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Spectroscopic Analysis and NLTE Radiative Cooling Effects in ICF Capsule Implosions with Mid-Z Dopants

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Abstract

K-shell emission spectroscopy is commonly used to diagnose the core temperature and density of ICF implosions. In addition to providing diagnostic information, mid-Z dopants can also change the implosion dynamics. Hydrodynamics simulations are performed with the code *HELIOS-CR*, which includes inline collisional-radiative, time-dependent, atomic kinetics. Calculations include the effects of bound-bound, bound-free, and free-free contributions to the plasma emission and opacity. In particular, we will address the impact of line radiation cooling on implosion dynamics and demonstrate the effect for characteristic target designs used at Z.

Calculated plasma core temperature and density distributions are then used to compute emission spectra. To this end, we utilize the multi-dimensional collisional-radiative, spectral analysis code *SPECT3D*. Comprehensive atomic models, including K-shell satellite and inner-shell transitions, are used so that very detailed spectra can be computed and compared with experimental spectra. Atomic level populations can be computed using time-dependent atomic kinetics, or a steady-state approximation. In this paper, we will discuss details of the calculations and compare our results against experimental data.

Keywords: Radiation hydrodynamics, radiation transport, NLTE atomic kinetics, high energy density plasmas.

1. Introduction.

The study of radiative properties of high-energy-density plasmas has a rich history. Over the years the development of x-ray spectroscopy techniques has allowed a better understanding of the radiative properties of these plasmas, the relevant kinetic processes, and radiative transfer. Fundamental information on plasma conditions can be obtained by analyzing line emission or absorption spectra. Detailed modeling of spectral formation can provide information on the plasma ionization balance, temperatures, and densities [1]. Thus, the radiative properties of these plasmas can be used to diagnose plasma conditions. Moreover, detailed measurement of the radiative properties of well characterized hot, dense plasmas in stable and reproducible experiments can serve as a test-bed for the verification and benchmarking of complex hydrodynamic simulations. In this paper we present hydrodynamic simulations and spectroscopic analysis of a typical capsule implosion driven by z-pinch dynamic hohlraum x-rays [2], [3]. Recent advances in spectroscopic instrumentation, such as time and space resolved spectrometers and imagers, allow for detailed studies of the imploded core structure based on emission signatures from dopants. Additionally, even small amounts of dopants can significantly change the implosion dynamics. Modeling radiative cooling due to mid-Z dopants is a challenging problem that requires accurate treatment of plasma radiative properties. In order to calculate plasma temperature and density distribution at the time of Ar emission, we performed a series of simulations with the one-dimensional Lagrangian radiation-hydrodynamic code *HELIOS-CR* with inline collisional-radiative atomic kinetics [4], using experimentally measured time-dependent drive temperatures to initialize implosion calculations. Plasma conditions obtained around the time of implosion stagnation were then used as an input for the spectral code *SPECT3D* [5]. In the next sections, we will provide detailed descriptions of our spectral model and general modeling capabilities, present results of the hydro simulations, and discuss comparisons between experimentally measured and computed spectral data.

2. Overview of collisional-radiative atomic kinetics modeling.

HELIOS-CR, SPECT3D, and *PrismSPECT* share the same physics algorithms to model atomic kinetics and radiation transport. *SPECT3D* is a versatile multi-dimensional collisional-radiative spectral analysis code that can be applied to a wide variety of plasma emission and absorption problems. Calculations include the effects of bound-bound, bound-free, and free-free contributions to the plasma emission and opacity. Comprehensive atomic models, including K-shell satellite and inner-shell transitions, are used so that very detailed spectra can be computed and compared with experimental spectra. Atomic processes include collisional ionization, recombination, excitation, and deexcitation; spontaneous emission; radiative recombination; autoionization, electron capture, and dielectronic recombination; and photoionization and photoexcitation. Occupation probability and continuum lowering models are also utilized. Radiation transport is based on a multi-angle short-characteristics algorithm. Lineshapes include the effects of natural, Doppler and Stark broadening.

PrismSPECT [5] is a zero-dimensional spectral code. It is used to gain better understanding of atomic processes involved in spectral formation of simpler uniform plasmas while using the same algorithms as *SPECT3D*.

HELIOS-CR is a 1-D Lagrangian radiation magnetohydrodynamics code with inline atomic kinetics. Conventionally, hydro codes employ diffusion algorithms and LTE multi-group opacities to compute radiation transport in plasmas. For ICF imploding capsules doped with mid-Z elements, however, this approximation may not be valid since the plasma is not diffusive and not necessarily in LTE [6]. It is known that, even in small quantities, line radiation contributes significantly to plasma cooling [7]. *HELIOS-CR* has a unique capability to model systems where non-LTE atomic kinetics is important with the same degree of sophistication as the spectral codes mentioned above. It is achieved by solving time-dependent atomic kinetics rate equations at every hydro time step. With populations computed, detailed radiation field and fluxes are generated and coupled to the plasma through heating and cooling rates. The complexity and accuracy of the inline collisional-radiative model results in substantial computational expense. To make the calculations more practical, *HELIOS-CR* has an option for flux-limited diffusion to be used instead of the short characteristics method. Simpler atomic models can also be used with a tremendous gain in computational speed while preserving most important advantages of inline atomic kinetics. In the next section, we will discuss the atomic models used in the calculations.

3. Energy level structure for Ar

We study the effects of the atomic energy level structure of Ar on radiative cooling of imploding capsules. We will first consider an idealized system to illustrate the difference between fine structure calculations and more approximate term-, configuration-, and super-configuration averaged levels. The argon atomic model includes ground and singly excited states up to n=6 for each ionization stage, since a vast variety of temperatures and densities is expected while the system goes from its initial state though implosion to the stagnation phase. Satellites to Lyα and Heα lines (with spectator electrons in n=2) are also considered, because they may affect K-shell emission and population distributions at stagnation [8].

Atomic level structure, collisional and radiative cross-sections and rates are computed with the code *ATBASE* [9]. The atomic data are usually computed for fine structure. The *Atomic Model Builder* code is used to select the atomic energy levels and transitions relevant to the problem under investigation. It can also be used to bundle fine structure levels together into terms, configurations, or super-configurations.

Population collapsing, or bundling, is a powerful technique that allows a significant reduction in computing time when dealing with complex atomic systems. The idea behind population collapsing is based on the observation that fine structure levels within the same configuration (or super-configuration) are close to each other in energy space. Super-configurations are groups of configurations which have the same number of electrons in each shell, regardless of the value of the orbital quantum number *l*. In the case of hot dense plasmas, these closely-spaced levels may be strongly coupled by collisional processes. Populations within each bundle are effectively governed by Boltzmann statistics, and groups of these levels can be treated as single entities. All the collisional and radiative processes between the groups can also be averaged to account for populating and depopulating mechanisms.

If the assumption of strong collisional coupling between the closely-spaced levels is valid, and the transitions between fine-structure levels cannot be resolved either because of substantial line broadening or finite instrumental resolution, then the approximation based on collapsing causes no significant degradation in the quality of the spectra. Computational costs, however, can be greatly reduced.

Atomic Model Builder supports four different levels of description for energy level structure: fine structure, term-, configuration-, and super-configuration averages. For example, the *1s2l2l'* super-configuration of Li-like Ar contains 3 configurations, 7 terms, and 14 fine-structure levels.

In order to illustrate the effect of population collapsing, we performed a set of simulations with various collapsing models. In the calculations, a uniform DD sphere doped with 0.1% Ar (number fraction) is allowed to cool radiatively. Hydrodynamic motion is turned off. The radius of the sphere is 100 microns (50 zones), the mass density is 1 g/cc, and the initial temperature is 1 keV. Atomic levels of hydrogen are collapsed to super-configurations. Atomic levels of Ar I through Ar XVI are also fully collapsed. For H and He-like Ar (including auto-ionizing states), we use fine-structure, term, configuration, and super-configuration schemes. As a reference, we also provide the results using multi-group diffusion (500 groups).

Figure 1 demonstrates the effect of collapsing on frequency-dependent radiative cooling rates at the beginning of the calculation for the extreme cases of fine structure and super-configurations. Overall, the rates computed with the fine-structure scheme do not display significant differences from super-configuration-averaged rates. Small differences can be observed for Lyα and Heα lines (note missing structure at the line centers, He-like satellites, and the absence of the inter-combination line in the case of super-configurations). Although these features may be important for spectroscopic analysis, they do not play an important role in energy transport. The gain in computational efficiency is, however, significant (~ factor of 20). Using appropriate atomic models, a typical calculation for Ar-doped capsule implosions can be completed in the order of hours on a desktop computer.

As illustrated in figure 1, multi-group opacity tables are not able to adequately resolve the structure of Ar K-shell emission. This has a profound impact on the plasma evolution. Starting at conditions described above, the plasma is allowed to cool radiatively for 100 ps. Multi-group diffusion significantly overestimates the cooling effect due to poorly-resolved line emission which results in much lower electron temperatures. Also, the temperature gradient is steeper in the case of the collisional-radiative model. This happens because the photons emitted by the optically thick alpha lines are trapped in the core center. In the case of multi-group diffusion, the lines are transported at Rosseland opacity allowing photons to escape.

Next, we study the importance of atomic levels with high principal quantum number *n*, and the autoionizing states. We performed a set of calculations using the nominal conditions in the most recent experiments: 2.0-mm-diameter CH-wall (40 micron thick) capsule with thin layers of PVA and Al. The capsule is filled with 20 atm of D_2 and tracer amounts of Ar and is embedded in a 14 mg/cc CH_2 foam. The target absorbs approximately 20 - 40 kJ of x-ray energy from the T~ 200 eV drive radiation as it implodes. The calculations run up to 1 ns after stagnation. The most detailed atomic model includes states with *n* up to 10 and autoionizing states (5459 levels total). Run time for this model is ~70 hours. Simpler models do not include autoionizing states (3309 levels, run time ~37 hours), and no states with $n>5$ (2847 levels, run time ~9.5 hours).

Our results indicate that, at the time around stagnation, high n states have very little effect on plasma conditions. The presence of autoionizing levels results in slightly lower temperatures (< 5%) and higher densities (~10%). Thus, simple atomic models result in a significant reduction of computing time, while making a modest impact on implosion dynamics.

4. Importance of non-LTE kinetics

For the systems described at the end of the last section, collisional-radiative atomic kinetics plays an important role. To illustrate the effect, we compare the results of the calculation using detailed non-LTE modeling with a simulation that uses the same energy level structure, but atomic populations are forced to be LTE. As indicated in figure 2, radiation flux at the fuel-pusher interface during the time of peak Ar emission is substantially higher in the case of LTE atomic kinetics. Therefore, the assumption of LTE for population kinetics overestimates the amount of radiation cooling. Figure 3 displays the time history of core-averaged electron temperature and mass density. At early time, there is no difference between either case. Excessive cooling due to LTE population kinetics starts playing a role at about 21 ns, when the plasma is hot enough to emit K-shell radiation. Lower temperatures, in turn, allow the plasma to compress more, resulting in higher density. The difference in temperature and density at the time of Ar spectra formation is high enough to affect experimentally observed spectra.

HELIOS-CR utilizes time-dependent atomic kinetics. To study the effect, we performed a set of *PrismSPECT* calculations for a uniform plasma using time-dependent temperatures and densities characteristic of the core center (a), near the pusher interface (b), and the core-averaged values (c). Also, at times of peak electron temperature, peak compression, and peak K-shell emission, we ran the calculations allowing populations to come to collisional-radiative equilibrium. During the time interval of the most intense Ar K-shell emission, there is very little difference in the emerging spectra and the population numbers between the steady-state and the time-dependent calculations for all plasma conditions. This result is important, since it validates traditional spectroscopic analysis of experimental spectra from imploded capsules based on the assumption of steady-state conditions. However, at different stages of core evolution, time dependent kinetics may be important. It may affect the spectral features and, potentially, the implosion dynamics. For example, with plasma conditions (b) at the time of peak compression, the flux from the time-dependent calculation was substantially larger as compared to the steady-state solution. Nevertheless, it would not change the observable spectra significantly since the emission was already fairly weak.

5. Analysis of experimental data

In this section, we discuss the analysis of experimental data recorded for shot 860 at the Sandia z-pinch facility [3]. A 1.7-mm-diameter CH-wall capsule filled with 2.8 atm CD_4 + 0.085 atm Ar absorbed approximately ~20 kJ of x-ray energy as it was imploded by the T~ 200 eV drive radiation. Time- and space-resolved spectra were recorded with the TREX elliptical crystal spectrometer. Time resolution is about 1 ns, and spatial resolution ~350 micron.

Initial analysis of the data was performed assuming uniform temperature and density distributions in the core, in order to obtain effective core parameters. This is done with the code *PrismSPECT*. The analysis is complicated, because for these fairly large targets and high Ar concentrations, opacity effects are strong. Opacity effects were carefully taken into account both for population distribution, and line transport. While fitting experimental data, we concentrated primarily on the spectral range from 3500 to 4200 eV that covers Ly and He beta and gamma transitions. For those lines, the optical depth is of the order of 1. The average temperature, estimated by fitting major spectral features, is about 1000 eV, and the electron density is about 1.5×10^{23} cm^{-3}. Figure 4 displays model sensitivity with respect to temperature and density variations. Optically thick (τ~200) alpha lines have also been analyzed, resulting in the same density, and slightly lower temperature (900 eV).

Above mentioned differences in temperature estimates most likely can be explained by the fact that experimental data, though space- and time-resolved, still contain contributions from non-uniform, rapidly varying plasmas. To address this issue, we performed a series of calculations with the radiation-hydrodynamics 1D code *HELIOS-CR*. Experimentally measured radiation dynamic hohlraum temperatures were used to drive the simulation. Plasma temperature and density distributions, obtained from the simulations, were then post-processed with *SPECT3D*. A synthetic spectrum, computed with these gradients, agrees well with the experimental data (Figure 5). Note, that this spectrum adequately fits most of the experimental features, which was not possible within the scope of uniform plasma calculations. Thus, we can infer that the hydro simulation results are characteristic of plasma conditions during Ar spectra formation.

6. Conclusions

We have shown that, in systems where radiative processes are important, the availability of time-dependent, collisional-radiative modeling is crucial. Though much more computationally intensive than commonly-used multi-group diffusion, collisional-radiative calculations provide more realistic treatment of line radiation. Computational efficiency can be improved dramatically by collapsing the atomic structure. The level of collapsing is problem specific. For the conditions discussed here, which are relevant to Ar-doped ICF capsule implosions, the most aggressive collapsing scheme, using the super-configuration average, is still a good approximation.

We performed hydrodynamic simulations and analysis of the Ar K-shell spectra from a capsule implosion driven by z-pinch dynamic hohlraum x-rays. The effective plasma temperature at the time of Ar spectra formation is estimated to be 1000 eV, and electron density ~ 1.5×10^{23} cm^{-3}. Discrepancies in temperature inferences suggest the importance of considering evolving non-uniform plasmas. By post-processing results of 1D radiation-hydrodynamics calculations, we generated spectra that agree well with the experiment. We emphasize that, for these experiments, accurate treatment of radiative cooling effects due to Ar line emission is important in order to obtain representative plasma conditions.

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Figure Captions

Figure 1. Radiation cooling rate for Ar K-shell emission region.

Figure 2. Radiation flux at fuel-pusher interface at 21.53 ns (time of peak Ar emission) for NLTE and LTE calculations.

Figure 3. Time dependence of core-averaged temperature and density for NLTE and LTE calculations.

Figure 4. Temperature and density sensitivity of Ar k-shell emission spectra.

Figure 5. Synthetic spectrum, obtained by post-processing hydro simulation compares well with the experimental data.

Figure 1. Golovkin et al, Spectroscopic Analysis…

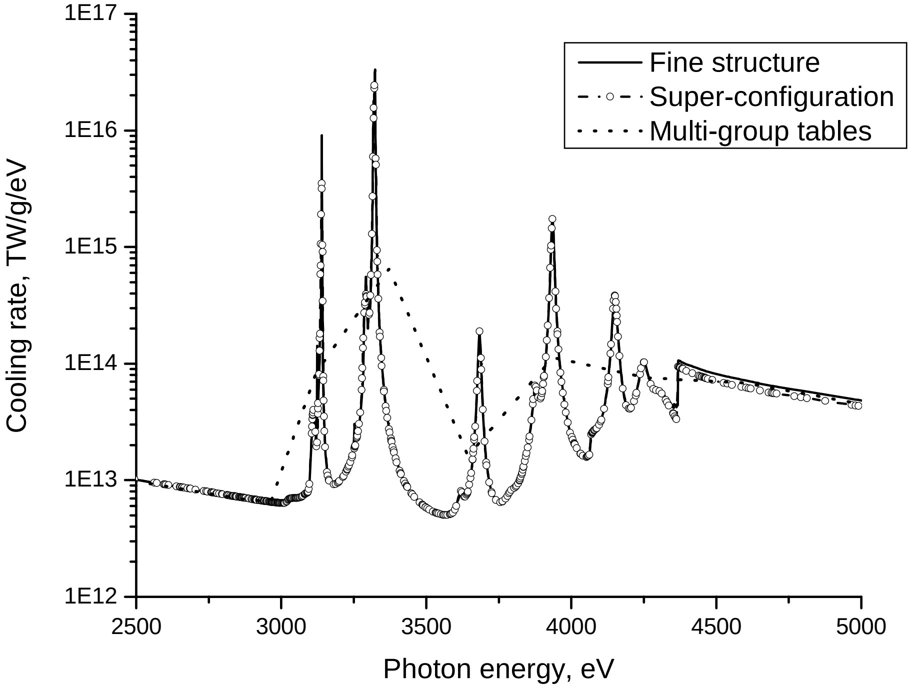

Figure 2. Golovkin et al, Spectroscopic Analysis…

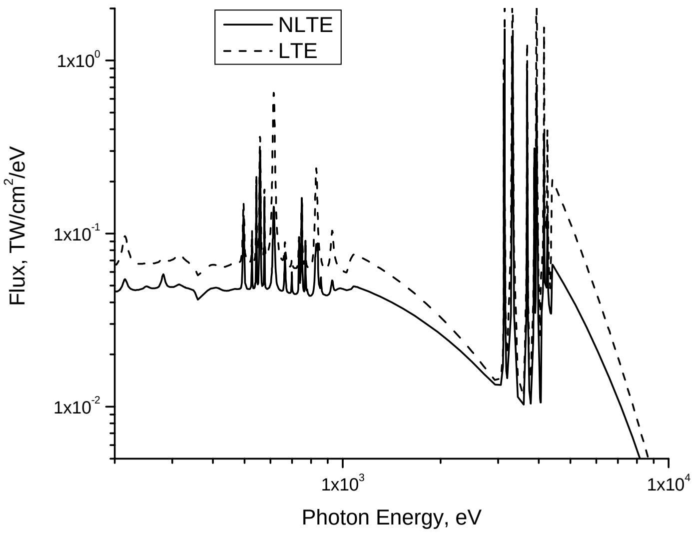

Figure 3. Golovkin et al, Spectroscopic Analysis…

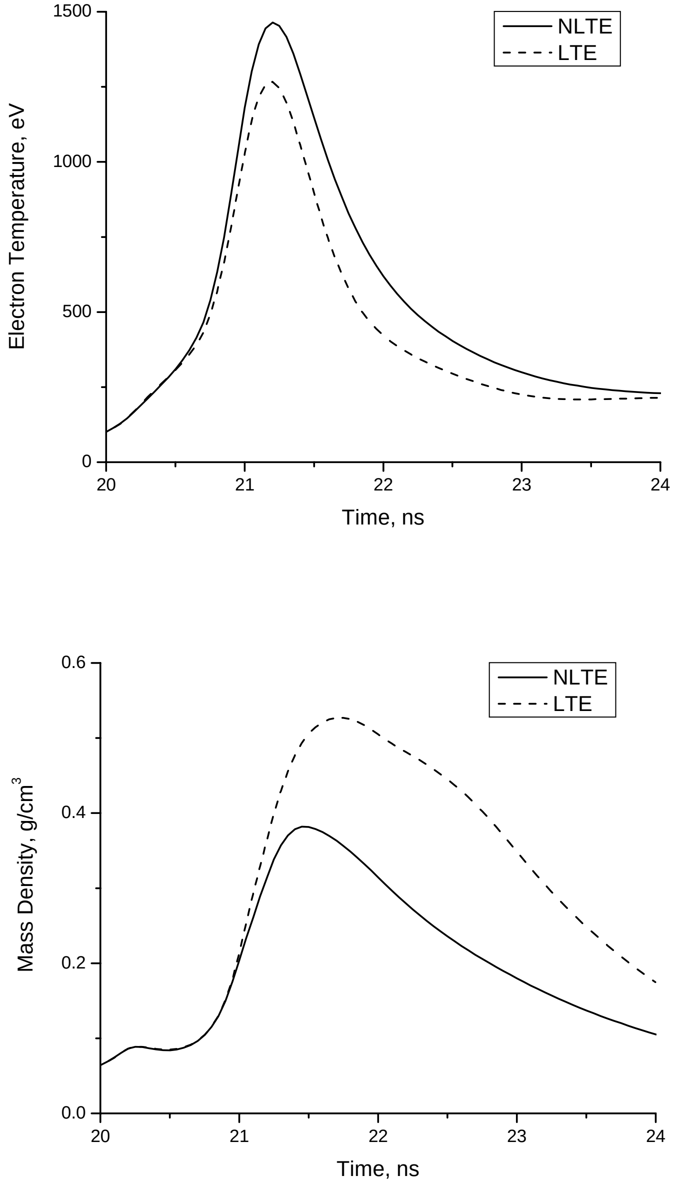

Figure 4. Golovkin et al, Spectroscopic Analysis…

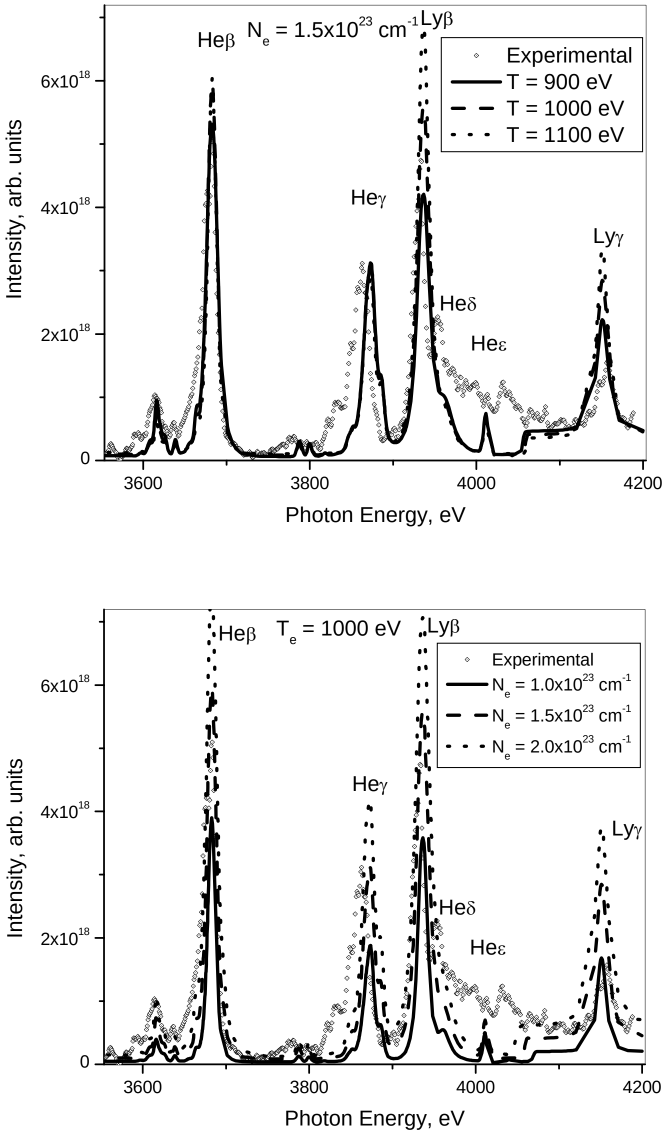

Figure 5. Golovkin et al, Spectroscopic Analysis…