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Ray and wave optics modeling of laboratory x-ray lasers

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ABSTRACT

Much progress has been made recently in characterizing the emission from neon-like Yttrium exploding foil x-ray lasers at Lawrence Livermore National Laboratory. Concomitant with that effort, we have carried out detailed modeling to enhance our understanding of the experiments and improve their design. Our modeling includes target hydrodynamics, calculation of gain, and both ray and wave optics propagation. We will describe our modeling of Yt x-ray lasers, including first simulations using a two transverse dimensional gain calculation. Our calculations indicate that the time-integrated signal is very sensitive to the time history of the gain, because of the rapid sweep of the beam in angle measured with respect to the plane of the foil. We have found that better agreement with experiment is achieved if the falloff of the gain with time is made slightly faster than our codes predict. In the vertical direction (normal to exploding foil direction), the experimental beam pattern is typically broader than we calculate. We find that ray and wave optics calculations are in good agreement. The coherence length obtained by a wave optics calculation is larger than seen in experiments; this is probably due to fluctuations and/or the smooth variation of the pump laser line focus. We discuss possible improvements to our modeling which would include such nonideal effects.

1. INTRODUCTION

The effective and efficient design of laboratory x-ray lasers depends crucially on the ability to accurately model proposed configurations of target and laser irradiance patterns. This is true because of the time and expense required for experimental shots on inertial confinement fusion class lasers such as NOVA at Lawrence Livermore National Laboratory (LLNL). We have therefore developed an XRL modeling capability, using an approach which consists of a series of post-processing steps to a basic hydrodynamic simulation of the pump laser-target interaction. These include calculations of gain and propagation, the latter using both ray and wave optics. To date we have concentrated most of our efforts on the neon-like Yttrium exploding foil x-ray laser.

We have chosen to model the Yt laser because of its importance in coherence experiments at LLNL¹. The Yt laser is well characterized: it is highly monochromatic, with the $J = 2 \rightarrow 1$ 155 Å line dominating; gain-lengths of about 13 are readily achievable; and its pointing character (beam refraction angle) is consistently reproducible. Furthermore, Mo:Si multilayer mirrors are available with normal incidence reflectivity of 50% or higher, and bandwidths as large as 7% (making large numerical aperture curved optics possible). For these reasons, the Yt laser has served as a building block in double target experiments, where one x-ray laser ("oscillator") seeds a second ("amplifier") to achieve a low effective Fresnel number. A variety of experimental data is available, including beam footprints (farfield), gain curves (XRL energy vs. target length), and time-resolved coherence diagnostic data. The last is a

measurement of the diffraction from a uniformly redundant random slit array which samples many spatial frequencies simultaneously.

Several considerations are important in modeling the Yt XRL. Because the electron density and gain vary on the time scale of the x-ray laser pulse, the calculations must use time-dependent density and gain profiles. In addition, retardation effects may be important, particularly for longer targets. Because an isolated amplifier XRL is highly multimode, with Fresnel number $k \times (\text{width})^2 / \text{length} \approx 150$, ray optics should be a good approximation for the intensity distribution. On the other hand, inherently wave optical properties such as coherence require a wave optics calculation.

In light of the above considerations, we use four codes to model the XRL emission, representing three computational steps which are decoupled to an excellent approximation: hydrodynamics, gain and propagation. The Lagrangian hydrodynamics code LASNEX² calculates the interaction of the optical pump laser with the foil target in a two-dimensional plane normal to the foil. Density and temperature data are then input to XRASER³, which computes the two dimensional atomic inversion kinetics, giving the small-signal gain for the 155 Å transition. Gain and density profiles are then passed to two propagation codes, CASER⁴ and WAVE⁵. The ray optics code CASER integrates the radiation transfer equation along three-dimensional rays to yield, among other things, nearfield patterns, farfield patterns, and gain curves. WAVE is a wave optics code which integrates the paraxial wave equation, treating spontaneous emission as a random source throughout the laser. In addition to quantities calculated by CASER, WAVE calculates coherence through the mutual coherence function at the output face of the laser. Both CASER and WAVE are fully time-dependent; WAVE also includes saturation. These codes will be described in more detail below.

Previously we have reported on simulations of Yttrium x-ray laser targets using two-dimensional gain distributions extrapolated from one-dimensional gain calculations along the symmetry axis of the foil⁶. These quasi-two dimensional calculations took the gain proportional to electron density, with cutoffs for large densities and low temperatures. We were able to obtain farfield beam patterns which were in good agreement with experiment for lineouts in the horizontal (exploding foil) direction, with appropriate choice of cutoff values. In the present work, we have improved the model by using a full two-dimensional gain calculation.

We have organized this paper as follows. In section 2, we describe the basic geometry of the system. Section 3 gives results of the hydrodynamic simulation of the target. In section 4 we describe the gain calculations. In section 5 we describe the results of ray tracing calculations, and compare these with experiment. We also describe in this section the above mentioned modification to the time-dependent gain as a plausible emendation of the gain model. In section 6 we give results of wave optics simulations, including a calculation of the mutual coherence function. We conclude in section 7 with a summary and remarks on possible improvements to our modeling.

2. SYSTEM

The specific system we have modeled is our "nominal" Yt target: a 100 µg/cm² Yt foil illuminated from one side by a 120 µm wide line focused beam at a peak irradiance of 1.4×10^{14} W/cm² (Fig. 1). The pump laser pulse is Gaussian in time with a FWHM of 0.5 nsec. The foil is coated onto a substrate of 10 µg/cm² lexan and is overcoated with 5 µg/cm² carbon.

Figure 1. Problem geometry.

The length of the foil was varied in the experiments between 0.68 cm and 2.52 cm, at constant irradiance. We have modeled laser lengths of 1.5 cm and 2.5 cm at fixed line focus width of 120 μm , which approximates the experimental line focus width values of $\approx 100 \mu\text{m}$ and $\approx 150 \mu\text{m}$ for the two laser lengths, respectively.

3. HYDRODYNAMICS

We neglect all variation along the x-ray laser (z) axis, so we require density and gain in the two-dimensional x-y plane perpendicular to the foil. The LASNEX code² transports radiation by diffusion; the atomic physics is done using the average atom package XSN. Electron conduction is included, with a flux-limiter of 0.03. LASNEX calculations have been shown to give accurate electron density profiles for experiments on exploding foil targets⁷. The electron density profile given by LASNEX for the standard Yt foil at the peak of the optical pulse is shown in Fig. 2.

Historically, foil targets were designed to give a relatively flat electron density profile at the time of peak gain to minimize refractive loss⁷. However, the nominal Yt 100 $\mu\text{g}/\text{cm}^2$ foil depicted in fig. 2 is in fact not burned through at the time of peak emission and thus possesses considerable density gradients. Nevertheless, thinner foils which burn through earlier have been shown experimentally to yield smaller peak fluences than the nominal foil.

Figure 2. Electron density profile at the peak of the optical pulse from 2D LASNEX simulation.

Figure 3. 2D X-RASER gain at the peak of the optical pulse.

4. GAIN MODEL

The gain distribution in space and time was calculated using the atomic kinetics code XRASER⁷. XRASER uses electron density and temperature information supplied by LASNEX, along with a detailed atomic model for Yttrium, and computes the detailed inversion kinetics for the lasing species. As mentioned above, we have carried out a full two-dimensional gain calculation for the Yt foil. Such a calculation is computationally intensive, requiring nearly 16 hours of Cray-YMP time. In Fig. 3, we show the gain profile as calculated by XRASER at the peak of the optical pulse (p.o.p.). Fig. 4 shows the variation of the electron density and temperature at p.o.p., which indicates that strong density gradients are present at the position of peak gain. Fig. 5 shows the relaxation of the density profile and falloff of the gain at 70 psec after p.o.p.

Figure 4. Profiles of electron density, temperature, and gain at the peak of the optical pulse.

Figure 5. Profiles of electron density and gain at the peak of the optical pulse and after 70 psec

We make the assumption that the spatial and temporal variation of gain is described by the XRASER prediction only up to an overall multiplier, α , which is, for now, constant in space and time. (Later we will also allow α to vary slowly in time.) To determine the value of α , we calculate the time-integrated (angular) peak fluence in the x-ray laser pulse as a function of laser length through propagation calculations (described in § 5). This gives us the effective gain, which we then match to the experimentally measured gain.

5. RAY PROPAGATION

The code CASER⁴ is used for our ray optics calculations. CASER solves for three-dimensional ray trajectories in the paraxial approximation through the two-dimensional LASNEX generated density profiles. The code then integrates the radiation-transfer equation,

$dI/ds = g(I + \sigma)$, along each ray using the gain model as described above and a Doppler lineshape. The source term σ is taken to be constant in space and time. The emerging spectral intensity

$I_0(x, y, \theta_x, \theta_y, \nu, t, L)$ is thus obtained; it may be integrated over any combination of its arguments to replicate various experimental observables. CASER uses an adaptive integration algorithm which automatically selects dominant rays, thus minimizing the number of rays to calculate.

Figure 6. The refraction angle at the peak of the farfield signal, and the peak value, vs. time.

From a gain-length study, we found that the experimentally determined gain of 5.3 cm^{-1} was

reproduced by using a constant gain multiplier $\alpha = 0.5$ for the 2D XRASER data. CASER allows us to

follow the motion of the farfield XRL beam $I(\theta_x, \theta_y, L) = \iiint I_0(x, y, \theta_x, \theta_y, \nu, t, L) dx dy d\nu$ throughout the pulse. We illustrate the strong effect of refraction in fig. 6, where we plot the angular position $\theta_x(t)$ of the maximum intensity and the x-ray laser emission as a function of time, for a 2.5 cm target. We see that the peak emission occurs in a narrow window of 50-100 psec, during which time the beam sweeps at a rate of about 15 mrad per 100 psec.

In fig. 7, we plot the time-integrated farfield obtained by CASER for 1.5 cm and 2.5 cm targets, along with representative experimental data. The agreement between calculation and experiment is remarkably good for the shorter target, in both mean refraction angle ($\approx 12 \text{ mrad}$) and angular width of the beam ($\approx 15 \text{ mrad FWHM}$). For the longer target, however, the experimental shots consistently give a larger refraction angle, $\approx 12 \text{ mrad}$ compared with $\approx 8 \text{ mrad}$ predicted by CASER. In addition, the angular width predicted by CASER is about the same for both length targets, whereas the experiment shows a narrowing (to $\approx 10 \text{ mrad FWHM}$) in moving from 1.5 to 2.5 cm targets.

Figure. 7 The time-integrated horizontal farfield signal computed by CASER compared with experiment, for two laser lengths: (a) 1.5 cm; (b) 2.5 cm.

One of the possibilities we explored for the disparity with experiment shown in fig. 7(b) is that the gain in the experiments falls off more quickly in time than XRASER's prediction. The XRASER gain may remain higher because of an inaccurately high temperature calculation by LASNEX. From fig. 6, we see that a faster gain falloff would bias the signal toward earlier times, when refractive gradients are steeper. To test this idea in a phenomenological way, we studied the effect of multiplying the XRASER gain by a slowly decreasing function of time. We suppose that the gain falls off exponentially with time from the peak gain,

i.e., $g(x,t) = \alpha g_{XRASER}(x,t) \exp\left\{-(t - t_{peak}) / \tau\right\}$, $t > t_{peak}$. The effect of decreasing τ from 1.5 nsec to about 0.1 nsec is to move the angular position of the peak from the position shown in fig. 7 (b) to about 15 mrad. We found that setting $\tau=0.4$ nsec gives an angular distribution which is in reasonable agreement with the experimental signal (fig. 8). Notably, this represents only a 10% change in the gain over the 50 psec interval after peak signal when there is significant XRL output.

Another explanation for the disparity with experiment is our neglect of axial variation of the XRL plasma. Because the foil is irradiated by focusing a circular beam to a line, the intensity varies along the line focus, an effect which is partially but not entirely compensated for by overfilling the target with the line-focused beam. To illustrate the possible consequences of this effect, we show in fig. 9 LASNEX lineouts of electron density (along $y=0$ symmetry axis) for our nominal irradiance and one at 70% of nominal, at the peak of the optical pulse. At the lower irradiance the foil is not yet burned through, and clearly presents steep transverse gradients to refract rays exiting the region of higher intensity. We plan to quantify this effect by modifying our present code, and resolving the axial variation through a series of 2D LASNEX runs.

Figure 8. The time-integrated horizontal farfield signal for modified 2D gain model compared with experiment.

Figure 9. lineouts of electron density at the peak of the optical pulse for $I = I_0 = 1.4 \times 10^{14} \text{ W/cm}^2$ and for $I = 70\% I_0$.

A lineout through the time-integrated experimental data in the vertical (y) direction compared with the modeling prediction is shown in fig. 10; our modeling clearly predicts a narrower angular spread of the beam in this direction. This is particularly surprising since, as detailed in section 2, we modeled a somewhat wider line focus than used in the experiment. The angular width predicted by CASER is approximately geometric, whereas in the experiments the vertical divergence appears to be independent of geometry as the length and width are changed. While this discrepancy is not yet understood, the neglect of reduced irradiance at the end of the line focus described above may also be playing a role in refracting rays in the vertical direction.

Figure 10. The time-integrated vertical farfield signal for modified 2D gain model compared with experiment.

6. WAVE OPTICS

While ray optics is an excellent approximation for the x-ray lasers we have modeled, inherently wave properties such as coherence requires a wave optics treatment. We used a scalar optics code, WAVE⁵, which integrates the paraxial wave equation using the characteristic propagation coordinate $\xi = z - ct$. WAVE uses a second order accurate split-operator FFT marching scheme. Spontaneous emission is treated as a random source throughout the laser. WAVE can also include saturation effects, although saturation is not an issue here. WAVE has been used to calculate beam patterns for a one-transverse-dimensional model, based

on a 1D XRASER calculation. Zoning requirements prohibit a fully three dimensional calculation; we used 4096 transverse zones and 10 in the propagation direction. In fig. 11 we show the farfield pattern as calculated by WAVE for this gain model for a 3 cm laser, superposed with the result of a CASER calculation also based on 1D XRASER, but for a 2.5 cm laser. The two are in good agreement, as expected for this large Fresnel number system. The difference in the widths of these distributions is likely due to the difference in laser lengths.

WAVE also calculated the complex coherence function (ccf), defined by

$\gamma(x,0) = \langle E^*(x)E(0) \rangle / \sqrt{\langle |E(x)|^2 \rangle \langle |E(0)|^2 \rangle}$, at the output face of the laser; where the brackets denote a time average. Its magnitude, the degree of mutual coherence, is shown in fig. 12. We see that the coherence length l_c (defined by $|\gamma(l_c,0)| = 0.84$) is quite small compared to the laser width: $l_c \approx 1.25 \mu\text{m}$. Related by Fourier transform to the ccf is the aperture function (Van Cittert-Zernike theorem), whose spatial extent gives an effective source size, *i.e.*, the size of a wholly incoherent line source (in 2D) giving the same l_c . In our case we find $x_{\text{source}} \approx 50 \mu\text{m}$.

Figure 11. WAVE farfield calculation compared with experiment and CASER

Figure 12. The time-averaged degree of mutual coherence at the output face of the laser as computed by WAVE.

Experimentally, the coherence of the Yt XRL was assessed by diffraction from a uniformly redundant array of slits sampling spatial scales from $1 \mu\text{m}$ to 1 mm . The ratio of the Fourier transforms of the measured diffraction pattern and the autocorrelation function of the slit array is the ccf. An effective source size is determined in this case by fitting the Fourier transform of the ccf to a Gaussian, whose FWHM is taken to be x_{source} . The effective (time-integrated) source size determined in this way was found to be $x_c \approx 90 \mu\text{m}$. This value is larger than that calculated by WAVE, probably due to nonideal effects such as fluctuations and longitudinal variation of plasma conditions.

7. CONCLUSIONS

We have shown results we have obtained in calculating beam patterns and coherence for Yt XRLs, which we summarize here. We have found good agreement with experiment for a 1.5 cm target, but for a 2.5 cm target we predicted a smaller peak angle for the time-integrated farfield signal. We then explored the sensitivity of the beam pattern to the time-dependent gain, and showed that a slightly faster falloff of the gain after peak XRL emission ($\sim 10\%$ over 50 psec) caused a bias in the signal to earlier times and hence a

larger refraction angle consistent with experiment. We found a beam divergence in the horizontal direction which was consistently smaller than seen in experiments. We have shown that a wave optics calculation gives an intensity distribution consistent with ray optics, and predicts an effective source size which is smaller than an experimentally determined value.

While the first-principles calculation did not quantitatively reproduce all the experimental data, we have obtained some insight into the physics of the XRL emission. In particular, we have seen the relatively large effect of uncertainties in the gain on the calculated signal. This is particularly true for targets which are not completely burned through at the time of peak emission because of the strong effect of density gradients. For the target considered here, the beam refraction angle changes rapidly with time, so an accurate calculation of the time-integrated beam refraction angle depends critically on the faithful characterization of the relationship between the time-dependent gain and density. Therefore we have had to allow some interplay between simulation and experiment, through modification of the time-dependent gain profile, in order to faithfully reproduce what is seen in the laboratory.

Perhaps the most serious lack in our model is the effect of plasma density and gain variation in the propagation direction, as we have mentioned in §5 above. The Nova line-focus is known to have $\approx 10\%$ intensity fluctuations on a length scale of $100\text{ }\mu\text{m}$, as well as a smooth variation along the length due to the projection of the circular beam onto a line. The small scale inhomogeneities will certainly result in variations in electron density which will scatter x-rays; this could change the beam pattern (increase the angular spread), and will certainly degrade the coherence. Inclusion of these effects is the next step in our modeling program.

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