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by

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ABSTRACT

We review our methodologies in the design and analysis of soft x-ray laser experiments. We convolve large scale 2-D hydro code output with detailed atomic data bases in a kinetics code with 1-D or 2-D line transfer. The time and space dependent level population data is then post processed further with a beam transport code, including refraction, to predict actual experimental results. While mysteries do remain, we present many examples that show how this complex modeling procedure is crucial in explaining experimental results.

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I. Introduction

The production of a plasma medium that can serve as a suitable soft x-ray laser amplifier is a difficult task. Besides achieving the proper ionization state and population inversion, the medium must be uniform enough to support proper beam propagation. At LLNL these media are created by the interaction of a high power glass laser with a target. The optical laser heats the target, creating a plasma of free electrons and of ions stripped to the intended charge state. We must correctly calculate the hydrodynamics of this interaction, as well as the atomic physics of ionization and ultimately of population inversion. In this paper we show many instances of the need to do this calculation in as complete (and necessarily complex) manner as possible. A failure to do so can lead, at times, to erroneous conclusions. By no means do we belittle modeling efforts that are less complex. Indeed we appeal to simple models whenever we can safely get away with it. We point out here, however, cases when we could not.

In Section II we give an overview of the modeling methodology. In Section III we review our state of knowledge as to the hydrodynamic aspects of our Ne-like-Se exploding foil targets¹ which first demonstrated gain² in 1984. In Section IV we show evidence from Se dot spectroscopy that we are correctly modeling the ionization balance. In Section V we discuss the measured gains of many of the 3p-3s transitions in Se, and compare them to our calculations. In Section VI we discuss the timing of the 3p-3s line emissions including the Na-like lines. In Section VII analogous

data on Mo is discussed. In Section VIII we discuss the need for detailed modeling in order to account for the angular divergence of the beam pattern in Se. In Section IX we briefly touch upon issues for schemes designed to produce gain at a wavelength in the sub 44Å "water-window" needed for biological holography, and sum up in Section X.

II. Methodology

We use the LASNEX³ code to simulate the 2-D hydrodynamics of the target heated by the optical laser. Laser and target parameters are fed as input into LASNEX. Laser absorption, electron and radiation transport, average-atom atomic physics, and hydrodynamics are then calculated, yielding density, temperature, velocity and radiation field data in both time and two spatial dimensions. Along with a detailed atomic data file, these quantities are fed into the XRASER⁴ atomic kinetics code. The data file typically contains hundreds of detailed atomic energy levels,⁵ along with radiative and collisional excitation and ionization rates, as well as inner shell ionization and detailed dielectronic recombination rates. XRASER combines this atomic data with the LASNEX produced hydro quantities and calculates ionization state abundances, level populations, and gains including the effects of line transfer. A post processor SPECTRE creates synthetic spectra, using a ray trace method, that can be directly compared to data.

III. Ne-like-Se Hydrodynamics

Our success in 1984^{1,2} involved a 750Å thick Se foil (on 1500Å plastic backing for support) illuminated on both sides by a 0.53 μ laser for 1/2 ns in a line focus 200 μ m high by 1 cm long with an irradiance of about 4×10^{13} W/cm² per side. Although our purpose here is to discuss new data that illustrate the need for the complex modeling described in Section II, we first summarize our recent experimental milestones. We have a) increased the output at 206Å from 100 W to nearly 1 MW by increasing the length of the line focus past 4 cm;⁶ b) spatially (in 1D) and spectrally resolved the near-field beam patterns⁷ (the analysis of which is beyond the scope of this paper); c) produced significant double pass amplification and even triple pass amplification⁸ by use of multilayer mirrors; d) produced Gabor holograms of C fibers using the 206Å Se line,⁹ and e) produced measurable gain at a wavelength as low as 50Å in Ni-like Yb.¹⁰

Our usual method of determining how well we model the hydrodynamic expansion of the target is through holographic interferometry. Reference 11 displays our continued success in this regard. Another way to deduce both density and temperatures is from the stimulated Raman scattered spectrum. The short wavelength cutoff is due to Landau damping and is thus temperature sensitive. Figure 1 favorably compares the LASNEX predictions, at foil center, for the temporal evolution of the density and temperature with those derived from the time history of the SRS spectral cutoff.¹² The temperature inferred from this method is an upper limit. Nonetheless

we would like much more temperature data, derived in various ways, e.g., via spectroscopy.¹³

IV. Ionization Balance in Ne-like-Se

Typically we deduce ionization balance in these systems by comparing the F-like vs. Ne-like 3-2 x-rays. In actual amplifier geometries,¹ issues of optical depth and 2D gradients complicate the interpretation. To alleviate this problem we illuminated a 40 μ diameter 750Å thick Se dot on a 3000Å CH foil with 11J in 700 ps of 0.53 μ light at an irradiance of 2×10^{14} W/cm². Figure 2 shows the calculated 2-D isocontours of temperature and density at the time of peak x-ray emission. Note the remaining complicating feature of non-uniformity across the exploded dot. Figure 3 shows the 3-2 spectra at 2 different times and compares it with the theoretical spectra, produced in a properly convolved fashion as per the description of Section II. We note the general similarity and relative heights of the patterns of lines, giving us some confidence in the modeling. Satellite lines appearing in the data are not included in this calculation.

V. Gains in Ne-like Se

Figure 4 compares the measured to theoretically predicted gains¹⁴ in Ne-like-Se. The predicted gains are obtained by convolving the time and space varying gain data with ray tracing to produce a synthetic signal at a given amplifier length, and repeating the procedure at various lengths, to produce a synthetic

"length study", in order to obtain a gain coefficient in a manner directly analogous to the experimental procedure. We note rather excellent agreement for all lines except the $J=0$ to 1 line at $182.4\text{\AA}$. Other lines predicted to have measurable gain but are not observed include F-like line at $203\text{\AA}$ and a $2s$ hole $3d-3p$ line near $182\text{\AA}$. At the time of peak $J=2-1$ on-axis emission, we actually calculate the $J=0$ to 1 line to have only about $3/4$ of the gain of the $J=2$ to 1 line. However, earlier in time the gain on the $J=0$ to 1 is predicted to be much larger and despite refraction a large signal is expected. This points to the importance of correctly modeling both the time dependent gain and the refraction in detail and will be discussed in the next few sections. The excellent agreement for gain between theory and data for most of the lines could not have been achieved without the large and complex modeling procedure. In the realm of atomic data alone, we note the importance of detailed inclusion of dielectronic recombination into the kinetics.^{15,16}

VI. Timing of the Gain

In a recent paper¹⁷ we presented absolutely timed data that showed the $J=2-1$ emission peaking off axis early in the driving pulse. The beam then sweeps inward and lands on-axis near the peak of the drive pulse. The close agreement demonstrated there between that data and the prediction of the on axis signal was made possible by the detailed modeling, convolving the predicted time and spatial history of the gain and of the density profiles which affect both gain and propagation (refraction).

The timing data ruled out a scenario of lasing due to rapid cooling recombination after the drive laser turned off.¹⁸ A piece of data² that could be interpreted along those lines shows the J=2 emission increasing while the Na-like line increases implying recombination. We reproduce it here in Figure 5, but now with absolute timing, and theoretical predictions superposed. Note the close agreement. How can the Na-like line be increasing while the pump is still on and heating up the plasma? The answer, again, lies in the detailed modeling. Even though the system is only a few % Na-like, the Na-like line is optically thick along the axis, with a mean free path of about 1/2 mm. Therefore, as the foil expands during this time, the source area increases and so does the signal. Thus the Na-like emission rises even though the plasma has not started to recombine significantly.

This example points out the unique spectroscopic qualities of looking down a long tube of plasma. For example, even the simple notion of an optically thin free-bound continuum is inaccurate. Consider a 1 cm long exploding foil. A 1/2 ns time gated instrument, with 1200 resolving power, at 60 eV, collects 4.5×10^{-6} J/Sr. One usually assumes a fully exploded amplifier "end-cap" area of $.02 \times .02 \text{ cm}^2$ radiating for 500 ps, or $2.5 \times 10^7 \text{ W/cm}^2 \text{ Sr}$, which is a 50 eV black body equivalent brightness. But in reality much of the signal is due to a 500 eV black body radiating at $3 \times 10^8 \text{ W/cm}^2 \text{ Sr}$ for 250 ps from an area $.02 \times .003 \text{ cm}^2$, when the foil is hotter, denser, and optically thicker. Namely the free-bound emission first increases in time as the foil is optically thick, heats up and

expands its surface radiating area. When the density drops low enough for the foil to be optically thin to the continuum, then the emission drops because thin emission is proportional to (density)² which is falling. The total free-bound emission thus may not scale linearly with the foil's length, since the signal is not solely due to the foil emitting only in the optically thin limit.

VII. Ne-like Mo Analogs

Gain measurements analogous to those Ne-like Se have been performed for Mo.¹⁹ Before we discuss those, we mention an observation in Mo apropos of the previous discussions concerning on-axis spectroscopy. The Na-like line at 104Å is found to have a width of 120 mÅ, whereas the Ne-like line with gain at 106Å has an instrument resolution limited width of 60 mÅ. Thermal Doppler widths should be about 10 mÅ. With Na-like line optical depths of about 30, a $\sqrt{\ln \tau}$ optical depth broadening brings us only to 20 mÅ. So why is it 120 mÅ wide? The solution to this paradox may lie in 3-D effects. The end tips of the line focus illuminated region of the foil blow off not just perpendicular to our on-axis line of sight, but also into our line of sight since they are at the free edge of the foil. Thus there is bulk Doppler broadening (of about 100 mÅ), which convolved with the 60 mÅ instrument resolution could account for the observed 120 mÅ width. Moreover, quantitative estimates of the brightness of the region within .02 cm of the end of the foil (which is expected to have significant 3D expansion) is about equal to the brightness of the rest of the tube (which is optically thick after another .03 cm down the axis).

Returning to the gain measurements in Mo, we present Table 1 and wish to make two major points. Firstly we show that detailed models with dielectronic recombination and inner shell ionization²⁰ change the relative gain of the $J_U = 0$ and $J_U = 2$ lines. (Compare model N2 with A1). Indeed due to the relatively large fraction of Na-like ions, inner shell processes contribute greatly to $J=2$ gains. Secondly we note that our best model (N2), with line transfer shows the same relationship of its predictions for gain to the measured gain in Mo as it did in Se. In particular, the 182 $J=0$ equivalent is still misbehaving in Mo, while another $J=0$ (at 106Å) has a measured gain quite close to predictions! Once again we have used our most complex modeling procedures in order to obtain the generally good agreement with the data.

VIII. Ne-like Se Beam Pattern

As described in Section V, the beam refracts early in time when density gradients in the foil are relatively large. Later in time as the density and its gradient are reduced, the beam can propagate straight down the foil's axis. The point we wish to make here, however, is that refraction alone is not enough to quantitatively explain the observation that the time integrated beam pattern peaks off axis. Figure 6a points out the problem. With a reasonable assumption that the gain profile follows the density profile, the signal peaks on axis for all times, since the rays that skim along the top of the parabolic density profile have both maximum gain and length and exit near 0° from the axial direction.²¹

Figure 6b shows the key to solving the "off-axis-peak" problem. When the gain peaks off axis the rainbow shaped ray trajectories have maximum gain-length product (despite not having maximum length) and exit the plasma at an off-axis angle. Figure 7 shows detailed calculated profiles of density, temperature, ionization state fraction, and gain. Indeed the gain does peak off axis because the lower density there leads to less multi-step collisional excitation (which causes ionization), thus lowering the F-like fraction and increasing the Ne-like ion fraction. Figure 8 shows the subsequent calculated beam patterns at various times using the semianalytical method described in Ref. 20 and fitting the profiles to quartic functions, and shows off-axis peaks at the appropriate time. Integrating these patterns in time produces a beam pattern with a peak off axis at 10 mrad that is 1.3 times the on-axis signal.

IX. Shorter Wavelength XRL Schemes

The Ni like 4d-4p lasing scheme is an obvious analog to the Ne like 3p-3s scheme. Ni-like W can lead to gain at 43Å. Our recent success¹⁰ with J=0 lines at 66Å in Eu and 50Å in Yb have left us with several mysteries however. In Eu we also predicted²² the J=2 lines to have measurable gain but none was observed. We note here however that J=2 mysteries are, in principle, easier to explain away than J=0 ones. This is due to the statistical weight factors, $\Delta n_{0-1} = n_0 - 1/3 n_1$ vs. $\Delta n_{2-1} = n_2 - 5/3 n_1$. A 28% increase in n_1 can destroy an inversion on 2-1 while only lowering

the gain on O-1 by 20%. Thus the discrepancy may be resolved via improved calculations of trapping, plasma parameters, and/or the coupling of the 4s state to the lower 4p laser level, a channel for feeding the lower XRL state not present in Ne-like systems.

The second mystery is the relatively low gain of 1 cm^{-1} in the Yb^{23} vs. an expected 5 cm^{-1} . Since Ni-like targets are higher Z and denser than their Ne-like-Se cousins, radiative cooling may be more important and we may be miscalculating the effect and thus the temperature. This is under investigation.

We are also pursuing rapid cooling recombination targets. Short pulse H-like Al 3-2 schemes have been designed with predicted gains of about 4 cm^{-1} . We are also pursuing a line of investigation involving Li-like ions. We have been unable to correctly predict the high gains seen in 5-3 Li-like Al. We are nonetheless designing Ca (Li like 5-3) and Cr (Li like 4-3) targets which might show gain near 39Å.

X. Summary

We have discussed many examples in the analysis of laboratory XRL results at LLNL wherein the need for the most detailed complex modeling and subsequent convolved theoretical data syntheses have played a crucial role in solving mysteries. Of course many mysteries still remain. Further theoretical tools are required. The finite speed of light needs to be included in SPECTRE. After all, transit time down a 3 cm long foil is 100 ps, a time scale over which hydro-variables and gain changes. For holography applications

we need to model the coherence and phase properties of the lasers. The effects of turbulence on propagation and on line shapes need to be assessed. Atomic data including possible absorber lines in nearby ionization states might enable us to understand missing lasing lines. The ability to make synthetic spectra that includes satellite lines, along with more spectroscopic data would go far in temperature determination.

In any event, we have shown why "sweating-the-details" is often required in explaining XRL phenomenon. It is for this reason that our motto in soft XRL target design is: "No pain -- No gain".

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GAIN (cm ⁻¹)				MODELS	DATA		
On:	J _v	λ _{Theory}	λ _{Se equiv.}	A1 g.s.-g.s. only cos 4E-11	N2 detailed F-Ne Ne-Na	N2 with trapping	consistent with
7-3	1	139.6	221	1.3	2.5	2.3	2.9
20-10	0	138.5	182	3.7	2.8	2.6	—
23-10	2	132.9	209	1.9	4.0	3.7	4.2
8-3	2	131.3	206	1.7	4.1	3.8	4.1
11-3	0	105.4	167	2.8	2.2	2.0	2.2
<u>% Ionization-state: t = -200 ps → t = 0</u>							
Na				30-32	35-27	36-30	
Ne				45-40	43-46	40-45	
F				12-15	6-13	6-12	

Table 1. Ionization Balance and Ne-like gain in Molybdenum.

Fig. 1. (a) Electron Density and (b) Temperature of a Se exploding foil vs. time. X $\equiv$ Data inferred from SRS short wavelength cutoff. L $\equiv$ LASNEX prediction at center of the foil.

Fig. 2. (a) LASNEX Mesh Plot, (b) Electron Temperature and (c) Density isocontours for a Se dot in CH foil experiment. Snapshot is at a time of peak 3-2 x-ray emission. The Se region is shaded.

Fig. 3. Snapshots of 3-2 x-ray spectra at peak emission time and 200 ps later for Se dot of Figure 2. Top: data. Bottom: simulation.

Fig. 4. Comparison of predicted to measured gain on 6 3p-3s lines in Ne-like Se.

Fig. 5. Line emission vs. time for a J=2 to 1 Ne-like line, and a Na-like resonance line. Data: solid lines. Simulation: dotted lines.

Fig. 6. Comparison of beam patterns from a Se exploding foil. a) Gain profile follows density profile. b) Gain peaks off axis.

Nominal Se Foil; $t =$ driving laser peak - 120 ps.

Fig. 7. a) Density (solid) and temperature (dashed) profiles for a Se foil 120 ps before the peak of the driving pulse. b) Gain (solid) and ionization state fractions (dashed) profiles at the same time.

Fig. 8. Calculated beam patterns at three different times.