Two Novel Cases of Plasma Characterization Through Spectroscopic Modeling

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Two Cases of Spectroscopic Modeling

Plasmas Formed During Laser Ablation

- Most common laser produced plasma
- $I_{laser} = 1 \times 10^7 - 1 \times 10^{10}$ W/cm^2
- T_e = 1-3 eV
- Stoichiometrically complex targets
- Time-dep. atomic kinetics
- Opacity and lineshape
- Uniqueness/Topology/Search Tech.

Intense Ultrashort Laser Plasmas

- Non-Maxwellian FEEDF
- Time-dep. atomic and e^- kinetics
- $I_{laser} = 1 \times 10^{15} - 1 \times 10^{21}$ W/cm^2; $\tau = 20 - 300 fs$
- T_e= 1000-1500 eV (Final T.E.)
- Ar cluster targets
- Atomic kinetics and plasma physics?

Spectroscopic Modeling of a Collisionally Confined Laser-ablated Plasma Plume

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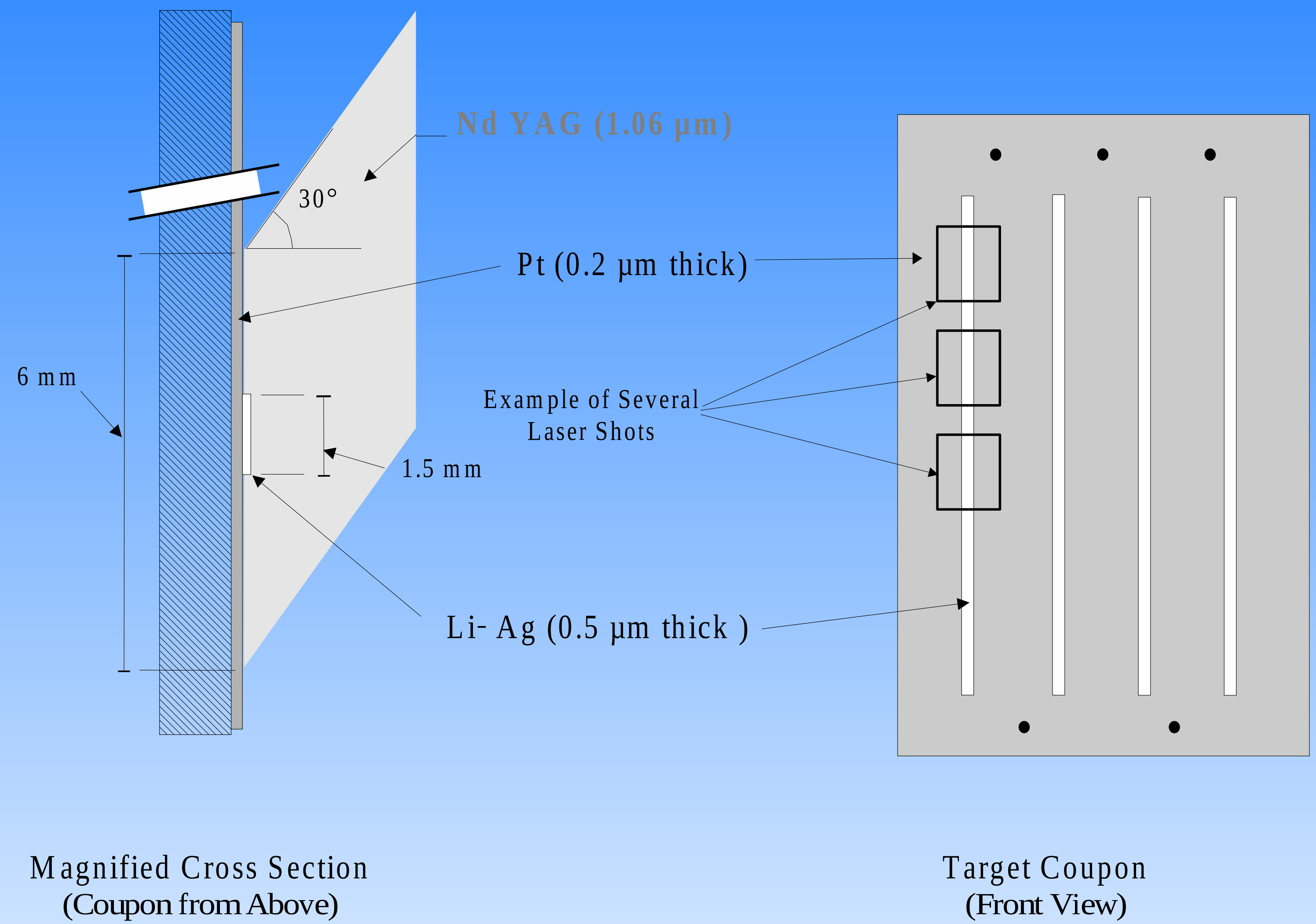


Figure 1: Target Design.

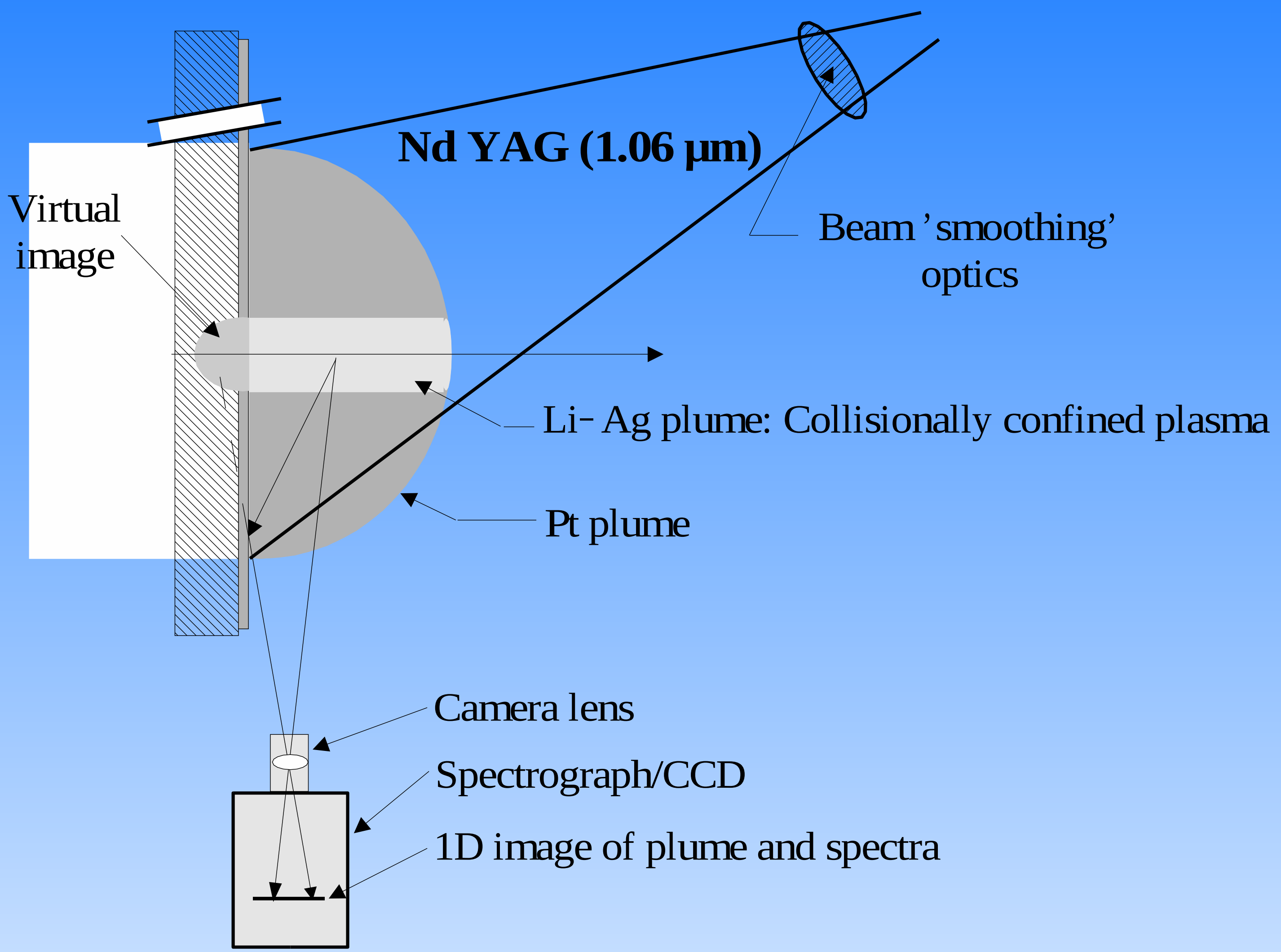


Figure 2: Experimental Configuration.

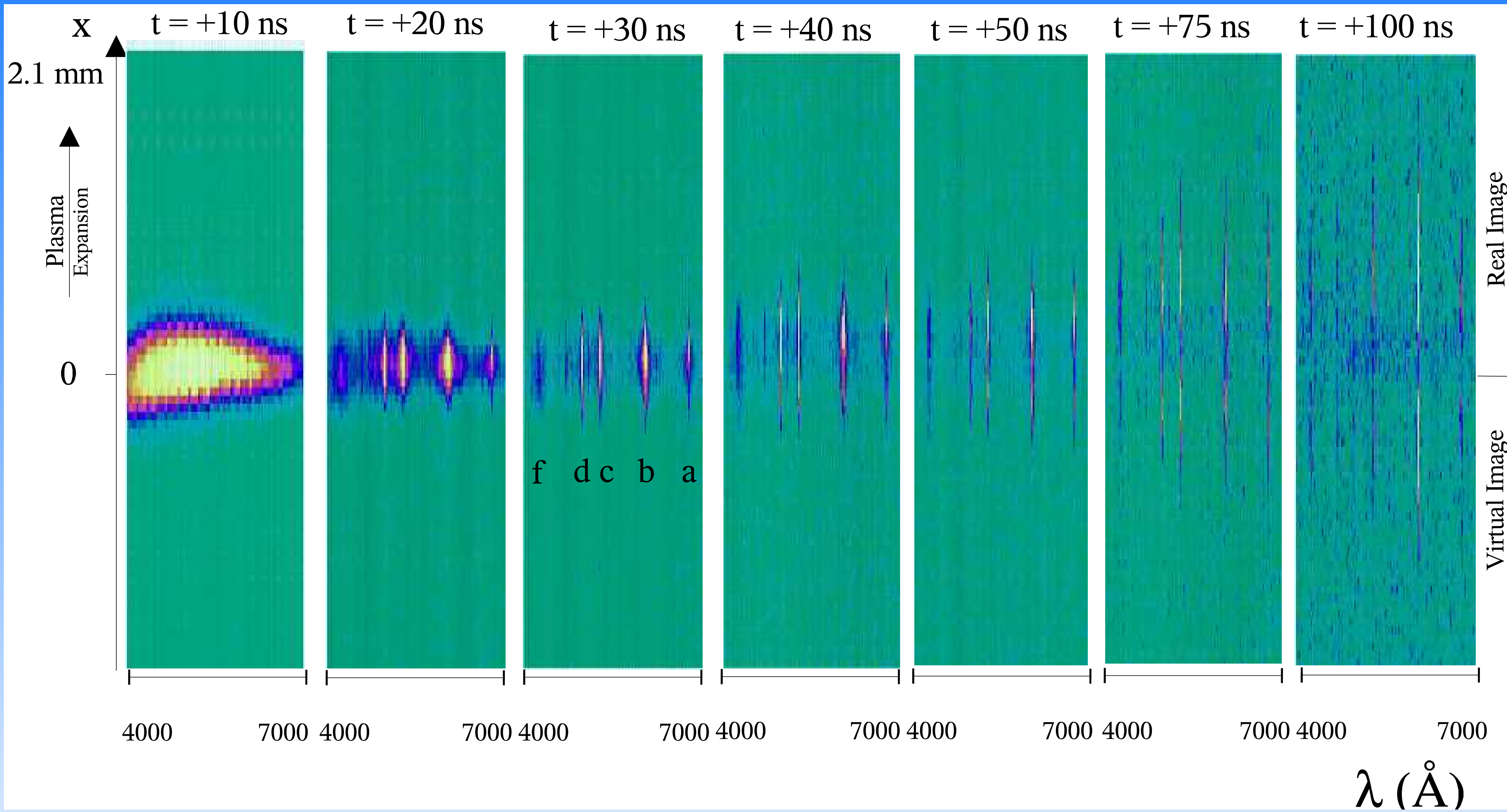


Figure 3: CCD Images.

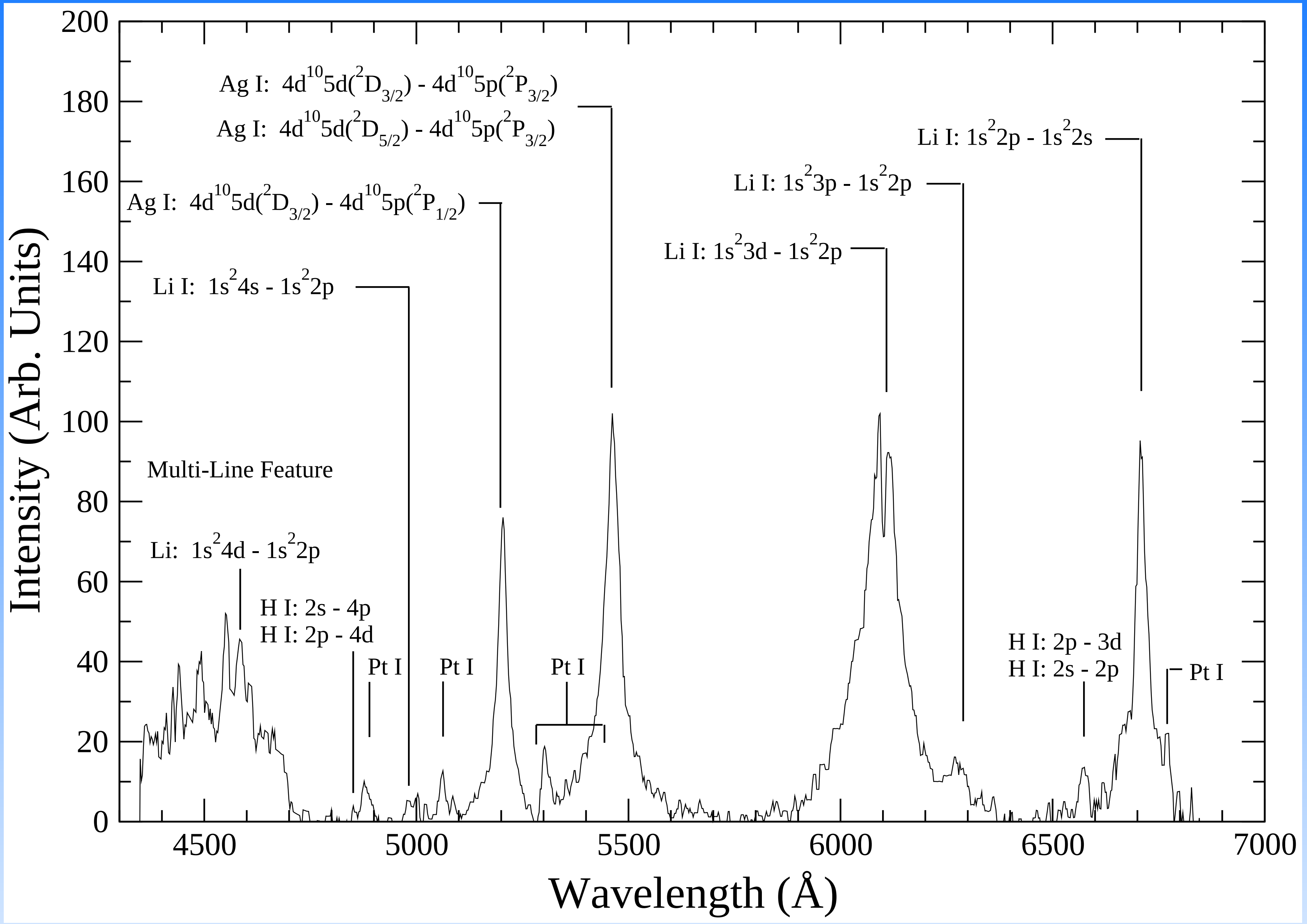


Figure 4: Early in time and close to the target surface, this lineout (x=28.8 μm, t=+20 nsec) displays the high density characteristics of Stark broadened line shapes.

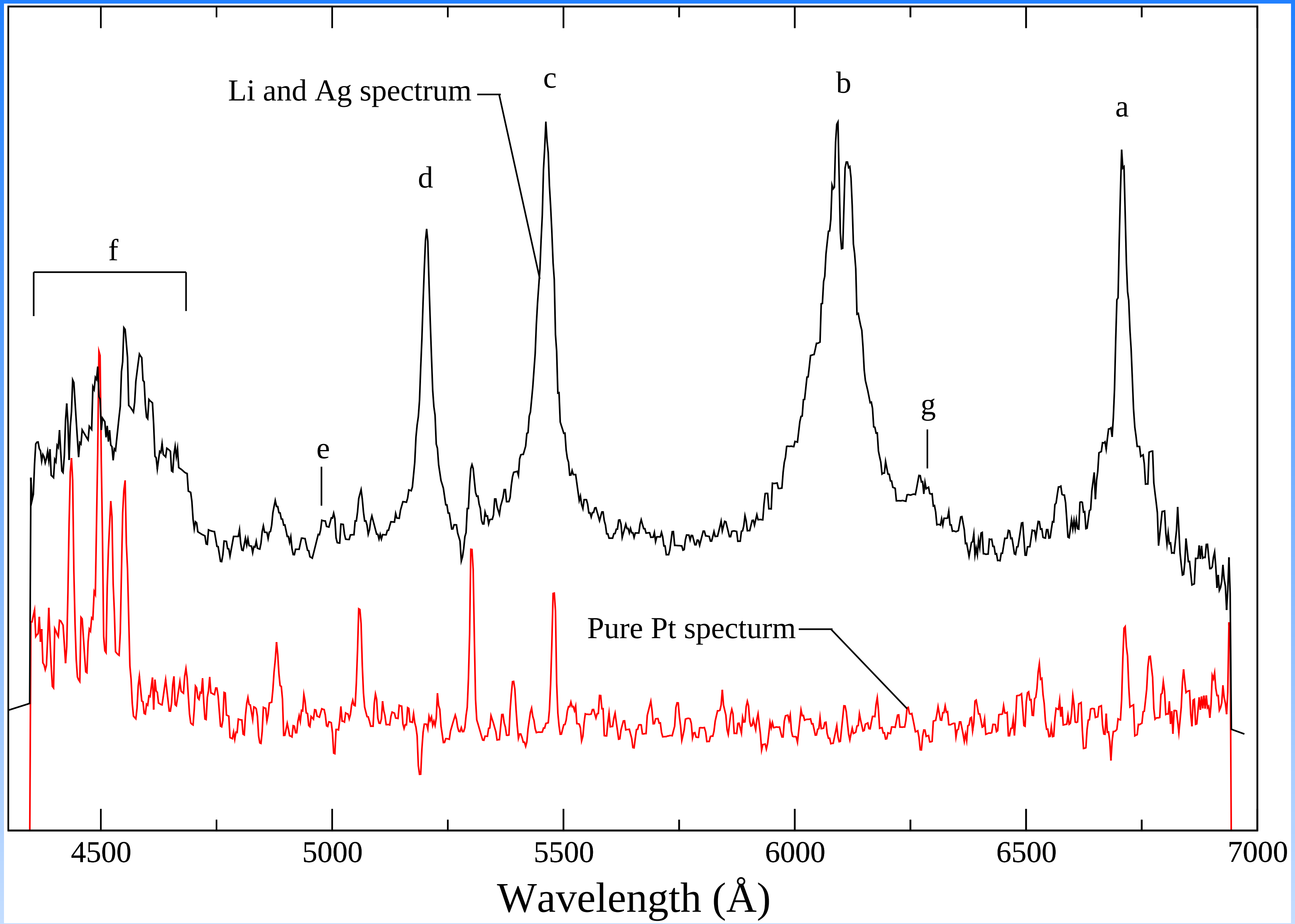


Figure 5: The superposition of two lineouts shows the location of platinum lines in the x=28.8 μm, t=+20 nsec spectrum. The spectrum of a pure platinum target was recorded during the Li-Ag trails at t=+50 nsec, x=56.7 μm from the surface with a 10 ns gate time.

Spectroscopic Model

Best Fit - Synthetic and Experimental Spectra

- Improving atomic structure calculations for high Z neutrals: energy levels and wavefunctions – cross sections and rates
- Reducing the number of calculated cross sections Ag^{+1}, Ag^{+2}, Ag^{+3}. - multi-representational model
- Multi-element collisional radiative model - common free $e-$ pool
- Local plasma effects on the radiator - detailed line shapes
- Non-local effects on the spectra - radiation transport accurate RTE solution
- Plasma gradients – self-reversal feature

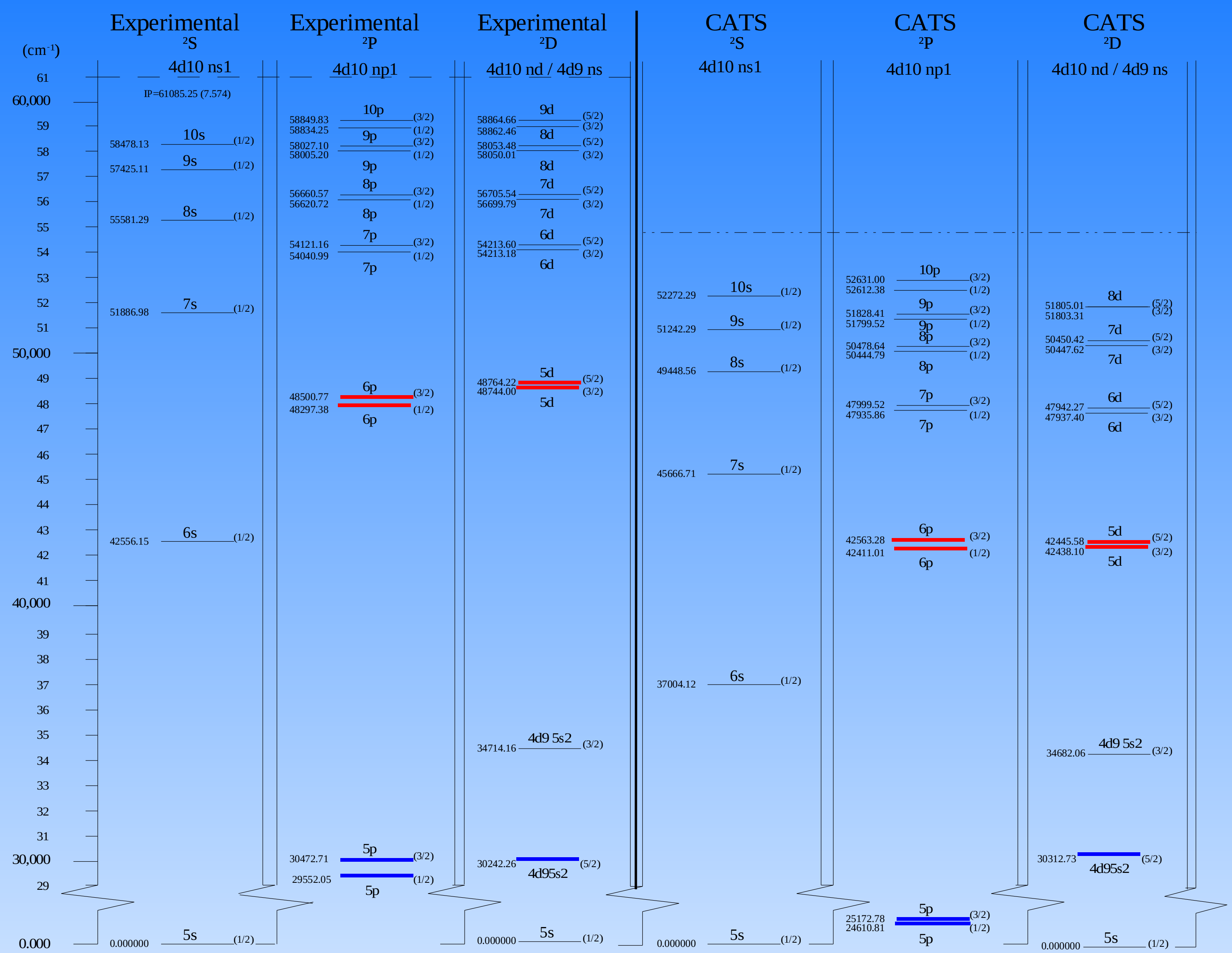


Figure 6: Comparison between experimentally obtained energy level structure (left) and that generated with Cowan's Atomic Structure code (CATS) (right) for neutral Ag.

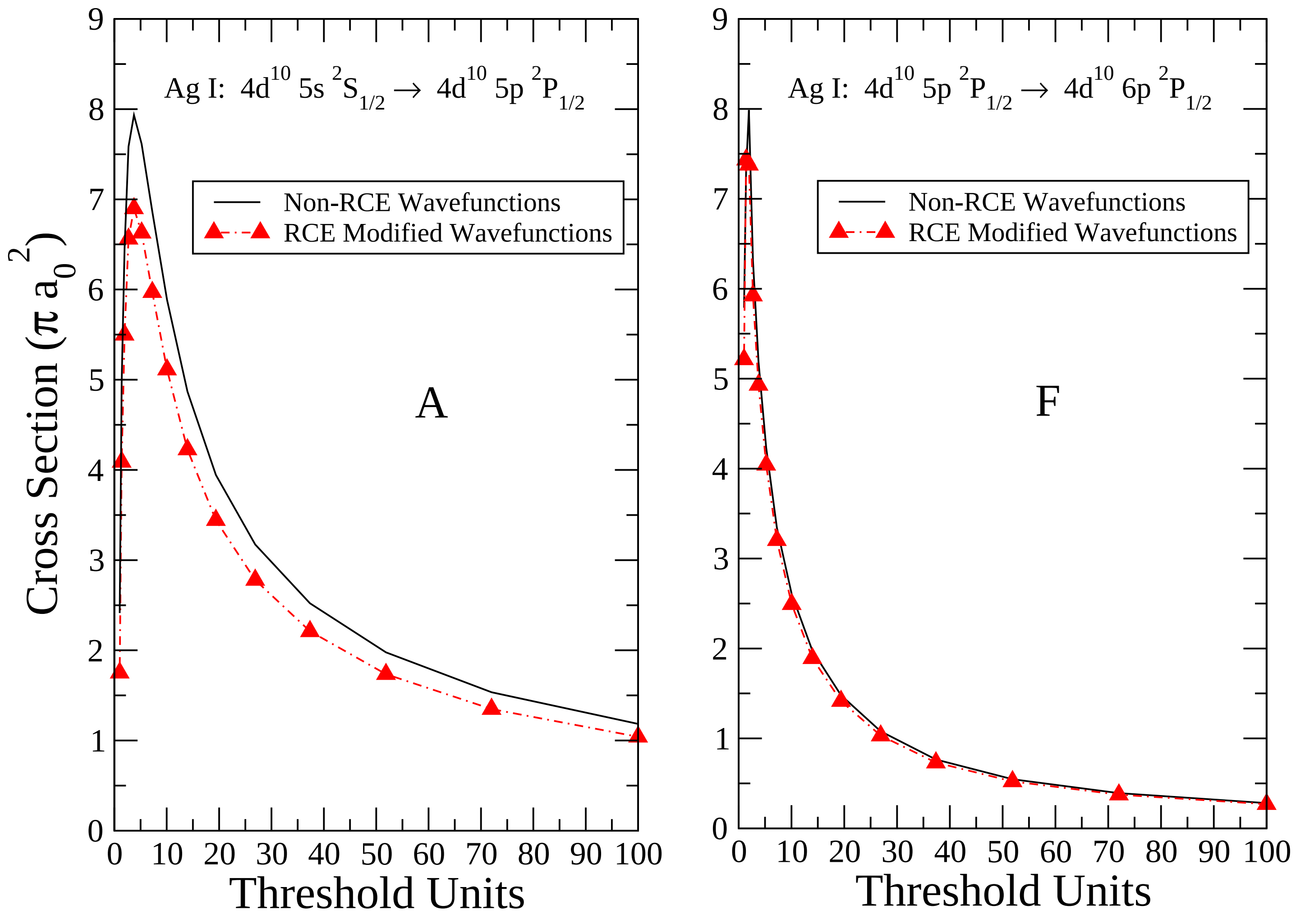


Figure 7: Comparison of electron impact excitation cross sections generated with and with RCE modifications of the wavefunctions. The two figures correspond to an allowed **A** (left) and forbidden **F** (right) transition.

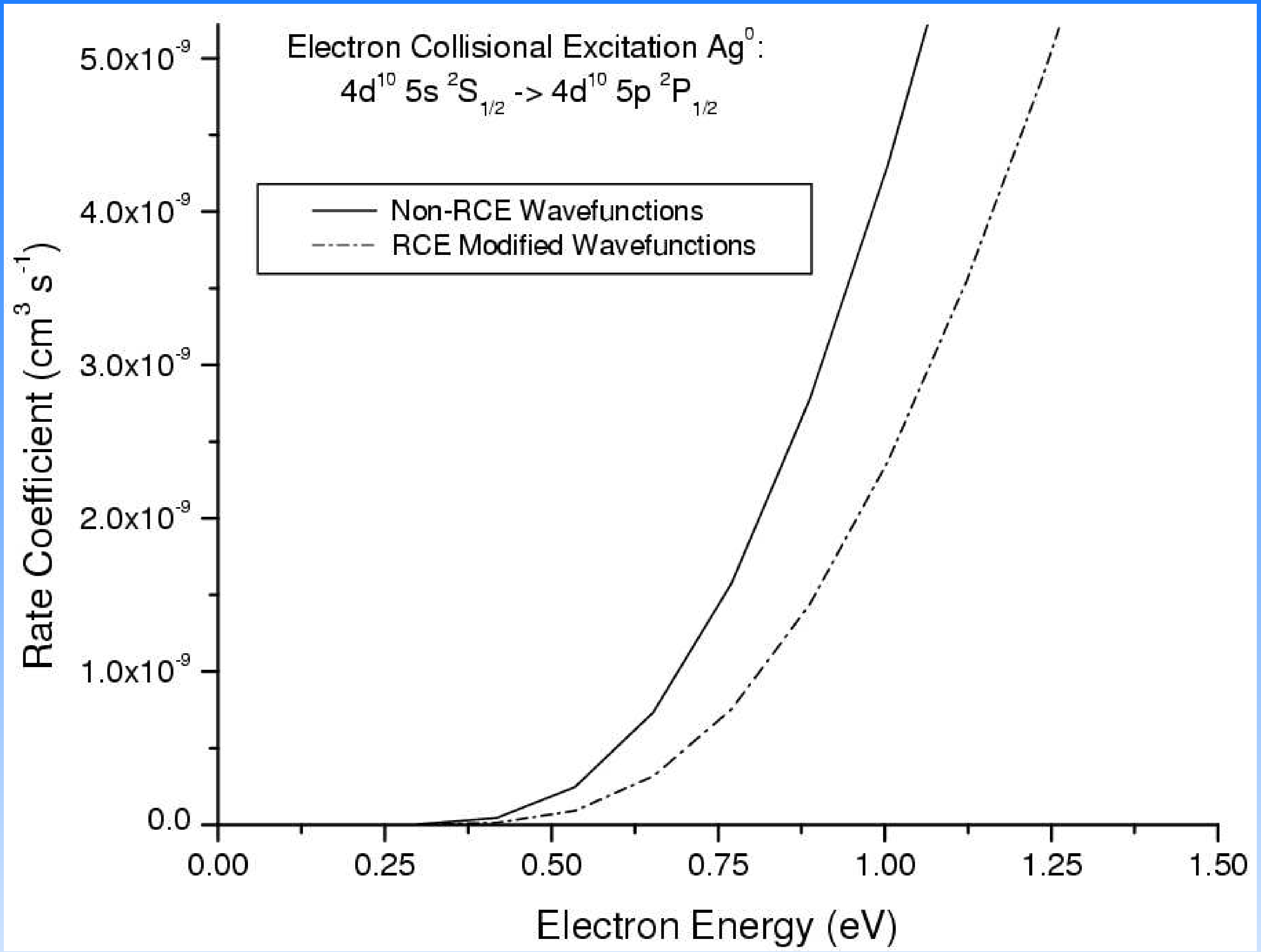


Figure 8: A comparison of an electron impact excitation rate for silver generated with and without wavefunction modifications by the RCE procedure.

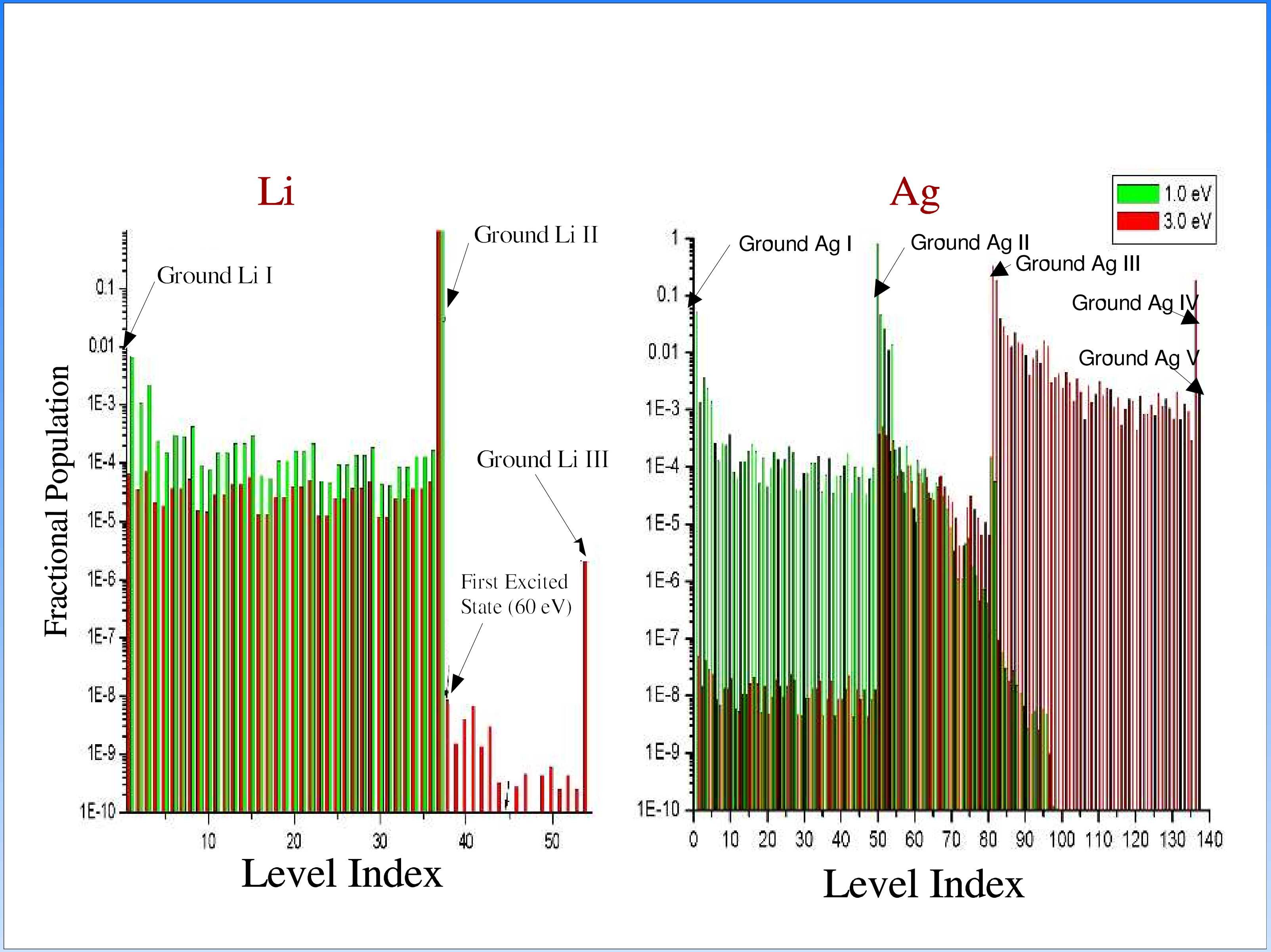


Figure 9: The effect of temperature on fractional level populations for three ionization stages in Li and five in Ag atoms, for an electron density of 1x10^{17} cm^{-3}.

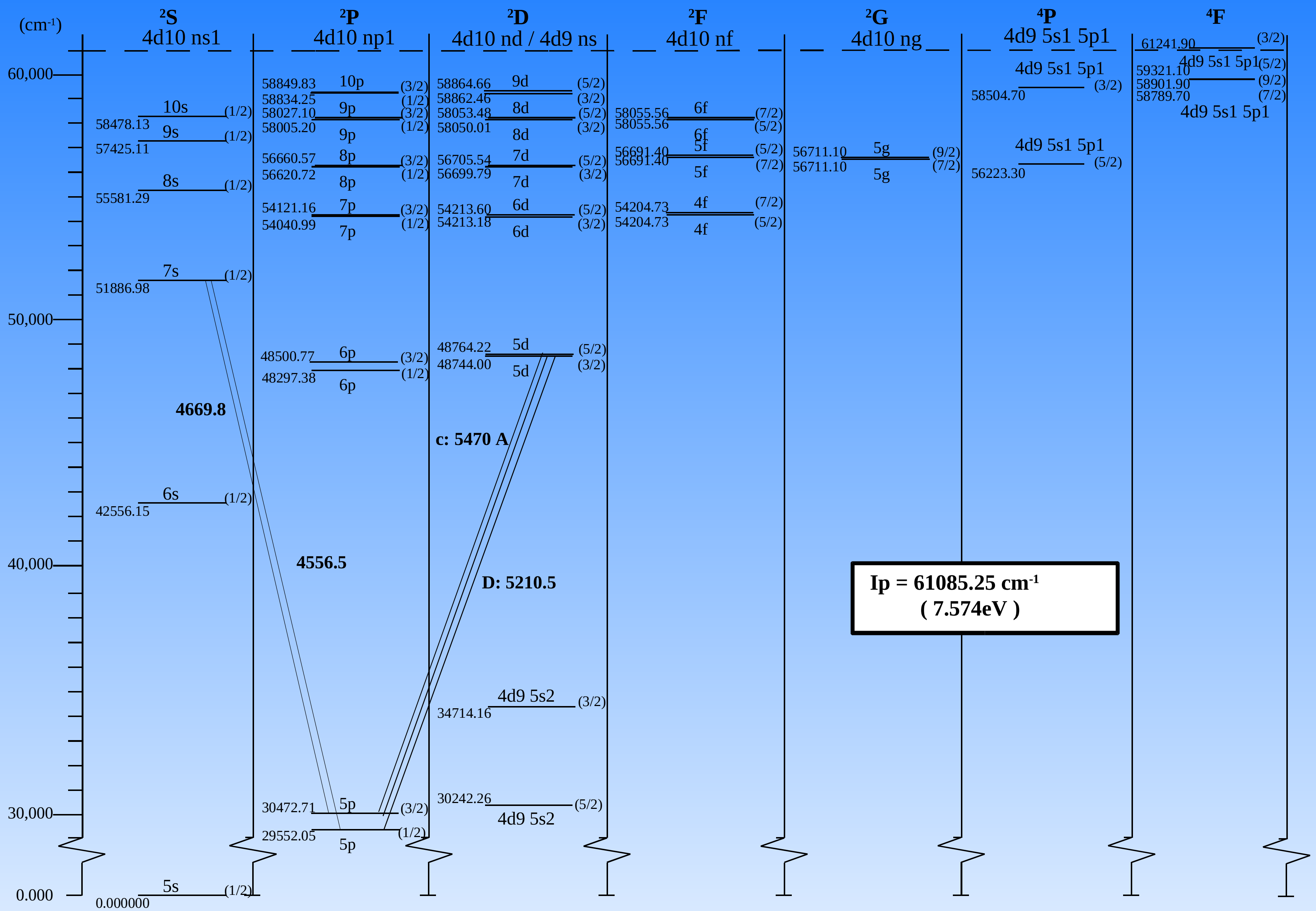


Figure 10: Ag I Grotrian diagram.

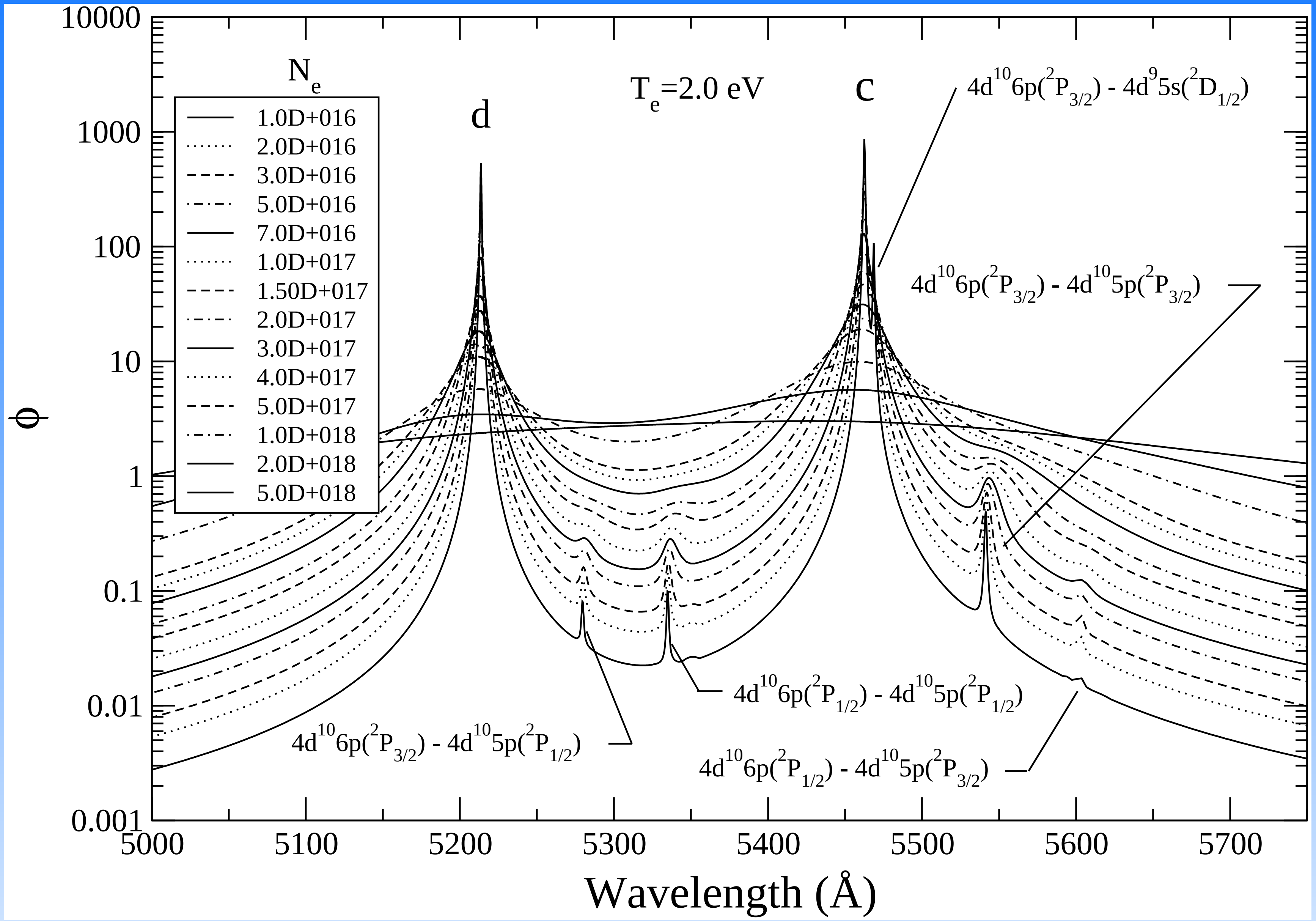


Figure 11: Neutral silver line profiles for various plasma electron densities with the two dominant $5d - 5p$ fine structure transitions.

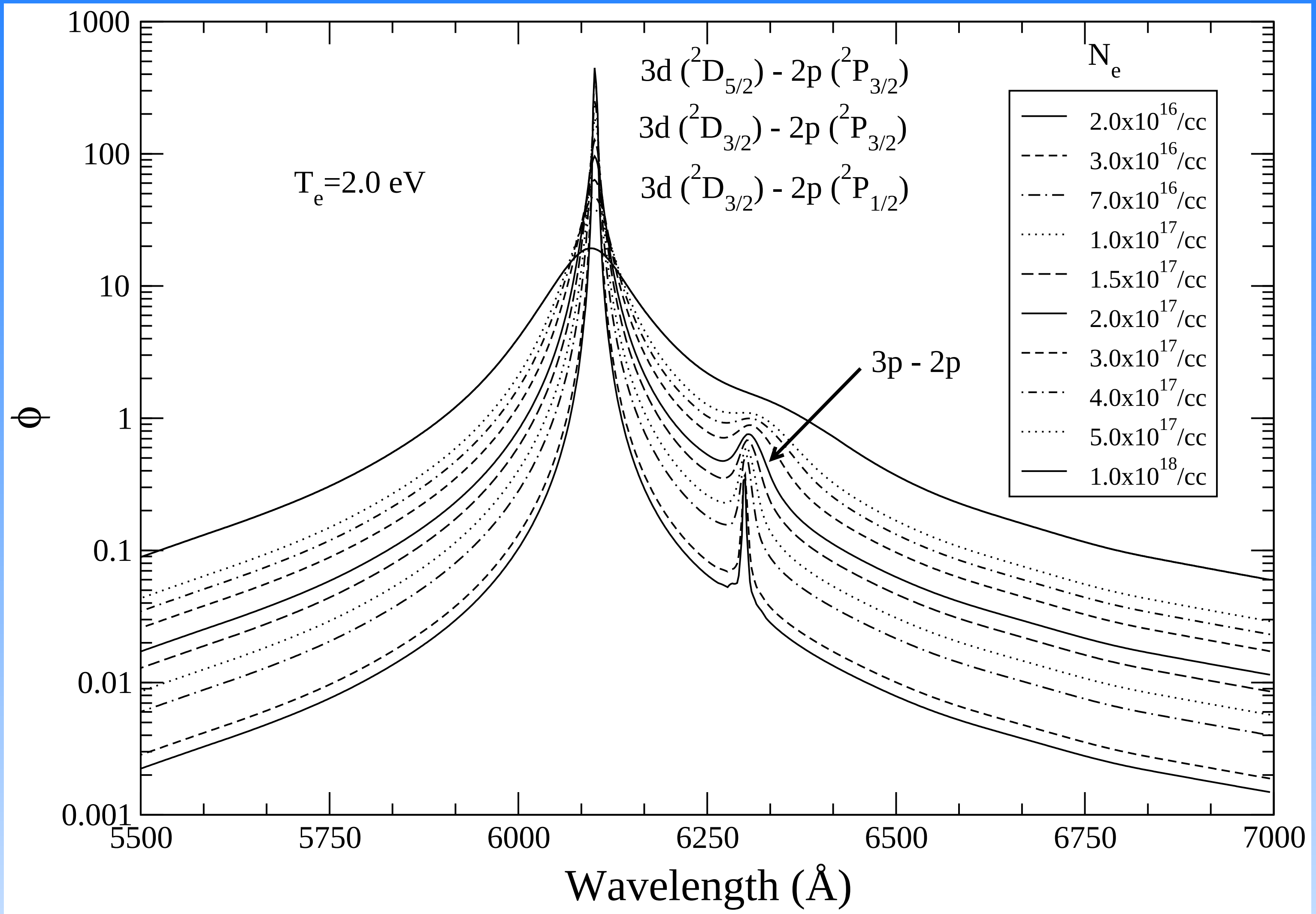


Figure 12: Neutral lithium line profiles at various plasma electron densities for the dominant $3d-2p$ transition. Note the asymmetry at the peak.

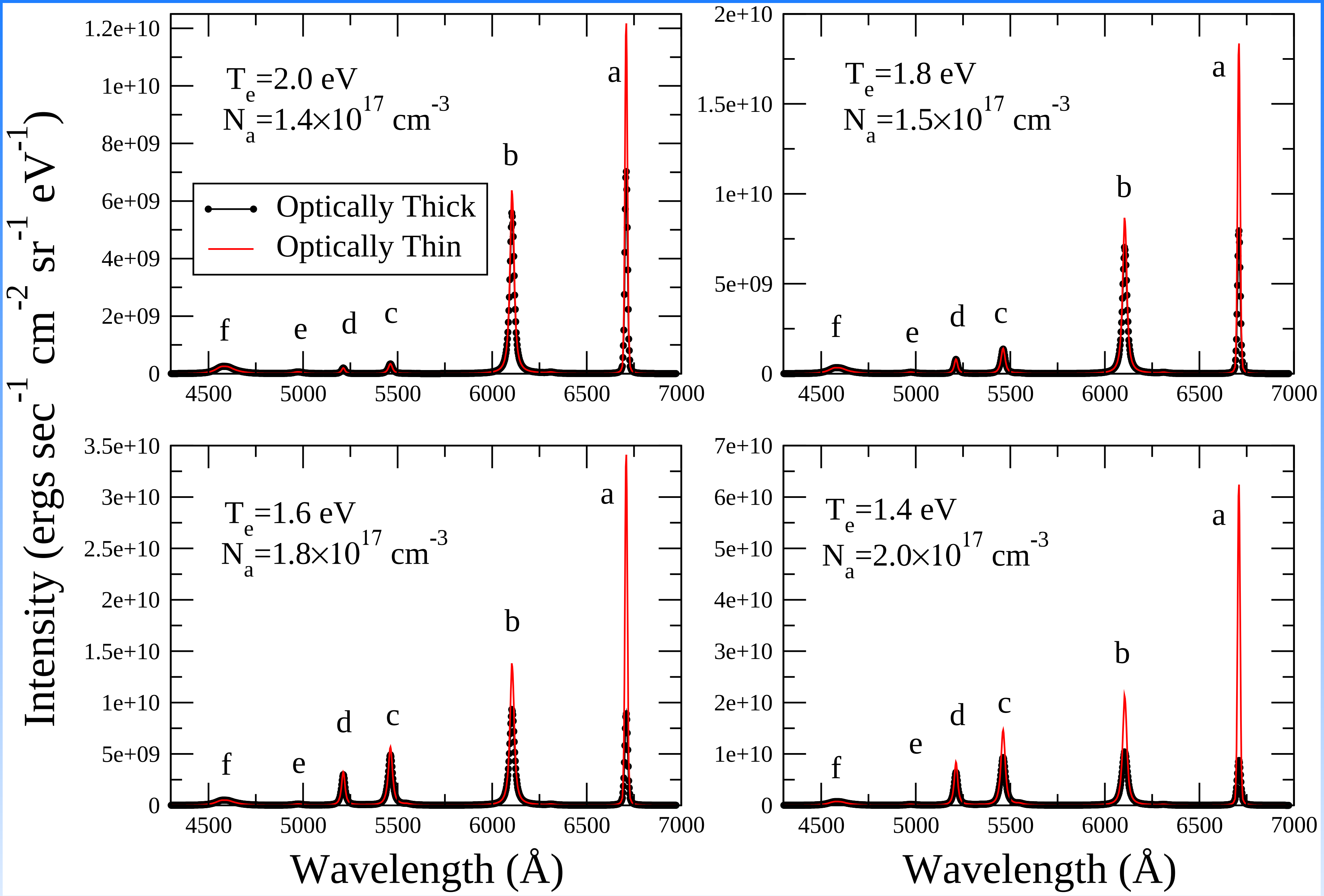


Figure 13: Superposition of optically thin and thick spectra for constant N_e series.

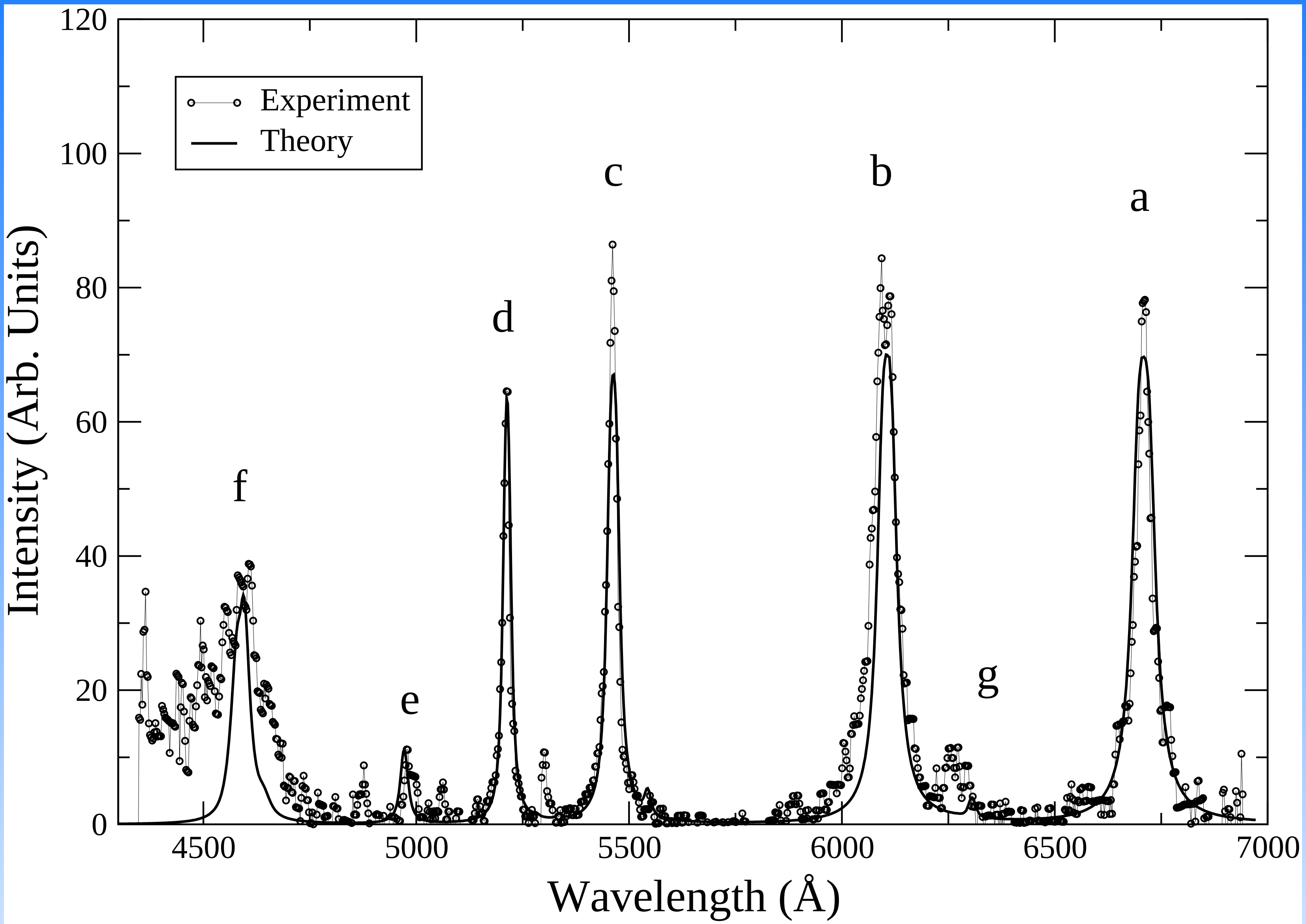


Figure 14: Experimental lineout at x=28.8μm and t=30 nsec with predicted T_e=0.8 eV and N_a=1.0x10^{17} cm^{-3} uniform synthetic spectra.

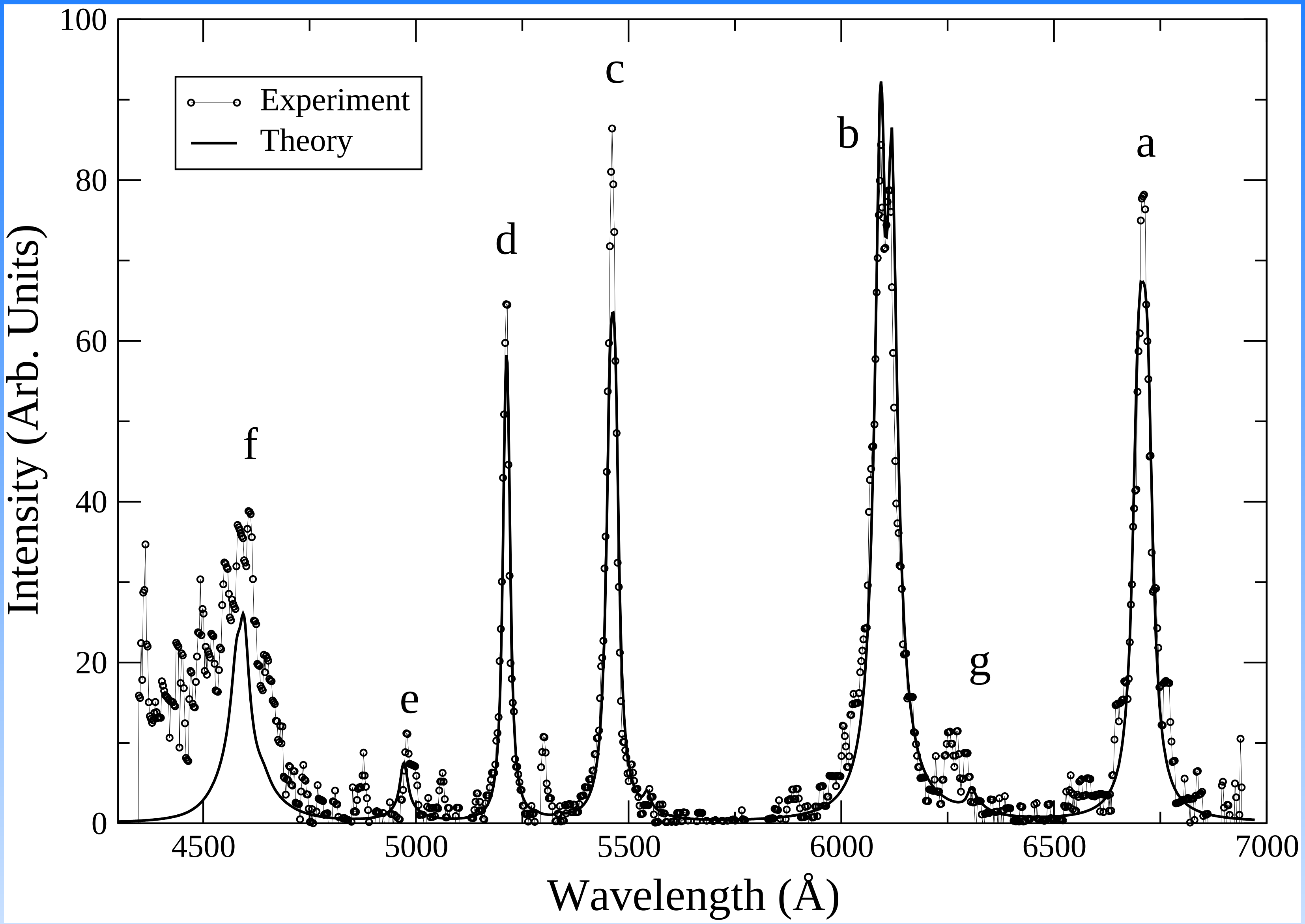


Figure 15: Experimental lineout at x=28.8μm and t=30 nsec with predicted T_e=[0.7, 1.8, 1.8, 0.7] eV and N_a=[1.0, 2.0, 2.0, 1.0] x10^{17} cm^{-3} 4-zone synthetic spectra.

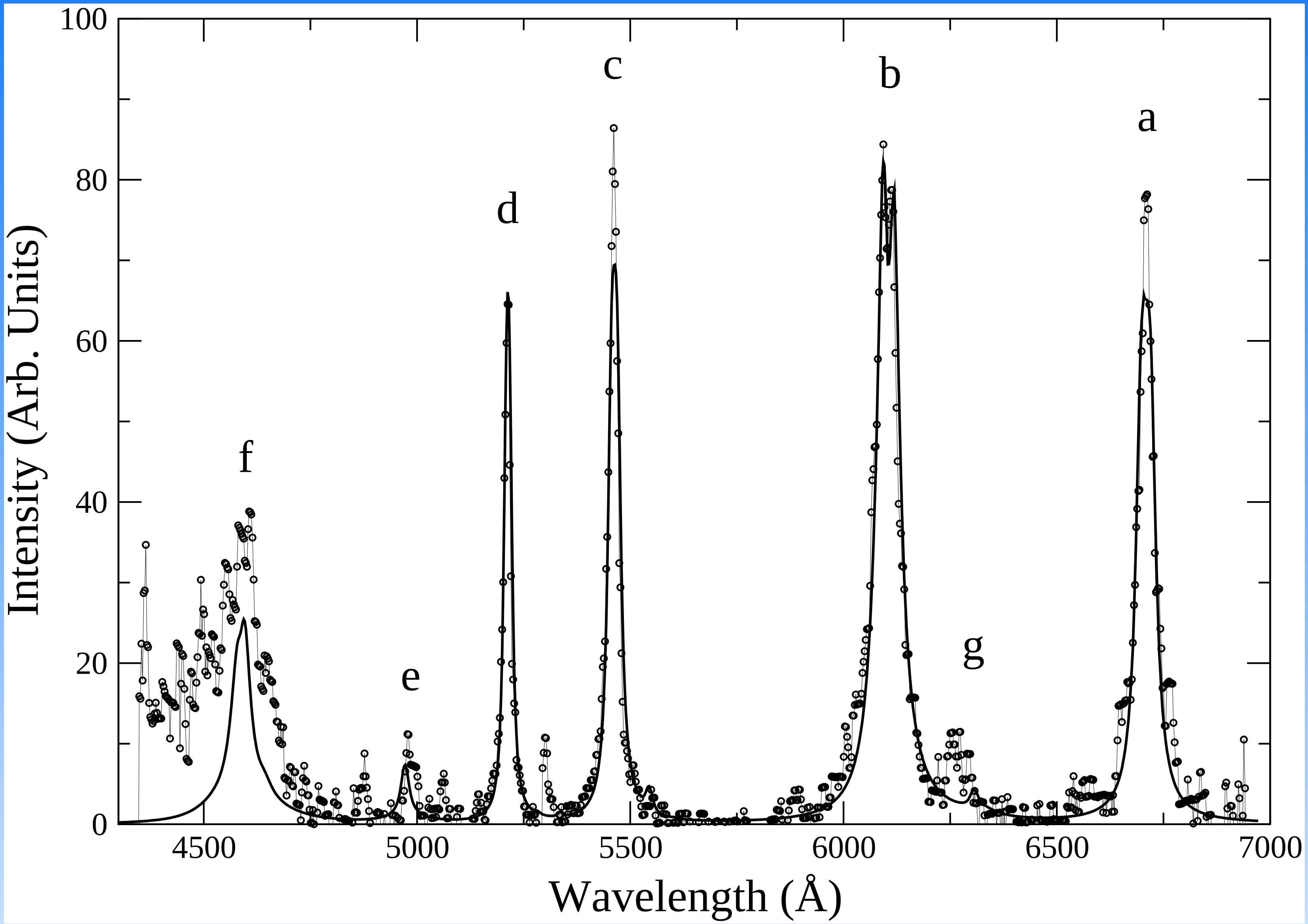


Figure 16: Experimental lineout at x=28.8μm and t=30 nsec with predicted T_e=[0.7, 0.8, 2.3, 2.3, 0.8, 0.7] eV and N_a=[1.0, 1.0, 2.5, 2.5, 1.0, 1.0] x10^{17} cm^{-3} 6-zone synthetic spectra.

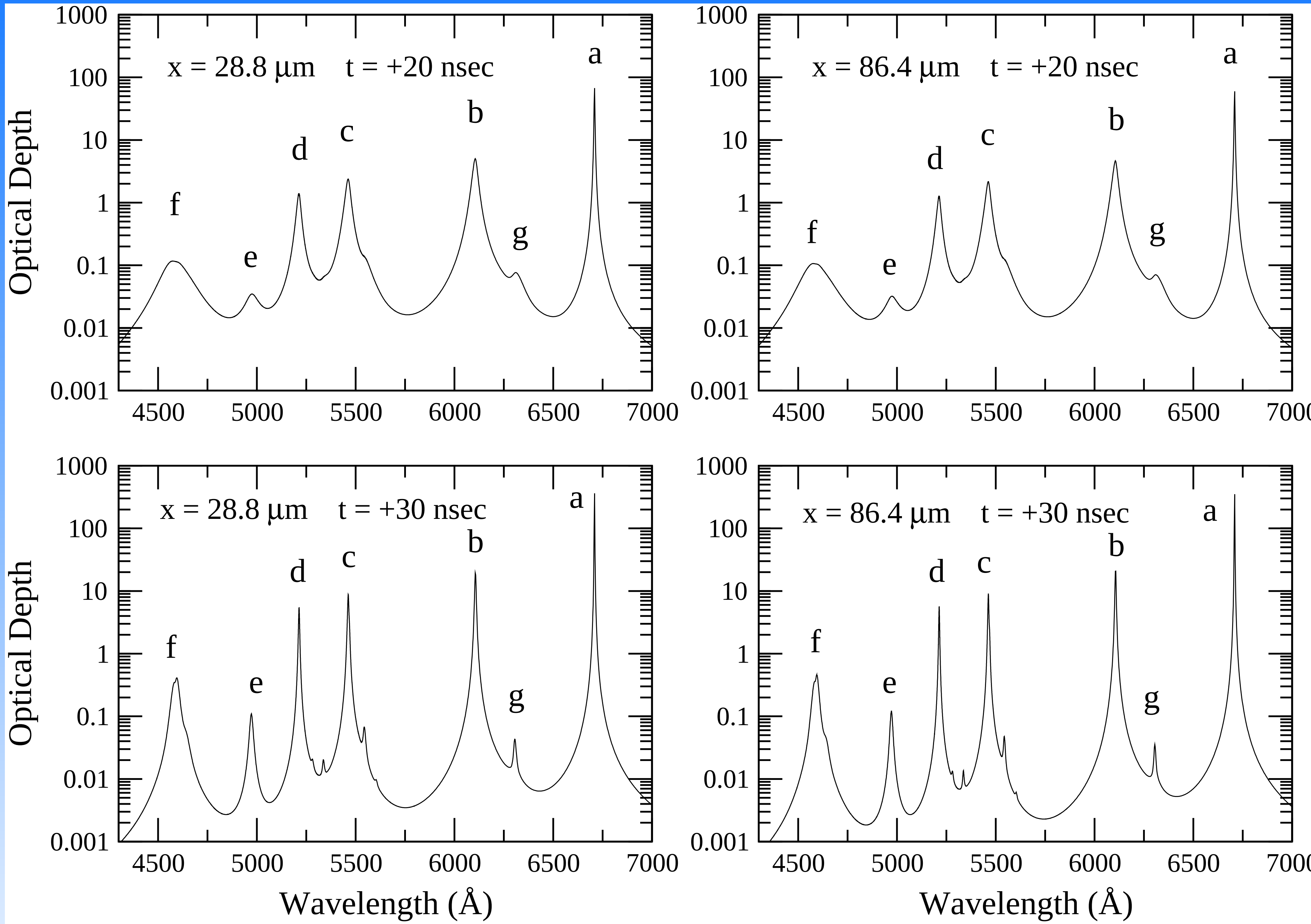


Figure 17: Optical depths for all four 6-zone synthetic spectra.

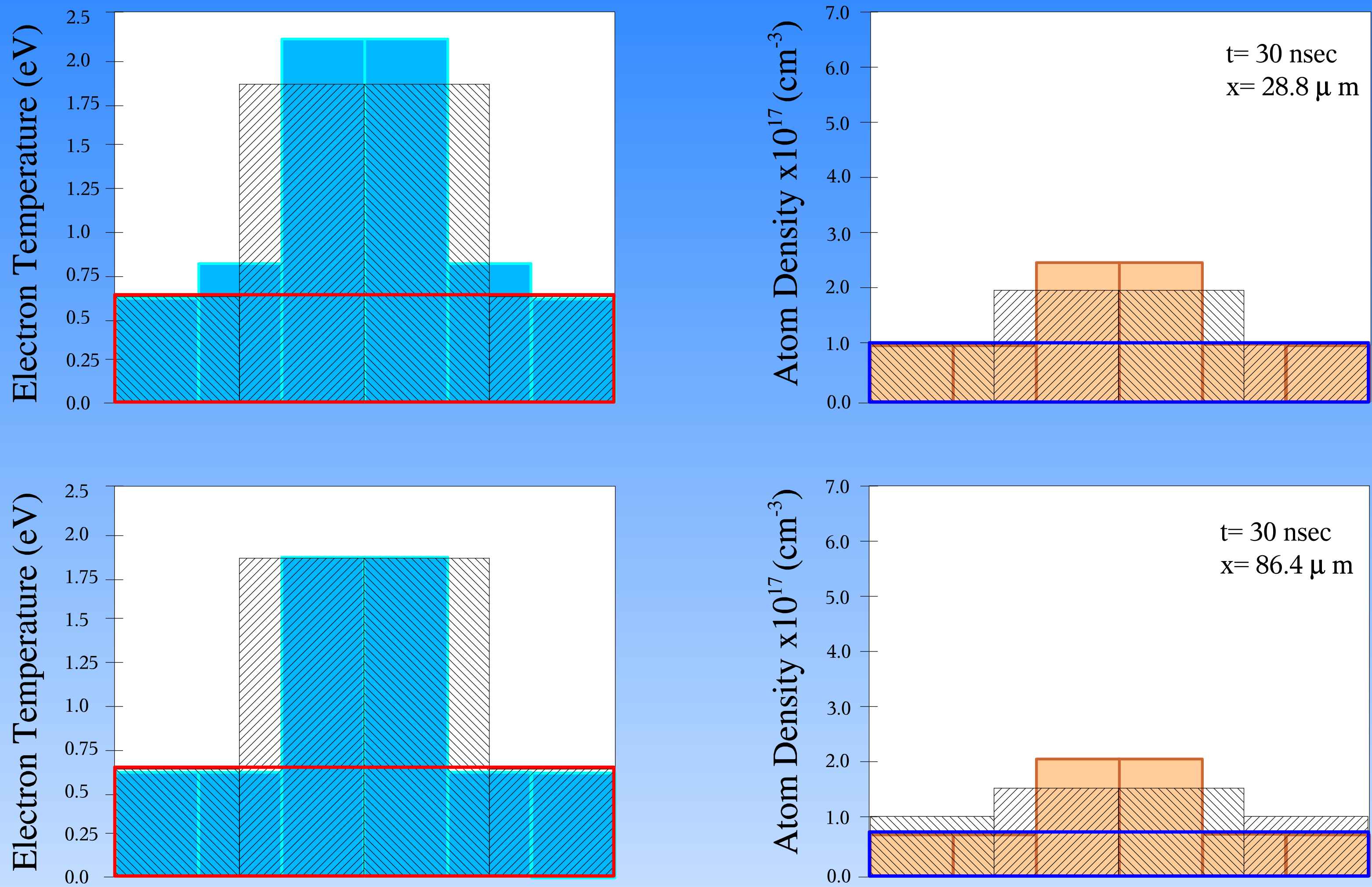
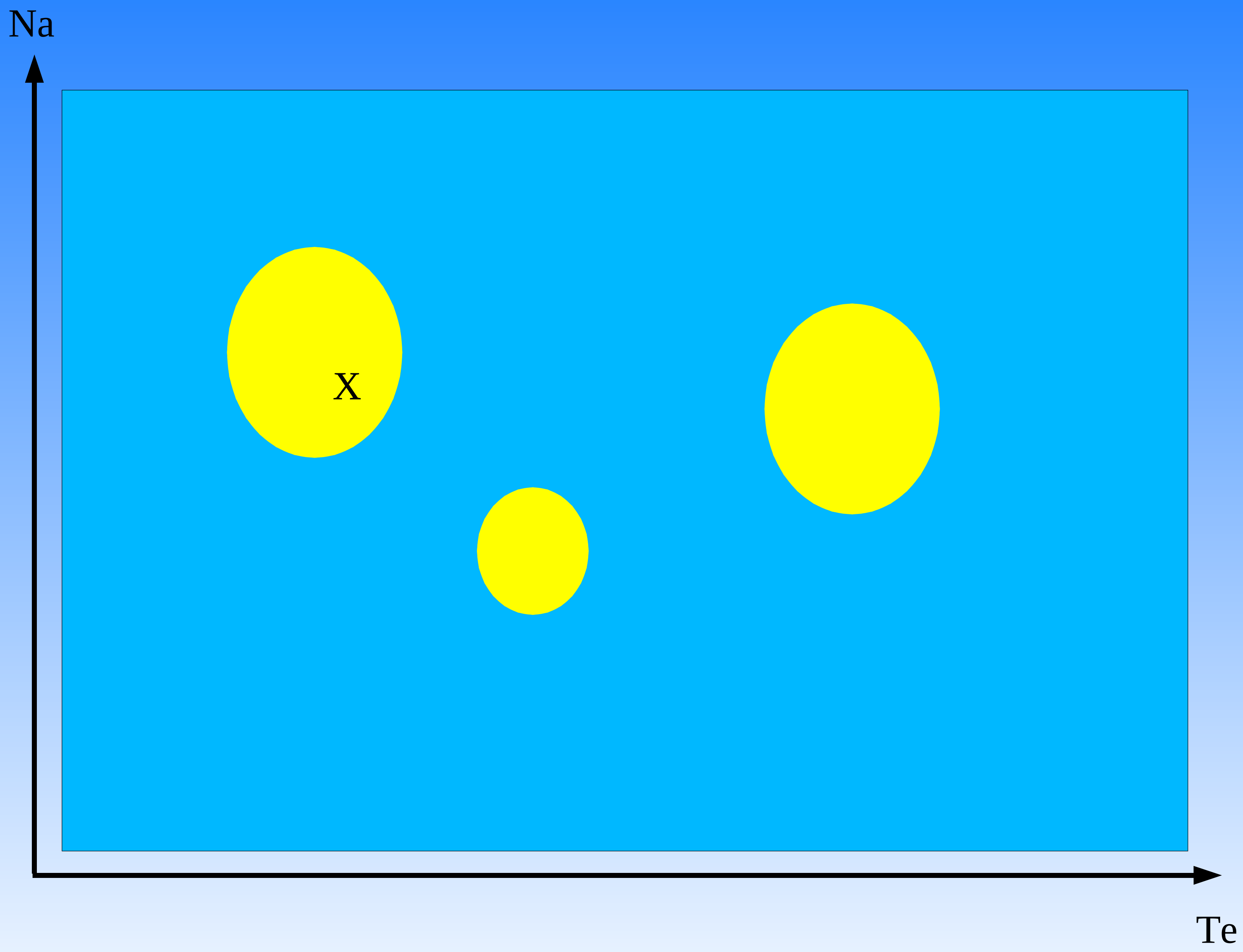


Figure 18: Uniform, 4 and 6 zone T_e and N_a profile results for t= +30 nsec synthetic spectra.

Summary & Insight

Concerning spectra whose features have a larger variation in optical depth

- REVERSE PROBLEM - Large optical depths reduces the sensitivity of the spectra and leads to ambiguity in plasma characterization.
- We see multiple acceptable solution domains.
- Solution space contains many plateaus - standard search techniques begin to fail.
- What does the best fit mean? What do the other plateaus mean?
- Brute force searches to establish this pattern.
- New search approach - mesh refinement: coarse to fine.


Na
X
Te

Coupled electron and atomic kinetics through the solution of the Boltzmann equation for generating time-dependent X-ray spectra

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Introduction

Problem Type

Spectral modeling of highly NON-EQUILIBRIUM PLASMAS (N_a=1.0$\times$10^{20} cm^{-3}).

Time-dependent systems where the electron energy distribution function (EEDF) is NON-MAXWELLIAN.

Implementation

- **Coupled electron and atomic kinetics**

  Stepping: EK solution is propagated to time $t+1$ with level populations from the AK at t. Then the AK are propagated to time $t+1$ with the EEDF from $t+1$. The $t+1$ level populations from the AK model are provided to the EK.

- **Simultaneous?**

  Too slow!

Introduction

- **Common Examples**

  Electron beam driven X-ray lamps for lithography

  Intense short pulse laser driven plasmas

Electron Kinetics

- **Boltzmann Transport Equation**

$$\frac{\partial f(\vec{r},\vec{p},t)}{\partial t} + \frac{\vec{p}}{m} \bullet \nabla_r f(\vec{r},\vec{p},t) + F \bullet \nabla_p f(\vec{r},\vec{p},t) = \left(\frac{\partial f(\vec{r},\vec{p},t)}{\partial t}\right)_{coll} \quad (1)$$

- **0-D Boltzmann Equation** - (Non-relativistic)

$$\frac{\partial f(E,t)}{\partial t} = \left(\frac{\partial f(E,t)}{\partial t}\right)_{coll} \quad (2)$$

Formalism

Following J.Bretagne et al[a] we write the Boltzmann equation for the free-electron distribution function in the following form,

$$\frac{\partial}{\partial t} f(E,t) = \left(\frac{\partial f}{\partial t}\right)_{el(e-e)} + \left(\frac{\partial f}{\partial t}\right)_{in} + A(t)S(E_p, E) \quad (3)$$

where

$$\left(\frac{\partial f}{\partial t}\right)_{in} = K_{ion} + K_{3BR} + K_{exc} + K_{de-exc} \,. \quad (4)$$

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[a] J. Phys. D, **14** pp. 1225-39

Formalism

Ionization Contribution

$$K_{ion}(E) = \sum_{iljm} K^{ion}_{iljm}(E) \tag{5}$$

where $K^{ion}_{iljm}(E)$ is the contribution to $K_{ion}(E)$ from the

$$e^- + (il) \longrightarrow e^- + e^- + (jm) \tag{6}$$

ionization process where (il) indices refer to the initial ion and its quantum state and (jm) to the final ion and its quantum state, respectively. $K^{ion}_{iljm}(E)$ can be given in the form,

$$\begin{aligned} K^{ion}_{iljm}(E) = N_{il} \Bigg[& \int_{E+E_0}^{2E+E_0} v' \sigma_{iljm}(E', E' - E_0 - E) f(E', t) \, dE' + \\ & + \int_{2E+E_0}^{E_{max}} v' \sigma_{iljm}(E', E) f(E', t) \, dE' + \\ & - v f(E, t) \int_0^{(E-E_0)/2} \sigma_{iljm}(E, E'') \, dE'' \Bigg] \end{aligned} \tag{7}$$

Formalism

Ionization Contribution: The total ionization cross section for a process will be denoted by $Q_{iljm}(E)$ (in units of cm^2) and thus it can be obtained from $\sigma_{iljm}(E, E'')$ via the formula,

$$Q_{iljm}(E) = \int_0^{(E-E_0)/2} \sigma_{iljm}(E, E'')\, dE'' \tag{8}$$

In the present work we assumed that $\sigma_{iljm}(E', E)$ can be written in the following form,

$$\sigma_{iljm}(E', E_1) = Q_{iljm}(E')\, \Omega(E', E_1) \tag{9}$$

where $\Omega(E, E_1)$ is described as follows (Astrophys. J, 381 pp 597-600 1991)

$$\Omega(E, E_1) = \frac{1}{(E - E_0)(E^2 + aE_0^2)} \times \left[2(a+1)E_0^2 + \frac{160(E + E_0)\left(E_1 - \frac{1}{2}(E - E_0)^4\right)}{(E - E_0)^3} \right] \tag{10}$$

and is normalized, that

$$\int_0^{(E-E_0)/2} \Omega(E, E_1)\, dE_1 = 1 \tag{11}$$

Numerical Solution of the Boltzmann Equation

Bin representation

The EEDF can be represented a series of constant values.

$$f(E,t) = f(E_u) \text{ for } E_u - w_u/2 \leq E \leq E_u + w_u/2 \tag{12}$$

where E_u is the midpoint of the uth bin, w_u is the width of the uth bin and N is the total number of bins.

Final Form of the Boltzmann Equation

$$\frac{d}{dt} f(E_u, t) = \sum_{v=1}^{N} M_{u,v}(t) f(E_v, t) \tag{13}$$

where the $M_{u,v}(t)$ matrix contains all the collisional contributions.

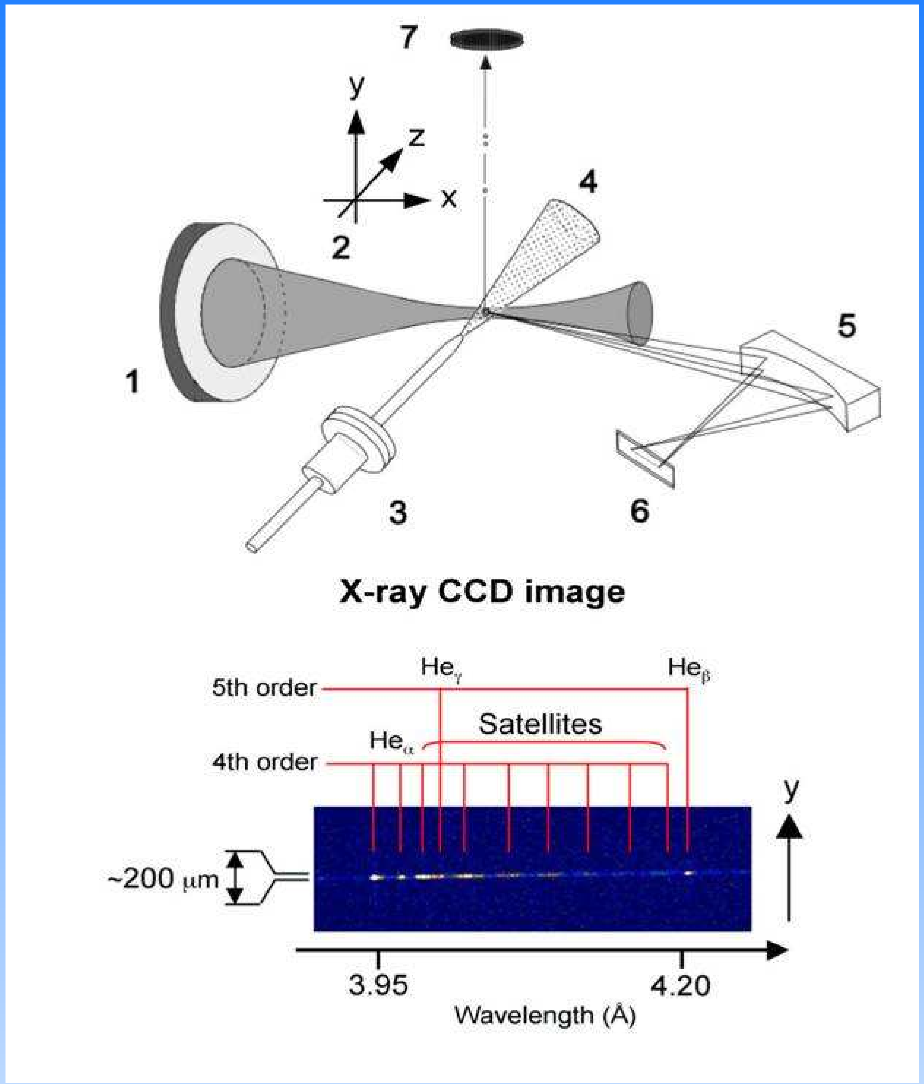

Figure 19: Laser: 200mJ, I=1.0e19 W/cm^2, 30 fs, Ti:sapphire laser. Prepulse: 1 ns duration 10^5 contrast ratio. Target: 1μm cluster target. FSSR:focusing spectrometers with spatial resolution, $\lambda/\delta\lambda =$1667 . Spectrum: 600 shots per spectrum.

Modeling the Experiment

- **Laser-Target Interaction**[a]

  Target 100K clusters in beam volume

  Beam more intense in the center, less on perimeter

- **Laser-Cluster Interaction**

  1 - 10 billion atoms

  1 μm cluster vs 10 μm main pulse

  3D - PROBLEM

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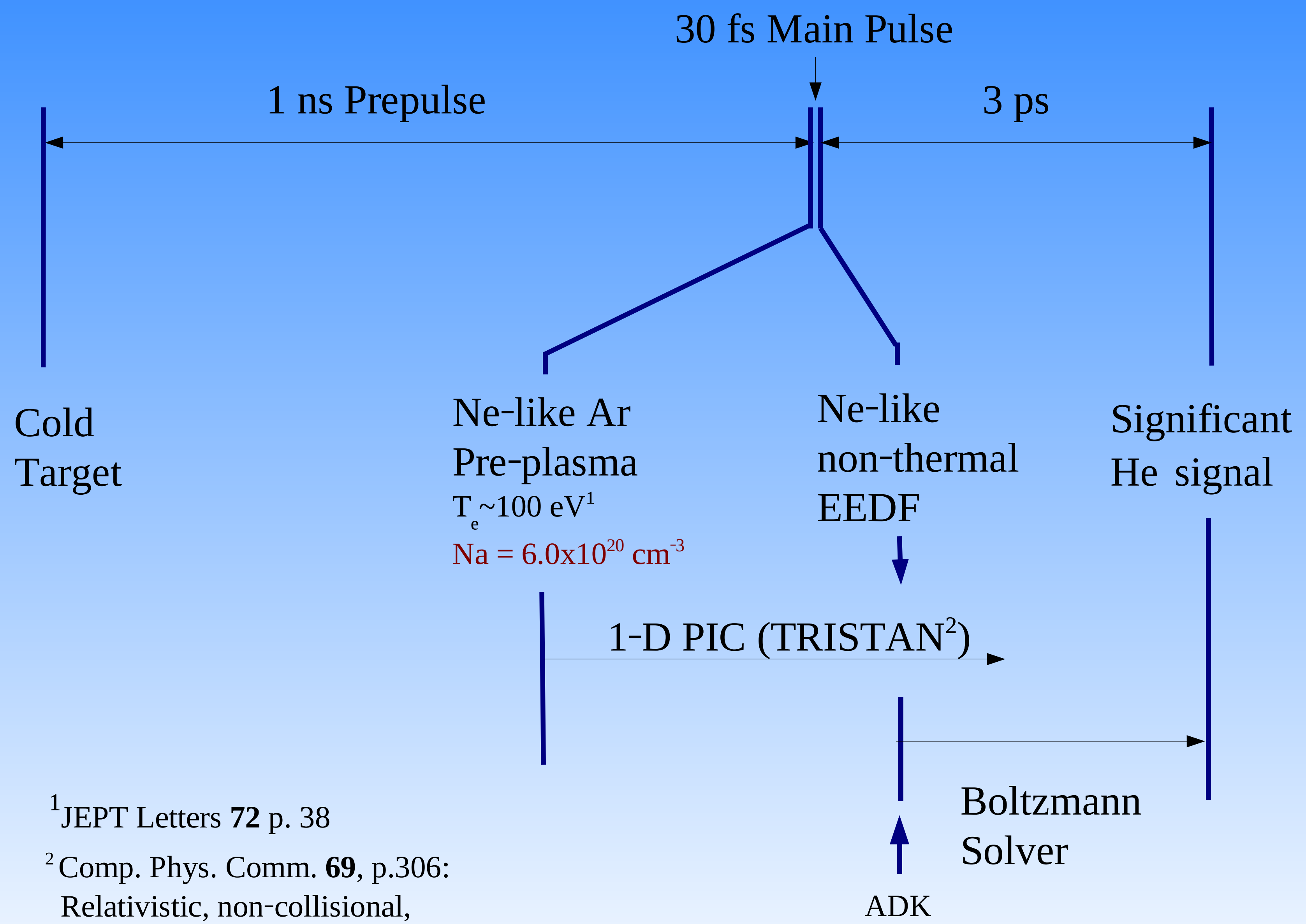
[a] JEPT Letters, **78** pp. 115-118

Plasma Evolution



[1] JEPT Letters **72** p. 38

[2] Comp. Phys. Comm. **69**, p.306: Relativistic, non-collisional, non-ionizing.

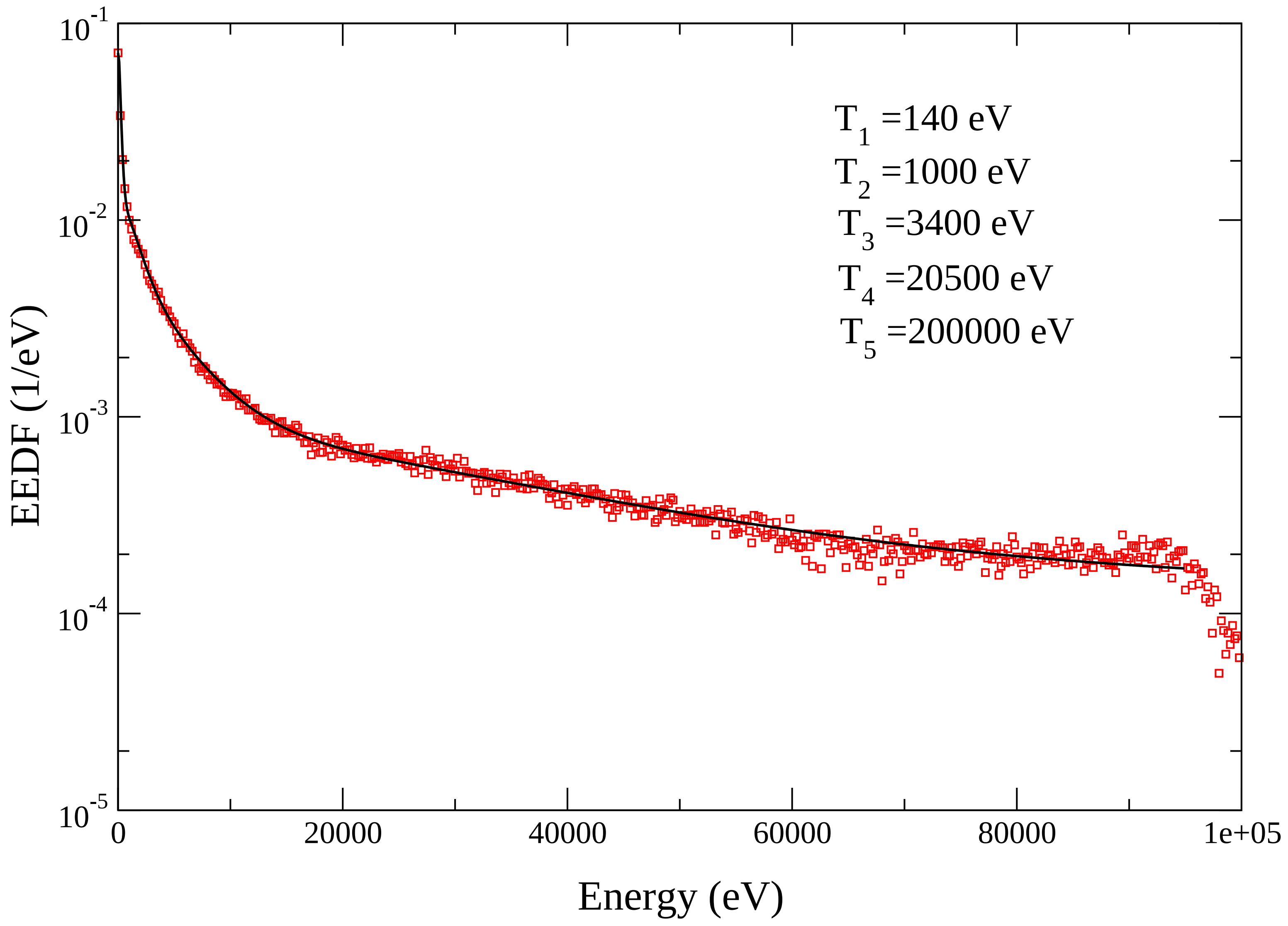
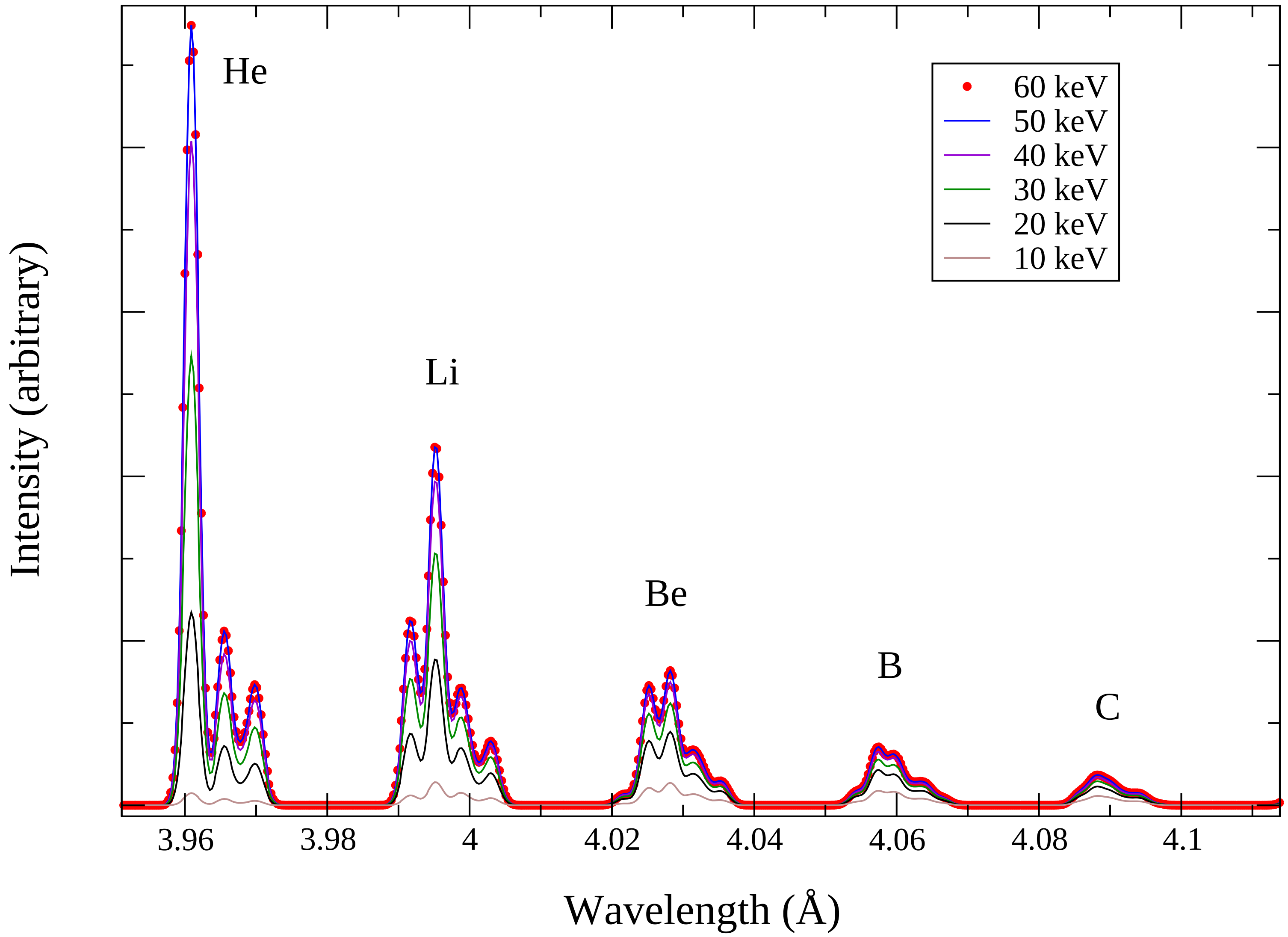
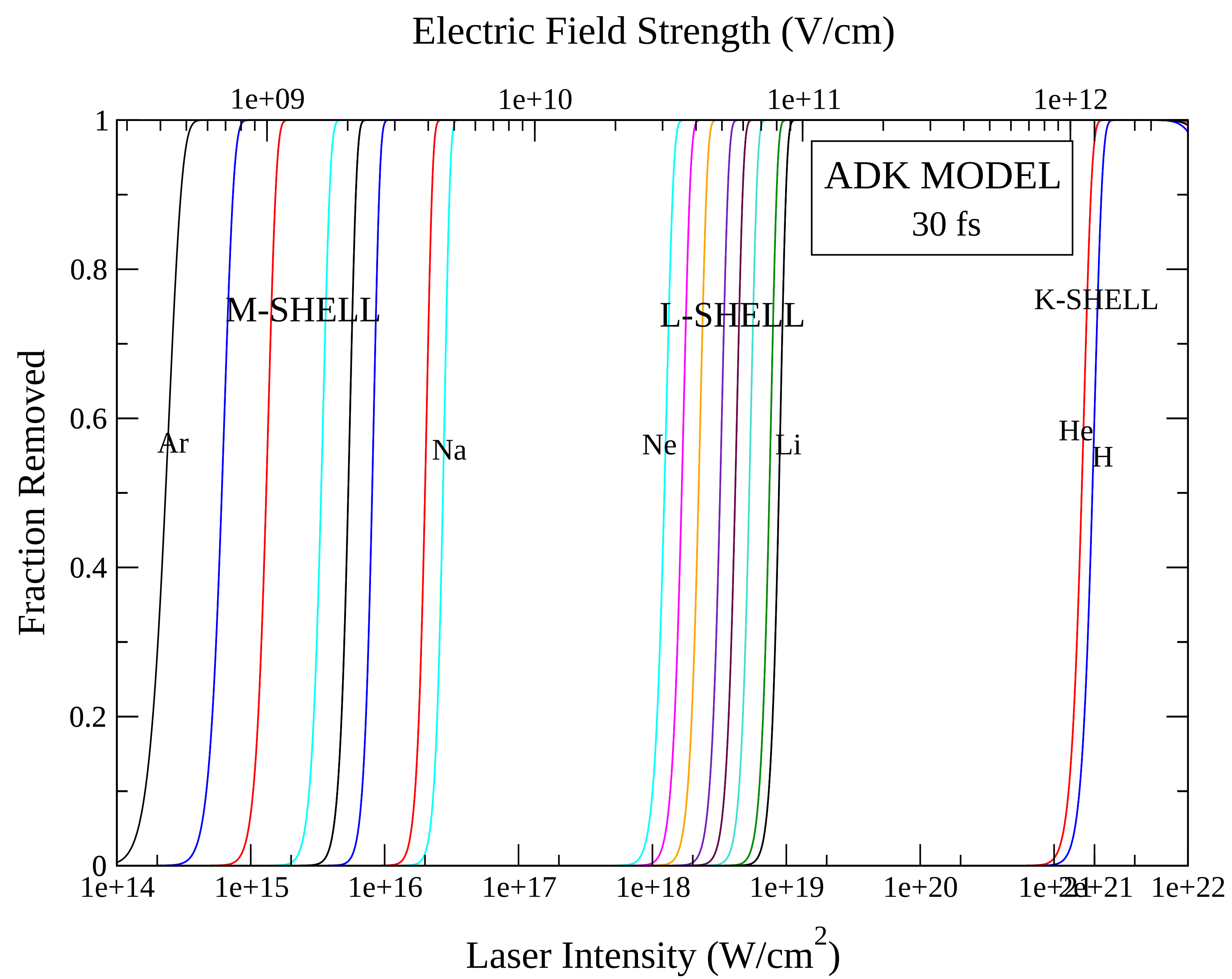


Figure 20: PIC produced EEDF at the end of the laser pulse.

EEDF Effects on Spectra





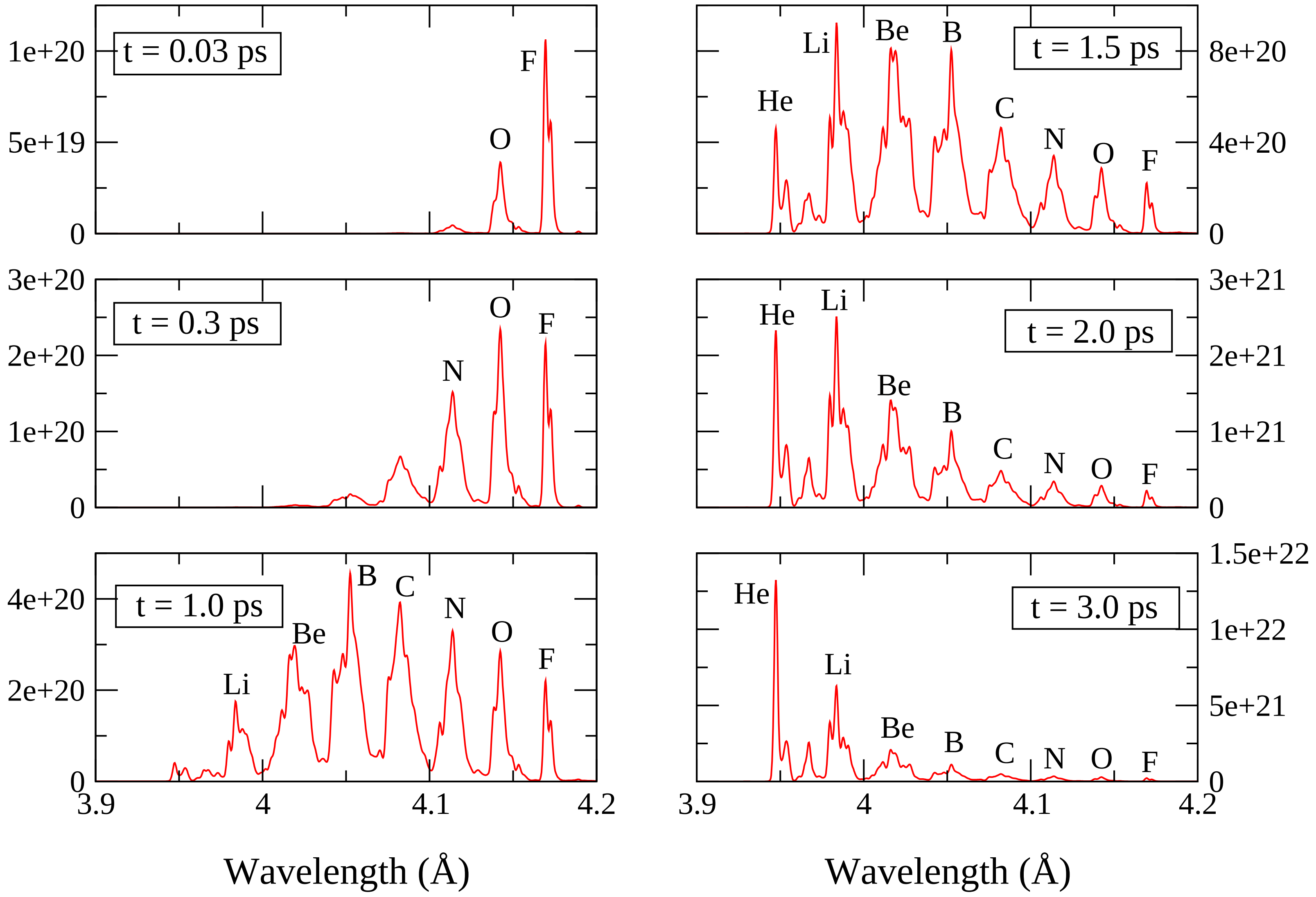
Electric Field Strength (V/cm)
1e+09
1e+10
1e+11
1e+12
ADK MODEL
30 fs
M-SHELL
L-SHELL
K-SHELL
Ar
Na
Ne
Li
He
H
Fraction Removed
0
0.2
0.4
0.6
0.8
1
1e+14
1e+15
1e+16
1e+17
1e+18
1e+19
1e+20
1e+21
1e+21
1e+22
Laser Intensity (W/cm2)

Plasma Evolution

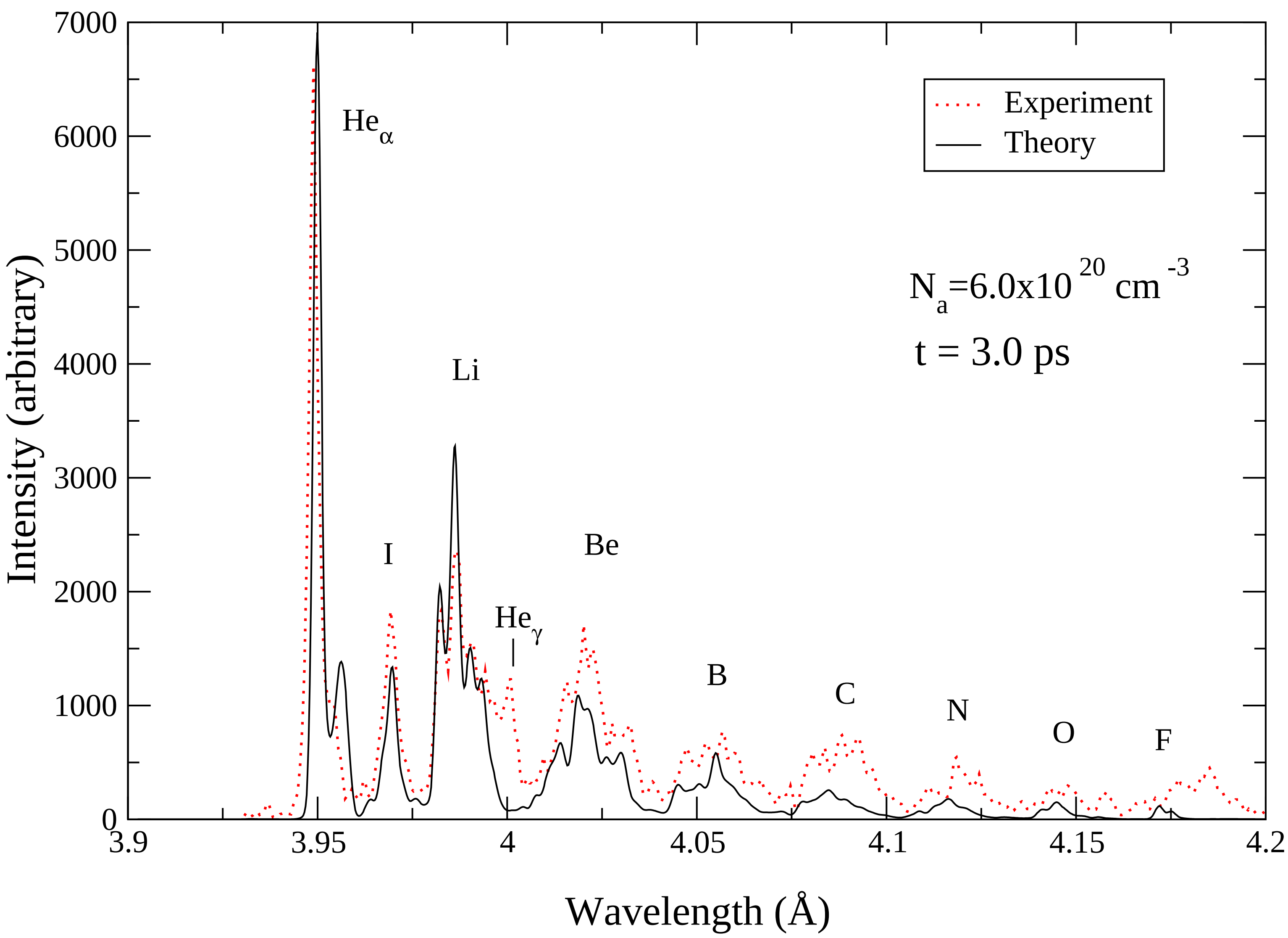
- CATS - Cowan’s Atomic Structure Code
- ACE - Collisional Excitation
- GIPPER - Collisional Ionization
- 3000 fine structure levels, Ne-like - H-like ionization stages.
- Configurations were truncated to principle number n=3.
- All possible n=1,n=2 X-ray transitions within the n=3 manifold.

Time Evolution of Integrated He_{α} Spectra

Intensity (arbitrary units)



Comparison of Time Integrated He_α Spectrum



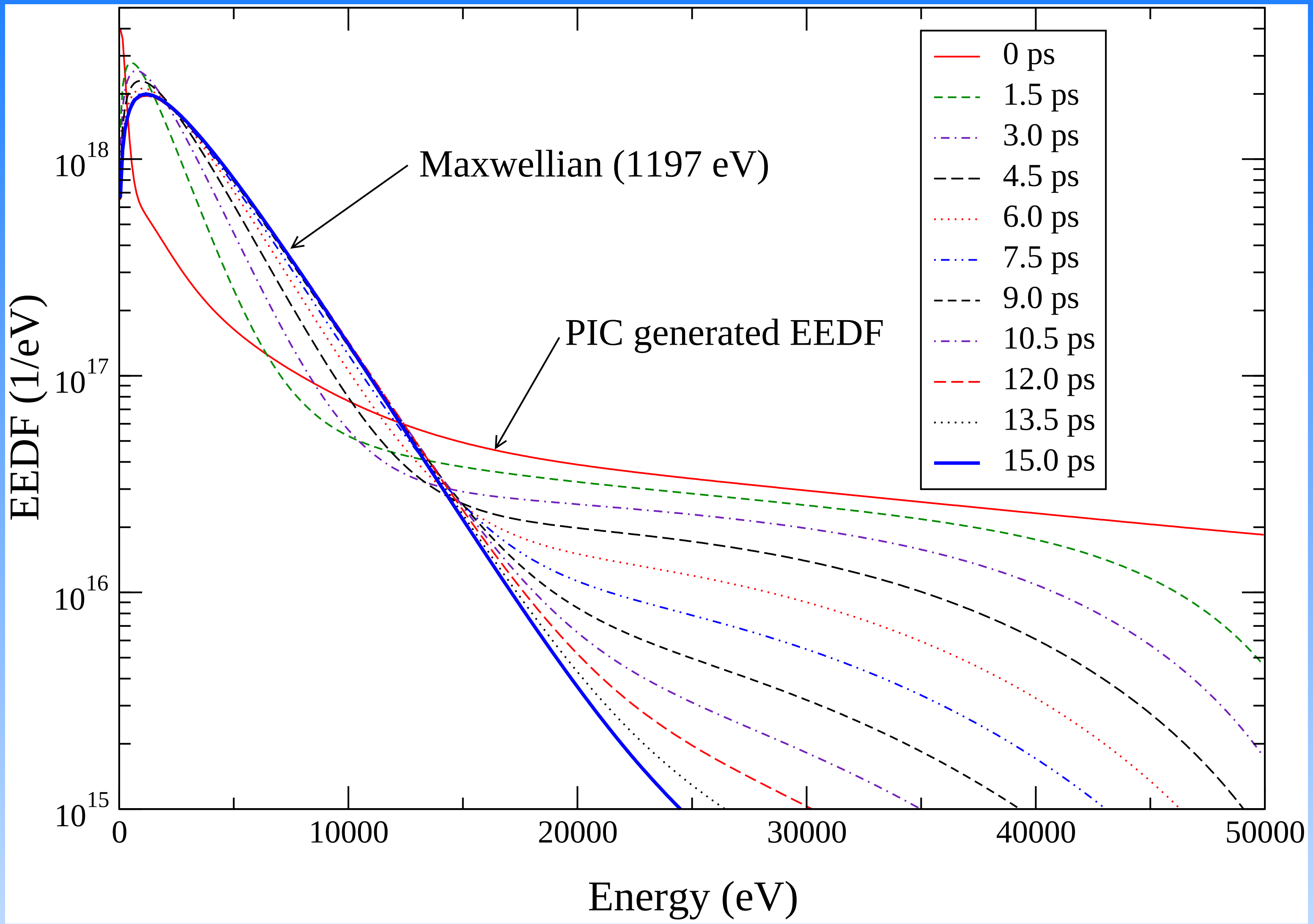


Figure 21: The time history of the EEDF, for times after the end of the laser pulse, computed by the Boltzmann solver for a constant atomic number density (N$_a$=6.0×10^{20} cm^{-3}). The system evolves into a Maxwellian (1197 eV) in approximately t=12.0 ps.

Conclusion/Summary

- Used 1-D particle-in-cell code to provide the initial EEDF of the Boltzmann solver.
- EEDF after 3 ps was far from equilibrated (13 ps)
- 50keV - 60keV of the EEDF is required to obtain a consistent spectra.
- From this model we predicted 6.0x10^{20} cm^{-3} represented an average density for the highly ionized contributions to the He$_{\alpha}$ spectrum.

Future Work

- Complete 3-body recombination
- Include autoionziation and dielectronic recombination
- Consider a non-constant volume approximation.
- Pursue comparisons between collisional PIC and Boltzmann Solver solutions.

Insight

Plasma and Atomic Physics

- Detailed description of the state of the plasma - The importance of plasma physics?
- Electron and Ion interaction?
- Emission spectra is of the order of the material expansion time - Coulomb explosion?
- Higher Z material and relativistic cross section - Plasma physicist assumption?