Photorecombination studies of highly charged tungsten ions at Shanghai EBIT

B. Tu, J. Xiao, K. Yao, X. Wang, Y. Shen, Y. Yang, D. Lu, L. Huang, C. Zhen, Y. Fu, B. Wei, R. Hutton, and Y. Zou
Shanghai EBIT Laboratory, Institute of Modern Physics, and Key Laboratory of Nuclear Physics and Ion-beam Application (MOE), Fudan University, Shanghai, China
E-mail: bingshengtu@fudan.edu.cn; keyao@fudan.edu.cn; zouym@fudan.edu.cn

Abstract. In this paper, we report studies on photorecombination (PR) processes for highly charged W ions. The experiment was performed at Shanghai electron beam ion trap by employing a fast electron beam-energy scanning technique. The KLL dielectronic recombination (DR) resonance strengths for He- up to O-like W ions were determined. The strong interference effect between DR and radiative recombination (RR) was observed and the Fano factor, which measures the interference degree, was determined for the main resonances of ground state He-, Be-, B-, C-, N-, and O-like W ions. In addition, we show experimentally that an autoionizing state can have both Fano and Lorentzian behavior naturally, depending on the processes involved. A fully relativistic configuration interaction method implemented in the flexible atomic code was employed to calculate DR, RR processes and also the interference effect.

1. Introduction
Dielectronic recombination (DR) of an ion is used to be considered a resonant two-step process. In the first step, a free electron is captured by the ion; at the same time a bound electron in the ion is promoted to form a multiply excited intermediate state sitting above the autoionization threshold. The second step is stabilization, in which photons are emitted so as to reduce the ion energy to below its ionization limit. DR is an important process in hot plasma physics as well as in atomic structure and collision theory [1]. It significantly affects the plasma temperature, the charge state distribution, ion level population, and produces some unresolvable satellites which may disturb line shape, line intensity, and line width, while the resolved satellite lines are very useful in electron temperature diagnostics [2]. Furthermore, DR of heavy ions contributes significantly to radiation energy loss in fusion plasmas, and thus leading to the severe problem on the quenching of fusion.

There is another non-resonant process called radiative recombination (RR), in which a free electron is captured by an ion and the excess energy is released by emitting a photon directly. Both DR and RR are electron-ion recombination processes with photon emissions, so they are classified as photorecombination (PR). If DR and RR have identical initial states, final states, and photon emissions, it is then impossible to distinguish through which process the recombination takes place, and interference would occur. As a consequence, asymmetric resonant line shape (Fano profile) appears. Such asymmetric resonances are ubiquitous in essentially many fields [3–5], through nuclear, atomic, molecular, and solid-state physics. Much work has been done to study PR processes, but only a very few studies have observed DR-RR interference [6–8].
due to the fact that most studies were for the cases where RR was much weaker than DR and the interference was negligible.

In this paper, we report the recent studies on PR processes for highly charged W ions at the upgraded Shanghai electron-beam ion trap (Shanghai-EBIT) [9]. The KLL DR resonance strengths as well as the DR-RR interference effect for He- up to O-like W ions were studied [10,11]. The dual Fano and Lorentzian line profile properties in an autoionizing state was also demonstrated via selecting the DR resonances which go through an intermediate state with decay channels to both the final states with no excited electrons and the final states with more than two electrons in the excited orbital [12]. The calculation was implemented through the method of relativistic configuration interaction (RCI) under the framework of Fano theory [13] by flexible atomic code (FAC) [14].

2. Experiment

The experiment was performed at Shanghai EBIT. The experimental setup was shown in Figure 1. During the experiment, the volatile organic compound W(CO)$_6$ was continuously injected into the trap region by a gas injection system. The electron energy was adjusted following the time sequence shown in Fig. 1, to produce the right charge states of W ions, and to scan through the DR resonances. To cover all the charge states from He-like to O-like W ions, we performed two sets of experiments with different parameters as listed in Table I. The narrower energy scanning region in Expt. B was for the resonances, which were not measured in Expt. A so that a relative higher detection efficiency can be achieved for these weak resonances.

![Figure 1. The sketch of experimental setup used in the PR measurement for W ions.](image)

In both experiments, the x-ray photons were detected by employing an ORTEC high purity germanium detector in the direction perpendicular to the electron beam. The event mode data acquisition system was triggered by an arrival x-ray photon. The photon energy and the corresponding electron beam energy were recorded simultaneously, forming the 2D scatter plots as shown in Fig. 2(a) and 2(b), respectively. In Fig. 2(a), the resonance peaks are from KLL DR events of He- up to C-like W ions. Those peaks lie in three distinct regions $39 \sim 40$ keV, $41 \sim 42$ keV, and $42.5 \sim 43.5$ keV, which are referred to as $KL_{12}L_{12}$, $KL_{12}L_3$, and $KL_3L_3$ manifolds, respectively. The events on the clear diagonal bands correspond to the RR processes with principal quantum number $n = 2$. In Fig. 2(b), $KL_3L_3$ DR peaks of Be- up to O-like are obtained. The $n = 2$ and $J = 1/2$ RR band is almost missing in this figure due to a lack of He- and Li-like ions. The raw data of recombination events were cut and then projected onto the electron beam axis to obtain the excitation function.
Table 1. Two sets of operating parameters in the experiments.

|                           | Expt. A | Expt. B |
|---------------------------|---------|---------|
| cooking energy (keV)      | 43.8    | 44.1    |
| Electron energy scanned (keV) | 39 $\sim$ 43.8 | 42.5 $\sim$ 44.1 |
| Electron beam current (mA) | 170     | 140     |
| Gas injection pressure (torr) | $5 \times 10^{-8}$ | $2 \times 10^{-7}$ |
| Trapping potential (V)    | 60      | 130     |
| Charge state obtained     | He- up to C-like | Be- up to O-like |

Figure 2. 2D scatter plots for PR measurements from Expt.A (a) and Expt.B (b), as a function of electron energy for the x-axis and photon energy for the y-axis. (Taken from [11])

3. Results and Discussion

The total recombination excitation function including both DR and RR cross section was used to fit the experimental data as following:

$$C(q, E) = D(E)f_q \frac{d\sigma_{RR}(q, E)}{d\Omega} + \sum_{idf} S_{idf} \times DR(q, E) \times W_{df}(90^\circ),$$

(1)

where $D(E)$ is the detection efficiency coefficient. $f_q$ is the ion abundance for the charge state $q$. $d\sigma_{RR}(q, E)/d\Omega$ is the differential cross section of RR at 90°. $W_{df}(90^\circ)$ is the angular distribution coefficient at 90° for electric dipole transition. $S_{idf}$ is the DR resonance strength from an initial state $i$ via a middle state $d$ to a final state $f$. $DR(q, E)$ is the energy distribution of the resonance profile. In the isolated-resonance and independent-processes approximation, DR resonance has an isolated Lorenzian line shape. However, a strong interference effect exists between DR and RR for heavy ions, which leads to an asymmetric line shape called Fano profile expressed as

$$F(E) = \frac{2}{\sqrt{2\pi\Gamma_d}} \frac{(Q + \epsilon)^2 + (B_a - 1)^2}{1 + \epsilon^2} - 1, \quad \epsilon = \frac{2(E_e - E_d)}{\Gamma_d}; \quad Q = \frac{2\langle i|V|d\rangle\langle d|R|f\rangle}{\Gamma_d\langle i|R|f\rangle},$$

(2)

where $\Gamma_d$ is the natural line width, $B_a = \Gamma_a/\Gamma_d$ is the autoionization branch ratio of the resonant state and $E_e$ is the incident electron energy. $\langle j|V|d\rangle$, $\langle d|R|f\rangle$ and $\langle j|R|f\rangle$ are the autoionization, spontaneous radiation and RR matrix element, respectively. $Q$ called fano factor, represents the degree of interference. Note that $L_F(E)$ is equivalent to Lorentzian when $Q$ tends to infinite. In an EBIT, the electron beam has an energy spread with a Gaussian profile. For comparison with the experiment results both the Lorentzian and Fano profile should be convoluted with a Gaussian distribution (details can be found in [10, 12]).
In the total recombination excitation function, $S_{idf}$, $D(E)$ and $f_q$ are the free parameters. All the other parameters are calculated using the relativistic configuration interaction (RCI) method by FAC. The PR excitation function for W ions, which were obtained by projecting the raw data of the 2D scatter plots to the electron energy axis, were then fitted by an iterative least-squares method with the theoretical $S_{idf}$ as the initial value.

**Table 2.** The total experimental resonance strength ($10^{-20}$cm$^{-2}$eV) of KLL DR W ions obtained by both Fano ($S_{\text{expt}}(\text{Fano})$) and Lorentz($S_{\text{expt}}(\text{Lorentz})$) line profile fitting, together with the theoretical data($S_{\text{theory}}$) results.

| Charge state | $S_{\text{expt}}(\text{Fano})$ | $S_{\text{expt}}(\text{Lorentz})$ | $S_{\text{theory}}$ |
|--------------|-------------------------------|-------------------------------|-------------------|
| He           | 22.99(2.13)                   | 23.26(2.35)                   | 22.35             |
| Li           | 14.31(1.20)                   | 12.58(1.08)                   | 13.70             |
| Be           | 10.17(0.77)                   | 10.16(0.88)                   | 9.95              |
| B            | 6.18(0.50)                    | 6.62(0.54)                    | 6.05              |
| C            | 2.85(0.27)                    | 3.18(0.28)                    | 2.81              |
| N            | 1.37(0.09)                    | 1.44(0.10)                    | 1.35              |
| O            | 0.41(0.03)                    | 0.46(0.04)                    | 0.43              |

**Figure 3.** The excitation function of He- up to O-like DR resonances for Expt. A in (a) and Expt. B in (b). The experimental data (solid black) is fitted by Fano profile (solid red) and Lorentzian (dash blue). The grey dot line shows the distribution of $n = 2$ RR. (Taken from [10])

The fitting results of the experimental excitation function for Expt.A and B are shown in figure 3(a) and 3(b), respectively. The black curves are the experimental data. The Fano profile fitting curves and Lorentzian curves are represented by red solid line and blue dash line, respectively. In figure 3(a), He- up to C-like DR resonance peaks including all the $KL_{12}L_{12}$, $KL_{12}L_3$, $KL_{3}L_3$ manifolds are well resolved. Other $KL_{3}L_3$ resonant peaks of Be-like up to O-like were shown in figure 3 (b). In figure 3(a), there is an explicit deficit on the left side and excess on the right side of $KL_{12}L_3$ manifold. Such an asymmetric Fano line profile is mainly caused by the interference effect between DR and RR of Be-like ions, which dominate the charge state distribution in Expt.A. Thus, the fitting curve of Fano profile is more tailored than the Lorentz fit. However, two line profile fitting curves show little difference in figure 3 (b). It is because that the resonant states in $KL_{3}L_3$ manifold have both Fano and Lorentzian profiles for B- up to O-like ions, consequently diluting the large degree of asymmetric line shape. In general, the experimental results from two different fitting functions for He- up to O-like resonance strengths agree with each other and with our calculation within the error bars as listed in Table II. Note that the results of Fano fit are much closer to the calculations than the Lorentz fit, and for some
charge states as Li-, C- and O-like the Lorentz fit also shows the deviation of about 10% from the Fano fitting results, however, due to the both experimental uncertainties also at this level, the advantage of Fano profile in the determination of resonance strengths is not conspicuously reflected in this case.

Table 3. The obtained resonance energies (\(E_d\)) and their corresponding measured Fano factors (\(Q_{\text{meas}}\)), calculation results (\(Q_{\text{cal}}\)) and (\(Q_{\text{aver}}\)), together with the measured energy shifts of the peak recombination cross sections.

| Label | Intermediate state | Final state | \(E_d\) (eV) | \(Q_{\text{meas}}\) | \(Q_{\text{cal}}\) | \(Q_{\text{aver}}\) | \(E_{\text{shift}}\) (eV) |
|-------|-------------------|-------------|---------------|----------------|----------------|----------------|-----------------|
| Be1   | \(1s^22s^22p_{3/2}\) | \(1s^22s^22p_{1/2}\) | 40917.8(1.9) | −12.3(1.8) | −13.2 | | |
| Be2   | \(1s^22s^22p_{3/2}\) | \(1s^22s^22p_{1/2}\) | 39897.7(2.0) | −12.3(1.9) | −13.3 | | |
| Be3   | \(1s^22s^22p_{3/2}\) | \(1s^22s^22p_{1/2}\) | 41442.1(1.9) | 12.7(1.7) | 14.9 | | |
| Be4   | \(1s^22s^22p_{3/2}\) | \(1s^22s^22p_{1/2}\) | 42888.3(1.2) | 17.4(2.4) | 15.2 | | |
| B1    | \(1s^22s^22p_{3/2}\) | \(1s^22s^22p_{1/2}\) | 41591(1.8) | 26.5(6.8) | 9.3 | | 27.4* |
| C1    | \(1s^22s^22p_{3/2}\) | \(1s^22s^22p_{1/2}\) | 43238.9(0.8) | 4.4(0.4) | 4.3 | | 9.8(0.8) |
| N1    | \(1s^22s^22p_{3/2}\) | \(1s^22s^22p_{1/2}\) | 43485(1.0) | 13.4(2.1) | 13.7 | | 3.5(0.6) |
| O1    | \(1s^22s^22p_{3/2}\) | \(1s^22s^22p_{1/2}\) | 43741(1.3) | 11.8(1.6) | 10.5 | | 4.3(0.8) |

* Obtained by averaging the Q values weighted with the branching ratios of the two transition channels.

Figure 4. The excitation functions of the \(KLL\) DR resonances for C-like W ions through the interference channel (a) and non-interference channel (b). The energy shift of the peak recombination cross section caused by the interference can be seen clearly in (c), comparing the peak position in (d). (Taken from [12])

In order to study the DR-RR interference effect in the isolated resonances, a state-selective method, which was introduced in [7,11,12], was used in data analysis. Figure 4a shows the resonant excitation function of the C-like W. The asymmetry is very clear, which indicates strong interference. The Fano line profile was used to fit the the excitation function. The result of the well resolved autoionizing state of \([1s^22s^22p_{1/2}(2p_{3/2})]_{5/2}\) shows a Fano factor of 4.4. Through the same method, the DR-RR interference effects in a total number of 9 isolated resonances in the PR measurements were studied and their Fano factors were obtained, as listed in Table III. All the experimental results, except that of Be2, agree very well with the calculation results. For B1 resonance, there are two inseparable stabilization channels with different Fano factors, so we tried to average the Fano factor weighted with the branching ratios of the two transition channels. The good agreement between the average Fano factor and the experimental result indicates that this treatment was appropriate.
In figure 4, the events marked as C(1) are from the DR processes of ground state C-like W ions through autoionizing states of \([1s^22s^2p_{1/2}^2(2p_{3/2}^2)]_{5/2}\), \([1s^22s^2p_{1/2}^2(2p_{3/2}^2)]_{3/2}\), and \([1s^22s^22p_{1/2}^2(2p_{3/2}^2)]_{1/2}\), to the final state of \([1s^22s^2p_{1/2}^2(2p_{3/2}^2)]_{3/2}\). Those designated as C(2) are through the same intermediate states, but to the final states with two electrons in the excited orbital of \(2p_{3/2}\), \([1s^22s^22p_{1/2}(2p_{3/2}^2)]_{3/2}\), \([1s^22s^22p_{1/2}(2p_{3/2}^2)]_{5/2}\), and \([1s^22s^22p_{1/2}(2p_{3/2}^2)]_{1/2}\). Figure 4a shows asymmetric line profiles, while 4b does not. It is obvious as C(1) sits on the RR band (shown in figure 2(b)) so interference occurs, while C(2) is located outside of the RR band and consequently no interfere with RR. The Fano profile fittings lead to a fano factor of 4.4 for the well-resolved resonance \([1s^22s^2p_{1/2}^2(2p_{3/2}^2)]_{5/2}\) in C(1), but infinite for the same resonance in C(2). The very different Fano parameters indicate that an autoionizing state can have both Fano and Lorentzian behavior naturally, depending on the processes involved. Comparing the peak positions of the interference and non-interference channel for \([1s^22s^2p_{1/2}^2(2p_{3/2}^2)]_{3/2}\) in figure 4a and 4b (for clearer, see figure 4c and 4d), the energy shift of the peak recombination cross section caused by the interference was obtained as 9.8 (0.8) eV (see in Table III). In the same treatment, for N-like and O-like autoionizing states of \([1s^22s^22p_{1/2}^2(2p_{3/2}^2)]_{3/2}\) and \([1s^22s^22p_{1/2}^2(2p_{3/2}^2)]_{1/2}\), the measured energy shifts are 3.5(0.6) and 4.3(0.8), respectively. For other resonances, due to the lack of non-interference channel for comparing with, the energy shift of the interference peak was not obtained.

4. Summary
In this report, we present the studies at Shanghai EBIT, of photorecombination of highly charged W ions, mainly from He-like up to O-like. This work determined the KLL total resonant strengths for the W ions of these charge states. The interference between DR and RR were observed, and it is quite strong in some cases, leading to the difference of the fitted resonant strengths between using Fano and Lorentzian profile as about 10% for some charge states. Our studies also revealed experimentally, that an autoionizing state can have both Fano and Lorentzian behavior, depending on the processes involved.

References
[1] Beiersdorfer P, May M, Scofield J and Hansen S 2012 High Energy Density Physics 8 271 – 283 ISSN 1574-1818
[2] Bitter M, Gu M F, Vainshtein L A, Beiersdorfer P, Bertschinger G, Marchuk O, Bell R, LeBlanc B, Hill K W, Johnson D and Roquemore L 2003 Phys. Rev. Lett. 91(26) 265001
[3] Eichmann U, Gallagher T F and Konik R M 2003 Phys. Rev. Lett. 90 233004
[4] Linn S H, Tzeng W B, Brom J M and Ng C Y 1983 J. Chem. Phys. 78 50
[5] Schmidt A R, Hamidian M H, Wahl P, Meier F, Balatsky A V, Garrett J D, Williams T J, Luke G M and Davis J C 2010 Nature 465 570
[6] Knapp D A, Beiersdorfer P, Chen M H, Scofield J H and Schneider D 1995 Phys. Rev. Lett. 74 54
[7] González Martínez A J, López-Urrutia J R C, Braun J, Brenner G, Bruhns H, Lapierre A, Mironov V, Soria Orts R, Tawara H, Trinczek M, Ulrich J and Scofield J H 2005 Phys. Rev. Lett. 94(20) 203201
[8] Nakamura N, Kavanagh A P, Watanabe H, Sakaue H A, Li Y, Kato D, Currell F J, Tong X M, Watanabe T and Ohtani S 2009 Phys. Rev. A 80(1) 014503
[9] Lu D, Yang Y, Xiao J, Shen Y, Fu Y, Wei B, Yao K, Hutton R and Zou Y 2014 Rev. Sci. Instrum. 85 093301
[10] Tu B, Xiao J, Shen Y, Yang Y, Lu D, Xu T H, Li W X, Chen C Y, Fu Y, Wei B and et al 2016 Physics of Plasmas 23 053301
[11] Tu B, Xiao J, Yao K, Shen Y, Yang Y, Lu D, Li W X, Qiu M L, Wang X, Chen C Y and et al 2016 Phys. Rev. A 93(3) 032707
[12] Tu B, Xiao J, Yao K, Shen Y, Yang Y, Lu D, Li W X, Qiu M L, Wang X, Chen C Y and et al 2015 Phys. Rev. A 91(6) 060502
[13] Fano U 1961 Phg. Rev. 124 1866
[14] Gu M F 2008 Cun. J. Phys. 86 675