Abstract—A scheme employing neonlike krypton ions is under intensive theoretical and experimental investigation to determine the feasibility of developing a pulsed power-driven laboratory X-ray laser. The scheme depends on discharging hundreds of kilojoules of electrical energy through coaxial cylindrical krypton gas puffs, generating a dense, hot, uniform, homogeneous, and highly ionized krypton plasma. The dynamics of energy absorption are such that self-generated magnetic fields compress and accelerate radially inward the outer plasma with speeds approaching $5 \times 10^7$ cm/s. When the outer plasma impinges and stagnates on the inner plasma shock waves are sent through the system as the plasma reverberates and bounces outward. Near the interface between the two interacting plasmas, and along the axis, conditions appear to be conducive to the establishment of a population inversion with the subsequent emission of coherent soft X-rays with measurable gain. The theory, analysis, and numerical simulations are based on a fully coupled, self-consistent, one-dimensional non-LTE radiation hydrodynamics model (including the effects of opacity and radiation transport). The multilevel ionization dynamics is evaluated in the collisional radiative equilibrium (CRE) approximation for the manifold of both ground and excited states distributed throughout the various stages of ionization. In addition, particular emphasis is placed on the atomic structure of the neonlike ionization stage which in our model consists of 48 excited levels in $J-J$ coupling. The evolution of the level populations as functions of the various atomic processes provides information on the conditions necessary to establish population inversion and the emission of coherent radiation in the lasing transitions. The spectral line profiles are represented by Voigt functions. A complete history of the implosion and radiation dynamics will be provided for the cases under investigation.

I. INTRODUCTION

X-RAY LASER research over the last 15 years has been based predominantly on lasing schemes involving laser-produced plasmas either as the gain medium or as a broadband X-ray source for photopumping another medium. In recent years this method has led to the successful demonstration of lasing in the ultraviolet and soft X-ray regimes [1], [2]. During this same time period pulsed power-driven Z-pinches were being developed as intense high-brightness broadband X-ray radiation sources for application in materials testing, spectroscopy studies, and X-ray lithography. Although these plasmas are excellent sources of high-energy radiation, their pathological behavior resulting in instabilities did not make them prime candidates for X-ray laser mediums. Part of the problem is that pulsed power-driven material loads have not enjoyed the benefits of detailed studies in target design—a hallmark of the laser fusion program. However, recent advances in the technology of load materials and configurations supported by an improved understanding of the dynamics has led to a revival of the usefulness of the Z-pinch plasma as a potential source of X-ray lasers. Experiments at both the Naval Research Laboratory (NRL) and Physics International Company (PI) have indicated the possibilities of this newly emerging technology. At NRL the sodium/neon system, which is the prototype of the line coincidence photopumping schemes, is under intensive investigation. Preliminary results appear to indicate that resonance fluorescence may have been achieved in the pumped transitions [3]. The scheme involves imploping and heating a sodium plasma on the GAMBLE II generator to temperatures commensurate with producing the sodium He-like resonance line to photopump the He-like $1s^2-1s4p^1P$ transition in a relatively cool neon plasma in a side-by-side configuration. These experiments are very encouraging and methods and techniques will continue to be investigated to try to increase the power in the pumping line to power levels sufficient to achieve measurable gain in the lasing transitions. Another series of pulsed power Z-pinch experiments at PI involves stagnating an outer gas-puff plasma onto a cylindrically symmetric coaxial core plasma located on the axis. Two different configurations have been investigated: the first involves concentric krypton gas puffs [4] and the second involves a neon puff-gas plasma stagnating onto an aluminum-coated parylene post on the axis [5]. The krypton design explores the possibility of creating an inversion and gain in the lasing transitions of neonlike krypton. The experimental results are somewhat uncertain because of the existence of line admixtures at the lasing wavelengths. On the other hand, the theory supports the existence of gain for a given set of implosion conditions discussed in the text. Preliminary experimental results from the second configuration strongly suggest gain in the lasing transitions in lithiumlike aluminum as aluminum plasma expands, cools, and recombines after collision with the inward-moving neon gas-puff plasma. All these new experimental results suggest that with proper design, Z-pinch plasmas have a promising future as a potential source for laboratory X-ray lasers.

There have also been a number of theoretical advances describing the dynamics of single wire, wire array, and gas-puff plasma implosions. These studies range from fusion plasmas to high-Z radiation source development to plasma flow opening switches. Depending on the specific application the theoretical models vary in their degree of complexity, ranging from the simple Bennett-pinch equi-
librium models to the sophisticated multidimensional MHD models. The emphasis of much of this work was on the hydrodynamics of the implosion/explosion phenomenon; i.e., implosion and thermalization times, density and temperature scale lengths, and the growth rates of the sausage and kink instabilities. For low-Z fully ionized plasmas, where radiation cooling is by bremsstrahlung, the MHD models do reasonably well in describing the plasmas’ evolution. However, for moderate- to high-Z plasmas these models are of limited value in that they neglect the major loss process, namely, radiation, which can have both a profound and subtle influence on the overall dynamics. In fact, the major improvement in these models in recent years has been the self-consistent inclusion of the radiation and radiation transport for the bound-bound, bound-free, and free-free transitions. The emphasis of much of this work was on the interplay and feedback between the atomic processes, radiation, and hydrodynamics are an extremely important and delicate interaction that ultimately determines whether or not lasing will occur.

In the spirit of our earlier work [6] we investigate the behavior of a krypton gas-puff plasma impinging and stagnating onto another krypton gas-puff plasma located on the axis. It has been found experimentally that upon collapse the inner plasma has a strong stabilizing influence on the outer plasma and appears to retard the development of plasma instabilities, creating a fairly uniform plasma in the interaction region where lasing may thus be expected to occur [4]. The strategy is to choose initial conditions such that in the interaction region between plasmas the temperature and density support the existence of sufficient quantities of neonlike krypton for times long enough for the various atomic processes to create a population inversion in the upper 3p and 3d levels, which will subsequently radiatively decay to the 3s and 3p levels, respectively, in the lasing lines. The model used to describe the implosion dynamics is a 1-D radiation hydrodynamics model including a self-consistent treatment of a) hydrodynamics and thermal conduction, b) atomic dynamics, and c) radiation emission and transport.

II. Theoretical Model

A. Hydrodynamics and Thermal Conduction

The basic hydrodynamic variables of mass, momentum, and total energy are transported in one dimension using a numerical scheme with a sliding-zone version of flux-corrected transport [6]. A special gridding algorithm is used that moves zones in a Lagrangian fashion and adjusts the mesh in order to resolve gradients in the flow. The hydrodynamic equations solved are

\[ \frac{D\rho}{Dt} = \frac{\partial p}{\partial t} + \nabla \cdot (u\rho) = 0 \]  
\[ \frac{D\rho u}{Dt} = -\nabla P + \epsilon \nabla \cdot \left( \eta \nabla T \right) \]

where \( \rho \) is mass density, \( u \) is velocity, \( P \) is pressure, \( \epsilon \) is total energy density, \( \epsilon \nabla \) is the rate of energy loss or gain resulting from radiation, \( \eta \) is the thermal conductivity, and \( N_j \) is the ion density. The thermal conduction is calculated implicitly, using an iterative Crank-Nicholson scheme.

Since the density generally did not exceed solid density in this study, a simple equation of state was assumed, i.e.,

\[ P = \frac{1}{3}(\epsilon - \frac{1}{2} \rho u^2 - \epsilon) \]

where \( \epsilon \) is the potential energy resulting from ionization and excitation. (A nonideal equation of state taking account of ionization energy and degeneracy pressure can be employed in cases where the density exceeds solid density.) A single temperature model was employed:

\[ kT = \frac{P}{(\rho + Z_\text{eff})} \]

where \( m_j \) is ion mass, and \( T \) is temperature. The ionization energy \( \epsilon \) and effective charge \( Z_\text{eff} \) are calculated from the ionization-radiation equations that are explained below. A single temperature assumption is valid in the core plasma, where the equilibration time is of the order of picoseconds, and it is adequate in the stagnation region, where the equilibration time can be of the order of nanoseconds, and the time scale for significant changes in temperature is about an order of magnitude longer. In the blowoff plasma it is a marginal approximation, but the consequences are minor since little radiation is emitted from this region and most of the thermal energy is carried by the electrons. The local rate of change of energy resulting from radiation transport, \( \epsilon \nabla \), will be discussed below.

Most gas-puff implosion experiments employ an azimuthal magnetic-field driver, whereas the calculations we will describe do not consider the effects of magnetic fields, but instead assign an initial radial velocity to the puff-gas plasma. This allows us to study the physics of imploding plasmas in an idealized framework without the complications of an external driver and coupled circuit, although we intend to consider more general configurations in future work. In a driven implosion with an optimized load we expect a nearly uniform velocity to be ultimately achieved, but density and temperature gradients will be produced in the puff, particularly near the outer edge, where Joule heating produces a layer of hot plasma.

B. Atomic Dynamics

The atomic level populations in the plasma are determined by a set of rate equations of the form

\[ \frac{df_i}{dt} = \sum_j W_{ij}f_j - \sum_j W_{ji}f_i \]
where \( f_i \) is the fractional population of atomic level \( i \), and \( W_{ij} \) is the net reaction rate describing the transition from initial state, \( j \), to final state, \( i \). An equation of this type is constructed for each of the atomic levels included in the model. For sufficiently dense plasmas the effective population and depopulation rates are generally fast compared with the hydrodynamic response. Under these circumstances an equilibrium assumption which involves dropping the explicit time dependence in (6) can be justified. The plasma is then said to be in collisional–radiative equilibrium (CRE), whereby the plasma ionization state responds instantaneously to changes in hydrodynamic quantities.

The rate coefficients that are used to calculate level populations, \( W_{ij} \), are calculated using various atomic calculational methods. The processes included in this calculation and the methods used in calculating the corresponding rate coefficients are summarized elsewhere [7].

Once the set of rate equations (including the optical pumping from the radiation field) has been solved for the fractional level populations, \( f_i \), the electron density can be calculated:

\[
N_e = \sum_i z_i f_i N_l
\]

where \( z_i \) is the ionic charge of level \( i \) and \( N_l \) is the total ion density.

The ionization and excitation energy can also be calculated by

\[
\epsilon_i = \sum \chi_i f_i N_l
\]

where \( \chi_i \) is the energy of level \( i \), measured from the ground state of the neutral atom.

The atomic model for krypton consists of 100 levels and about 300 emission lines. This includes all the ground states and selected excited states distributed throughout the \( M \)-, \( L \)-, and \( K \)-shells. In addition, a detailed neonlike model in \( J-J \) coupling containing an additional 48 excited levels was incorporated into the overall atomic model in order to provide a better picture of the dynamics of the neonlike levels and the lasing transitions. An abbreviated Grotrian diagram illustrating the lasing lines along with their wavelengths and spontaneous decay rates is shown in Fig. 1.

C. Radiation Emission and Transport

Radiation emission from and absorption by a plasma are dependent on the local atomic level population densities. Except for optically thin plasmas, however, the level populations depend on the radiation field since optical pumping via photoionization and photoexcitation can produce significant population redistribution. Thus, the ionization and radiation transport processes are strongly coupled and must be solved self-consistently. In this model an iterative procedure is used where level populations are calculated using the radiation field from the previous iteration, then using these populations to calculate a new radiation field and recalculating populations until convergence is reached.

A probabilistic radiation transport scheme is employed which forms local angle and frequency-averaged escape probabilities for each emission line and for each bound-free process. Free-free radiation is treated with a multi-frequency transport formalism. The escape probabilities calculated for the transport of bound-bound radiation take into account Doppler and Voigt line profiles. The method can treat comprehensive atomic models and provides good overall energetics but cannot calculate accurately certain spectral details and lines with very high optical depths.

Inner-shell opacities are included in the model since these processes are very important in the cool, dense plasma regions. Inner-shell photoionization cross sections for the neutral element are calculated as described in Dustin et al. [7], and the positions of the ionization-dependent absorption edges are taken from the Hartree-Fock calculations of Clementi and Roetti [8].

The local rate of energy change in zone \( j \), a result of radiation transport, is given by

\[
\dot{\epsilon}_{\text{rad}} = - \sum_P \left( F_{ PJ } - \sum_k C_{PK} F_{ PK } \right)
\]

where \( F_{ PK } \) is the rate of energy loss in zone \( k \) resulting from a discrete radiative process (or frequency group) \( P \), and \( C_{PK} \) is the radiative coupling of zone \( k \) to zone \( j \) for that process. The couplings are functions of opacity, integrated over the process and photon path. In the probabilistic model a matrix of couplings must be computed for each bound-bound, bound-free, and free-free process. In this way the net cooling and heating by radiation emission...
and absorption between the various zones of the plasma is accurately taken into account.

III. Results

The numerical simulations were performed for an outer hollow cylindrical annular krypton puff gas with a Gaussian mass density distribution of 140 $\mu$gm/cm$^3$, with its centroid located 15 mm from the origin, and an inner coaxial cylindrical krypton puff gas with a Gaussian mass distribution of 20 $\mu$gm/cm$^3$ with its centroid located 1 mm from the origin. The configuration is schematically illustrated in Fig. 2. The initial temperature and particle density of the puff gas and core plasma are 2.5 eV and $2 \times 10^{17}$ cm$^{-3}$ and 0.5 eV and $2 \times 10^{18}$ cm$^{-3}$, respectively. A tenous background plasma was placed between the puff and core plasmas with a mass density of $5 \times 10^{-7}$ gm/cm$^3$. The results of the simulation are insensitive to this value, which was chosen for numerical expediency. Finally, the outer gas-puff plasma is given an initial kinetic energy corresponding to a radial implosion velocity of $4.5 \times 10^7$ cm/s.

The outer plasma continues to move radially inward until its leading edge makes contact with the boundary of the core plasma where it stagnates onto and begins to cause compression of the core. During this phase of the implosion the kinetic energy of run-in is redistributed into thermal, ionization, radiation, and kinetic energy associated with the generation and propagation of weak shocks and rarefaction waves. As energy is converted during the stagnation process photons are emitted over a broadband spectrum extending from the visible to the soft X-ray regime, preheating the core plasma which itself begins to radiate. The interface region between the interacting plasmas and, especially, the compressed core plasma is where we expect conditions conducive to lasing to occur.

The phenomenology of the assembly phase of the implosion dynamics is best characterized by the behavior of the hydrodynamic variables, particularly the temperature, density, velocity, pressure, and the cooling rate by radiation. Specifically focusing on the times corresponding to the first assembly phase, we present in Figs. 3-5 the temporal variation of these variables as a function of displacement, extending from the origin out to 0.08 cm. The ordinate is normalized in order to illustrate the behavior of all the variables on a single figure. The scale factor for each variable is given by density $\times 1 \text{ gm/cm}^3$, temperature $\times 1 \text{ eV}$, pressure $\times 10^{12} \text{ erg/cm}^3$, velocity $\times 10^{11} \text{ cm/s}$, and $\dot{r}_{\text{rad}} \times 10^{27} \text{ erg/s-cm}^3$. Fig. 3, at 33 ns, illustrates the situation during the assembly phase when the plasma is still stagnating on axis. Fig. 4, at 34.22 ns, gives evidence of complex motion as the plasma begins to rebound. Fig. 5, at 35.0 ns, shows the off-axis stagnation which occurs as plasma rebounding from the compression along the axis collides with plasma which is still imploding. A more comprehensive history of the implosion can be obtained from the contour plots in radius and time of the ion density and electron temperature, which are discussed below. As the inward propagating shock reaches the central axis at about 28 ns, there is strong heating near the axis. The temperature reaches about 750 eV bu radiation cooling and hydrodynamic effects quickly reduce the temperature on axis. Ion number density monotonically increases at the origin until about 34 ns at which time the temperature decreases. The plasma remains quite warm, however, a short distance from the
origin where the density falls off sharply. By 33 ns the temperature at the origin has dropped to about 150 eV; however, at about 0.025 cm the temperature peaks in excess of 700 eV. From the velocity gradients at this time, it is evident that the plasma is compressing in the vicinity of the hot shell. Notice that the velocity is negative (directed toward the origin) everywhere at 33 ns. Actually, by referring to the contour plot of temperature over space and time, it will be seen how the shell of warm krypton evolves. Also note that because the gradients in temperature and density are in opposite directions, the radiation cooling rate is subject to relatively large variations over relatively small gradient scale lengths. Just after 33 ns, plasma near the origin begins to expand in a complicated fashion: parts of the plasma move outward while other parts are moving inward. This behavior produces compressions and rarefactions in the core plasma leading to heating and cooling in localized regions. At 34.22 ns, it is seen on Fig. 4 that plasma which is a short distance (0.008 cm) from the origin is expanding radially, while plasma is moving radially inward elsewhere. The contour plot of temperature will clearly exhibit the localized regions of rapid heating and cooling from 33 to 36 ns. The relief of the very large pressure gradient built up at 34.22 ns is evident at 35 ns in Fig. 5, where it has caused a virtual stagnation at about 0.035 cm. Plasma is now moving radially outward within the region and colliding with imploding plasma. As a result, a fairly broad shell of hot plasma (1 keV) has been produced. Since the ion density is fairly small over much of this region, the radiative cooling rate is correspondingly reduced.

A novel way of presenting the results of the numerical simulations is to illustrate by contour plots the behavior of the hydrodynamic variables. The contour plots complement our earlier figures as well as provide a better picture of the course of events. In the contour plots time runs along the vertical axis from 27 to 36 ns and displacement or radius runs along the horizontal axis from the origin out to 0.08 cm. The various shades of light and dark are coded to the right of the figures. There are several ways to understand and interpret the results. One of the easiest is to choose a time and then observe how the parameters vary from larger to smaller displacements and simply repeat the process for increasing times. Also, much of what has already been said is repeated here in order to provide commentary with the results. The radial temperature history is shown on Fig. 6 over distances mainly confined to the compressed core plasma and the interaction region. The brighter regions are primarily the result of compressional wave heating or weak shocks. The expanding darker regions later in time extending from the axis outward reflect the effects of radiative cooling while the brighter regions from 34 ns on indicate heating due to weak shocks moving outward. The temperature peaks at around 1 keV in this region. The ion density is shown on Fig. 7, where it is seen that as time increases the density along the axis increases where the plasma is compressing. These high pressures near the origin slow down the incoming plasma. Thus, kinetic energy is constantly being thermalized in this region, commencing just after the on-axis assembly. Radiation cooling in this region falls off sharply with the radius following the corresponding density falloff. Just after 33 ns the plasma near the origin exhibits both inward and outward flowing plasma. This produces compressions and rarefactions leading to heating and cooling in localized regions. Just after 34 ns the plasma at about 0.008 cm from the origin is expanding radially while elsewhere the plasma is moving radially inward. From the contour plot of temperature shown on Fig. 6 it can be seen that alternating rapid cooling and heating is produced from 33 to about 36 ns in localized regions. The large pressure gradient is relieved, producing a virtual stagnation at about 0.035 cm. Plasma is now moving
Fig. 6. Temperature contours as a function of displacement and time.

Fig. 7. Ion density contours as a function of displacement and time.
Fig. 8. Neonlike ion fraction contours as a function of displacement and time.

Fig. 9. Gain/cm contours of the 172 Å line as a function of displacement and time.
Fig. 10. Gain/cm contours of the 170 Å line as a function of displacement and time.

Fig. 11. Gain/cm contours of the 184 Å line as a function of displacement and time.
radially outward from this point and colliding with imploding plasma. This results in the formation of a fairly broad shell of hot plasma (about 1 keV).

The fraction of neonlike krypton ions in the ground state is shown on Fig. 8. Since the fractional abundance of neonlike ions is strongly temperature dependent and only weakly density dependent, it is not too surprising to observe that the number of neonlike ions tracks the temperature. The greater abundances occur for temperatures in excess of about 400 eV, which is about the temperature commensurate with the appearance of neonlike krypton. Shown on Fig. 8 are a number of localized regions where the fractional abundance of neonlike ions exceeds 50 percent and a few regions where it is upwards of about 70 percent, i.e., in those regions of the plasma anywhere from 50 to 70 percent of all the ions are in the neonlike ground state. A very propitious situation, indeed, for our proposed X-ray laser scheme!

Conditions conducive to a population inversion leading to a gain in the lasing transitions were achieved for three of the lines: the 172, 170, and 184 Å lines, respectively. These results are shown on Figs. 9, 10, and 11, respectively. Reference to Fig. 1 shows the wavelengths of the respective transitions. Gains of one or more occur in highly localized regions eventually achieving values in excess of 9/cm for the 172 Å line; 5/cm for the 170 Å line; and 3/cm for the 184 Å. The atomic processes contributing to the gain are predominantly due to recombination and electron impact excitation. The gain for the 172 Å line extends over the largest radial region extending from the origin out to about 0.048 cm from 28 to 29 ns. A more localized region occurs from 34 to 36 ns. The gain for the 170 Å line occurs at the same time but is confined to smaller regions. Finally, gain for the 184 Å line, which is due predominantly to electron collisions, is confined to an even smaller region peaking around 35 ns. Note that on the scale to the right of the gain profiles some of the values represented are negative numbers and correspond to the absorption of radiation.

IV. Conclusion

The results of the numerical simulations support the notion that it is theoretically possible to achieve a population inversion and gain in three of the lasing lines provided that the appropriate plasma conditions are realized. The final confirmation of whether this approach is feasible is currently unfolding with the analysis of the experimental observations.

References