

The LANL atomic kinetics modeling effort and its application to W plasmas

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Overview of LANL suite of atomic physics codes

- The LANL suite of atomic physics codes can be used to model a broad range of applications
- Various levels of detail
 - Non-relativistic configuration average kinetics (nI^w) + UTA spectra
 - Relativistic configuration average kinetics (nIj^w) + UTA spectra
 - Mixed UTA (MUTA)
 - Configuration average kinetics
 - Spectra composed of mixture of UTAs and fine-structure features
 - Fine-structure levels

The LANL Suite of atomic modeling codes

Atomic Physics Codes

Atomic Models

ATOMIC

CATS: Cowan Code

RATS: relativistic

ACE: e⁻ excitation

GIPPER: ionization

<http://aphysics2.lanl.gov/tempweb>

fine-structure
config-average
UTAs
MUTAs
energy levels
gf-values
e⁻ excitation
e⁻ ionization
photoionization
autoionization

LTE or NLTE
low or high-Z
populations
spectral modeling
emission
absorption
transmission
power loss

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

CATS atomic structure code

- 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

RATS relativistic atomic structure code

- 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

ACE collisional excitation code

- Provides plane-wave-Born, 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 ionization code

- Provides collisional, photo and autoionization cross sections
- 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

ATOMIC kinetics modeling code

- ATOMIC has been in use over the past ~7 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

Recent code modifications/improvements

- Parallel version of semi-relativistic CATS code in use
- Allows significantly larger fine-structure calculations to be performed
- CATS can also now perform fine-structure calculations including 55 interacting subshells
- Addition of multipole transitions to kinetics modeling capabilities
- Speed ups implemented for RATS code
- Magnetic sub-level structure and collision capability added

The LANL suite of atomic physics codes has been applied to a broad range of applications

- Fundamental cross section experiments (EBIT, etc)
 - E.g. Inner-shell electron-impact ionization expts of Luo et al: Colgan, Fontes & Zhang, Phys. Rev. A **73**, 062711 (2006)
- High density plasmas
 - Inertial confinement fusion
 - Z-pinch opacities (Sandia Z machine) → see next example
 - Pulsed-laser experiments
- Medium density plasmas
 - Magnetic fusion energy
- Low density plasmas
 - Astrophysical plasmas (solar corona power loss, supernova emission, etc)

A specific application: The mixed UTA (MUTA) approach

- MUTA method was used to calculate the NLTE-6 tungsten test case
- Mazevet and Abdallah, JPB **39**, 3419 (2006)
- Configuration-average model is used to generate ionization balance and configuration populations
- A mixture of fine-structure lines and UTA features are used to generate an emission spectrum
- Only dipole allowed (E1) radiative transitions are currently implemented when calculating an MUTA spectrum

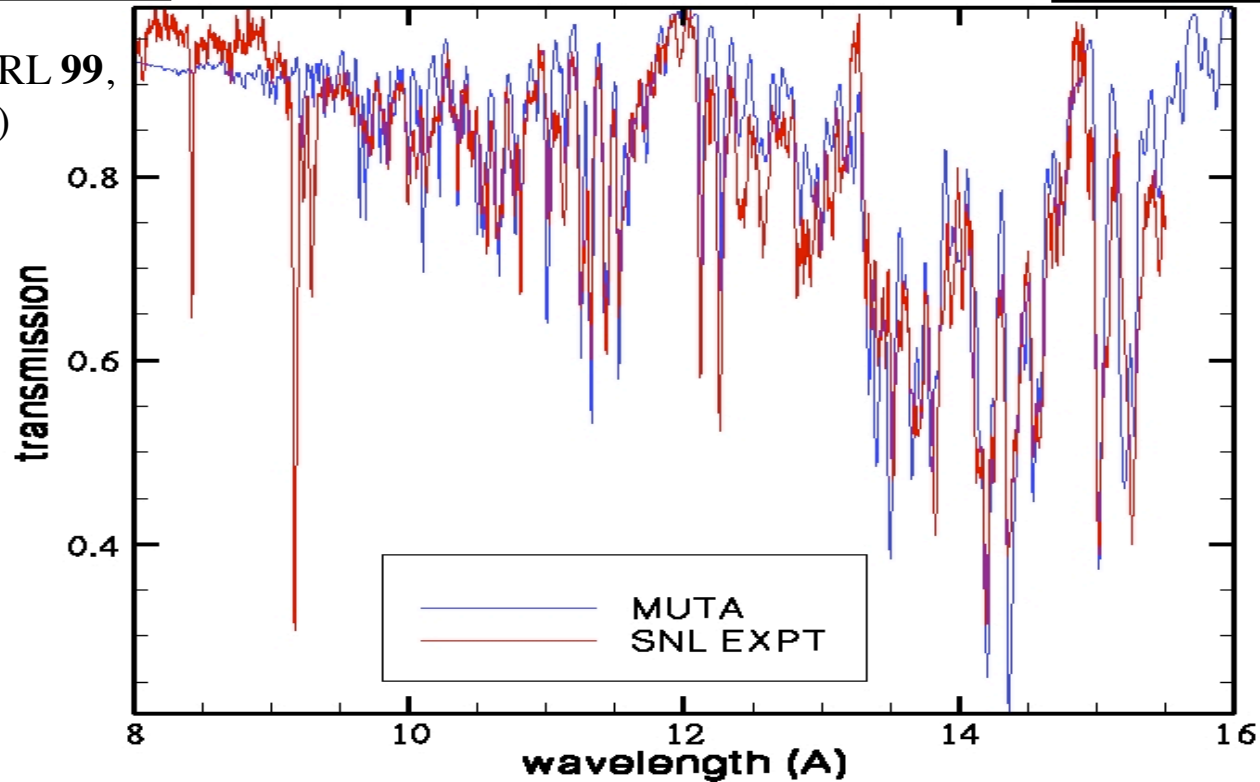
Comparison of LANL MUTA model with Sandia-Z iron opacity experiments; Very good agreement!

Data provided by
Jim Bailey, SNL

$$kT=160 \text{ eV}, N_e=1.5 \times 10^{22} \text{ cm}^{-3}$$

Calculations by
Joe Abdallah, LANL

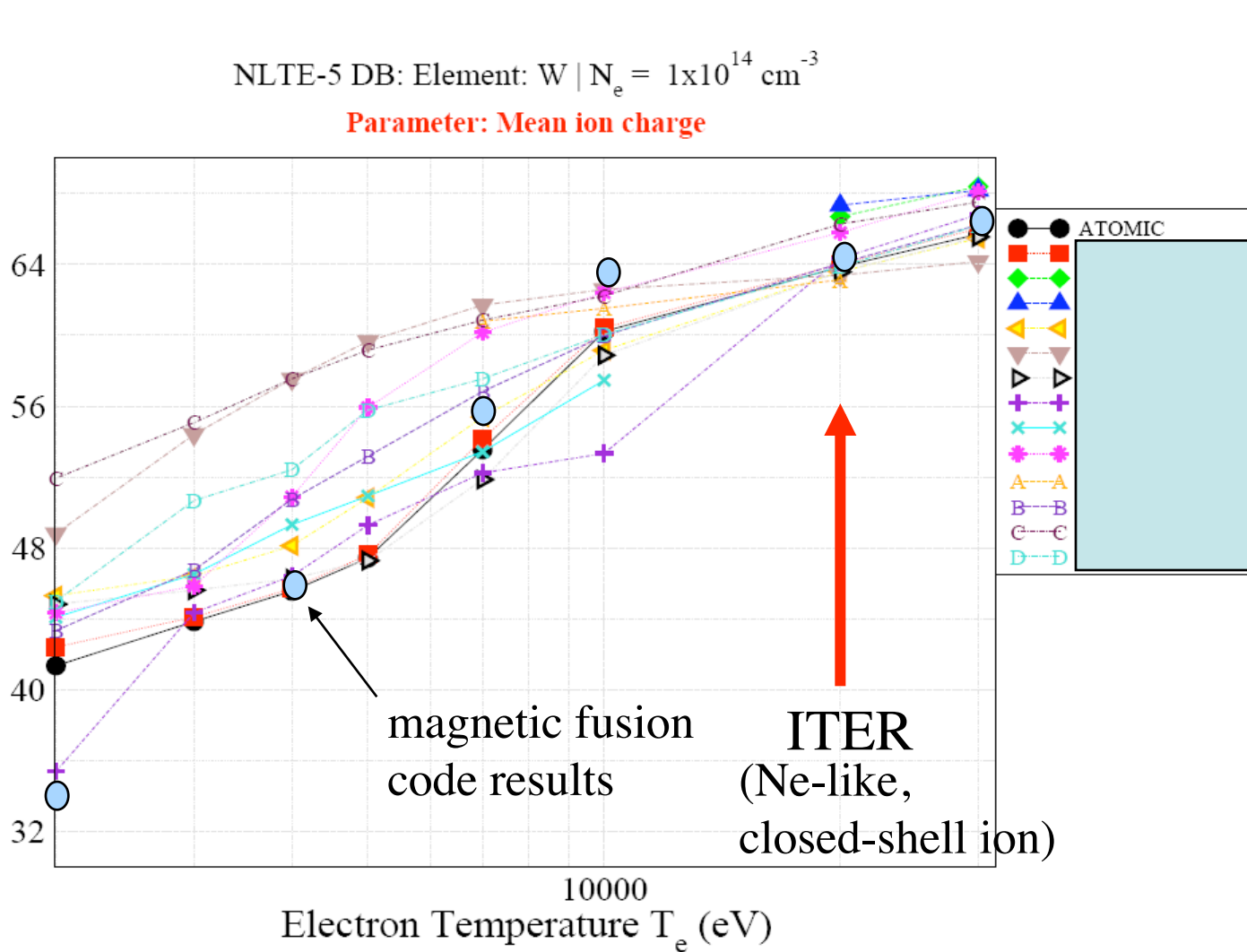
Bailey et al, PRL **99**,
265002 (2007)



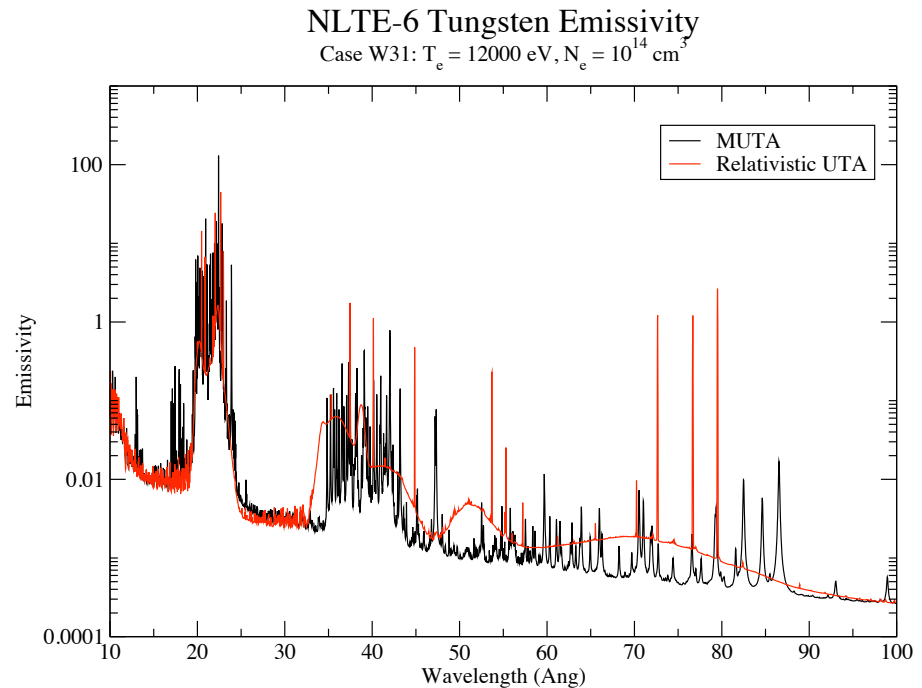
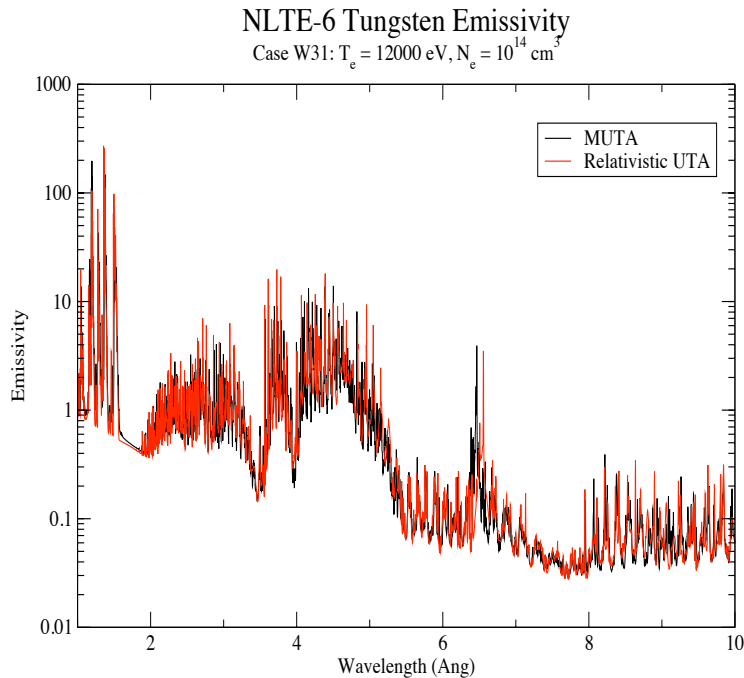
LANL work on Tungsten

- LANL has participated in the recent NLTE workshops
- The last two of these included W as a test case
- LANL configuration-average/MUTA calculations were used to compute plasma properties, including emission spectra, at 20 keV and typical MFE electron densities
- Agreement between various code submissions was reasonable when plasma conditions were dominated by a closed-shell ion, but significant differences remain for more complicated cases.

Tungsten mean ion charge for ITER conditions



Tungsten spectra at 12 keV



- We compare ATOMIC MUTA and ATOMIC relativistic UTA calculations.
- The MUTA calculation shows more spectral features due to its detailed line treatment, but the rel-UTA calculation captures the main trends in the spectra.

Tungsten work currently underway at LANL

- We are checking the 15-year-old LANL atomic data on W on the IAEA web servers
 - Much larger calculations are now possible so we can assess the accuracy of the older data
- We aim to investigate low-temperature W processes, since W at temperatures of a few eV is expected to be present in the divertor region
 - Modeling will assess sensitivity of the power loss and emission spectra to quality of the atomic data
- We hope that interaction with other CRP participants will stimulate further modeling efforts
- Please contact us with any questions/comments!