file
1.e+18	file
1.e+19	file
1.e+20	file
1.e+21	file
1.e+22	file
1.e+23	file
1.e+24	file

The radiative loss rates show the similar coronal behavior up to $N_e=10^{17}$ and the rate/N_e stays constant. As N_e increases, the rate/N_e decreases from the coronal value

Example: Gold ionization balance in high temperature hohlraum (HTH) experiments

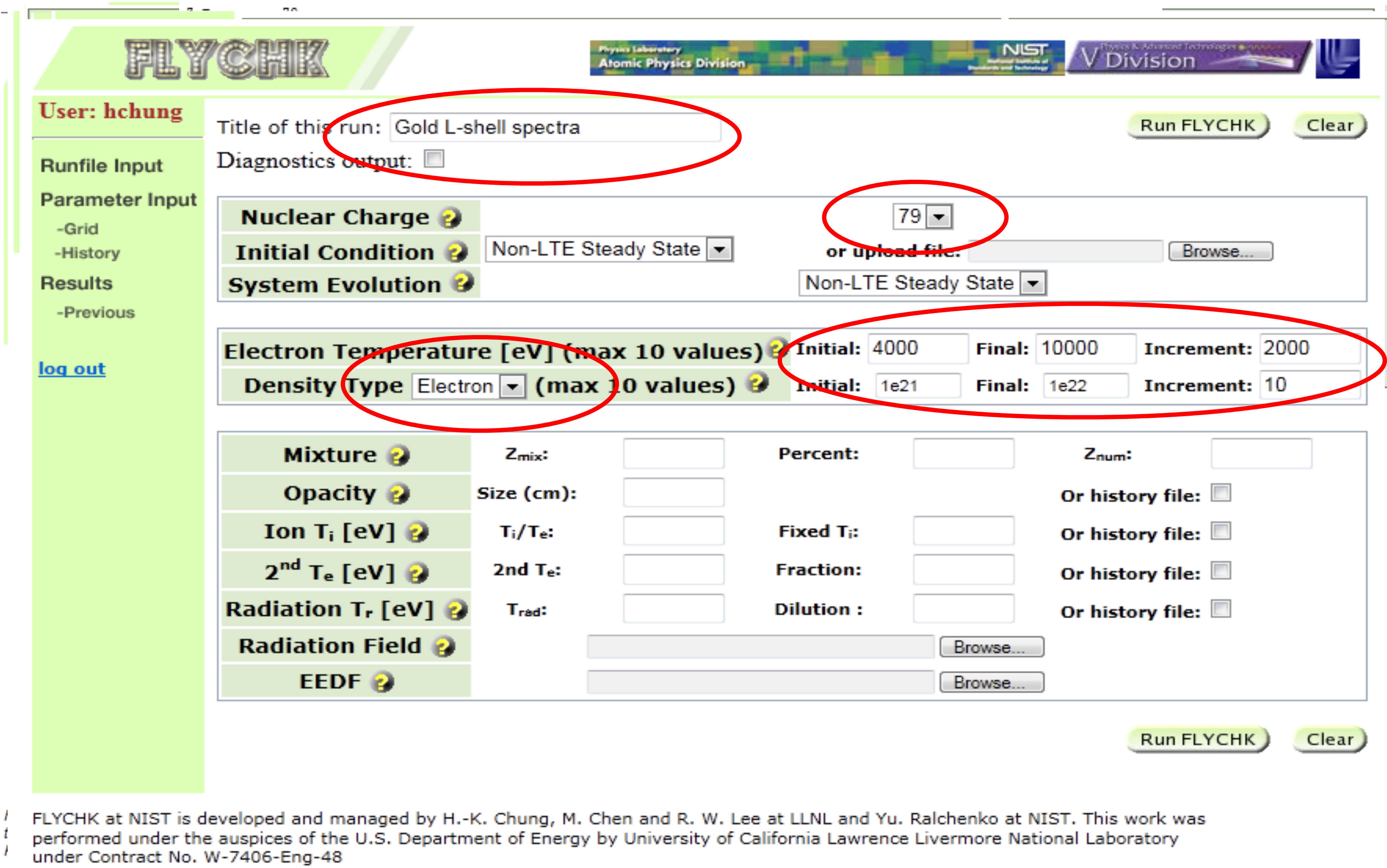
- High-T hohlraum reach temperatures: ~ 10 keV
- Spectrum from $n_e \sim 4\times10^{21}$ cm^{-3}, $T_e \sim$ 7-10 keV measured for first time


L-shell gold spectra (K. Widmann)


Spectroscopic data and calculation

FLYCHK gives an estimate of Gold L-shell spectra

Long pulse laser plasmas:
Gold L-shell spectroscopy



User: hchung

Title of this run: Gold L-shell spectra

Diagnostics output: ☐

Nuclear Charge: 79

Initial Condition: Non-LTE Steady State

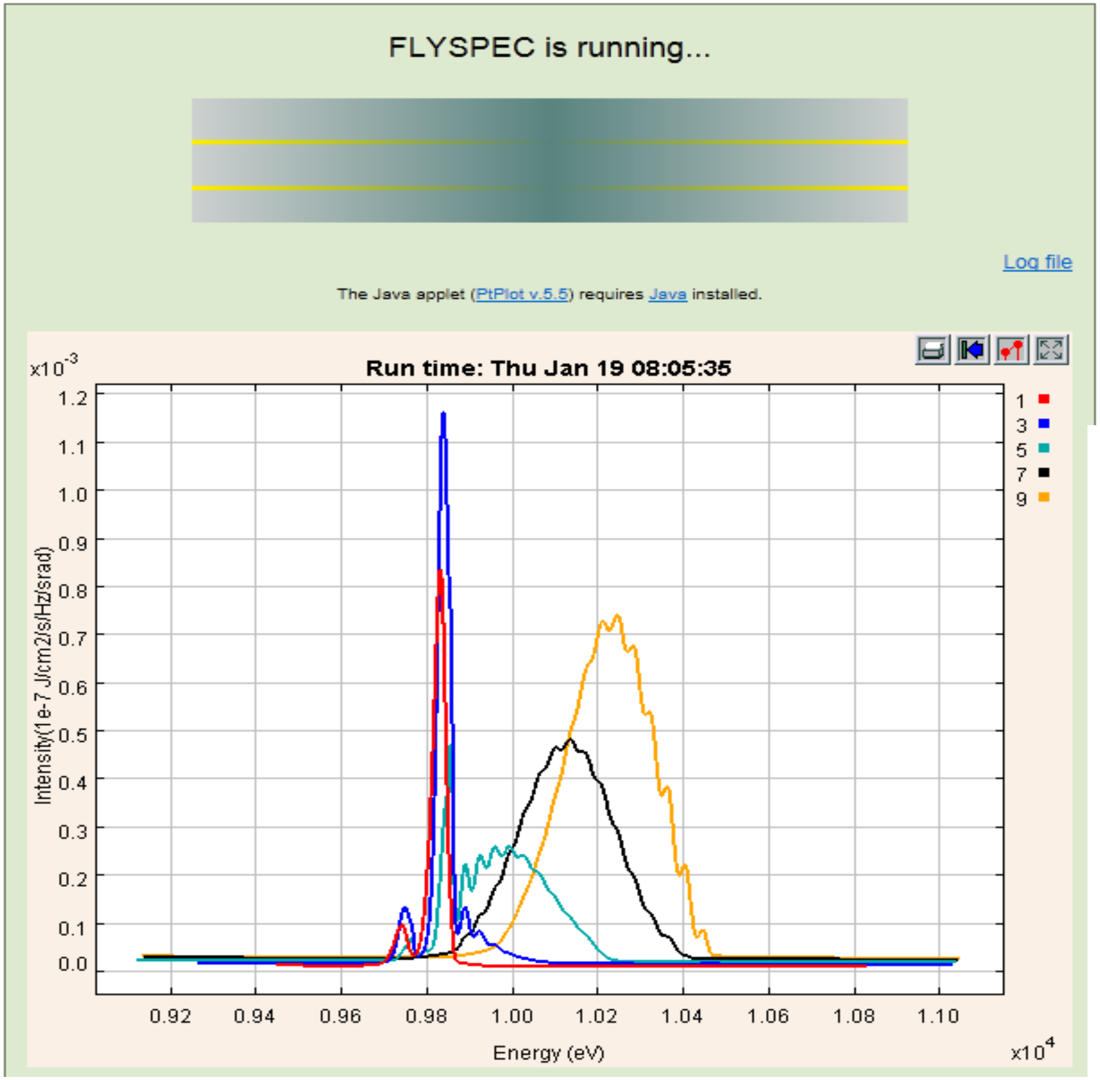
System Evolution: Non-LTE Steady State

Electron Temperature [eV] (max 10 values) Initial: 4000 Final: 10000 Increment: 2000

Density Type Electron (max 10 values) Initial: 1e21 Final: 1e22 Increment: 10

FLYCHK at NIST is developed and managed by H.-K. Chung, M. Chen and R. W. Lee at LLNL and Yu. Ralchenko at NIST. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract No. W-7406-Eng-48

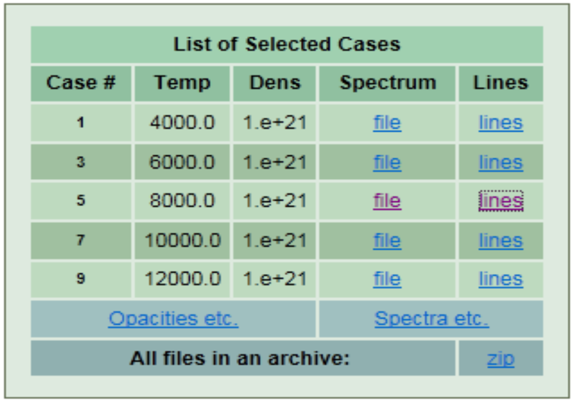
STA spectra compared with configuration-average spectra



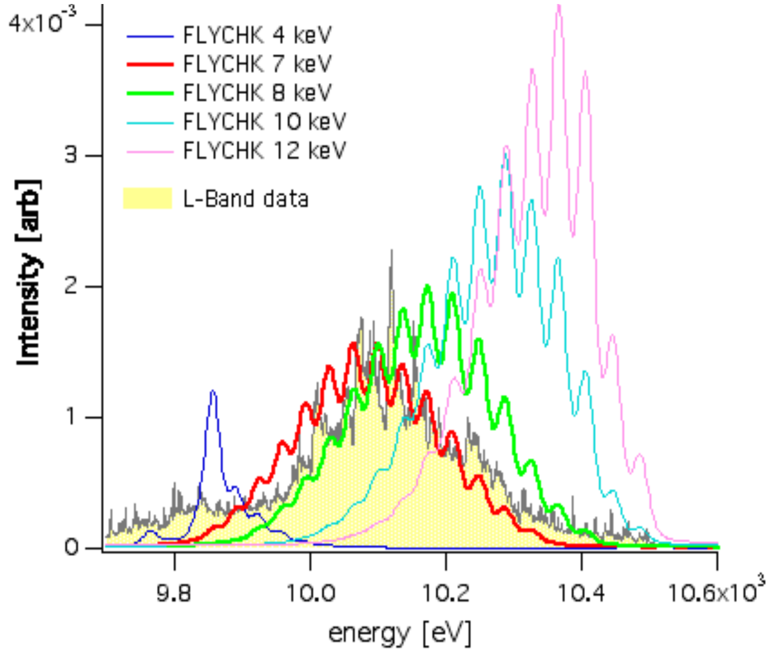
FLYSPEC is running...

Log file

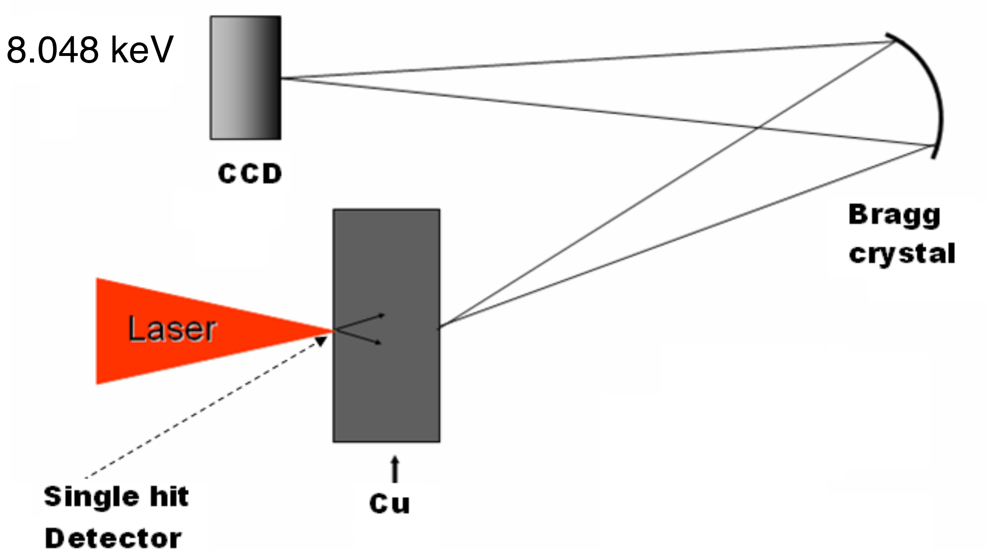
The Java applet (PtPlot v.5.5) requires Java installed.

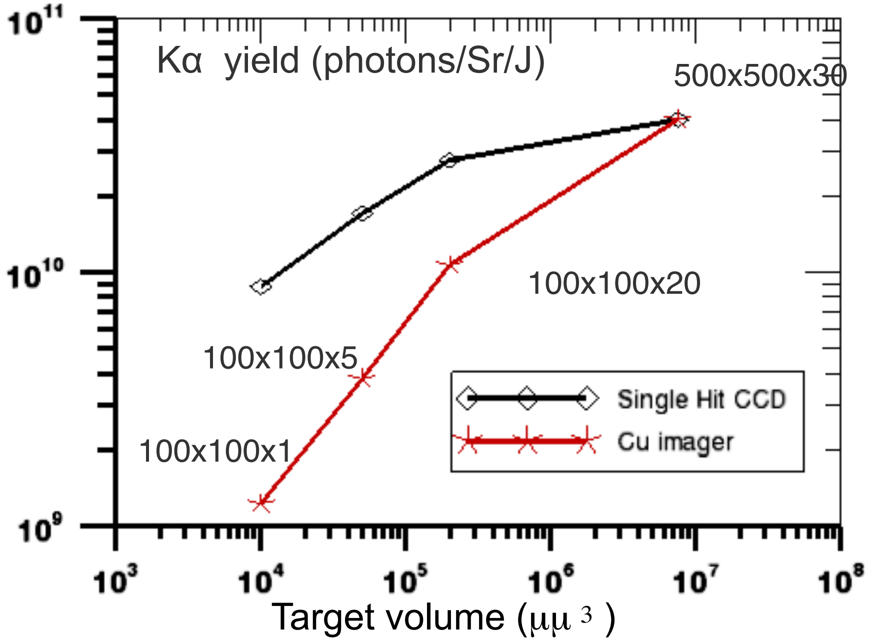


List of Selected Cases				
Case #	Temp	Dens	Spectrum	Lines
1	4000.0	1.e+21	file	lines
3	6000.0	1.e+21	file	lines
5	8000.0	1.e+21	file	lines
7	10000.0	1.e+21	file	lines
9	12000.0	1.e+21	file	lines
Opacities etc.			Spectra etc.	
All files in an archive:				zip



Example: Cu Kα radiation measured by single hit CCD spectrometer and 2-D imager for T_e diagnostics



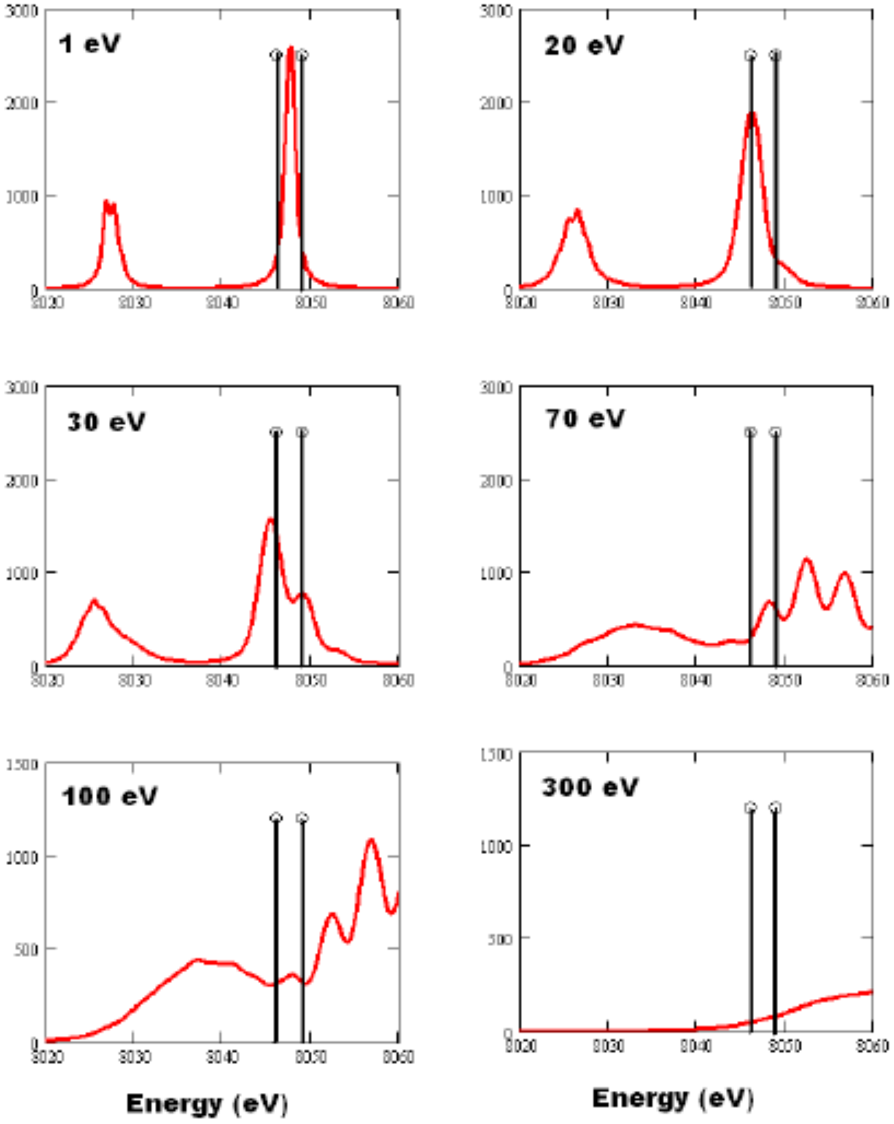


Single Hit CCD Kα yield is higher than that of 2-D imager for smaller target volumes :

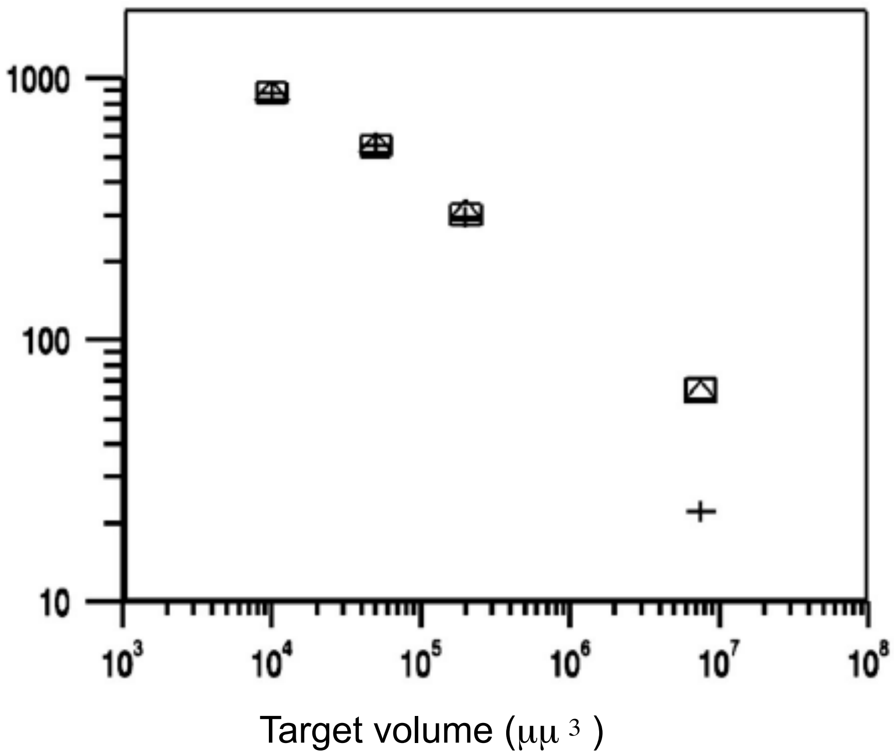
An experimental evidence of shifting and broadening of Kα emission lines in small targets with high temperatures

Shifts and Broadening of Kα emission as a function of electron thermal temperature

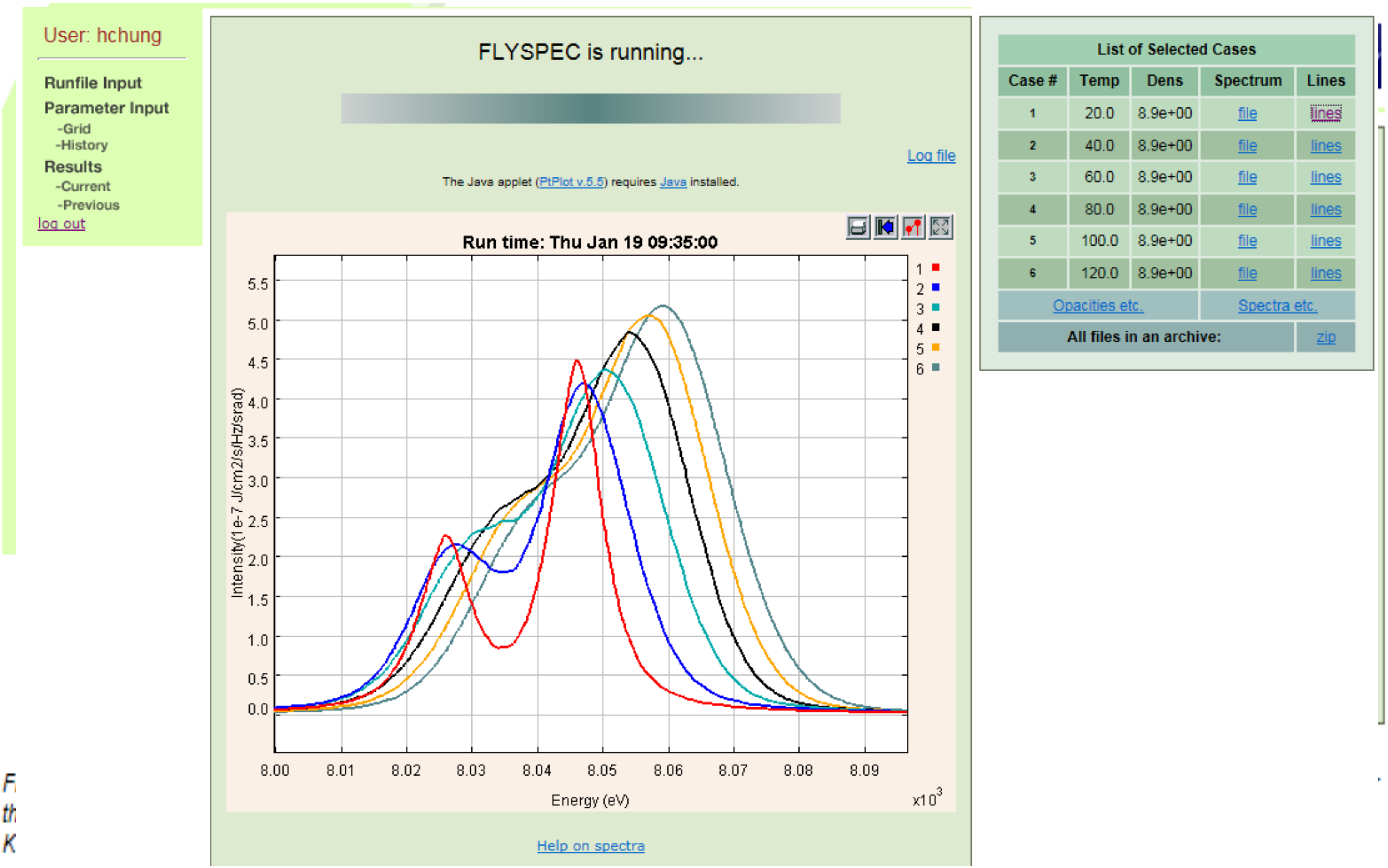
FLYCHK simulations



Average T_e(eV) of targets



Short pulse laser plasmas: Cu Kα Spectroscopy



User: hchung

Runfile Input

Parameter Input

- -Grid
- -History

Results

- -Current
- -Previous

log out

FLYSPEC is running...

Log file

The Java applet (PtPlot v.5.5) requires Java installed.

Run time: Thu Jan 19 09:35:00

Help on spectra

List of Selected Cases

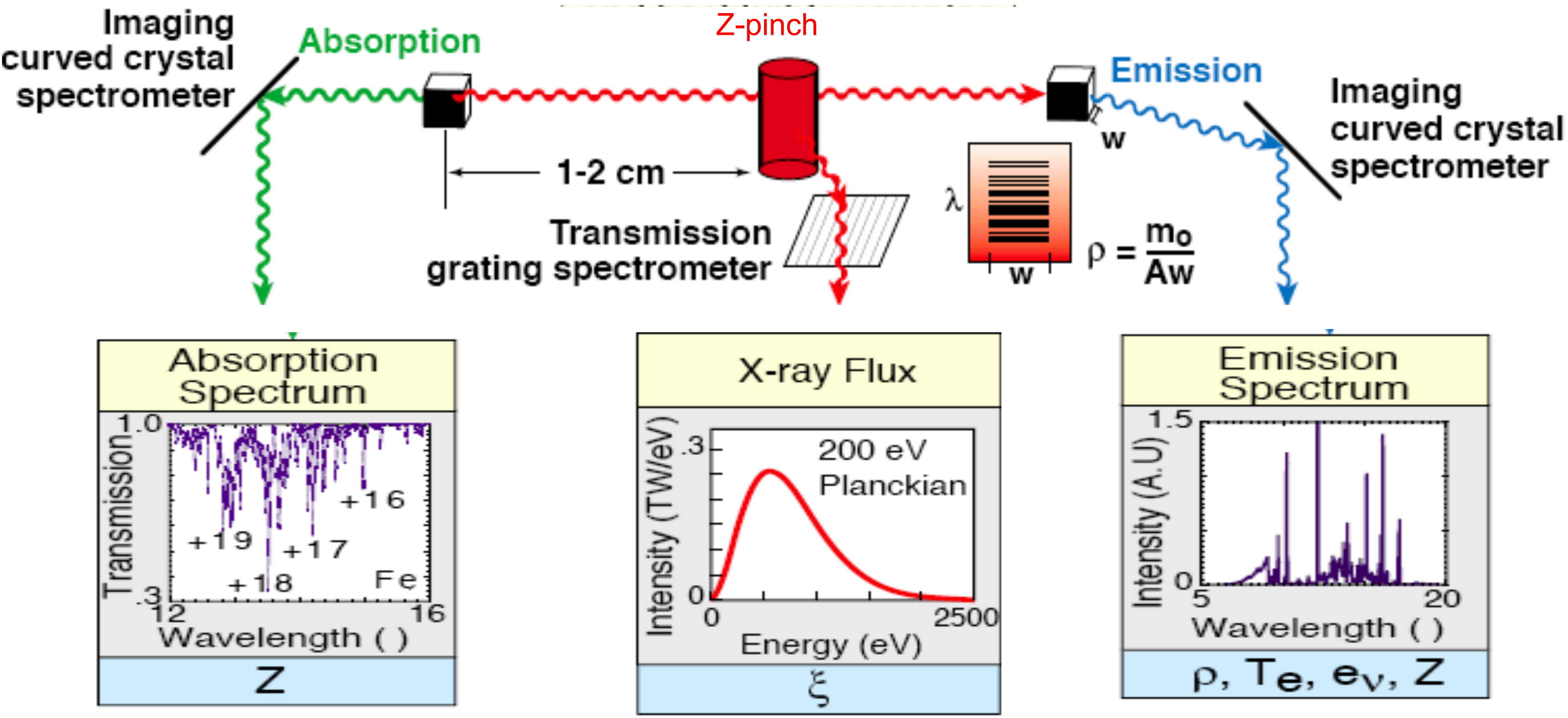
Case #	Temp	Dens	Spectrum	Lines
1	20.0	8.9e+00	file	lines
2	40.0	8.9e+00	file	lines
3	60.0	8.9e+00	file	lines
4	80.0	8.9e+00	file	lines
5	100.0	8.9e+00	file	lines
6	120.0	8.9e+00	file	lines

Opacities etc. | Spectra etc.

All files in an archive: zip

F
th
K

Example: Photoionized plasmas produced by Z-Machines – Astrophysical model benchmark

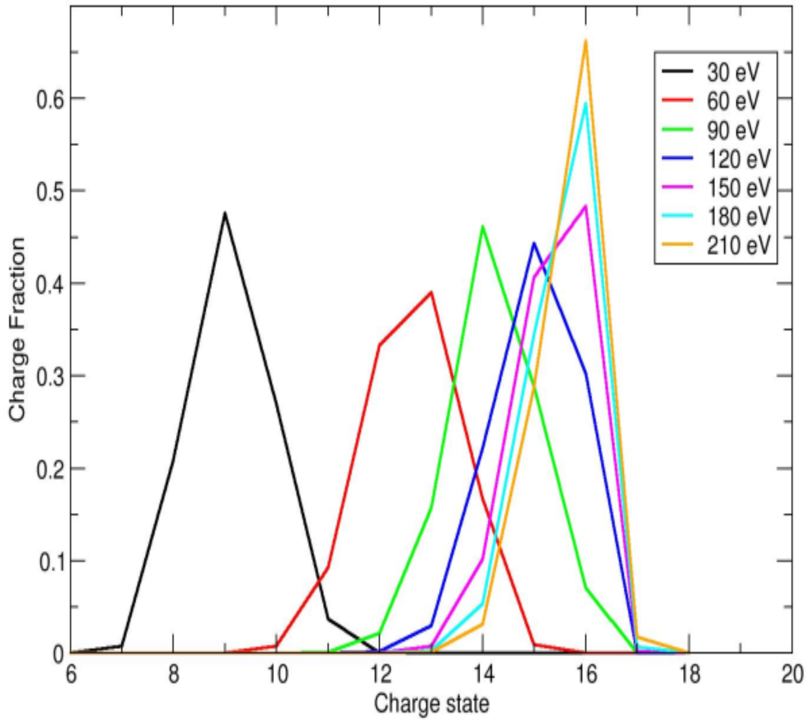


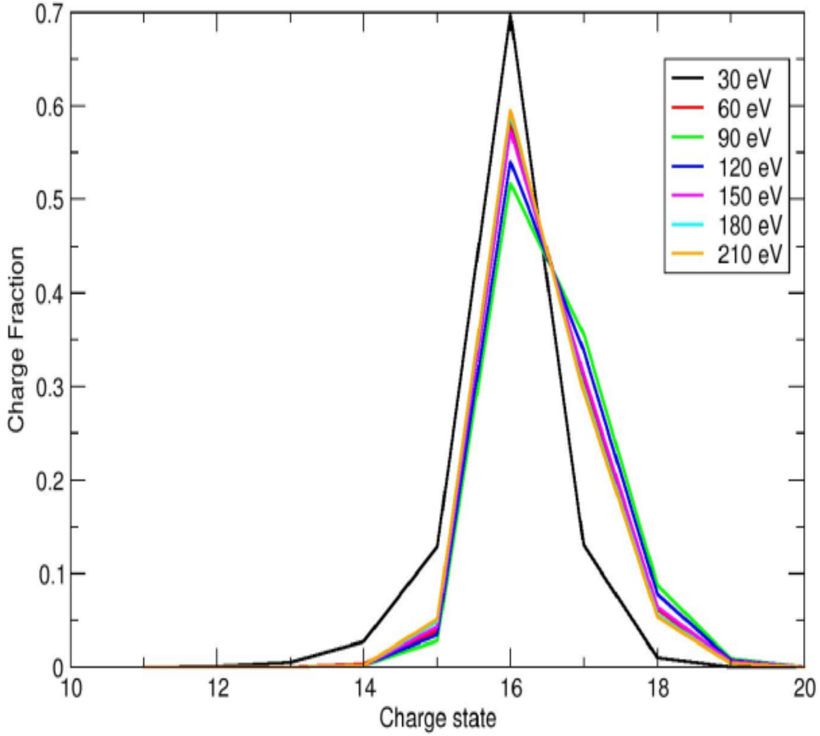
ξ=20-25 ergs-cm/s

Charge state distribution is a function of N_e and Radiation field strength

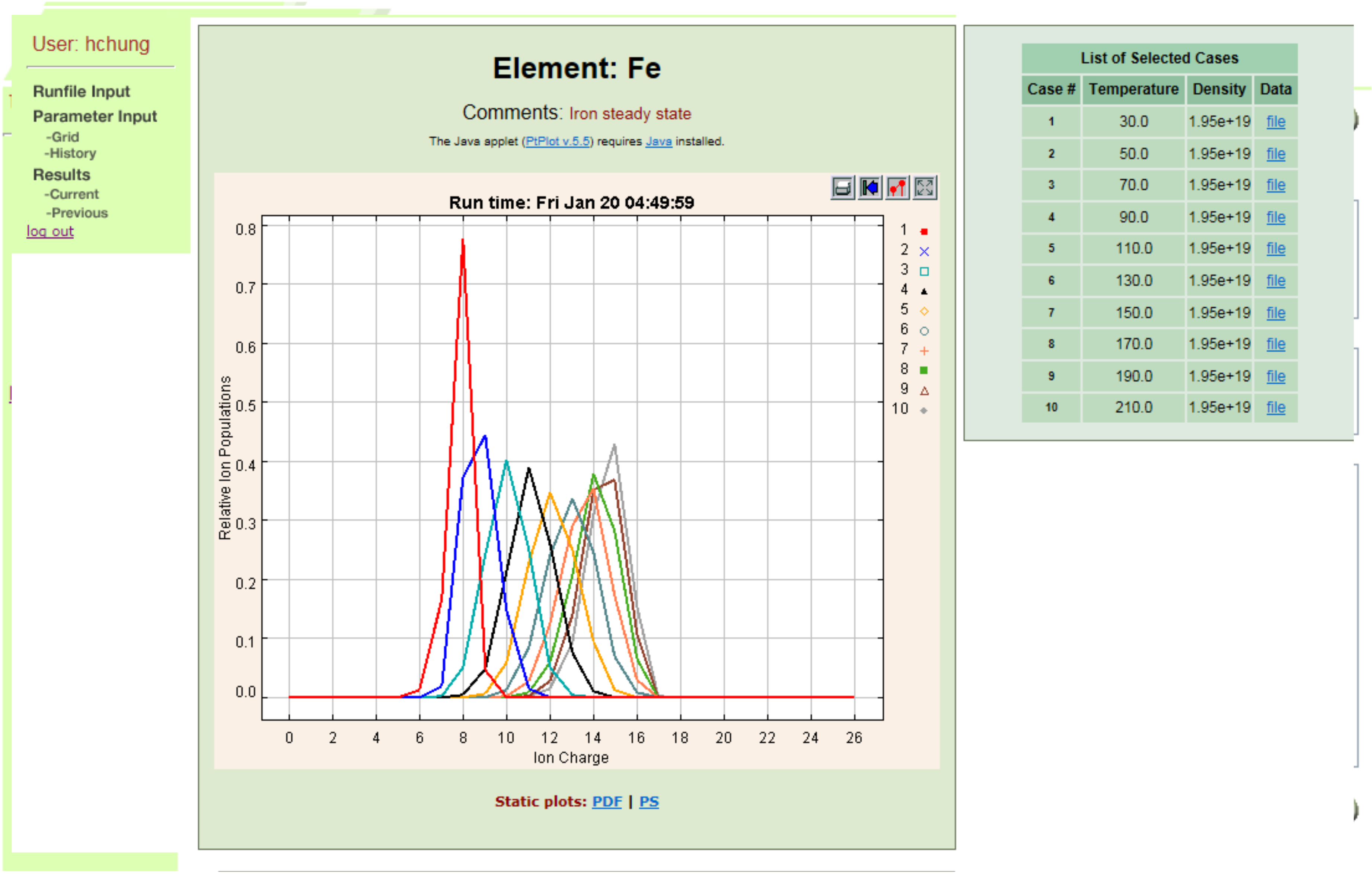
N_e =1.95E19cm^{-3}

Radiation field of 165 eV and 0.01 dilution





Photoionization equilibrium plasmas: Fe Z-Pinch Plasma



User: hchung

Runfile Input
Parameter Input
-Grid
-History
Results
-Current
-Previous
log out

Element: Fe

Comments: Iron steady state

The Java applet (PtPlot v.5.5) requires Java installed.

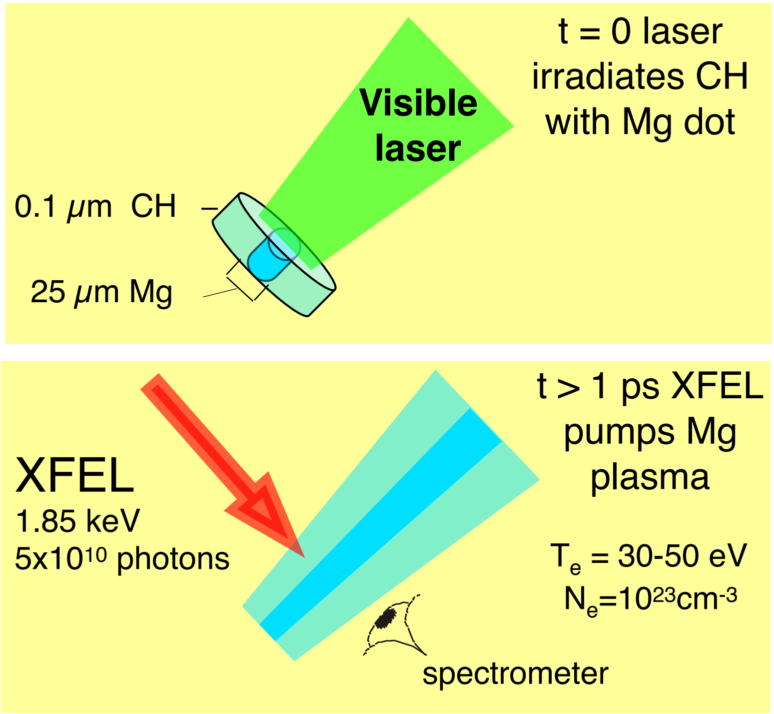
Static plots: PDF | PS

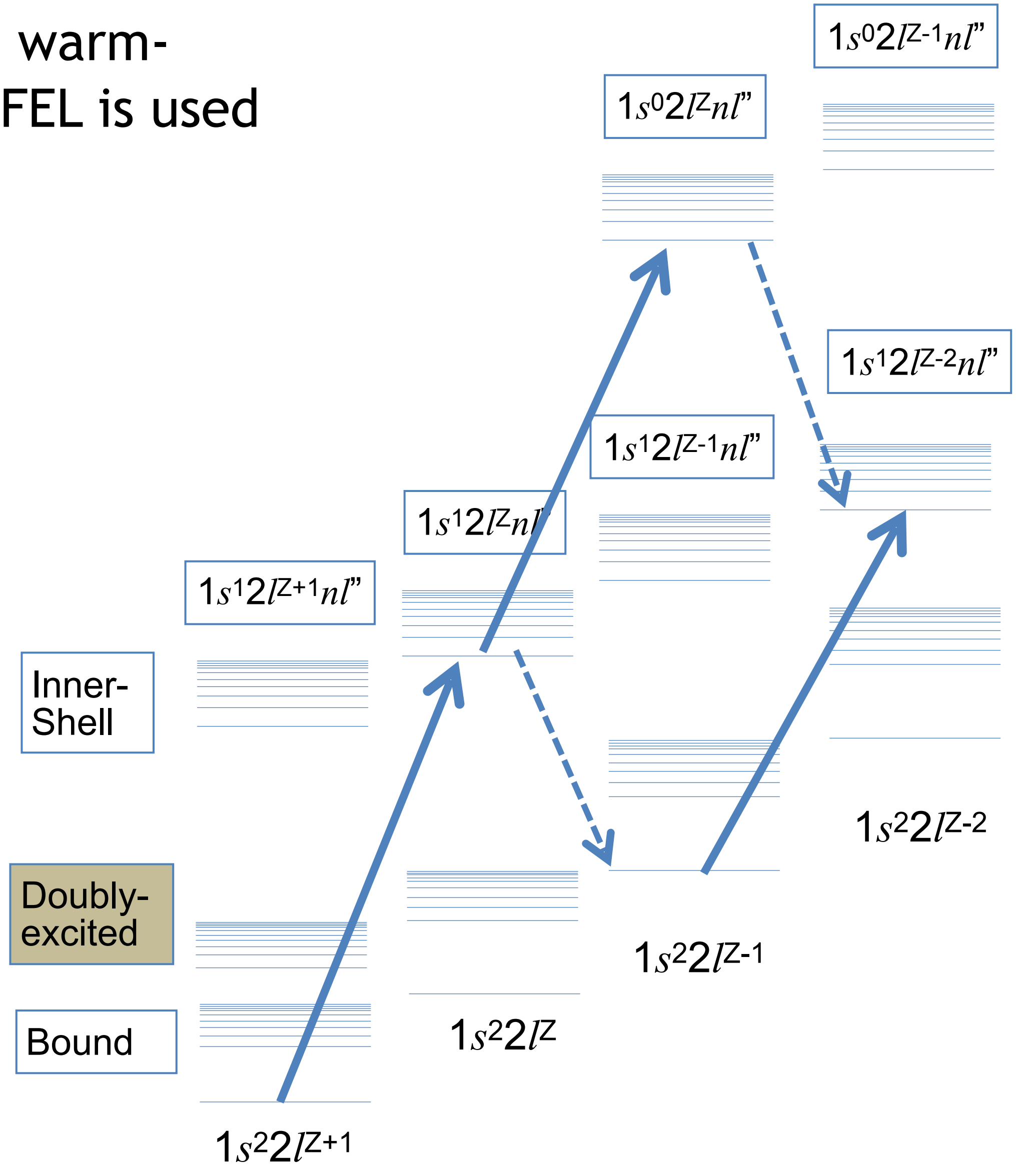
List of Selected Cases

Case #	Temperature	Density	Data
1	30.0	1.95e+19	file
2	50.0	1.95e+19	file
3	70.0	1.95e+19	file
4	90.0	1.95e+19	file
5	110.0	1.95e+19	file
6	130.0	1.95e+19	file
7	150.0	1.95e+19	file
8	170.0	1.95e+19	file
9	190.0	1.95e+19	file
10	210.0	1.95e+19	file

Example: XFEL provides an opportunity for HEDS plasma spectroscopy

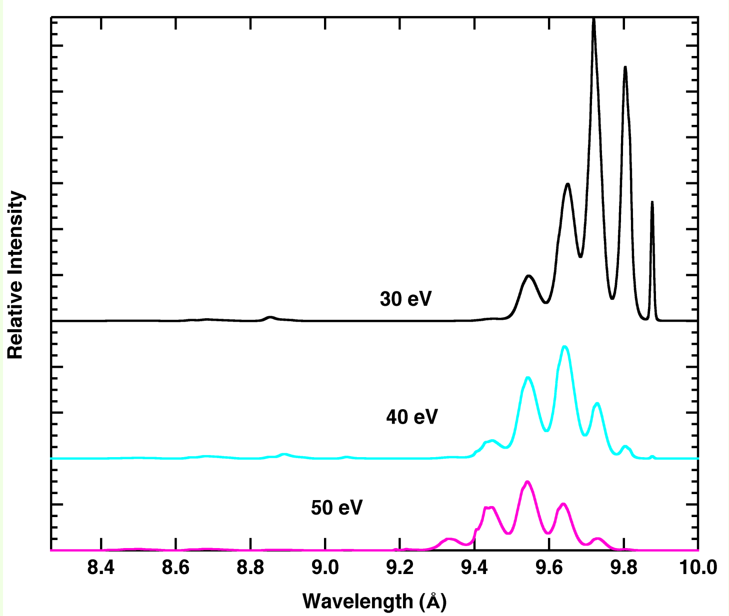
Long-pulse laser is used to create warm-dense-matter plasmas and then XFEL is used to probe the internal state.



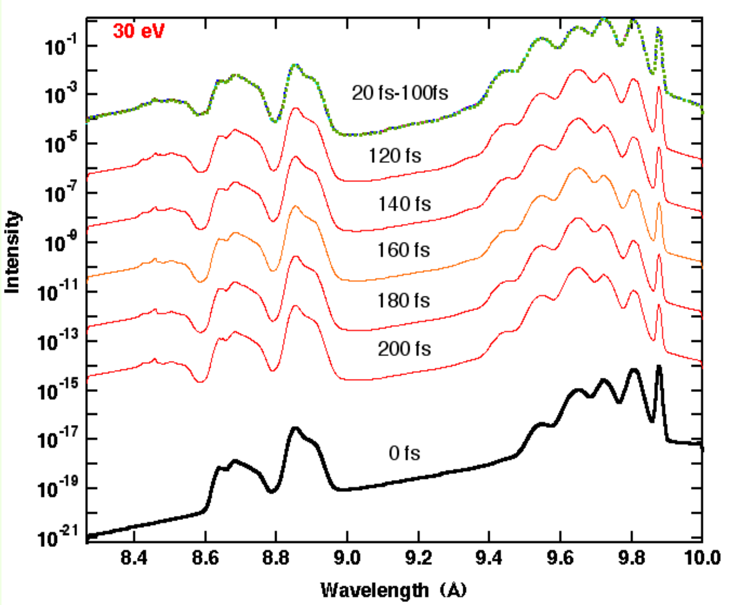


In Warm Dense Matter regime the hollow ions provide time-resolved diagnostic information

- XFEL forms unique states ***and*** provides *in situ* diagnostics with ~100 fs res.
  - 5×10^{10} 1.85 keV photons in 30 μm spot into a **$n_e=10^{23}$ cm^{-2}** plasma
  - Strong coupling parameter, Γ_{ii} = Potential/Kinetic Energy ~ 10



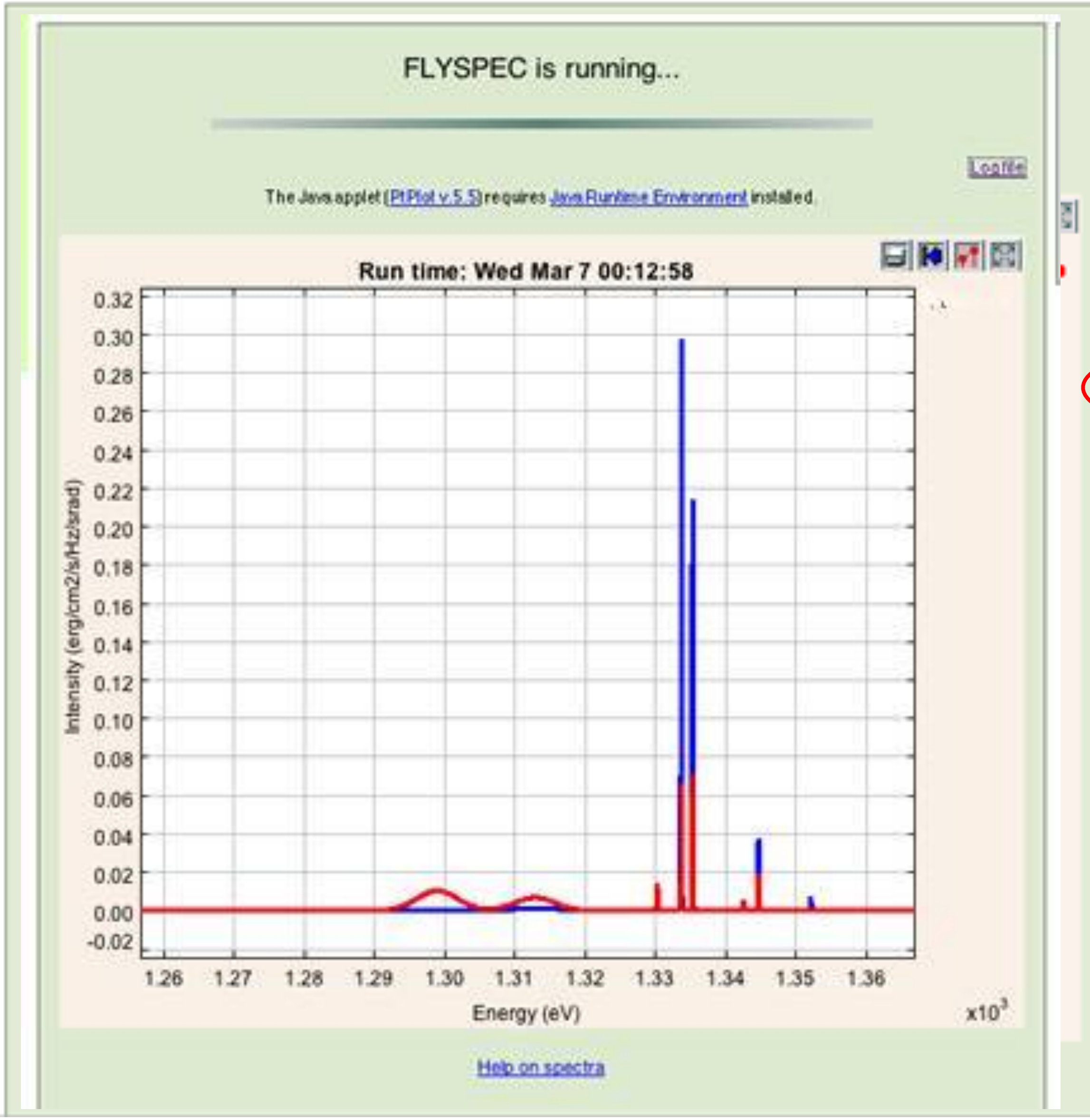
- Steady-state Spectra at various T_e



- At high n_e emisson lasts ~100 fs

XFEL ionized plasma:

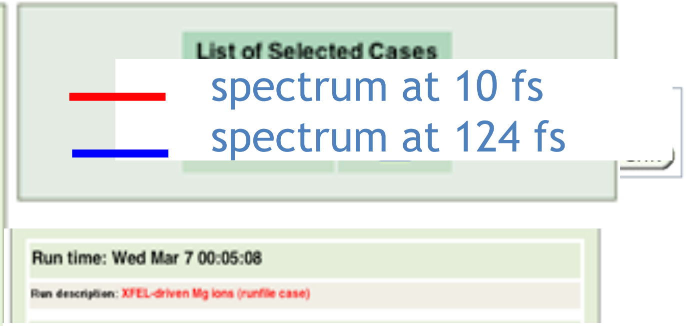
Mg time-dependent K-shell spectroscopy



FLYSPEC is running...

The Java applet (PtPlot v.5.5) requires Java Runtime Environment installed.

Run time: Wed Mar 7 00:12:58



- 🟥 spectrum at 10 fs
- 🟦 spectrum at 124 fs

Run time: Wed Mar 7 00:05:08

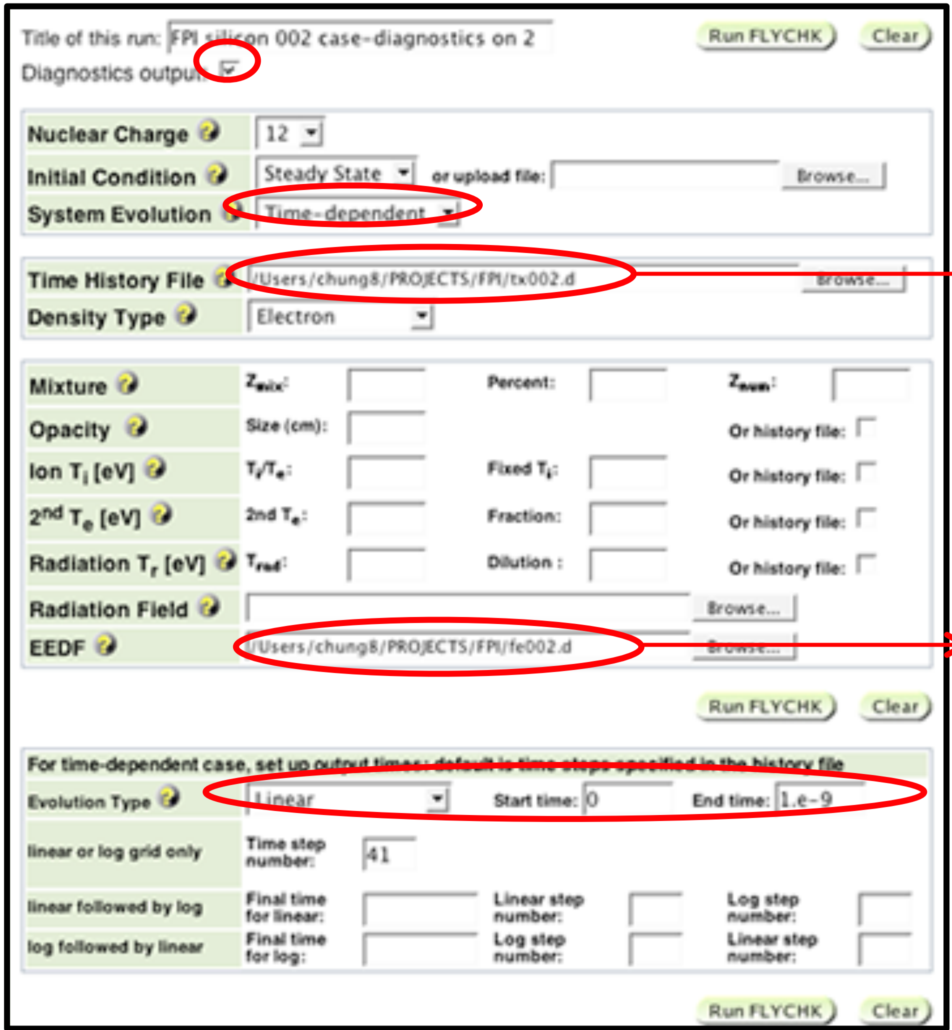
Run description: XFEL-driven Mg ions (runfile case)

Even with 3.1 keV photons, the <Z> and hence the ionization distribution do not change significantly in 1000 fs. However, the details in the K-shell spectrum can change to reflect the change in K-hole state population. This can lead to a pump diagnostics

The zigzag behavior can happen when the IPD (ionization potential depression) removes a highly excited states. Unless the fluctuation is not an order of a charge, it is not a serious concern.

Postprocessing electron kinetic simulation

- SiO_2 aerogel targets doped with Ge or Ti for X-ray backlighter development
- 1-D e- kinetic code FPI shows Non-maxwellian energy functions due to strong laser heating and nonlocal electron heat flow -- J-P. Matte & K.B. Fournier


Title of this run: FPI silicon 002 case-diagnostics on 2
Diagnostics output ☑

Nuclear Charge	12				
Initial Condition	Steady State	or upload file:			
System Evolution	Time-dependent				
Time History File	/Users/chung8/PROJECTS/FPI/tx002.d				
Density Type	Electron				
Mixture	Z_{mix}:	Percent:		Z_{num}:	
Opacity	Size (cm):			Or history file:	☐
Ion T_i [eV]	T_i/T_e:	Fixed T_i:		Or history file:	☐
2nd T_e [eV]	2nd T_e:	Fraction:		Or history file:	☐
Radiation T_r [eV]	T_{rad}:	Dilution :		Or history file:	☐
Radiation Field					
EEDF	/Users/chung8/PROJECTS/FPI/fe002.d				

For time-dependent case, set up output times: default is time steps specified in the history file

Evolution Type	Linear	Start time:	0	End time:	1.e-9
linear or log grid only	Time step number:	41			
linear followed by log	Final time for linear:	Linear step number:		Log step number:	
log followed by linear	Final time for log:	Log step number:		Linear step number:	

History input always includes thermal T_e

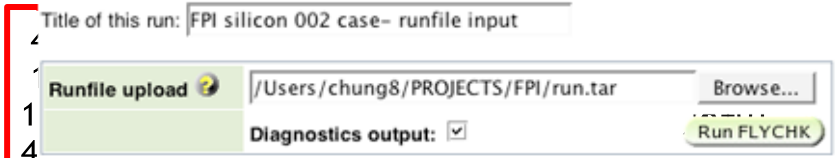
EEDF is added as additional e- source

Runfile input can specify

EEDF to be the only e- source

```
      time        te          ne
  0.0000E-21  9.9786E+00  2.4806E+20
  2.5000E-10  1.8787E+03  8.3812E+20
  3.7600E-10  2.2745E+03  8.6984E+20
  7.0000E-10  2.9818E+03  9.0895E+20
  7.2500E-10  3.0262E+03  9.1025E+20
  7.5000E-10  3.0695E+03  9.1140E+20
```

```
 6.89062E+01 8.26562E+01 9.76562E+01 1.13906E+02
1.31406E+02 1.50156E+02 1.70156E+02 1.91406E+02
2.13906E+02 2.37656E+02
 2.62656E+02 2.88906E+02 3.16406E+02 3.45156E+02
3.75156E+02
5.07656E+02 5.43906E+02
 5.81406E+02 6.20156E+02 6.60156E+02 7.01406E+02
7.43906E+02 7.87656E+02 8.32656E+02 8.78906E+02
9.26406E+02 9.75156E+02
 1.02516E+03 1.07641E+03 1.12891E+03 1.18266E+03
1.23766E+03 1.29391E+03 1.35141E+03 1.41016E+03
1.47016E+03 1.53141E+03
```


Title of this run: FPI silicon 002 case– runfile input

Runfile upload: /Users/chung8/PROJECTS/FPI/run.tar

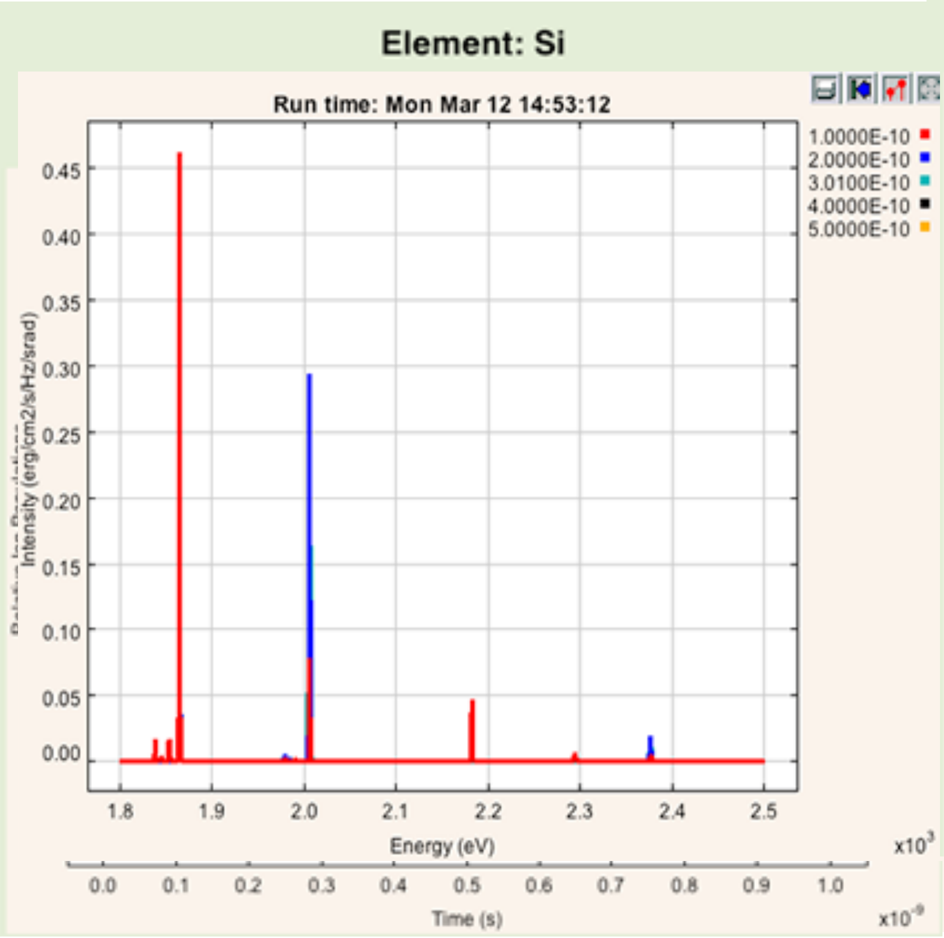
Diagnostics output: ☑

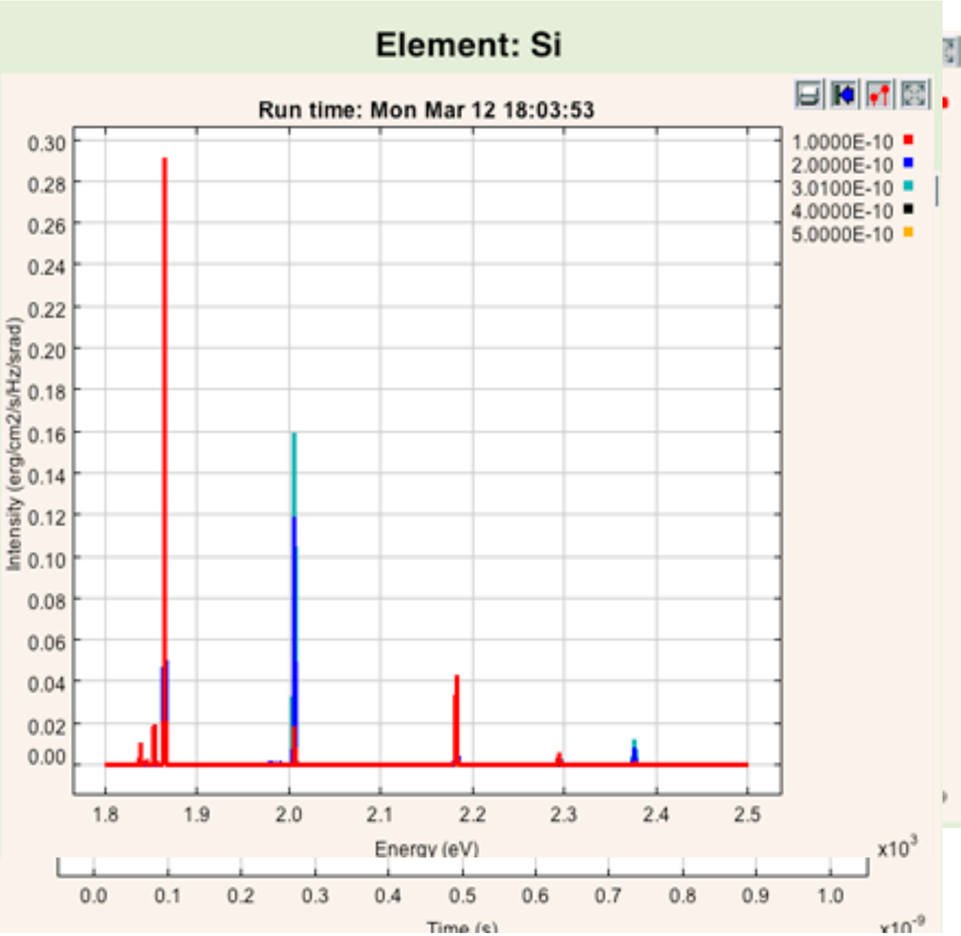
```
c Te and Ne should be always included
c for continuum lowering model
c even though they do not come into play
c in kinetics and rate equations
z 14
outfile fe.dat
initial ss
evolve td
fe fe002.d only
history tx002.d te ne
.....
time 0. 1.e-9 41
end
```

Output: <Z> is quite similar with/without thermal e-

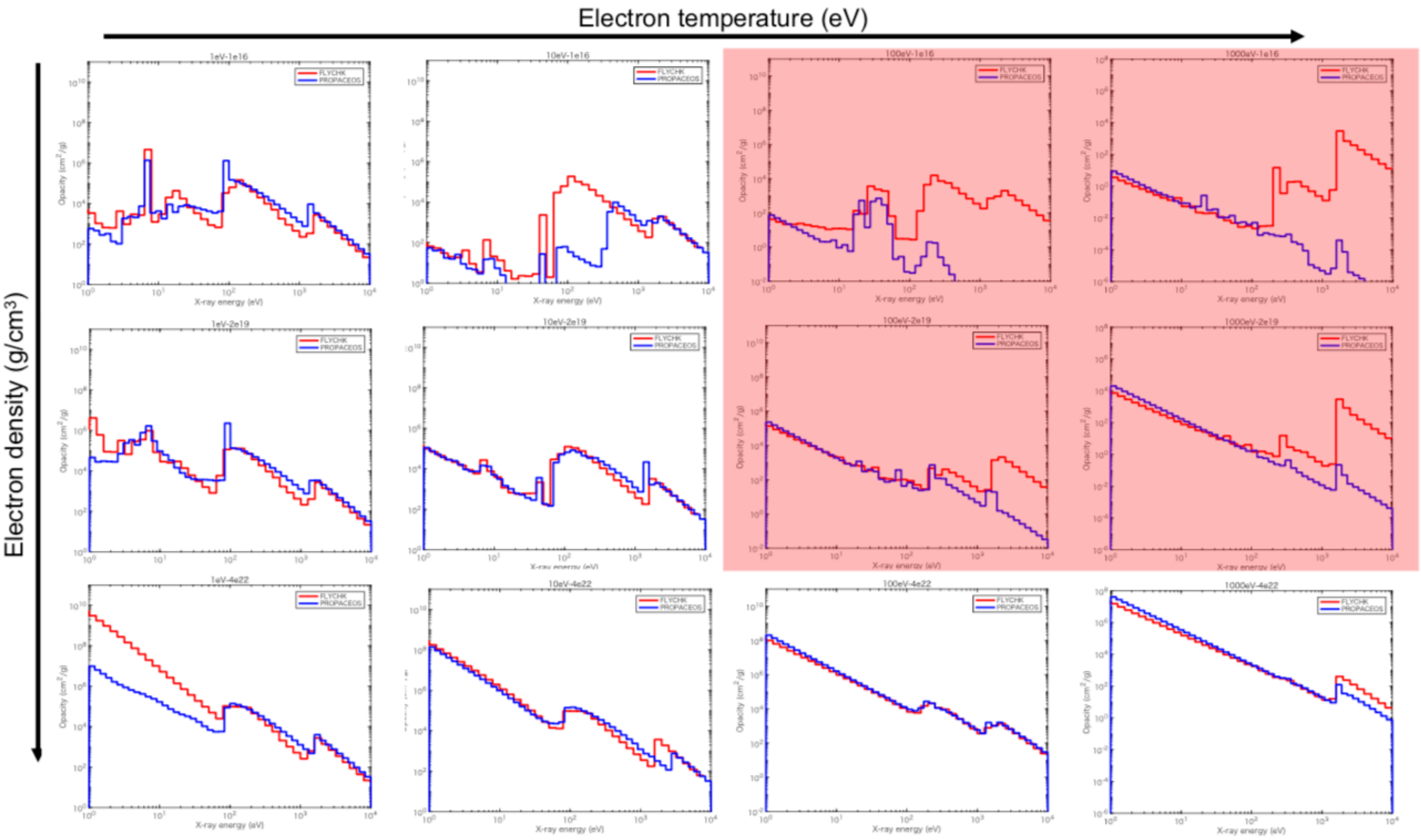
Using fe(E) with thermal e-

Using fe(E) only without thermal e-



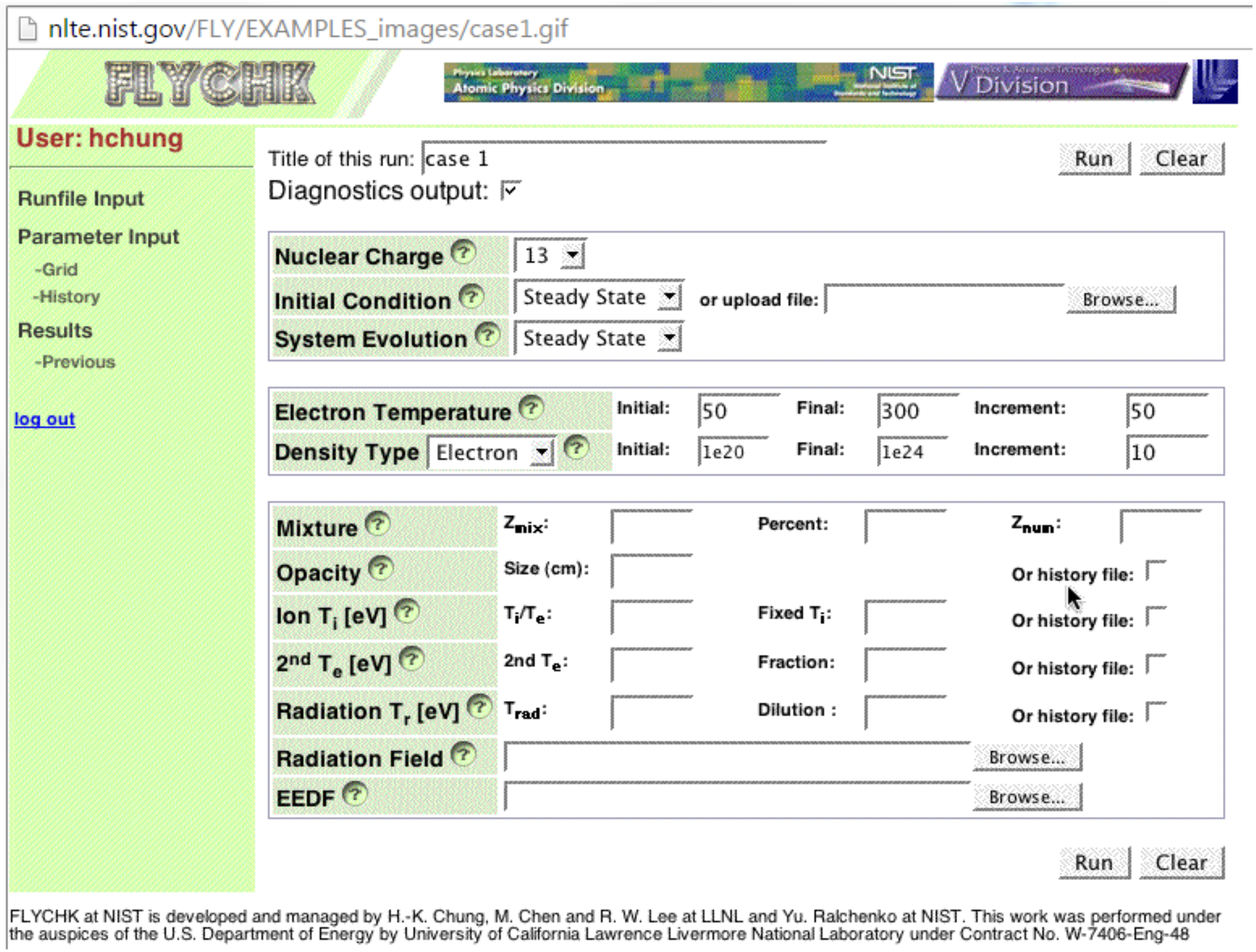


Aluminum Opacity (NIST data)



Useful Examples http://nlte.nist.gov/FLY/EXAMPLE.html

Please check the Screen shot of each case



User: hchung

Title of this run: case 1

Diagnostics output: ☑

Nuclear Charge	13				
Initial Condition	Steady State	or upload file:			
System Evolution	Steady State				

Electron Temperature	Initial:	50	Final:	300	Increment:	50
Density Type: Electron	Initial:	1e20	Final:	1e24	Increment:	10

Mixture	Z_{mix}:		Percent:		Z_{num}:	
Opacity	Size (cm):				Or history file:	☐
Ion T_i [eV]	T_i/T_e:		Fixed T_i:		Or history file:	☐
2^{nd} T_e [eV]	2nd T_e:		Fraction:		Or history file:	☐
Radiation T_r [eV]	T_{rad}:		Dilution :		Or history file:	☐
Radiation Field						
EEDF						

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Thank you!