SHORT WAVELENGTH LASER CALCULATIONS IN THE Be I, B I AND C I ISOELECTRONIC SEQUENCES
U. Feldman, J. Seely, G. Doschek

To cite this version:

HAL Id: jpa-00225869
https://hal.archives-ouvertes.fr/jpa-00225869
Submitted on 1 Jan 1986

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
SHORT WAVELENGTH LASER CALCULATIONS IN THE Be I, B I AND C I ISOELECTRONIC SEQUENCES

U. FELDMAN, J.F. SEELY and G.A. DOSCHEK

E.O. Hulburt Center for Space Research, Naval Research Laboratory, Washington, DC 20375-5000, U.S.A.

Abstract - Short Wavelength Laser Calculations in the Beryllium, Boron and Carbon Isoelectronic Sequences - Level populations of the 2s3p, 2s2p3p and 2s2p3p configurations in ions of the Be I, B I and C I isoelectronic sequences can be inverted with respect to populations of the 2s3s, 2s2s and 2s2p3s configurations by electron collisional pumping. In the case of B I and C I ions, the process is analogous to the process for Ne-like ions which has lately received considerable attention. In the case of Be I ions, the inversion is a consequence of the slow radiative decay of the 2s3p 3P2 and 2s3p 3P0 levels. Level populations are calculated for Be-like, B-like and C-like ions with atomic number Z between 18 and 36 and for electron densities from 10^{15} to 10^{22} cm^{-3}. For each of the Be I and B I isoelectronic sequences, 20 levels are involved with principal quantum number n equal either to 2 or 3. For the C I isoelectronic sequence 46 levels are involved. Using the level populations, gain coefficients are calculated for transitions of the type 2s3s - 2s3p, 2s2s - 2s2p and 2s2p3s - 2s2p3p. The calculated gain coefficients are compared to previous calculations. At high electron densities where collisional mixing of the excited levels becomes important, the intensities of the X-ray transitions from the 2s_{k=0}^{2p}m_{p=0,1} levels decrease relative to the X-ray transitions from the 2s_{k=1}^{2p}m_{3} and 2s_{k=2}^{2p}m_{3} levels where k=1, m=0 or k=2, m=0,1. The density dependence of these X-ray line ratios is calculated elsewhere /16,17/. These line ratios represent a promising diagnostic for electron density. Finally, the opacities of the 2s2p - 2s3s, 2s2p - 2s3s and 2s2p - 2s2p3s transitions are discussed for plasma parameters for which a reasonable gain can be achieved.

I. INTRODUCTION

The idea of using transitions of the type 2s_{k=0}^{2p}m_{p=0,1} levels - 2s_{k=0}^{2p}m_{p=0,1} where k = 0-5
for the generation of VUV and X-ray laser radiation originally appeared in the literature a decade ago. By using a simple three level model, Elton/1/ concluded that it is possible to extrapolate near UV ion laser transitions into the vacuum UV. In a subsequent paper, Palumbo and Elton/2/ carried out calculations of electron pumping in carbonlike ions. Zherikhin et al. /1/ found that significant amplification can be achieved for 3s–3p transitions in neonlike ions. Vinogradov et al. /3/ investigated population inversion of transitions in neonlike ions with atomic numbers \( Z = 7-15 \) and found that a steady state gain of \( \alpha = 20 \text{ cm}^{-1} \) may be expected for a particular transition \( 2s^22p^53s \, ^1p_1 - 2s^22p^53p \, ^1s_0 \). Depending on the atomic number, this transition is expected to appear in the 400-800 Å range. They also concluded that radiation trapping by the resonance lines \( 2s^22p^6 \, ^1S_0 - 2s^22p^53s \, ^1p_1 \) may drastically alter the gain. Several years later Vinogradov and Shlyaptsev/4/ calculated the population level inversions and gains in a stationary plasma containing neonlike ions allowing for radiative collision relaxation between all the 27 levels involving the four configurations \( 2s^22p \), \( 2s^22p^3s \), \( 2s^22p^3p \), and \( 2s^22p^3d \). They performed the calculations for a number of ions between Mg III and Fe XVII. According to them, the most important conclusion is that a steady state inversion with a gain higher than 0.1 cm\(^{-1}\) is found for a number of transitions.

Experiments with laser-produced calcium plasma have been reported by Iljukhin et al./5/. In rare shots, the evidence of gain at 600 Å has been observed; however shot to shot reproducibility has not been achieved and therefore the demonstration of lasing in these experiments is questionable.

Dahlback et al./6/ discussed the possibility of obtaining gain from neonlike krypton at 144 Å, using the discharge of the 5 TW Pithon electrical generator. Feldman et al./7/ used a similar approach to the one used to calculate the neonlike spectra of Krypton (Kr XXVII). They have shown that in a steady state plasma, the largest gain is expected from the \( 2s^22p^3s \, ^3p_1 - 2s^22p^53p \, ^1s_0 \) transition, and at an electron density of \( N_e = 10^{22} \text{ cm}^{-3} \) it can be as high as \( \alpha = 35 \text{ cm}^{-1} \) for a 1 keV plasma and twice this value for a 3 keV plasma. However, at lower electron densities \( (N_e = 10^{21} \text{ cm}^{-3}) \), several other transitions, e.g., \( 2s^22p^53s \, ^3p_1 - 2s^22p^53p \, ^3D_2 \) and the \( 2s^22p^3s \, ^1p_1 - 2s^22p^3p \, ^3S_1 \), can have gains which are within a factor of 1.5-2 of the one with the largest gain.

In a subsequent paper, Feldman et al./8/ have used the same approach to calculate the population inversions between the same configurations of neonlike ions with atomic numbers \( Z = 14 \) (Si V), 18 (Ar IX), 22 (Ti XIII),
It was shown that population inversions occur over a wide range of electron temperatures and electron densities from $10^{17}$ cm$^{-3}$ for Si V to $10^{22}$ cm$^{-3}$ for Kr XXVII. For all ions studied, the maximum value of population inversion ($N_{3p}/g_{3p} - N_{3s}/g_{3s}$) for the best transition involving the $2s^22p^53p$ $^1S_0$ level was found to be approximately equal to $4 \times 10^{-3} N_i$ where $N_i$ is the total density of neonlike ions. With the exception of Si V, laser gains greater than 1 cm$^{-1}$ are possible for all ions that were considered, and the gain increases with the atomic number $Z$ and reaches values of 2 to 30 cm$^{-1}$ for ions Ar IX through Kr XXVII. For a given value of electron density, there exists an optimum value of atomic number $Z$ which results in the highest gain. Figure 1 shows the gain as a function of density for the three transitions $2s^22p^53s^1P_1 - 2s^22p^53p^1S_0$, $2s^22p^53s^1P_1 - 2s^22p^53p^1D_2$, and $2s^22p^53s^3P_1 - 2s^22p^53p^3P_2$ marked by the numbers 1, 2, and 3.

![Diagram showing gain as a function of density for different ions](image)

**Fig. 1** - Calculated gain for the three transitions $2s^22p^53s^1P_1 - 2s^22p^53p^1S_0$, $2s^22p^53s^1P_1 - 2s^22p^53p^1D_2$, and $2s^22p^53s^3P_1 - 2s^22p^53p^3P_2$ marked by the numbers 1, 2, and 3. The adopted electron temperatures are approximately 50% of the ionization potentials.
A demonstration of gain from neonlike selenium was reported by Matthews et al./9/ and Rosen et al./10/ by using a 11 mm long target which was composed of a 750 Å layer of selenium and illuminated by green light (λ = 0.532 Å) along a line focus with dimensions of 0.02 x 1.12 cm. They reported gains of as much as 5.5 ± 1.0 cm⁻¹. The gain was seen on two transitions at 206.3 Å and at 209.6 Å. These transitions were not expected to show the largest gain. Surprisingly, they did not see any gain from the 2s²2p⁵3s¹p₁ - 2s²2p⁵3p¹s₀ transition at 183 Å which was expected to show the strongest gain. Moreover, they did not see any line at the expected wavelength. They also reported gain in yttrium foils. In a later presentation, Rosen et al./11/ reported repeating the selenium experiment with a longer line focus (3 cm) and at that time they saw the 183 Å line; however, at an intensity less than expected from the calculations discussed above.

II. LEVEL POPULATIONS AND GAIN

Level populations near ionization equilibrium are calculated by solving the coupled rate equations

\[
N_j \left[ \sum_{i<j} A_{ji} + N_e \left( \sum_{i<j} c_{ji} + \sum_{i>j} c_{ij} \right) \right] =
\]

\[
= N_e \left( \sum_{i<j} N_i c_{ij} + \sum_{i>j} N_i c_{ij} \right) + \sum N_i A_{ij}
\]

(1)

where

\[
\sum_{i=1}^{n} \left( \frac{N_i}{N_I} \right) = 1
\]

(2)

and \( N_e \) = electron number density (cm⁻³), \( N_i \) = population number density of level, \( N_I \) = the total number density of all levels of the ion, \( A_{ji} \) = spontaneous decay rate from level \( j \) to level \( i \) (s⁻¹), \( c_{ij} \) = electron impact excitation (deexcitation) rate coefficient from level \( j \) to level \( i \) (cm³ s⁻¹). The process of radiative recombination from the next higher ionization stage is ignored because near ionization equilibrium this process will be negligible compared to excitation within the ion in question. The excitation rate coefficients are calculated from collision strengths \( Q_{ij} \) using the equation
\[ c_{ij}^e = \frac{8.63 \times 10^{-6} \Delta E_{ij}}{g_i \, k \, T_e^{3/2}} \int \frac{Q(E_{ij}) \exp(-E/kT)}{\Delta E_{ij}} \, dE \]  

where \( \Delta E_{ij} \) = the transition energy (ergs), \( g_i \) = statistical weight of level \( i \), \( k \) = Boltzmann's constant, and \( T_e \) = electron temperature.

The atomic data used by us for all of the isoelectronic sequences discussed in the following sections, including energy levels, collision strengths, and spontaneous decay rates, have been obtained using a computer package developed at the University College London. A complete set of references for the computer package can be found in reference 7.

The actual number density of a level is obtained from the identity

\[ N_j = \frac{N_j}{N_i} \frac{N_i}{N_T} \frac{N_T}{N_e} \]  

where \( N_T \) is the total number density of all ionization stages. For a Doppler broadened spectral line, the gain coefficient is given by

\[ \mathcal{A} = \frac{\lambda_{ul} \, A_{ul}}{8 \pi} \left( \frac{M}{3\pi kT_i} \right)^{1/2} \frac{N_e}{N_i} \frac{N_i}{N_T} \left( \frac{N_i}{N_e} - \frac{N_i}{N_T} \right) \]  

where \( M \) = ion mass, \( \lambda_{ul} \) = wavelength of the transition, \( T_i \) = ion temperature and \( u \), \( \ell \) = upper and lower levels of the transition.

III. GAIN CALCULATIONS

The Berylliumlike Ions

A schematic energy level diagram of a typical berylliumlike ion is shown in Figure 2. The six lowest configurations \( 2s^2, 2s2p, 2p^2, 2s3s, 2s3p, \) and \( 2s3d \), which have a total of 20 levels, are the ones that primarily dominate the level populations of interest for an inversion based on a \( 3s-3p \) system. Level populations and gains were calculated for a number of different temperatures and electron densities using these six configurations. The calculations were then repeated for the same 20 levels, but with configuration interactions taken into account due to the \( 2p3s, 2p3p, \) and \( 2p3d \) configurations. The atomic data that included the interactions due to
the three additional configurations for Ar XV, Ti XIX, Ni XXV, Ge XXIX, and Kr XXXIII have been published by Bhatia et al.\cite{12}.

Reduced populations as a function of density, with and without the configuration interactions, are shown in Figure 3. The inversions occur because the $2s3p^2P_0$ and $2s3p^2P_2$ levels cannot decay fast or cannot decay at all to the $2s^21S_0$ level. At low densities, the population density is proportional to electron density. At these densities, excitation into excited states is followed immediately by radiative decay, and collisional mixing of excited levels can be ignored. At intermediate densities, collisional depopulation will become comparable to radiative decay for the $2s3p^2P_0$ and $2s3p^2P_2$ levels, and their populations will increase less rapidly than the density and eventually they will reach a plateau at about $1 \times 10^{-5}$. However, the populations of the other levels of the $2s3p^2$ configurations will continue to increase proportionally to the electron density, and at some high electron density the populations of the two sets of levels will equilibrate. At this electron density, population inversion will disappear.
Fig. 3 - Reduced populations, i.e., fractional level populations per unit statistical weight, for selected levels of Ti, Fe, Ge and Kr ions in the Be I isoelectronic sequence. The solid (dashed) lines are for the calculations with 6 (9) configurations. The adopted electron temperatures are approximately 670 eV (Ti XIX), 970 eV (Fe XXIII), 1500 eV (Ge XXIX) and 2000 eV (Kr XXXIII).

Results for the gain coefficient $\mathcal{J}$ are shown in Figure 4. In the gain calculations, the fractional abundances of the number densities of the berylliumlike ions were assumed to be one-fourth for all elements, and the electron temperature was taken to be one-half of the ionization temperature. The behavior of gain coefficient with atomic number can be understood by considering the fact that the gain is proportional to the product of the electron density and the difference of the reduced populations between the particular lasing levels.

The additional three configurations $2p3s$, $2p3p$ and $2p3d$ change the level populations as a function of density. As can be seen from the dashed lines in Figure 3, at the high density limit the reduced populations of the $^3P_2$ and $^3P_0$ levels change little while the reduced population of the $^3S_2$ level is lowered. As a result, the collisional limit is moved to higher electron densities. Since the gain is proportional to the difference of the reduced populations between the $^3P_2$ and $^3S_2$ levels, and since at the high density limit the populations of $^3P_2$ and $^3S_2$ are almost equal, a lower $^3S_2$ population will result in a higher gain. Moreover, a particular high density gain will appear for elements with lower atomic numbers than is the case without the additional three configurations. These results are seen in the dashed curves of Figure 4.
Figs. 4a,b - Calculated gain coefficient as a function of ion for fixed values of electron density between $10^{18}$ and $10^{22}$ cm$^{-3}$. The solid (dashed) lines are for calculations with 6 (9) configurations.
At the low density limit the picture is different. The populations of the \(3\text{p}_2\) level, and to a lesser extent, the \(3\text{p}_0\) level, are lower by a factor of \(\approx 3\), and as a result the gain is also lower for those densities.

In conclusion it is believed that additions of configurations to the basic ones will modify the calculations substantially. However, the basic picture remains unchanged.

At densities of \(10^{22} \text{ cm}^{-3}\), nickel and heavier elements have a gain of \(3 \text{ cm}^{-1}\) in the line \(2\text{s}3\text{s}^3\text{S} - 2\text{s}3\text{p}^3\text{P}_2\). The gain for the same transition decreases to about \(1 \text{ cm}^{-1}\) at a density of \(10^{21} \text{ cm}^{-1}\); however, at such densities, population inversion is already achieved for titanium and all the higher \(Z\) elements in the beryllium sequence. The \(2\text{s}3\text{s}^3\text{S}_1 - 2\text{s}3\text{p}^3\text{P}_0\) transition also shows gain; however, this gain is smaller by an order of magnitude. A complete description of gain calculations for berylliumlike ions in the six configuration case can be found in Feldman et al./13/.

The Boronlike Ions

A schematic energy level diagram of a typical ion in the boron isoelectronic sequence is shown in Figure 5. There are six configurations to consider: \(2s^22p\), \(2s2p^2\), \(2p^3\), \(2s^23s\), \(2s^23p\), and \(2s23d\). As for the berylliumlike ions, the lowest six configurations in the boronlike sequence have a total of 20 levels. The two transitions of interest in the gain calculations are \(2s^23s^2\text{S}_{1/2} - 2s^23p^2\text{P}_{3/2}\) and \(2s^23s^2\text{S}_{1/2} - 2s^23p^2\text{P}_{1/2}\). As in the case of the berylliumlike ions, the reduced populations of the two inverted levels reach a plateau somewhere below \(1 \times 10^{-4}\) (see Figure 6). The atomic data for the boron isoelectronic sequence, including Ar XIV through Kr XXXII, can be found in Bhatia et al./14/. The gain calculations of the boronlike ions are shown in Figure 7. Generally the calculated gains are similar to the results obtained from ions in the berylliumlike sequence. For nickel and higher \(Z\) ions, the gain of the \(2s^23s^2\text{S}_{1/2} - 2s^23p^2\text{P}_{3/2}\) transition is \(1 \text{ cm}^{-1}\) at a density of \(10^{22} \text{ cm}^{-3}\) and is \(0.6 \text{ cm}^{-1}\) at a density of \(10^{21} \text{ cm}^{-3}\). The gain of the second transition under similar conditions is a factor of \(\approx 2\) lower. For details see Feldman et al./13/.

The Carbonlike Ions

A partial schematic energy level diagram of a typical ion in the carbonlike isoelectronic sequence (Kr XXXI) is shown in Figure 8. The six lowest configurations \(2s^22p^2\), \(2s2p^3\), \(2p^4\), \(2s^22p3s\), \(2s^22p3p\) and \(2s^22p3d\) consist of
Fig. 5 - Schematic diagram of energy levels of the boronlike ion Kr XXXII.

Fig. 6 - Reduced populations of selected levels for Ti, Fe, Ge, Kr ions of the B I isoelectronic sequence. The adopted electron temperatures are approximately 600 eV (Ti XVIII), 900 eV (Fe XXII), 1400 eV (Ge XXVII) and 1900 eV (Kr XXXII).
Figs. 7a,b - Calculated gain coefficient as a function of ion for fixed values of electron density between $10^{17}$ and $10^{22}$ cm$^{-3}$.
Fig. 8 - The energy levels of Kr XXXI, the radiative decay rates, and the collisional excitation rate coefficients at an electron temperature of 1.8 keV. Only 20 of the 46 levels included in the model are shown here. The numerical keys assigned to the levels are also indicated. The upper levels of the transitions that have the highest calculated gain are levels 30 and 33.

46 levels. The collision strengths and radiative decay rates connecting the 46 levels have been published in Bhatia et al. 15/. The levels of most interest for population inversion and gain, the 2s2p3p 3D and 2s2p3p 3P levels, are shown in Figure 8 with some of the atomic data associated with them. At electron densities for which collisional mixing to other excited levels is unimportant, the populations of many of the 2s2p3p 3D and 3P levels are relatively high and actually exceed the populations of many of the 2s2p3s and 2s2p3d levels. This is illustrated in Figure 9 where the reduced populations of one representative level from each of the six configurations are presented. In Kr XXXI at an electron density of 10^{19} cm^{-3}, collisional depopulation of the 2s2p3d 3D level to the other excited levels becomes important and collisional equilibration of the n = 3 levels is nearly complete above 10^{22} cm^{-3}. For Kr XXXI, the electron density region from 10^{19} cm^{-3} to 10^{22} cm^{-3} is of interest for 3s-3p population inversions. For lower Z ions, the region of interest occurs at lower electron densities owing to the Z scaling of the atomic data. In general, the reduced populations of the inverted levels reach a plateau at a value somewhat lower than 10^{-4}, a value similar to those obtained in the beryllium and boronlike sequences.
Gain calculations of some transitions in Ar XIII, Ti XVII, Fe XXI, Zn XXV, Se XXIX and Kr XXXI are shown in Figure 10. The transitions that typically have the highest gain are between level numbers 30-23 and 33-24 in Kr XXXI. These transitions are \(2s^22p^33p^3 P_2 - 2s^22p^33p^3 D_2\) and \(2s^22p^33s^1 P_1 - 2s^22p^33p^3 D_2\) respectively. As is the case in beryllium and boronlike sequences at electron densities of \(10^{22}\) cm\(^{-3}\), the gain is \(Z = 2-3\) cm\(^{-1}\) for elements of \(Z > 28\). At a density of \(10^{21}\) cm\(^{-1}\) the gain is reduced by a factor of 3-10. Our calculated gains for transitions in Ar XIII are smaller than the ones calculated by Palumbo and Elton/2/. For a detailed description of the carbonlike gain calculation see Feldman et al./16/.

Optical Depths of the Resonance lines in Be I, B I and C I Sequences

One of the difficulties in obtaining population inversions in the \(3s-3p\) type transitions is the effect of opacity in increasing the population of the \(3s\) levels. Considering boronlike ions as an example, at the electron densities required for the production of X-ray lasers, both of the transitions that connect the lower laser level \(2s^23s^2S_{1/2}\) to the levels of the ground configuration \(2s^22p^2P_{1/2}, 2p^3/2\) can become optically thick. The opacity of these transitions results in an enhanced population of the \(2s^23s\) levels. In the case of the Ne I sequence there is only a single ground level, i.e., \(2s^22p^61S_0\), in which most of the ion population is concentrated. However in beryllium and boronlike ions, and even more so in
Fig. 10 - The calculated gain coefficients for transitions of the type \(3s-3p\) between levels designated 23 and 30 \((2s^22p3s^2P_2 - 2s^22p3p^3D_3)\) and between levels 24 and 33 \((2s^22p3s^1P_1 - 2s^22p3p^3P_2)\). Smooth curves have been drawn through the data points calculated for ions with atomic numbers \(Z = 18, 22, 26, 30, 34, \) and 36.

As examples of the magnitudes of the opacities involved, we calculate opacities at line center for selected transitions assuming a cylindrical geometry. The opacity is defined to be the opacity from the center of the cylinder out to the surface of the cylinder along the radius of the cylinder. The radius of the cylinder is determined by adopting a value of 5 for the product of the gain coefficient for a specific transition times the length of the cylinder, and by assuming that the radius of the cylinder is \(1/20\) of the length. Thus, the opacities we calculate depend on the value of a gain coefficient for a particular transition as well as on the

carbonlike ions, the number of low lying levels keeps increasing and the population density of each level is reduced. Since the opacity in a line is proportional to the population density of the lower level, one can expect that for some particular set of conditions the opacities in beryllium, boron and carbonlike ions will be somewhat reduced relative to the ions in the neon like sequence.
electron density. Examples of the magnitude of opacities involving the lower level of the transition with highest gain in krypton ions at an electron density of $10^{21}$ cm$^{-3}$ are given in Table I. In the neonlike selenium experiment described by Rosen et al./10/ and Matthews et al./9/ the ratio of the radius of the cylinder to the length was approximately 1/100. Under such conditions opacity is of little importance.

IV. CONCLUSIONS

The theoretical study of 3s-3p lasing transitions has been extended from the neonlike and carbonlike sequence calculations to include the berylliumlike and boronlike sequences, and a more thorough study of the carbonlike sequence. All of these sequences contain promising transitions for lasing. In addition, density diagnostic line ratios have been identified. However, much work remains to be done. Also, no published calculations yet exist for the N I and O I sequences; these sequences will certainly contain promising lasing transitions. Finally, under actual experimental conditions, lasing can occur in a non-ionization equilibrium situation. In this case additional processes, such as radiative, three-body, and dielectronic recombination, and perhaps resonances, can significantly affect level populations. No detailed study of how the effects of these processes scale with $Z$ has yet appeared in the literature, although specific calculations including these processes have been carried out for certain ions./10/ Perhaps one of the important deficiencies in our present knowledge is the lack of good, high resolution spectra that unambiguously reveal 3s-3p transitions in different isoelectronic sequences. These spectra are very difficult to obtain, because the 3s-3p lines are weak if they are not amplified, and they fall next to much stronger resonance lines of lower ionization stages, e.g., the neonlike lines fall near strong sodiumlike lines.

We stress that an important reason for considering the possibility of lasing transitions in 3s-3p type sequences other than neonlike is that the addition of these sequences greatly increases the number of lines in the same general wavelength range for which amplification can be achieved. Even though the neonlike sequence has several advantages over the other sequences in the presently available experiments, in the future the possibility of cavities or better target designs will greatly improve the X-ray amplifiers and may result in a more or less equivalence between lasing lines of different sequences. In this admittedly speculative situation, the presence of many lines from several sequences and elements
would allow the 3s-3p laser to be tunable over a rather broad wavelength range, which should increase its value for certain applications.

REFERENCES