

Dielectronic recombination of He-like to C-like iodine ionsH. Watanabe,^{1,2,*} H. Tobiya,¹ A. P. Kavanagh,³ Y. M. Li,⁴ N. Nakamura,¹ H. A. Sakaue,⁵ F. J. Currell,³ and S. Ohtani^{1,2}¹*Institute for Laser Science and Department of Applied Physics and Chemistry, University of Electro-Communications, Chofu, Tokyo 182-8585, Japan*²*CREST, Japan Science and Technology Agency, Chofu, Tokyo 182-8585, Japan*³*Queen's University Belfast, Belfast BT7 1NN, United Kingdom*⁴*Institute of Applied Physics and Computational Mathematics, P. O. Box 8009, Beijing 100088, China*⁵*National Institute for Fusion Science, Toki, Gifu 509-5292, Japan*

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KLL dielectronic recombination resonances, where a free electron is captured into the *L* shell and at the same time a *K* shell electron is excited into the *L* shell, have been measured for open shell iodine ions by measuring the detected yield of escaping ions of various charge states and modeling the charge balance in an electron beam ion trap. In the modeling, the escape from the trap and multiple charge exchange were considered. Extracted ions were used to measure the charge balance in the trap. The different charge states were clearly separated, which along with the correction for artifacts connected with ion escape and multiple charge exchange made the open shell highly charged ion measurements of this type possible for the first time. From the measured spectra resonant strengths were obtained. The results were $4.27(39) \times 10^{-19} \text{ cm}^2 \text{ eV}$, $2.91(26) \times 10^{-19} \text{ cm}^2 \text{ eV}$, $2.39(22) \times 10^{-19} \text{ cm}^2 \text{ eV}$, $1.49(14) \times 10^{-19} \text{ cm}^2 \text{ eV}$ and $7.64(76) \times 10^{-20} \text{ cm}^2 \text{ eV}$ for the iodine ions from He-like to C-like, respectively.

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I. INTRODUCTION

Dielectronic recombination (DR) is the resonant electron capture of a free electron via a doubly excited state accompanied by photon emission. It was first considered by Massey and Bates [1] to explain atomic processes relating to O^+ ions in the upper atmosphere. However, the importance of this process had not been realized for two decades until Burgess [2] pointed out that it had a large recombination rate in high temperature plasmas, in which the electron temperature was larger than one-fifth of the excitation energy of the first optically allowed transition of the recombining ion. The understanding of the DR process is considered very important nowadays due to the progress of the plasma research. For example, in fusion plasmas it is well known that the ions of heavy elements such as tungsten exist due to the sputtering of the wall materials of the vessel. The DR of such heavy ions is one of the primary sources of the radiation energy loss. Also, heavy elements such as xenon are introduced into the diverter of a fusion reactor. Radiative energy dissipation by highly charged ions reduces the concentration of the heat load due to the collisions of high energy ions to the diverter plates.

DR of highly charged ions has been measured with ion storage rings [3–5] and electron beam ion traps (EBITs) [6–12]. The atomic data of DR for open shell ions are relevant to the understanding of charge balances of practical plasmas, because such plasmas consist of various charge states of ions. In the case of EBIT experiments, the experimental method where x rays are measured with a solid state detector while the electron energy is scanned has been widely used [7–12]. When the electron energy matches DR

resonant energies, the x rays due to DR are measured. In this method, since it is practically impossible to produce a plasma in which a single charge state ion dominates, the x-ray spectrum obtained is sometimes a mixture of the x rays from different charge state ions. Therefore, extraction of atomic data such as resonant strengths from the obtained spectra is not straightforward. Alternatively, a crystal spectrometer can be used instead of the solid state detector [6]. With this method, the x rays from different charge state ions can be distinguished due to the higher energy resolution, making the open shell DR measurements possible. However, the crystal spectrometer has different sensitivity to the two polarization components of x-ray emission, so consideration of the polarization of x rays is required to obtain the cross sections and the resonant strengths. Furthermore, the sensitivity of this method is very low, requiring long run times, even for the strongest resonances.

We measured DR into open shell targets by measuring extracted ions from the EBIT, following the method used by Ali *et al.* [13,14] for DR of He-like Ar^{16+} with the addition of a procedure to account for ion escape from the trap and multiple charge exchange with neutrals. Here, multiple charge exchange means multiple electron captures from a neutral into a highly charged ion by a single collision. If extracted ions are used, the different charge state contributions can be easily separated and the correction of the polarization needed for the x-ray measurement is not required.

II. CHARGE BALANCE EQUATION

When equilibrium is achieved in the trap, the following relationship holds if the rates for ion escape from the trap and multiple charge exchange with neutrals are small [13,14]:

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$$n_{q-1}/n_q = \sigma_q^{DR}/\sigma_{q-1}^{EI} + [\sigma_q^{RR} + (e/j)n_0\sigma_q^{CX}\bar{v}_q]/\sigma_{q-1}^{EI}, \quad (1)$$

where n is the number density of ions in the trap, σ^{EI} , σ^{DR} , σ^{RR} , and σ^{CX} are the cross sections of electron impact ionization, DR, radiative recombination (RR), and single electron capture from neutrals, respectively, n_0 is the density of neutrals, \bar{v} is the mean velocity of the ions, e is the unit charge, and j is the electron current density. The subscript denotes the charge state of the ions.

The escape rate and the transport efficiency of the beam line can be considered to be the same for the adjacent charge state ions, because the electromagnetic effect caused by a single charge difference would be negligible for very highly charged ions of heavy elements. Thus, n_{q-1}/n_q is equal to the ion count ratio N_{q-1}/N_q , where N is the detected counts of the extracted ions over a fixed interval. The first term in the right hand side of the equation changes sharply with the electron energy around resonances, while the second term is slowly varying. If the ion count ratio is plotted with respect to the electron energy, the peaks appearing on the smooth background are from DR. Therefore, if the energy dependent portion of the ion count ratio is obtained, the DR spectra scaled with ionization cross sections are obtained. However, in the case of highly charged ions of heavy elements, escape from the trap and multiple charge exchange are not negligible with respect to the other processes. We modify Eq. (1) as shown below, taking the effect of ion escape from the trap and the multiple charge exchange into account:

$$n_{q-1}/n_q = (\sigma_q^{DR} + \sigma_q^{RR})/\sigma_{q-1}^{EI} + (e/j) \sum_{i=q}^{q_{\max}} (n_0\sigma_i^{CX(i-q+1)}\bar{v}_i + \epsilon_i) \times (n_i/n_q)/\sigma_{q-1}^{EI}, \quad (2)$$

where $\sigma^{CX(i)}$ is total cross section for more than $i-1$ electron capture from neutrals, ϵ the ion escape rate, and q_{\max} the maximum charge state in the trap. $\sigma^{CX(i)}$ can be written as $\sigma^{CX(i)} = \sum_{j=i}^{q_{\max}} \sigma_j^{CX}$, where σ_j^{CX} is the j electron capture cross section from neutrals. As one can recognize from the equation, additional structures could appear on the smooth background. Each term in the summation includes a factor n_i/n_q , a term which can rapidly vary with energy, giving rise to artifacts which are not connected with the DR resonance of interest. For example, consider the case when the beam energy passes through a resonance which reduces the population of charge state n_i for a particular value of i (i.e., DR into charge state $i-1$). Then, one of the terms in the summation of Eq. (2) will also reduce through reduction in the value of n_i/n_q , leading to a corresponding reduction in the ratio n_{q-1}/n_q . Therefore, the smooth background may show dips caused by the strong number density variation of higher charge state ions through the effects of ion escape and multiple charge exchange, which themselves do not have a strong energy dependence.

III. EXPERIMENT

The Tokyo-EBIT [16] at the University of Electro-Communications was used for the present measurement. The ions which escaped over the trap potential were extracted

into a beam line with 3 kV electrostatic potential. They were then dispersed with a sector magnet depending on their charge states. These ions were then introduced into an observation chamber equipped with a microchannel plate with a position sensitive resistive anode, so the ions with different charge states were measured simultaneously, to eliminate all effects originating from the fluctuation of the EBIT plasma. The electron energy was scanned from 19.5 keV to 22.5 keV with a 6 eV step. The electron current was 45 mA. The electron energy was increased every 10 s. We checked the time dependence of $N_{\text{Li-like}}/N_{\text{He-like}}$ at the resonance for this 10 s. No obvious time dependence was observed. Therefore, it is considered that the equilibrium was quickly achieved after the increase of the electron energy. However, the counts obtained during first 2 s were not used in the analysis to guarantee the charge equilibrium had been established. The electron energy was obtained by measuring the outputs of the power supplies which determine the electron energy with a voltage divider. The measured voltages were corrected by the calculated space charge potential of the electron beam. Because of this procedure, the accuracy of the absolute energy values are rather low and there would be the error of about a few tens of an eV. On the other hand, the error of the relative energy values is small, and is estimated to be 1.2%.

The assumption that the escape rate and the transport efficiency of the beam line were the same for the adjacent charge state ions was confirmed experimentally. We measured RR x-ray intensities of bare and H-like ions with a Ge detector. The count rates for RR into $n=1$ for these two charge states can clearly be resolved and in each case it is proportional to the number density of the trapped ions. The ratio of RR intensity of bare ions to twice that of H-like ions was calculated. This ratio is equal to the ratio of the number densities of the trapped ions, since the RR cross section of bare ions is twice that of H-like ions. This ratio was 0.077(2). At the same time, the ratio of the extracted bare ions to the H-like ions was measured, which gave 0.081(2). These ratios were consistent within the range of the uncertainties. Therefore, this assumption that escape rate and transport efficiency is the same for neighboring high charge states is justified.

IV. DATA REDUCTION

To obtain actual DR spectra, the effect of the ion escape and the multiple charge exchange should be estimated and artifacts connected with them removed from the data. Equation (2) can be rewritten as

$$\sigma_q^{DR}/\sigma_{q-1}^{EI} = n_{q-1}/n_q - \sum_{i=0}^{q_{\max}-q} \alpha_i n_{q+i}/n_q, \quad (3)$$

where $\alpha_0 = \sigma_q^{RR}/\sigma_{q-1}^{EI} + (e/j)(n_0\sigma_q^{CX}\bar{v}_q + \epsilon_q)/\sigma_{q-1}^{EI}$ and $\alpha_i = (e/j)(n_0\sigma_{q+i}^{CX(i+1)}\bar{v}_{q+i} + \epsilon_{q+i})/\sigma_{q-1}^{EI}$ ($i \geq 1$). The left hand side of the equation is 0 in the off-resonance regions. Then, Eq. (3) becomes

$$f(n_{q-1}, n_q, \dots, \alpha_0, \alpha_1, \dots) \equiv n_{q-1} - \sum_{i=0}^{q_{\max}-q} \alpha_i n_{q+i} = 0. \quad (4)$$

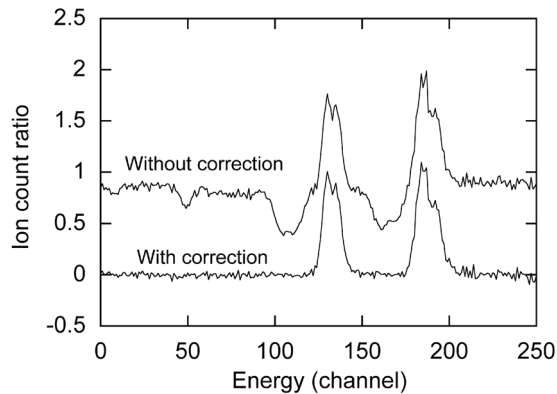


FIG. 1. The ion count ratios of B-like iodine ions with and without the correction for ion escape and multiple charge exchange. Dips in the uncorrected trace are artifacts connected with these processes as described in the main text.

Therefore, if the set of α_i which satisfies Eq. (4) is obtained in the off-resonance regions, the effect of the ion escape and the multiple charge exchange is corrected. In this study, α_i were estimated with the maximum likelihood method. We assumed that the number density $n_{k,l}$, where k specified the charge state of the ions and l specified the set of n_k at each electron energy, followed the normal distribution whose parent mean was $\mu_{k,l}$ and parent variance was $\sigma_{k,l}^2$. The likelihood function is defined as

$$L = \sum_{l=1}^{\nu} \sum_{k=q-1}^{q_{\max}} \left[-\frac{(n_{k,l} - \mu_{k,l})^2}{2\sigma_{k,l}^2} + \lambda_l f_l \right], \quad (5)$$

where ν is the total number of sets, $s_{k,l}$ is the estimate of $\sigma_{k,l}$, λ_l is the Lagrange multiplier, and $f_l = f(\mu_{q-1,l}, \mu_{q,l}, \dots, \alpha_0, \alpha_1, \dots)$. We determined μ , λ , and α so as to maximize L under the conditions $f_l = 0$ ($l = 1, \dots, \nu$). Once values for the α_i were computed by the maximum likelihood method in the off-resonance regions, they were used to subtract the terms $\alpha_i n_i / n_q$ from n_{q-1} / n_q , thereby automatically removing all artifacts, even if they are blended with the DR resonance peaks.

The ion count ratios of B-like ions with and without the corrections for the ion escape and the multiple charge exchange are shown in Fig. 1. The horizontal axis is the channel of the multichannel analyzer used in the measurement, which corresponds to the beam energy. The vertical axis is the ion count ratio. The dips under the baseline of the spectrum are clearly seen in the spectrum which was not corrected. These dips are examples of artifacts connected with ion escape and multiple charge exchange. For the ion count ratio corrected by the method detailed above, the effects of ion escape and multiple charge exchange were well corrected.

V. RESULTS AND DISCUSSION

The DR spectra are shown in Fig. 2. These spectra were obtained by multiplying the electron impact ionization cross sections which we calculated to the ion count ratios which

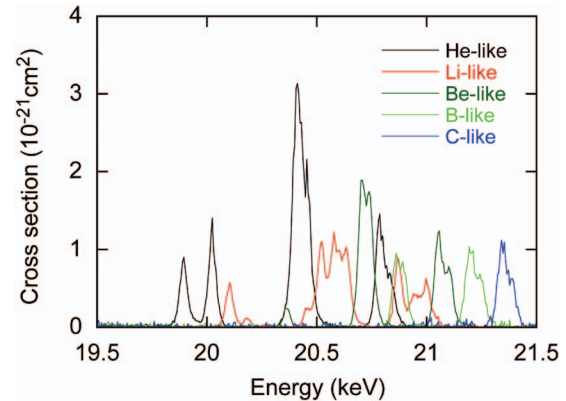


FIG. 2. (Color) The *KLL* DR spectra of He-like to C-like iodine ions.

were corrected by the method detailed in the previous section. It should be noted again that the absolute energy scale of the spectra has an error of about a few tens of an eV, while the error of the relative scale was estimated to be 1.2%. The electron impact ionization cross sections were calculated by using a distorted wave method. The structures of initial and final states were calculated with the GRASP code [15]. The self-consistent potential of the initial calculation was taken to be the distorted potential with which Dirac type distorted wave equations were solved to obtain wavefunctions of continuous states. The generalized Breit interaction effect was omitted, because its contribution was less than 1% in our test calculation.

From the spectra we obtained resonant strengths. The resonant strength can be obtained by integrating the DR cross section with respect to the electron energy:

$$S_q = \int \sigma_q^{DR} dE = \int \sigma_{q-1}^{EI} (N_{q-1}/N_q)' dE = \sigma_{q-1}^{EI} S'_q, \quad (6)$$

where $(N_{q-1}/N_q)'$ is the electron energy dependent portion of the ion count ratio and $S'_q = \int (N_{q-1}/N_q)' dE$, which we call the scaled resonant strength. σ^{EI} can be treated as a constant over the narrow energy width of the resonances and, thus, it can be put outside the integral. The scaled resonant strengths are listed in Table I for future convenience, because the accuracy of the resonant strengths depends, in part, on that of the electron impact ionization cross sections. The values in the parentheses are experimental errors, which are estimated from statistical uncertainties (0.6–4%) and the relative electron energy scale of the spectra (1.2%). The escape rate and the transport efficiency of the beam line were treated as the same for the adjacent charge state ions. This assumption was verified because the ratio of the trapped ions and that of the extracted ions were the same within the range of the experimental error, as has been explained in the previous section. This error (8%) was also added in the errors of the scaled resonant strengths although this is rather conservative and might lead to overestimating the final error.

TABLE I. Scaled resonant strengths, theoretical electron impact ionization cross sections, and resonant strengths. The values in the parentheses are the experimental errors.

Ion	S'_q (10^3 eV)	σ_{q-1}^{EI} (10^{-22} cm 2)	S_q (10^{-19} cm 2 eV)
He-like	2.40(20)	1.78	4.27(39)
Li-like	0.816(66)	3.57	2.91(26)
Be-like	0.371(30)	6.43	2.39(22)
B-like	0.158(13)	9.44	1.49(14)
C-like	0.0583(53)	13.1	0.764(76)

We obtained the resonant strengths by multiplying the scaled resonant strengths by theoretical electron impact ionization cross sections. The resonant strengths are listed in Table I together with the theoretical electron impact ionization cross sections for the *KLL* resonance of He-like to C-like iodine ions. The errors shown in the parentheses were obtained by including the uncertainties of the electron impact ionization cross sections (4%) together with those of the scaled resonant strengths. These results are also shown in Fig. 3. The resonant strengths increase sharply with the increase of the charge state. This increase mainly comes from the increase of *L* shell vacancies, since the number of the states available to the intermediate doubly excited states increases.

The *KLL* resonant strengths of He-like ions which have been obtained so far [6–8,10–12,14] are summarized in Fig. 4 together with the result obtained in the present measurement. The solid circles are experimental values [6,10–12,14], while the open circles are theoretical values [7,8]. There are several measurements for low *Z* elements. As shown in the figure, the resonant strengths become smaller with increasing *Z* except for Ar. The electron capture into the doubly excited states becomes more difficult as *Z* increases, which makes the resonant strengths smaller with increasing *Z*. However, for Ar, Auger processes which compete with radiative processes become significant and the doubly excited states could decay through the Auger processes to a significant extent.

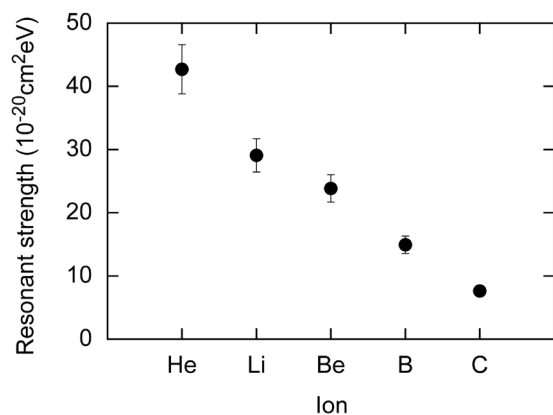


FIG. 3. The resonant strengths for *KLL* DR into He-like to C-like iodine ions.

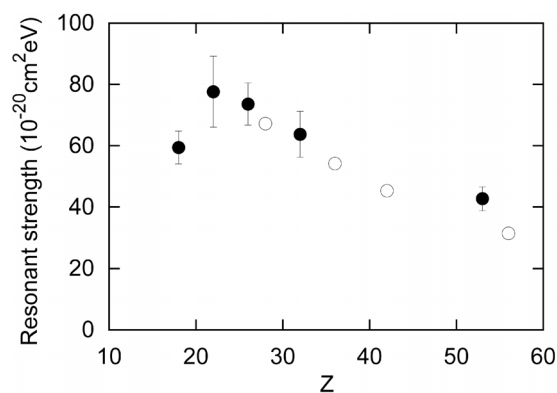


FIG. 4. The resonant strengths of the *KLL* resonance of He-like ions. The solid circles are experimental results and the open circles are theoretical results. I^{51+} is the present result. The other data are Ar $^{16+}$ [14], Ti $^{20+}$ [11], Fe $^{24+}$ [6], Ni $^{26+}$, Mo $^{40+}$, and Ba $^{56+}$ [7], Ge $^{30+}$ [12], and Kr $^{34+}$ [8].

This makes the resonant strength smaller. In the high *Z* region above *Z*=32, no experimental resonant strength has been reported, though there are theoretical results which were verified by comparing the spectra composed with the theoretical resonant strengths and those measured by the EBIT. In these experimental spectra, the contamination of the lower charge state ions was serious due to the limitation of the electron energy which was not enough to make He-like ions dominate the charge balance. This fact might make the extraction of the experimental resonant strengths difficult and would generally lead to an underestimate of the measured resonant strengths. Our data can be compared with the theoretical data for Mo and Ba, which were reported by Knapp *et al.* [7]. These data are significantly smaller than our present result. More experimental resonant strengths are required to judge high *Z* behavior of the *KLL* resonant strengths.

VI. SUMMARY

DR of highly charged iodine ions has been measured with the EBIT. From the electron energy dependence of the extracted ion count ratio between the adjacent charge state ions, DR spectra were obtained. From the spectra the resonant strengths of the *KLL* resonance were obtained for He-like to C-like iodine ions to be $4.27(39) \times 10^{-19}$ cm 2 eV, $2.91(26) \times 10^{-19}$ cm 2 eV, $2.39(22) \times 10^{-19}$ cm 2 eV, $1.49(14) \times 10^{-19}$ cm 2 eV, and $7.64(76) \times 10^{-20}$ cm 2 eV, respectively.

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