Modeling of fast capillary-discharge for soft x-ray lasers

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Abstract. In this work we present the results of the numerical investigations of the one-dimensional single-fluid magneto-hydrodynamics (MHD) model, with separate electron and ion temperatures, of a capillary-discharge collisional soft x-ray laser. The MHD equations are solved by the Lagrangian cylindrical geometry approach. The effects of the gas filling pressure on the plasma densities and temperatures, and implosion-pinch phase for soft x-ray lasing conditions have been analyzed. The results are compared with experimental measurements of the operating pressure ranges.

1. Introduction

Soft x-ray lasers are invaluable tools for studying high-density plasmas and permitting one to see smaller features in microscopy, to write finer patterns in lithography and to generate shorter pulses. These lasers have applications for the materials science community, both inside and outside the laboratory, by supplying detailed information about the atomic structure of new and existing materials. These in turn lead to new scientific understandings, perhaps through surface science, chemistry and physics, providing feedback to the enabling technologies. Development of soft x-ray spectral region is presently in a rapid growth and there is much interplay between the science associated technologies.

In 1984, soft x-ray lasers were first demonstrated in plasmas generated by powerful laser drivers in large laboratories \cite{1, 2}. However, the large pump lasers used for this kind of soft x-ray laser experiments are only available at a few large laser facilities in the world due to their large size, complexity, and extremely high cost. Therefore the demonstration of a capillary discharge soft x-ray laser operating in the transition of Neon (Ne)-like ions by Rocca et al \cite{3} in 1994 opened the possibility to develop compact, efficient and simpler soft x-ray laser. This similar demonstration had then been only repeated by Ben-kish et al \cite{4} in 2001, followed by the work of Niimi et al \cite{5} and Kukhlevsky et al \cite{6} in the following year. The quest for improving these systems still continues by parallel efforts involving theory and computer simulations of the experiments to understand the laboratory observation and to optimize the resulting energy density. Even after more than a decade, systems with improved performance and efficiency are still being reported \cite{7}.

In this paper, the capillary discharge soft x-ray laser described by Tan and Kwek \cite{8} is modeled using two-temperature, one dimensional single-fluid magneto-hydrodynamics (MHD) equations. The details of the governing equations and the computational simulation will be applied and shown. The model was then utilized to numerically evaluate the time and radial dependences of capillary plasma characteristics of fast capillary discharges with current rise time of around 50 ns and peak currents 16 kA in a capillary 3 mm in diameter filled with pre-ionized argon (Ar) gas. The results were then
compared with experimental data [8] from different initial argon filled pressures. The effects of the gas filling pressure on the plasma densities and temperatures, during implosion-pinch phase for soft x-ray lasing conditions were analyzed.

2. Magneto-hydrodynamics model
The basic MHD equations used are described below. The continuity equation (mass conservation) is given by

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \]

where \( \rho \) is mass density and \( \mathbf{u} \) is the plasma fluid velocity. Generally, in any steady state process, the rate at which mass enters a system is equal to the rate at which mass leaves the system. In this numerical scheme, the continuity equation is automatically satisfied.

The momentum conservation equation is solved in the one-fluid approximation where the plasma electrons and ions are assumed to flow together as a single fluid. The momentum equations is governed by

\[ \rho \frac{d\mathbf{u}}{dt} = -\nabla P + \mathbf{J} \times \mathbf{B}, \]

where \( P_e \) and \( P_i \) are the thermal pressure due to electrons and ions, respectively, \( \mathbf{B} \) denotes the magnetic field induced by the axial current and \( \mathbf{J} \) is the axial component of the electric current density. Here, \( q \) is the von Neumann artificial viscosity. The artificial viscosity, which in included in the equation of motion to handle shocks, effectively smoothes the shock over a small number of zones.

The energy balance for electrons and ions is described by

\[ \frac{dE_{\alpha}}{dt} = \nabla \cdot (\kappa_{\alpha} \nabla T_{\alpha}) + \psi_{\text{joule}} - \frac{dE_{\alpha}}{dV} \frac{dV}{dt} - \frac{(T_e - T_i)}{t_{eq}}, \]

where \( C_{\alpha e}, T_{\alpha e}, E_{\alpha e}, P_{\alpha e} \) and \( \kappa_{\alpha} \) are, respectively, the specific heat, temperature (in eV), specific internal energy, pressure and thermal conductivity, of the electrons (\( \alpha = e \)) and ions (\( \alpha = i \)). While \( V \) is the specific volume, \( \psi_{\text{joule}} \) is joule heating term and \( t_{eq} \) is the electron-ion collisional coupling term.

The difference between the temperature diffusion equations for the electrons and ions is the absence of the Joule heating term in the ion equation. Since the currents are mainly due to the lighter electrons, the energy is transferred to the ions through the collision specified by the term involving \( t_{eq} \).

The magnetic field transport and diffusion equation reads

\[ \frac{d\mathbf{B}}{dt} = \frac{\eta}{4\pi} (\nabla \cdot \nabla) \mathbf{B} - (\nabla \cdot \mathbf{u}) \mathbf{B}, \]

where \( \eta \) is defined as the plasma electrical resistivity. This equation is obtained using Maxwell equations and generalized Ohm’s law neglecting the time variation of the electric field [9].

These MHD equations have been adopted in the Lagrangian reference frame using the specific volume expression. The position of each cell and the velocity on cell boundary are determined by

\[ \frac{dr}{dt} = u. \]

All dynamical values in the equations evolve as a function of position \( r \) from the capillary axis at a time \( t \).
3. The requirement characteristic of populations and gains in neon-like argon

As a first estimation of absolute gain of this transition, the fractional abundance of charge states is evaluated using steady-state ionization model.

The atomic physics PrismSPECT code [10] solves the equation of state and provides radiative properties for plasma in local thermodynamic equilibrium (LTE) state. The ionization population fractions in the range $T_e \in 1 – 1000$ eV for a given electron density $N_e \sim 2.0 \times 10^{18}$ cm$^{-3}$ are depicted on the figure 1. This value has been chosen because of the value of the pinch electron density of the case study will be studied in next section. The maximum ionization population fraction of neon-like Ar$^{8+}$ ion, $f^{8+} \approx 0.95$ is accomplished at temperature $T_e \approx 40$ eV. The temperature range of Ne-like ionization state is approximately between 10 – 200 eV. It should be kept in mind that the steady-state ionization model does not depend on ionization dynamics, namely, ionization plasma history.

![Figure 1](image1.png)

**Figure 1.** Argon ionization fractions dependences on plasma electron temperature for atom density $N_0 = 2 \times 10^{18}$ cm$^{-3}$.

Figure 2 presents a contour plot of gain against $N_e$ and $T_e$ computed using steady-ion ionization model. The effect of reabsorption of the resonance radiations on the distribution of population density of excited-states has been neglected (optically-thin plasma assumption). It has been assumed that $T_e = T_i$. This assumption generally sets the upper limit of gain in capillary-discharge.

Figure 2 indicates that a large gain formed for $N_e \approx 2 \times 10^{18}$ cm$^{-3}$. For the regime $N_e > 10^{20}$ cm$^{-3}$, collisional depopulation exceeds the radiative decay rates. Hence, the populations become distributed according to the Boltzmann distribution function and the collisional quench of the population inversion occurs (i.e., unsuitable gain regime). Although, the fractional abundance of Ne-like Ar becomes a maximum at $T_e \approx 40$ eV using the steady-state approximation for ionization model, the optimum regime of gain is approximately at $T_e \approx 60$ eV, as shown in figure 2. This fact shows a mismatch between electron temperature that maximizes gain and fractional abundance of Ne-like Ar ion, in which is a general problem of Ne-like x-ray lasers [11]. The mismatch arises because the excitation energy into the $n = 3$ levels is typically three-quarters of the ionization energy and thus a
temperature which gives large ground-state excitation rates will lead to large ionization rates if the electron density is sufficient (the relaxation time for the ionization balance $\approx 10^{11} \text{s}^{-1}$) [12].

The collisions between particles in the plasma transfer energy from particle to particle in a random fashion, thereby heating the plasma and ionizing the atoms. Generally, multiple ionization states are formed, each with its own characteristic emission lines, leading to a rich spectrum of lines. By carefully controlling the temperature and density of the plasma, the population of specific ionization species can be preferentially established. Generally, such high temperatures and densities are established at or close to pinch radius.

![Figure 2](image)

**Figure 2.** The contour of gain in $3p \ ^1S_0 \rightarrow 3s \ ^1P_1$ transition as function of the electron temperature and density.

Under certain plasma conditions (electron density of $0.1 - 4 \times 10^{19} \text{ cm}^{-3}$, and electron temperature $\approx 40 - 90 \text{ eV}$, as in results from figure 2), collisional electron impact excitation of the ground state Ne-like ions produces a population inversion between the $3p \ (J=0)$ and the $3s \ (J=1)$ levels resulting in amplification at the 46.9 nm wavelength.

4. Results and discussion

Using the general physical model outlined in section 2, the discharge channel can be simulated with specific values of the controlling parameters. The parameters of a working discharge x-ray laser reported in reference [8] are used. Here the radius of the capillary has been fixed at 0.15 cm, and current rise time is about 50 ns. For this basic situation, the filling pressures and the current profiles are varied to investigate the impact of these variations on the plasma. Initially, the pre-ionized plasma is assumed to be uniformly distributed with $T_e = T_i = 1 \text{ eV}$. For the simulations, we use the HELIOS-CR code described in reference [13]. It is a modeling platform that can handle LTE and non-LTE plasmas in one dimension. The peak discharge current 16 kA is used in this paper. These are the typical values used in the laser of reference [8].

Figure 3 presents the calculated results for a capillary discharge with a peak current of 16 kA and 0.15 mbar gas filling pressure. The temporal evolution of the trajectories of argon plasma elements
inside the channel of this configuration is illustrated in figure 3(a). The blue line represents the discharge current. Figure 3(b) shows contour plots of the logarithm of the electron density measured in cm$^{-3}$ while figure 3(c) shows the electron temperature measured in eV. These figures also provide quantitative information about the distribution of the plasma parameters inside the channel at different times. Some characteristics features are discussed below.

The dynamics of a Z-pinch plasma can be described by the balance between the thermal pressure and the magnetic pressure. In the early stages ($t < 20$ ns) the plasma is not compressed immediately but actually tries to expand due to the fact that the plasma pressure exceeds other forces. However, this expansion is constrained by the rigid wall of the capillary. The pressure in the outer zones of the plasma is due to both the initial filling pressure and Joule heating. Generally, the current tends to flow in the outer part of the cylindrical plasma, and Joule heating occurs due to current passing through the plasma. This heating results in an increase in pressure which can be sufficiently high for the outer regions of the plasma to initially expand before being accelerated inward by the magnetic piston.

When the discharge current has reached a value such that the magnetic pressure is larger than the thermal pressure ($t > 20$ ns), the plasma is compressed inward onto the axis. At the same time, a

**Figure 3.** Basic parameters of discharge in capillary with diameter of 3 mm filled with argon at an initial gas filling pressure of 0.15 mbar for $I_0 = 16$ kA and rise time 50 ns. (a) The plasma time-space flow diagram; blue line corresponds to the discharge current at outer boundary; (b) contour lines of the decimal logarithm of the electron density (measured cm$^{-3}$) on the ($t$, $r$) plane; (c) contour lines of the electron temperature (measured in eV).
vacuum region appears near the wall and a converging shock wave is formed which propagates towards the channel axis. The shock waves eventually meet at the axis, and are subsequently reflected. During compression, the plasma becomes hotter due to Joule and shock heating, and the thermal pressure increases. Although, before the time 50 ns, when the total current has been increasing towards the maximum value, the discharge current is high, and the Lorentz force dominates. Thus, the compression stops. When the thermal pressure balances the magnetic pressure, the plasma stagnates ($t \approx 43.5$ ns) and then expands ($t > 43.5$ ns). During the compression, a high density and temperature plasma on the axis is produced, as shown in figure 3(b) and 3(c). The temperature $T_e$ reaches the value of 70 eV and continues to heat up to 160 eV during the expansion phase. This is because the inner zones of plasma continue to compress again after the first pinch. The value of electron density $N_e$ at the pinch is about $3 \times 10^{18}$ cm$^{-3}$. A hot plasma core with the radial dimension $r_{\text{core}} = 0.266$ mm and central mass density $\rho_{\text{core}} = 1.22 \times 10^{-4}$ g/cm$^3$ is formed.

At the stage of expansion the MHD instabilities may break the uniformity of the plasma column, leading to turbulent mixing, enhanced heat transport and resistance. However, from the theory of the classical pinch effect, MHD instabilities begin to evolve when the expansion velocity begins to decrease [14]. If the lasing occurs during the few first nanoseconds after the reflection of the shock wave, MHD instabilities have no time to evolve. The validity of this description of the plasma behavior in the capillary discharge ends at the moment when the diverging shock wave reaches the capillary wall.

The time dependence of small signal gain factor $G$ is determined by the time dependences of both laser level populations $n_{3p3S}^{8s}$ and $n_{3s3P}^{8s}$. In this case above (a non-ablating alumina capillary with radius $r_0 = 1.5$ mm filled with initial gas filling pressure of 0.15 mbar, current pulse with $T_{1/4} = 50$ ns and current peak value $I_{\text{max}} = 16$ kA) the gain factor has a shape of very short peak with maximum value $G(t_G) = 0.8$ cm$^{-1}$ at the time $t_G = 44.5$ ns (see figure 4). The peak value of gain is achieved during the pinch time.

![Figure 4. The spatial and temporal evolution of gain](image)

5. Comparison with experiments
The simulations of the capillary discharge dynamics for $r_0 = 1.5$ mm, $T_{1/4} = 50$ ns, $I_{\text{max}} = 16$ kA and various initial gas filling pressure $p_0$ of argon have been performed here. For given capillary radius $r_0$ and current waveform, the peak value of gain factor $G(t_G)$ may be expressed as a function of the
initial gas filling pressure (see figure 5). The gain curve shows that the measurable gain factor for \( r_0 = 1.5 \) mm, \( T_{1/4} = 50 \) ns, \( I_{\text{max}} = 16 \) kA is found in the pressure range \( 0.11 \) mbar < \( p_0 < 0.29 \) mbar.

**Figure 5.** Dependence of gain factor peak value on the initial gas filling pressures.

**Figure 6.** Comparison between experimental data and simulation data. The main discharge current is 16 kA.

From the MHD simulation, the electron densities and temperatures that fulfilled the plasma conditions and high gain factors obtained are in between 0.11 to 0.29 mbar. These results have been further computed which included refraction effect due to electron density gradient. The simulation output of the intensity are compared with the experimental data [8] shown in figure 6. The dotted lines
are the range of gas filling pressures that are computed by MHD simulation. The soft x-ray lasers (experimental data) have been produced in the range of 0.12 to 0.28 mbar (the solid line) which show good agreement if compared to simulation data.

6. Conclusions
The results from an MHD modeling of a fast capillary-discharge for soft x-ray lasers have been compared with experiment results. The effects of the gas filling pressure on the plasma densities and temperatures, and implosion-pinch phase for soft x-ray lasing conditions resulting in high gain factors have been analyzed. Our findings indicate that the simulations performed gave reasonably good agreement with experiment.

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References
[1] Matthews D L et al. 1985 Demonstration of a soft x-ray amplifier Phys. Rev. Lett. 54 110
[2] Suckewer S, Skinner C H, Milehberg H, Keane C and Voorhees D 1985 Amplification of stimulated soft x-ray emission in a confined plasma column Phys. Rev. Lett. 55 1753
[3] Rocca J J, Shlyaptsev V, Tomasel F G, Cortázar O D, Hartshorn D and Chilla J L A 1994 Demonstration of a Discharge Pumped Table-Top Soft-X-Ray Laser Phys. Rev. Lett. 73 2192
[4] Ben-Kish A, Shuker M, Nemirovsky R A, Fisher A, Ron A and Schwob J L 2001 Plasma Dynamics in Capillary Discharge Soft X-Ray Lasers Phys. Rev. Lett. 87 015002
[5] Niimi G, Sakamoto N, Nakajima M, Hayashi Y, Watanabe M, Okino A, Horioka K and Hotta E 2002 Study of low current capillary discharge for compact Soft x-ray laser. AIP Conf. Proc.: AIP) pp 103-6
[6] Kukhlevsky S V, Ritucci A, Kozma I Z, Kaiser J, Shlyaptseva A, Tomassetti G and Samek O 2002 Atomic Model Calculations of Gain Saturation in the 46.9 nm Line of Ne-like Ar Contr. Plasm. Phys. 42 109-18
[7] Heinbuch S, Grisham M, Martz D and Rocca J J 2005 Demonstration of a desk-top size high repetition rate soft x-ray laser Opt. Express 13 4050
[8] Tan C A and Kwek K H 2007 Influence of current prepulse on capillary-discharge extreme-ultraviolet laser Phys. Rev. A 75 043808
[9] Burnett N H and Offenberger A A 1974 Magnetohydrodynamic behavior of a laser-heated solenoid J. Appl. Phys. 45 2155-62
[10] MacFarlane J J, Golovkin I E, Woodruff P R, Welch D R, Oliver B V, Mehlhorn T A and Campbell R B 2003 Inertial Fusion Sciences and Applications (American Nuclear Society)
[11] Holden P B and Pert G J 1996 Long-wavelength, prepulsed driving as a means to greatly increase the gain in low-Z Ne-like XUV lasers J. Phys. B: At. Mol. Phys. 29 2151
[12] Whitten B L, London R A and Walling R S 1988 Scaling of neonlike lasers using exploding foil targets J. Opt. Soc. Am. B 5 2537-47
[13] MacFarlane J J, Golovkin I E and Woodruff P R 2006 HELIOS-CR - A 1-D radiation-magnetohydrodynamics code with inline atomic kinetics modeling J. Quant. Spectrosc. Radiat. Trans. 99 381-97
[14] Vrba P, Vrbová M, Bobrova N and Sasorov P 2005 Modelling of a nitrogen x-ray laser pumped by capillary discharge Cent. Eur. J. Phys. 3 564-80