The KLL dielectronic recombination processes for highly charged krypton, iodine and barium ions*

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The KLL dielectronic recombination (DR) processes of ions from highly charged helium-like to oxygen-like krypton, iodine and barium ions are studied systematically in the relativistic distorted-wave approximation with configuration interaction. The KLL DR resonant energies, the corresponding resonant strengths and the theoretical spectra for each highly charged ion species are obtained. The results accord well with other available values. The behaviour of KLL resonant strengths for He-like ions with atomic number Z is analysed.

Keywords: KLL dielectronic recombination, resonant strength, cross section
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1. Introduction

Dielectronic recombination (DR) is a fundamental electron–ion collision process of known importance in hot and low-density plasmas. The DR process has been widely studied by employing different methods in recent years.[1−6] In the isolated resonance and independent-process approximation, the DR may be described as a two-step process. In the first step, a doubly excited state is formed in the recombined ion through a resonant process involving the capture of a free electron and the simultaneous excitation of a bound electron, i.e. a reverse Auger process. In the second step, if the doubly excited state decays due to the emission of a photon, the DR process is completed. The DR process is usually denoted by labels KLL, KLM, and so on. For example, KLL means that a free electron is captured into the L shell and the concurrent excitation of a K-shell electron to the L shell. Schematically, for a He-like ground-state target ion, the KLL DR process is given as

$$1s^2 + e \rightarrow 1s2l^2 \rightarrow 1s^2 2l + h\nu. \quad (1)$$

The KLL DR process provides the greatest sensitivity for the determination of ionization equilibrium in astrophysical and laboratory plasmas.[7] Recently, several KLL DR processes for highly charged ions have been studied in experiment with an electron beam ion trap (EBIT).[1,8−13] Zhang *et al.*[1] calculated the KLL DR resonant strengths of the ions from highly charged He-like to C-like germanium ions employing the flexible atomic code (FAC). Shi *et al.*[2,3] studied the KLL DR process of highly charged mercury, uranium and iodine ions by employing the multiconfiguration Dirac–Fock (MCDF) method.

The krypton ion is increasingly used as an injected impurity for diagnosing tokomak fusion plasmas, such as the international thermonuclear experimental reactor (ITER). Several measurements and calculations on KLL DR resonance of Kr have been reported. Fuchs *et al.*[14] reported on the measurement of DR cross sections via the KLn (n = 2,...,5) resonance for highly charged He-like, Li-like, Be-like krypton ions, and also gave theoretical results by employing the Hebrew University Lawrence Livermore Atomic Code (HULLAC). Zhang *et al.*[4] calculated the DR cross sections of KLL resonance for the He-like Kr ion by using the MCDF method. Shi *et al.*[15,16] calculated DR cross sections of the He-like Kr ion by employing the FAC. The Auger transition rates from $1s2s(^3S)2p\ ^2P_{1/2}$ to $1s^2\ ^0S_1$, obtained by different methods, are very different.[4,14−17] Recently, Hu *et al.*[13] measured the KLL resonant strengths for the ions from highly charged He-like to C-like Kr ions by using the Shanghai-EBIT for the first time. Though the DR cross sections and the resonant strengths of

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KLL resonance for the highly charged krypton ion have been widely calculated by employing different methods, there are no comprehensive theoretical results to confirm the resonant strengths for the highly charged krypton ion.

Watanabe *et al.*[11] studied the KLL DR processes of the ions from highly charged He-like to C-like iodine ions by using the Tokyo-EBIT for the first time recently, where all relevant cross sections were obtained for differently charged ions in the KLL region. Shi *et al.*[3] studied the KLL DR processes of the ions from highly charged He-like to C-like iodine ions by using the MCDF method. However, the difference in resonant energy between the experimental results obtained by using the Tokyo-EBIT and the calculations is about 420 eV. It is necessary to calculate, systematically, the KLL DR processes of highly charged iodine ions by employing different methods.

Barium is perhaps the easiest element to study in the EBIT because it is a primary dopant in the electron gun cathode, and sufficient barium atoms evaporate from the heated cathode to provide an abundant source for the trap.[18] Knapp *et al.* measured the DR cross section for He-like Ba^{54+} with an EBIT at the Lawrence Livermore National Laboratory and obtained the theoretical KLL DR resonance strength for He-like Ba^{54+} by using the MCDF method in 1993.[19] To our knowledge, only the KLL DR resonance strength for He-like Ba^{54+} is available. In order to predict the effect of injected barium on the EBIT, it is necessary to study the KLL DR resonance strength for highly charged barium ions.

The DR cross sections of KLL resonance for different charge states are needed to determine charge state distribution in plasmas. In the present paper, we perform a systematical study on the KLL DR processes of the ions from highly charged He-like to O-like krypton, iodine and barium ions by using the FAC.

2. Outline of theory

The DR cross section for an individual resonance, involving excitation from an initial state i via a doubly excited state j, to a final state k, can be given by the following equation in the framework of the isolated resonance approximation:

$$\sigma_{ijk}^{\mathrm{DR}} = \sigma_{ij}^{\mathrm{DC}} \cdot B_{jk}^{\mathrm{r}}, \tag{2}$$

where $\sigma_{ij}^{\mathrm{DC}}$ is the cross section for the resonance capture process from i to j, and B_{jk}^{r} is the radiative branching ratio for the process from j to k. The quantities $\sigma_{ij}^{\mathrm{DC}}$ and B_{jk}^{r} can be written as

$$\sigma_{ij}^{\mathrm{DC}} = \frac{\pi^2\hbar^3}{m_{\mathrm{e}}\varepsilon_{ij}} \frac{g_j}{2g_i} A_{ji}^{\mathrm{a}} \delta(\varepsilon - \varepsilon_{ij}) \tag{3}$$

and

$$B_{jk}^{\mathrm{r}} = \frac{A_{jk}^{\mathrm{r}}}{\sum\limits_{k'} A_{jk'}^{\mathrm{r}} + \sum\limits_{i'} A_{ji'}^{\mathrm{a}}}, \tag{4}$$

where g_i and g_j are the statistical weights of states i and j, respectively; A_{ji}^{a} is the autoionization rate from j to i; ε_{ij} is the difference in energy between levels i and j, i.e. the resonant energy of the doubly excited state j ; $\sum\limits_{i'} A_{ji'}^{\mathrm{a}}$ and $\sum\limits_{k'} A_{jk'}^{\mathrm{r}}$ are the total Auger decay rate and the total radiative decay rate of the doubly excited state j. $\delta(\varepsilon - \varepsilon_{ij})$ is a delta function that implies the matching of free electron energy ε to ε_{ij}.

The DR strength S_{ijk}^{DR} is

$$\begin{aligned} S_{ijk}^{\mathrm{DR}} &= \int_{-\infty}^{+\infty} \sigma_{ijk}^{\mathrm{DR}} \mathrm{d}\varepsilon \\ &= \frac{\pi^2\hbar^3}{m_{\mathrm{e}}\varepsilon_{ij}} \frac{g_j}{2g_i} A_{ji}^{\mathrm{a}} \frac{A_{jk}^{\mathrm{r}}}{\sum\limits_{k'} A_{jk'}^{\mathrm{r}} + \sum\limits_{i'} A_{ji'}^{\mathrm{a}}}, \end{aligned} \tag{5}$$

and the total DR strength may be obtained by summing S_{ijk}^{DR} over all possible intermediate states (j) and final states (k). In order to make a comparison between the calculated results with experimental results, the calculated cross section should be convoluted by assuming the electron energy distribution in the beam to be a Gaussian distribution, i.e.

$$\sigma_{\mathrm{total}}^{\mathrm{DR}}(\varepsilon) = \sum_{j,k} \frac{S_{ijk}^{\mathrm{DR}}}{\Delta\sqrt{\pi}} \exp\left[-\frac{(\varepsilon - \varepsilon_{ij})^2}{\Delta^2}\right], \tag{6}$$

where $\Delta = \omega/(2\sqrt{\ln 2})$ and ω is the full-width-at-half-maximum (FWHM) of the beam energy spread.

Systematic study of the DR process should include the determination of energies, Auger and radiative transition rates for atomic states in the recombined ion. These parameters are obtained by using the FAC, which integrates various atomic processes within a unified theoretical framework, ensures self-consistency between different parts, and provides a uniform, flexible, and user-friendly interface for accessing all computational tasks.[20–22] The atomic structure calculation in FAC is based on the relativistic configuration interaction method. The continuum processes, such as direct excitation and autoionization, are treated in the distorted wave (DW) approximation. Special attention has been paid to the long-range contributions to the continuum–continuum radial integral by using a phase-amplitude method for

the continuum wave functions. Systematic application of the factorization-interpolation method of Bar–Shalom makes the code highly efficient for large scale calculations. Recently, the FAC has been widely used to deal with DR processes.[1,15,16,23] In our calculation, we consider all single and double excitations from the reference configurations up to the $n = 3$ shell as the interacting configurations. Furthermore, the Breit interaction involving all bound and continuum states is included. Vacuum polarization and self-energy corrections are treated in the screened hydrogenic approximation. All stabilizing radiative decays including electric dipole, electric quadrupole, magnetic dipole and magnetic quadrupole are taken into account.

3. Results and discussion

In order to predict the effect of injected krypton ion on the ITER performance and explore its benefit for diagnostic applications, accurate cross sections for ionization and recombination are needed. In Tables 1 and 2, we compare the Auger and total radiative transition rates of some strong KLL resonances for Kr^{34+} calculated using FAC, MCDF and HULLAC respectively.

Table 1. Auger transition rates of some strong KLL resonances for Kr^{34+} (s^{-1}). The a[b] represents a×10^b.

config. and term	this work	HULLAC[14]	MCDF1[4]	MCDF2[17]	FAC1[15]	FAC2[16]
$1s2s^2\ ^2S_{1/2}$	1.70[14]	1.46[14]	1.56[14]	1.59[14]	1.50[14]	1.50[14]
$1s2s(^3S)2p\ ^2P_{1/2}$	9.88[13]	7.85[13]	1.00[14]	9.74[13]	7.51[13]	7.53[13]
$1s2s(^1S)2p\ ^2P_{1/2}$	4.98[13]	4.89[13]	4.84[13]	4.58[13]		
$1s2s(^1S)2p\ ^2P_{3/2}$	1.16[14]	1.10[14]	1.14[14]	1.11[14]		
$1s2p^2\ ^4P_{5/2}$	7.06[13]	7.11[13]	7.16[13]	7.08[13]	7.24[13]	7.30[13]
$1s2p^2\ ^2D_{3/2}$	1.19[14]	1.23[14]	1.21[14]	1.19[14]	1.24[14]	1.24[14]
$1s2p^2\ ^2D_{5/2}$	9.95[13]	9.91[13]	9.93[13]	9.98[13]	9.78[13]	9.71[13]
$1s2p^2\ ^2P_{3/2}$	4.15[13]	4.75[13]	4.04[13]	4.11[13]		
$1s2p^2\ ^2S_{1/2}$	3.02[13]	3.13[13]	2.70[13]	3.06[13]		

Table 2. Total radiative transition rates of some strong KLL resonances for Kr^{34+} (s^{-1}). The a[b] represents a×10^b.

config. and term	this work	HULLAC[14]	MCDF1[4]	MCDF2[17]	FAC1[15]	FAC2[16]
$1s2s^2\ ^2S_{1/2}$	5.79[13]	5.05[13]	5.33[13]	5.11[13]	5.47[13]	5.39[13]
$1s2s(^3S)2p\ ^2P_{1/2}$	7.84[14]	6.08[14]	7.63[14]	7.40[14]	7.71[14]	7.57[14]
$1s2s(^1S)2p\ ^2P_{1/2}$	1.03[15]	1.07[15]	1.06[15]	9.79[14]		
$1s2s(^1S)2p\ ^2P_{3/2}$	4.09[13]	1.84[13]	5.56[13]	2.96[13]		
$1s2p^2\ ^4P_{5/2}$	4.06[14]	3.50[14]	3.78[14]	3.87[14]	3.91[14]	3.89[14]
$1s2p^2\ ^2D_{3/2}$	1.54[15]	1.45[15]	1.55[15]	1.46[15]	1.54[15]	1.52[15]
$1s2p^2\ ^2D_{5/2}$	5.35[14]	5.26[14]	5.42[14]	5.09[14]	5.44[14]	5.32[14]
$1s2p^2\ ^2P_{3/2}$	2.09[15]	2.08[15]	2.15[15]	1.97[15]		
$1s2p^2\ ^2S_{1/2}$	1.02[15]	1.00[15]	1.04[15]	9.60[14]		

As can be seen from Tables 1 and 2, our calculations are in good agreement with other calculations. The main reason for the difference in Auger transition rate in Table 1 between our results and the previous calculations by using the FAC comes from the different considerations of configuration interaction. Our present total radiative transition rates are larger than the previous calculations by using FAC in Table 2, which is mainly because we consider all stabilizing electric dipole, electric quadrupole, magnetic dipole, and magnetic quadrupole radiative decays.

Figure 1 shows the plots of the KLL DR cross section ($\sigma^{\rm DR}$) as a function of electron beam energy (ε) for the ions from He-like to O-like krypton ions and compares KLL DR cross sections with the HULLAC calculations of Fuchs *et al.*[14] The difference between the two results is within 6%.

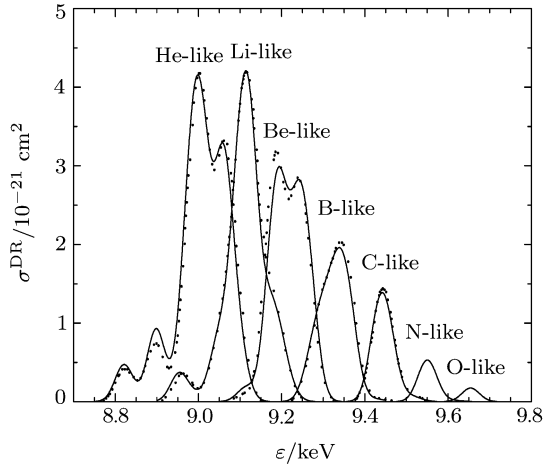


Fig. 1. KLL DR cross sections for the ions from He-like to O-like krypton ions. The cross sections are generated by applying a 50-eV FWHM Gaussian to resonance strengths $S_{ijk}^{\rm DR}$ calculated from Eq. (5). The solid lines are for the present results and the dot lines are for the theoretical results calculated by Fuchs *et al.*[14]

Recently, the KLL DR spectra of the ions from He-like to C-like iodine ions have been studied theoretically and experimentally.[3,11] However, the difference in resonant energy between theoretical calculations by employing the MCDF[3] and experimental results by using the Tokyo-EBIT[11] is about 420 eV.

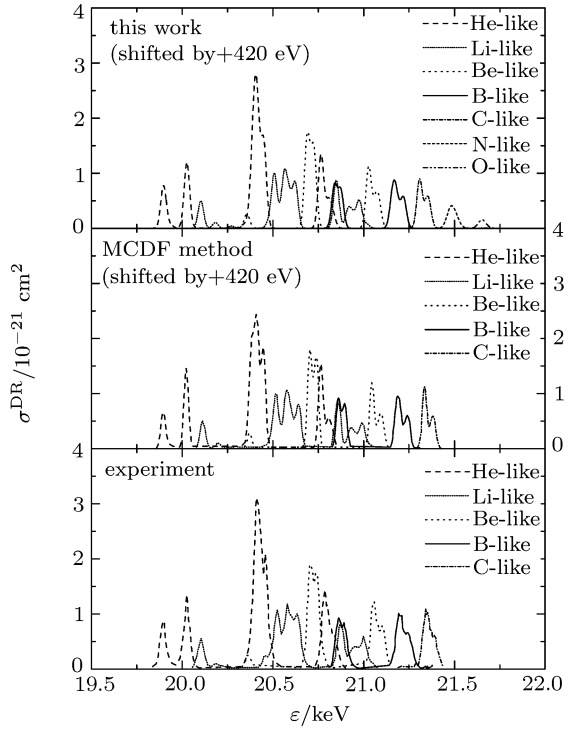


Fig. 2. KLL DR cross sections for the ions from He-like to O-like iodine ions. The cross sections are generated by applying a 36-eV FWHM Gaussian distribution to resonance strength $S_{ijk}^{\rm DR}$ calculated from Eq. (5).

To understand the difference between them, in this research, we employ the FAC to study the KLL DR process of the highly charged iodine ions systematically. In Fig. 2, we plot our present KLL DR cross sections ($\sigma^{\rm DR}$) as a function of electron beam energy (ε) with FWHM = 36 eV. The theoretical results cited from Ref. [3] and the experimental results cited from Ref. [11] are both shown in Fig. 2. The amplitudes of the cross sections and the line shapes show good agreement between our present results and available theoretical and experimental results. Both our present resonant positions and the resonant positions from Ref. [3], shifting 420 eV, match well with the experimental results. As the scanning electron beam energy in EBIT experiment is determined by theoretical results,[9] the resonant positions of KLL DR experimental spectra should be checked.

Barium is a component of the electron gun structure, emitted as a permanent trap contaminant. In Fig. 3, we plot our present KLL DR cross sections ($\sigma^{\rm DR}$) for the ions from He-like to O-like Ba as a function of electron beam energy (ε) with FWHM = 50 eV.

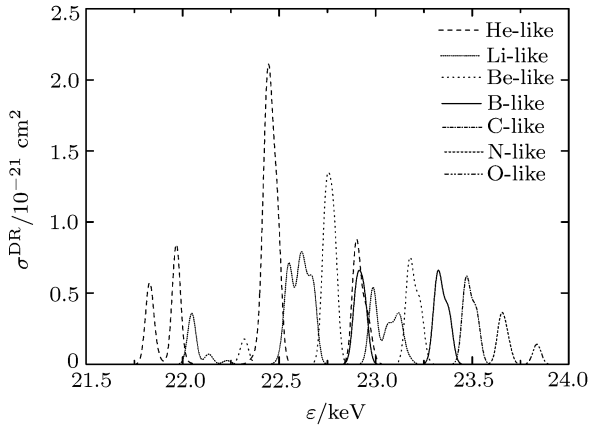


Fig. 3. The KLL DR cross sections for the ions from He-like to O-like Ba ions with 50-eV FWHM.

The present calculated total KLL DR resonant strengths for the ions from He-like to O-like krypton, iodine and barium ions are listed in Table 3, together with the other different theoretical results and experimental results with EBIT. As shown in Table 3, the present total KLL DR resonant strengths for the highly charged krypton ion are in good agreement with the previous experimental results[13] and theoretical calculations obtained by employing the HULLAC[14] within their accuracy. For each differently charged iodine ion, the present total KLL DR resonant strengths are in good agreement with the theoretical calculations obtained by employing the MCDF method[3] and smaller than the available experimental results[11]

within around 20%. Considering the fact that our present results of the KLL DR for the highly charged krypton ion are in agreement with recent experimental results, and that our results are consistent with the theoretical results from Ref. [3], the inaccuracy of Ref. [11] may be large and should be improved. The difference in KLL DR resonant strength for He-like barium between the present result and the result obtained by the MCDF method[19] is 3%. The resonant strengths increase sharply with the increase of the charge state. This increase mainly comes from the increase of L shell vacancy number, as the number of the states available to the intermediate doubly excited states increases. For instance, there are twenty intermediate doubly excited states in a Li-like ion, but only eight in a Be-like ion.

Table 3. Total KLL DR resonant strengths (in 10^{-19} cm^2·eV) for the ions from He-like to O-like krypton, iodine and barium ions. The values in parentheses are the experimental errors.

	krypton ions			iodine ions			barium ions	
	FAC	HULLAC[14]	experiment[13]	FAC	MCDF[3]	experiment[11]	FAC	MCDF[19]
He-like	5.58	5.42	5.41(27)	3.51	3.41	4.27(39)	3.25	3.15
Li-like	4.29	4.39	4.33(26)	2.32	2.32	2.91(26)	2.11	
Be-like	3.53	3.61	3.59(22)	1.99	1.86	2.39(22)	1.80	
B-like	1.95	2.05(25)	1.20	1.18	1.49(14)	1.09		
C-like	0.93	0.98(15)	0.58	0.59	0.764(76)	0.52		
N-like	3.10			0.27			0.24	
O-like	0.92		0.08		0.07			

By defining radiative transition rate $A^{\rm r}(Z)$, autoionization rate $A^{\rm a}(Z)$ and resonance energy $E(Z)$ each as a function of Z, the KLL He-like resonance strengths may be scaled as

$$S = \frac{1}{m_1 Z^2 + m_2 Z^2}, \tag{7}$$

where m_1 and m_2 are fitting parameters determined from fits to the previous measurements and cited from Ref. [24] respectively. The KLL resonant strengths ($S^{\rm DR}$) for He-like ions are plotted as a function of atomic number (Z) in Fig. 4. The curve shows the variation of resonant strength obtained from Eq. (7) with atomic number. Our theoretical results for Kr^{34+}, I^{51+} and Ba^{54+} are shown with open squares, the solid circles with error bars represent experimental results,[1,11,13,24–26] while the open circles refer to theoretical values.[19] It is clear that this scaling formula provides a good fit to the available experimental and theoretical results. Our present results are in good agreement with the results from this scaling formula.

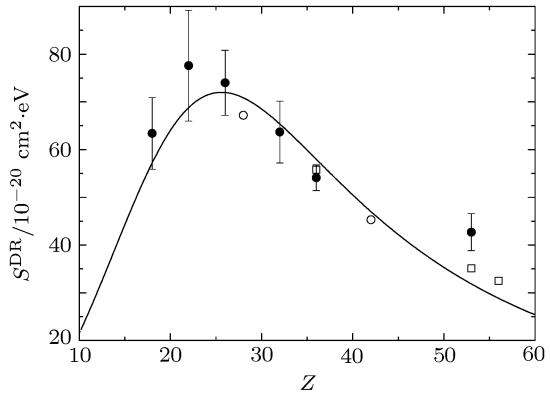


Fig. 4. Comparison between total KLL DR resonant strengths for He-like ions. The data with error bars represent experimental results: Ar^{16+},[25] Ti^{20+},[26] Fe^{24+},[24] Ge^{30+},[1] Kr^{34+},[13] I^{51+},[11] while the open circles denote theoretical results: Ni^{26+}, Mo^{40+},[19] the open squares refer to the present results: Kr^{34+}, I^{51+}, Ba^{54+}.

4. Conclusions

The resonant strengths and cross sections of the KLL DR process for ions from highly charged helium-like to oxygen-like krypton, iodine and barium ions are calculated in the relativistic distorted-wave approximation with configuration interaction. Theoretical DR spectra for each highly charged ion species are obtained in the KLL region. The present KLL DR spectra for the ions from helium-like to carbon-like krypton ions accord well with the results calculated from the HULLAC code. The relative difference between the total KLL DR resonant strength for the highly charged krypton ion in the present results and the results from the HULLAC code is less

than 6%. Within the experimental inaccuracy, the results of the total KLL DR resonant strengths for the ions from highly charged He-like to C-like krypton ions, obtained from the present calculation and experimental measurements, are in agreement. For highly charged iodine ions, the present calculated KLL DR spectra accord well with the results from the MCDF method, and the resonant positions of experimental simulated spectra should decrease around 420 eV. The present calculated KLL resonant strengths for the ions from He-like to C-like iodine ions accord well with the results from the MCDF method, and the inaccuracy of recent experimental results[11] may be large, and should be improved. Moreover, the behaviour of the KLL resonant strengths varying with Z is analysed for He-like ions in particular. The KLL resonant strengths for He-like krypton, iodine and barium ions are very consistent with the results calculated from the scaling formula.

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