Line intensities and Collisional-Radiative Modeling

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(many slides from Y. Ralchenko & J. Seely presentations at ICTP-IAEA School in 2017)
http://indico.ictp.it/event/7950/other-view?view=ictptimetable
https://www-amdis.iaea.org/Workshops/ICTP2017/

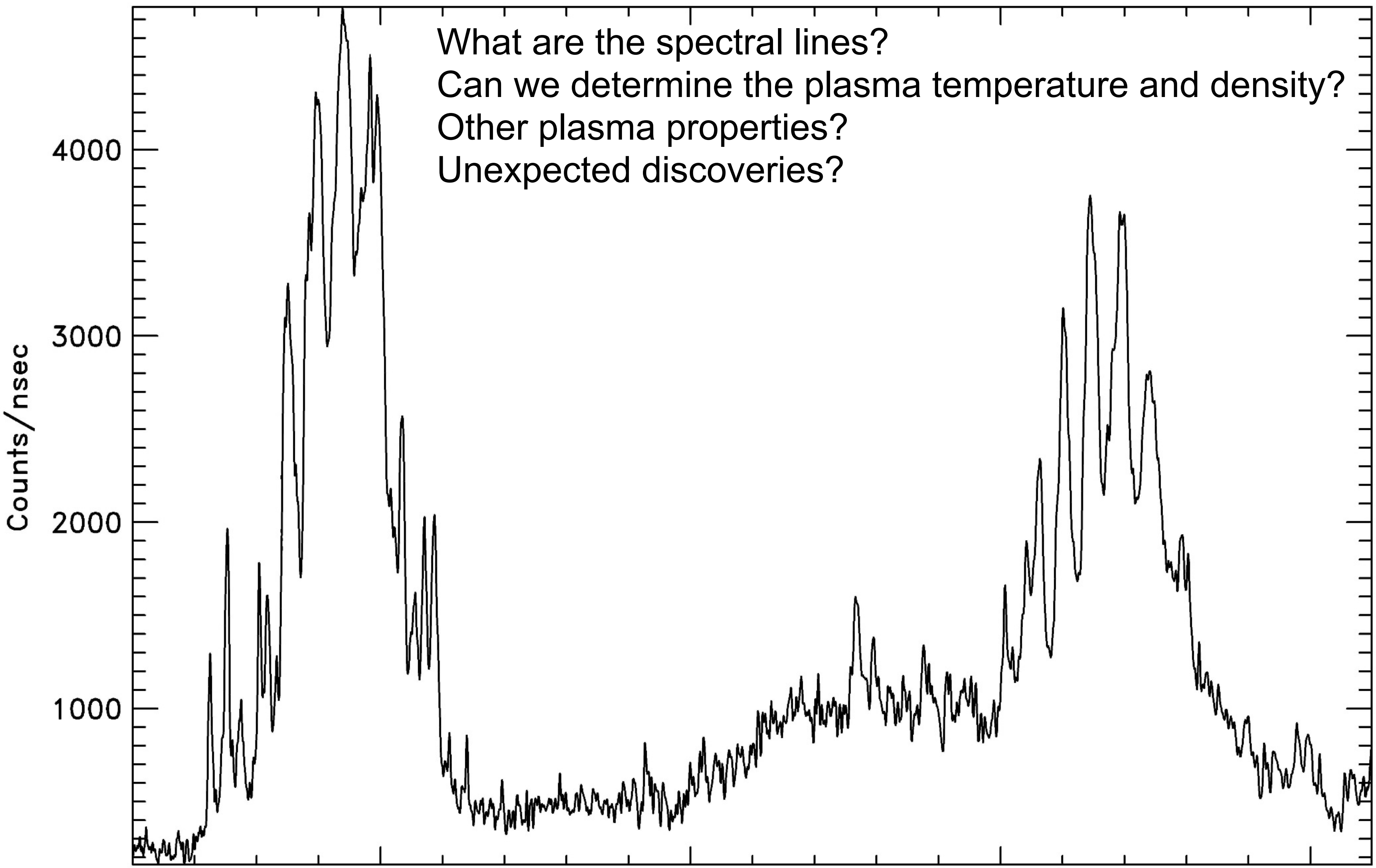
May 8th, 2019

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

Spectroscopic observables of matter states

INTRODUCTION

Experimental X-Ray Spectra



Spectral Line Intensity (optically thin)

$$I_{ij} = N_j \cdot A_{ij} \cdot h\nu_{ij}$$

Upper state density (cm^{-3})

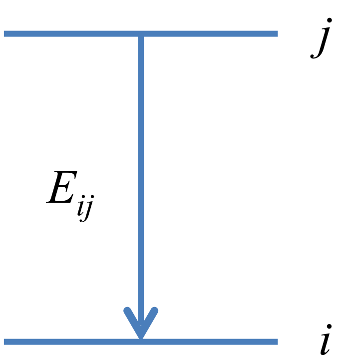
Einstein coefficient or transition probability (s^{-1})

strongly depends on plasma conditions

(*almost*) purely atomic parameters

Energy emitted due to a specific transition from a unit volume per unit time

Photon energy (J)

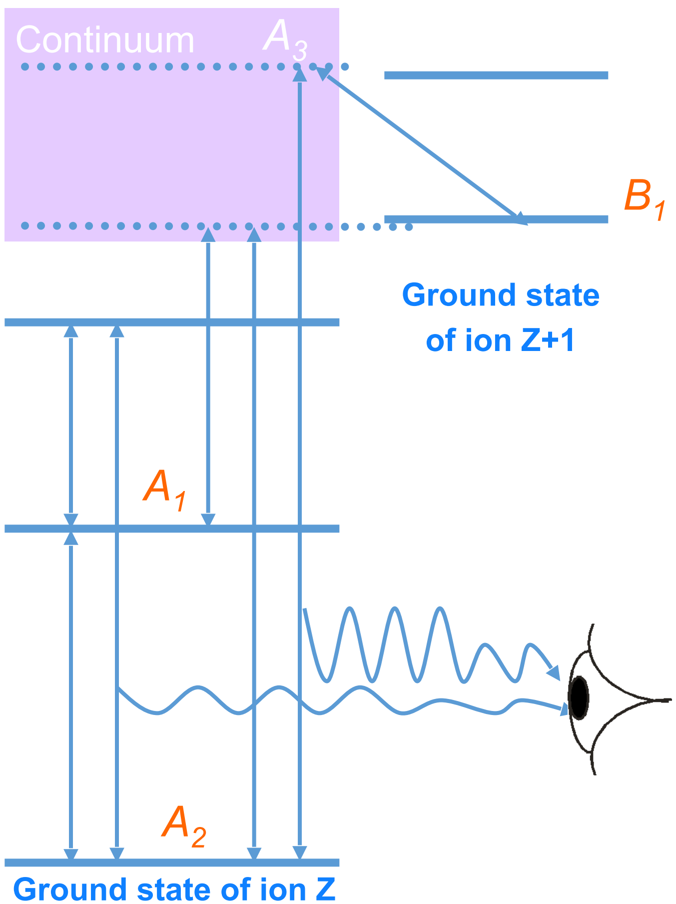


5 fields of expertize to constitute plasma spectroscopic analysis

INGREDIENTS OF SPECTROSCOPIC ANALYSIS

1) A Complete Set of Atomic Data

Energy levels of an atom



BOUND-BOUND TRANSITIONS

$A_1 \rightarrow A_2 + h\nu_2$ Spontaneous emission

$A_1 + h\nu_1 \leftrightarrow A_2 + h\nu_1 + h\nu_2$ Photo-absorption or emission

$A_1 + e_1 \leftrightarrow A_2 + e_2$ Collisional excitation or deexcitation

BOUND-FREE TRANSITIONS

$B_1 + e \rightarrow A_2 + h\nu_3$ Radiative recombination

$B_1 + e \leftrightarrow A_2 + h\nu_3$ Photoionization / stimulated recombination

$B_1 + e_1 \leftrightarrow A_2 + e_2$ Collisional ionization / recombination

$B_1 + e_1 \leftrightarrow A_3 \leftrightarrow A_2 + h\nu_3$ Autoionization / Dielectronic Recombination (electron capture + stabilization)

Atomic Physics Codes: FAC, HULLAC, LANL, GRASP-2K

2) Population Kinetics Modeling

The key is to figure out how to manage the infinite set of levels and transitions of atoms and ions into a model with a tractable set of levels and transitions that represents a physical reality!

(Completeness + Tractability + Accuracy)

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

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

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

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

3) Radiation Transport

Radiation field carries the information on atoms in plasmas through population distributions

- Radiation intensity *I(r,n,v,t)* is determined self-consistently from the coupled integro-differential radiation transport and population kinetic equations

$$[c^{-1}(\partial / \partial t) + (\mathbf{n}\cdot\nabla)]I(\mathbf{r},\mathbf{n},\nu,t) = \eta(\mathbf{r},\mathbf{n},\nu,t) - \chi(\mathbf{r},\mathbf{n},\nu,t)I(\mathbf{r},\mathbf{n},\nu,t)$$

- Emissivity $\eta(r,n,v,t)$ and Opacity $\chi(r,n,v,t)$ and are obtained with population densities and radiative transition probabilities

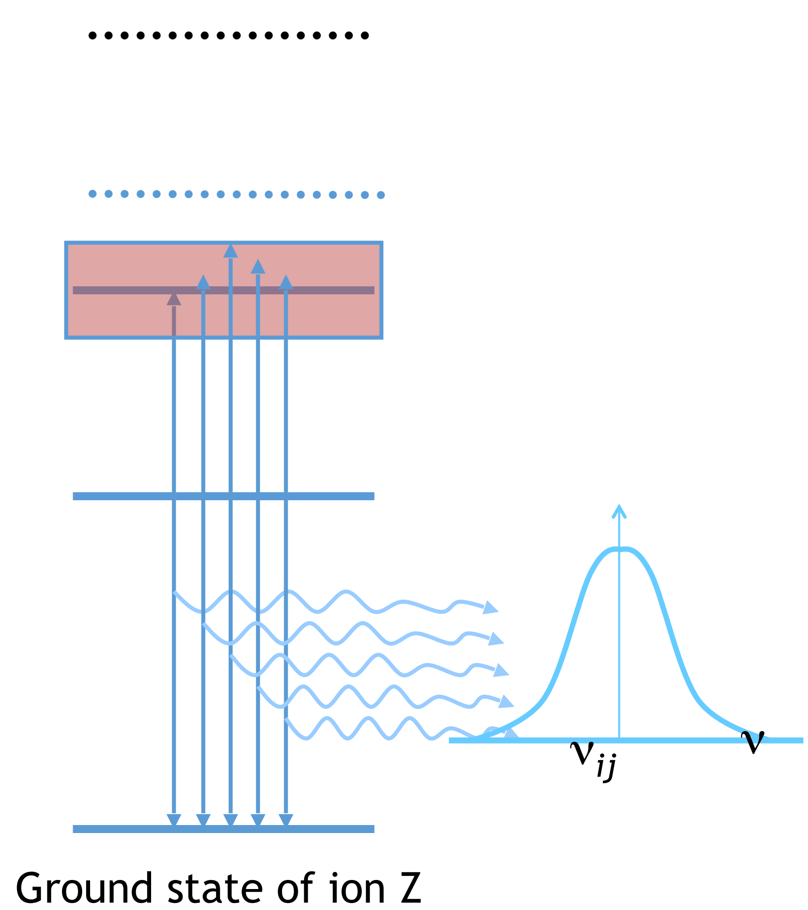
$$\eta_\nu = (2h\nu^3/c^2)\left[\sum_i\sum_{j>i}(g_i/g_j)n_j\alpha_{ij}(\nu) + \sum_i n_i^* e^{-h\nu/kT}\alpha_{i\kappa}(\nu) + \sum_\kappa n_e n_\kappa \alpha_{\kappa\kappa}(\nu,T)e^{-h\nu/kT}\right]$$

$$\chi_\nu = \sum_i\sum_{j>i}[n_i - (g_i/g_j)n_j]\alpha_{ij}(\nu) + \sum_i (n_i - n_i^* e^{-h\nu/kT})\alpha_{i\kappa}(\nu) + \sum_\kappa n_e n_\kappa \alpha_{\kappa\kappa}(\nu,T)(1-e^{-h\nu/kT})$$

4) Line Shape Theory for Radiation Transport

- Line shape theory is a theoretically rich field incorporating quantum-mechanics and statistical mechanics

- Line shapes have provided successful diagnostics for a vast range of plasma conditions
  - Natural broadening (intrinsic)
  - Doppler broadening (T_i)
  - Stark broadening (N_e)
  - Opacity broadening
  - Resonance broadening (neutrals)



5) Particle Energy Distribution

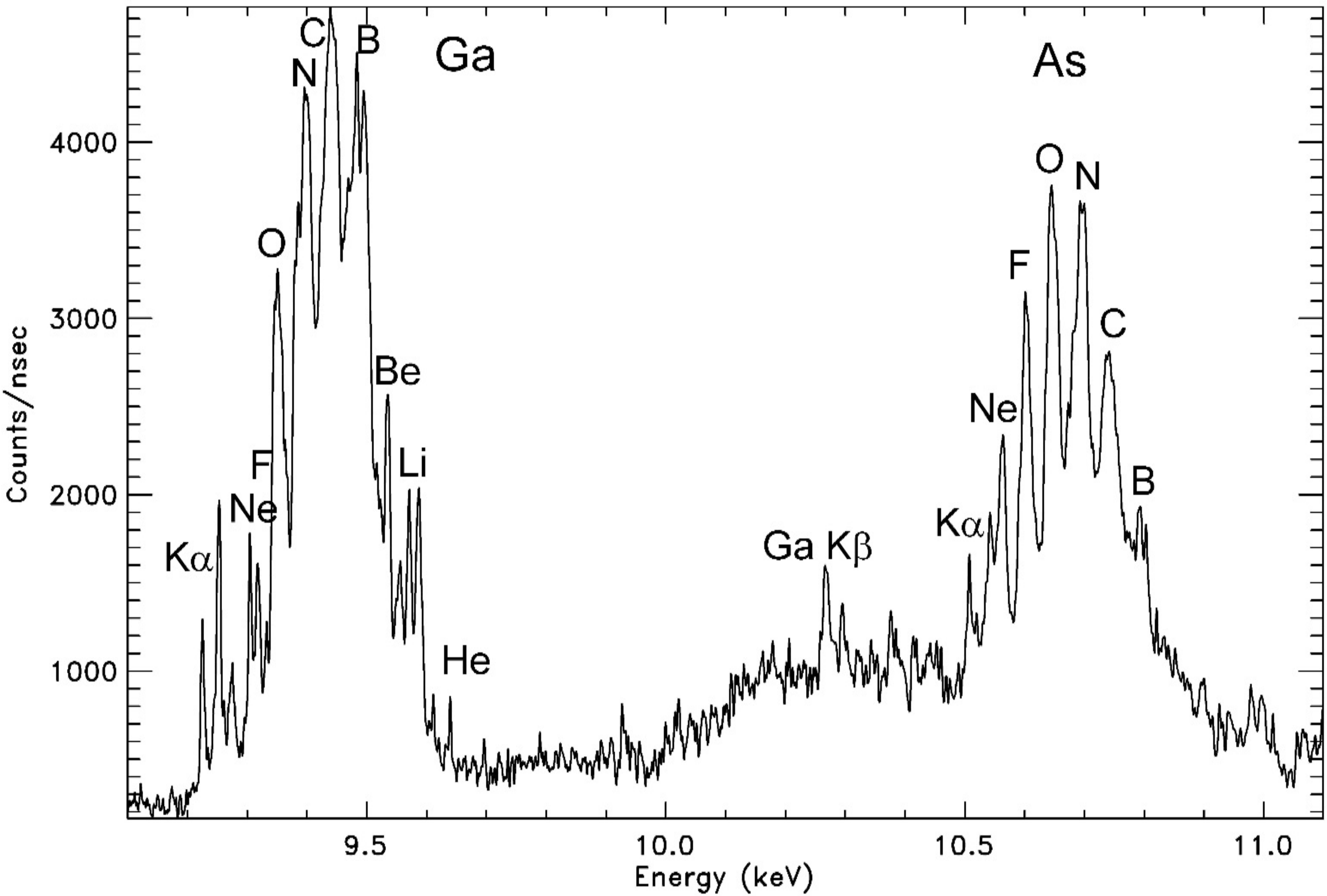
- Time scales are very different between atomic processes and classical particle motions : separation between QM processes and particle mechanics

→ Is this a valid assumption?

- Radiation-Hydrodynamics simulations
  - Fluid treatment of plasma physics
    - Mass, momentum and energy equations solved
  - Plasma thermodynamic properties
  - LTE (Local Thermodynamic Equilibrium) (assumed)

- PIC (Particle-In-Cell) simulations
  - Particle treatment of plasma physics
    - Boltzmann transport and Maxwell equations solved
  - Electron energy distribution function
  - Simple ionization model (assumed)

First, identify lines and then obtain line intensities using a kinetics code and determine the temperature and density of the plasma emission region.



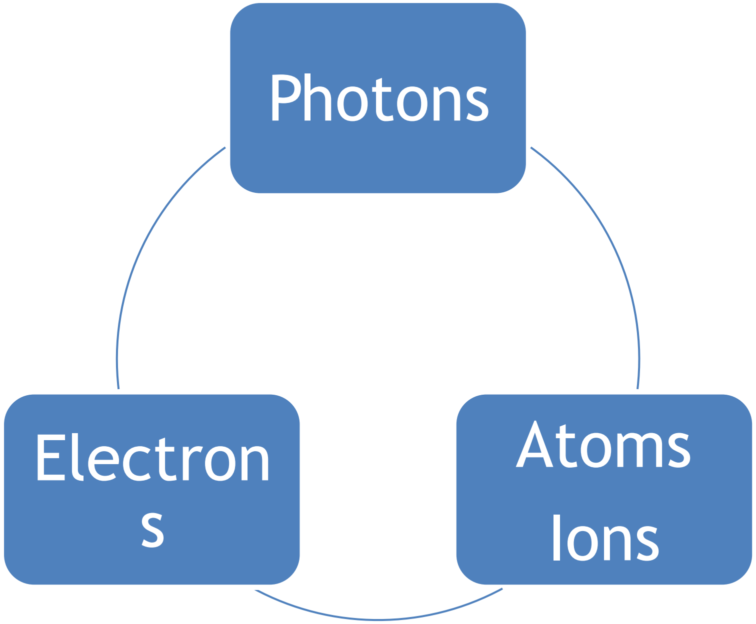
Statistical Distributions of Electronic Level Population Density

3 Representative Models

POPULATION KINETICS MODELS

(1) Thermodynamic equilibrium

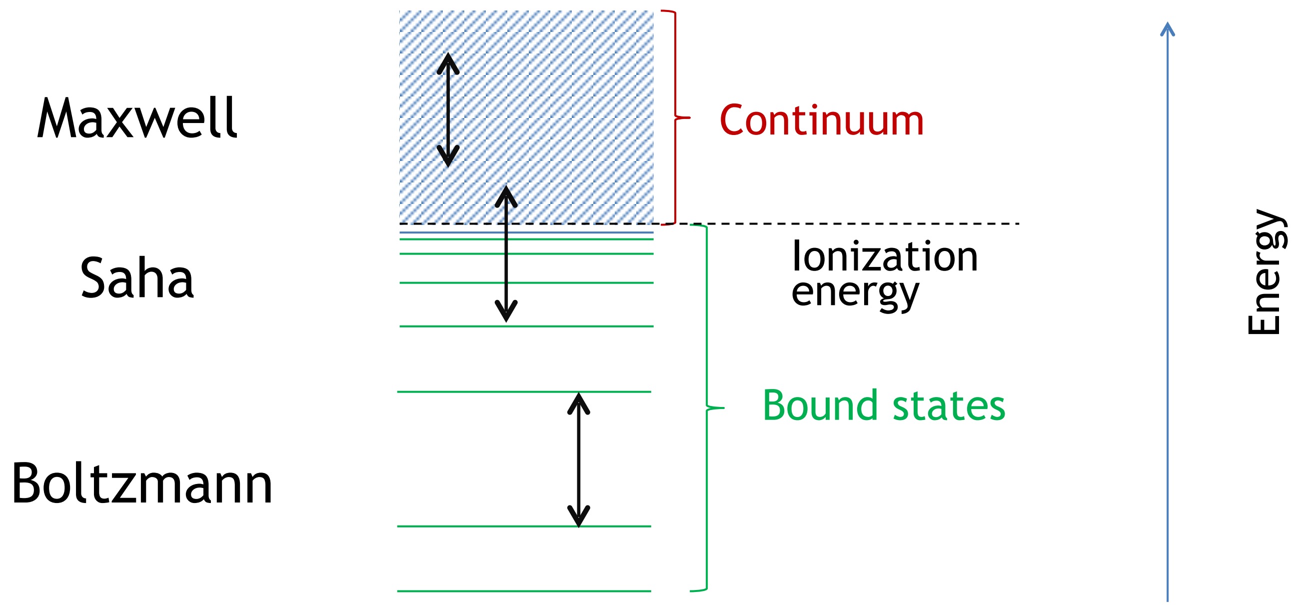
- Principle of detailed balance
  - ***each direct process is balanced by the inverse***
    - radiative decay (spontaneous+stimulated) ↔ photoexcitation
    - photoionization ↔ photorecombination
    - excitation ↔ deexcitation
    - ionization ↔ 3-body recombination
    - autoionization ↔ dielectronic capture



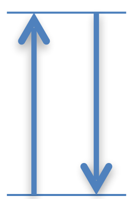
TE: distributions

- Four “systems”: **photons**, **electrons**, **atoms** and **ions**
- Same temperature $T_r = T_e = T_i$
- We know the equilibrium distributions for each of them
  - Photons: Planck
  - Electrons (free-free): Maxwell
  - Populations within atoms/ions (bound-bound): Boltzmann
  - Populations between atoms/ions (bound-free): Saha

TE: energy scheme



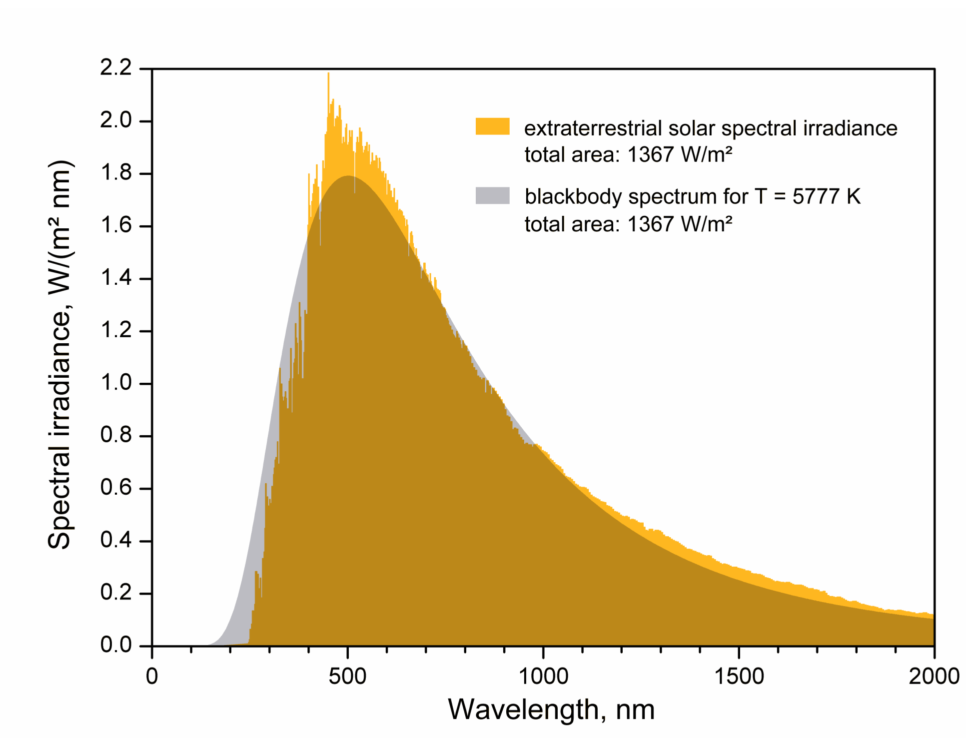
Boltzmann: $$\frac{N_1}{N_2} = \frac{g_1}{g_2}\exp\left(-\frac{E_1 - E_2}{T_e}\right)$$



Planck and Maxwell

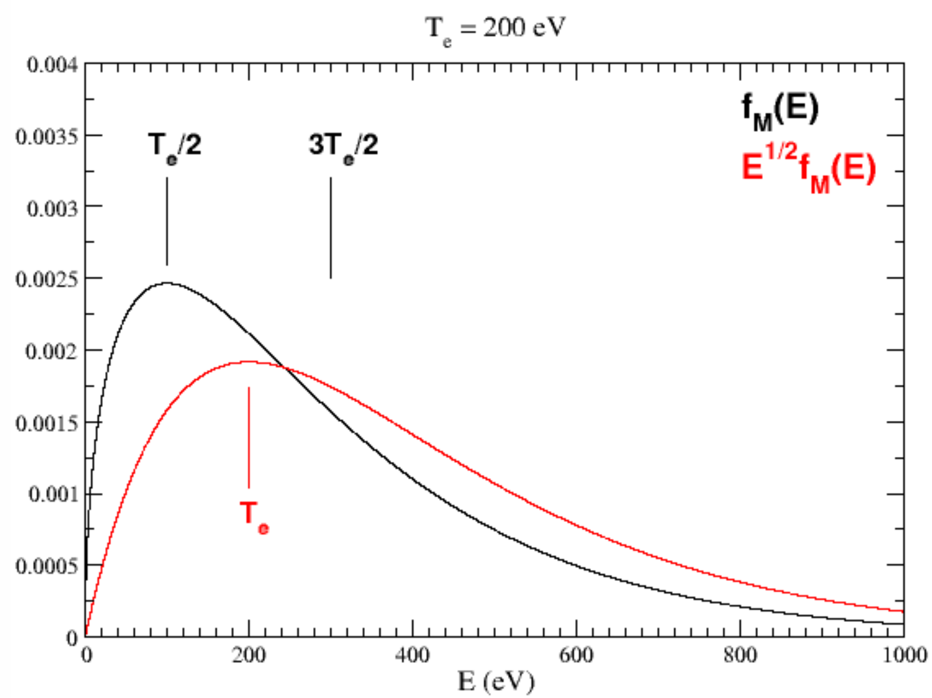
- Planck distribution

$$B(E) = \frac{2E^3}{h^2c^2}\frac{1}{e^{E/T}-1}$$



- Maxwell distribution

$$f_M(E)dE = \frac{2}{\pi^{1/2}T_e^{3/2}}E^{1/2}\exp\left(-\frac{E}{T_e}\right)dE$$

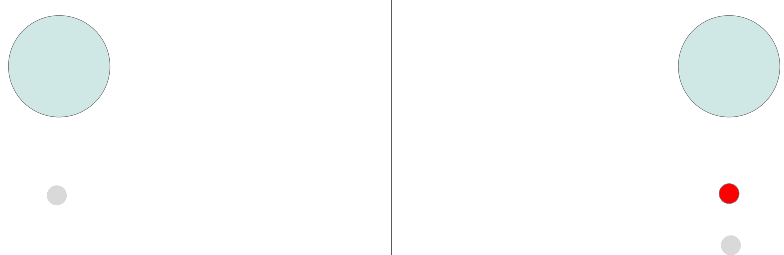


Saha Distribution

$A_Z\ (+\ e) \leftrightarrow A_{Z+1} + e\ (+\ e)$

Z

Z+1



ionization ↔ 3-body recombination

autoionization ↔ dielectronic capture

$$\frac{N^{Z+1}}{N^Z} = \frac{g_{Z+1}}{g_Z} 2 \left(\frac{2\pi m T_e}{h^2} \right)^{3/2} \frac{1}{N_e} e^{-\frac{I_Z}{T_e}}$$

$$g_Z = \sum_i g_{Z,i} e^{-\frac{E_i - E_0}{T_e}}$$

Which ion is the most abundant?

$$\frac{N^{Z+1}}{N^Z} = 1 \qquad \frac{I_Z}{T_e} >> 1 (\sim 10)$$

Local Thermodynamic Equilibrium

- **(Almost) never complete TE:** photons decouple easily…therefore, let's forget about the photons!
- LTE = Saha + Boltzmann + Maxwell

- Griem's criterion for Boltzmann: *collisional rates > 10*radiative rates*

$$N_e\left[cm^{-3}\right] \geq 1.4\times10^{14}\left(\Delta E_{01}\left[eV\right]\right)^3\left(T_e\left[eV\right]\right)^{1/2} \propto Z^7$$

H I (2 eV): 2×10[17] cm[-3]
C V (80 eV): 2×10[22] cm[-3]

- Saha criterion **for low T_e**:

$$N_e\left[cm^{-3}\right] \geq 1\times10^{14}\left(I_z\left[eV\right]\right)^{5/2}\left(T_e\left[eV\right]\right)^{1/2} \propto Z^6$$

H I (2 eV): 10[17] cm[-3]
C V (80 eV): 3×10[21] cm[-3]

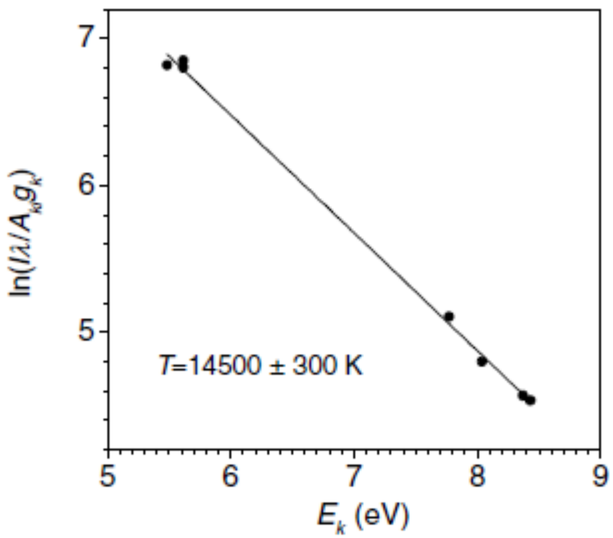
LTE Line Intensities

- ***No atomic transition data*** (only energies and statistical weights) are needed to calculate populations
- Intensity ratio $$\frac{I_1}{I_2} = \frac{N_1 \Delta E_1 A_1}{N_2 \Delta E_2 A_2} = \frac{g_1 \Delta E_1 A_1}{g_2 \Delta E_2 A_2} \exp\left(-\frac{E_1 - E_2}{T_e} \right)$$
- Or just plot the intensities on a log scale:

Boltzmann plot

$$I = N \cdot A \cdot E = \frac{g_i}{G} AE \exp(-E_i / T_e)$$

$$\ln(I / g_i AE) = -E_i / T_e - \ln(G)$$



Aragon et al, J Phys B **44**, 055002 (2011)

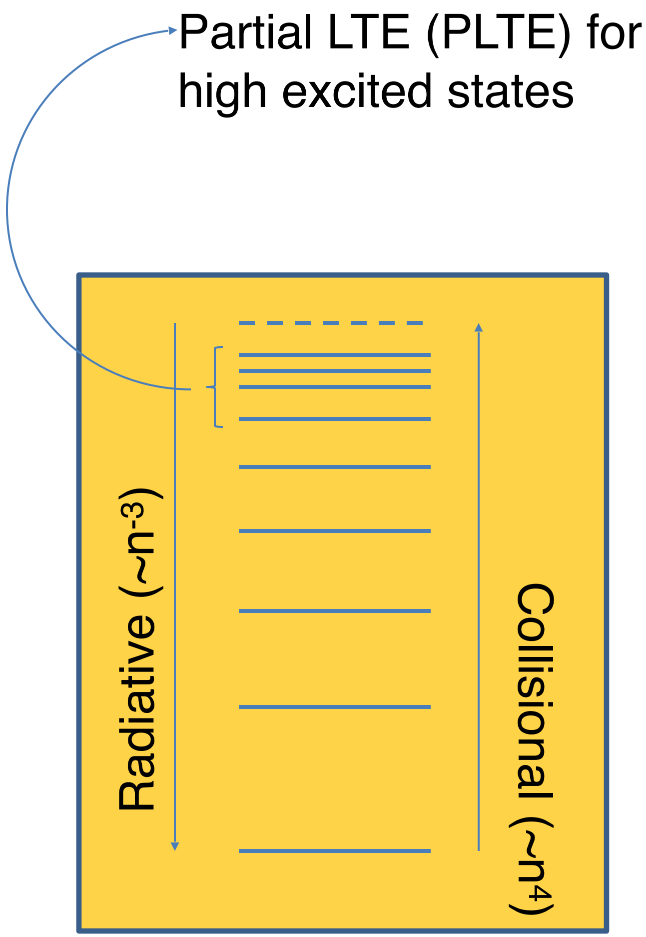
Saha-LTE conclusions

- Collisions >> radiative processes
  - Saha between ions
  - Boltzmann within ions
- Since collisions decrease with Z and radiative processes increase with Z, higher densities are needed for higher ions to reach Saha/LTE conditions
  - H I: 10^{17} cm^{-3}
  - Ar XVIII: 10^{26} cm^{-3}

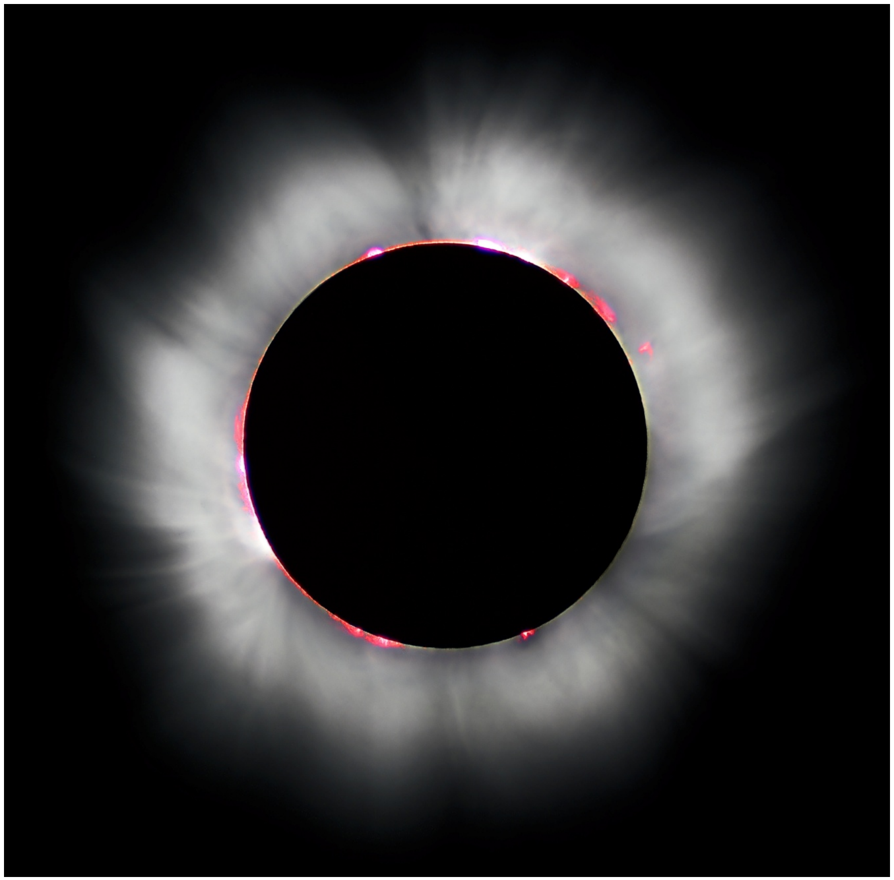
ASD: can calculate Saha/LTE spectra!!!

Deviations from LTE

- Radiative processes are non-negligible
  - LTE: coll.rates (~n_e) > 10*rad.rates
- Non-Maxwellian plasmas
- Unbalanced processes
- Anisotropy
- External fields
- …

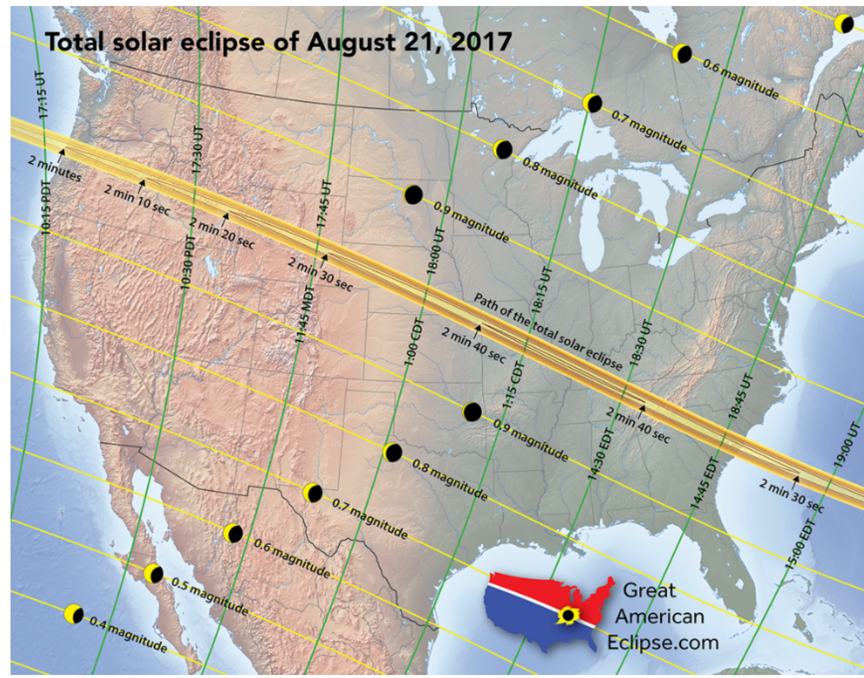


(2) The other limiting case: Coronal Equilibrium



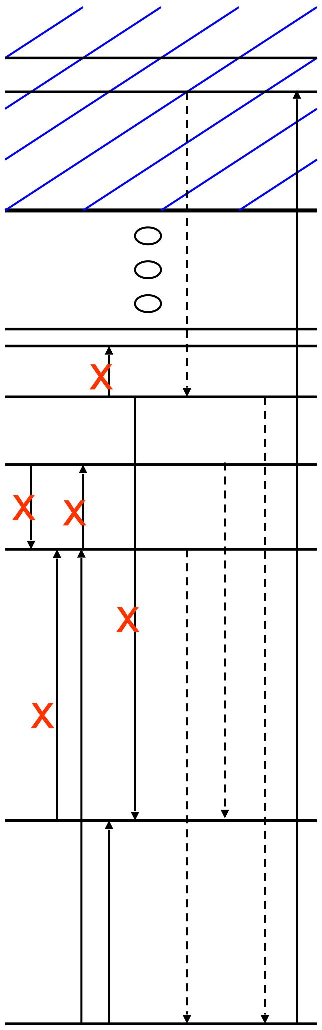
Low electron densities!

Aug 21, 2017



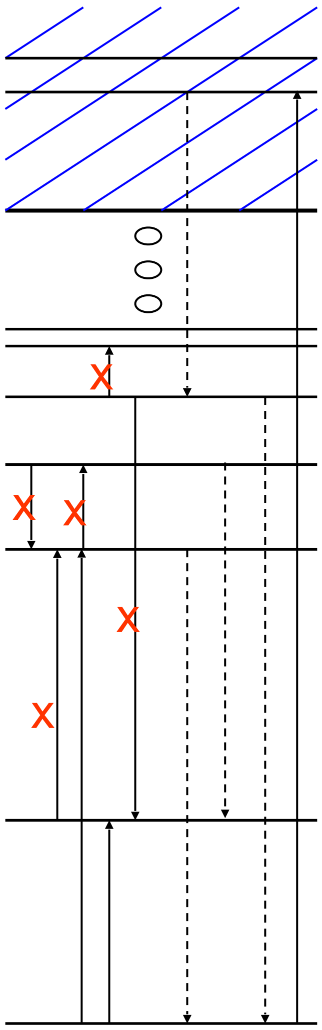
Coronal Model

- High temperature, low density and optically thin plasmas ($J_\nu = 0$)
- Excitations (and ionization) only from ground state…
- …and metastables
- Does require a complete set of collisional cross sections
- Do we have to calculate all direct and inverse processes?..

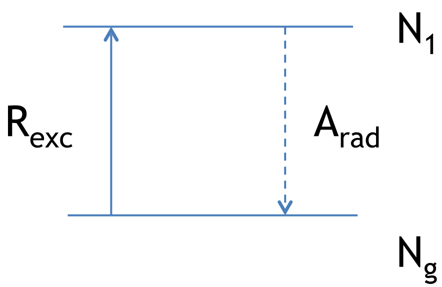


Coronal Model

- Rates (N_e^2) << Rates (N_e) << Rates (spontaneous)
  - 3-body recombination not important
  - Collisional processes from excited levels dominated by spontaneous radiative decays
  - Left with collisional processes from ground levels and radiative processes from excited levels
- Atomic processes:
  - Collis. ionization (including EA),
  - Radiative recombination (including DR)
  - Collisional excitation
  - Radiative decay (including cascades)
- Ions basically in their ground state
- Ionization decoupled from excitation



Line Intensities under CE



Balance equation:

small populations!

$$N_g R_{exc} = N_1 A_{rad}$$

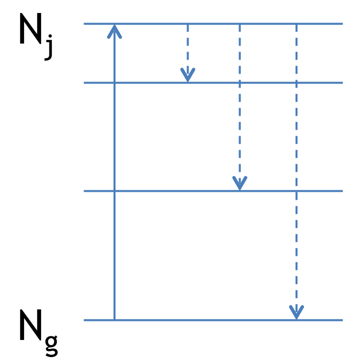
$$N_1 = \frac{N_g R_{exc}}{A_{rad}} = \frac{N_g N_e \langle v\sigma \rangle}{A_{rad}}$$

$$I = N_1 A_{rad} E = \underline{N_g R_{exc}} E$$

Line intensity does NOT depend on A_{rad}!

$I \propto N_e$

If more than one radiative transition:



$$N_g R_{exc} = N_j \sum_{i<j} A_{ij}$$

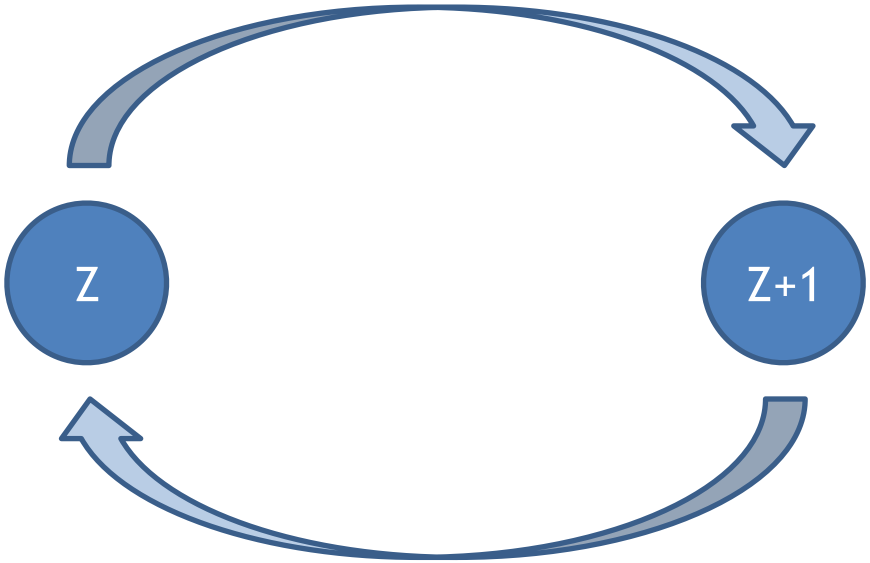
$$N_j = \frac{N_g R_{exc}}{\sum_{i<j} A_{ij}} = \frac{N_g N_e \langle v\sigma_{jg} \rangle}{\sum_{i<j} A_{ij}}$$

$$I_{ij} = N_j E_{ij} A_{ij} = N_g N_e \langle v\sigma_{jg} \rangle \frac{A_{ij}}{\sum_{k<j} A_{kj}}$$

Also cascades may be important

Ionization Balance in CE

Electron-impact ionization: $\propto N_e$



$$\frac{N_{Z+1}}{N_Z} = \frac{N_e \langle v\sigma \rangle_{ion}}{N_e \langle v\sigma \rangle_{RR} + N_e \langle v\sigma \rangle_{DR}}$$

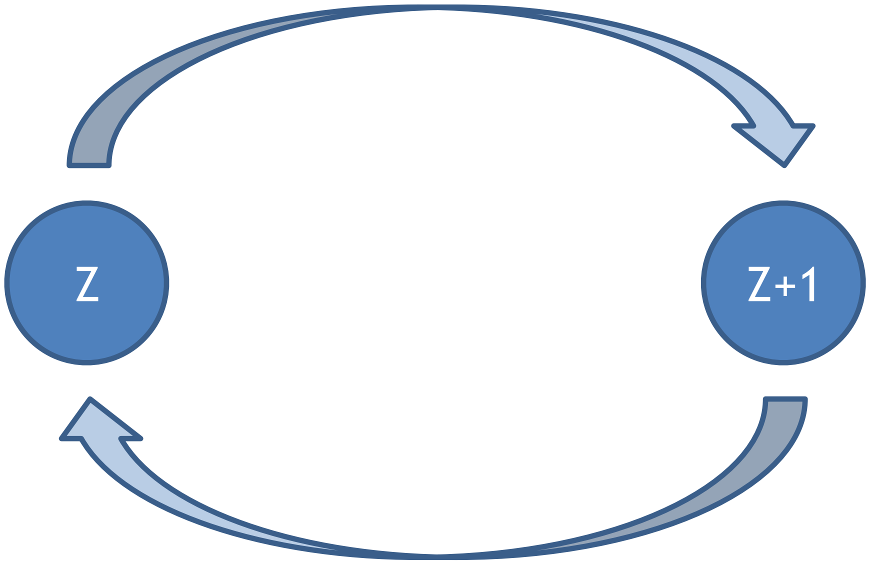
Independent of N_e!

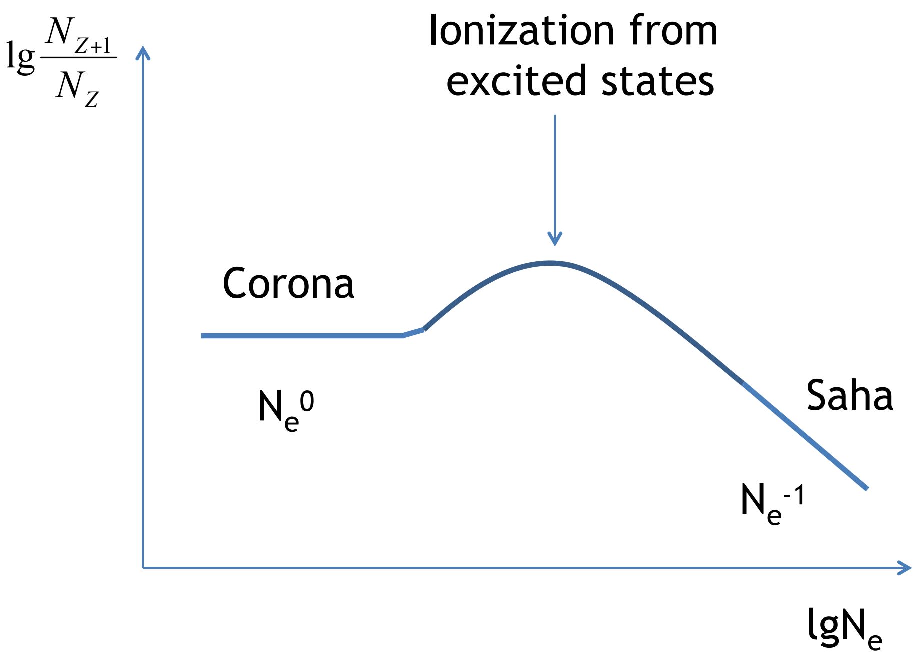
Photo recombination and Dielectronic recombination: $\propto N_e$

Most abundant ion: $\frac{I_Z}{T_e} \sim 3 \ (Z_N < 30)$

Ionization Balance in a General Case

Electron-impact ionization: $\propto N_e$

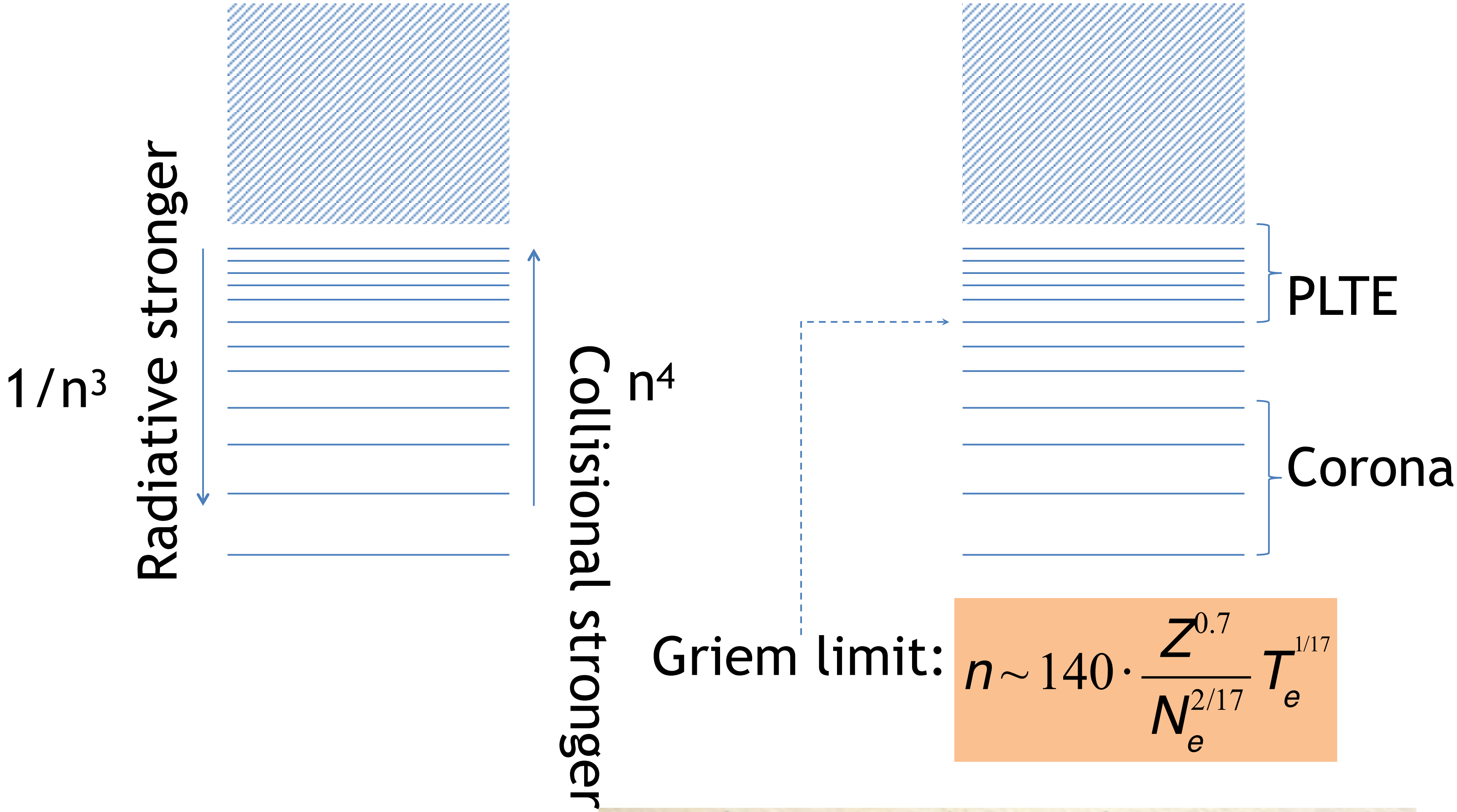




Photorecombination and Dielectronic recombination: $\propto N_e$

3-body recombination: $\propto N_e^2$

From Corona to PLTE



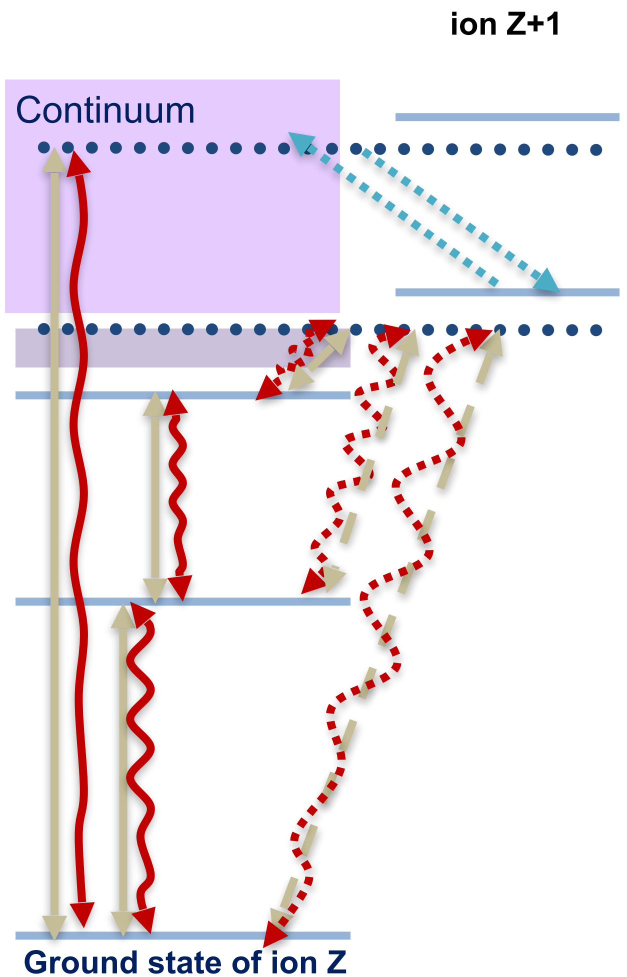
Griem limit: $n \sim 140 \cdot \frac{Z^{0.7}}{N_e^{2/17}} T_e^{1/17}$

Results in another Wilson criterion

$n_e < 4\times10^{21}\, q^{-1}(kT/1\mathrm{keV})^4\ \mathrm{cm}^{-3}$

(3) Collisional-Radiative Model

- Population distribution is obtained by rate equations considering collisional and radiative processes, along with plasma effects
- *Excited states* are substantially populated and *increase the total ionization* by step-wise ionization processes
- The 3-body recombination to these states is proportional to n^4 and N_e^2 and excited states can significantly *enhance the total recombination*.
- Plasma effects such as non-local radiation transport, fast particle collisions and density effects should be included in the model.
- Self-absorption (radiation pumping) should be included for treating radiative processes involving optically thick lines.



Collisional-Radiative Model

Basic rate equation

$$\hat{N} = \begin{pmatrix} \cdots \\ N_{Z,i} \\ \cdots \end{pmatrix}$$

Vector of atomic states populations

$$\frac{d\hat{N}(t)}{dt} = \hat{A}\left(t, \hat{N}(t), N_e, N_i, T_e, T_i \ldots\right) \hat{N}(t) + \hat{S}(t)$$

Rate matrix

Source function

Off-diagonal: total rates of all processes between two levels
Diagonal: total destruction rates for a level

Basic rate equation (cont'd)

$$\frac{dN_{Zi}}{dt} = \sum_{j<i} N_{Z,j}\left(R_{Z,ji}^{e-exc} + R_{Z,ji}^{h-exc} + B_{Z,ji}^{p-exc}\right)$$

$$+ \sum_{j>i} N_{Z,j}\left(R_{Z,ji}^{e-dexc} + R_{Z,ji}^{h-dexc} + A_{Z,ji}^{sp-rad} + B_{Z,ji}^{st-rad}\right)$$

$$+ \sum_{Z'>Z}\sum_{k\in Z'} N_{Z',k}\left(\alpha_{Z'k,Zi}^{3b} + \alpha_{Z'k,Zi}^{rr} + \alpha_{Z'k,Zi}^{dc} + \alpha_{Z'k,Zi}^{cx}\right)$$

$$+ \sum_{Z'<Z}\sum_{k\in Z'} N_{Z',k}\left(S_{Z'k,Zi}^{e-ion} + S_{Z'k,Zi}^{i-ion} + S_{Z'k,Zi}^{p-ion} + S_{Z'k,Zi}^{cx}\right)$$

$$- N_{Z,i} \times$$

$$\left(\sum_{j>i}\left(R_{Z,ij}^{e-exc} + R_{Z,ij}^{h-exc} + B_{Z,ij}^{p-exc}\right) + \sum_{j<i}\left(R_{Z,ji}^{e-dexc} + R_{Z,ji}^{h-dexc} + A_{Z,ji}^{sp-rad} + B_{Z,ji}^{st-rad}\right)\right.$$

$$+ \sum_{Z'<Z}\sum_{k\in Z'}\left(\alpha_{Zi,Z'k}^{3b} + \alpha_{Zi,Z'k}^{rr} + \alpha_{Zi,Z'k}^{dc} + \alpha_{Zi,Z'k}^{cx}\right)$$

$$\left. + \sum_{Z'<Z}\sum_{k\in Z'}\left(S_{Zi,Z'k}^{e-ion} + S_{Zi,Z'k}^{i-ion} + S_{Zi,Z'k}^{p-ion} + S_{Zi,Z'k}^{cx}\right)\right)$$

$$+ S_i$$

CR model: features

1. Most general approach to population kinetics
2. Depends on detailed atomic data and requires a lot of it…
3. Should reach Saha/LTE conditions at high densities and coronal at low
4. May includes tens up to millions of atomic states

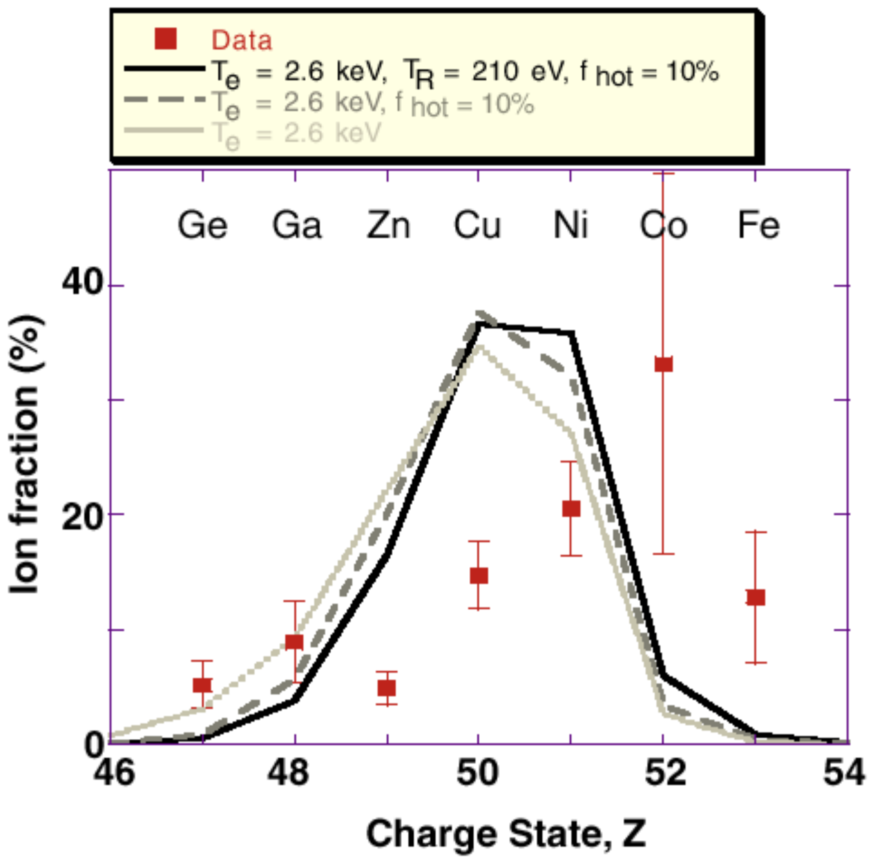
CR model: questions to ask

1. What state description is relevant?
2. Which level of data accuracy is sufficient for this particular problem?
3. How to calculate the rates? What is the source of the data?
4. What are the most (and not so) important physical processes?
5. Which plasma effects are important? Opacity? IPD?

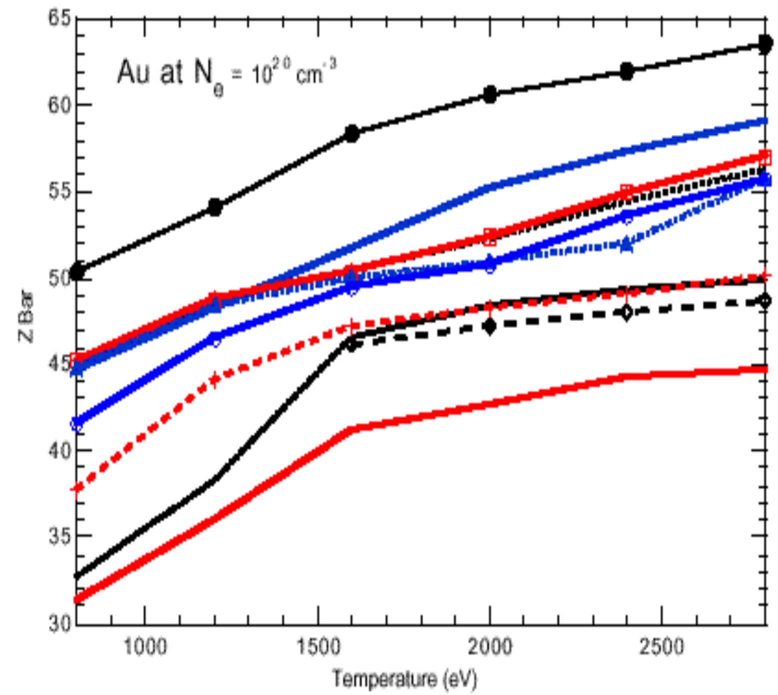
There is NO universal CR model for all cases

Non-LTE plasmas have well documented problems for experiment and theory

Au M-shell emission
Glenzer et al. PRL (2001)



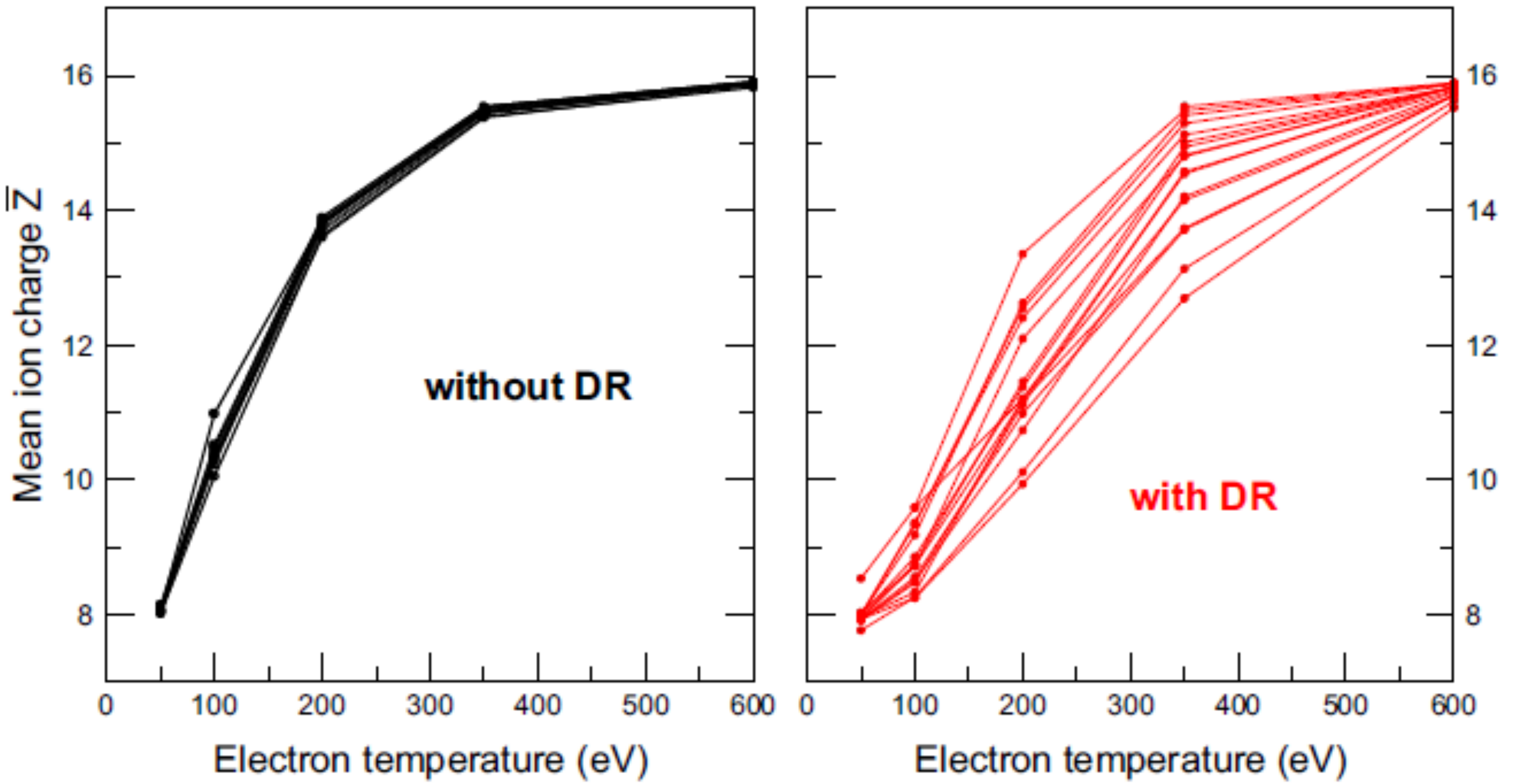
1st Non-LTE workshop (1996) documented large differences between codes for Au



- Note the wide range of predicted average ionization state

Dielectronic Recombination and Excitation Autoionization

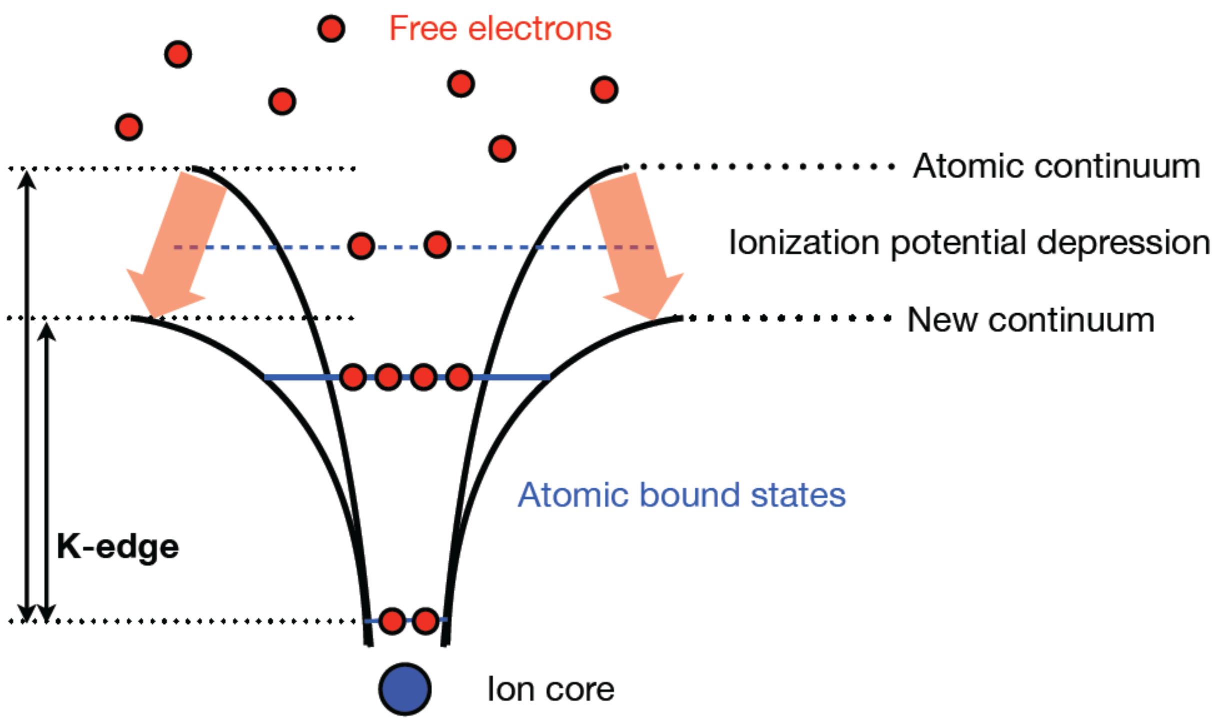
NLTE 6&7 Mean ion charges for Ar case, $n_e = 10^{12}\ cm^{-3}$



NLTE Workshops 6&7, Chung et al. HEDP 9, 645 (2013)

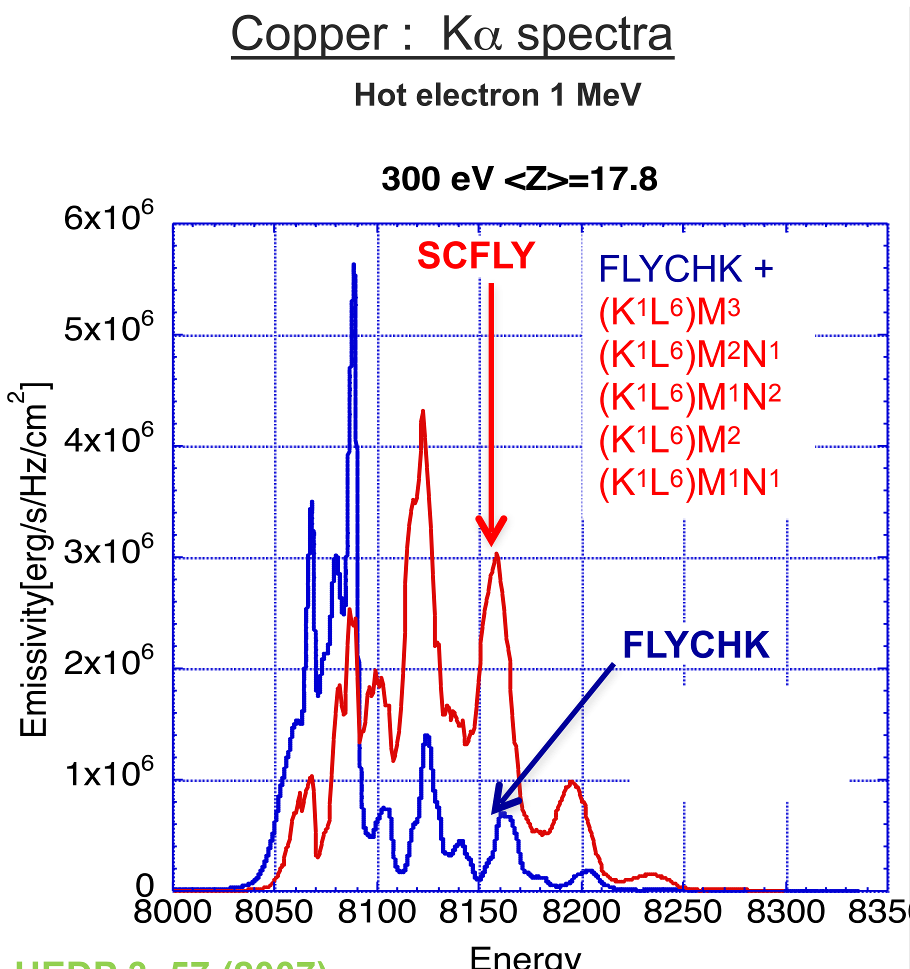
Pressure ionization / Ionization Potential Depression of HED matter

- For dense plasmas, high-lying states are no longer bound due to interactions with neighbouring atoms and ions leading to a "pressure ionization"
- Ionization potentials are a function of plasma conditions

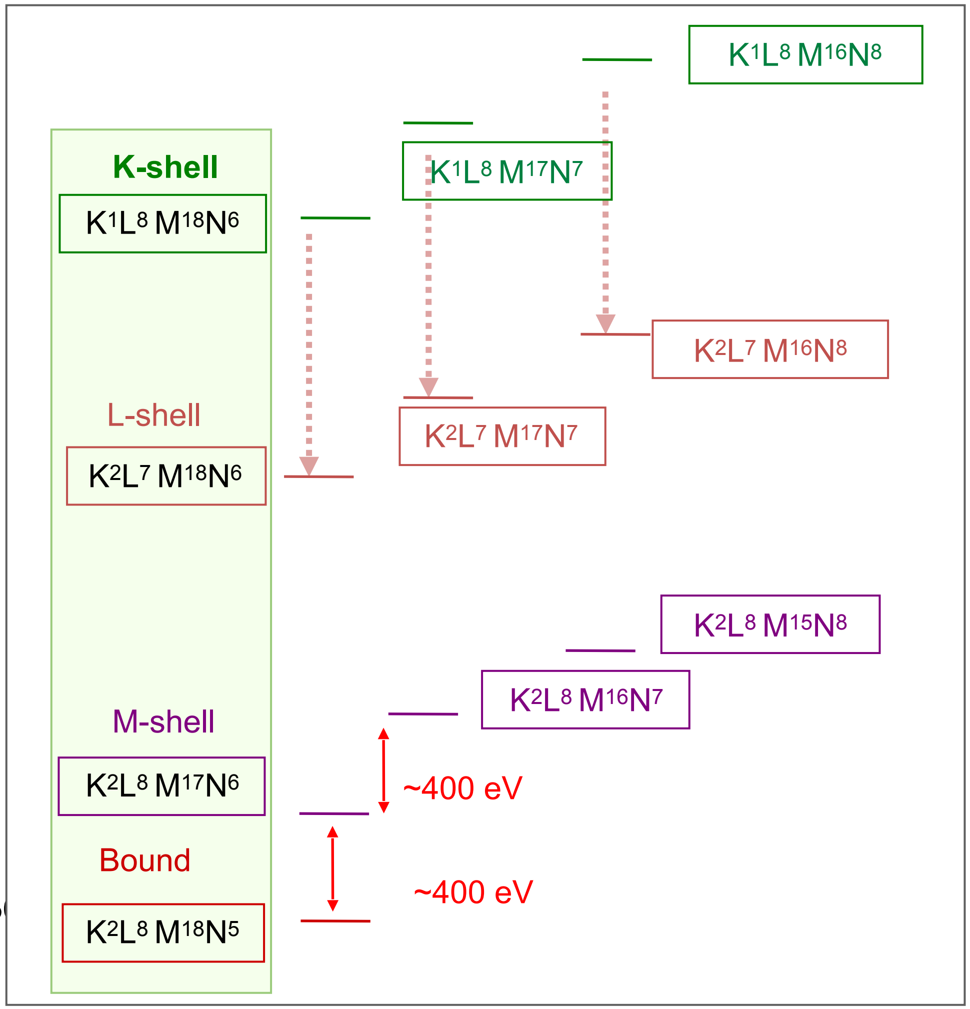


Completeness in Level Configurations

- FLYCHK uses the minimal set of configurations for NLTE plasmas
- For WDM matter the set of configurations need to be expanded

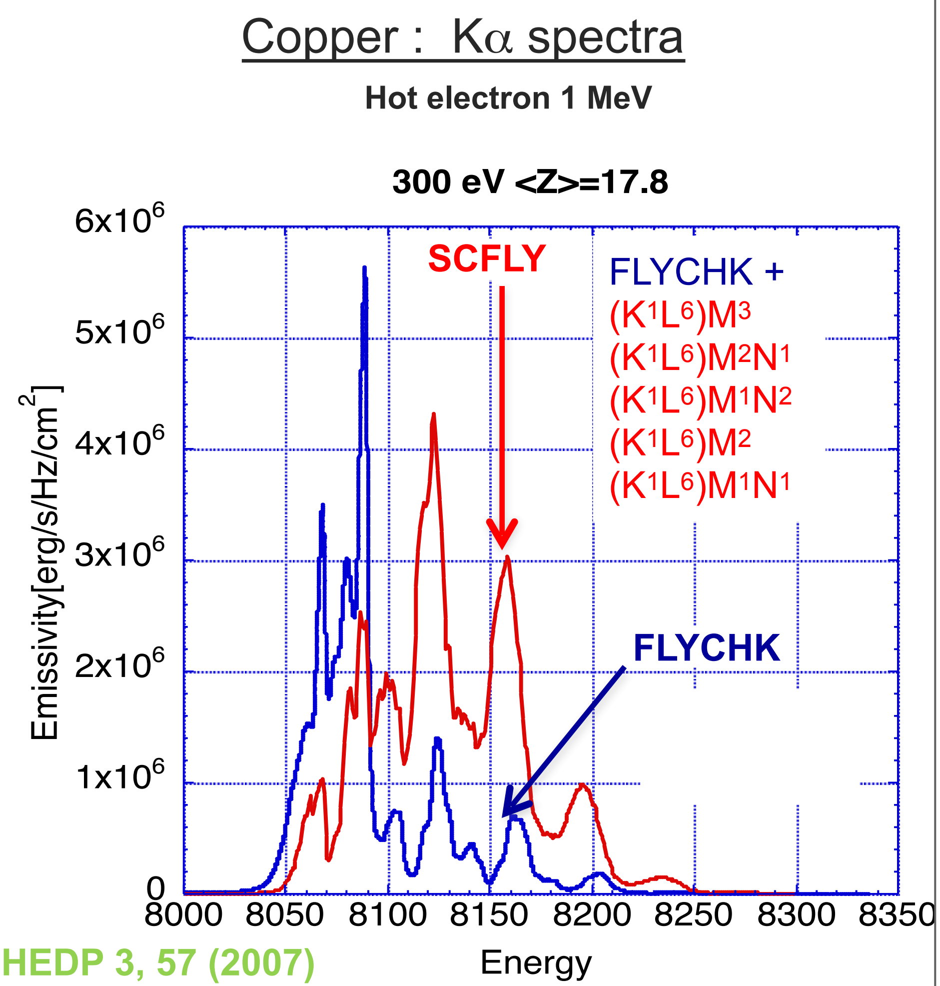


HEDP 3, 57 (2007)

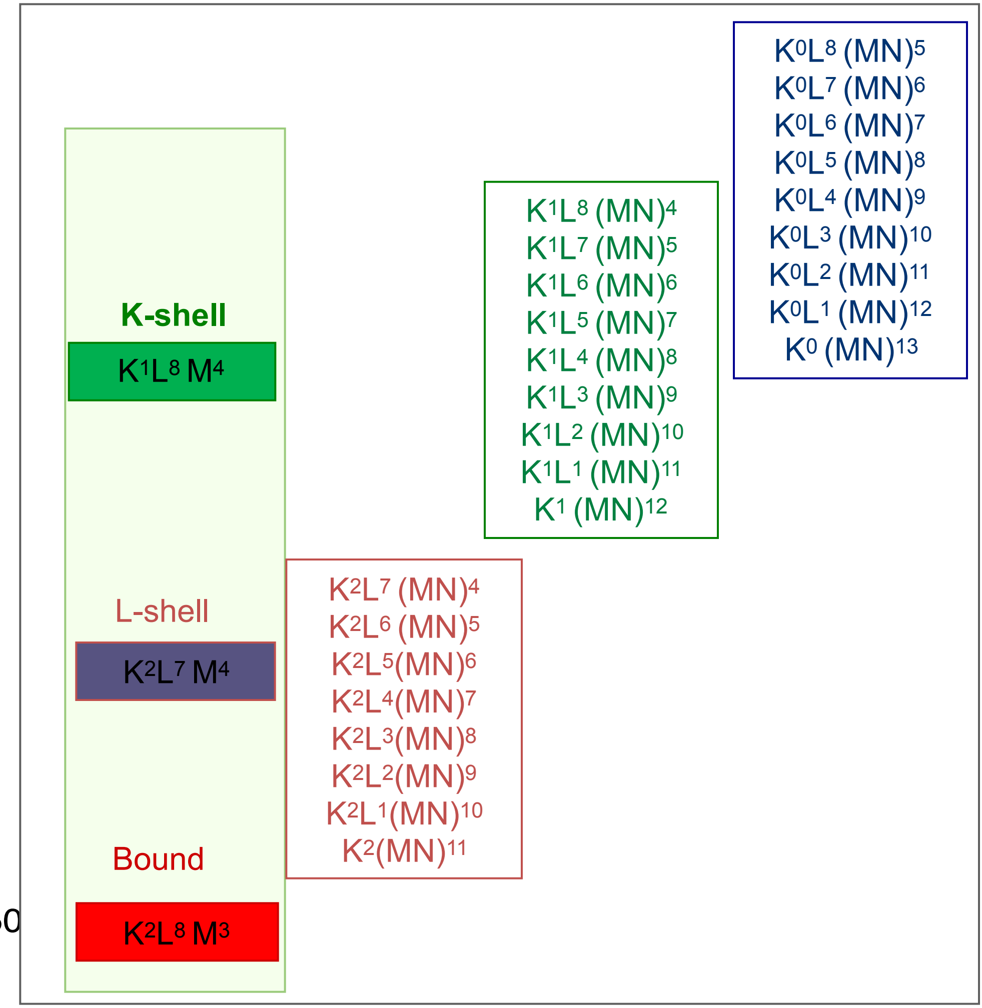


Completeness in Level Configurations for Dense Matter

- FLYCHK uses the minimal set of configurations for NLTE plasmas
- For WDM matter the set of configurations need to be expanded



HEDP 3, 57 (2007)

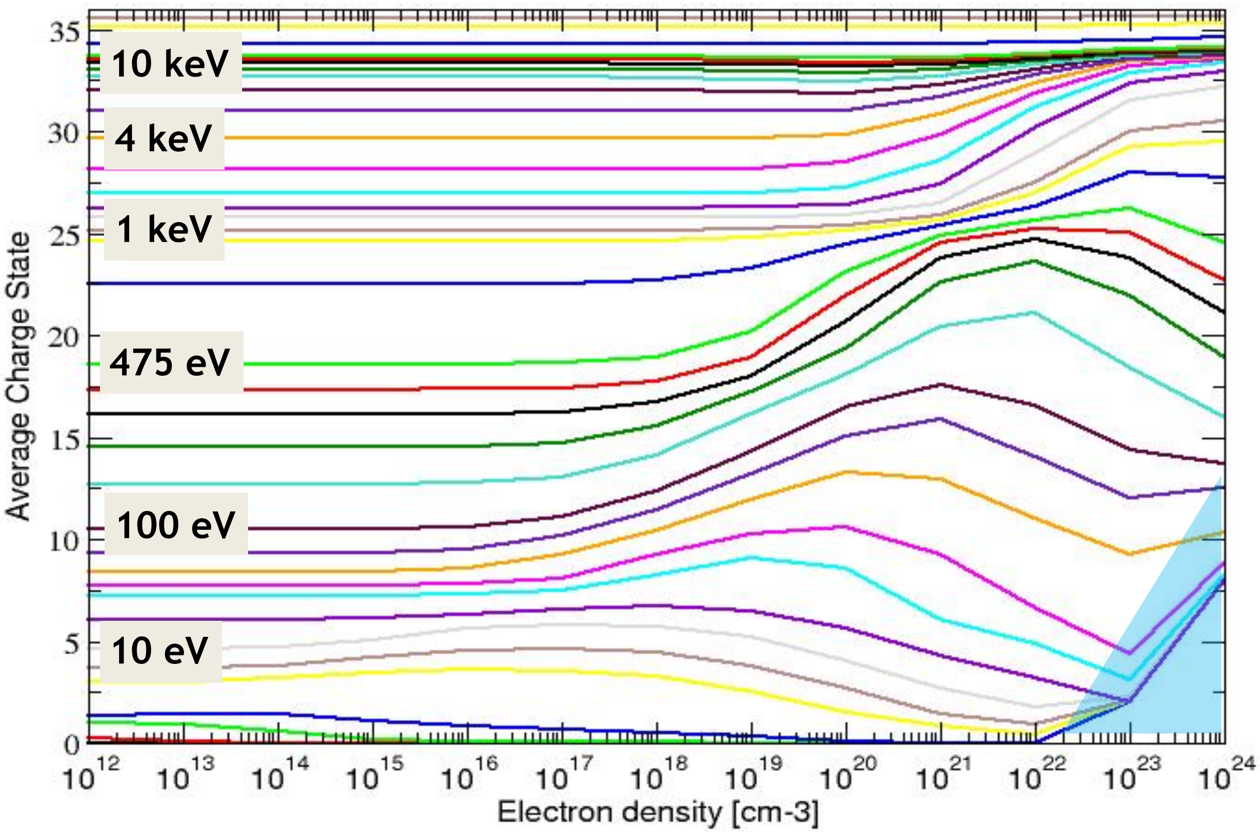


Average charge states as a function of electron density

Stepwise excitation via excited states → <Z> increase

3-body recombination via Rydberg states → <Z> decrease

Pressure ionization of excited states and ionization potential depression → <Z> increase



Krypton

FLYCHK

T_e=0.5 eV-100 keV

$N_e=10^{12}$-10^{24} cm^{-3}

LINE INTENSITY RATIO ANALYSIS

Spectral Line Intensity (<u>optically thin</u>)

Upper state density (cm^{-3})

Einstein coefficient or transition probability (s^{-1})

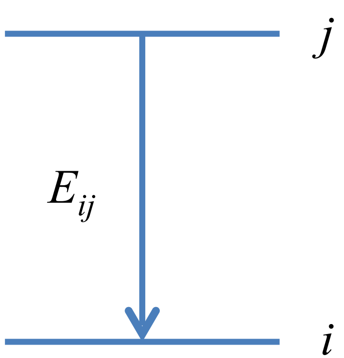
strongly depends on plasma conditions

$$I_{ij} = N_j \cdot A_{ij} \cdot h\nu_{ij}$$

(*almost*) purely atomic parameters

Energy emitted due to a specific transition from a unit volume per unit time

Photon energy (J)



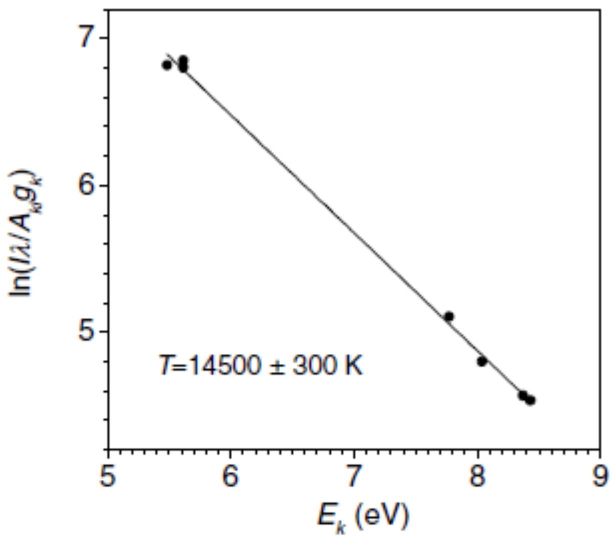
(partial-) LTE Line Intensities

- ***No atomic transition data*** (only energies and statistical weights) are needed to calculate populations
- Intensity ratio $$\frac{I_1}{I_2} = \frac{N_1 \Delta E_1 A_1}{N_2 \Delta E_2 A_2} = \frac{g_1 \Delta E_1 A_1}{g_2 \Delta E_2 A_2} \exp\left(-\frac{E_1 - E_2}{T_e}\right)$$
- Or just plot the intensities on a log scale:

Boltzmann plot

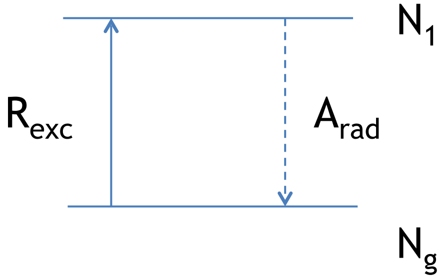
$$I = N \cdot A \cdot E = \frac{g_i}{G} AE \exp(-E_i / T_e)$$

$$\ln(I / g_i AE) = -E_i / T_e - \ln(G)$$



Aragon et al, J Phys B **44**, 055002 (2011)

Line Intensities under CE



Balance equation:

$$N_g R_{exc} = N_1 A_{rad}$$

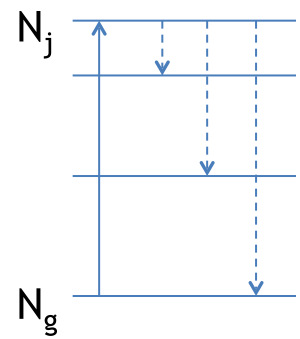
$$N_1 = \frac{N_g R_{exc}}{A_{rad}} = \frac{N_g N_e \langle v\sigma \rangle}{A_{rad}}$$

$$I = N_1 A_{rad} E = \underline{N_g R_{exc}} E$$

Line intensity does NOT depend on A_{rad}!

$I \propto N_e$

If more than one radiative transition:



$$N_g R_{exc} = N_j \sum_{i<j} A_{ij}$$

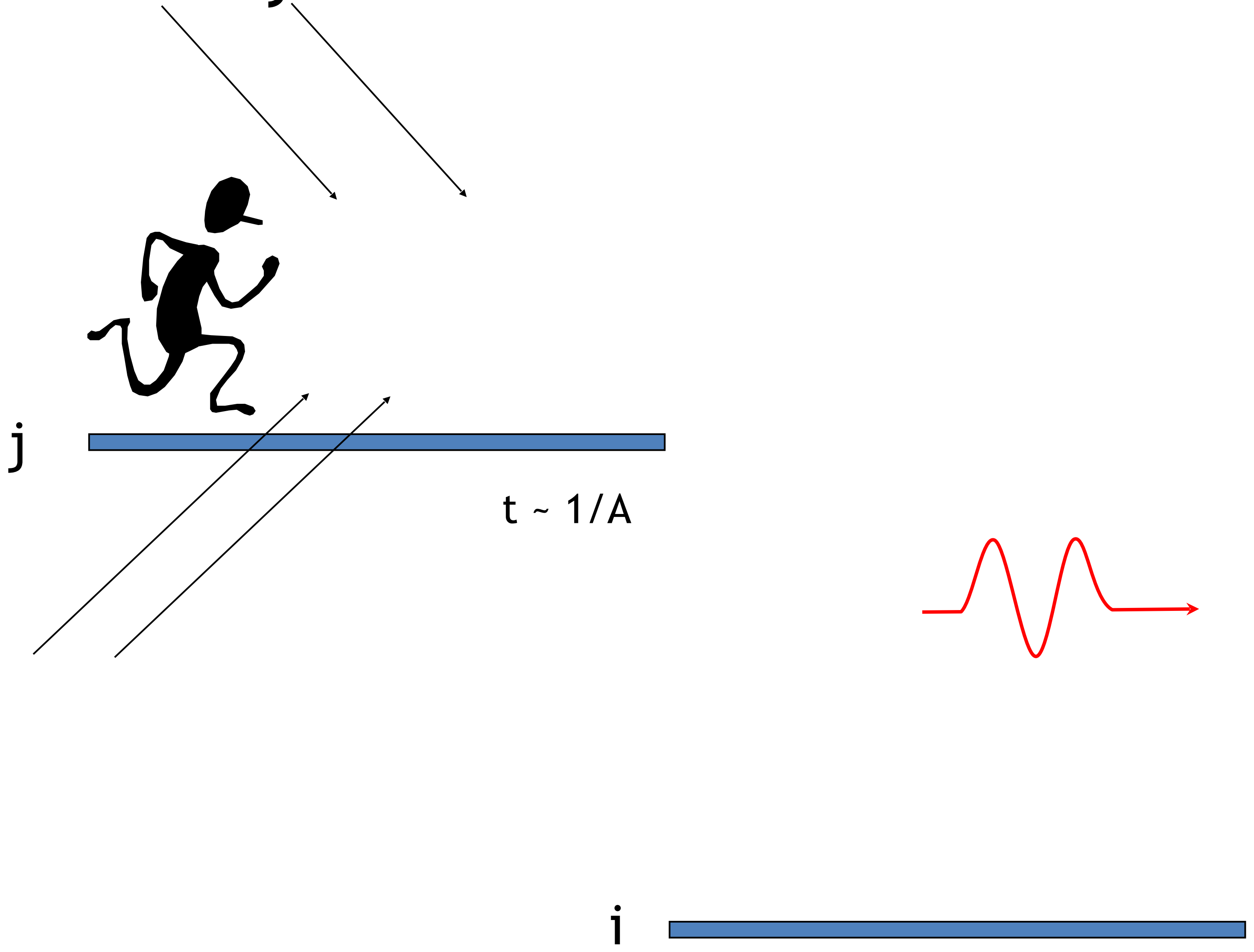
$$N_j = \frac{N_g R_{exc}}{\sum_{i<j} A_{ij}} = \frac{N_g N_e \langle v\sigma_{jg} \rangle}{\sum_{i<j} A_{ij}}$$

$$I_{ij} = N_j E_{ij} A_{ij} = N_g N_e \langle v\sigma_{jg} \rangle \frac{A_{ij}}{\sum_{k<j} A_{kj}}$$

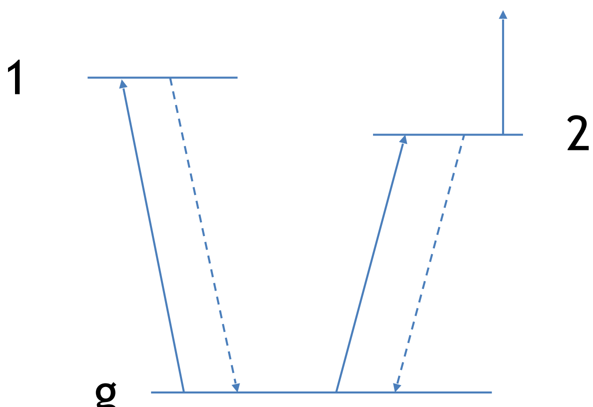
General ideas for line intensity ratio diagnostics

- Electron density
  - Collisional dumping (density-dependent outflux)
  - Density-dependent influx
- Electron temperature
  - Different parts of Maxwellian populate different lines (upper levels)

Why are the forbidden lines sensitive to density?



Let put him into a formula:



Strong transition

$$N_g n_e \langle \sigma v \rangle_{g1} = N_1 A_1$$

$$N_g n_e \langle \sigma v \rangle_{g2} = N_2 A_2 + N_2 n_e \langle \sigma v \rangle_2$$

$$N_1 = \frac{N_g n_e \langle \sigma v \rangle_{g1}}{A_1}$$

$$N_2 = \frac{N_g n_e \langle \sigma v \rangle_{g2}}{A_2 + n_e \langle \sigma v \rangle_2}$$

$$\frac{N_1 A_1}{N_2 A_2} = \frac{\langle \sigma v \rangle_{g1}}{\langle \sigma v \rangle_{g2}} \cdot \frac{A_2 + n_e \langle \sigma v \rangle_2}{A_2}$$

E.g., resonance to intercombination lines in He-like ions

Dielectronic satellites

1s^2 – *1s2p*: resonance lines in He-like ions

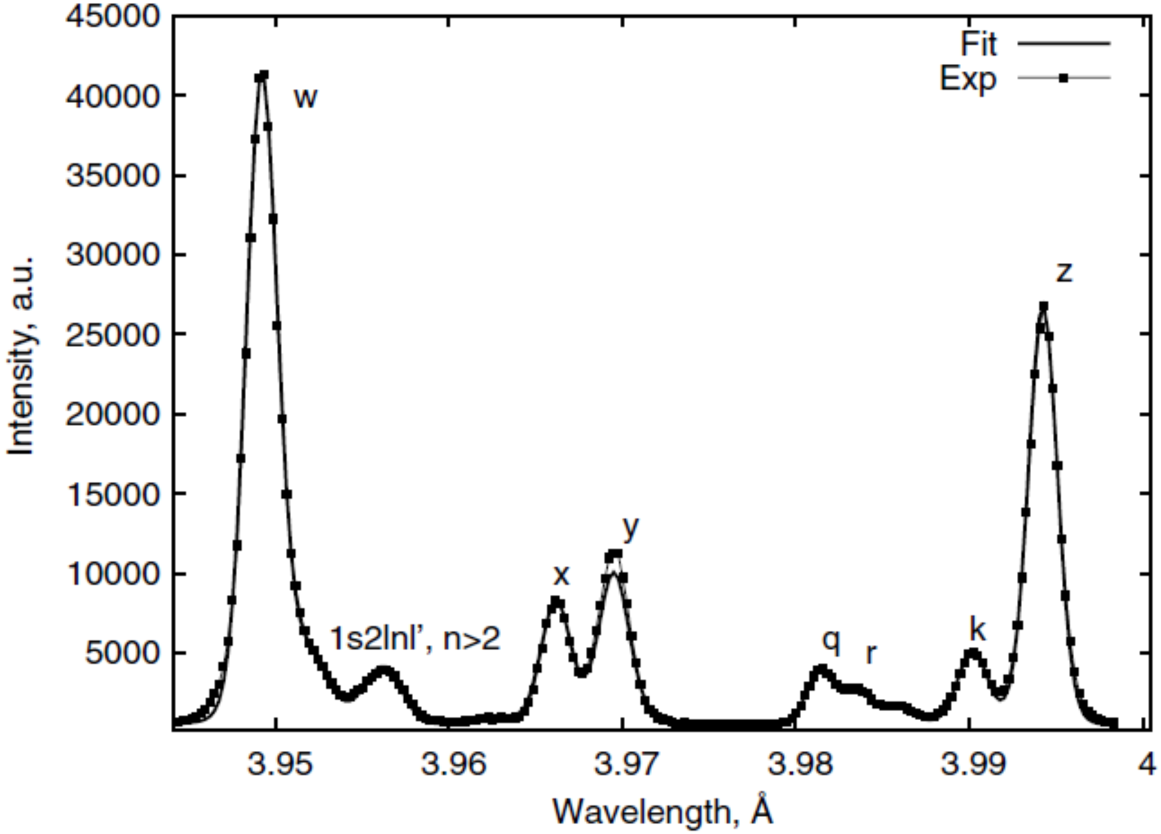
1s^2*nl* – *1s2pnl*: satellite to a resonance line (Li-like ion)

Main population mechanism:
dielectronic capture (resonance process!)

$$1s^2 + e \rightarrow \quad 1s2lnl' \rightarrow \quad 1s^2nl' + h\nu$$

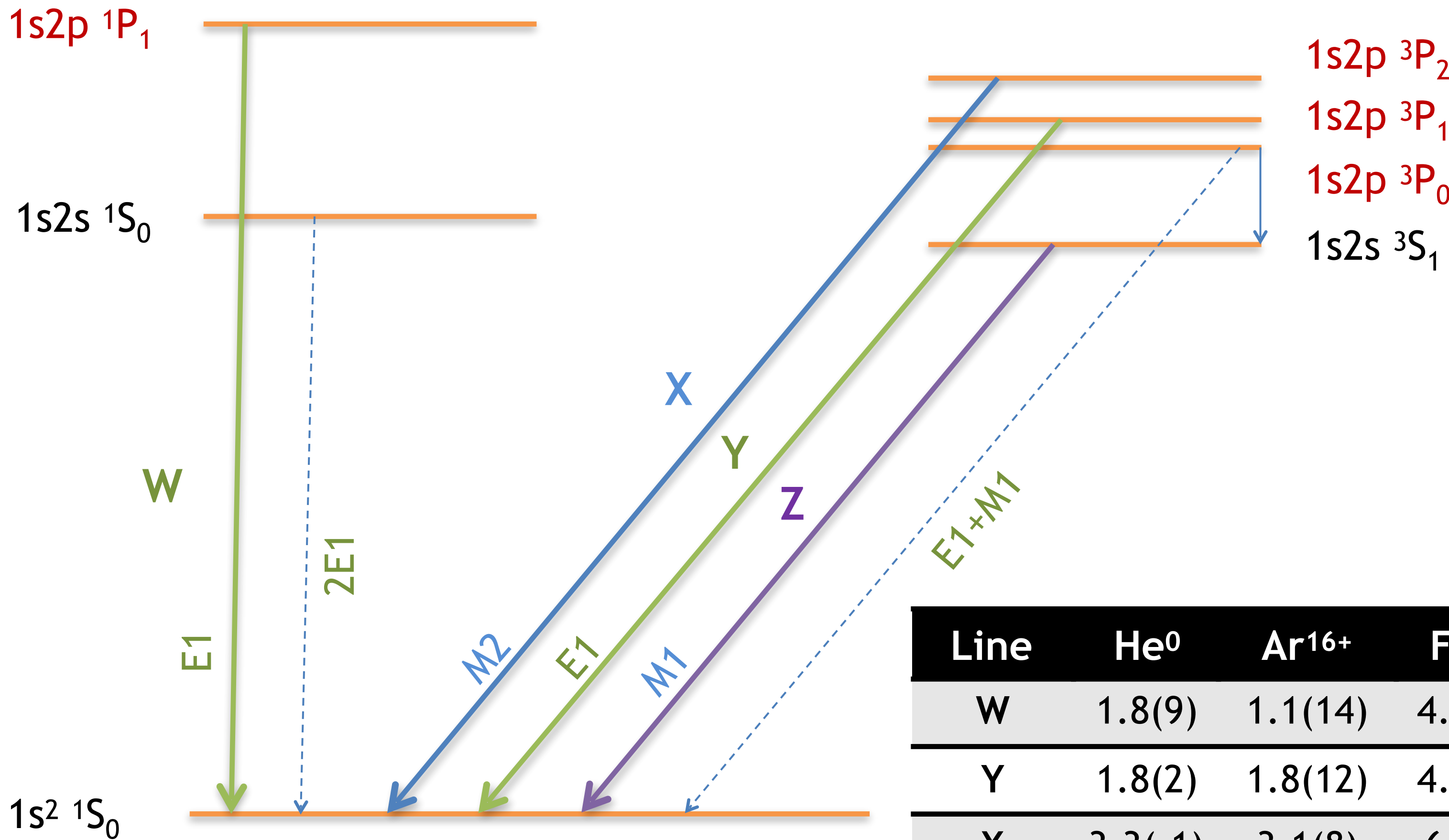
Also in H-like and other ions

He-like lines and satellites



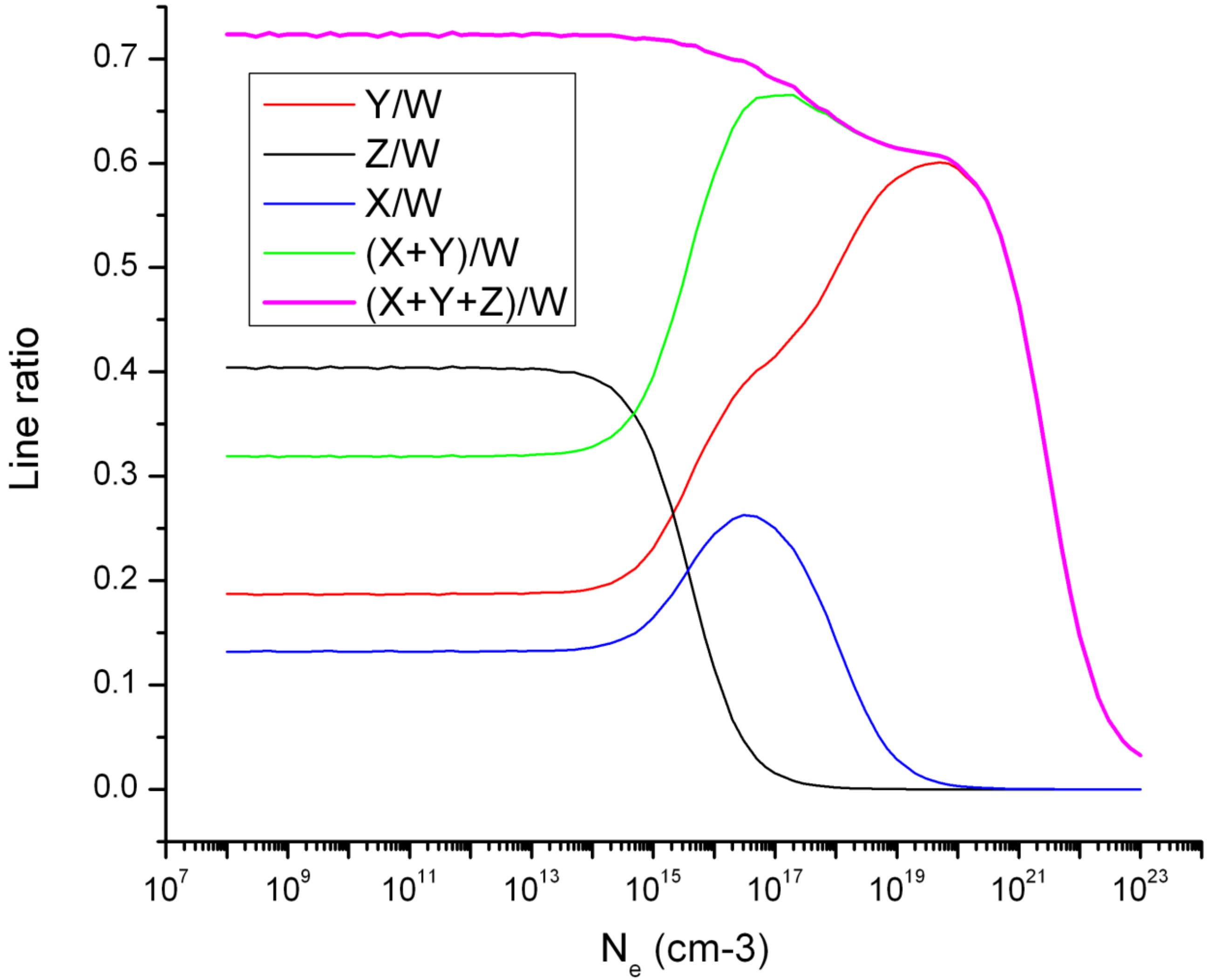
O.Marchuk et al, J Phys B 40, 4403 (2007)

He-like Ar Levels and Lines

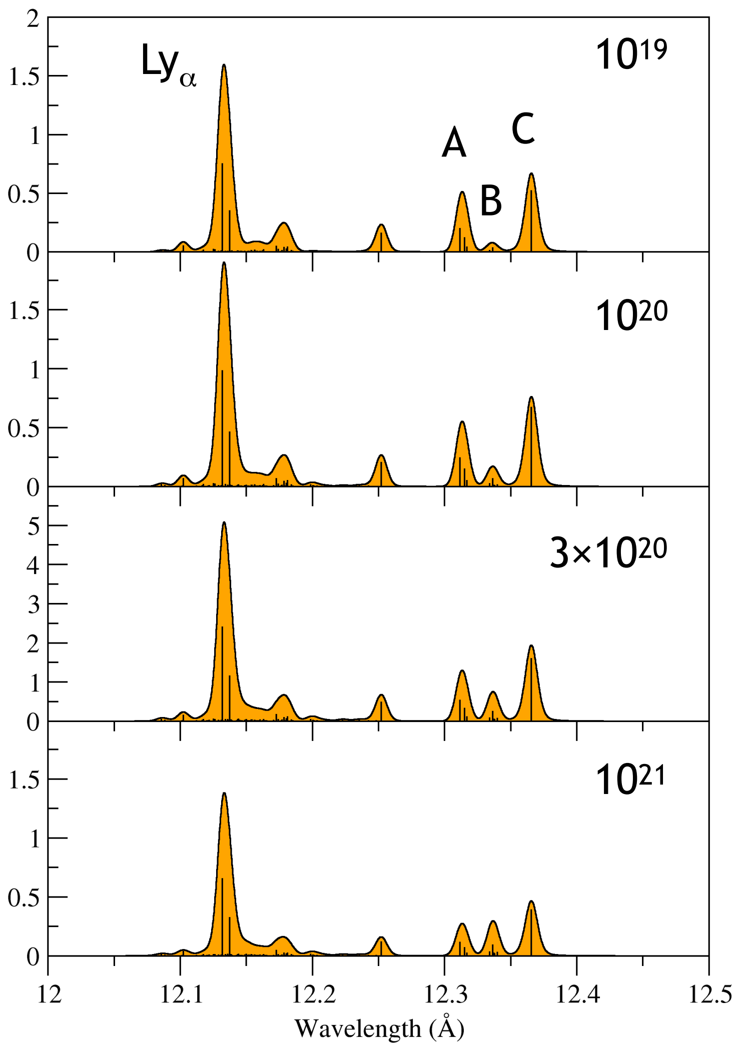


Line	He^0	Ar^{16+}	Fe^{25+}	Kr^{34+}
W	1.8(9)	1.1(14)	4.6(14)	1.5(15)
Y	1.8(2)	1.8(12)	4.4(13)	3.9(14)
X	3.3(-1)	3.1(8)	6.5(9)	9.3(10)
Z	1.3(-4)	4.8(6)	2.1(8)	5.8(9)

Ar XVII Line Ratios



Density Dependence

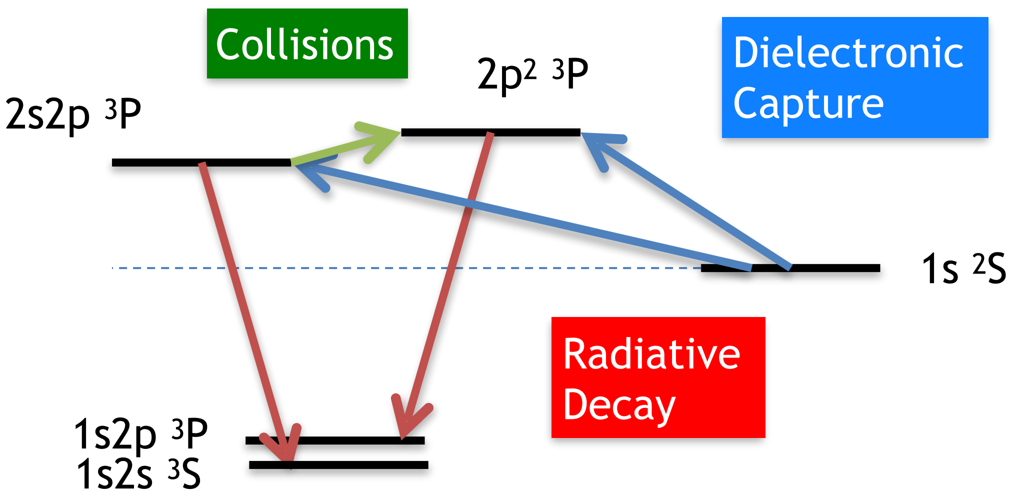


Ne X Ly_α and satellites *1snl-2pnl*

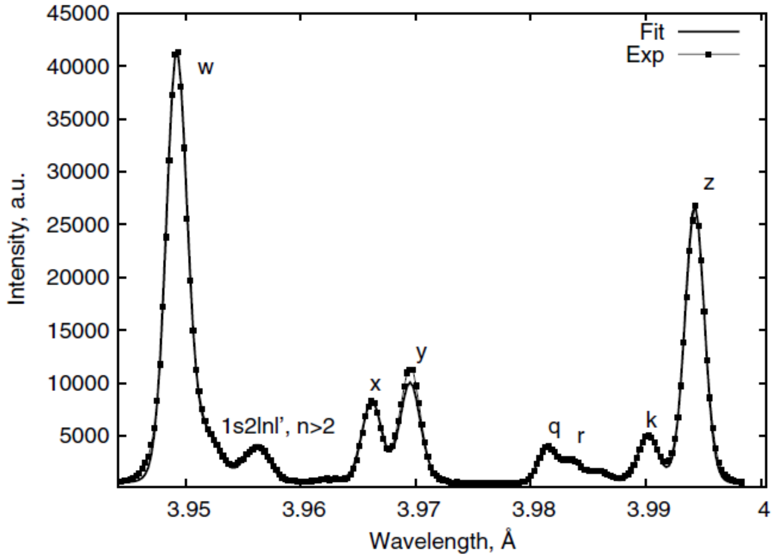
A. $1s2s\ ^3S_1 - 2s2p\ ^3P_{0,1,2}$

B. $1s2p\ ^3P_{0,1,2} - 2p^2\ ^3P_{0,1,2}$

C. $1s2p\ ^1P_1 - 2p^2\ ^1D_2$ (J satellite)



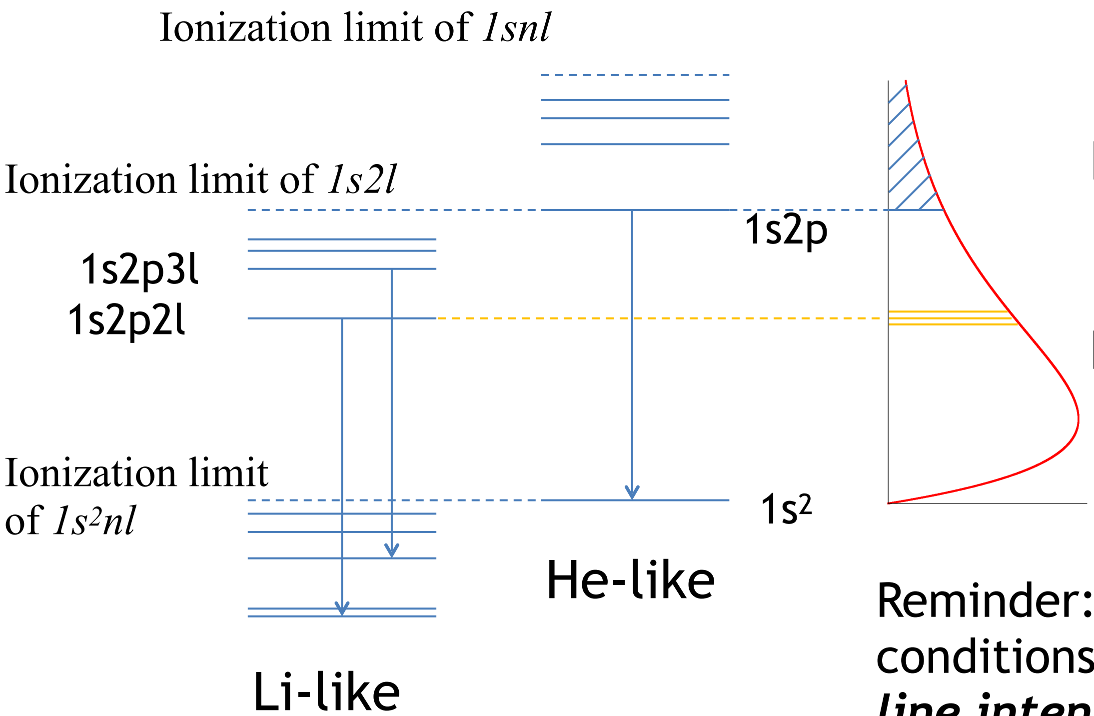
1*s*2*lnl* satellites



- 1l2l2l'
  - 1s2s2p - 1s2s^2 $^2S_{1/2}$:
    - 1s2s2p(^{1}P) $^2P_{3/2}$ (*s*), $^2P_{1/2}$ (*t*)
    - 1s2s2p(^{3}P) $^2P_{3/2}$ (*q*), $^2P_{1/2}$ (*r*)
    - 1s2s2p(^{3}P) $^4P_{3/2}$ (*u*), $^4P_{1/2}$ (*v*)
  - 1s2p^2 - 1s^{2}2p $^2P_{1/2,3/2}$:
    - 1s2p^2(^{1}D) $^2D_{3/2,5/2}$ (*j*,*k*,*l*)
    - 1s2p^2(^{3}P) $^2P_{1/2,3/2}$; $^4P_{1/2,3/2,5/2}$
    - 1s2p^2(^{1}S) $^2S_{1/2}$

- 1s2lnl' (n>2)
  - Closer and closer to *w*
  - Only 1s2l3l can be reliably resolved
  - Contribute to *w* line profile

Temperature diagnostics with Dielectronic Satellites



Excitation rate for 1s2p ~ $\dfrac{e^{-\frac{E_W}{T}}}{T^{1/2}}$

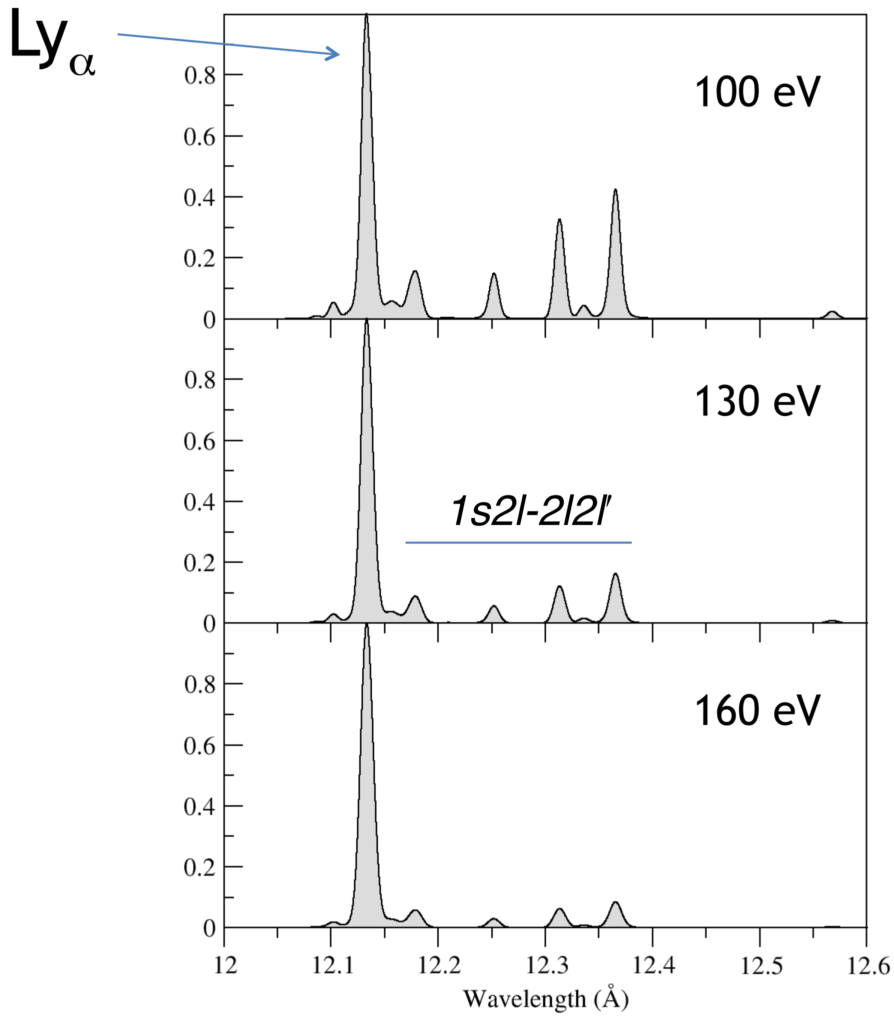
DC rate for 1s2l2l′ ~ $\dfrac{e^{-\frac{E_s}{T}}}{T^{3/2}}$

Reminder: for (low-density) coronal conditions
line intensity = population influx

Therefore: $$\frac{I_s}{I_W} \propto \frac{\exp\left(-\frac{\Delta E}{T}\right)}{T} \sim \frac{1}{T}$$

Independent of ionization balance since the initial state is the same!

Temperature Dependence: Ly_α satellites



H-like Ne X

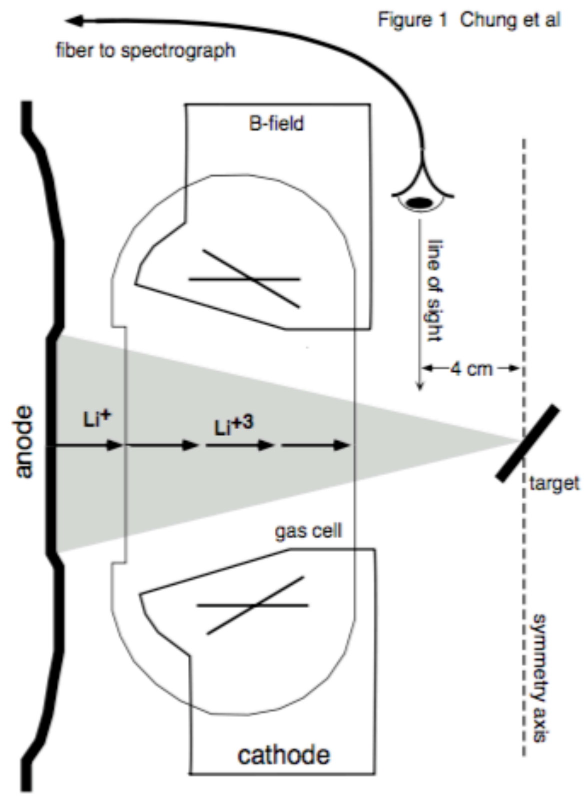
$1s_{1/2}$-$2p_{1/2}$

$1s_{1/2}$-$2p_{3/2}$

1snl-2l′nl, n=2,3,4,...

SPECTROSCOPIC ANALYSIS OF ION-BEAM PRODUCED NON-MAXWELLIAN ARGON PLASMAS

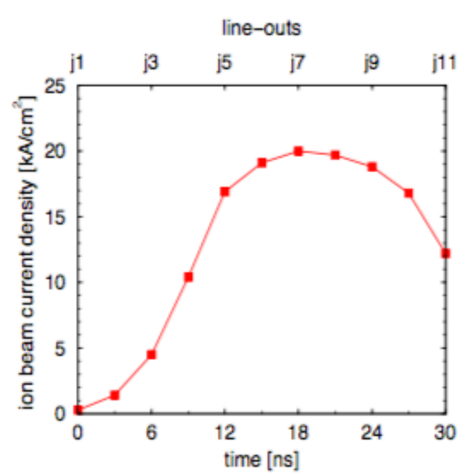
PBFA-II Experiments Explore Plasma Formation Processes Using High Intensity Ion Beam of ICF-Parameter.

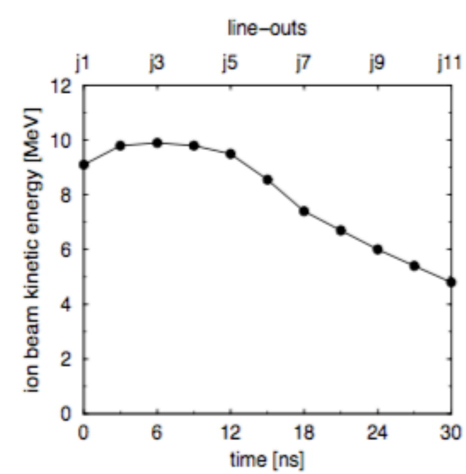


J. E. Bailey *et al.* Phys. Rev. Lett. **82**, 739 (1999)

- This research assists heavy-ion research by **benchmarking simulations (IPROP) of the plasma formation** and **developing diagnostic methods** which may be used in higher-intensity heavy-ion experiments.

- A High-intensity Li^{+3} (9 MeV, 20kA/cm^2) beam deposits 8TW/g in 2-Torr Ar, which is 40 times higher specific deposition than previous experiments.

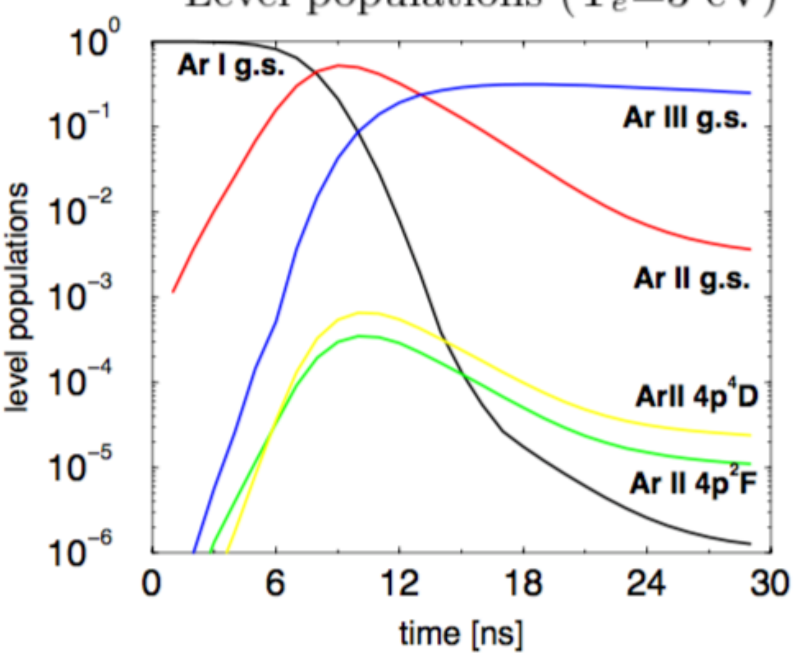


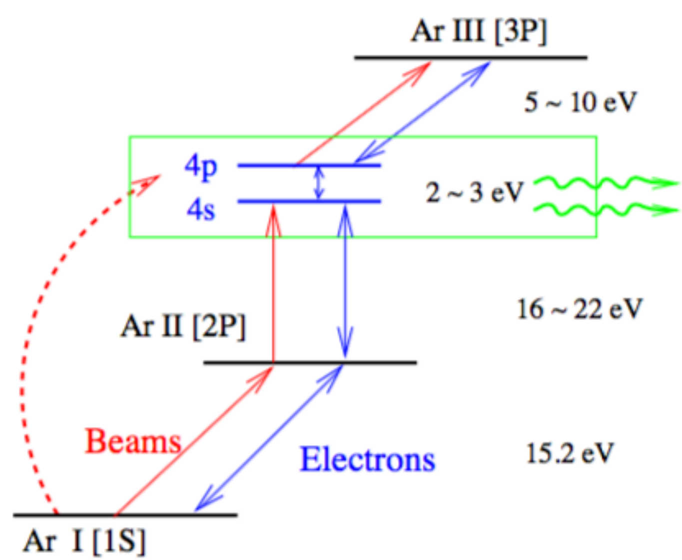


Ionization dynamics of beam-produced plasmas

- Ionization dynamics is driven by upward-collisional processes.
  - ▷ Beam ions and non-thermal electrons
  - ▷ Thermal electrons
- Closely-spaced levels reach LTE even in presence of non-thermal particles.
  - ▷ Detailed balance due to high collisional rates with thermal electrons
  - ▷ Possible Boltzmann plot analysis for thermal electron temperatures

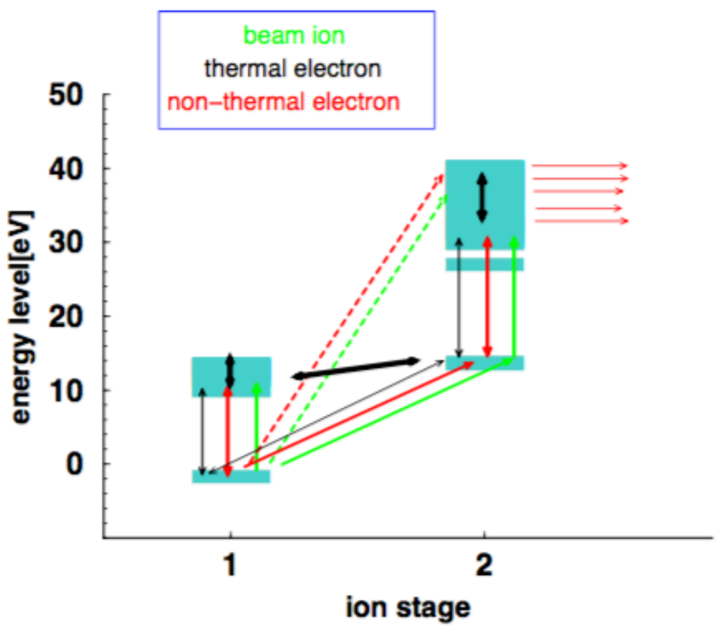
Level populations (T_e=3 eV)





Atomic Level Populations Are Calculated By CR Model.

- Include total of 627 Ar levels from Ar I-Ar VII ionization stages.
- Use ion beam energy and current density from experiments, non-thermal electron distributions from IPROP results as input parameters.
- Use electron temperature determined from line-ratio methods.
- Time-dependent electron densities are computed self-consistently.



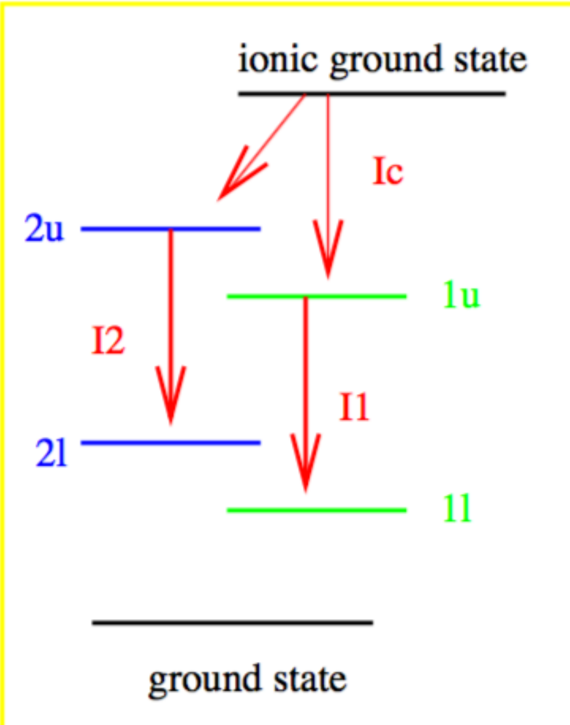
- Energetic particles are effective in high ΔE transitions.
  - One-Step Ionization/Excitation
  - Simultaneous Ionization/Excitation
  - Multi-Ionization/Inner-Shell Ionization
- Thermal electrons effective in low $\Delta E \sim \mathrm{T}_e$.
  - Stepwise Excitation/Deexcitation
  - Stepwise Ionization/Recombination

Spectral Modeling Of Beam-Produced Plasmas

- Electron temperature measurement ⇒ Line ratio analysis
  - Non-LTE at early times : Line ratio analysis exploiting CR calculations
  - LTE at later times : Boltzmann plot analysis
- Electron density measurement ⇒ Line broadening analysis
  - Non-LTE at early times : Line ratio analysis with CR calculations
  - LTE at later times : Stark broadening analysis
- Measured spectra are significantly affected by Opacity effect.
  - Boltzmann plot analysis : Reduction of measured intensities
  - Line broadening analysis : Opacity broadening

Spectral Intensity Methods

- Ratios of line radiation (Bound-Bound transitions)



In a homogeneous optically-thin plasma,

$$I_1 = \frac{1}{4\pi}\int n_{1u}(s)A_1 h\nu_1 ds = \frac{1}{4\pi} n_{1u} A_1 h\nu_1 l$$

$$\frac{I_2}{I_1} = \frac{n_{2u}}{n_{1u}}\frac{A_2}{A_1}\frac{h\nu_2}{h\nu_1} = \frac{A_2}{A_1}\frac{h\nu_2}{h\nu_1}\frac{g_{2u}}{g_{1u}} exp\left[-\frac{E_{2u}-E_{1u}}{kT_e}\right]$$

$$log\left(\frac{I_2}{g_{2u}A_2 h\nu_2}\right) - log\left(\frac{I_1}{g_{1u}A_1 h\nu_1}\right) = -\frac{E_{2u}-E_{1u}}{kT_e}$$

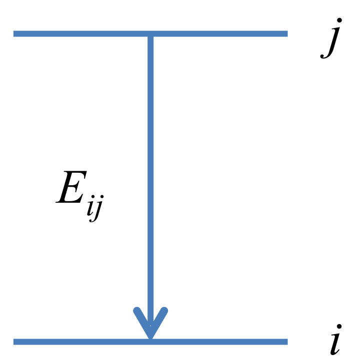
- Slope of continuum radiation (Bound-Free or Free-Free transitions)

$$I_c(h\nu) \sim exp\left[-\frac{h\nu}{kT_e}\right]$$

Spectral Line Intensity (optically thick)

$$I_{ij} = N_j \cdot A_{ij} \cdot h\nu_{ij} \cdot P_e$$

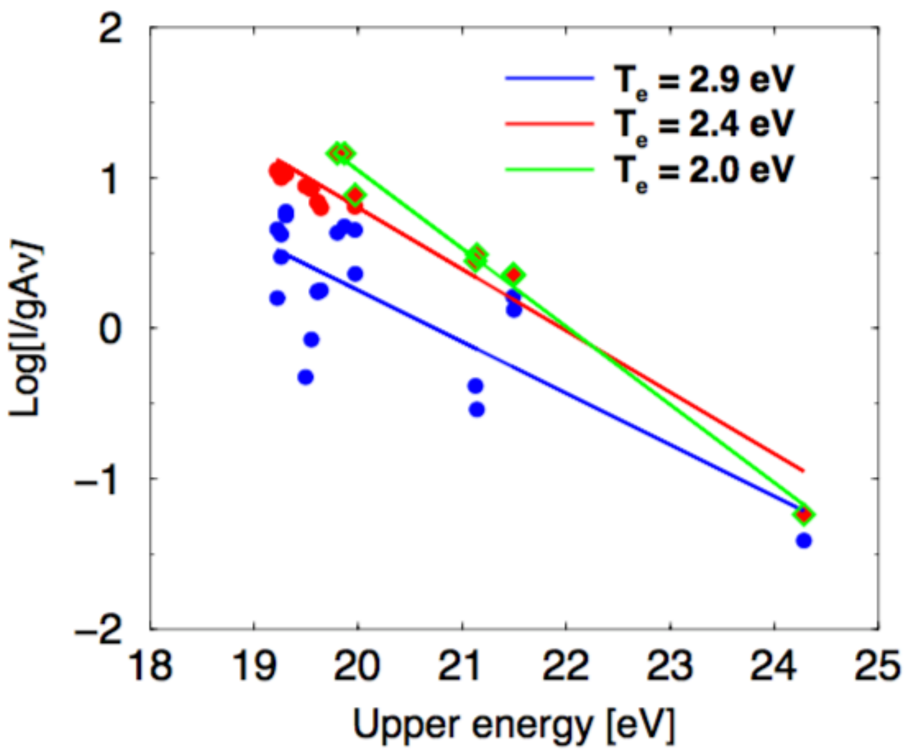
- Upper state density (cm^{-3})
- Einstein coefficient or transition probability (s^{-1})
- strongly depends on plasma conditions
- (*almost*) purely atomic parameters
- Energy emitted due to a specific transition from a unit volume per unit time
- Photon energy (J)
- Radiation escape Probability



Boltzmann Plot Analysis

- Find lines from levels in LTE
- Include a radiation transport effect (Escape probability)
- For optically-thick lines with escape probabilities(P_e)

$$log(\frac{I_2}{g_{2u}A_2h\nu_2P_{e2}}) - log(\frac{I_1}{g_{1u}A_1h\nu_1P_{e1}}) = -\frac{E_{2u}-E_{1u}}{kT_e}$$



Slope = - $1/T_e$ (T_e = 2 eV)

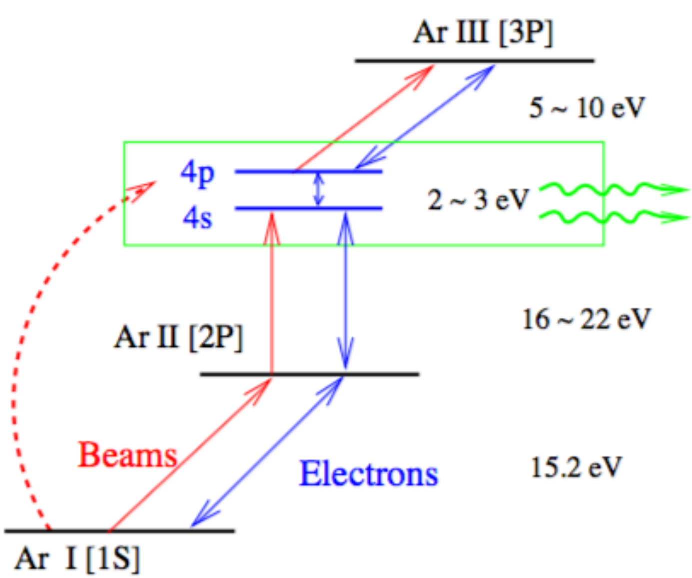
Blue curve : No opacity effect

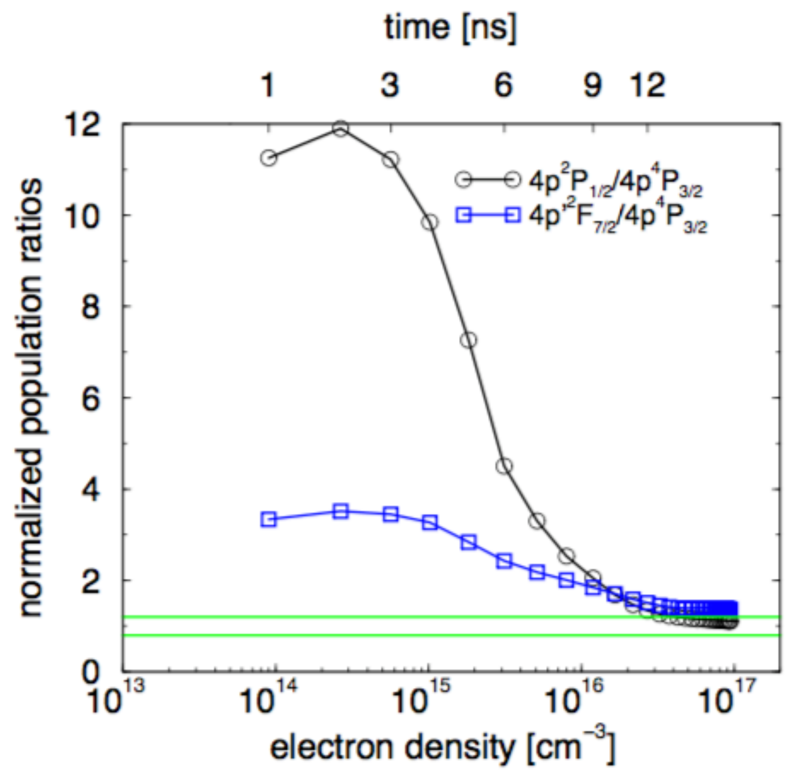
Red curve : opacity effect

Green curve : opacity effect and no quartet lines

Ar II Levels Are Populated From Ar II Excited Levels By Thermal Electrons, Ar I and II Ground States By Energetic Particles.

- Simultaneous ionization/excitation by energetic particles leads to Non-LTE initially due to preferential population of doublet 4p levels.
- As thermal electrons increases, collisional equilibration leads to LTE among excited levels.

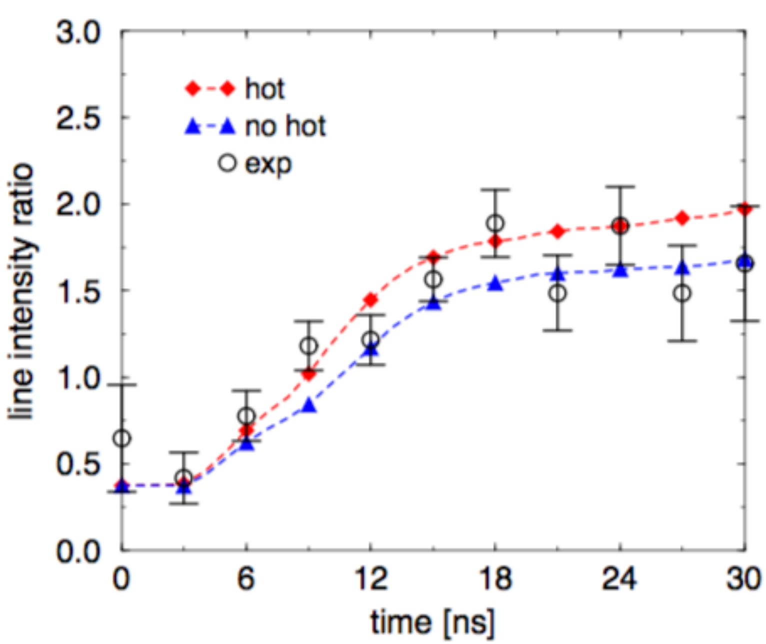


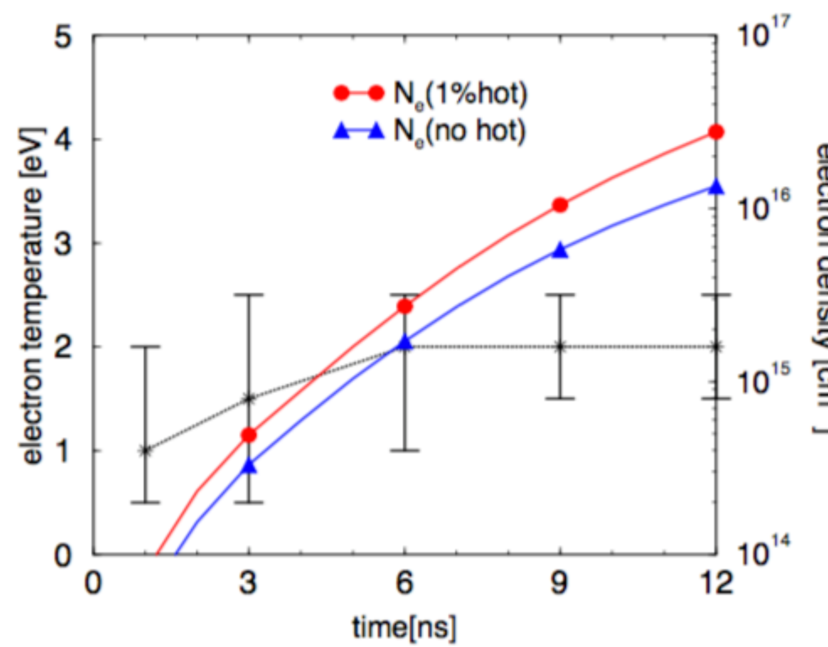


(Sanchez, PRA, v41, p1392 (1990), Koozekanani, IEEE J.QE, vQE-2,p770 (1966))

Line Ratio Analysis Are Insensitive To Existence Of Non-Thermal Electrons.

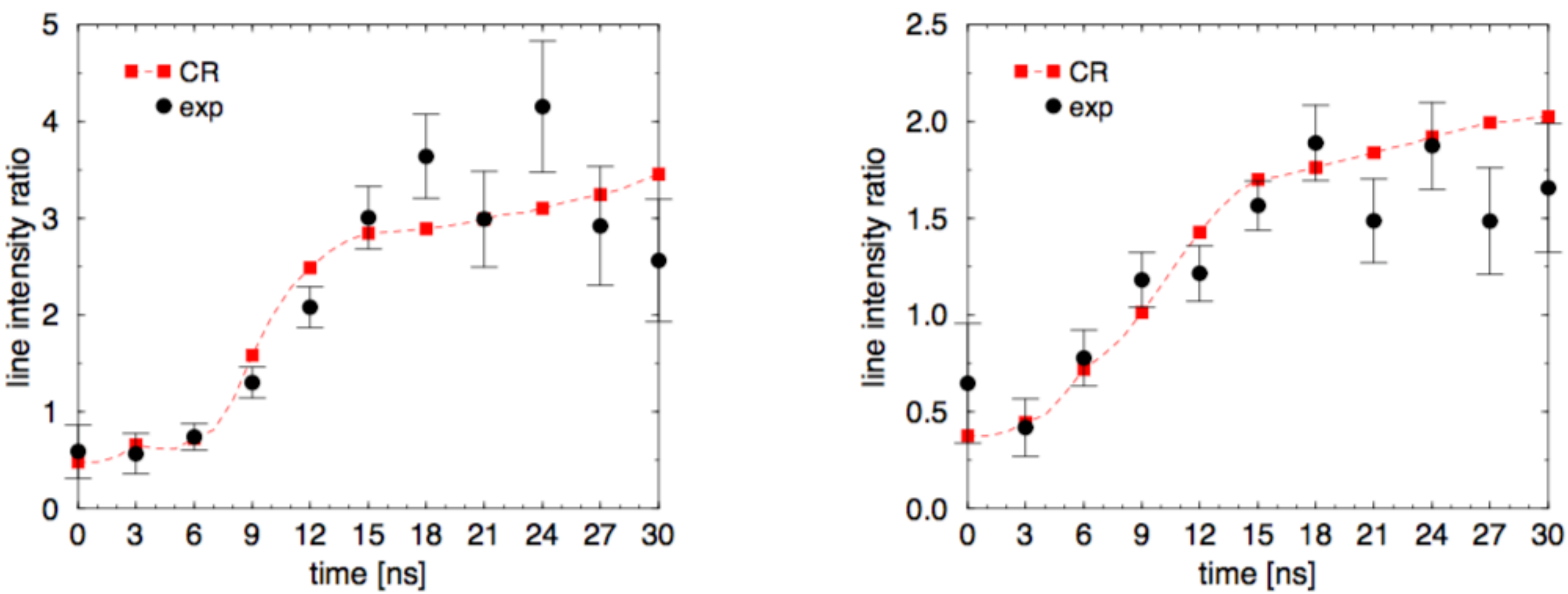
- IPROP calculations predict that a fraction of electrons, 1%, exist as the non-thermal electron component in the energy distribution.
- Non-thermal electron fractions less than 5% are consistent with experiments.





Line Ratio Analysis Exploits CR Calculations For T_e.

- Relative populations and line intensities strongly depend upon electron temperature and density prior to reaching equilibrium.
- We determine the plasma conditions that give the best agreement between measured and calculated line ratios.
- Line ratios $\frac{4348\mathring{A}(4p^4D_{7/2})}{4657.9\mathring{A}(4p^2P_{1/2})}$ and $\frac{4348\mathring{A}(4p^4D_{7/2})}{4609\mathring{A}(4p'^2F_{7/2})}$ are compared.



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Line Broadening Methods

- Natural Broadening : Finite radiative lifetimes

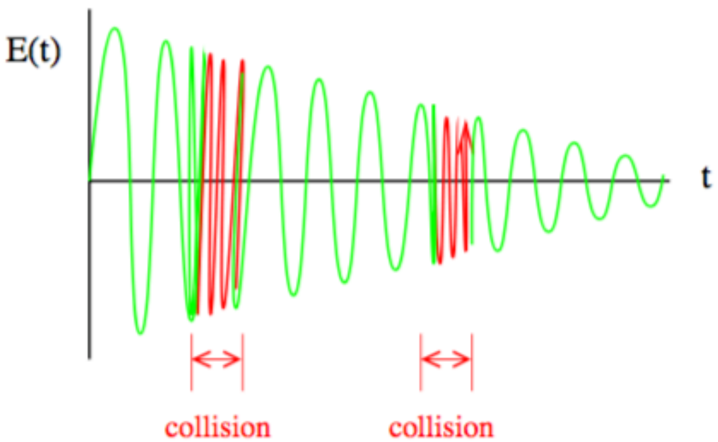
$$E(\omega) = \int E(t) e^{-i\omega t} dt \qquad I(\nu) \propto E(\omega)\cdot E^*(\omega) \propto \frac{\frac{\Delta\nu}{2\pi}}{(\nu-\nu_0)^2 + (\frac{\Delta\nu}{2})^2}$$

- Stark Broadening : Electron density measurement

Hydrogen $\Delta\nu \propto N_e^{2/3}$

Heavier elements

$$\Delta\nu \propto f(N_e, T_e) N_e$$



- Doppler Broadening : Ion temperature measurement

$$I(\nu)d\nu \propto exp(-(\nu-\nu_o)^2/\nu_D^2)d\nu \qquad \nu_D = (2kT/m)^{1/2}\nu_0/c$$

- Opacity Broadening : Optically thick plasmas

Spectra Can Be Predicted From Radiation Transport Equation.

In a plane-parallel geometry, for an intensity $I(\nu)$ at a frequency ν normally emerging from a radiating medium,

$$\frac{dI(\nu)}{dx} = \eta(\nu) - \chi(\nu)I(\nu)$$

Emissivity

$$\eta(\nu) = n_u A_{lu} \frac{h\nu}{4\pi}\phi(\nu) = n_u \frac{g_l}{g_u}\left(\frac{2h\nu^3}{c^2}\right)\left(\frac{\pi e^2}{mc}\right) f_{lu}\phi(\nu)$$

Opacity

$$\chi(\nu) = \left[n_l - n_u \frac{g_l}{g_u}\right]\left(\frac{\pi e^2}{mc}\right) f_{lu}\phi(\nu).$$

in terms of the upper and the lower level population densities n_u and n_l, an absorption oscillator strength f_{lu} or a spontaneous decay rate A_{lu} and intrinsic line profile $\phi(\nu)$. In terms of a source function $S(\nu) = \eta(\nu)/\chi(\nu)$ and an optical depth $d\tau(\nu) = -\chi(\nu)dx$,

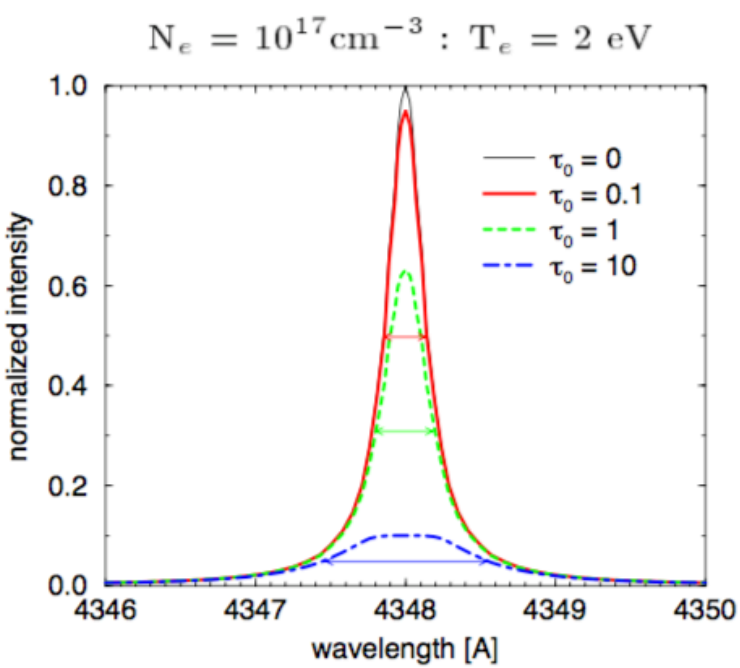
$$\frac{dI(\nu)}{d\tau(\nu)} = I(\nu) - S(\nu).$$

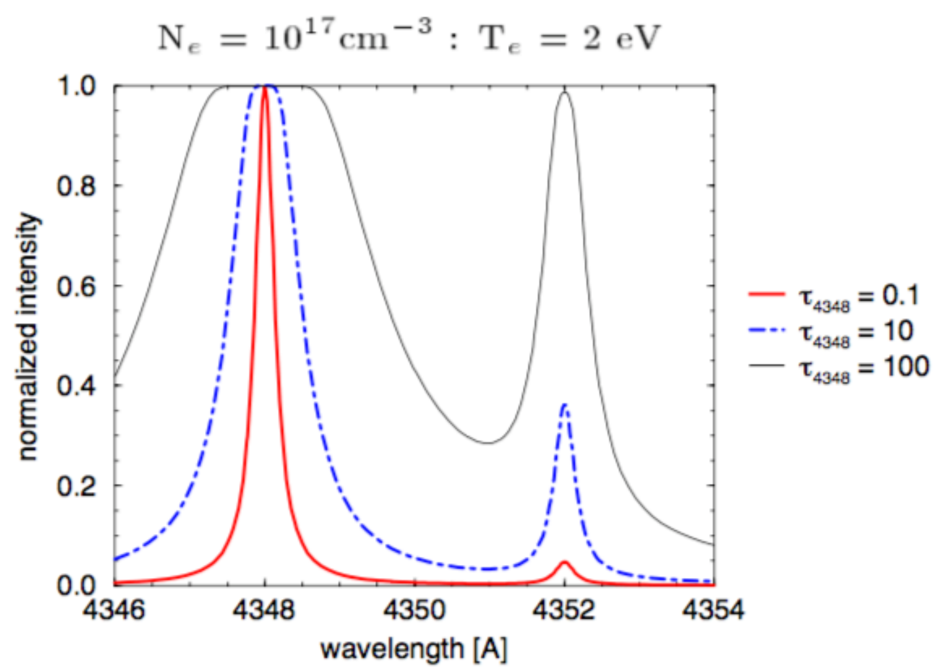
Opacity Broadening May Be Important In Line Broadening.

- Optically Thick Lines Have Higher FWHM.
- Intensities Increases With Opacity For Finite-Sized Plasmas.

$$I(\nu) = S(\nu)(1 - e^{-\tau(\nu)}) \begin{cases} I(\nu) = S(\nu)\tau(\nu) & \text{if } \tau \ll 1 \\ I(\nu) = S(\nu) & \text{if } \tau \gg 1 \end{cases}$$

- Relative Peak Intensities/FWHM Reflect Opacity Effects.



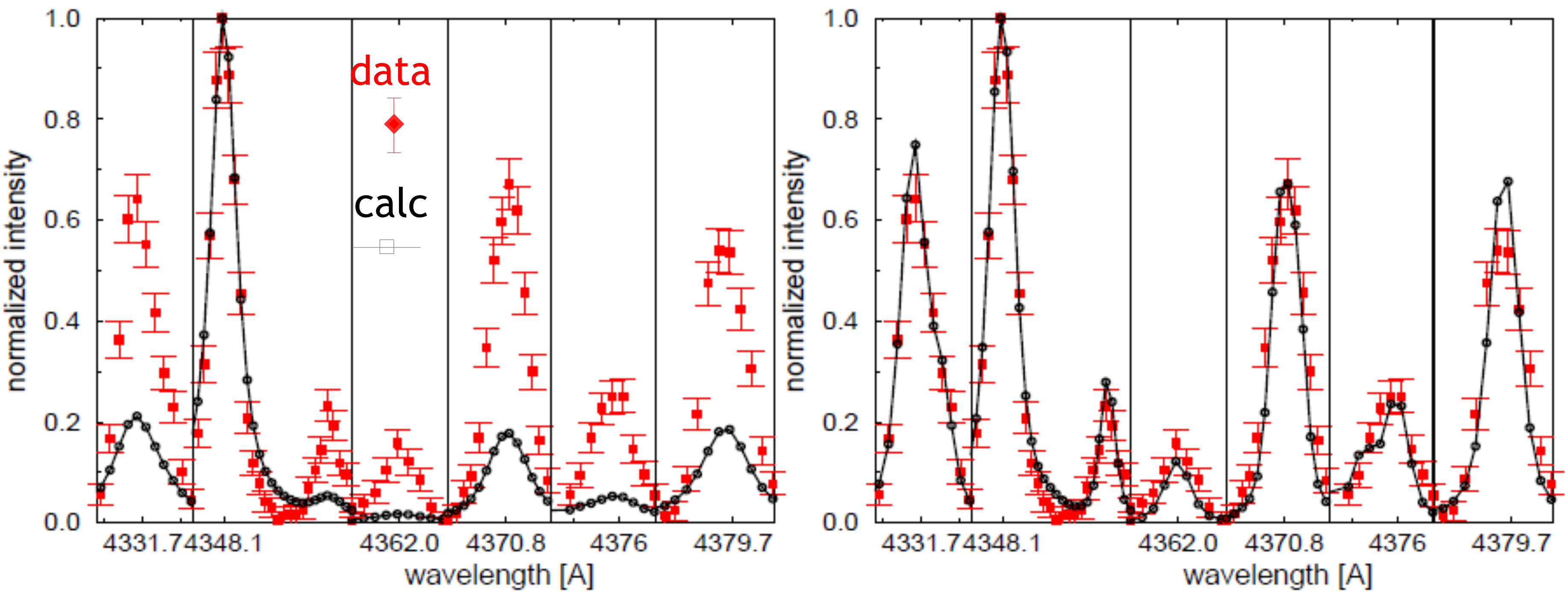


Line Width Analysis of argon plasma influenced by opacity effects

- n_e diagnostics are derived from Stark broadened line widths
- Population kinetics needed for correct optical depths

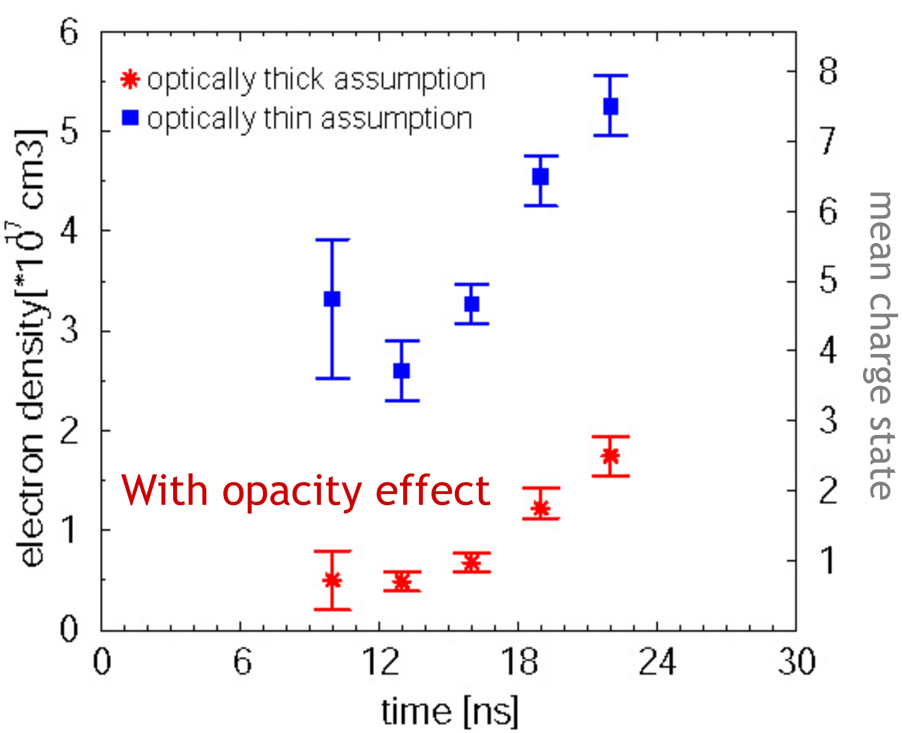
Statistical Fitting Analysis of Opacity- and Stark-Broadened Ar^{+2} Line Profiles Measured in Ion Beam Transport Experiments H.K. Chung et al, JQSRT, vol. 65, p. 135 (2000)

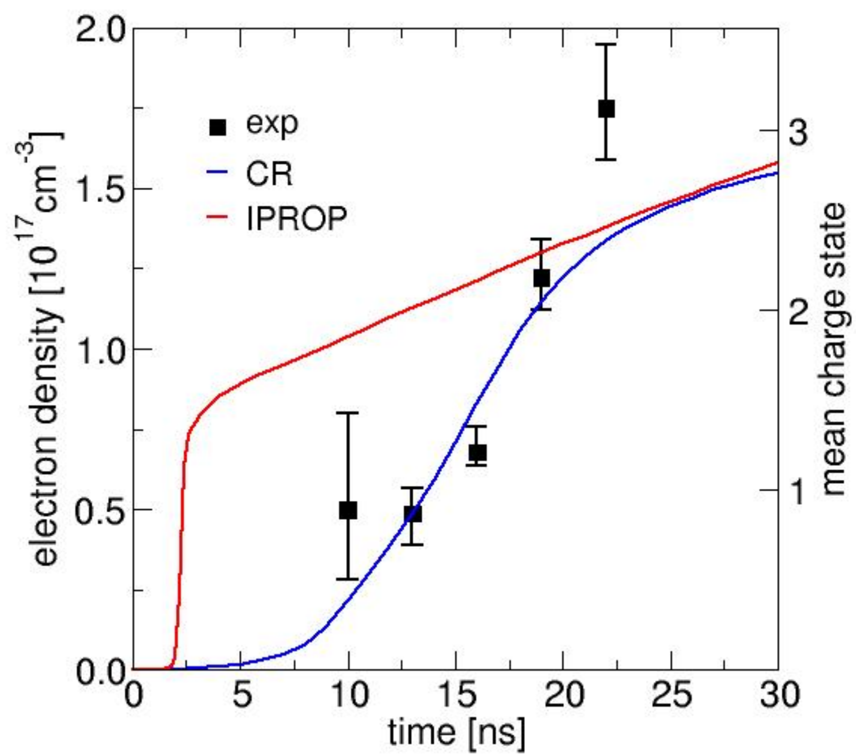
Without Opacity | With Opacity



Line intensity and width analysis should include opacity effects

- Analysis of measured spectra from the initial phase of the ion-beam plasma formation using NLTE populations reveals that ***IPROP*** (a PIC/ Fluid hybrid code) using simple population model overestimates T_e
- Note that IPROP uses a simple breakdown ionization model



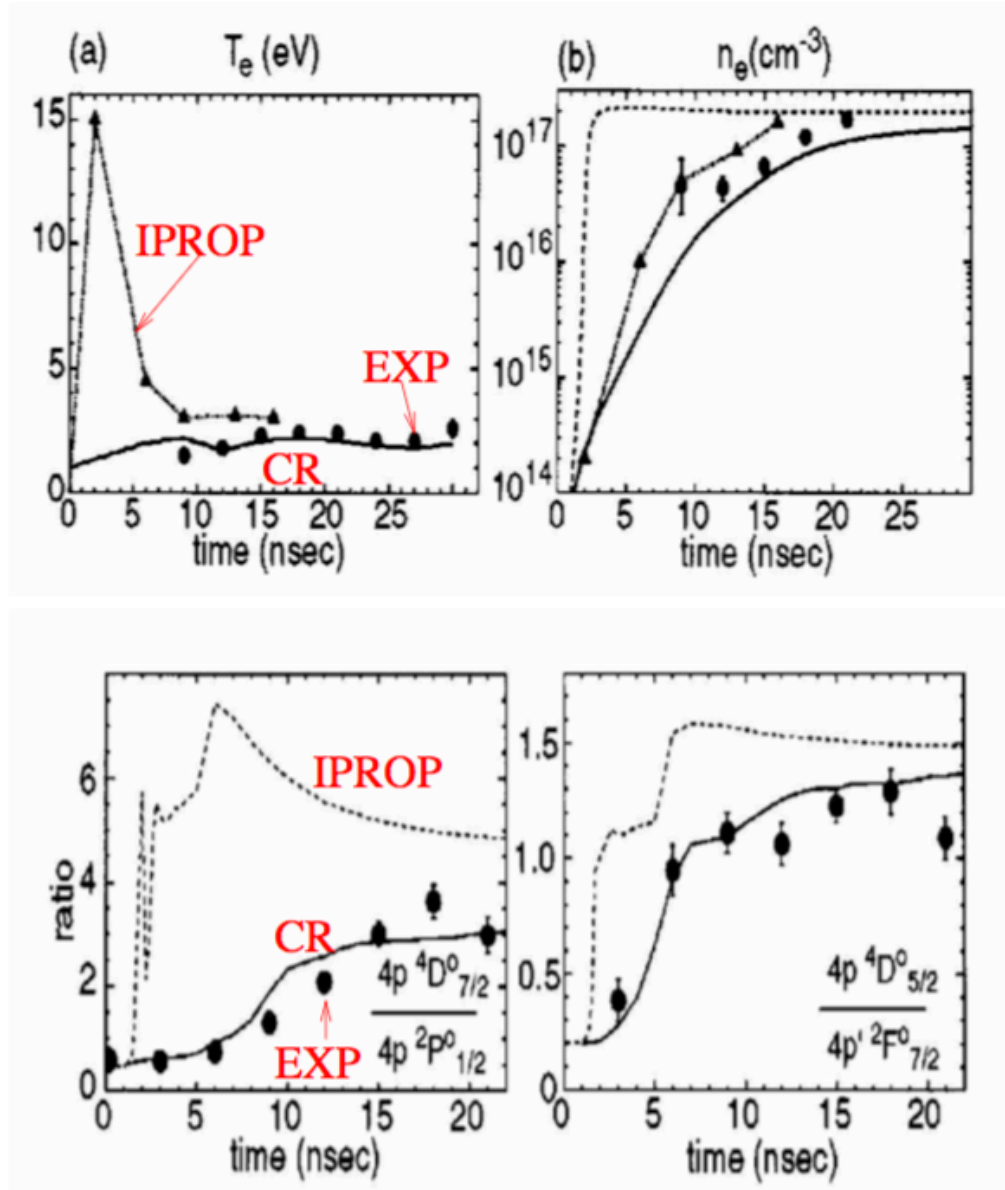


Comparisons of Measurements/IPROP/CR Calculations

- IPROP-predicted high temperature, however, is inconsistent with measured temperatures from high-intensity lithium beam transport experiments.

- CR calculations suggest that the inconsistency may be due to the lack of an appropriate atomic model in IPROP. (Beam-deposited energy partition to gas internal energy and stepwise ionization may not be appropriately considered.)

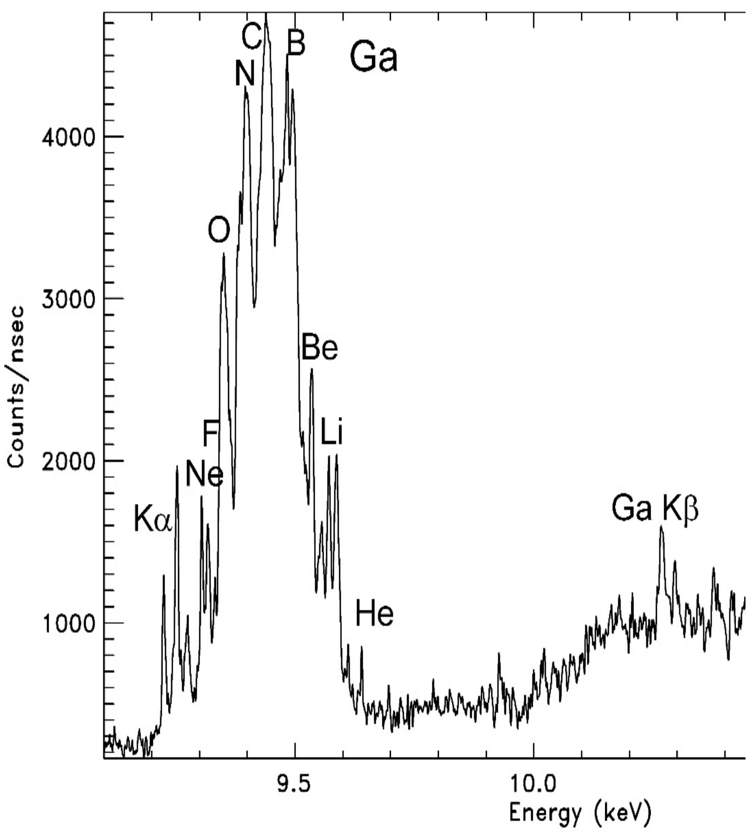
$$\frac{3}{2}n_eT_e = \int n_b v_b \frac{dE}{dx}dt - U_{gas}$$

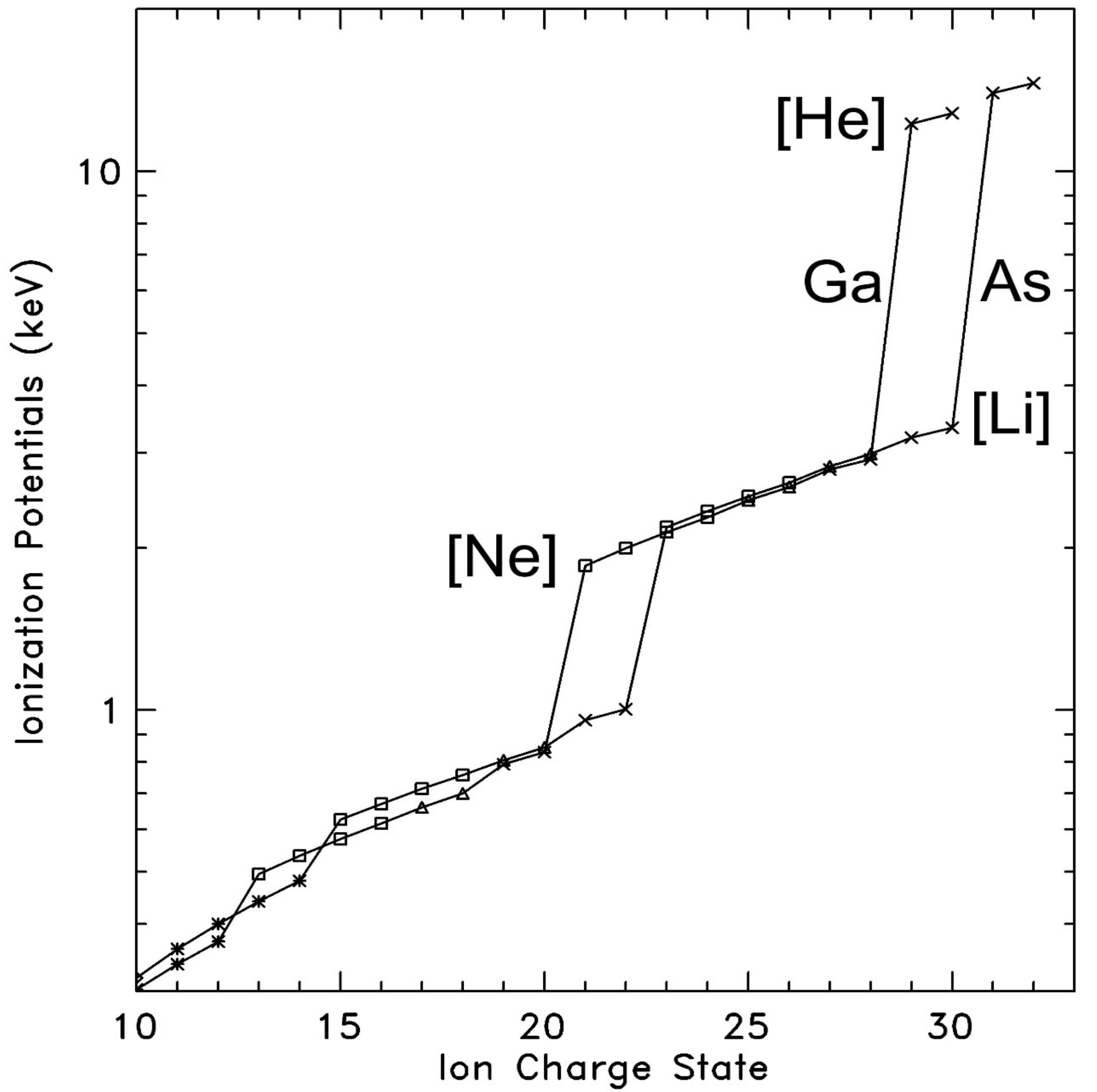


Using FLYCHK simulations:

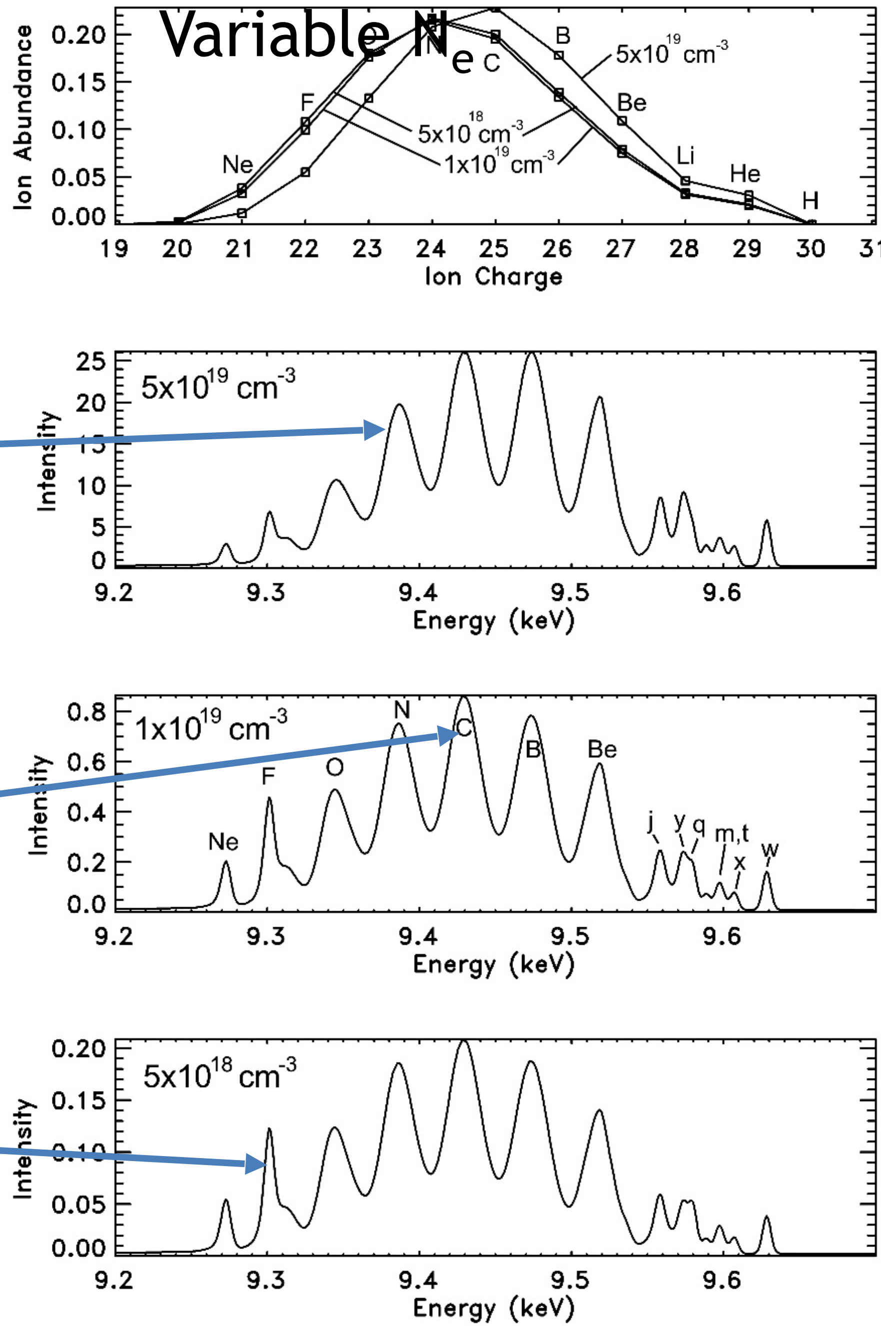
What T_e and N_e to choose for the spectrum simulations?

We know that the most abundant charge states in a thermal plasma have ionization potential ≈ $3T_e$, so choose T_e ≈ 2 keV (1 keV?).





FLYCHK Simulations of the Ga Spectrum with T_e = 2 keV and Variable N_e

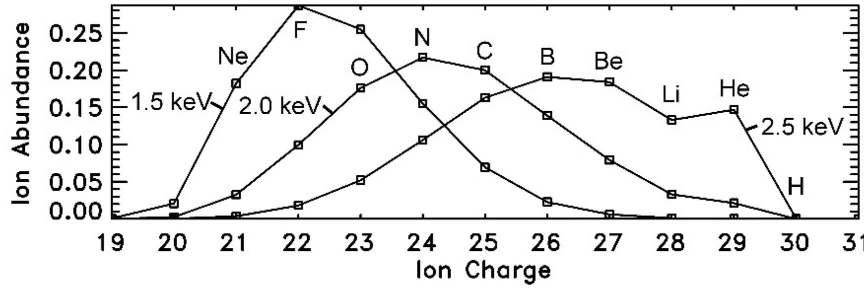


Low charge states too low

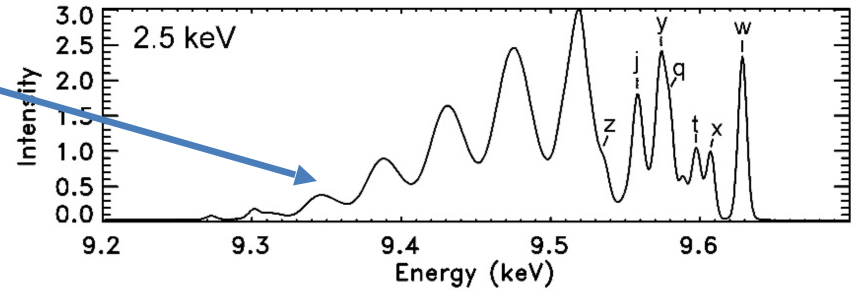
C is highest. Good

Lower charge states too high

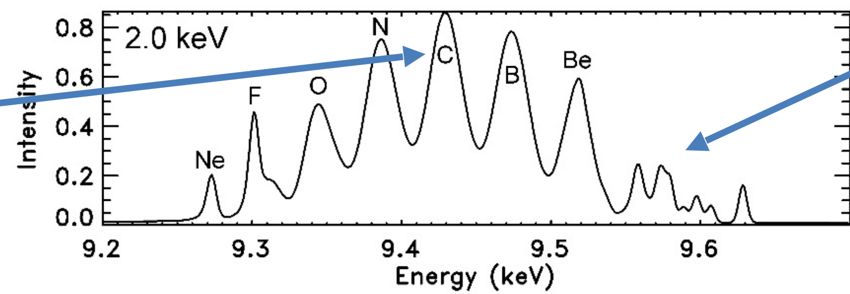
FLYCHK Simulations of the Ga Spectrum with Variable T_e and $N_e = 1\times10^{19}$ cm^{-3}



Low charge states too low

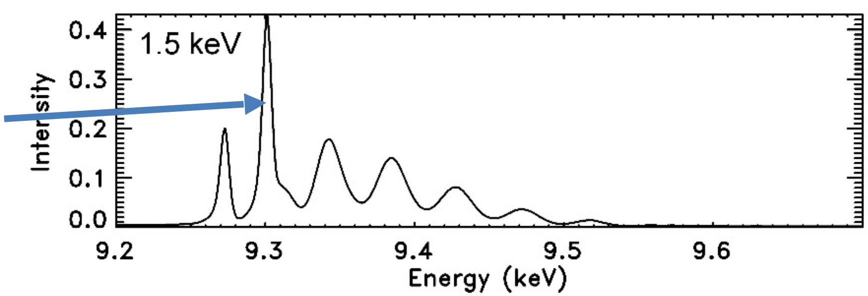


C is highest. Good

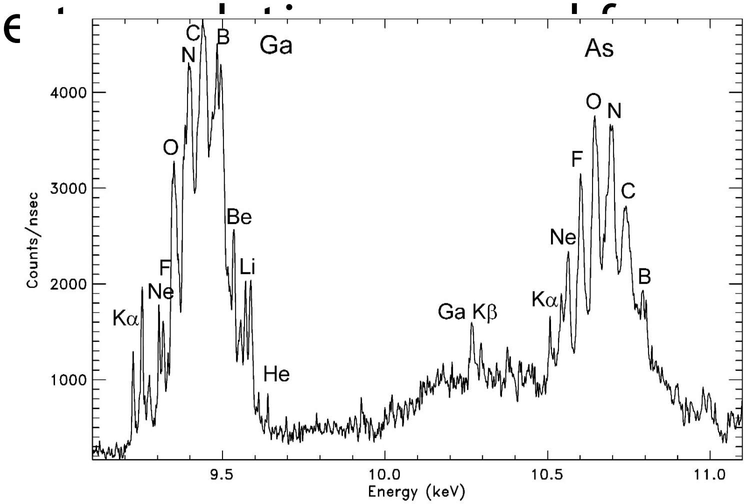


He-like transitions and Li-like satellites have good intensities.

Lower charge states too high



FLYCHK simulations of the Ga spectrum were performed with variable T_e, N_e, and hot electron fraction. The correlations between the calculated and experimental spectra were calculated. The highe



T_e = 1100 eV ± 5%

N_e = 3x10^{19} cm^{-3} ± 50%

Fraction of hot electrons = 0.025 ± 0.005