COMPUTATIONAL DESIGN OF SHORT PULSE LASER DRIVEN IRON OPACITY MEASUREMENTS AT STELLAR-RELEVANT CONDITIONS

By

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To my family and friends who supported me during my academic journey.
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Opacity is a critical parameter in the simulation of radiation transport in systems such as inertial confinement fusion capsules and stars. The resolution of current disagreements between solar models and helioseismological observations would benefit from experimental validation of theoretical opacity models. Short pulse lasers can be used to heat targets to higher temperatures and densities than long pulse lasers and pulsed power machines, thus potentially enabling access to x-ray emission spectra at conditions relevant to the radiative zone of the sun. The radiation-hydrodynamic code HYDRA is used to investigate the effects of separately modifying laser energy, laser pulse length, and target dimensions on the plasma conditions, x-ray emission, and inferred opacity of a buried layer iron target. The plasma conditions are controlled by the laser energy and tamper thickness while the accuracy of the opacity inference is sensitive to tamper emission and optical depth effects. As an extension of the single parameter studies, a process using Lawrence Livermore National Laboratory’s Uncertainty Quantification Pipeline has been developed to simultaneously optimize laser and target parameters to meet a variety of design cases. Two sets of design cases were explored: a set focused on conditions relevant to the radiative zone of the sun (electron temperatures of 200 to 400 eV and densities greater than 1/10 of solid density) and a set focused on reaching temperatures consistent with deep within the radiative zone of the sun (500 to 1000 eV) at a fixed density. Optimized designs of a buried layer iron target were found. It was
determined that the appropriate dopant, for inferring plasma conditions, depends on the
temperature reached: magnesium for up to 300 eV, aluminum for 300 to 500 eV, and
sulfur for 500 to 1000 eV. The optimal laser energy and buried layer thickness increase
with goal temperature. The accuracy of the opacity inference is limited to between 12 %
and 26 %, depending on the design. Overall, short pulse laser heated iron experiments
reaching stellar-relevant conditions have been designed with consideration of minimizing
tamper emission and optical depth effects while meeting plasma condition and x-ray
emission goals.
CHAPTER 1
INTRODUCTION

A plasma is a quasi-neutral gas, consisting of both charged and neutral particles, that exhibits collective behavior. Plasmas are commonly characterized by electron temperature $T_e$ (in eV or keV where 1 K $\approx 8.618 \times 10^{-5}$ eV) and electron density $N_e$ (in m$^{-3}$ or cm$^{-3}$), as indicated in Figure 1-1. High electron temperatures and high electron densities are indicative of the plasmas found in both stars and inertial confinement fusion. Inertial confinement fusion (ICF) is an approach to controlled nuclear fusion that uses laser energy to heat and compress a fusion target. Radiation plays an important role in the energy transfer of these high energy density (HED) systems. Radiation transfer is a multi-step process, which includes photon emission by matter, transport in matter, and interaction with matter (either by absorption or scattering). This process is generally modeled by the radiative transfer equation - a differential equation for the variation of radiation intensity.

Figure 1-1. Typical plasmas for different $T_e$ and $N_e$. [This image is used with permission from the Contemporary Physics Education Project (Ref. 2).]
as it propagates through space. This equation includes terms for emission and loss of radiation due to interactions with matter. The absorption of radiation is represented by the opacity. Larger opacities lead to less efficient radiation transfer. Both stars and ICF targets are typically optically thick systems, meaning there are many radiation interactions within the plasmas. In stars, energy generated by fusion in the core is transported from the center to the stellar surface through both radiative and convective heat transfer. The opacity of the ICF target materials plays a large role in the efficiency of energy transport during the target implosion.

Both ICF and stellar physics require the use of computational models to describe energy transport. ICF targets and laser pulses are designed through the use of radiation hydrodynamic codes. Solar models are mathematical representations of the sun, most often treated as a spherically symmetric plasma, that rely on energy transport models. Typically, numerical methods to solve the radiation transport equation incorporate opacity in either theoretically based formulas or tables. Opacity values are computed using theoretical models based on the atomic transitions that occur when matter interacts with photons. Two main types of atomic transitions are relevant to HED plasmas: continuous transitions and line transitions. Continuous transitions, such as free-free and bound-free transitions, occur for a range of photon energies. In a free-free transition, a free electron gains more energy by absorbing a photon. In a bound-free transition, the absorption of a photon by an atom or ion causes a bound electron to be ejected from the atom or ion. Bound-bound transitions only occur for discrete photon energies and are often called “line transitions.” A bound-bound transition involves a bound electron being excited to a higher energy level by the absorption of a photon with energy equal to the difference between the electron’s new energy level and original energy level. The atomic models that calculate these types of transitions depend on the ionization structure and excited states of each ionization stage of each element in the system’s plasma. Elements with large numbers of ionization stages and excited states are complex and may require statistical methods.
to create an atomic model. The assumed simplifications made in an statistical method may make an atomic model, using that method, less certain. Experimental validation of opacity for such elements and conditions is particularly important. It is impractical to test every set of conditions and elements used in theoretical opacity models due to the volume of data and degrees of freedom in the problem. Therefore, opacity measurements for a subset of plasma conditions are desired to test and validate the physical assumptions used in opacity models. It is assumed that, if the model can be validated experimentally, extrapolation to other conditions and elements may be justified.

There are currently disagreements between parameters based on solar models and helioseismological observations that would benefit from the experimental validation of theoretical opacity models at stellar-relevant electron temperatures and densities. As shown in Figure 1-2, the energy produced by nuclear fusion in the sun’s core is transported through the radiative zone, where radiation transport is dominant, and the convective zone, where convective heat transfer is dominant, to the sun’s surface. A thin radiative zone at the sun’s surface transports energy to the space outside of the sun. An important component in solar structure is the abundances of various elements. Grevesse and Sauval calculated the standard abundances of elements in the sun based on photospheric spectroscopy data and time independent 1-dimensional solar atmosphere models.\textsuperscript{4} Several years later, these abundances were updated using time-dependent 3-dimensional models of the solar atmosphere.\textsuperscript{5,6} This resulted in the decrease in the abundances for many elements in the sun. While these new abundances alleviated some existing astrophysical issues, they also created a set of new ones. Parameters calculated using solar models based on the lower abundances disagree with helioseismological observations.

The lower abundances suggest the convective zone boundary is not as deep as helioseismological data indicate.\textsuperscript{7} In addition, it has been found that the sun’s calculated sound speed and density profiles conflict with the profiles inferred from observations.\textsuperscript{8}
Figure 1-2. Zones of the solar interior. Energy generated by nuclear fusion in the sun’s core is transported to the surface through different zones, named for their dominate forms of energy transport. At the surface of the sun there is a thin radiative zone that transport energy to the space outside of the sun. [This image is used with permission from the Heliophysics and Planetary Science Group of NASA/Marshall Space Flight Center (Ref. 3).]

The effect of increasing opacity values for stellar-relevant materials on the disagreement between the calculated and observed parameters has been studied by several groups. Basu and Anita suggested that an increase in opacity of 19 % would place the sun’s calculated density profile within the uncertainty of helioseismological data. Basu and Anita suggested that an increase in opacity of 19 % would place the sun’s calculated density profile within the uncertainty of helioseismological data. Bahcall et al. concluded that an increase of 21 % in the opacity near the base of the convective zone would align the calculated and observed parameters for the base of the convective zone. They also suggested that a broad increase in the opacity by 11 % would give better agreement of the calculated and observed parameters for the sun overall. These suggestions were not based on theoretical calculations or experimental measurements of opacity and were more of an ad hoc adjustment to align calculated and observed data.
Efforts to revise the opacity used in solar models only resulted in a minor increase (<5 %), which is not sufficient to resolve these types of disagreements.\textsuperscript{11} For example, Bahcall \textit{et al.}, using revised opacities from the Opacity Project, which were 2.5 % larger than a commonly used theoretical opacity code, OPAL, found that the calculated parameters still disagreed with observations.\textsuperscript{12} Basu and Anita pointed out that there were no laboratory measurements of opacities for relevant conditions, which made it difficult to estimate theoretical errors.\textsuperscript{11} It was suggested that experimental opacity measurements for electron temperatures greater than 100 eV and densities larger than a fraction of solid density are needed in order to investigate the uncertainties in theoretical opacity models for stellar-relevant materials.\textsuperscript{13} These conditions are relevant to the base of the convective zone and radiative zone of the sun. Oxygen, iron, and neon significantly contribute to the opacities at the base of the convective zone, while iron, sulfur, silicon, and oxygen significantly contribute to the opacities in the radiative zone of the sun.\textsuperscript{11}

In this dissertation, the computational design of iron opacity measurements at conditions representing the radiative zone of the sun will be investigated. Figure 1-3 shows the plasma temperatures and densities that represent the convective zone’s base and radiative zone of the sun. Experiments reaching temperatures of 200 - 400 eV and electron densities of $10^{23} - 10^{24}$ cm$^{-3}$ have been designed in this project. In addition, experiments reaching higher temperatures (500 - 1000 eV) at a constant density which aim to study how opacity scales with temperature, have also been designed. In order to conduct opacity measurements at stellar-relevant conditions, the target must be heated into a high energy density plasma. This was not achievable until the invention of high powered lasers and high pulsed-power machines. Three approaches to creating HED plasmas have been explored: long pulse laser driven, pulsed power driven, and short pulse laser driven. Each approach and previous experiments are discussed in Chapter 2. Short pulse laser driven experiments can create plasmas at conditions representing the radiative zone of the sun and will be the approach considered in this dissertation.
This research presents further computational design of short pulse laser driven iron opacity measurements based on the approach established in London and Castor.\textsuperscript{14} Since temperatures of 10 - 200 eV and densities of $10^{18} - 10^{22}$ cm$^{-3}$ for iron have already been well explored (Chapter 2), this project focuses on temperatures larger than 200 eV and densities of $10^{23} - 10^{24}$ cm$^{-3}$, which are representative of the radiative zone of the sun. Few iron experiments have been performed in this regime. Computational design includes optimizing target dimensions, dopant material for temperature/density measurements, and incident laser pulses. The intensity of the target emission spectrum
and inferred opacity is simulated and optimized to reach design goals with consideration of design constraints. Measurements at plasma conditions consistent with the radiative zone of the sun may be used to investigate the validity of existing theoretical opacity models and may resolve some of the discrepancy between solar parameters calculated from solar models and helioseismological observations. In addition, short pulse driven iron measurements at higher temperatures and densities would complement the existing iron opacity measurements performed at Sandia National Laboratories’ Z facility.\textsuperscript{15-18}

The computational design and analysis of short pulse laser driven opacity experiments for temperatures and densities representing the radiative zone of the sun will provide valuable information for other applications. Since this study will analyze the validity of opacity models at these regimes, the physical understanding gained can be applied to other materials at similar temperatures and densities. These high energy density regimes are important not only to stellar physics, but also inertial confinement fusion and stewardship science. In addition, knowledge gained from this investigation will serve to validate and/or help inform future opacity calculations.
CHAPTER 2
BACKGROUND

Over the past several decades, three main approaches to measuring opacity have
been explored. The first approach, discussed in Section 2.1, uses long pulse lasers to
either irradiate a target directly or to heat a high Z-material causing the high Z-material
to emit x-rays, which are used to radiatively heat a target. As discussed in Section 2.2,
the second approach uses pulsed power drive, such as a Z-pinch machine, to radiatively
heat a target. The third approach, discussed in Section 2.3, uses short pulse lasers to
directly irradiate the surface of a target producing hot electrons that transport through
the target, volumetrically heating the target. In a short pulse laser driven experiment, it is
assumed that the opacity can be inferred from the emission spectra. The emission spectra
is related to the atomic structure and ionization of the heated plasma. In Section 2.3, we
also discuss radiation transport and atomic physics modeling as they relate to short pulse
laser heated opacity measurements.

2.1 Long Pulse Driven Experiments

The majority of long pulse laser driven opacity experiments use the laser to irradiate
either a high-Z foil or a high-Z cavity, known as a hohlraum, geometrically arranged
so that the x-rays emitted by the irradiated high-Z material can heat the target. For
experiments that use a hohlraum, the target can be placed either within the cavity or
at an opening in the hohlraum, while for experiments using a foil, the target is placed
adjacent to the foil. In addition, all long pulse driven opacity measurements make use
of absorption spectroscopy techniques. A backlighter is used to probe the target plasma
so that the attenuated backlighter spectrum can be used to determine the absorption
of the target plasma. This requires the use of a short duration backlighter, so that the
recorded spectrum represents a snapshot in time. In addition, the backlighter’s spectrum
must cover the spectral range of interest, lack features, and have intensity larger than the
self-emission of the target. In point projection spectroscopy, a commonly used method,
a point source of x-rays is used to project a radiographic image of the target on film or an electronic detector. The point source of x-rays is projected through the heated sample and then spectrally dispersed using a Bragg crystal. The unattenuated backlighter spectrum is also measured so that the opacity of the target plasma can be deduced from the ratio between the attenuated and unattenuated backlighter spectrum.

There have been many long pulse laser driven measurements that cover a variety of different target materials, plasma temperatures, and plasma densities. One of the earliest was completed by Davidson et al. (Ref. 21), which used HELEN (a 0.53 μm, 60 J, 200 ps laser) to irradiate a thin gold foil which, heated an aluminum foil buried within plastic. The plastic tamper is intended to limit the aluminum foil’s expansion and produce a more uniform density throughout the experiment. The experiment used point projection spectroscopy with another laser beam incident on a samarium-coated fiber or a titanium-niobium alloy wire to generate the backlighter x-ray source. The plasma conditions ($T_e = 30 - 40$ eV and $\rho = 0.015 \text{ g/cm}^3$) were inferred from hydrodynamic simulations. Davidson et al. suggested the need for separate diagnostic measurements of temperature and density to alleviate the dependence of analysis on hydrodynamics simulations.

Balmer et al. sought to alleviate the dependence on hydrodynamic simulations by using the optical depth, calculated from the measured transmission spectra, to infer the ground state number density of He-like aluminum ions (ions consisting of two electrons), which allowed for simulation independent estimates of the plasma temperature and ionization balance.\textsuperscript{22} This type of research progressed into developing techniques to determine electron temperatures and densities from the K-shell (principal quantum number $n = 1$) and L-shell (principal quantum number $n = 2$) absorption lines which are related to the ionic populations.\textsuperscript{23-25} The dominant ion populations indicate the electron temperature and density of the plasma. Later experiments used radiographs to measure the target expansion and measured the Stark-broadened widths of He-like ions to infer
As a result of this collective research, most opacity experiments make use of spectral lines from a low-Z dopant material to infer the density (from the Stark-broadened line widths) and the temperature (from the line intensities which suggest ionic populations). For example, Perry et al. (Ref. 29) determined the opacity, temperature ($\approx 40 \text{ eV}$), and density ($\approx 0.012 \text{ g/cm}^3$), simultaneously, from the absorption spectra of germanium samples doped with aluminum. The methodology of inferring plasma temperature and density from spectral lines of a low-Z dopant is used in all three approaches to conducting opacity measurements. Knowing the plasma conditions well is necessary because electron temperature and density are needed to calculate theoretical opacities to compare the to measured values.

Of the materials important to opacity in the radiative zone of the sun, there have been several long pulse driven iron opacity experiments. Da Silva et al. (Ref. 30) performed both absorption and emission spectroscopy experiments with plastic (CH) tamped iron targets. The emission spectra of the iron and plastic were subtracted from the absorption spectra. The measured iron transmission spectra were in agreement with OPAL, a commonly used stellar opacity code. The spectral lines measured are indicative of a large range of plasma temperatures and densities ($10 - 40 \text{ eV}$ and $10^{-5} - 10^{-2} \text{ g/cm}^3$). Springer et al. (Ref. 28) measured the absorption spectra of Lexan tamped iron targets where the iron was mixed with sodium fluoride. The electron temperature ($\approx 60 \text{ eV}$) was inferred by the sodium fluoride lines, while the density ($\approx 0.0113 \text{ g/cm}^3$) was inferred from the radiographic measurements of target expansion. Winhart et al. inferred the temperature ($\approx 20 \text{ eV}$) and density ($\approx 0.01 \text{ g/cm}^3$) of a carbon tamped iron absorption spectroscopy experiment from the lines of a separate aluminum measurement at similar heating conditions. In an experiment reaching similar temperatures ($\approx 20 \text{ eV}$) and densities ($2 - 4 \times 10^{-3} \text{ g/cm}^3$), Chenais-Popovics et al. (Ref. 33) used point projection spectroscopy to measure the absorption spectra of carbon tamped iron targets and then compared the results to several different opacity codes. In other absorption spectroscopy
studies of carbon tamped iron targets, temperatures of 15 - 25 eV and densities of 2 - 10 \times 10^{-3} \text{ g/cm}^3 \text{ were reached.}^{34,35} \text{ While these experiments studied iron, they only reached temperatures up to 60 eV and densities up to 0.01 g/cm}^3 \text{ which are too low to be consistent with the radiative zone of the sun. These conditions are consistent with the top of the convective zone of the sun. A current effort at the National Ignition Facility (NIF) is focused on creating a platform that can reach conditions consistent with the base of the convective zone of the sun in order to conduct iron opacity measurements comparable to those performed at Sandia National Laboratories’ (SNL) Z facility (discussed in Section 2.2). Much effort has been put into hohlraum,\textsuperscript{36} backlighter,\textsuperscript{37,38} spectrometer,\textsuperscript{39–41} and platform design.\textsuperscript{42–45} Other proposals include long pulse driven carbon, nitrogen, and oxygen opacity experiments at the NIF, also designed to reach temperatures consistent with the base of the convective zone of the sun.\textsuperscript{46,47}

2.2 Pulsed Power Driven Experiments

Pulsed power driven opacity experiments can also reach conditions consistent with the base of the convective zone of the sun. This technique requires heating and backlighting a target with x-rays produced by a pulsed-power machine such as a Z-pinch. There have been a series of iron opacity measurements completed at SNL’s Z facility that use the dynamic hohlraum x-ray source.\textsuperscript{15–18} In order to create a dynamic hohlraum,\textsuperscript{48} a voltage is supplied to the electrodes sending a current through tungsten wires. This creates a magnetic pressure that accelerates the tungsten wires into the low density foam placed on the Z-pinch axis. The collision of the tungsten with the foam launches a shock that travels inward to the axis of the hohlraum and is trapped by the tungsten plasma, creating a “dynamic” hohlraum. The dynamic hohlraum compresses the foam and can be used to radiatively heat opacity targets placed at the aperture. In this configuration the dynamic hohlraum x-rays both heat and backlight the opacity target. Both the unattenuated and attenuated backlighter spectra, are measured and the data analysis is similar to that of long pulse laser driven experiments.
The first iron opacity measurements performed at SNL Z facility reached electron temperatures around 156 eV and densities around $7 \times 10^{21}$ cm$^{-3}$. These experiments were for plastic (CH) tamped iron targets doped with magnesium. The lines from He-like magnesium ions were used to infer the temperatures and densities. A computational study sought to increase the density in these experiments by increasing the back tamper layer thickness, which was confirmed by experiment. Another computational study investigated the development of a spectral model that will solve for the temperature and density gradient in the target that establishes a best fit of simulated spectra and measured spectra based on the line shapes and ratios of the low-Z dopant. However, experimental measurements did not indicate a significant axial temperature gradient. In a Nature article, Bailey et al. (Ref. 18) described a thorough comparison of stellar-relevant iron opacity measurements (electron temperatures of 160 - 200 eV and electron densities of 0.7 - $4 \times 10^{22}$ cm$^{-3}$) to a variety of opacity models. Compared to the base of the convective zone of the sun, the maximum temperature reached was $\approx 4\%$ larger, while the maximum electron density reached was a factor of 2 lower. However, the charge state distribution reached is similar to that of the base convective zone of the sun. Bailey et al. concluded that the measured opacity is 30 to 400% larger than predicted values, which explains approximately 50% of the discrepancy between calculated solar parameters using the revised lower element abundances and helioseismological observations. This suggests there may be some physical concepts not incorporated into the existing opacity models or the approximations used to speed up computational efficiency do not provide enough detail for this regime.

2.3 Short Pulse Driven Experiments

In order to reach conditions consistent with the radiative zone of the sun, temperatures and densities must be higher than those reached by pulsed power driven and long pulse laser driven experiments. This is achievable with the use of short pulse lasers. As discussed in Section 2.3.1, a short pulse driven opacity measurement requires inferring
an opacity from the emission of the heated target. This is fundamentally different from the previously discussed absorption spectroscopy experiments. At the temperatures reached by short pulse lasers, the self-emission of the target is substantial, making it difficult to design a backlighter with sufficient signal.

2.3.1 Experimental Concept*

In this section, we discuss short pulse laser driven experiments in which a layer of material is tamped by a low-Z material such as plastic (Figure 2-1). The high intensity short pulse laser irradiates one side of the tamper, where the laser light is absorbed predominantly through collisionless processes such as resonance absorption, vacuum heating, relativistic $j \times B$ heating, and the anomalous skin effect.$^{53,54}$ These processes create hot electrons near the surface of the target, which are typically characterized by a Maxwellian distribution at temperature $T_h$. The scaling of $T_h$ with laser intensity has been studied using simulation and experiment.$^{55-58}$ The hot electrons move through the target, heating the background plasma by collisions and by the Ohmic heating of the return current of cold electrons.$^{59,60}$ After the initial transit through the target, the hot electrons begin to recirculate (also known as reflux) between the back and front of the target because of the electric sheaths created at the front and back.$^{61-67}$ With each pass through the target, the hot electrons heat the background plasma through collisions. Recent theoretical studies suggest that the collisional damping of plasma waves, created by relativistic electron bunches, can provide enhanced heating of the background plasma.$^{68,69}$ As the background plasma is heated it emits x-rays, which are recorded, preferably, with a time-resolved spectrometer.

* This section is reprinted from Martin et al., Physics of Plasmas 24, 022705 (2017), with permission of AIP Publishing (Ref. 52).
Figure 2-1. Schematic of a short pulse laser driven experiment. A laser pulse creates a source of high energy electrons at the target surface. The electrons move through the target, heating the materials and causing the emission of x-rays, which are recorded by a spectrometer. The measured x-ray emission is used to infer the frequency dependent opacity of the buried layer.

The radiation transfer equation, which describes the emission from the target, is written as:

$$\frac{1}{c} \frac{\partial}{\partial t} \left( I_\nu(\vec{r}, t; \vec{\Omega}, h\nu) \right) + \frac{\partial}{\partial s} \left( I_\nu(\vec{r}, t; \vec{\Omega}, h\nu) \right) = \eta_\nu(\vec{r}, t; \vec{\Omega}, h\nu)$$

$$- \chi_\nu(\vec{r}, t; \vec{\Omega}, h\nu) I_\nu(\vec{r}, t; \vec{\Omega}, h\nu). \quad (2-1)$$

The specific intensity, $I_\nu(\vec{r}, t; \vec{\Omega}, h\nu)$, represents the radiant energy per unit time, solid angle, area, and photon energy moving in the direction $\vec{r}$. The emissivity, $\eta_\nu(\vec{r}, t; \vec{\Omega}, h\nu)$, represents the emitted energy. The opacity coefficient, $\chi_\nu(\vec{r}, t; \vec{\Omega}, h\nu)$, represents the absorption per unit length. In Eq. (2–1) the temporal and spatial change in radiation
intensity balances the emission and loss of radiation intensity. For target dimensions of
10 - 100 μm and heating pulses of the order of 1 - 10 ps, we may assume steady state and
1D-planar geometry. Assuming steady state and constant properties, the solution of the
radiation transfer equation is

\[ I_\nu = \frac{\eta_\nu}{\kappa_\nu} \left( 1 - e^{-\kappa_\nu \rho \Delta l} \right) \tag{2.2} \]

where \( \kappa_\nu \) is the opacity, \( \rho \) is the plasma density, and \( \Delta l \) is the thickness of the buried
layer. If we assume local thermodynamic equilibrium (LTE), the ratio of emissivity to
opacity is given by the Planck function \( (B_\nu(T)) \),

\[ \frac{\eta_\nu}{\kappa_\nu} = B_\nu(T) = \frac{2\hbar \nu^3}{c^2} \left( \frac{1}{\exp \left( \frac{\hbar \nu}{k_B T} \right) - 1} \right) \tag{2.3} \]

where \( \hbar \) is Planck’s constant, \( \nu \) is the radiation frequency, \( c \) is the speed of light, \( k_B \) is the
Boltzmann constant, and \( T \) is the temperature. Assuming LTE, Eq. (2.2) becomes

\[ I_\nu = B_\nu(T) \left( 1 - e^{-\kappa_\nu \rho \Delta l} \right) \tag{2.4} \]

By measuring \( I_\nu \), \( T \), and \( \rho \Delta l \), we can determine the frequency dependent opacity by
inverting Eq. (2.4),

\[ \kappa_\nu = -\ln \left( \frac{1 - \frac{I_\nu}{B_\nu(T)}}{\rho \Delta l} \right) \tag{2.5} \]

This solution for \( \kappa_\nu \) assumes that the plasma emitting x-rays is in LTE. The departure
from LTE is typically quantified by comparing LTE and non-LTE models, as discussed in
Section 3.2.3.

As suggested in Figure 2-1, a dopant material is needed in the iron layer so that
the plasma temperature and density can be inferred. The plasma temperature \( (T) \) can
be inferred by comparing the relative strengths of different atomic transition lines. The
electron density can be inferred by analyzing the Stark broadened line widths. In the 1D
approximation, the areal density \( (\rho \Delta l) \) is conserved and determined by its initial value.
In order to use well established kinetic models to determine the temperature and density,
the dopant material should be K-shell ionized at the conditions of the experiment. More information on the use of K-shell emission to diagnose plasma conditions is found in books such as Griem\textsuperscript{71} and Lochte-Holtgreven.\textsuperscript{72} As explained in this section, the frequency dependent opacity can be inferred in an emission measurement from the specific intensity of a doped layer target.

Short pulse laser driven emission experiments have been completed for several different materials. The majority of the existing experiments were done with aluminum targets. They have reached temperatures from 200 to 700 eV and densities from $10^{23}$ - $10^{24}$ cm$^{-3}$.\textsuperscript{73-79} Another material fairly well researched is germanium, for which short pulse laser drive experiments have reached temperatures from 250 to 800 eV and densities approximately $10^{23}$ cm$^{-3}$.\textsuperscript{76,80-82} The only stellar-relevant material that has been investigated is iron. There have been only a few short pulse laser driven iron opacity measurements published. Nazir \textit{et al.} (Ref. 83) performed the first iron emission experiment using short pulse lasers and concluded that synthetic x-ray spectra calculated using an LTE opacity model agreed with the main features of the experimental x-ray spectra. They inferred the temperature ($\approx 600$ eV) and density ($\approx 10^{24}$ cm$^{-3}$, near solid density) from 1-dimensional hydrodynamic simulations. In a similar experiment, Shahzad \textit{et al.} (Ref. 84) inferred temperatures of 360 to 700 eV and densities of $10^{22}$ to $10^{24}$ cm$^{-3}$. There have also been a few computational studies done on the application of short pulse laser driven opacity measurements. Davidson \textit{et al.} (Ref. 85) investigated the concept of doping the buried layer with a low-Z element to use as a temperature and density diagnostic. The use of a low-Z dopant was not incorporated in the few published short pulse laser driven iron opacity measurements. London and Castor have modeled the mechanisms by which short pulse lasers heat planar buried layer targets to temperatures of approximately 500 eV and densities near solid density for aluminum and iron.\textsuperscript{14} The temperatures and densities that can be reached using short pulse lasers are consistent with the radiative zone of the sun ($> 200$ eV and $> 10^{23}$ cm$^{-3}$).
2.3.2 Interactions with Matter

The radiation transfer equation (Eq. (2–1)) considers the net total emission, absorption, and scattering of radiation within an HED system. The emissivity, \( \eta_\nu(\vec{r}; t; \Omega, h\nu) \), represents all the processes by which the particles in the plasma can emit or scatter radiation. The opacity coefficient, \( \chi_\nu(\vec{r}; t; \Omega, h\nu) \), includes absorption opacity and scattering opacity although typically in HED plasmas the scattering opacity is negligible.

Photon-matter interactions most important in HED plasmas occur via three different types of atomic processes: free-free, bound-free, and bound-bound transitions. In free-free transitions, a free electron gains or loses energy by interacting with an ion or photon. Two common free-free transitions include bremsstrahlung emission, in which an electron gains energy by an interaction with another charged particle resulting in photon emission, and inverse bremsstrahlung absorption, in which the absorption of a photon increases the energy of a free electron. In bound-free transitions, a bound electron’s energy is increased enough to excite it above the ionization energy and into the continuum. In photoionization, a bound-free process, a bound electron absorbs a photon, causing the bound electron to become free. In recombination, a free electron is absorbed by an ion, resulting in a photon being emitted. Both free-free and bound-free transitions contribute to continuum emission and absorption spectra. Line emission and absorption spectra arise from bound-bound transitions. In bound-bound transitions, a bound electron is either excited to higher energy level by absorbing a photon or decays to a lower level by emitting a photon. Bound-bound transitions result in spectral lines with energies equal to the energy difference between the two electron energy levels.

The atomic models used to calculate these types of transitions depend on the electronic structure of the material present in the HED system. For a given material, the number of potential ionization stages is given by one plus the total number of electrons in a neutral atom. For each ionization stage, there is a set of electron energy levels for which atomic transitions can take place. As more ionization stages are required to model
an HED plasma, atomic modeling becomes more computationally expensive and may require statistical methods. The next section will further discuss the role of atomic physics modeling in predicting x-ray emission and absorption spectra.

2.3.3 Atomic Physics Modeling

Plasma properties such as emissivity and opacity depend on the populations of each energy level within all of the ionization stages in a given plasma. The most general approach to calculating such plasma properties would be to include all of the possible atomic transitions for every electron energy level. Thus, for each energy level, an equation for the rates of each atomic transition would need to be constructed. The populations of the ionization stages are determined by solving the system of rate equations. This approach is referred to as detailed line accounting (DLA). For plasmas with many ionization stages and many energy levels, solving large sets of rate equations is difficult and computationally expensive. In an alternative approach, referred to as detailed configuration accounting (DCA), a set of energy levels is grouped into a single configuration with averaged quantities and rate equations are constructed for each configuration. This allows a large number of energy levels to be grouped into a smaller number of configurations, for which solving a system of rate equations is more tractable. If solving a system of rate equations for a number of configurations is still computationally difficult, configurations can be grouped into superconfigurations and super transition arrays can be used to represent transitions between superconfigurations. More information regarding the determination of atomic energy levels, configurations, and superconfigurations can be found in books such as Bauche et al. (Ref. 86) and Cowan (Ref. 87).

In a plasma in local thermodynamic equilibrium (LTE) the population of each ionization stage can be determined from Saha-Boltzmann statistics and does not require solving a system of rate equations. In LTE, only the electron energy level structure is required. Either DLA or DCA can be used to determine the energy level structure.
In DLA, the energy levels are treated individually and the population of each level is calculated using Saha-Boltzmann statistics. In DCA, the energy levels are grouped into a set of configurations and the population of each configuration is calculated using Saha-Boltzmann statistics. For a non-LTE plasma the populations of each ionization stage must be calculated by solving a system of atomic transition rate equations. Atomic transition cross sections can be tabulated from transition rates and ion populations. Transition cross sections are used to calculate the emissivity and opacity used in the radiative transport equation. As mentioned in Chapter 1, both ICF and stellar physics research use computational models that include radiation energy transfer. In such computational models, the opacity and emissivity are either calculated in-line using some theoretical approach to atomic physics modeling or taken from tables that have been previously calculated from atomic physics theory. How the atomic energy levels are grouped, e.g. individually or in configurations, will affect the calculation of radiation transport. Simulated spectra based on radiation transfer models will be sensitive to what atomic physics modeling was used in determination of the emissivity and opacity. This can drastically affect the line emission or line absorption spectra, which are related to the number of individual levels or configurations contributing to the bound-bound atomic transitions.

In a short pulse laser driven opacity experiment, the opacity is inferred from the x-ray emission spectra as discussed in Section 2.3.1. Comparisons of measured x-ray emission spectra to simulated spectra are dependent on the assumed atomic physics modeling in the simulated spectra. The plasma temperature and density diagnosis from the dopant material’s K-shell emission relies on the detailed modeling of the material’s K-shell ionization. In addition, the measured emission from the material of interest will need to be compared against the simulated emission calculated using opacity models that apply different strategies to compute the ion populations. For the design studies in this dissertation, the DCA approach was used to calculate opacity and emissivity. As discussed
in Section 3.2.3, for temperatures of 200 - 400 eV consistent with the radiative zone of the sun, plasma conditions are near enough to LTE such that LTE DCA can be used. For temperatures larger than 400 eV, non-LTE DCA must be used.
CHAPTER 3
SINGLE PARAMETER STUDIES FOR IRON AND IRON-MAGNESIUM BURIED LAYERS*

This chapter will focus on the computational design of short pulse laser driven iron opacity measurements that are at temperatures (200 - 400 eV) and densities ($N_e = 10^{23} - 10^{24}$ cm$^{-3}$ and $\rho = 0.8 - 7.88$ g/cm$^3$) characteristic of the upper radiative zone of the sun. Computational design is needed to determine target and laser parameters such that specific plasma conditions and emission spectra are achieved. The HYDRA$^{88}$ code was used to study the effects of laser irradiance and target dimensions on plasma conditions, x-ray emission, and opacity inference for iron and iron-magnesium buried layer targets.

3.1 Simulation Methodology

Computational design simulations spanning a range of input parameters describing the target and the laser pulse have been studied. The goal is to determine the parameters that produce plasmas with a desired range of temperature (200 - 400 eV) and density ($N_e = 10^{23} - 10^{24}$ cm$^{-3}$ and $\rho = 0.8 - 7.88$ g/cm$^3$) for, preferably, a duration that is several times longer than the time resolution of a spectrometer. In addition, the emitted x-ray spectra are simulated and examined in the context of assessing how well opacity inferred from the simulated emission matches the opacity included in the model.

3.1.1 HYDRA Assumptions

We used the HYDRA$^{88}$ radiation hydrodynamics code for the simulations. The models reported here assume 1D geometry, use electron conduction with Lee and More$^{89}$ conductivities and a flux limiter of 0.05, multigroup diffusion for radiation transport, and detailed configuration accounting (DCA)$^{90,91}$ for atomic structure and opacity. The HYDRA-DCA package$^{92}$ includes non-LTE time-dependent atomic kinetics from CRETIN$^{93}$. Results were not sensitive to changes in the flux limiter. Radiation

* This chapter, with the exception of Section 3.1.4, is reprinted from Martin et al., Physics of Plasmas 24, 022705 (2017), with permission of AIP Publishing (Ref. 52).
hydrodynamics can be approximated using 1D geometry for experiments where the laser focal spot size is much larger than the target thickness, especially larger than the buried layer which is responsible for the bulk of the emission. These one-dimensional models are most applicable to experiments where a microdot is surrounded by tamper material on all sides and the laser focal spot overfills the lateral radius of the microdot. The use of the diffusion model for radiation transport is supported by comparisons between discrete ordinates and diffusion radiation calculations, in which changes of less than 7 % in plasma variables were found. Running HYDRA with diffusion radiation transport saves more than 50 % computation time over using discrete ordinates radiation transport. A Thomas-Fermi based\textsuperscript{94,95} equation of state (EOS) is used for tamper materials. Iron only buried layer models used a Purgatorio\textsuperscript{96,97} based equation of state. Purgatorio is a planewave density functional theory code for an average atom treatment of the electronic structure of a material. It more accurate than the Thomas-Fermi model because it includes shell structure. Mixed iron-magnesium buried layer models used an in-line quotidian equation of state (QEOS)\textsuperscript{95} model because comparisons with an externally calculated constant Thomas-Fermi pressure based mixed EOS model\textsuperscript{1} yielded very similar (< 2 % different) average plasma conditions in the buried layer. All of these EOS models assume LTE, which is valid for plasma conditions considered in this chapter (200 - 400 eV). For larger temperatures (> 400 eV), non-LTE atomic structure and EOS should be included. Non-LTE effects are further discussed in Section 3.2.3. The physics assumed in the HYDRA parameter studies are justified for the plasma conditions explored in this chapter.

3.1.2 Energy Deposition Source

While HYDRA has a laser propagation and deposition package, it is tailored for moderate intensity, long pulses. It does not include either collisionless absorption

\textsuperscript{1} P. Sterne, private communication (2015)
processes,\textsuperscript{54,98} which are dominant for intensities larger than $10^{16}$ W/cm\textsuperscript{2}, or hot electrons, which are generated with energies of 10s - 100s of keVs at these intensities. Modeling of high intensity, short pulse laser-matter interactions is often done with particle-in-cell codes.\textsuperscript{99} Since such modeling is difficult and computationally expensive, we take a simple parametric approach, representing the target heating as a specified time-dependent internal energy source. In keeping with the approximate nature of this approach, we do not consider a laser pre-pulse and its effect on hot electron generation.

Our model contains two essential assumptions about the space and time dependence of the heating. The first is of a Gaussian time dependence, with a duration equal to the duration of the laser pulse. In reality, heating may be longer due to electron recirculation and other effects, as suggested by time-dependent K\textsubscript{α} spectroscopy measurements\textsuperscript{67,100–103} from solid targets. The second assumption is that the heating rate per unit mass is constant in space. The total energy deposited in the target is specified as a fraction (or conversion efficiency) of the laser energy, (\textit{ϵ}). This accounts for the conversion of absorbed laser light into hot electrons and the fraction of hot electron energy deposited within the laser focal spot, since there maybe lateral spreading of hot electron energy beyond the focal spot. Previous studies suggest a large variety of laser light absorption efficiencies (20 - 60 \%)\textsuperscript{104–107} and hot electron energy conversion efficiencies (5 - 50 \%).\textsuperscript{99,100,108–115} For our parameter studies, we have assumed a conversion efficiency (\textit{ϵ}) of 5 \%, which is consistent with similar modeling completed to assist with analysis of previous iron experiments at Comet\textsuperscript{116} and aluminum experiments at Orion.\textsuperscript{117}

Specifically, our energy source assumes that the maximum internal energy is proportional to the average laser energy per unit mass, which is related to the laser irradiance. The peak laser irradiance (\textit{I}) is

$$I = 2 \sqrt{\frac{\ln 2}{\pi}} \frac{E}{(t_{\text{FWHM}})ab\pi}$$

(3–1)
where $E$ is the laser energy, $t_{\text{FWHM}}$ is the full width half maximum of the laser pulse, $a$ is the semi-major axis, and $b$ is the semi-minor axis of an elliptical laser focal spot. The maximum internal energy ($U_{\text{max}}$) is

$$U_{\text{max}} = \epsilon \left( \frac{E}{M_{\text{target}}} \right)$$  \hfill (3-2)

where $\epsilon$ is the conversion efficiency and $M_{\text{target}}$ is the total mass of the target. The Gaussian heating pulse is described by

$$P(t) = 2 \sqrt{\frac{\ln 2}{\pi}} \frac{U_{\text{max}}}{t_{\text{FWHM}}} \exp \left( -\frac{(4 \ln 2)(t - \bar{t})^2}{t_{\text{FWHM}}^2} \right)$$  \hfill (3-3)

where $t$ is time and $\bar{t}$ is the time of peak power. The pulse is centered ($\bar{t} \gtrapprox 1.5 \ast t_{\text{FWHM}}$) such that the total integral of the Gaussian pulse is greater than 99% of the maximum internal energy ($U_{\text{max}}$). The incremental internal energy source supplied to HYDRA is the cumulative integral of the Gaussian heating pulse and is deposited into the target’s electrons. Each layer’s ions gain energy through collisions with electrons. Both tampers and the buried layer are assumed to have the same internal energy source, meaning that the hot electrons deposit the same energy per unit mass into the entire target. Further analysis into the stopping power of hot electrons for different materials and how best to incorporate that into modeling will be addressed in future work. As described here, for specific laser and target parameters, the internal energy source characterizes the heating of the target by the short pulse laser.

### 3.1.3 Validation with Experiments

To validate our methodology, we simulated two published short pulse heated experiments. Shahzad et al. (Ref. 84) presented experimental results for thin buried layer iron targets. They modeled their experiments, using HYADES, by depositing 0 - 10% of the mass weighted laser energy. To model their experiment with our methodology, we assumed a conversion efficiency of 3% for a 2 J, 2 ps, 20 \(\mu\)m diameter focal spot laser incident on a target consisting of a 77 nm iron layer buried between two parylene-N layers.
of 740 nm and 240 nm thicknesses. Our model reaches similar peak electron temperatures (780 - 830 eV), similar peak average ionization (23 - 24), and slightly lower peak electron densities (0.7 - 1 x 10^{24} \text{ cm}^{-3}) in the iron layer to those predicted and inferred by Shahzad et al. We also simulated buried layer aluminum experiments by Hoarty et al. (Ref. 78). They measured an x-ray pulse duration of approximately 20 ps, inferred an electron temperature of 600 eV, and inferred a density of 1.5 ± 0.5 g/cm^3. We assumed a 3 % conversion efficiency for a 100 J, 0.5 ps, 50 \mu m diameter focal spot laser incident on a 0.15 \mu m Al layer buried between two parylene-N layers of 10 \mu m and 12 \mu m thicknesses. Our model reaches a peak average electron temperature of 610 eV and a coincident density of approximately 2 g/cm^3. For the spectral energy range of the experimental time-resolved measurements, 1.75 to 2.2 keV, we predict an x-ray pulse duration of approximately 20 ps. Our comparisons with these two experiments suggest that this methodology can be used to predict peak plasma conditions and reasonable x-ray pulse durations. Even so, the parameters describing the target heating in our model, i.e. the conversion efficiency and the pulse length, are only approximate. We expect that values of these parameters can be adjusted to best match plasma conditions for a particular experiment. We fix the conversion efficiency (\epsilon = 5 \%) and the pulse length (equal to the laser pulse length) for the studies discussed in this chapter.

3.1.4 Verification of Methodology

The HYDRA development team follows a quality assurance plan that includes tests and nightly checks to compare the algorithms included in HYDRA with problems that have known results.\(^2\) Generally, most errors in coding are detected before a HYDRA version is deployed for use. The quality tests check the performance of both the radiation transport and hydrodynamic algorithms we use in our methodology. When developing our methodology we completed a convergence study of the zoning in the material mesh

\(^2\) M. M. Marinak, private communication (2017)
in order to determine the minimum areal density per zone required to converge the
plasma conditions to within 5 - 10%. The minimum areal density for each material in
the problem is fixed such that thicker layers require more zones. In addition, we explored
different options for radiation transport, equation of state, and opacity. As discussed in
Section 3.1.1, use of both diffusion and discrete ordinates radiation transport yielded
similar plasma conditions. Comparisons of different equation of states for iron and iron
mixtures are discussed in Section 3.1.1. Simulations using a Thomas-Fermi based\textsuperscript{94,95} EOS
table, an in-line QEOS\textsuperscript{95} calculation, and a Purgatorio\textsuperscript{96,97} based EOS table for tamper
materials yielded similar plasma conditions. Including non-LTE EOS results in higher
densities and lower pressures because of the ion-sphere coulomb correction.\textsuperscript{118} Externally
calculated electron pressures, including the ion-sphere correction, agree with the electron
pressure output by HYDRA simulations using non-LTE EOS. HYDRA simulations
using opacities from two different models, VISTA\textsuperscript{3} and DCA,\textsuperscript{90,91} yielded similar plasma
conditions but different, as expected, opacities, emissivities, and multigroup radiation
energy densities because of the atomic structure and transitions included in each opacity
model. We also verified the Yorick\textsuperscript{121} function that calculates the x-ray emission along a
user-specified ray by comparing it with the analytical solution to the radiation transport
equation for a simple slab. Our comparison identified a long standing error in the Yorick
function that double counted the part of the ray in zone containing the ray’s starting
point. All identified errors were addressed before applying our methodology to the studies
included in this dissertation.

Our methodology also yields results reasonably similar to the results described in
London and Castor (Ref. 14), which used a different radiation-hydrodynamics code named
LASNEX. Instead of a parametric internal energy source, London and Castor include the

\textsuperscript{3} VISTA is a LTE opacity code developed by M. H. Chen based on the STA theory
(Ref. 119 and Ref. 120).
transport and coupling of hot electrons by a multigroup diffusion model. They simulated a 0.1 μm Fe layer buried between two 4.5 μm layers of CH heated by a hot electron intensity of 2.4 x 10^{17} W/cm^2. The simulation reached peak conditions of approximately 300 eV, 4.5 x 10^{23} electrons/cm^3, and average ionization of 15 - 19. The peak x-ray emission over the L-shell Fe range varies from 2 to 6.5 x 10^{13} W/cm^2/str/keV and the opacity varies from 0 - 2 x 10^4 cm^2/g. Using our methodology, we simulated a 0.2 μm Fe layer sandwiched between two 5 μm CH tampers heated by a 5 J, 1 ps, and 30 μm diameter focal spot laser assuming a 5 % conversion efficiency. Our model reached peak conditions of approximately 280 eV, 6 x 10^{23} electrons/cm^3, and average ionization of 17. Over the L-shell Fe range, the x-ray emission varies from 4 - 15 x 10^{13} W/cm^2/str/keV and the opacity varies from 0.2 - 1.3 x 10^4 cm^2/g. The x-ray emission in our simulation is larger because we have twice the amount of iron as in London and Castor’s simulation. Overall, the plasma conditions, x-ray emission, and opacity are similar between the two methodologies suggesting that our methodology yields reasonable results.

### 3.2 Results and Analysis

We have investigated the effects of varying a single laser or target parameter on plasma conditions, x-ray emission, and inferred opacity while fixing all other parameters. The HYDRA results are analyzed and compared using Yorick, an interpreted language for scientific simulations and calculations. A Yorick function calculates the x-ray emission using a solution to the radiation transfer equation (Eq. (2-1)), along a specified line of sight, and uses the opacity, emissivity, density, and thickness from HYDRA. The effects of changing the laser energy, the laser pulse length, the buried layer thickness, and the tamper thicknesses, as well as the effects of departure from LTE and including a dopant material, are discussed in this section. The propagation of experimental uncertainties in the opacity inference and an example design reaching conditions relevant to the radiative zone of the sun are also discussed.
3.2.1 Base Model

Our base model represents a peak laser irradiance of $10^{18}$ W/cm$^2$ with 8 J of laser energy, a 1 ps pulse length ($t_{\text{FWHM}}$), and a 30 μm diameter focal spot incident on a planar target consisting of 0.2 μm of iron sandwiched between 5 μm of parylene-N (CH) on either side. This model used non-LTE DCA opacities for electron temperatures larger than 75 eV. The internal energy source is calculated as described in Section 3.1 using initial densities of 1.11 g/cm$^3$ for parylene-N and 7.88 g/cm$^3$ for iron. Figure 3-1, shows that rapid heating of the target within the first 2 ps results in an increase in the electron temperature. This heating causes the layer to expand into the tamper material, which is demonstrated by a widening of the layer boundaries and a decrease in the material density. As the layer expands, a pressure wave is launched in the tamper layers causing a small increase in the tamper density near the layer starting around 2 ps. At around 7 ps, the layer recompresses. The recompression is caused by radiative cooling of the layer, known as a radiative collapse.\textsuperscript{122-126} Since the CH tampers are mostly transparent to the x-rays radiating from the layer, that energy escapes the target. The layer will cool to a temperature that is lower than that of the surrounding tamper material, causing a pressure differential at the interface that drives the tampers to recompress the layer. During this process, conductive heat transfer between the layer and tampers somewhat counteracts the radiative collapse by smoothing out the temperature difference and thus limiting the pressure differential at the interface. Therefore the interplay between radiative losses and conduction controls how much the layer recompresses. After the layer recompresses, between 12 ps and 30 ps, the layer remains at a relatively constant density before the target ultimately expands.

The streak plots in Figure 3-1 also show that the variation of plasma temperature and density across the layer changes with time. For approximately the first picosecond, the plasma conditions are constant across the layer. The largest spatial gradients in electron temperature and density occur while the layer is being heated, expanded, and
recompressed. Once the layer is recompressed, the temperature and density remains constant across the layer. The same general temporal and spatial behavior is seen for all models, but the timing of the buried layer expansion and recompression, the period of constant density, and the magnitudes of electron temperature and density depend on the specific laser and target parameters.
3.2.2 Parameter Variations

3.2.2.1 Laser energy

In order to reach plasma conditions consistent with the radiative zone of the sun, we investigated the effect of varying the laser energy on plasma conditions and x-ray emission. We fixed the laser pulse length (1 ps), laser focal spot size (30 μm diameter), and target dimensions (5 μm CH - 0.2 μm iron - 5 μm CH). All models used non-LTE DCA opacities for electron temperatures larger than 75 eV. The internal energy source is increased in proportion to the laser energy. Figure 3-2 displays the time history of the average buried layer electron temperature for laser energies of 5 J, 8 J, and 19 J. The 5 J and 8 J models reach electron temperatures consistent with the radiative zone of the sun (290 - 390 eV) while the 19 J model reaches temperatures similar to the center of the sun (1 keV). For all models, the electron temperature rapidly peaks at approximately 2 ps then drops as the target cools. The ion temperature qualitatively exhibits a similar temporal shape, but peaks after the electron temperature and reaches a smaller (5 % for 5 J to 14 % for 19 J) peak as shown in Figure 3-2 for the 19 J laser. As most evident for peak temperature, the average electron and ion temperatures increase with increasing laser energy. These three models were selected to demonstrate a range of electron temperatures that may be achieved using a short pulse laser.

As shown in Figure 3-3, the initial rapid drop in the iron layer’s average density represents the early buried layer expansion. Characterized by the increase in the slope of the initial density drop, the rate of the layer expansion increases with increasing laser energy. In addition, the minimum average layer density after initial expansion decreases with increasing laser energy. After the initial density drop, an increase in the average density corresponds to the radiative collapse of the layer, as discussed in Section 3.2.1. In all three models, there is some period of time for which the iron density remains steady before decreasing with the ultimate expansion of the target. The duration of this time period of relatively constant density decreases with increasing laser energy,
being approximately 20 ps for the 5 J model, 14 ps for the 8 J model, and 4 ps for the 19 J model. Taking multiple time-resolved measurements at relatively constant plasma conditions will be more difficult with increasing laser energy.

The simulated x-ray emission at normal incidence from the target is shown in Figure 3-4. This, and all subsequent, simulated x-ray emission includes time-dependent atomic kinetics from the HYDRA-DCA package. The emission is shown at the time of peak average electron temperature in the layer, when the x-ray emission is strongest. The frequency range 0.7 keV to 1.9 keV captures the iron L-shell emission. The specific intensity and ionization increase with increasing laser energy due to higher layer temperatures. The increase in ionization shifts the line emission to higher energy ranges. Therefore, increasing the laser energy results in higher electron temperatures and x-ray emission, which will improve spectrometer signal, but will also shift the line emission of the iron L-shell, which will affect the required spectrometer frequency range.
3.2.2.2 Dopant

As an example that reaches conditions relevant to the radiative zone of the sun, a 5 J, 1 ps, 30 μm focal spot diameter laser model with LTE opacities (Section 3.2.3 for discussion of LTE and non-LTE) is adapted to include a Mg dopant in the buried layer as a plasma diagnostic. All remaining subsections of Section 3.2.2 will discuss models that use LTE opacities. The Mg Hydrogen-like (H-like) and Helium-like (He-like) lines should be discernible in the simulated emission spectra. The model assumes a target consisting of 5 μm of CH on either side of a 50 % Fe and 50 % Mg by atom (“doped”) layer. The initial material density of the doped layer is calculated by

$$\rho_{BL} = \frac{1}{\frac{w_{Fe}}{p_{Fe}} + \frac{w_{Mg}}{p_{Mg}}}$$  \hspace{1cm} (3-4)
Figure 3-4. Simulated x-ray emission, at the time of peak electron temperature, at normal incidence from the target. The spectral resolution is 2 eV per bin. Average ionization of the iron layer at this time is included in the legend. The bracketed notation lists the atomic transitions represented in that range of frequencies.

where $w_{Fe}$ and $w_{Mg}$ are the mass fractions of Fe and Mg in the buried layer. The mass fraction of either Fe or Mg is given by

$$w_i = \frac{\gamma_i A_i}{\gamma_{Fe} A_{Fe} + \gamma_{Mg} A_{Mg}}$$

(3-5)

where $i$ is either Fe or Mg, $\gamma_i$ is the atom fraction, and $A_i$ is the atomic mass (in g/mol). The layer thickness is 0.6 $\mu$m to keep the number of Fe atoms the same as the undoped layer. Consistent iron and doped buried layer models are compared to assess the effects of including a dopant material on the plasma conditions and emission. Including Mg in the iron layer did not significantly affect the plasma temperature. Doped and iron layers experience the same qualitative behavior, initial expansion followed by recompression.
followed by late time expansion, but the doped layer reaches lower densities than the iron layer.

The simulated x-ray emission at the time of peak electron temperature, in Figure 3-5, shows additional lines for H-like and He-like Mg from the doped layer. It is important

Figure 3-5. Simulated x-ray emission at normal incidence from the target and the time of peak electron temperature for the iron and doped layers. The average ionization of the layer is included in the legend.

that the Fe and Mg spectra are separated, with Fe emission between 0.7 - 1.25 keV and the Mg emission between 1.25 - 1.8 keV. The iron emission (0.7 - 1.4 keV) from the doped layer is different than the emission from the pure iron layer due to differences in ionization and density. The iron in the doped layer is slightly more ionized than the pure iron layer because the electron density in the doped layer is lower (≈ 35 %) than that of the pure iron layer. The time of peak electron temperature, displayed in Figure 3-5, occurs when the target is still expanding. At later times, when the target is more hydrodynamically
stable, the electron densities and iron ionizations in the two layers are more similar thus the ionization difference is not dominant in the spectra.

3.2.2.3 Pulse length

We used a doped layer model, which reached conditions relevant to the radiative zone of the sun, to study the effects of laser pulse length. We increased the pulse length \( t_{\text{FWHM}} \) from 1 to 15 ps and kept the laser energy (5 J), the focal spot size (30 \( \mu \text{m} \) diameter), the tamper thicknesses (5 \( \mu \text{m} \) on either side), and the buried layer (0.3 \( \mu \text{m} \) doped) constant. The average electron temperatures in the layer, for each model, are shown in Figure 3-6A. In all these cases, the peak electron temperature occurs at approximately twice the \( t_{\text{FWHM}} \) of the pulse, a time which corresponds to \( > 90 \% \) of the energy deposition. The peak temperature decreases with increasing pulse length, but remains within our range of interest (200 - 400 eV). Increasing the laser pulse also increases the duration for which the average electron temperature remains similar to the peak temperature before the target begins to cool. All of these effects are attributed to the same average energy deposition per unit mass being spread out over a longer period of time. Pulse length can be used to control the value and duration of the peak electron

Figure 3-6. Average plasma conditions in the buried layer for different pulse lengths. A) Electron temperature (eV). B) Density (g/cm\(^3\)).
temperature. Longer pulse lengths allow for multiple time-resolved emission measurements during a period of relatively constant electron temperature.

Increasing the pulse length delays the initial expansion of the layer as shown in Figure 3-6B. Even though the expansion is delayed, the minimum density before recompression remains similar for all pulse lengths. Overall, increasing the laser pulse length delays the initial heating and expansion of the layer while decreasing the peak electron temperature. These calculations indicate that a set of experiments for several pulse lengths could be used to explore emission for different electron temperatures at similar densities. All four models reach temperatures (> 200 eV) and densities (60 % of solid density, \( \approx 2.3 \text{ g/cm}^3 \)) relevant to the radiative zone of the sun.

3.2.2.4 Buried layer thickness

We studied the effects of varying the buried layer thickness from 0.1 \( \mu \text{m} \) to 0.5 \( \mu \text{m} \) on plasma conditions, emission, and optical depth. We fixed the laser pulse (5 J, 5 ps, and 30 \( \mu \text{m} \) focal spot diameter), the tamper thickness (5 \( \mu \text{m} \) on either side), and the buried layer material (50 % Fe - 50 % Mg). Increasing the layer thickness is expected to increase the Fe and Mg emission because there is more material to be heated and emit x-rays. However, increasing the layer thickness will also increase the optical depth, which may affect the Fe and Mg emission depending on the plasma conditions reached.

Increasing the buried layer thickness has a small effect on the electron temperature in the layer: the peak electron temperature slightly decreases from 245 eV for the 0.1 \( \mu \text{m} \) layer to 235 eV for the 0.5 \( \mu \text{m} \) layer. The decrease in temperature is due to the assumption that the total deposited energy is fixed at a constant laser energy. Increasing the layer thickness increases the target mass slightly, reducing the energy per unit mass, and therefore the temperature. A stronger effect is seen on the average material density in the buried layer. Increasing the layer thickness decreases the initial expansion rate, which delays the minimum density before recompression but does not affect the densities reached in the model.
Increasing the layer thickness generally increases x-ray emission, as in Figure 3-7, except for the He-\(\alpha\) Mg line, which decreases. The decrease in Mg’s He-\(\alpha\) line emission for

![Graph](image)

Figure 3-7. Simulated emission at normal incidence from the target and the time of peak electron temperature for different layer thicknesses. A) Fe emission. B) Mg emission.

the 0.3 and 0.5 \(\mu\)m layers demonstrates the sensitivity of the emission to optical depth and temperature gradients in the layer. The optical depth of the layer is

\[
\tau = \kappa_\nu \rho \Delta l
\]  

(3-6)

where \(\kappa_\nu\) is the opacity, \(\rho\) is the plasma density, and \(\Delta l\) is the thickness of the layer. The layer’s optical depth increases with increasing layer thickness, as shown in Figure 3-8. The emission from the layer is characteristic of plasma conditions within approximately 1 optical depth into the layer. With increasing optical depths, the emission becomes characteristic of plasma conditions closer to the edge of the layer instead of the entire layer. For increasing layer thickness, the edges of the layer become cooler. The decrease in emission of Mg He-\(\alpha\) is due to the lower edge temperatures of the thicker layers.

While not as evident as in the Mg He-\(\alpha\) line, the optical depth of the thickest layer also affects the Fe emission. Comparing the 0.3 and 0.5 \(\mu\)m layers, the 0.78 - 1.0 keV Fe
emission \((1 \lesssim \tau \lesssim 5)\) increases less than the 1.0 keV - 1.25 keV Fe emission \((\tau \lesssim 1)\). The more optically thick lines do not increase as much because their emission is characteristic of a portion of the layer instead of the entire layer, as is the case for the optically thin lines. As the optical depths increase, the emission will saturate such that additional layer thickness will no longer increase emission. This saturation limit will be reached at smaller layer thicknesses for the optically thick lines and larger layer thicknesses for the optically thin lines. It is important to avoid this saturation effect in the frequency range of interest by using a thin layer. The sensitivity of the inferred opacity to optical depth effects and uncertainty in the measured emission is further discussed in Section 3.2.4.

In addition to affecting the emission, temperature gradients in the layer will affect the inferred opacity. Figure 3-9 shows the inferred opacities for different choices of the temperature in Eq. (2-5) for the 0.5 \(\mu m\) layer model. Also shown is the mass weighted average (“model”) opacity of the 0.5 \(\mu m\) layer. The optically thick lines from 0.78 - 1.0 keV are most affected by temperature gradients. The opacity inferred using the electron temperature at the layer’s center over-predicts the model opacity because it is colder than the temperature contributing most to the model opacity. The opacities inferred using
the average temperature and the temperature at the layer’s edge both under-predict the model opacity for the 0.8 keV line, indicating those temperatures are hotter than the temperature contributing most to that line. For 0.84 - 0.92 keV the opacity inferred using the average temperature matches the model opacity well. For 1 - 1.25 keV, where the optical depths are less than 1, the inferred opacity using all temperatures matched the model opacity well. As the buried layer thickness and optical depth increase, the inferred opacity becomes more sensitive to temperature gradients in the layer.

Overall, increasing the buried layer thickness, and thus the amount of Fe and Mg, slows initial expansion of the layer, increases optical depth, and increases emission if the target is optically thin. Increasing the buried layer thickness also increases the sensitivity of the inferred opacity to temperature gradients in the layer. Provided the target remains optically thin for the frequency range of interest, increasing the layer thickness can be used to increase emission without drastically changing plasma conditions.
3.2.2.5 Tamper thickness

We studied the effects of varying the tamper thickness on plasma conditions, x-ray emission, and inferred opacity by comparing different target configurations with a constant internal energy per unit mass. The maximum internal energy ($U_{\text{max}}$) and conversion efficiency ($\epsilon = 5\%$) are fixed for varying tamper thickness, and thus varying target mass ($M_{\text{target}}$). The laser energy ($E$) is given by

$$E = \frac{U_{\text{max}} M_{\text{target}}}{\epsilon}.$$  \hspace{1cm} (3-7)

We fixed the laser pulse length (5 ps), the focal spot size (30 $\mu$m diameter), and the buried layer (0.3 $\mu$m doped), while we varied both the tamper thicknesses from 1 $\mu$m to 5 $\mu$m.

The initial heating of the layer happens in approximately the same amount of time, but the peak electron temperature slightly decreases ($< 4\%$ of 240 eV) with decreasing tamper thicknesses. The layer cools more rapidly for thinner tampers. The initial expansion of the layer is similar for all tampers. The thicker tampers recompress the buried layer to larger densities for a longer duration than the thinner tampers. After recompression, the thinner targets expand earlier than the thicker targets and this contributes to the more rapid cooling of the layer. Therefore, thicker tampers will better limit the expansion of the layer. The plasma conditions at the time of peak electron temperature, which occurs before the layer recompresses, are similar for all tamper thicknesses. The simulated x-ray emission at the time of peak electron temperature generally decreases with decreasing tamper thickness because the CH emission component is reduced. Even though thinner tampers allow the layer to expand more, they also reduce the CH contribution to the measured emission, which results in emission spectra that are more representative of the layer.

In an experiment, the layer opacity will be inferred from the measured x-ray emission and plasma conditions using Eq. (2-5). The inferred opacity uses the average electron temperature and areal density in the layer. The opacity inference should be more accurate
for thinner tampers since the CH emission component is reduced. For three different tamper thicknesses, the opacity inferred from the simulated x-ray emission and the layer’s model opacity are shown in Figure 3-10. The inferred opacity over-predicts the model opacity for 5 μm and 3 μm tampers, while the inferred opacity generally matches the model opacity for 1 μm tampers. For the 1 μm tampers, the inferred opacity under-predicts the model opacity for 0.8 - 0.82 keV, which is an optical depth effect. At that frequency, the optical depth is greater than 1, so the simulated x-ray emission is more indicative of plasma conditions near the boundary of the layer. The average layer temperature, which is used to infer the opacity, is higher than the temperature near the surface, which contributes most to the x-ray emission for 0.8 - 0.82 keV. Therefore, the inferred opacity is larger than the model opacity. Overall, the inferred opacity approaches the model opacity as the tamper thicknesses are decreased because the CH emission component is reduced. We conclude that thicker tampers can be used to slow the cooling and expansion of the layer, but will also increase tamper emission, which limits the accuracy of the opacity inference.
3.2.3 Departure from LTE

It is desirable to produce plasmas with LTE conditions to best mimic the conditions inside stars and to compare measured opacities to the best theoretical opacities, which assume LTE. LTE is generally achieved by a combination of high density, low temperature, large optical depth and slow time variation. Since such conditions are not necessarily obtained in plasmas created by short pulse laser heating, our simulations have utilized more general non-LTE models. In this section, we examine how close to LTE our conditions are and to what extent departures from LTE introduce errors in an opacity measurement.

The non-LTE effects were studied using a 5 J model that reaches a peak electron temperature of approximately 290 eV and densities near 2 g/cm$^3$ (Figure 3-2 and Figure 3-3). Comparing a model using LTE opacities with the non-LTE model previously discussed in Section 3.2.2.1, we find small differences in electron temperature ($< 3\%$), material density ($< 1\%$), average ionization ($< 1\%$), electron density ($< 2\%$), and radiation temperature ($< 5\%$). While there are moderate differences between the two models in the opacities ($< 18\%$), emissivities ($< 30\%$), and multigroup radiation energy density ($< 17\%$), the largest differences occur at times when the target is heating (1 - 2.3 ps) and the buried layer’s electron temperature is rapidly changing (between 75 eV and 290 eV). For other times, differences are smaller (mostly $< 7\%$). For a time-resolved measurement, the non-LTE effects on opacities and emissivities are most important for times of strongest emission. The emitted intensity during the period of strongest emission, between 1.5 and 4 ps, is shown in Figure 3-11.

As suggested by Eq. (2-3), departure from LTE is demonstrated by how the ratio of emissivity ($\eta_\nu$) to opacity ($\kappa_\nu$) differs from the Planck function for the appropriate electron temperature. The departure is characterized by the function, $1 - \frac{\eta_\nu}{\kappa_\nu} \frac{1}{B_\nu(T)}$. Figure 3-12 shows the departure from LTE of the layer’s center with respect to time (for 1 - 4 ps) and frequency. Departure from LTE is small for 0 - 1 ps and 2.5 - 60 ps ($< 3\%$) and moderate
Figure 3-11. Simulated x-ray emission at normal incidence from the target with respect to frequency and time for 1 to 4 ps.

for 1 - 2.5 ps (< 17 %), indicating only a portion of the peak emission time (1.5 - 4 ps) is characterized by moderate departures from LTE. The time integrated emission is not sensitive to the departures from LTE near peak emission time because the time integrated emission is dominated by times between 4 and 20 ps, when the non-LTE effects are small. However, for 1.6 - 2.5 ps where the departure from LTE is largest, differences between simulated LTE and non-LTE time-resolved x-ray emission are moderate (< 12 %). The ability to distinguish this difference in experimental data depends on the experimental uncertainty in the x-ray emission. For uncertainties larger than 12 %, non-LTE effects will not cause an experimentally distinguishable difference in x-ray emission for designs with peak temperatures near or less than 300 eV.

In order to establish the non-LTE effects on inferred opacity separate from temperature gradient, optical depth, and tamper thickness effects, the specific intensity was calculated for a single zone in the layer using Eq. (2-2) with constant properties. The calculated zone
specific intensity was then used in Eq. (2-5) to determine an inferred opacity. The opacity inference equation assumes LTE conditions, so the difference between the inferred opacity and the model’s zone opacity quantifies the non-LTE effects on the inferred opacity.

For the 5 J model, the center zone was used because it represents an upper bound of the departure from LTE. The relative differences in the inferred opacity and the model opacity with respect to time and frequency are very similar to the departures from LTE in Figure 3-12. The largest differences (7 - 17 %) occur from 1 - 2.5 ps. At the time of peak electron temperature (2.1 ps, 287 eV), the largest departure from LTE is approximately 14 % which corresponds to an approximately 12 % error in the inferred opacity. Figure 3-13 shows the inferred opacity and model opacity for the center zone at the time of peak electron temperature. In general, the inferred opacity under-predicts the model opacity.
Overall, the non-LTE effects on inferred opacity are similar in relative magnitude to the departures from LTE.

A similar comparison using an 8 J model suggests that, for temperatures 300 to 400 eV, non-LTE effects have a small impact on plasma conditions but moderate impacts on emissivity, opacity, and time-resolved x-ray emission. A similar comparison for a 19 J model, reaching temperatures near 1 keV, non-LTE effects significantly alter the plasma conditions, time-resolved, and time integrated x-ray emission. For plasma conditions representative of the upper radiative zone of the sun (200 - 400 eV, $\rho = 0.8 - 7.88$ g/cm$^3$), conditions are near enough to LTE. For higher temperatures, consideration of non-LTE effects should be included in analysis and design.

### 3.2.4 Propagation of Uncertainty in Opacity Inference

In this section, we examine how uncertainties in the measured quantities affect the accuracy of the inferred opacity. This analysis assumes constant relative uncertainties
for each spectrally resolved intensity measurement and that there are no correlations in the uncertainties between the intensity measurements, inferred electron temperature, and areal density. For experimental uncertainties in the intensity ($\sigma_{I_e}$), the inferred electron temperature ($\sigma_T$), and the areal density ($\sigma_{\rho \Delta l}$), the propagated uncertainty in the inferred opacity is

$$\sigma^2_{\kappa_\nu} = \left( \frac{\partial \kappa_\nu}{\partial I_\nu} \right)^2 \sigma^2_{I_\nu} + \left( \frac{\partial \kappa_\nu}{\partial B_\nu} \right)^2 \left( \frac{\partial B_\nu}{\partial T} \right)^2 \sigma^2_T + \left( \frac{\partial \kappa_\nu}{\partial \rho \Delta l} \right)^2 \sigma^2_{\rho \Delta l}. \quad (3-8)$$

Including all the partial derivatives, using Eq. (2-4) for intensity, and Eq. (3-6) for optical depth, Eq. (3-8) becomes

$$\left( \sigma^\text{rel}_{\kappa_\nu} \right)^2 = \left( \frac{1 - e^{-\tau}}{\tau^2 e^{-2\tau}} \right) \left( \sigma^\text{rel}_{I_\nu} \right)^2 + \frac{1}{B^2_\nu} \left( \frac{2 \hbar^2 \nu^3}{c^2 (k_B T)^2} \left( \exp \left( \frac{h \nu}{k_B T} \right) - 1 \right)^2 \left( \sigma^\text{rel}_T \right)^2 (k_B T)^2 \right) + \left( \sigma^\text{rel}_{\rho \Delta l} \right)^2. \quad (3-9)$$

We define $\sigma^\text{rel}_j$ as the relative uncertainty in parameter $j$ such that $\sigma_j = j \sigma^\text{rel}_j$.

The effect of increasing optical depth on the propagated uncertainty is demonstrated in Figure 3-14, which shows the optical depth and relative standard deviation in the inferred opacity assuming $\sigma^\text{rel}_{I_\nu} = 10\%$, $\sigma^\text{rel}_T = 5\%$, and $\sigma^\text{rel}_{\rho \Delta l} = 10\%$ for four different layer thicknesses. For all of these models, an internal energy source was selected such that the plasma conditions were consistent with the radiative zone of the sun (near 230 eV, 2.1 g/cm$^3$). Overall, increasing the buried layer thickness increases the relative standard deviation in the inferred opacity. The effect is most drastic for 0.76 - 0.98 keV, where the optical depth is highest. The propagated uncertainty in the inferred opacity will be larger at frequencies for which optical depths are high because, as in Eq. (3-9), the experimental uncertainties in the intensity ($\sigma^\text{rel}_{I_\nu}$) and the temperature ($\sigma^\text{rel}_T$) are multiplied by a coefficient that exponentially increases with optical depth. For frequencies where the optical depth is low (0.98 - 1.25 keV), increasing the buried layer thickness increases the uncertainty less than for frequencies for which the optical depth is high (0.76 - 0.98 keV).
Figure 3-14. Optical depth and propagated experimental uncertainties at the time of peak temperature for four different buried layer thicknesses. Models assume laser pulses with approximately 3 J of energy, a 5 ps pulse length, and a 30 μm diameter focal spot incident on a target consisting of 3 μm tampers of either side of a doped layer. A) Optical depth. B) Propagated experimental uncertainties.

Increasing the buried layer thickness will increase optical depths, which will increase the propagated uncertainty in the inferred opacity.

For a given set of plasma conditions, a set of different buried layer thickness targets could be designed to maximize the x-ray emission of a specific set of frequencies, while minimizing the optical depth effects on propagated experimental uncertainties. Ideally, it would be best to have more buried layer material and thus higher x-ray emission over the entire iron L-shell emission frequency range, but optical depth effects limit the accuracy of the inferred opacity. Alternatively, using a thin buried layer might result in x-ray emission barely above the continuum for higher frequencies. In addition to the relative uncertainty in measured intensity, we expect an absolute uncertainty, which will produce inaccuracy at low values of intensity. Focusing on a subset of the iron L-shell could allow one to select a thinner layer for an optically thick frequency range and a thicker layer for an optically thin frequency range. For example, given electron temperature of near 230
eV and density near 2.1 g/cm$^3$, a 0.3 μm layer might be sufficient for 0.98 - 1.25 keV, where the maximum propagated uncertainty is approximately 36%. However, for 0.76 - 0.98 keV, a 0.1 μm layer would be needed to obtain a maximum propagated uncertainty below 40%. The specifics of a set of such targets would depend on the desired plasma conditions, ionization, and emission frequency range.

Recent investigation indicates that spectroscopic measurements can differ by up to 30% in electron density and 4% in electron temperature, depending on the choice of the spectral model. Such an uncertainty in the electron temperature can be incorporated in our analysis by increasing $\sigma_T^{\text{rel}}$, which will increase the propagated uncertainty in the opacity inference. An uncertainty in the electron density is important when experimental opacities are compared with theoretical opacities. In order to isolate the effect of such an uncertainty on an emission-based opacity experiment, we compared the opacity of Fe-Mg mixtures with electron densities of $4 \times 10^{23}$ and $5 \times 10^{23}$ cm$^{-3}$ at a fixed electron temperature of 230 eV. Over the 0.7 - 1.25 keV spectral range, the opacities differed by up to ±45% with an average difference of ±20%. Therefore, assuming a 25% uncertainty in the electron density may limit the comparison of measured opacities with theoretical opacities to ±20% on average. In order to better constrain comparisons between experimental and theoretical opacities, improvements must be made to line shape theories. More thorough investigation into how the uncertainties in plasma diagnostic techniques relate to the uncertainties in the measured quantities should be completed for each experiment.

3.2.5 Example Design

As an example that reaches plasma conditions consistent with the upper radiative zone of the sun (230 eV, 1.8 g/cm$^3$ for 1.2 ps), a 0.7 J, 5 ps laser pulse with a 30 μm diameter focal spot incident on a target consisting of 0.5 μm CH tampers on either side of a 0.05 μm doped buried layer minimizes tamper emission and optical depth effects. The period of relatively constant temperature and density can be increased by using a longer
laser pulse, a thicker buried layer, or some combination of both. As discussed previously, increasing the laser pulse length spreads out the energy deposition, resulting in a smaller and delayed peak electron temperature, as well as delayed initial expansion of the layer. Increasing the buried layer thickness also delays the initial expansion of the layer, but less so than increasing the laser pulse length. Combining these two effects allows for aligning periods of relatively constant temperature and density. From Figure 3-14, a target with a 0.05 \( \mu \text{m} \) doped layer is optically thin and has reasonable propagated uncertainties (24 - 36 \%\) for the entire iron L-shell frequency range (0.7 - 1.25 keV). However, the targets in Figure 3-14 have 3 \( \mu \text{m} \) tampers on each side of the layer. The example design discussed here has thinner tampers (0.5 \( \mu \text{m} \)) to reduce the CH emission and thus increase the accuracy of the inferred opacity. In general, the thinner the layer, the thinner the tampers need to be in order to reduce the effect of CH emission on the accuracy of the inferred opacity.

As previously discussed, thinner tampers result in lower layer densities since there is less surrounding material to inhibit the expansion of the layer. Figure 3-15 shows the contribution of the tampers to the x-ray emission and the inferred opacity. The difference between the model opacity and the inferred opacity is mostly from the CH contribution to the continuum x-ray emission, shown as a red dash in Figure 3-15A. The average relative difference between the inferred opacity and the model opacity over the iron emission (0.77 - 1.25 keV) is 25 \%\) for 0.5 \( \mu \text{m} \) tampers and 210 \%\) for 3 \( \mu \text{m} \) tampers. The relative error is highest in the opacity valleys, where the opacity is low (\(< 5 \times 10^3 \text{ cm}^2/\text{g} \) in Figure 3-15B), which weights the average relative error. The relative error is particularly large around 1.1 keV where there is an opacity valley and the x-ray emission is close to the continuum emission. The relative error is lowest at the opacity peaks (\(> 1 \times 10^4 \text{ cm}^2/\text{g} \) in Figure 3-15B). The moderate relative errors between the inferred and model opacities could be mitigated in an experiment by subtracting out the tamper emission before inferring opacity. This example design is a thin buried layer, which requires thin...
Figure 3-15. Comparison of the x-ray emission and opacity for an example design reaching conditions consistent with the upper radiative zone of the sun. A) The x-ray emission at normal incidence from the target and tampers at the time of peak electron temperature for an example design. B) The opacity inferred from the emission for the entire target and the model opacity.

tampers to mitigate CH emission effects on the accuracy of the inferred opacity. However, as discussed in Section 3.2.4, for the 0.98 - 1.25 keV frequency range, where the opacity is low, a thicker buried layer could be used to ensure adequate signal and reasonable propagated uncertainties. In the thicker buried layer case, thicker tampers could be used and still reduce the effect of CH emission on the accuracy of the inferred opacity. Overall, using an emission-based measurement to infer opacity is sensitive to optical depth effects, tamper emission, and experimental uncertainties, all of which must be considered when designing experiments.
In this chapter, we discuss an automated design process for iron buried layer targets that allow for single and multiple parameters variations. While, in Chapter 3, we presented an example design that mitigated effects seen in a series of single parameter studies, the example design was not selected using a formal optimization process. As such, we developed an automated process which includes optimizing design parameters to meet specific design cases. An automated process enables us to explore a broader parameter space than can be explored in a series of single parameter studies. Optimization in a broad parameter space enables us to determine globally optimized designs for specific design cases that address a variety of goals. We defined a cost function to solve an unconstrained optimization problem for each specific design case. We used the process to find optimized designs of buried iron sulfide (FeS$_2$) targets. The choice of iron sulfide is motivated by experiments at Atomic Weapons Establishment’s Orion Laser Facility in June 2017, which were originally proposed to use 0.3 μm iron sulfide sandwiched between two 3 μm layers of parylene-N. The experiments were planned to use a 0.53 μm wavelength laser beam with a pulse length of 0.5 ps, focused to 20 - 50 μm diameters, and laser energies up to 100 J. We explored two sets of design cases using the automated process. The first set focused on the range of plasma conditions relevant to the radiative zone of the sun: $T = 200$ eV, $T = 300$ eV, and $T = 400$ eV, each with $\rho > 1/10$ of solid density. The second set focused on reaching higher plasma temperatures at a fixed density and will be valuable for investigating how iron opacity scales with temperature: $T = 500$ eV, $T = 750$ eV, and $T = 1000$ eV, each with $\rho = 4.2$ g/cm$^3$. In this chapter, we discuss the automated design process and its application to these six design cases.

### 4.1 Automated Design Process

We developed an automated design process using the LLNL Uncertainty Quantification Pipeline (UQP) to manage and analyze ensembles of HYDRA simulations. Figure
Figure 4-1. Flow chart of the automated design process we developed.

4.1.1 Optimization Formulation

An ideal design would be one in which the simulated inferred opacity agrees with the opacity supplied to HYDRA and meets design constraints at peak temperature. We defined a general design optimization that minimizes the average relative difference between inferred and model opacity, while satisfying a number of constraints. The average relative difference is represented by

$$\sigma_{\kappa}^{\text{rel}} = \frac{\text{abs}(\kappa - \kappa^{\text{model}})}{\kappa^{\text{model}}} \quad (4-1)$$

and the design constraints are summarized in Table 4-1. The design constraint forms are normalized by the relevant design constraint value, indicated with “*”, so that
the equations are unitless. In each constraint form, the variable indicated as “peak” refers to the appropriate single value metric, at peak temperature, to compare with the design constraint value. Our constrained optimization problem can be converted to an unconstrained problem through the use of a penalty function.\textsuperscript{133,134} The cost function is

\[ \beta \sigma_{\kappa}^{\text{rel}} + \sum_{i=1}^{m} \phi(\alpha_i, g_i) \]  

(4-2)

where \( \beta \) is a coefficient, \( \sigma_{\kappa}^{\text{rel}} \) is defined in Eq. (4-1) and \( \phi(\alpha_i, g_i) \) are penalty functions with parameters \( \{\alpha_i\} \) and constraint functions \( \{g_i\} \). We used the following penalty function form in this study:

\[ \phi(\alpha_i, g_i) = \begin{cases} 
0, & g_i < 0 \\
\alpha_i g_i^2, & g_i \geq 0 
\end{cases} \]  

(4-3)

where the constraint functions \( g_i \) are the left hand side of the constraint forms in Table 4-1. Our selected penalty function form penalizes the cost function of a design that violates at least one design constraint. We set the constraint functions, penalty parameters, and relative difference coefficient for each design case. We calculate the cost function (Eq. (4-2)) for each ensemble simulation then use quantitative optimization techniques (Section 4.1.3.2) to find the design parameters that yield the global minimum cost function.

\subsection*{4.1.2 HYDRA Simulations}

We used HYDRA\textsuperscript{88} radiation hydrodynamics code for the simulations included in each ensemble. The assumptions are the same as in Section 3.1.1 and Section 3.1.2 with a few exceptions, which are outlined here. All simulations discussed in this chapter used DCA\textsuperscript{91,92} non-LTE atomic models for the opacities and equations of state for electron temperatures larger than 300 eV. The switch to non-LTE physics was chosen because, as discussed in Section 3.2.3, non-LTE effects have moderate impacts on emissivity, opacity, and time-resolved x-ray emission at temperatures larger than 300 eV. At temperatures less than 300 eV, we assumed DCA LTE opacities, a Thomas-Fermi based\textsuperscript{94,95} equation of
Table 4-1. Design constraints at the time of peak temperature included in the general optimization problem

<table>
<thead>
<tr>
<th>Constraint no.</th>
<th>Design constraint description</th>
<th>Constraint form</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>peak $T^{\text{peak}}$ is larger than -5% of goal $T^*$</td>
<td>$0.95 - \frac{T^{\text{peak}}}{T^*} \leq 0$</td>
</tr>
<tr>
<td>2</td>
<td>peak $T^{\text{peak}}$ is less than +5% of goal $T^*$</td>
<td>$\frac{T^{\text{peak}}}{T^*} - 1.05 \leq 0$</td>
</tr>
<tr>
<td>3</td>
<td>$\rho^{\text{peak}}$ is larger than minimum design $\rho$</td>
<td>$1 - \frac{\rho^{\text{peak}}}{\rho^*} \leq 0$</td>
</tr>
<tr>
<td>4</td>
<td>period of constant $T$ and $\rho$ ($\Delta t^{\text{peak}}$) is larger than minimum design period ($\Delta t^*$)</td>
<td>$1 - \frac{\Delta t^{\text{peak}}}{\Delta t^*} \leq 0$</td>
</tr>
<tr>
<td>5</td>
<td>variation in $T$ across buried layer ($\Delta T^{\text{peak}}$) is less than maximum design variation ($\Delta T^*$)</td>
<td>$\Delta T^{\text{peak}} - \Delta T^* \leq 0$</td>
</tr>
<tr>
<td>6</td>
<td>variation in $\rho$ across buried layer ($\Delta \rho^{\text{peak}}$) is less than maximum design variation ($\Delta \rho^*$)</td>
<td>$\Delta \rho^{\text{peak}} - \Delta \rho^* \leq 0$</td>
</tr>
<tr>
<td>7</td>
<td>optical depth ($\tau^{\text{peak}}$) is larger than design minimum ($\tau_{\text{min}}^*$)</td>
<td>$1 - \frac{\tau^{\text{peak}}}{\tau_{\text{min}}^*} \leq 0$</td>
</tr>
<tr>
<td>8</td>
<td>optical depth ($\tau^{\text{peak}}$) is less than design maximum ($\tau_{\text{max}}^*$)</td>
<td>$\frac{\tau^{\text{peak}}}{\tau_{\text{max}}^*} - 1 \leq 0$</td>
</tr>
<tr>
<td>9</td>
<td>x-ray emission ($I^{\text{peak}}_v$) larger than minimum signal ($I_v^*$) required for spectrometer</td>
<td>$1 - \frac{I^{\text{peak}}_v}{I_v^*} \leq 0$</td>
</tr>
<tr>
<td>10</td>
<td>dopant H-α to He-α line ratio ($R^{\text{peak}}<em>{\alpha}$) is larger than minimum design ratio ($&gt; R</em>{\alpha}^{*,\text{min}}$)</td>
<td>$1 - \frac{R^{\text{peak}}<em>{\alpha}}{R</em>{\alpha}^{*,\text{min}}} \leq 0$</td>
</tr>
<tr>
<td>11</td>
<td>dopant H-α to He-α line ratio ($R^{\text{peak}}<em>{\alpha}$) is less than maximum design ratio ($&lt; R</em>{\alpha}^{*,\text{max}}$)</td>
<td>$\frac{R^{\text{peak}}<em>{\alpha}}{R</em>{\alpha}^{*,\text{max}}} - 1 \leq 0$</td>
</tr>
<tr>
<td>12</td>
<td>dopant H-β to He-β line ratio ($R^{\text{peak}}<em>{\beta}$) is larger than minimum design ratio ($&gt; R</em>{\beta}^{*,\text{min}}$)</td>
<td>$1 - \frac{R^{\text{peak}}<em>{\beta}}{R</em>{\beta}^{*,\text{min}}} \leq 0$</td>
</tr>
<tr>
<td>13</td>
<td>dopant H-β to He-β line ratio ($R^{\text{peak}}<em>{\beta}$) is less than maximum design ratio ($&lt; R</em>{\beta}^{*,\text{max}}$)</td>
<td>$\frac{R^{\text{peak}}<em>{\beta}}{R</em>{\beta}^{*,\text{max}}} - 1 \leq 0$</td>
</tr>
<tr>
<td>14</td>
<td>dopant H-α line emission signal ($S^{\text{peak}}<em>{H-\alpha}$) is larger than minimum signal required for spectrometer ($&gt; S</em>{H-\alpha}^{*,\text{min}}$)</td>
<td>$1 - \frac{S^{\text{peak}}<em>{H-\alpha}}{S</em>{H-\alpha}^{*,\text{min}}} \leq 0$</td>
</tr>
<tr>
<td>15</td>
<td>dopant He-α line emission signal ($S^{\text{peak}}<em>{\text{He-\alpha}}$) is larger than minimum signal required for spectrometer ($&gt; S</em>{\text{He-\alpha}}^{*,\text{min}}$)</td>
<td>$1 - \frac{S^{\text{peak}}<em>{\text{He-\alpha}}}{S</em>{\text{He-\alpha}}^{*,\text{min}}} \leq 0$</td>
</tr>
<tr>
<td>16</td>
<td>dopant H-β line emission signal ($S^{\text{peak}}<em>{H-\beta}$) is larger than minimum signal required for spectrometer ($&gt; S</em>{H-\beta}^{*,\text{min}}$)</td>
<td>$1 - \frac{S^{\text{peak}}<em>{H-\beta}}{S</em>{H-\beta}^{*,\text{min}}} \leq 0$</td>
</tr>
<tr>
<td>17</td>
<td>dopant He-β line emission signal ($S^{\text{peak}}<em>{\text{He-\beta}}$) is larger than minimum signal required for spectrometer ($&gt; S</em>{\text{He-\beta}}^{*,\text{min}}$)</td>
<td>$1 - \frac{S^{\text{peak}}<em>{\text{He-\beta}}}{S</em>{\text{He-\beta}}^{*,\text{min}}} \leq 0$</td>
</tr>
</tbody>
</table>
state (EOS) for tamper materials and an in-line quotidian equation of state (QEOS)\textsuperscript{95} for all buried layer materials. For the FeS\textsubscript{2} mixed buried layer, we used a mixture with 33.3 % of and 66.7 % of S by atom with an initial density of 4.8 g/cm\textsuperscript{3}. We used the energy source discussed in Section 3.1.2, with an assumed conversion efficiency ($\epsilon$) of 3 %, in all simulations presented in this chapter. We simulated a previous Orion Laser Facility short pulse heated buried layer experiment\textsuperscript{78} using our energy source with a 3 % conversion efficiency and, as discussed in Section 3.1.3, the results showed good agreement with peak plasma conditions and x-ray pulse durations. With the exception of the specific details described here, all other assumptions discussed in Section 3.1.1 and Section 3.1.2 are the same for simulations in this chapter.

4.1.3 Process Flow and Integration with UQP

4.1.3.1 UQP ensemble management

As outlined in Figure 4-1, we used the UQP to manage ensembles of HYDRA simulations. We created a set of configuration files that guide the management of the ensembles. The UQP samples design parameters, based on a sampling strategy specified in the configuration files, then launches an ensemble of simulations using those sampled parameters. The UQP manipulates general HYDRA input files to include the appropriate set of sampled parameter values for each simulation. We created general HYDRA input files that define the energy source, spatial grid, time step control, and results output structure based on the sampled parameters. The UQP schedules and monitors the simulations, including restarting simulations that failed to finish within the allocated time. Once a simulation is completed, the UQP executes a post-simulation analysis process. In the post-simulation analysis process, we included a Yorick analysis script that saves HYDRA data to binary files and saves single value metrics, which will later be used to create a cost function for optimization, to text files. Once all of the simulations in the ensemble are completed, the UQP compiles the ensemble results into a set of text files. We created the UQP configuration files, the general HYDRA input files, and the Yorick
analysis script. The UQP automatically managed the sampling of design parameters, execution and analysis of ensemble simulations, and summarizing of ensemble results.

4.1.3.2 User-controlled ensemble analysis

As indicated in Figure 4-1, we analyzed the ensemble separate from the UQP ensemble management. We created a Python script to read the ensemble data file(s) and calculate the cost function given a set of design constraints and the ensemble results. Our Python script adds the design constraints, cost function coefficients, and calculated cost function to the ensemble data files. We used the UQP to create a surrogate of the cost function using Gaussian process regression (GPR).\(^{135}\) In Gaussian process regression the prediction (estimated cost function values) interpolates the ensemble observations (true cost function values) using a regression function and a Gaussian correlation model. By using GPR, we assume that the correlation is strong between nearby observations and weak between far apart observations. We tested the surrogate by comparing the predicted cost function values with the true cost function values for a subset of ensemble observations held separate from the observations used to train the surrogate. The UQP saves the resulting surrogate model as a Python shelve file.\(^{136}\) We created a surrogate to interpolate cost function on areas of the parameter space in between ensemble simulations which allows us optimize across the entire parameter space.

We created another Python script to find the optimal design parameters which minimize the surrogate cost function. We used two existing Python functions to find local minima of the surrogate cost function: basin hopping\(^ {137}\) and brute force.\(^ {138}\) Basin hopping evaluates the cost function surrogate for a subset of the parameter space around an initial guess. The smallest surrogate value becomes the new guess. The algorithm evaluates the surrogate for a randomly determined subset of the parameter space around the new guess. If there is another guess with a smaller surrogate value, it is accepted as the new guess and the process repeats. The process ends when the same guess is found for 50 iterations. We repeated basing hopping for at least 100 random initial guesses to find local minima.
and compared the local minima to find the global minimum. As a secondary approach, we used the brute force algorithm. Brute force evaluates the cost function surrogate on grid within the parameter space that has more points than the number of simulations in the ensemble. The point in the grid with the minimum cost function surrogate value is identified as the global minimum. The brute force method is tractable for the small parameter spaces explored in this study. However, as the number of parameters increase, the brute force method will become computationally expensive and may not be tractable.

Once an optimized design is found, we evaluate the quality of that design by executing a HYDRA simulation with the optimized design parameters. We calculate the cost function from the simulation results, then examine the cost function and the constraints. We accept the design if the design meets the constraints sufficiently well. If the design does not meet constraints well, we evaluate why the design failed to meet constraints. If the cost function was too sensitive, or not sensitive enough, to a specific design constraint, we adjust the cost function coefficients and repeat the ensemble analysis. For example, if the optimized design reaches a temperature 50% larger than the goal temperature, the coefficient for the temperature constraint is increased to increase the sensitivity of the cost function to that constraint. If the cost function is adequate, but consideration of the entire ensemble parameter space indicates that the global minimum was not reached, we adjust the parameter space and sampling then repeat the entire design process.

4.2 Results and Analysis

We used the automated design process to conduct single and multiple design parameter studies of FeS$_2$ buried layer targets. Our energy deposition source, described in Section 3.1.2, deposits a fraction of the laser energy (conversion efficiency) into the entire target assuming a Gaussian time dependance. In addition, the peak heating power is proportional to the laser energy per unit mass. For the parameter studies in this chapter, only laser energy and laser pulse length are considered variable laser
parameters because, for a fixed laser pulse length, a given energy source is consistent with different combinations of conversion efficiency, laser energy, and laser focal spot size. The conversion efficiency is assumed to be 3 %, as discussed in Section 4.1.2, and the laser focal spot size is fixed at a 50 μm diameter. The variable target parameters are buried layer and tamper thicknesses. For both single and multiple parameter studies, we considered two sets of design cases: a set focused on conditions relevant to the radiative zone of the sun and a set focused on pushing to higher temperatures. For all design cases, we fixed a subset of the constraint values which are summarized, along with their motivation, in Table 4-2.

4.2.1 Single Parameter Ensembles

We generated ensembles varying laser energy \((E = 0.1 - 100 \text{ J})\), laser pulse length \((t_{\text{FWHM}} = 10 \text{ fs} - 15 \text{ ps})\), buried layer thickness \((\Delta l_{\text{BL}} = 10 \text{ nm} - 1 \text{ μm})\), and tamper thicknesses \((\Delta l_{\text{CH}} = 10 \text{ nm} - 10 \text{ μm})\) individually using the ensemble management step of the automated design process. For each ensemble, the UQP sampled 20 samples uniformly between the upper and lower bounds of the variable parameter. When not being varied, the fixed values of laser energy, laser pulse length, buried layer thickness, and tamper thicknesses were 14 J, 0.5 ps, 0.3 μm of FeS2, and 3 μm of parylene-N, respectively. We analyzed the ensemble for two sets of design cases and the design case-specific constraint values are described in Table 4-3. For the design set pushing to higher temperatures at a fixed design density, we changed the minimum density constraint (no. 3) to two inequalities in order to constrain the density within ± 10 % of the design density goal:

Constraint no. 3:

\[
0.9 - \frac{\rho_{\text{peak}}}{\rho^*} \leq 0
\]

\[
\frac{\rho_{\text{peak}}}{\rho^*} - 1.1 \leq 0
\]

For each design case, we used visual optimization, instead of quantitative optimization, by plotting the cost function value versus variable parameter. As an example, Figure 4-2,
<table>
<thead>
<tr>
<th>Constraint no.</th>
<th>Design constraint value</th>
<th>Motivation for value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>$\Delta t^* = 2.0$ ps</td>
<td>consistent with temporal resolution of existing x-ray streak spectrometers$^{75,79,139}$</td>
</tr>
<tr>
<td>5</td>
<td>$\Delta T^* = 5%$</td>
<td>less than the uncertainty in inferred temperature in previous short pulse heated experiments$^{76,78,79,81,82}$</td>
</tr>
<tr>
<td>6</td>
<td>$\Delta \rho^* = 10%$</td>
<td>less than the uncertainty in inferred density in previous short pulse heated experiments$^{76,78,79,81,82}$</td>
</tr>
<tr>
<td>7</td>
<td>$\tau_{\text{min}}^* = 0.03$</td>
<td>selected to avoid regions of low opacity that might cause emission to be too close to the continuum emission</td>
</tr>
<tr>
<td>8</td>
<td>$\tau_{\text{max}}^* = 0.64$</td>
<td>selected to limit the effect of optical depth on the propagation of experimental uncertainties by limiting the coefficient of the first term in Eq. (3-9)</td>
</tr>
<tr>
<td>9</td>
<td>$I^*_\nu = 10^{13}$ W/cm$^2$/str/keV</td>
<td>selected to capture a minimum intensity that could be measured on existing spectrometers$^{78,79}$</td>
</tr>
<tr>
<td>10</td>
<td>$R^*_{\alpha,\text{min}} = 0.1$</td>
<td>selected to give a wide range of potential ratios since parameter studies will explore a large temperature regime</td>
</tr>
<tr>
<td>11</td>
<td>$R^*_{\alpha,\text{max}} = 10.0$</td>
<td>same as constraint 10</td>
</tr>
<tr>
<td>12</td>
<td>$R^*_{\beta,\text{min}} = 0.1$</td>
<td>same as constraint 10</td>
</tr>
<tr>
<td>13</td>
<td>$R^*_{\beta,\text{max}} = 10.0$</td>
<td>same as constraint 10</td>
</tr>
<tr>
<td>14</td>
<td>$S^*_{\text{H-}\alpha,\text{min}} = 10^{12}$ W/cm$^2$/str</td>
<td>selected to match models for which the dopant line begins to have significant signal</td>
</tr>
<tr>
<td>15</td>
<td>$S^*_{\text{He-}\alpha,\text{min}} = 7 \times 10^{11}$ W/cm$^2$/str</td>
<td>same as constraint 14</td>
</tr>
<tr>
<td>16</td>
<td>$S^*_{\text{H-}\beta,\text{min}} = 6 \times 10^{11}$ W/cm$^2$/str</td>
<td>same as constraint 14</td>
</tr>
<tr>
<td>17</td>
<td>$S^*_{\text{He-}\beta,\text{min}} = 5 \times 10^{11}$ W/cm$^2$/str</td>
<td>same as constraint 14</td>
</tr>
</tbody>
</table>
Table 4-3. Design constraint values for design cases considered in this chapter

<table>
<thead>
<tr>
<th>Constraint no.</th>
<th>Design constraint values for the radiative zone design set</th>
<th>Design constraint values for the higher temperature design set</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 &amp; 2 ($T^*$ in eV)</td>
<td>200 300 400 500 750 1000</td>
<td></td>
</tr>
<tr>
<td>3 ($\rho^*$ in g/cm$^3$)</td>
<td>0.48 0.48 0.48 4.2 4.2 4.2</td>
<td></td>
</tr>
</tbody>
</table>

shows how the cost function varies for each variable parameter for the 300 eV design case. For all single parameter ensembles, the 300 eV design case cost function initially decreases, but then increases with increasing design parameter. Therefore the optimal design parameter can be visually estimated from the minimum of the cost function. From the scales in Figure 4-2, we conclude the cost function is most sensitive to laser energy and target dimensions (buried layer and tamper thickness) and is least sensitive to laser pulse length. The sensitivity of the cost function to laser energy and target dimensions is because the cost function is most sensitive to the goal temperature and optical depth constraints. The temperatures reached are dominantly controlled by laser energy while the optical depth is controlled by the buried layer thickness. The tamper thickness also effects the temperatures reached because the energy source in the model is related to a fraction of the laser energy per unit mass. The general behavior described above was also seen in the visual analysis of the other design cases.

The optimized parameters for each design case are listed in Table 4-4. For the variable laser energy ensemble, the temperatures increases (80 eV to 2.1 keV) with increasing laser energy (0.1 to 100 J). The optimal laser energy increased with increasing goal temperature because higher laser energies reach higher temperatures. The variable laser pulse length ensemble reached temperatures ranging from 360 eV to 200 eV, for the pulse lengths of 10 fs to 15 ps, respectively. The variable buried layer thickness ensemble reached temperatures ranging from 300 eV to 250 eV for thicknesses of 10 nm to 1 \( \mu \)m, respectively. The laser pulse length and buried layer thickness ensembles are not well suited for finding optimized designs for the 400 - 1000 eV design cases. The variable tamper thickness ensemble reached temperatures between 1.4 keV and 180 eV, for tamper
thicknesses of 10 nm to 10 μm. The increase in temperature with decreasing tamper thickness is because the energy source assumes a peak power proportional to a fraction of the laser energy per unit mass. Overall, these single parameter ensembles demonstrate the sensitivity of the cost function to the temperatures reached.

Table 4-4. Optimized designs for the single parameter ensembles

<table>
<thead>
<tr>
<th>Design Parameter</th>
<th>200 eV design</th>
<th>300 eV design</th>
<th>400 eV design</th>
<th>500 eV design</th>
<th>750 eV design</th>
<th>1000 eV design</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (J)</td>
<td>10.0</td>
<td>16.0</td>
<td>21.0</td>
<td>26.0</td>
<td>40.0</td>
<td>50.0</td>
</tr>
<tr>
<td>$t_{FWHM}$ (ps)</td>
<td>1.2</td>
<td>0.7</td>
<td>0.7</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td>$\Delta l_{BL}$ (μm)</td>
<td>0.5</td>
<td>0.4</td>
<td>0.35</td>
<td>0.35</td>
<td>0.35</td>
<td>0.35</td>
</tr>
<tr>
<td>$\Delta l_{CH}$ (μm)</td>
<td>3.8</td>
<td>2.6</td>
<td>1.8</td>
<td>1.0</td>
<td>0.5</td>
<td>0.5</td>
</tr>
</tbody>
</table>
The laser energy ensemble is most applicable to targets proposed for an Orion campaign in June 2017. The optimized design for the laser energy ensemble gives an idea of what laser energies are needed to reach different electron temperatures (assuming 3% conversion efficiency and 50 μm diameter focal spot size). The application of the other single parameter ensembles to the June campaign is limited. Both the laser pulse length and buried layer thickness ensembles are only applicable to reaching temperatures under 400 eV. The temperature increases with decreasing tamper thickness because the energy source assumes a peak deposition proportional to the average energy per unit mass. Overall, the set of single design parameter ensembles demonstrates the impact of the interplay of design parameters on the temperature and the cost function. We consider multiple design parameter ensembles in order to further examine the effect of the interplay between parameters on the cost function and optimal designs.

4.2.2 Two Parameter Ensemble

We created an ensemble varying laser energy from 0.1 to 100 J and buried layer thickness from 10 nm to 1 μm of FeS₂ using the automated design process. We fixed the laser pulse length (0.5 ps) and the tamper thicknesses (3 μm of parylene-N). The UQP managed an ensemble of 768 simulations for parameters selected by Latin Hypercube sampling. Latin Hypercube sampling subdivides the range of each parameter into a specified number (N = 768 in this case) of equally probable intervals, then randomly selects a value within each interval. The selected values of each parameter are combined randomly such that the resulting set of sample values has only one sample in each combination of design parameter intervals. Latin Hypercube sampling provides a pseudo-random sampling of multidimensional spaces. We analyzed the ensemble for the two sets of design cases described in Table 4-3.

We iterated values of the relative difference coefficient ($\beta$) and penalty parameters ($\{\alpha_i\}$) because the initial optimized designs had peak temperatures much larger (> 50 %) than the goal temperature. We increased the penalty parameters for the temperature
constraints (no. 1 & 2) to increase the cost function’s sensitivity to the goal temperature. After iteration, we selected a standard set of coefficients and penalty parameters because the optimized designs became less sensitive to the changes and met most design constraints. We selected the following penalty parameters for the radiative zone design set: 100 for the temperature constraints (no. 1 & 2) and 2 for all other constraints (no. 3 - 17). We selected the same penalty parameters for the higher temperature design set, except we selected 100 for the density constraint (no. 3). For both design sets, we selected 25 for the relative difference coefficient.

4.2.2.1 Surrogate quality

We created surrogates for each cost function in the radiative zone design set \((T = 200 - 400 \text{ eV})\), by training the surrogate using 691 of the simulations and testing the surrogate using 77 of the simulations. Training the cost function surrogates, for the higher temperature design set, using the same 691 simulations created poor surrogates because the cost function becomes more sensitive to large optical depths as the goal temperature increases. We removed simulations with large optical depths \((\tau > 5)\) in order to create better performing surrogates. Removing simulations with large optical depths trimmed the edges of the parameter space with high cost function values. The trimmed edges are areas where optimized designs would not be found. For the 1000 eV design case, removing the simulations with large optical depths did not yield a quality surrogate. In addition, we removed simulations with an average relative difference between the inferred and model opacity larger than 100 \%, which further trimmed the edges of the parameter space with high cost function values. Again, the trimmed edges are areas where an optimized design would not be found. We trained the 500 eV and 750 eV design case surrogates using 706 simulations and tested the surrogates using 70 simulations. We trained the 1000 eV design case surrogate using 622 simulations and tested the surrogate using 62 simulations. A summary of the surrogate quality metrics for each design case surrogate is included in Table 4-5. These quality metrics were calculated for a comparison between the
test simulations’ true cost function values and the cost function values predicted by the surrogate. The $R^2$ metric is the coefficient of determination\textsuperscript{141} and provides the percentage of the variation in the surrogate predictions that can be explained by the relationship between the surrogate and the true cost function. The correlation score\textsuperscript{142} gives the percentage of the surrogate predictions that fit a linear response between the surrogate predictions and true cost function values. We defined quality surrogates as having a $R^2$ and correlation score larger than 90%. The $L-1$\textsuperscript{143} relative error is the average absolute relative difference between the surrogate predictions and the true cost function values. For the 200, 300, and 400 eV design cases, the quality of the surrogates decrease as indicated by the decreasing $R^2$ and correlation scores as well as the increasing $L-1$ relative error. The increasing $L-1$ relative error suggests that some area of the parameter space is not fit well by the surrogate. The areas of the parameter space not well fit by the surrogate are the edges of the parameter space with large optical depths and thus high cost function values. We could trim those areas to improve the $L-1$ relative error but we did not because the surrogate predicts the areas of low cost function values well. The surrogates referenced in Table 4-5 are the surrogates used to find optimized designs.

Table 4-5. Surrogate quality metrics for all design cases examined using the variable laser energy and buried layer thickness ensemble

<table>
<thead>
<tr>
<th>Quality metric</th>
<th>200 eV design</th>
<th>300 eV design</th>
<th>400 eV design</th>
<th>500 eV design</th>
<th>750 eV design</th>
<th>1000 eV design</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R^2$ (%)</td>
<td>99.8</td>
<td>99.1</td>
<td>96.5</td>
<td>98.8</td>
<td>92.2</td>
<td>95.3</td>
</tr>
<tr>
<td>Correlation score (%)</td>
<td>99.9</td>
<td>99.5</td>
<td>98.3</td>
<td>99.4</td>
<td>96.1</td>
<td>97.8</td>
</tr>
<tr>
<td>L-1 relative error (%)</td>
<td>21.4</td>
<td>41.2</td>
<td>67.8</td>
<td>27.2</td>
<td>25.6</td>
<td>14.1</td>
</tr>
</tbody>
</table>

4.2.2.2 Optimized designs

The basin hopping method found two local minima for each design case surrogate. In addition, the brute force method found one global minimum that agreed with one of the local minima found by the basin hopping approach. Figure 4-3 shows the cost function surrogate for the 300 eV and 750 eV design case. The circles indicate the design parameter values of the ensemble simulations. The white squares mark the design parameter values
of the local minima calculated by both the basin hopping and brute force approach. For
all design cases, the quantitative optimization approaches yielded designs that were in
the areas where the surrogate values are small indicating the quantitative approaches
successfully identified the areas where local minima occur.

In general, the areas of high cost function surrogate values are dominated by the
failure to meet temperature constraints (no. 1 & 2) and failure to meet optical depth
constraints (no. 7 & 8). Figure 4-4 shows the surrogates for peak electron temperature
and maximum optical depth over the Fe emission range for the 300 eV design case. The
color scale in Figure 4-4A is limited to 100 - 500 eV and the thin white region indicates
the area of the parameter space where the temperature constraints are met (285 - 315 eV).
The color scale in Figure 4-4B is limited to 0.03 - 1 and the areas with values between
0.03 and 0.64 meet the optical depth constraints. The white region indicates values
between 0.48 - 0.52. Based on the surrogates in Figure 4-4, it is predicted that neither of
the local minima found from the optimization process met the temperature and optical
depth constraints. However, the thinner local minimum more closely meets both the

Figure 4-3. Cost function surrogates for two design cases. The cost function surrogate
values are indicated in the color bar. The circles mark the design parameter
values of the ensemble simulations. The white squares mark the design
parameter values of the local minima yielded by optimization process. A) 300
eV design case B) 750 eV design case.

Figure 4-4. Cost function surrogates for peak electron temperature
and maximum optical depth over the Fe emission range for the 300 eV design case. The
color scale in Figure 4-4A is limited to 100 - 500 eV and the thin white region indicates
the area of the parameter space where the temperature constraints are met (285 - 315 eV).
The color scale in Figure 4-4B is limited to 0.03 - 1 and the areas with values between
0.03 and 0.64 meet the optical depth constraints. The white region indicates values
between 0.48 - 0.52. Based on the surrogates in Figure 4-4, it is predicted that neither of
the local minima found from the optimization process met the temperature and optical
depth constraints. However, the thinner local minimum more closely meets both the
temperature and optical depth constraints. The thicker local minimum has a temperature approximately a third higher than the goal temperature (300 eV) and an optical depth larger than 1. Similar results are found for the other design cases, but the region of the parameter space where the temperature constraints are met, shifts with goal temperature. It spans a lower laser energy range for the 200 eV design case and increasingly higher laser energy ranges for the 400 to 1000 eV design cases. The maximum optical depth surrogate remains similar for the other design cases.

Figure 4-4. Surrogates for peak temperature and maximum optical depth for the 300 eV design case. The surrogate values are indicated in the color bar. The circles mark the design parameter values of the ensemble simulations. The yellow squares mark the design parameter values of the local minima yielded by optimization process. A) Peak temperature (eV). The color scale is limited to 100 - 500 eV. B) Maximum optical depth over Fe emission range. The color scale is limited to 0.03 - 1.0.

For each local minimum, we executed a HYDRA simulation with the design parameters found by the quantitative optimization approaches. We calculated the single value metrics, constraint, and cost function using the HYDRA simulation results. We examined the cost function and constraints to determine which of the minima best satisfies the design constraints. For all design cases, the optimization approaches yield one minimum with a lower laser energy and thinner buried layer and one with a higher laser energy and thicker buried layer. For the 200, 300, and 400 eV design cases, both minima
failed to satisfy the temperature constraints because they reached temperatures that were too high. The thicker buried layer minima violated the temperature constraint more severely than the thinner minima. The minima do not satisfy the temperature constraints because the sulfur constraints (ratios and signals) are better met as the temperature increases. Therefore optimizing the cost function favors higher temperatures. For goal temperatures of 500 eV or larger, the sulfur constraints are met and the optimization approaches found minima that met the temperature constraints. For each design case, we compared the design constraints and cost function values of each minimum. We select the design with either the smallest cost function value or, in the case of very similar cost function values, with the smallest optical depth as the optimal design.

The optimal designs and how well they met each design constraint are described in Table 4-6. In general, the relative difference between inferred opacity and model opacity ranges from 10 - 40 %. The lower temperature design cases yielded optimized designs with temperatures larger than the goal temperature because the sulfur dopant constraints push the optimization of the cost function toward higher temperatures. None of the optimized designs met the desired time period of constant temperature and density. In order to increase that period, we would need to increase the laser pulse length. The variation in density was higher than the desired 10 %, but was still less than the uncertainty in some densities inferred from K-shell line widths in existing experiments.\textsuperscript{78,79,127} For the designs in which the optical depth was outside the desired range, optical depth effects are still limited because the maximum optical depth was less than or equal to 1. The iron emission signal was sufficient for all optimized designs, but the sulfur line ratios and sulfur emission signals were only satisfied for the 750 and 1000 eV designs. The 500 eV design does have sufficient signal for the He-like emission, which may be useful for determining plasma temperature and density.

The fact that the sulfur line ratios and emission signals were only satisfied for the higher temperature designs suggests that sulfur is not a good dopant for lower
Table 4-6. Optimized designs for the variable laser energy and buried layer thickness ensemble

<table>
<thead>
<tr>
<th></th>
<th>200 eV design</th>
<th>300 eV design</th>
<th>400 eV design</th>
<th>500 eV design</th>
<th>750 eV design</th>
<th>1000 eV design</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (J)</td>
<td>12.8</td>
<td>17.5</td>
<td>20.6</td>
<td>27.5</td>
<td>38.6</td>
<td>55.8</td>
</tr>
<tr>
<td>$\Delta l_{BL}$ (μm)</td>
<td>0.17</td>
<td>0.22</td>
<td>0.26</td>
<td>0.26</td>
<td>0.28</td>
<td>0.41</td>
</tr>
<tr>
<td>$\sigma_{rel}^{\rho}$ (%)</td>
<td>39</td>
<td>32.1</td>
<td>13</td>
<td>20</td>
<td>20</td>
<td>15</td>
</tr>
<tr>
<td>Met $T^*$?</td>
<td>37 % larger</td>
<td>22.7 % larger</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Met $\rho^*$?</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Met $\Delta t^*$?</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>Met $\Delta T^<em>$ and $\Delta \rho^</em>$?</td>
<td>$\rho$ varies 15 %</td>
<td>$\rho$ varies 15 %</td>
<td>$\rho$ varies 14 %</td>
<td>$\rho$ varies 16 %</td>
<td>$\rho$ varies 17 %</td>
<td>$\rho$ varies 18 %</td>
</tr>
<tr>
<td>Within $\tau_{min}$ and $\tau_{max}$?</td>
<td>max 0.85</td>
<td>Yes</td>
<td>Yes</td>
<td>min 0.02</td>
<td>min 0.01, max 1</td>
<td>min 0.01</td>
</tr>
<tr>
<td>Met $I_t$?</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Within $R^{<em>,min}$ and $R^{</em>,max}$?</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Only $\alpha$ ratio</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Met $S^{*,min}$?</td>
<td>No</td>
<td>Only He-α</td>
<td>Only He-α</td>
<td>Only He lines</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Cost function value</td>
<td>32</td>
<td>20</td>
<td>9</td>
<td>7.5</td>
<td>9.2</td>
<td>7.5</td>
</tr>
</tbody>
</table>

temperatures. Particularly for temperatures of 200 - 400 eV, only the sulfur He-α line emits sufficient signal. Two options for alternative dopant materials are magnesium and aluminum. Magnesium H- and He-like emission ranges from 1.25 - 1.8 keV, while aluminum emission ranges from 1.57 - 2.1 keV. An appropriate dopant material should not overlap the iron emission range because the overlap would complicate analysis of the dopant line ratios. The 200 eV design has Fe emission from 0.75 - 1.3 keV, but the emission from 1.25 - 1.3 keV is small and would be dominated by Mg K-shell emission (similar to Figure 3-5). The 300 eV and 400 eV designs have Fe emission from 0.76 - 1.5 keV, which overlaps Mg K-shell emission but not Al K-shell emission. The overlap of the Fe emission with Mg emission is shown in Figure 4-5. The emission from 1.25 - 1.5 keV would have a component coming from the Fe, making plasma temperature and density inference from the Mg K-shell lines more difficult. For the 300 eV and 400 eV designs,
an Al dopant would be more appropriate since there is no overlap between the Fe and Al emission.

![Graph showing x-ray emission spectra](image)

Figure 4-5. Simulated x-ray emission, at the time of peak electron temperature, at normal incidence from the target for the 300 eV design. The black indicates the Fe emission, the red indicates the Al emission, and the blue indicates the Mg emission.

We executed a HYDRA simulation with the S dopant replaced by either Al or Mg for each of the lower temperature designs. For iron-magnesium buried layers, we used a mixture of 50 % Fe and 50 % Mg by atom. For iron-aluminum buried layers, we used a mixture of 58.5 % Fe and 41.5 % Al by atom. Both mixed buried layers had an initial density calculated using equation Eq. (3-4). Using the results from the HYDRA simulations, we calculated the cost function, constraints, and single value metrics. The revised optimal designs and how well they met each design constraint are described in Table 4-7. Overall, these revised designs met the dopant ratio and line emission constraints, however had slightly increased optical depths. The optical depths are still less
than 1, which yield reasonable propagated uncertainties in the inferred opacity. Ideally, the ensemble should be repeated for both an iron-magnesium and an iron-aluminum buried layer because the optimization analysis might yield different designs than the ones included in Table 4-7. In particular, since the sulfur is replaced with a dopant that meets signal and ratio requirements at lower temperatures, the optimized design is likely to have a closer match to goal temperatures of 200 - 400 eV. We have left the application of the design process described in this chapter to variable buried layer and laser energy ensembles for iron-magnesium and iron-aluminum buried layers for future work.

Table 4-7. Optimized designs for the variable laser energy and buried layer thickness ensemble with revised dopant materials

<table>
<thead>
<tr>
<th></th>
<th>200 eV design</th>
<th>300 eV design</th>
<th>400 eV design</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (J)</td>
<td>12.8</td>
<td>17.5</td>
<td>20.6</td>
</tr>
<tr>
<td>Dopant</td>
<td>Mg</td>
<td>Al</td>
<td>Al</td>
</tr>
<tr>
<td>$\Delta l_{BL}$ (μm)</td>
<td>0.17</td>
<td>0.22</td>
<td>0.26</td>
</tr>
<tr>
<td>$\sigma_{rel}^{\nu}$ (%)</td>
<td>22</td>
<td>26</td>
<td>12</td>
</tr>
<tr>
<td>Met T*?</td>
<td>43 % larger</td>
<td>18 % larger</td>
<td>Yes</td>
</tr>
<tr>
<td>Met $\rho$*?</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Met $\Delta t$*?</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>Met $\Delta T$* and $\Delta \rho$*?</td>
<td>$\rho$ varies 11 %</td>
<td>$\rho$ varies 17 %</td>
<td>$\rho$ varies 15 %</td>
</tr>
<tr>
<td>Within $\tau_{\min}^<em>$ and $\tau_{\max}^</em>$?</td>
<td>max 0.7</td>
<td>max 0.96</td>
<td>max 0.95</td>
</tr>
<tr>
<td>Met $I_r$?</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Within $R^{<em>,\min}$ and $R^{</em>,\max}$?</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Met $S^{*,\min}$?</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Cost function value</td>
<td>22.2</td>
<td>11</td>
<td>7.89</td>
</tr>
</tbody>
</table>

The inferred and model opacity for the optimal 300 eV and 750 eV designs are shown in Figure 4-6. The figures are limited to the appropriate iron emission range for each design. The plot in Figure 4-6B is on a linear-log scale so that the differences between the inferred and model opacity are clearer. Both designs have decent agreement between the inferred and model opacity ($\sigma_{rel}^{\nu} < 26 \%$). For the 300 eV design, the difference between the inferred and model opacity for 0.76 - 0.86 keV is due to tamper emission. The under-prediction of the inferred opacity from 0.92 - 1.2 keV is an optical depth effect similar to the one in Figure 3-10C. The optical depth over 0.92 - 1.2 keV is larger than 0.7 but less than 1, indicating that the opacity inference for this design
is fairly sensitive to optical depth. For the 750 eV design, the difference in the opacity valleys is due to the tamper emission. There is a small under-prediction of the inferred opacity at the opacity peaks from 1.05 - 1.15 keV, but the difference in the opacity valleys contributes more to the average relative difference than the under-prediction.

In an experiment, subtracting out the tamper emission before inferring the opacity could reduce the moderate relative difference between inferred and model opacities. We examined the propagated experimental uncertainties (as in Section 3.2.4) assuming a 10 % uncertainty in the measured x-ray emission, a 5 % uncertainty in the temperature, and a 10 % uncertainty in the areal density. For both designs, the propagated experimental uncertainties were less than 30 % across the appropriate iron emission range. As suggested by the comparison in Section 3.2.4, propagated uncertainties can get very large for designs with large optical depths and a 30 % propagated uncertainty is reasonable. Overall, these designs provide a good trade-off between minimizing optical depth and tamper emission effects while reaching the goal plasma conditions and ensuring adequate iron and dopant signals.
All designs presented in this chapter yield very small periods of constant plasma conditions (0.2 - 0.4 ps). These periods are less than the temporal resolution of previous experiments (≈ 1 - 2 ps), meaning that the measured emission would capture a range of plasma conditions. Based on the studies in this dissertation, there are two possible ways to increase the period of constant plasma conditions. The first is increasing laser pulse length which elongates the duration of constant plasma conditions at the time of peak electron temperature. The second, is to focus the design optimization on a time, after buried layer recompression, during which the density is relatively constant. The duration of constant recompressed density decreases with increasing laser pulse (Section 3.2.2.1) and increases with increasing tamper thickness (Section 3.2.2.5). A design optimization focusing on aligning periods of constant temperature with the period of constant recompressed density could be created. This type of design optimization would be focused on when the target is cooling, and the temperature is dropping, which will complicate the ability to reach goal temperatures. Nonetheless, the design process developed in this chapter could be applied to such an approach. Future work should include the application of the automated design process to a variable laser energy, laser pulse length, and buried layer thickness aimed at optimizing at the time of peak electron temperature and at the time of constant recompressed density.
CHAPTER 5
SUMMARY AND CONCLUSIONS

This dissertation explores the computational design of short pulse laser driven iron opacity experiments. In such experiments, target materials can be heated to several hundreds of eVs while maintaining densities 1/10 of solid to solid density. This enables access to conditions relevant to the upper radiative zone of the sun (200 - 400 eV and densities larger than 1/10 of solid density). It also enables access to higher temperatures consistent with the deep radiative zone of the sun (up to 1000 eV), however, at lower electron densities. Spectroscopic measurements at temperatures of 200 - 1000 eV and densities of 1/10 of solid to solid density would investigate the validity of theoretical opacity models at stellar-relevant conditions. Such measurements may aid in resolving the current disagreement between solar parameters calculated from model and observations.

We used one-dimensional radiation hydrodynamic simulations to individually study the effects of changing the laser energy, the laser pulse length and the target dimensions on the plasma conditions, x-ray emission, and inferred opacity. We specified an energy source with the same time dependence as the laser pulse and with peak power proportional to a fraction of the laser energy per unit mass. Our energy source is proportional the assumed laser and target parameters in each simulation.

* Studying the effects of changing the laser energy, the laser pulse length, and the target dimensions provides insight into how plasma conditions and x-ray emission might be controlled by design. Peak electron temperatures increase with increasing laser energy and decrease with elongating laser pulse. Increasing the tamper thickness slows the late time cooling of the target, resulting in larger late time electron temperatures. The initial expansion of the layer is accelerated by increasing the laser energy and delayed

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* This paragraph is reprinted from Martin et al., Physics of Plasmas 24, 022705 (2017), with permission of AIP Publishing (Ref. 52).
by elongating the laser pulse or increasing the buried layer thickness. Manipulation of
the laser pulse length and the layer thickness could be used to align periods of constant
electron temperature and density, thus enabling multiple time-resolved measurements at
similar conditions. The recompression of the layer is dominantly controlled by the tamper
thickness. Thicker tampers will increase the density to which the layer is recompressed
and the duration of recompression. Increasing the tamper thickness will also increase
the CH continuum emission, which makes the opacity inference less accurate. Therefore
the density and emission effects of the tamper thickness must be considered in design.
The amount of x-ray emission is drastically increased by increasing the laser energy but
can also be moderately increased by increasing the buried layer thickness if the target is
sufficiently optically thin. In addition, the propagated uncertainty in the inferred opacity
increases with increasing layer thickness and thus increasing optical depth. Therefore
the target must be sufficiently optically thin to limit the propagated uncertainty in the
opacity inference. The interplay of all these parameters can be optimized to design a set
of experiments reaching conditions consistent with the upper radiative zone of the sun
(200 - 400 eV, $\rho = 0.8 - 7.88 \text{ g/cm}^3$). An example design that reaches such stellar-relevant
conditions, reduces tamper emission effects, and reduces optical depth effects over the iron
L-shell emission range was discussed.

The example design presented as a result of the individual laser and target parameter
studies was not selected by optimization. Instead, it was manually selected from the
effects in the single parameter studies which examined a limited range of the full design
parameter space. In order to find globally optimized designs, we developed an automated
design process using Lawrence Livermore National Laboratory’s (LLNL) Uncertainty
Quantification Pipeline (UQP). The UQP manages ensembles of one-dimensional
radiation hydrodynamic simulations where each simulation assumes a set of design
parameters. The LLNL UQP samples the design parameters, executes the ensemble of
simulations, analyzes the ensemble of simulations, and creates ensemble data files. We
then analyze the ensemble data files to find optimized designs for a range of design cases. The optimization aims to minimize the relative difference between the inferred and model opacity, while also meeting design constraints. The design constraints focus on meeting desired plasma conditions, limiting optical depth effects, and meeting iron and dopant emission requirements. We define a cost function that penalizes the relative difference between inferred and model opacity for each unsatisfied design constraint. For multiple design parameter ensembles, we use the UQP to create a surrogate for each design case cost function. We then use the cost function surrogate to find optimized designs. Once an optimized design is found, we execute a radiation hydrodynamic simulation for the optimized design and then analyze the cost function and design constraints for that simulation. If the design has a reasonable difference between inferred and model opacity while meeting constraints sufficiently, the design is considered a “good” design.

We used the automated design process to find optimized designs for single and multiple parameters ensembles of FeS$_2$ buried layer targets. We selected FeS$_2$ because an experimental campaign at Atomic Weapons Establishment’s Orion Laser Facility was planned to use a short pulse laser (0 - 100 J, 0.5 ps, 20 - 50 µm diameter focal spot) to heat 0.3 µm FeS$_2$ sandwiched between 3 µm of parylene-N. We explored a set of design cases relevant to the radiative zone of the sun: $T = 200$ eV, $T = 300$ eV, and $T = 400$ eV, each with $\rho > 1/10$ of solid density. In addition, we explored a set of design cases for higher temperatures at a constant density: $T = 500$ eV, $T = 750$ eV, and $T = 1000$ eV, each with $\rho = 4.2$ g/cm$^3$. Ensembles individually varying laser energy, laser pulse length, buried layer thickness, and tamper thicknesses demonstrated that the cost function is most sensitive to the goal temperature and optical depth constraints. The laser energy ensemble suggested that, in order to reach temperatures of 200 - 1000 eV, laser energies of 10 - 50 J, respectively are needed. We created ensembles simultaneously varying laser energy and buried layer thickness. For each design case, we used the UQP to generate a surrogate which we used to find optimized designs. For the 200 - 400 eV design cases,
sulfur failed to satisfy the dopant ratio and emission constraints. Magnesium was an appropriate alternative dopant for the 200 eV design case because its emission range (1.25 - 1.8 keV) did not overlap with the iron emission range (0.75 - 1.3 keV). Aluminum was an appropriate alternative dopant for the 300 and 400 eV design cases because its emission range (1.57 - 2.1 keV) did not overlap with the iron emission range (0.76 - 1.5 keV). Both magnesium and aluminum met the dopant constraints for the 200 - 400 eV design cases. Sulfur was found to be an appropriate dopant for 500 - 1000 eV. For all optimized designs, the average relative difference between the inferred and model opacity was reasonable (< 26 %). However, the time period of constant plasma conditions (0.2 - 0.4 ps) was significantly smaller than the temporal resolution of previous experiments (1 - 2 ps). Within the design optimization outlined in this dissertation, the period of constant plasma conditions could be increased by increasing laser pulse length. Alternatively, a design optimization focused on a time during constant recompressed density could be done to maximize the duration of constant plasma conditions. Overall, we used the automated process to design experiments at stellar-relevant conditions while minimizing tamper emission, minimizing optical depth effects, meeting plasma condition goals, and meeting x-ray emission goals.

All of the work in this dissertation assumes a simple parametric energy source to account for the absorption of laser energy, the conversion of absorbed energy into hot electrons, and the deposition of hot electron energy into the target materials. We assume that the heating time dependence is Gaussian with a duration equal to the pulse length of the laser. We also assume that the total energy is uniformly deposited into the target and proportional to a fraction of the average laser energy. Using our assumed energy source to model previous experiments has been shown to predict peak plasma conditions and reasonable x-ray pulse durations. However, we recognize that our methodology does not address the experimental evidence suggesting that heating may be longer than the laser pulse length and that hot electron heating laterally spreads outside of the laser focal
spot size. In addition, our 1D modeling does not include experimental details, which may cause 2D effects, such as: roughness of layers, spatial speckling of the laser spot, and spatial inhomogeneities in mixed buried layers. Also, all mixed buried layers in this dissertation assume an atom mixture between two materials, which may not be physically achievable. In such a case, it is common for the buried layer to be made of a series of alternating layers between the desired materials. Our methodology could be applied to such a target by including the individual layers into the model. While we believe that our methodology is useful for designing experiments, more detailed modeling would likely be needed to analyze experimental results. Specifically, more detailed modeling that better captures the temporal and spatial dependence of short pulse laser heating mechanisms may be needed. One idea is to couple the results of a high resolution particle-in-cell simulation of the short pulse laser absorption with a hot electron transport simulation that includes the recirculation of hot electrons, then create an interface between the hot electron transport simulation and a radiation hydrodynamic simulation such that heating source is informed by the hot electron transport. Such a coupled calculation would take a while to develop, complete, and analyze, limiting its use as relatively quick design tool. We developed a computational design process that allows for the relatively quick determination of optimized designs given some design goal and constraints. Particularly, the process focuses on designing short pulse laser driven iron opacity experiments at stellar-relevant conditions. Experiments of this nature would investigate the validity of opacity theory at such conditions and may help resolve current disagreement between solar models and observations.
REFERENCES


BIOGRAPHICAL SKETCH

Madison received a Doctor of Philosophy in nuclear engineering sciences from the University of Florida (UF) in August 2017. She completed her doctoral research at Lawrence Livermore National Laboratory (LLNL) as a graduate scholar. Her research project included the computational design of short pulse laser driven iron opacity measurements.

She received a Bachelor of the Arts in mathematics and physics from Florida Atlantic University’s Harriet L. Wilkes Honors College in May 2010. After that, she spent a year working on the Turkey Point 6 & 7 licensing team at Florida Power & Light. It was her experience working on the licensing effort for a new nuclear project that inspired her to pursue a technical degree in nuclear engineering. She received a Master of Science in nuclear engineering sciences from UF in December 2012. Her non-thesis project explored the existing research related to continuous energy adjoint Monte Carlo simulation applied to neutron transport and the implementation of such a technique in existing neutron transport codes. She spent the summer of 2013 working at Lawrence Livermore National Laboratory, investigating the effect of different x-ray drives that compress inertial confinement fusion capsules on ignition performance and instability growth.

Madison was actively involved in Lawrence Livermore Postdoc Association where she acted as vice president and graduate student liaison. Before conducting her research at LLNL, she served as an officer in the UF student sections of American Nuclear Society and Women in Nuclear. In addition, she was a representative of the Nuclear Engineering Program on the Engineering Graduate Student Council, which serves as a forum for graduate students to express concerns regarding graduate student life and academics to the Herbert Wertheim College of Engineering at University of Florida. In addition to her research and involvement in organizations, Madison participated in a variety of science outreach programs while at both UF and LLNL.