Gain Coefficients for Possible 4d-4p X-ray Lasers of Ni-like Nd, Sm, Eu, Gd, Ta and W Ions

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Abstract. Populations of the 249 levels belonging to the ground configuration $3s^23p^63d^{10}$ and those of single excitations of a $3d$, $3p$ and $3s$ electron to the orbitals of $n=4$ and $5$ have been calculated for Nickel-like Nd, Sm, Eu, Gd, Ta and W ions for temperatures from 300 to 2000 eV and densities of $1.0 \times 10^{21}$ and $1.0 \times 10^{22}$cm$^{-3}$. The gain coefficients for possible x-ray laser lines have also been calculated at these plasma conditions. The possible laser lines are transitions from levels $(3d_{3/2}^14d_{3/2})_0$ and $(3d_{5/2}^14d_{5/2})_0$ to levels of $(3d_{3/2}^14p_{1/2})_l$, $(3d_{5/2}^14p_{3/2})_l$ and $(3d_{3/2}^14p_{3/2})_l$. Estimation is made on the optimum plasma condition for x-ray laser gain.

Introduction

Researchers have been trying to realize a shorter wavelength x-ray laser for holography of biological living cell specimens within the water window. Much lower pump energy is required for the electron collisional excitation scheme of Ni-like ions than that of Ne-like scheme due to the higher quantum efficiency of the former. This makes the Ni-like scheme more promising to scale down to a shorter wavelength than the latter one. Collisional pumped x-ray laser in Ni-like ions due to 4d-4p transitions in laser plasmas of high atomic number elements have been demonstrated by various workers [1-4]. It has been proven to be the most successful method to date of producing lasing in the soft x-ray region. The efficiency of this scheme has been significantly improved since the first demonstration of lasing over a decade ago.

Saturated x-ray laser output has been demonstrated for Ni-like Ag, Sm and Dy [1,3,5]. Take Ni-like Sm as an example. Zhang et al. [1] reported a saturated laser beam output at a wavelength of 7.3 nm with an output energy of 0.3 millijoule in 50-picosecond pulses. The laser line at a wavelength of 6.8 nm was also visible. Lin et al. [2] carried out a systematic study of double pulse pumping at 7.3 nm. They found that Ni-like Sm x-ray laser output can change by orders of magnitude when the intensity ratio of the pumping pulses and their relative delay are varied. To model x-ray lasers and their gains, a better understanding of atomic physics and plasma kinetics is essential.

For x-ray lasers, Ni-like Nd ($Z=60$), Sm ($Z=62$), Eu ($Z=63$), Gd ($Z=64$), Ta ($Z=73$), and W ($Z=74$) ions are of particular interest. In the present work we first study the population inversion between the levels of possible 4d-4p x-ray lasers by solving the rate equation and then calculate the gain coefficients of the possible x-ray lasers for these ions at different temperatures and densities. The atomic data required in the rate equation have been obtained from Flexible Atomic Code (FAC). Estimation has been made for the optimum electron temperature of maximum x-ray laser gain. Practical calculations show that more x-ray laser lines should be visible for these Ni-like ions than those have been demonstrated.
Theoretical Method

The level populations have been obtained by solving the set of coupled steady-state rate equations

\[ N_j \left( \sum_{i<j} N_i A_i + \sum_{i>j} C_i + \sum_{i=j} C_i \right) = \sum_{i<j} N_i A_i + n_e \left( \sum_{i<j} N_i C_i + \sum_{i=j} N_i C_i \right) \]  

(1)

Where \( N_j \) is the number density of level \( j \), \( A_i \) is the spontaneous decay rate, \( n_e \) is electron density and the superscript \( e \) and \( d \) refer to electron excitation and de-excitation, respectively. The populations are calculated for each of the 249 levels belonging to the configurations of \( 3s^23p^63d^{10} \), \( 3s^23p^63d^9nl \), \( 3s^23p^53d^{10}nl \), and \( 3s^23p^63d^{10}nl \) \( (n=4, \ 5; \ l=0, \ ..., \ n-1) \) of Ni-like Nd, Sm, Eu, Gd, Ta and W ions. To obtain the populations, one needs the energy levels, radiative decay rates and electron impact collision strengths. These atomic data connecting the 249 levels of Ni-like ions were calculated by many authors. A fully relativistic approach based on the Dirac equation is used to obtain the atomic data. Interactions among the above configurations have been included in the calculations of the energy levels, radiative decay rates and collision strengths. The collision strengths were calculated with relativistic distorted wave approximation. To ensure the convergence of the collision strengths, large angular momentum contributions (the maximum partial waves up to 50) have been taken into account. Higher partial wave contributions have been included using the Coulomb-Bethe approximation [6]. The collisional rate coefficients required in the rate equation are obtained from the collision strengths assuming a Maxwell distribution. It is assumed that the plasma is near ionization equilibrium and that recombination is negligible in obtaining the populations.

The gain coefficient \( G \) for a Doppler-broadened laser transition, dominant in high-temperature plasmas, is given by

\[ G = \frac{\lambda^3}{8\pi} A_i \frac{M}{2\pi k T} (N_e - N_i g_j) \frac{N_j}{g_j} \]  

(2)

Where \( \lambda \) is the wavelength of the transition between the upper and lower levels, \( A_i \) is the rate of spontaneous emission from the upper level \( u \) to lower level \( l \), \( N_i \) is the ion population density in the level \( j \) having statistical weight \( g_j \), \( k \) is the Boltzmann constant, \( M \) is the ion mass, and \( T_i \) is the ion temperature. It is assumed to be equal to the electron temperature in the present work.

The populations of the upper and lower laser levels are obtained from the identity

\[ N_j = \left( \frac{N_j}{N_i} \right) \left( \frac{N_i}{N_j} \right) N_i \]  

(3)

Where \( N_i \) is the total number density of all the levels of the ion under consideration, and \( N_j \) is the total number density of all ionization stages. Since the populations calculated from Eq. (1) are normalized such that

\[ \sum_{j=1}^{249} \left( \frac{N_j}{N_i} \right) = 1 \]  

(4)

The quantity actually obtained from Eq. (1) is the fractional populations \( N_j / N_i \). We assume that 1/4 of the ions are in the Ni-like ionization stage. The ratio of the electron density to the total ion density \( N_e / N_i \) is set equal to the degree of ionization of the Ni-like ions.

Results and Discussions

Table 1 shows the five levels which may be connected with the x-ray lasers of Ni-like Nd, Sm, Eu, Gd, Ta and W ions on the \( 3d^24d J=0 \rightarrow 3d^24p J=1 \) transitions. \( 3d^2 \) means a hole in the 3d sub-shell. Table I also lists the theoretical relative energies to the ground level \( (3s^23p^63d^{10} 1S_0) \). With the increasing of atomic number \( Z \), the energy interval between the levels of configurations \( 3d^24p \) and \( 3d^24d \) becomes larger, which means the wavelength of the possible x-ray lasers gets shorter. Fig. 1
shows the variations of the reduced population fractions $n_i / g_j$ with the temperature at an electron density of $1.0 \times 10^{19}$ cm\(^{-3}\) for the six Ni-like ions. The numbers labeled in the plots refer to the No. given in Table I. As can be seen from Fig. 1, the population inversion can be occurred between the upper level of $(3d^7_{5/2}4d_{3/2})_2$ (No.5) and all those lower levels of $(3d^7_{5/2}4p_{3/2})_2$ (No.1), $(3d^7_{5/2}4p_{5/2})_2$ (No.2), and $(3d^7_{5/2}4p_{5/2})_1$ (No. 3) for all six ions. The most favorable population inversion occurs between levels of Nos.5 and 2. Most of the experiments which have demonstrated x-ray lasers observed laser line by this transition. For example, this laser line for Ni-like Sm corresponds to wavelength of 7.3 nm. It has been experimentally demonstrated by Zhang et al. [1] and Lin et al. [2]. For the population inversion of level No. 4 and those belonging to the configuration of $3d^74p$ whose angular momentum is 1, the situation is different. For Ni-like Nd, Sm, Eu, and Gd ions, population inversion can only be occurred between levels of Nos.4 and 2 at the given electron density. However, population inversion can be occurred between levels of Nos.5 and 1, 2, and 3. Note that the difference of population from level No.4 are much smaller than that from level No.5, X-ray lasers caused from level No.4 have not been observed experimentally so far. One of the possible reasons may be that the population inversion is too small, and therefore the gain is also too small.

Table I. The energy levels (in eV) relative to the ground level related to the 4d-4p x-ray lasers of Ni-like Nd, Sm, Eu, Gd, Ta, and W ions.

<table>
<thead>
<tr>
<th>No</th>
<th>Designation</th>
<th>J $\pi$</th>
<th>Nd</th>
<th>Sm</th>
<th>Eu</th>
<th>Gd</th>
<th>Ta</th>
<th>W</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>$3d^7_{5/2}4p_{5/2}$</td>
<td>1$^e$</td>
<td>932.15</td>
<td>1032.57</td>
<td>1084.50</td>
<td>1137.56</td>
<td>1664.28</td>
<td>1728.05</td>
</tr>
<tr>
<td>2</td>
<td>$3d^7_{5/2}4p_{3/2}$</td>
<td>1$^e$</td>
<td>942.45</td>
<td>1045.06</td>
<td>1098.23</td>
<td>1152.65</td>
<td>1697.56</td>
<td>1764.17</td>
</tr>
<tr>
<td>3</td>
<td>$3d^7_{5/2}4p_{5/2}$</td>
<td>1$^e$</td>
<td>964.44</td>
<td>1071.22</td>
<td>1126.67</td>
<td>1183.52</td>
<td>1757.87</td>
<td>1828.72</td>
</tr>
<tr>
<td>4</td>
<td>$3d^7_{5/2}4d_{3/2}$</td>
<td>0$^e$</td>
<td>1059.23</td>
<td>1170.64</td>
<td>1228.33</td>
<td>1287.35</td>
<td>1877.96</td>
<td>1950.17</td>
</tr>
<tr>
<td>5</td>
<td>$3d^7_{5/2}4d_{5/2}$</td>
<td>0$^e$</td>
<td>1106.13</td>
<td>1220.35</td>
<td>1279.50</td>
<td>1340.03</td>
<td>1946.89</td>
<td>2021.30</td>
</tr>
</tbody>
</table>

Figure 1. Variation of level population fractions for Ni-like Nd, Sm, Eu, Gd, Ta and W ions with the temperature at an electron density of $1.0 \times 10^{19}$ cm\(^{-3}\).

Let us focus on the population inversion between levels of Nos.5 and 2. For Ni-like Nd, Sm, Eu, and Gd, the fraction of population of level 5 increases with the increasing atomic number $Z$. At a given temperature, the fraction of level 5 is the largest among all the possible laser lines. However, it
is on the opposite trend for level 2. At a given temperature, the fraction of level 2 decreases with the increasing atomic number \( Z \). As a result, the most favorable population inversion occurs for Ni-like Gd ion which has the largest atomic number. For Ni-like Ta and W, the fractions of both levels 5 and 2 are decreased compared with those of Ni-like Nd, Sm, Eu, and Gd at a given temperature. Therefore, the difference of their populations has also been decreased for these two ions.

![Figure 2](image_url)

**Figure 2.** Gain coefficients for transitions of \( \frac{1}{2} - \frac{1}{2} \) (No.5), \( \frac{3}{2} - \frac{1}{2} \) (No.1), \( 
\frac{3}{2} - \frac{1}{2} \) (No.2) and \( \frac{3}{2} - \frac{1}{2} \) (No.3) at an electron density of \( 1.0 \times 10^{15} \text{ cm}^{-3} \).

Fig. 2 shows the variation of gain coefficients for the possible x-ray lasers of six Ni-like ions with the temperature at the same electron density as that in Fig.1. As can be seen from the figure, the variation trend of gains is basically the same for Ni-like Nd, Sm, Eu and Gd ions. For these four ions, the laser line 5-2 has the largest gain among all possible laser lines, while the gains of 5-1 and 5-3 laser lines are much smaller than that of 5-2. For the strongest laser line 5-2, the gain of all four ions increase with temperature and then reaches a maximum value. From the temperature of the maximum gain, the gain decreases with the temperature. The turning point of temperature occurs at 700-800 eV for the four ions. This behavior of variation means that there is an optimized plasma condition for x-ray laser gain at a given electron density. On the other hand, at a given temperature, the gain decreases with the atomic number \( Z \). This is understandable because with the increasing of the atomic number, \( N_e/N \), in eq. (3) decreases with \( Z \). For Ni-like Sm, Zhang et al. [1] experimentally demonstrated the x-ray laser of transition 5-2. They measured the gain coefficient to be 8.4 cm\(^{-1}\) for this laser line at 7.3 nm. In view of the reabsorption in the experiment, our simulated gain coefficient at the density of \( 1.0 \times 10^{15} \text{ cm}^{-3} \) agrees reasonable well with the experiment. The maximum gain predicted by theory occurs at about 800 eV and it is 18 cm\(^{-1}\). This shows that the plasma condition in the experiment should be close to the optimum plasma condition of creating favorable x-ray laser. For other two ions, i.e., Ni-like Ta and W, the trend of gain variation with the temperature is different from the four ions. As mentioned above, there are six possible x-ray laser lines for these two ions, while there are only four lines for Ni-like Nd, Sm, Eu and Gd. In Fig. 2, we only give the gains of the four lines whose gains are relatively large. The gain increases fast with temperature at low temperatures, whereas it becomes very smooth when the temperature is higher than about 1000 eV.
Such a result implies that there is a wide temperature range for the optimum plasma condition of favorable x-ray laser.

Figure 3. The variation trend of the gain coefficients with the atomic number Z at a temperature of 1000 eV and an electron density of $1.0 \times 10^{21}$ cm$^{-3}$.

The trend of the gain variation with the atomic number Z mentioned above can easily be seen from Fig. 3, which shows the gain for the 5-2 laser line of the six Ni-like ions at a temperature of 1000 eV and an electron density of $1.0 \times 10^{21}$ cm$^{-3}$.

Figure 4. Gain coefficients for Ni-like x-ray laser lines at an electron density of $1.0 \times 10^{22}$ cm$^{-3}$.

Practical calculations show that at the electron density of $1.0 \times 10^{20}$ cm$^{-3}$, the gains of all possible laser lines for the six ions are below 1 cm$^{-1}$. This means that either a very long gain medium or supplemental heating must be used to boost the gain-length product to interesting values. Therefore, it is difficult to demonstrate efficient x-ray lasers near the electron density of $1.0 \times 10^{20}$ cm$^{-3}$. With the increase of electron density, the gains will become larger. Fig. 4 shows the gain coefficients at an electron density of $1.0 \times 10^{22}$ cm$^{-3}$. At this density, the behavior of the gains is different from that of at an electron density of $1.0 \times 10^{20}$ cm$^{-3}$, which are shown in Fig. 2. Firstly, the gains for Ni-like Ta and W are
much larger than in Fig. 2, while the gains for Ni-like Nd, Sm, Eu and Gd do not increase so much. Such a result shows that saturated output has been obtained at some density between $1.0 \times 10^{21} \text{cm}^{-3}$ and $1.0 \times 10^{22} \text{cm}^{-3}$. Secondly, the trend of the gain variation with the atomic number Z is on the opposite at the electron densities of $1.0 \times 10^{21} \text{cm}^{-3}$ and $1.0 \times 10^{22} \text{cm}^{-3}$. At the electron density of $1.0 \times 10^{21} \text{cm}^{-3}$, the gain decreases with the atomic number Z, while the gain increases with the atomic number Z at the electron density of $1.0 \times 10^{22} \text{cm}^{-3}$. Thirdly, for Ni-like Ta and W, the gains for laser lines of 5-1 and 5-2 are very close at the density of $1.0 \times 10^{21} \text{cm}^{-3}$, which is not the case at the density of $1.0 \times 10^{22} \text{cm}^{-3}$. Furthermore, 5-1 laser line has the largest gain at the density of $1.0 \times 10^{21} \text{cm}^{-3}$ among all the possible laser lines. At the density of $1.0 \times 10^{22} \text{cm}^{-3}$, 5-2 laser line has the largest gain for Ta while line 5-1 has the largest gain for W. From the results shown in Figs. 2 and 4, one can conclude that gain behavior is complex with the plasma condition (temperature and density). Favorable plasma condition is important in the experiment of x-ray lasers. An important unexpected anomaly was reported by Elton et al. [7] who could not demonstrate the x-ray laser gain from 3p-3s transitions of Ne-like copper plasmas. The possible reason might be that population inversion did not occur in the experiment or that the laser gain was too small to be observed.

Summary

In conclusion, the level populations for Ni-like Nd, Sm, Eu, Gd, Ta and W ions have been calculated for plasma conditions of variant temperatures and densities. Population inversion and gain coefficient have been calculated for possible x-ray laser lines of transitions 4d-4p $J=0-J=1$. For Ni-like Nd, Sm, Eu, Gd, the x-ray laser line which has the largest gain is due to the transition from level $(3d^{10}4d_{5/2})_h$ to $(3d^{10}4p_{3/2})_h$. For Ni-like Ta and W, however, the x-ray laser line of the largest gain may be the transition from $(3d^{10}4d_{5/2})_h$ to $(3d^{10}4p_{3/2})_h$, or to $(3d^{10}4p_{1/2})_h$, depending on the electron density of the plasma. At higher electron density, the gain is very close for these two laser lines. The favorable plasma condition for the output of x-ray laser can be determined. However, it is difficult to obtain efficient laser output below the electron density of $1.0 \times 10^{21} \text{cm}^{-3}$ for the six Ni-like ions.

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