High gain inner-shell x-ray lasers pumped by X-ray Free-electron laser system FLASH in DESY

J. Zhao1†, Q. L. Dong1, S. J. Wang1, L. Zhang1 and J. Zhang1,2‡
1Beijing National laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China
2Department of Physics, Shanghai Jiao Tong University, Shanghai 200240, China
E-mail: †zhaoj@aphy.iphy.ac.cn, ‡jzhang@aphy.iphy.ac.cn

Abstract. The feasibility of generating high gain inner-shell x-ray lasers photo-ionization pumped by the DESY/XFEL facility is studied. The gain characteristics are analyzed for the two representative schemes of inner-shell x-ray transitions, the self-terminated x-ray lasing (1s)−1→(2p)−1 (λ=4.5 nm) in carbon (Z=6) and the quasi-stationary x-ray lasing (2p)−1→(3s)−1 (λ=4.1 nm) in calcium (Z=20). When the third harmonic XFEL pumping pulses of 10 fs at 284 eV and 360 eV with the pumping intensities of 6×10^{14} W/cm^2 and 1×10^{17} W/cm^2 for C and Ca are available, respectively, a net gain of 120 cm^{-1} are predicted with quite short durations of 10 fs and 2 fs. Our studies show that DESY/XFEL facility is sufficient to generate the high gain photo-ionization pumped $K_{\alpha}$ radiations in low Z atoms.

1. Introduction
First proposed by Duguay and Rentzepis [1] in 1967, the photo-ionization-pumped inner-shell x-ray laser (ISXRL) is one of the promising way for generating coherent ultra-short (∼10 fs) x-ray lasing at short wavelength within the “water window” (2.3 – 4.4 nm) or even shorter than 1 nm. Vast theoretical studies have been performed on the gain characteristics of inner-shell transitions in various atomic systems pumped by different sources (blackbody and Larmor radiations, electron beams) [2, 3, 4, 5]. However, the lasing has not been demonstrated experimentally, because of the critical requirement for high intense x-ray source with short rise time due to the fast Auger decay of inner-shell holes and the huge reabsorption as the stimulated line emission propagates.

Recently, the x-ray free-electron lasers (XFEL), operating at tunable fundamental wavelengths from 6 to 30 nm, delivering ultra-short (10 ~ 50 fs), high-power laser flashes, has been established at the DESY research center in Hamburg in 2005 [6]. In this paper, we theoretically discuss the feasibility of the production of the photo-ionization pumped ISXRL, using the XFEL as an x-ray source. Two characteristic atomic systems (carbon, calcium) with representative inner-shell transition processes of (1s)^{-1}→(2p)^{-1} (λ=4.5 nm), (2p)^{-1}→(3s)^{-1} (λ=4.1 nm), are studied. We use the Flexible Atomic Code (FAC) [7] to generate the atomic data like the energy levels (j-j coupling) and the rates of photoionization, electron collisional ionization and radiative decay. The Auger or Coster-Kronig rates are taken from the calculations carried out by McGuire [8].

2. Model Analysis
Figure. 1 shows the pumping scheme with the main inner-shell vacancy levels (IVL’s) (the ground
state of the neutral atom 0, and the upper and lower states 2 and 1) and atomic processes considered in the photo-ionization pumped ISXRL. Initial population inversion is achieved by the direct photoionization of the upper energy level \( N_2 \) with a hole in 1s (C) or 2p (Ca) inner-shell by an x-ray source with the energy just above the ionization threshold. The photon energy of 284 or 360 eV maximizes the photoionization cross section of the 1s or 2p inner-shell electron in carbon or calcium, and minimizes the secondary electrons production by the photoionization of outer-shell electrons. Much of the population of the upper state is depleted through the subsequent Auger decay. And the energetic Auger electrons (280 eV, 300 eV, respectively) collisionally ionize the outer-shell electrons 2p (C) or 3s (Ca) of the neutral atoms and thereby produce the lower state. This destroys the inversion for the (1s)\(^{-1} \rightarrow 2p\)\(^{-1}\) \((\lambda = 4.5 \text{ nm})\) transition in carbon, for the lower state (2p)\(^{-1}\) does not decay. However, the lower state (3s)\(^{-1}\) of calcium that undergoes the fast Coster-Kronig decay has the decay rate significantly larger than that of the deeper vacancy state (2p)\(^{-1}\). A quasi-stationary population inversion can be expected in calcium.

The gain coefficient is calculated through the rate equations concerning the lasing transitions:

\[
\dot{N}_0 = -N_0(R^e_{\text{total}} + R^p_{\text{total}}) \tag{1}
\]
\[
\dot{N}_2 = N_0(R^e_{02} + R^p_{02}) - D_2N_2 \tag{2}
\]
\[
\dot{N}_1 = N_0(R^e_{01} + R^p_{01}) - D_1N_1 \tag{3}
\]

The ground state of the neutral atom is the state 0, and the upper and lower states of the single ionic stage are the states 2 and 1, respectively. \( N_k \) is the population for each state \( k \); \( R^e_{0k} = n_e\sigma_{0k}\nu_e \) is the electron impact ionization rate (considering only monoenergetic Auger electrons), \( R^p_{0k} = I\sigma(\nu)/h\nu \) the photoionization rate with the spectral bandwidth of the XFEL \( \Delta\nu/\nu \ll 1 \) considered; \( R_{\text{total}} \) is the total rates summed over all the single ion levels; \( D_k \) the decay rate including radiative, Auger and Coster-Kronig processes, photo-ionization and electron collisional ionization from single ions to all the possible double ions. The gain of x-ray lasing between the inner-shell vacancies is given by \( G_{\text{inv}} = \sigma_g(N_2 - gN_1). \) \( g = g_2/g_1 \) is the ratio of the statistical weights and \( \sigma_g = A_{ul}\frac{\lambda^3}{8\pi\hbar c\Delta\nu} \) is the stimulated emission cross section. The effective gain \( G_{\text{eff}} \) is the difference between \( G_{\text{inv}} \) and the absorption of the lasing line by neutrals and ions: \( G_{\text{eff}} = G_{\text{inv}} - \alpha_{\text{abs}}. \) The approximation of the absorption coefficient is \( \alpha_{\text{abs}}(\text{cm}^{-1}) = \mu(\text{cm}^2/\text{gm})*\rho(\text{gm}/\text{cm}^3), \) where \( \mu(\text{cm}^2/\text{gm}) \) is the photoabsorption cross section, taken from a synthesis of the currently available experimental data and theoretical calculations.

3. FEL pumping
The temporal intensity profile of XFEL pulses is assumed as

\[
I(t) = \begin{cases} 
I_p\sin^2(\pi t/2\tau) & 0 \leq t \leq 2\tau \\
0 & t > 2\tau 
\end{cases} \tag{4}
\]

\( t \) is the time, \( \tau \) is the full width at half-maximum intensity (FWHM) and \( I_p \) is the peak intensity.
3.1. Self-terminated inner-shell lasing in Carbon

Figure 2 shows ions population and gain evolution for the XFEL pumping radiation at 284 eV with a peak intensity of $3 \times 10^{14}$ W/cm$^2$ and FWHM of $\tau = 20$ fs. The initial neutral density of carbon is $2.28 \times 10^{21}$ cm$^{-3}$. The pumping pulse starts at time $t = 0$. The time evolution of the populations of single IVL’s (1s)$^{-1}$, (2s)$^{-1}$, (2p)$^{-1}$ is shown in Fig. 2(a). Figure 2(b) shows that $G_{inv}$ is obtained from the beginning of the third harmonic XFEL pulses. The value of $G_{inv}$ reaches its maximum ($140$ cm$^{-1}$) at the peak time ($t = 20$ fs) of the pumping radiation and rapidly decreases when excessive Auger electrons are produced.

We also investigated the influence of the XFEL pulse width, shown in Fig. 3. Compared to the XFEL pulse radiation with $2\tau = 40$ fs, the pulse with a shorter duration $2\tau = 20$ fs (half radiation energy) gives higher gain coefficient $G_{inv}$. With the same pumping power, the shorter pulse $2\tau = 10$ fs produces larger gain coefficient. Because of the fast Auger decay of the inner-shell upper state, the ultrashort ($\sim 10$ fs) pumping radiation is necessary in achieving high gain ISXRL in carbon. Figure 3 shows sufficient high net gain $\simeq 120$ cm$^{-1}$ can be reached with a FWHM of 5 fs for the inner-shell $K_{\alpha}$ transitions of carbon, pumped by an XFEL radiation pulse with a peak intensity of $6 \times 10^{14}$ W/cm$^2$ and a pulse duration $2\tau = 10$ fs. Assume the focal spot of $1 \mu$m, the flux energy of the third harmonics at 284 eV is estimated to be $\sim 4$ nJ.
3.2. Quasi-stationary inner-shell lasing in Calcium

The initial neutral density of Ca is set as $1.2 \times 10^{21}$ cm$^{-3}$. The absorption coefficient of the lasing line is approximately 480 cm$^{-1}$. Figure 4 gives the gain performance pumped of two different pumping conditions. Compared to the self-terminated $K_\alpha$ transitions in carbon ($Z = 6$), more complicated energy levels are included in the atomic processes and more pumping power is required to get sufficient population inversion. From Fig. 4(b), a shorter (10 fs) and smaller pumping power ($I_p = 1 \times 10^{17}$ W/cm$^2$) can generate a higher net peak gain $\approx 120$ cm$^{-1}$. But the duration of net gain is quite short about 2 fs.

4. Conclusion

According to our simulations, the net gain of 120 cm$^{-1}$ can be obtained for the self-terminated $(2p)^{-1} \rightarrow (3s)^{-1}$ (λ = 4.1 nm) transitions in carbon ($Z = 6$) and the quasi-stationary population inversion scheme transitions $(2p)^{-1} \rightarrow (3s)^{-1}$ (λ = 4.1 nm) in calcium ($Z = 20$) pumped by the 10 fs third harmonics from the XFEL’s at 284 eV and 360 eV with the intensities of $6 \times 10^{14}$ W/cm$^2$ and $1 \times 10^{17}$ W/cm$^2$, respectively. The gain has short durations of 10 fs and 2 fs. We find that high gain photo-ionization pumped $K_\alpha$ radiations in low Z atoms could be realized using DESY/XFEL facility as a pumping source.

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References

[1] Duguay M A and Rentzepis G P 1967 Appl. Phys. Lett 10 350
[2] Moon S J and Eder D C 1998 Phys. Rev. A 57 1391
[3] Moribayashi K, Sasaki A and Tajima T 1999 Phys. Rev. A 59 2732
[4] Hooker S M 2000 Opt. Commu 182 209
[5] Kim D, Son S H, Kim J H, Toth C and Barty C P J 2001 Phys. Rev. A 63 023806
[6] Jeandron M 2005 Phys. World 18 8
[7] Gu M F 2003 Astrophys. J 582 1241
[8] McGuire E J 1972 Phys. Rev. A 5 1052