Characteristics of populations and gains in neon-like argon (Ar IX)

Dong-Eon Kim a)
Department of Physics, Pohang University of Science and Technology, Pohang, 790-784, Korea

Dae-Soon Kim
Department of Office Automation, Youngwol Institute of Technology, Youngwol, Kangwon-Do 230-800, Korea

Albert L. Osterheld
Lawrence Livermore National Laboratory, L-41, P.O. Box 808, Livermore, California 94551

(Received 21 January 1998; accepted for publication 20 August 1998)

I. INTRODUCTION

Since Zherikhin et al.1 recognized that the populations of some levels in the 2p 53p configuration can be larger than those in the 2p 53s configuration for proper electron densities and temperatures, the x-ray laser schemes using transitions between the 2p 53p and 2p 53s configurations have been studied both theoretically and experimentally.2–4 Palumbo and Elton5 predicted the results of gains on the 3p 1S 0–3s 1P 1, 3p 3P 2–3s 1P 1, and 3p 3D 2–3s 3P 1 transitions for the density between 10 18 and 10 19 cm–3. The effect of the opacity of the 2p 1S 0–3s 3P 1, 2p 1S 0–3s 1P 1, 2p 1S 0–3d 3D 1, 2p 1S 0–3d 1P 1, and 2p 1S 0–2s3p 1P 1 transitions becomes important for a density higher than 10 18 cm–3 and even increases the gain on the 3p 1S 0–3s 1P 1 transition for the opacity of the 2p 1S 0–3s 3P 1 transition up to 2.

II. MODEL FOR CALCULATION

The rate equation for the population N i l of an excited level l in the i th ionization stage is given by

\[
\frac{dN_i^l}{dt} = \sum_u R_{ul}^i N_u^l - n_e Q_{il}^{i+1} N_1^{i+1} + n_e C_{ul}^e, \quad (1)
\]

with

\[
R_{ul}^i = n_e C_{ul}^e, \quad l > u, \\
R_{ul}^i = n_e C_{ul}^e + A_{ul}, \quad l < u, \quad (2)
\]

where \(n_e\) is the electron density, \(C_{ul}^e\) the electron excitation (deexcitation) rate coefficient, and \(A_{ul}\) the radiative transition rate from a state u to a state l. The terms \(I_{l}^i\) and \(Q_{l}^{i+1}\) represent the electron collisional-ionization rate coefficient from a level l and the total recombination rate coefficient to the level, respectively.

Since an equilibrium between the excited levels is readily established due to their short lifetimes, the quasi-steady-state approximation has been adopted in our calculation:

\[n_e = \text{constant} \]

abundance of the Ne-like ionization stage is expected to be highest for an electron temperature near a half the ionization potential. The collisional-radiative model used here has been used for analyzing atomic population kinetics in non-local-thermodynamic-equilibrium (non-LTE) plasmas at these electron densities.

In the Sec. II, the model and approach in our simulation are described: i.e., the quasi-steady-state collisional-radiative model, atomic model, and the treatment of the opacity. The simulation results are presented and discussed in the Sec. III.

---

a)Electronic mail: kimd@vision.postech.ac.kr
Furthermore, the recombination and ionization processes between neighboring ionization stages can be ignored because these processes are negligibly slow compared to the excitation and deexcitation processes within the Ne-like ionization stage under the densities and temperatures of our interest. Then, the level populations in a single ionization stage of interest are determined by the balance of collisional and radiative transitions. In the present calculation the level populations are normalized in such a way that

\[
m_i = \frac{N_i}{N_1}, \quad \sum_i m_i = 1, \tag{4}
\]

where \(N_1\) is the total population of all the levels considered. The relative level populations are calculated by solving the coupled rate equations Eq. (1) under the conditions of Eqs. (3) and (4). The coupled rate equations can then be rewritten in the matrix form:

\[
m = \begin{pmatrix}
m_1 \\
m_2 \\
m_3 \\
\vdots \\
m_n
\end{pmatrix}
= \begin{pmatrix}
1 & 1 & 1 & \cdots & 1 \\
R_{21} & R_{22} & R_{23} & \cdots & R_{23} \\
R_{31} & R_{32} & R_{33} & \cdots & R_{33} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
R_{n1} & R_{n2} & R_{n3} & \cdots & R_{nn}
\end{pmatrix}
\begin{pmatrix}
1 \\
0 \\
0 \\
0
\end{pmatrix},
\]

where

\[
\begin{align}
N_l &= \sum_i N_i, \\
N_u &= \sum_i N_i, \tag{5}
\end{align}
\]

In this study, the 37 levels of the \(2p^6, 2p^53s, 2p^53p, 2p^53d, 2s2p^63s, 2s2p^63p,\) and \(2s2p^63d\) configurations in Ne-like Ar have been considered. All the radiative and collisional processes between the 37 levels have been taken into account. The necessary atomic data were obtained from the Hebrew University-Lawrence Livermore Atomic Code package (HULLAC). In the atomic structure calculation, the wavefunctions, energy levels, and all the important radiative decay rates were obtained from a relativistic configuration interaction treatment based on a parametric potential model.\(^{15}\) Electron impact excitation cross sections were calculated in the semirelativistic, distorted-wave approximation using the techniques of Ref. 16. In this approach, the cross section is factorized into a radial part involving wavefunctions only, and an angular factor depending only on the target states. The semirelativistic approximation treats the continuum electron nonrelativistically, while retaining a fully relativistic treatment of the bound electrons. The cross sections were averaged over a Maxwellian velocity distribution with a temperature \(T_e\) to obtain excitation rate coefficients. The electron excitation rate coefficients were approximated by the five-parameter fit:\(^{17}\)

\[
C_{iu}^e = \langle \sigma v \rangle = 1.58 \times 10^{-5} \frac{P(b_{iu})}{b_{iu}^3} e^{-b_{iu}} \text{cm}^3/\text{s}, \tag{6}
\]

where

\[
b_{iu} = \frac{E_{iu}}{\gamma}, \tag{7}
\]

and

\[
\ln p(b_{iu}) = c_0 + c_1 \ln b_{iu} + c_2 \ln^2 b_{iu} + c_3 \ln^3 b_{iu}, \tag{8}
\]

where \(E_{iu}\) is the transition energy (in eV) and \(\gamma = T_e\) the electron temperature (in eV). The deexcitation rate coefficient is obtained using the detailed-balance relation

\[
C_{iu}^d = \frac{g_l}{g_u} e^{b_{iu}} C_{iu}^e. \tag{9}
\]

For a Doppler-broadened spectral line, the gain coefficient on a radiative transition between an upper level \(u\) and a lower level \(l\) is given by

\[
G = \frac{1}{8\pi} \frac{M}{2\pi kT_{\text{ion}}} \frac{1}{A_{ul} \lambda_{ul}^3 N_u} \left( \frac{N_u}{g_u} - \frac{N_l}{g_l} \right) = \sigma_{\text{gain}} \left( \frac{N_u}{g_u} - \frac{N_l}{g_l} \right), \tag{10}
\]

where \(M\) is the atomic mass of the ion, \(k\) the Boltzmann constant, \(T_{\text{ion}}\) the ion temperature, \(\lambda_{ul}\) the wavelength of the transition, \(g_u\) and \(g_l\) the statistical weights of the levels, \(N_u\) and \(N_l\) the population of the levels \(u\) and \(l\), respectively, and \(\sigma_{\text{gain}}\) the gain cross section. Ion temperature \(T_{\text{ion}}\) were chosen to be approximately equal to electron temperature \(T_e\); however, \(T_{\text{ion}}\) may be smaller than \(T_e\).

Using the relative populations, Eq. (10) can be rewritten as follows:

\[
G_{ul}/N_l = 9.98 \times 10^{-32} A_{ul} \lambda_{ul}^3 \frac{1}{T_e^2} \frac{1}{g_u} \left( \frac{m_u}{g_u} - \frac{m_l}{g_l} \right) \text{cm}^4, \tag{11}
\]

where \(\lambda\) is given in angstrom, \(T_e\) in eV. The right-hand side of Eq. (11) consists of terms only related to Ne-like Ar. Hence, it represents inherent characteristics of gain on a transition in Ne-like Ar for a given electron temperature and density.

A rapid radiative decay of the lower level is crucial to the formation of the population inversion between the two levels. Thus, the radiation from the lower level should freely escape from a plasma. In other words, the plasma must be optically thin to the transition from the lower level, at least in the transverse direction. We have also investigated the opacity effect on gains. The opacity \(\tau\) on a radiative transition between the levels \(l\) and \(m\) is defined by

\[
\tau_{lm} = k_{im}(\lambda) L, \tag{12}
\]

where \(L\) is the effective length of the plasma medium and \(k_{im}(\lambda)\) the absorption coefficient, which is given by

\[
k_{im}(\lambda) = \frac{e^2 f_{im}}{m_e c^2 \left( 2kT_{\text{ion}} \right)^{1/2}} N_{l} \lambda_{im}, \tag{13}
\]

where \(f_{im}\) is the absorption oscillator strength between the levels \(l\) and \(m\), \(m_e\) the electron mass, and \(e\) the electron charge. The opacity has the effect of increasing the population of the upper level involved. High opacity on the resonance transitions between the \(2p^6\) and \(2p^53s\) configurations eventually results in the increase of the level populations in the \(2p^53s\) configuration, leading to the decrease of gains on the transitions between the \(2p^33s\) and \(2p^33p\) configurations.
The relative sublevel populations as a function of electron density for Ne-like Ar (not to scale). The $J=0$→$1$ transition (I) was observed to have gain and be strongly amplified at proper conditions (Ref. 10).

![FIG. 1. A schematic diagram of several energy levels under interest in Ne-like Ar (not to scale). The J=0→1 transition (I) was observed to have gain and be strongly amplified at proper conditions (Ref. 10).](image)

The escape probability method used in our calculation approximates this by the effective reduction of the radiative decay rates. In our case, the radiative decay rate of a relevant transition was replaced by the effective rate given by $E(\tau)A$, where $E(\tau)$ is the escape probability for a given $\tau$ and $A$ the original radiative transition rate. For the escape probability $E(\tau)$, we have used the following polynomial fit to tabulated values of $E(\tau)$ calculated by Zemansky: 18

for $0<\tau\leq4.5$,

$$E(\tau) = 0.999003 - 0.697745\tau + 0.266529\tau^2 - 0.061906\tau^3 + 0.008106\tau^4 - 0.000453\tau^5,$$  \hspace{1cm} (14)

and for $\tau>4.5$,

$$E(\tau) = \frac{1}{\tau\sqrt{\pi}\ln\tau}. \hspace{1cm} (15)$$

### III. RESULTS AND DISCUSSION

The relative sublevel populations ($m_i/g_i$) have been calculated by solving the 37 coupled rate equations given by Eq. (5). The gains have then been calculated for the following transitions between the $2s^22p^53p$ and $2s^22p^53s$ levels that have large radiative transition rates (see Fig. 1):

(A) $2p^53p\; ^3D_2\rightarrow2p^53s\; ^3P_1,$

(B) $2p^53p\; ^3D_1\rightarrow2p^53s\; ^3P_1,$

(C) $2p^53p\; ^1D_2\rightarrow2p^53s\; ^3P_1,$

(D) $2p^53p\; ^3P_0\rightarrow2p^53s\; ^3P_1,$

(E) $2p^53p\; ^1S_0\rightarrow2p^53s\; ^3P_1,$

(F) $2p^53p\; ^3P_1\rightarrow2p^53s\; ^1P_1,$

(G) $2p^53p\; ^3P_2\rightarrow2p^53s\; ^1P_1,$

(H) $2p^53p\; ^1P_1\rightarrow2p^53s\; ^1P_1,$

(I) $2p^53p\; ^1S_0\rightarrow2p^53s\; ^1P_1,$

In Fig. 2, the relative sublevel populations of the relevant levels are presented as functions of electron densities at given two-electron temperatures of 50 and 200 eV. As shown in Fig. 2, the relative sublevel populations grow with the electron density and the temperature due to the increase of collisional excitation rates. For a given temperature, in the region of low electron density, the populations of the $3s\; ^3P_1$ and $^1P_1$ levels are smaller than those of other levels under consideration due to their strong radiative decay; however, in the region of high electron density, the populations become distributed according to Boltzmann distribution because the collisional deexcitation rates exceed the radiative transition rates. Due to the close collisional coupling of the $2p^53p\; ^1S_0$ level to the ground level, the level is most largely populated; however, its inversion against the $2p^53s\; ^3P_1$ level destroyed around $N_e=10^{19} \text{cm}^{-3}$. The density dependence of the population distribution is maintained for temperatures between 50 and 200 eV. The populations of the $2p^53p\; ^1P_1$, $^3P_1$, and $^3D_1$ levels are very close to one another as those of the $2p^53p\; ^1P_2$ and $^3D_2$ level are due to the balance of radiative decay and collisional processes. The population of the $3p\; ^3P_0$ level is also very close to that of the $3s\; ^3P_1$ level and its population inversion with respect to the $3s\; ^3P_1$ level is destroyed above the middle of $10^{17} \text{cm}^{-3}$. This can be

![FIG. 2. Relative sublevel populations as a function of electron density for given temperatures: (a) and (c) for $T_e=50 \text{eV}$; (b) and (d) for $T_e=200 \text{eV}$.](image)
times smaller than that of the $3p\,^1S_0$ level. Transitions A and G have gain cross sections 3.1 and 4.6 times larger than transition I, respectively.

In Rocca’s experiment, the discharge device was operating at 700 mTorr of Ar, which corresponds to the density of about $2.3 \times 10^{16}$ cm$^{-3}$ at room temperature. The gain on the transition I was observed at the electron density of about or less than $1 \times 10^{19}$ cm$^{-3}$. The present calculation shows a gain per particle density on transition I of $1.5 \times 10^{18}$ cm$^{-4}$ for an electron density of $1 \times 10^{18} - 1 \times 10^{19}$ cm$^{-3}$ [Fig. 3(d)] and results in a gain of 0.35–0.4 cm$^{-1}$ for Rocca’s experimental conditions, which is in fairly good agreement with the observed value of 0.6 cm$^{-1}$ in that the present calculation did not take into account hydrodynamics. The present calculation also shows a reasonable gain on transition G, the amplification of which was also noticed by Rocca but its gain measurement was not pursued due to the complication of the spectral line being blended with other lines from different ionization stages.

We have also studied the opacity effect. In the calculation, the opacities of the following fast transitions were taken into account: $2p\,^1S_0 - 3s\,^3P_1$, $2p\,^1S_0 - 3s\,^3P_1$, $2p\,^1S_0 - 3d\,^3D_1$, $2p\,^1S_0 - 3d\,^3P_1$, and $2p\,^1S_0 - 2s\,3p\,^3P_1$. These transitions have larger opacities than other transitions. For a given opacity of a transition $\alpha$, the opacity of another transition $\beta$ can be related by

$$\tau_\beta = \frac{\lambda_\beta}{\lambda_\alpha} \frac{f_\beta}{f_\alpha},$$

which only depends on atomic properties. In the calculation, the $2p\,^1S_0 - 3s\,^3P_1$ transition was used as a reference: the values of $\tau$ given in Fig. 4 are for the transition. The opacities of the other four transitions were calculated according to Eq. (16). Figure 4 shows the opacity effect on the transitions $3p\,^1S_0 - 3s\,^3P_1$ and $3p\,^3D_2 - 3s\,^3P_1$. Below the electron density of $10^{18}$ cm$^{-3}$, the opacity effect is rather small for $\tau$ up to 2. The opacity effect becomes important for an electron density larger than $10^{18}$ cm$^{-3}$ or opacity larger than 4. For a density higher than $10^{18}$ cm$^{-3}$, the opacity up to 2 increases the gains. The increase is larger for higher temperature. The opacities in transitions $2p\,^1S_0 - 3d\,^3D_1$, $2p\,^1S_0 - 3d\,^3P_1$, and $2p\,^1S_0 - 2s\,3p\,^3P_1$ reduce their radiative decay rates, leading to the effective increase of the population of the $3p\,^1S_0$ level via collisional and radiative cascades. When their opacities are intentionally neglected, the gain in the $3p\,^1S_0 - 3s\,^3P_1$ transition unexpectedly decreases as shown in Fig. 4(c). The opacity has a larger effect in low temperature than in high temperature: i.e., when the pumping rate is small as in low temperature, even a slight reduction of the decay rate leads to a significant change of the population distribution. It is noted that the $3p\,^3D_2 - 3s\,^3P_2$ transition is less affected than the $3p\,^1S_0 - 3s\,^3P_1$ transition.

IV. CONCLUSION

We have studied the characteristics of the populations of the levels in the $2s^22p^33s$ and $2p^22p^33p$ configurations and the gains on the fast transitions between them. The $3p\,^3D_2 - 3s\,^3P_1$, $3p\,^3P_2 - 3s\,^3P_1$, and $3p\,^1S_0 - 3s\,^3P_1$
transitions have large gains. The calculated gain on the $3p^1 S_0 - 3s^1 P_1$ transition was found to be in good agreement with the experimental observation. The maximum of the gain on each transition occurs around $N_e = 10^{18} \text{ cm}^{-3}$. The density dependences of the gains at low and high temperatures are similar.

The effect of the gains due to reabsorption seems negligible if the opacity on the $2p^1 S_0 - 3s^1 P_1$ is less than 2 and the electron density is smaller than $10^{18} \text{ cm}^{-3}$. For a higher density than $10^{18} \text{ cm}^{-3}$, the opacity even increases the gains because the reduced radiative decay rates of the transitions between the $2s^2 2p^5 3d$, $2s 2p^6 3p$, and $2s^2 2p^6$ configurations eventually result in the increase of the population of the $3p^1 S_0$ level via collisional and radiative cascades.

ACKNOWLEDGMENTS

This work has been supported in part by POSTECH/BSRI special fund, the Basic Science Research Institute Program, Ministry of Education (Project No: BSRI-97-2439), Korea Research Foundation in 1997 and Korea Science Engineering Foundation (Contract No: 951-0205-01702).