Collisional-radiative modeling of Tungsten at temperatures of 1200-2400 eV

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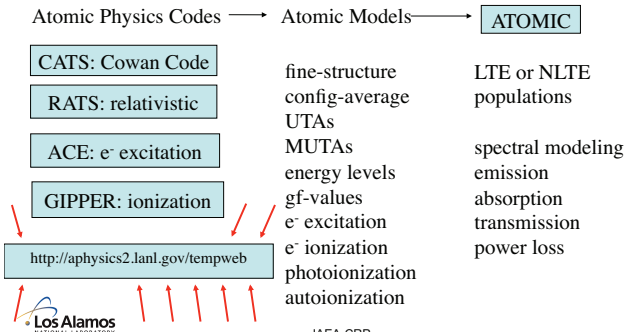
Outline of talk

- The LANL suite of atomic physics codes
  - structure codes
  - collision codes - updates
  - ATOMIC: collisional-radiative modeling
- Collisional-radiative modeling of W at moderate temperatures
  - Studied in recent NLTE8 workshop
  - We discuss LANL contributions:
    - Completeness of configuration lists
    - Semi-relativistic configuration-average model
    - Relativistic configuration-average model
    - Semi-relativistic MUTA calculations – includes fine-structure detail
    - Calculations that include full configuration-interaction – how far can this be pushed?
- Conclusions

The LANL suite of atomic modeling codes



General code features

- Simple input format for handling arbitrarily complex problems
- Various physical approximations:
  - Atomic structure: Hartree-Fock (semi-relativistic) or Dirac-Fock-Slater (fully relativistic)
  - Collision/Photo cross sections: distorted-wave, Coulomb-Born or plane-wave-Born
- Data are stored in a random-access binary format called IPCRESS (Independent of Platform and Can be Read by Existing Software Subroutines)
- Easy to create very detailed configuration-average and fine-structure models

Code features

- Atomic structure and collision codes form a mature platform (20+ years in development) that has been rigorously tested
  - Comparisons of atomic data with measurement and other codes have been performed for a wide range of systems
- Most important aspect that LANL atomic physics codes provide are consistency and completeness
- It is straightforward to compute large-scale sets of atomic data at a well-defined level of approximation in a fully consistent manner
  - Data provided are in a compact, easily accessed binary format for use in CR modeling
  - One may then straightforwardly assess convergence with respect to the number of states within a CR model in a methodical manner

Structure codes

- Semi-relativistic atomic structure code named CATS
  - Hartree-Fock code based on Cowan's ATomic Structure code
  - Generates wavefunctions, energies, oscillator strengths in the semi-relativistic approximation (spin-orbit interaction, mass-velocity term, Darwin term)
  - Generates plane-wave-Born excitation cross sections
  - May be run via webserver: http://aphysics2.lanl.gov/tempweb
- Fully-relativistic structure code named RATS
  - Dirac-Fock-Slater code based on fractional occupation number (FON) method from Sampson and Zhang's Penn State University code [see recent Physics Reports (2009) article]
  - Generates wavefunctions, energies, oscillator strengths in a fully relativistic manner
  - Generates relativistic plane-wave-Born excitation cross sections

Collision codes

- ACE code provides PWB, Coulomb-Born and distorted-wave (first-order many-body theory) electron-impact excitation cross sections
  - Accepts semi-relativistic/relativistic type data from CATS/RATS
  - Excitation cross sections are computed consistently with the type of input atomic structure data
  - Any ACE cross sections will supercede CATS/RATS PWB cross sections when solving the rate matrix for populations in the ATOMIC code
- GIPPER code provides collisional, photo and autoionization cross sections
  - Also accepts semi-relativistic/relativistic type data from CATS/RATS
  - Ionization cross sections are computed consistently with the type of input atomic structure data
  - Two kinds of collisional ionization data are typically generated: "scaled-hydrogenic" [Sampson et al] and distorted-wave
  - Photo and autoionization data are usually generated with continuum orbitals determined from a distorted-wave approach

New collision strength calculations

- Recent improvement to the 'top-up' procedure used in computing fully relativistic PWB collision strengths for highly charged ions
  - C.J. Fontes & H.L. Zhang, Phys. Rev. A **76**, 040703(R) (2007).
- New fully-relativistic top-up is most important for:
  - Δn=0 dipole allowed transitions
  - high Z values
  - high incident energies

New collision strength calculations

- All calculations consider dipole allowed transitions
  - Can be strongly affected by more accurate RPWB top-up approach
- Be-like ions: n=2; 26 ≤ Z ≤ 92; ADNDT 99, 416 (2013)
- B-like ions: n=2; 26 ≤ Z ≤ 92; ADNDT 100, 802 (2014)
- C-like ions: n=2; 26 ≤ Z ≤ 92
  - Accepted for publication in ADNDT
  - Also considers forbidden transitions
- N-like ions: n=2; 26 ≤ Z ≤ 92; ADNDT 100, 1292 (2014)
- O-like ions: n=2; 26 ≤ Z ≤ 92
  - Accepted for publication in ADNDT

ATOMIC kinetics modeling code

- ATOMIC has been in use over the past ~10 years
- Combines and improves two previous Los Alamos codes:
  - FINE: non-equilibrium spectral modeling code (b-b, b-f physics)
  - LEDCOP: physics packages (free-free, Thomson and Compton scattering, Stark and collisional broadening, conductive opacities)
- Accepts input from CATS/RATS, ACE and GIPPER
- Builds rate matrix, solves for populations and computes spectra and energy losses
- Also recent work using ATOMIC to generate new low-Z opacity tables, which should be publically available soon (Z=1-30)

ATOMIC: MUTA approach

- A mixed UTA (unresolved transition array) approach has been used in recent years in attempts to provide fine-structure detail to emission (or opacity) calculations at a much smaller computational cost
  - Structure calculations are performed in which fine-structure calculations are performed only for transition arrays (TAs) that include a tractable number of lines
  - For other TAs only the strongest lines in a transition array are retained
  - For very large TAs, only UTA parameters are computed
  - The fine-structure calculations include intermediate-coupling, but not configuration-interaction
  - One can easily vary the threshold for which TAs are included in detail or not
- The kinetics calculation is still, however, performed within the configuration-average approximation – an implicit assumption thus made that the levels from a given configuration are populated statistically

ATOMIC: Tungsten modeling - motivation

- Recent NLTE8 workshop examined tungsten at temperatures of 1200-2400 eV.
- Motivated by paper of Pütterich et al where the emission spectrum of W was examined for "cold" and "hot" plasma regions

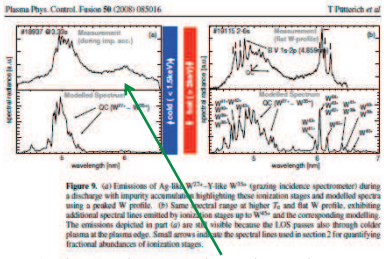
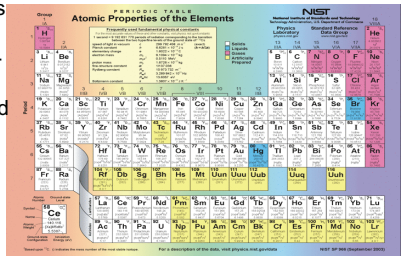


Figure 9. (a) Emissions of Ag-like W^{33+}–Y-like W^{29+} (grazing incidence spectrometer) during a discharge with impurity accumulation highlighting these ionization stages and modelled spectra using a peaked W profile. (b) Same spectral range at higher T_e and flat W profile, exhibiting additional spectral lines emitted by ionization stages up to W^{36+} and the corresponding modelling. The emissions depicted in part (a) are not visible because the LOS passes also through colder plasma at the plasma edge. Small arrows indicate the spectral lines used in section 2 for quantifying fractional abundances of ionization stages.

An interesting 'quasi-continuum' feature observed in the spectra around 6 nm

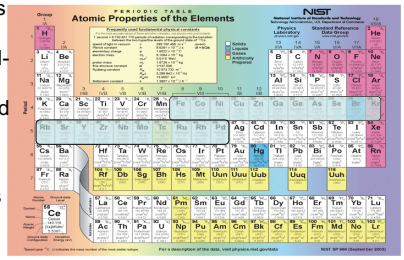
ATOMIC calculations for Tungsten

- For tungsten at temperatures of a few keV, ionization stages from ~ Fe-like (26 electrons through Pd-like (46 electrons) need to be considered



ATOMIC calculations for Tungsten

- For tungsten at temperatures of a few keV, ionization stages from ~ Fe-like (26 electrons) through Pd-like (46 electrons) need to be considered
- Implies a lot of ionization stages and a lot of configurations to deal with open p and d-shell systems!



W test case for NLTE8: LANL contribution

- Two relativistic and two semi-relativistic models for W were constructed
- The two relativistic models were run in configuration-average mode, one with E1-only radiative transitions and the other one with higher-order multipole transitions (E1-M3)
  - Advantages: configuration-average is much faster than fine-structure; relativistic theory can generate all possible higher-order multipole rates, so can be used to determine if multipole transitions are important
  - Disadvantages: configuration-average does not provide accurate populations; no fine-structure lines in the spectra; more computing time required to run relativistic configurations compared to semi-relativistic configurations

W test case: semi-relativistic model

- The two semi-relativistic models were constructed from configurations that are much more extensive than the relativistic case (for example, n_{max} = 10 vs 8, more doubly excited states)
- The populations for the two semi-relativistic models were also obtained in configuration-average mode, but for the MUTA model, these populations were statistically split into fine-structure populations to obtain a detailed spectrum
  - Advantages: MUTA model leads to very detailed spectra (~$4x10^9$ fine-structure transitions per temp/density point); MUTA fine-structure calculation is tractable compared to an explicit calculation
  - Disadvantages: statistical splitting may not agree with actual metastable populations; no higher-order multipole radiative transitions; no configuration interaction (but does include intermediate coupling)

W test case: semi-relativistic model

- Example configuration list for W^{34+} (super-shell notation):

Zr-like (40 electrons)
$[Ar]3d^{10}4s^24p^64d^4$

3[18] 4[12]
3[18] 4[11] (5-10)[1]
3[18] 4[10] 5[2]
3[18] 4[10] 5[1] (6-10)[1]
3[18] 4[9] 5[3]
3[18] 4[9] 5[2] (6-10)[1]
3[17] 4[13]
3[17] 4[12] (5-10)[1]

- This implies > 100,000 configurations for this ion stage
- We use > 10^6 configurations for all the ion stages considered in the semi-relativistic calculations
- Tests on this number of configurations suggest that convergence has been reached with this model

W test case: semi-relativistic model

- Example configuration list for W^{34+} (super-shell notation):

No more than 6 electrons permitted in 4f subshell

Allowing 2-electron excitations into n=6 subshells did not significantly change ionization balance

3[18] 4[12]
3[18] 4[11] (5-10)[1]
3[18] 4[10] 5[2]
3[18] 4[10] 5[1] (6-10)[1]
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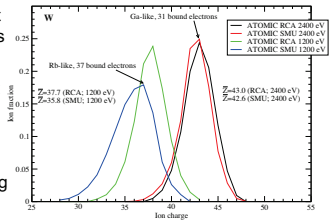
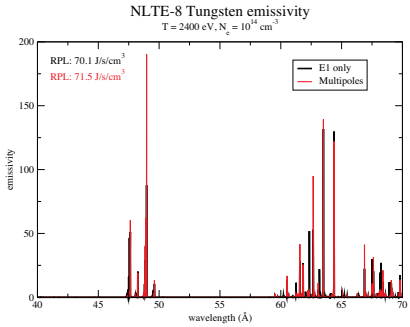
W test case: ionization balance

- For the higher temperature (2400 eV) the relativistic and semi-relativistic models predict very similar ionization balances
- At the lower temperatures the two approaches show different ionization balances, with the average ionization differing by almost 2 units of charge
- This may be due to the differing number of configurations considered in each model



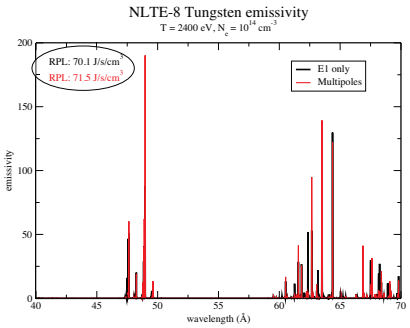
W test case: fully relativistic config-average

- Consider highest temperature case (T_e=2400 eV)



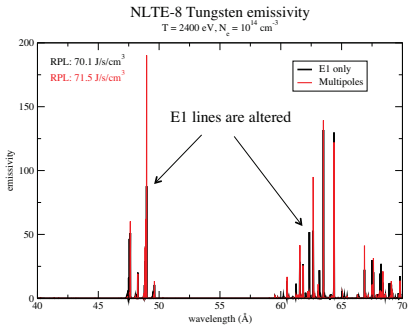
W test case: fully relativistic config-average

- Consider highest temperature case (T_e=2400 eV)
- RPL is very similar



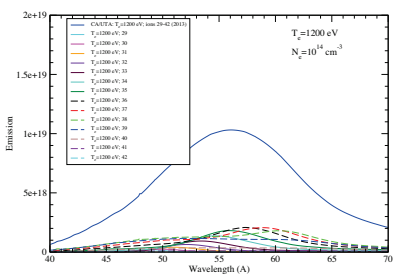
W test case: fully relativistic config-average

- Consider highest temperature case (T_e=2400 eV)
- RPL is very similar
- But some E1 lines are strongly altered when multipole transitions are included



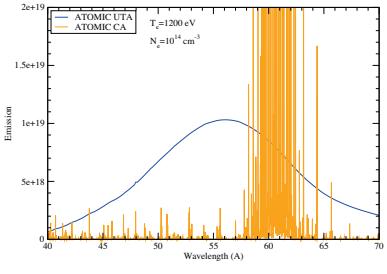
W test case: semi-relativistic model

- Illustration of UTA spectrum (T_e=1200 eV)
- Many ion stages contribute in a significant manner to the total emission



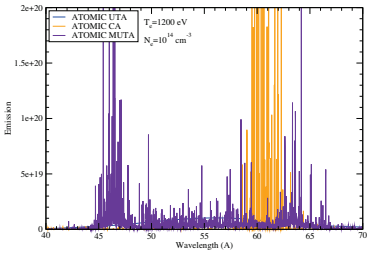
W test case: semi-relativistic model

- Illustration of UTA vs pure configuration-average (CA) spectrum (T_e=1200 eV)
- Because UTA is relatively featureless, we decided to examine a pure CA model
- CA model produces significantly more detail
- UTA produces a single, broad feature in a location that indicates that some fine-structure features should appear to the left



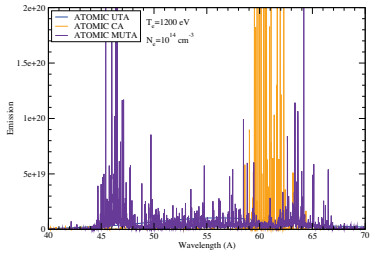
W test case: semi-relativistic model

- Illustration of MUTA vs UTA vs pure CA spectrum (T_e=1200 eV)
- CA model produces significantly more detail
- UTA produces a single, broad feature in a location that indicates that some fine-structure features should appear to the left
- MUTA produces significant fine-structure features at lower wavelengths, consistent with UTA location



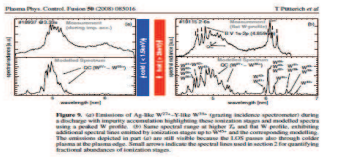
W test case: semi-relativistic model

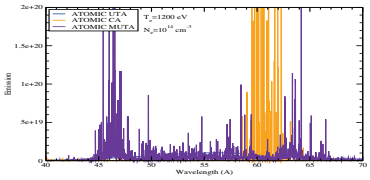
- How accurate are line positions in MUTA calculations?
- These calculations include intermediate-coupling but not full configuration-interaction (CI) – does this matter?
- We can explore this by considering smaller calculations that include full CI



W test case: semi-relativistic model

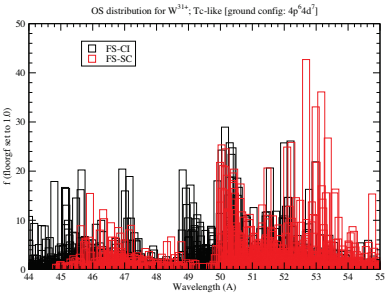
- Qualitative agreement with main features of measurement
- Increased emission in the 6-7 nm range
- Although one would likely have to average over multiple temperatures to make a detailed comparison with measurement





W test case: semi-relativistic model

- Illustration of configuration-interaction effect
  - SC=single-configuration
  - CI=configuration-interaction
- SC gf values stronger at higher wavelengths
- CI gf values stronger at lower wavelengths



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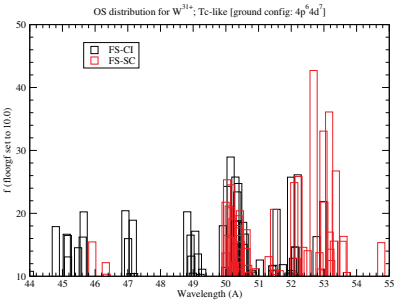
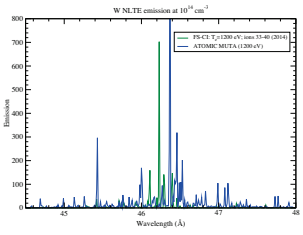


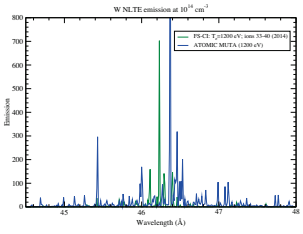
W test case: semi-relativistic model

- We constructed full CI calculations that only include ~ 10 configs per ion stage but generate 1000s of levels
  - We considered only permutations within the n=4 shells, since 4-4 transitions dominate the emission in the 5 nm region
  - However the mixing between configurations that contain open 4p and/or 4d, 4f subshells is very strong and large numbers of levels are generated
- The full CI calculations cannot produce an accurate <Z>, but the emission can inform us as to the accuracy of some line positions



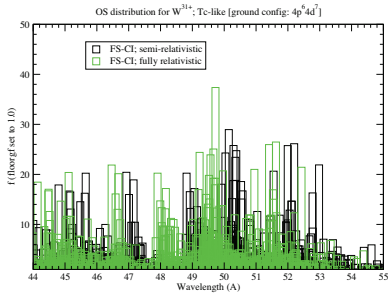
W test case: semi-relativistic model

- We find that some of the strong lines observed in the MUTA calculations are shifted by CI effects
  - a shift of around 0.1 nm
  - Some line strengths also differ
- Clearly it would be desirable to have full CI calculations for such ion stages, as well as large enough configuration sets to ensure correct populations, but such calculations may be computationally out of reach at present



W test case: semi-relativistic model

- Comparison of fully and semi-relativistic gf values with configuration-interaction
- Features are very similar, but there is a small shift in line positions



Conclusions

- Los Alamos codes form a useful suite for which to generate large-scale atomic data sets for use in plasma modeling
  - Structure and collision codes form a consistent, well-tested and mature base from which to perform collisional-radiative modeling calculations
  - Several new atomic data sets are now available
- The ATOMIC CR code is also a mature platform with which to perform plasma modeling
- We have started a study of W at moderate temperatures – a problem for which the complexity is formidable
  - Tungsten is ionized to ions that have complex structure
  - Large numbers of configurations need to be considered
  - Detailed (more detailed than CA) calculations are needed to properly predict emission spectra from such ions
  - Computational effort is considerable for such calculations

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