Vol 18 No 8, August 2009
1674-1056/2009/18(08)/3409-05

Chinese Physics B

© 2009 Chin. Phys. Soc.
and IOP Publishing Ltd

# Dielectronic recombination of Co-like tantalum*

Zhou Li(周 莉)[a)b)], Meng Fan-Chang(孟凡昌)[a)b)], Huang Min(黄 敏)[a)b)], Chen Chong-Yang(陈重阳)[a)b)†], and Wang Yan-Sen(王炎森)[a)b)]

[a)] *The Key Laboratory of Applied Ion Beam Physics, the Ministry of Education, Shanghai* 200433, *China*

[b)] *Shanghai EBIT Laboratory, Modern Physics Institute, Fudan University, Shanghai* 200433, *China*

(Received 25 September 2008; revised manuscript received 4 November 2008)

*Ab initio* calculation of the total dielectronic recombination (DR) rate coefficient from the ground state of Co-like tantalum is performed using the relativistic distorted-wave approximation with configuration interaction. The contributions to the total DR rate coefficients are explicitly calculated from the complexes of Ni-like tantalum: $3s^23p^63d^3_{3/2}3d^6_{5/2}n'l'$, $3s^23p^53d^{10}n'l'$, $3s3p^63d^{10}n'l'$, $3s^23p^63d^84ln'l'$, $3s^23p^53d^94ln'l'$ and $3s3p^63d^94ln'l'$ with $n' \leq 25$, and $3s^23p^63d^85ln'l'$ with $n' \leq 9$. The $l'$ and $n'$ dependences of partial DR rate coefficients are investigated. The contributions from higher $n'$complexes are evaluated by a level-by-level extrapolation method. The total DR rate coefficients mainly come from the complex series $3s^23p^63d^84ln'l'$, $3s^23p^53d^94ln'l'$ and are fitted to an empirical formula with high accuracy. Comparison of the present results with those of other works shows that the previously published data underestimate significantly the DR rates of Co-like tantalum.

**Keywords:** dielectronic recombination, rate coefficient, Co-like tantalum
**PACC:** 3480L

## 1. Introduction

Knowledge of accurate dielectronic recombination (DR) rate coefficients of heavy ions is crucial for the study of ionization balance of highly ionized elements in hot plasmas[1] and is also essential for research into x-ray lasers, especially for calculation of the population and depopulation of lasing levels.[2] For instance, in the theoretical simulation of a Ni-like x-ray laser, Co-like DR processes can populate the upper x-ray levels and affect the x-ray amplification and x-ray transfer.[3,4]

Due to the complexity of Co-like ions with open $M$-shell, there have only been a few calculations of DR rates through the low-lying doubly excited Ni-like configurations. Yan *et al* [5] calculated the DR rates of Co-like Ag and Ta ions through Ni-like $3l^{-2}4l4l'$ configurations and studied the configuration-interaction effects on DR of the Co-like Xe ion.[6] Zhang *et al* [7] presented the DR rates of Co-like Pd ions through doubly excited Ni-like states $3l^{-2}4l4l'$ and $3l^{-2}4l5l'$. The above calculations[5−7] all employed a semi-relativistic multi-configuration Hartree–Fock method in conjunction with the distorted-wave approximation.

Gu[8−10] developed a fully relativistic configuration interaction code, i.e. the flexible atomic code (FAC), which integrated various atomic processes within a unified theoretical framework. The atomic structure calculation in FAC is based on the relativistic configuration interaction method. The continuum processes are treated in the distorted-wave (DW) approximation. The systematic application of the factorization interpolation method of Bar–Shalom[11] makes the code highly efficient for large scale calculations. Employing FAC, we recently computed the total excitation rate coefficients with resonance contributions for Ni-like tantalum and tungsten,[12,13] the DR rate coefficients of Ni-like gold through the doubly excited Cu-like configurations $3d^94l4l'$ and $3d^94l5l'$,[14] and the DR rate coefficients of Co-like gold.[15]

Here, also by employing FAC, we present the *ab initio* level-by-level calculations of the total DR rate coefficients for Co-like tantalum from the ground state $(3s^23p^63d^9)_{J=5/2}$. An elaborate discussion about the physical factors affecting the DR rate coefficients is presented. To conveniently use the present results, the total DR rate coefficients are fitted to an empirical formula. In addition, the present DR rates are compared with those from Yan *et al*.[5]

*Project supported by the National Natural Science Foundation of China (Grant No 10574029) and the Chinese Association of Atomic and Molecular Data and National High-Tech ICF Committee in China. It is also partially supported by Shanghai Leading Academic Discipline Project (Grant No B107).

†Corresponding author. E-mail: chychen@fudan.edu.cn

## 2. Outline of the theory

In the isolated resonance and independent-process approximation, and neglecting the profile of the resonances, one can obtain the DR strength using the detailed balance principle:

$$S_{ij} = \frac{\pi^2\hbar^3}{m_{\rm e}E_{ij}}\frac{g_j}{2g_i}A^a_{ji}B^{\rm DR}_j, \tag{1}$$

where $j$ represents a doubly excited intermediate state, $i$ represents the initial state of dielectronic capture (DC). $E_{ij}$ is the resonant energy, $g_i$ and $g_j$ are the statistical weights of states $i$ and $j$ respectively. $A^a_{ji}$ is the autoionization rate from level $j$ to $i$. The DR branching ratio $B^{\rm DR}_j$ is defined iteratively as

$$B^{\rm DR}_j = \frac{\sum\limits_f A^r_{jf} + \sum\limits_{f'} A^r_{jf'} + \sum\limits_{j'} A^r_{jj'}B^{\rm DR}_{j'}}{\sum\limits_k A^a_{jk} + \sum\limits_f A^r_{jf} + \sum\limits_{f'} A^r_{jf'} + \sum\limits_{j'} A^r_{jj'}}, \tag{2}$$

where $A^a$ and $A^r$ are the Auger and radiative rates, respectively. In the present work, only electric dipole transitions are taken into account. $k$ is the possible autoionizing channel of the doubly excited level $j$. The levels $f$, $f'$ and $j'$ represent the singly excited, nonautoionizing doubly excited and low-lying autoionizing doubly excited states of Ni-like ions, respectively. $B^{\rm DR}_{j'}$ is the DR branching ratio of state $j'$ and is defined similarly to Eq.(2). The four terms in the denominator of Eq.(2) are the total autoionizing rates and the total radiative transition rates from the autoionizing level to singly excited states (resonant stabilizing transitions, RS), to doubly excited states (non-resonant stabilizing transitions, NRS) and the total radiative rates of decays to autoionizing levels followed by radiative cascade (DAC), respectively. In this work we employ FAC[8−10] to calculate all the basic atomic data including energy levels, autoionizing and radiative transition rates.

Assuming a Maxwellian velocity distribution of the thermal plasma electrons exists, the DR rate coefficient is defined as

$$\begin{aligned}\alpha_i(T) &= \frac{h^3}{(2\pi m_{\rm e}kT_{\rm e})^{3/2}} \\ &\quad\times\sum_j \frac{g_j}{2g_i}A^a_{ji}B^{\rm DR}_j\exp\left(-\frac{E_{ij}}{kT_{\rm e}}\right) \\ &= \sum_j \beta^c_{ij}B^{\rm DR}_j,\end{aligned} \tag{3}$$

where $\beta^c_{ij}$ is the dielectronic capture rate coefficient to form the level $j$ from initial state $i$.

## 3. Calculation procedure

In the present work we include explicitly the DR contributions through seven autoionizing doubly excited configuration complex series of Ni-like tantalum: $3s^23p^63d^3_{3/2}3d^6_{5/2}n'l'$, $3s^23p^53d^{10}n'l'$, $3s3p^63d^{10}n'l'$, $3s^23p^63d^84ln'l'$, $3s^23p^53d^94ln'l'$ and $3s3p^63d^94ln'l'$ with $n' \le 25$, and $3s^23p^63d^85ln'l'$ with $n' \le 9$, which are respectively associated with the $\Delta n = 0$ ($3d_{3/2}$–$3d_{5/2}$, $3p$, $3s$–$3d$), $\Delta n = 1$ ($3d$, $3p$, $3s$–$4l$), and $\Delta n = 2$ ($3d$–$5l$) core-excitations. The configuration-interaction within the same complex is considered. The RS and NRS transitions are fully included. The possible important DAC transitions are also considered. The DAC transitions from $(3s^23p^63d^{10})^{-1}n'l'$ configurations are fully taken into account. For $(3s^23p^63d^{10})^{-2}4ln'l'$, the DAC transitions to $(3s^23p^63d^{10})^{-2}4l4l''$ configurations are considered. For $3s^23p^63d^85ln'l'$, the DAC transitions of the $5l$ and $n'l'$ electrons, towards $M$- and $N$-shells are taken into account. In addition, all possible autoionizing channels of the doubly excited states are included in the calculation.

Within the selected $n'$ complexes, the dependences of partial DR rate coefficients at an electron temperature of 1000 eV on the orbital angular momentum $l'$ are plotted in Fig.1. It can be seen that the contributions through the resonant configurations with $l' > 12$ and $l' > 8$, respectively, formed by $\Delta n = 0$ and $\Delta n = 1, 2$ core excitations, are expected to be negligible. Hence, only the configurations with $l' \le 12$ for $\Delta n = 0$ core excitations and $l' \le 8$ for $\Delta n = 1, 2$ core excitations are included in the present calculation.

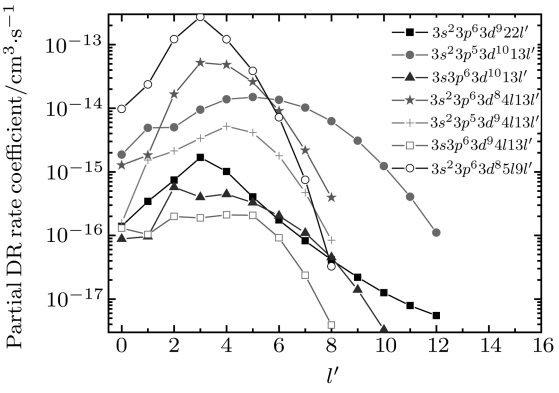



**Fig.1.** Partial DR rate coefficients at an electron temperature of 1000 eV, as a function of $l'$.

The partial DR rate coefficients of the ground state $Ta^{46+}$ through the seven core-excitations, multiplied by $(n')^3$, without and with the inclusion of DAC

transitions, are respectively plotted as a function of the primary quantum number $n'$ of the outer captured electron in Figs.2(a) and 2(b), at an electron temperature of 1000 eV. Some results can be seen from Fig.2 as follows: (i) In the range of low $n'$ values there are irregularities in the behavior of the partial rate coefficients. As pointed out in Ref.[16], they are due to the opening of new DR channels, the closing of radiative stabilization channels, and the opening of new autoionization channels. For instances, the abrupt increase at $n' = 9$ for the partial DR rates through the $3s^2 3p^5 3d^{10} n'l'$ complex series is due to the opening of new DR channels associated with the $3p_{3/2}$–$3d_{5/2}$ core-excitation. And the large decrease at $n' = 9$ for the partial DR rates through the $3s^2 3p^5 3d^9 4l n'l'$ complex series is due to the closing of radiative stabilization channels, i.e. the decays to $3s^2 3p_{1/2}^2 3p_{3/2}^3 3d^{10} 9l'$. (ii) The inclusion of DAC transitions breaks down the usual $(n')^{-3}$ scaling law (first proposed by Hahn[17]) of the DR rates through the resonances associated with $3s$–$3d$ core excitation. (iii) For relatively high values of $n'$, the partial DR rates through the resonances associated with $3d_{3/2}$–$3d_{5/2}$ and $3d$–$4l$ core-excitations scale as $(n')^{-3}$, whereas the $(n')^{-3}$ scaling law does not take place for the other core-excitations.

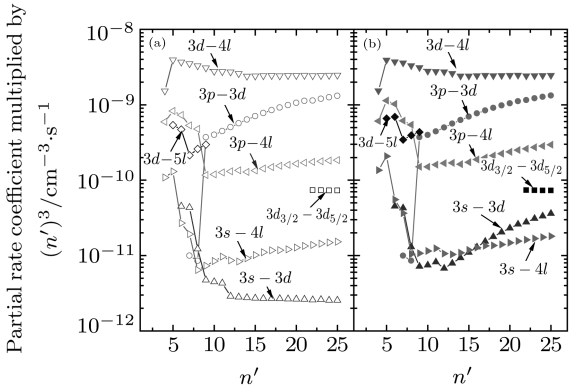



**Fig.2.** The partial DR rate coefficients through different core-excitations, multiplied by $(n')^3$, without and with the inclusion of DAC transitions, plotted respectively as a function of the primary quantum number $n'$ of the outer captured electron in Figs.(a) and (b), at an electron temperature of 1000 eV.

The DR contributions through the resonances, with $n' > 25$ and $n' > 9$ associated with $\Delta n = 0, 1$, and $3d$–$5l$ core-excitations, respectively, should be included in the extrapolation procedure. In the present work, we employ the level-by-level extrapolation method developed in Ref.[15], in which the DAC transitions could be taken into account. The calculations show: (i) The influence of DAC and high $n'$ contributions are negligible at electron temperature below 100 eV. (ii) The relative contributions from high $n'$ resonances to the total DR rate coefficients increase with increasing temperature and reach about 7% at 100 keV. (iii) The effects of considering DAC transitions also increase with increasing temperature, they enlarge the total DR rates by a factor of about 10% at 100 keV.

# 4. Results and discussion

Figure 3 shows the DR rate coefficients through the seven core-excitations and the total DR rate coefficients of Co-like tantalum. As can be seen from the figure, in the whole range of electron temperature the dominant DR contributions come from the doubly-excited configurations $3s^2 3p^6 3d^8 4l n'l'$ and $3s^2 3p^5 3d^9 4l n'l'$ which are associated with $3d$–$4l$ and $3p$–$4l$ core-excitations, respectively. The relative contributions through $3d$–$4l$ core-excitation of the total DR rates are 87% at 10 eV, then decrease smoothly, and become 65% at 100 keV. The contributions through $3p$–$4l$ core-excitation are 5% at 10 eV, and are about 10% at electron temperature above 100 eV. At low electron temperatures ($< 10$ eV), the contributions through $3s$–$3d$ and $3d_{3/2}$–$3d_{5/2}$ core excitations to the DR rate coefficients are about 10%. And at high temperatures ($> 1000$ eV), the relative contributions through $3d$–$5l$ core excitation are about 10%. Unlike in the case of Co-like gold,[15] in which the $3s^2 3p^5 3d^{10} n'l'$ complex series may make significant contributions (up to 19%) to the total DR rates, here the contributions from the $3s^2 3p^5 3d^{10} n'l'$ peak at 200 eV have a value of 8%. The contributions from $3s 3p^6 3d^9 4l n'l'$ configurations are less than 2% in the whole range of electron temperature.

In order to conveniently use the present results, the calculated total DR rate coefficients are fitted to an empirical formula. The DR rate coefficients at low temperatures ($< 10$ eV) are extremely sensitive to the exact position (in energy) of the resonances, which cannot be calculated accurately enough in the present work, hence we only fit the DR rates in the range of 10 eV–100 keV to the following formula (in units of cm$^3$·s$^{-1}$):

$$\alpha^{\mathrm{DR}}(kT_{\mathrm{e}}) = 10^{-6} \times (kT_{\mathrm{e}})^{-3/2} \sum_{i=1}^{5} A_i \mathrm{e}^{-B_i/kT_{\mathrm{e}}}, \quad (4)$$

in which both $A_i$ and $B_i$ are adjustable parameters, $kT_{\mathrm{e}}$ is in units of eV. Using the parameters listed in Table 1 we can reproduce the present total DR rate coefficients to within 1% at most electron temperatures. The largest deviation between the fitted and calculated values is about 1.7% at 100 keV.

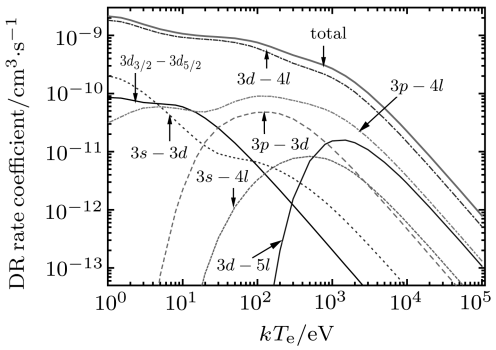



**Fig.3.** The partial DR rate coefficients through the seven core-excitations and the total DR rate coefficients of Co-like tantalum.

**Table 1.** The fit parameters of the total DR rate coefficient (see Eq.(4)).

| $I$ | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| $A_i$ | 0.11831 | 0.72943 | 2.0596 | 4.9457 | 17.125 |
| $B_i$ | 12.752 | 68.260 | 202.00 | 655.94 | 1604.3 |

Figure 4 shows the comparison of the present results with those from Yan *et al.*[5] By employing the semi-relativistic multi-configuration Hartree–Fock method in conjunction with the distorted-wave approximation, Yan *et al* [5] calculated the DR rate coefficients through the complexes $(3s^23p^63d^{10})^{-2}4l4l'$ for the ground state of Co-like tantalum. The dotted-line in Fig.4 shows the present DR contributions from $(3s^23p^63d^{10})^{-2}4l4l'$ configurations. Also plotted in Fig.4 are the present DR rates from the complex series $(3s^23p^63d^{10})^{-2}4ln'l'$ and the total DR rates. It can be seen that the agreement between the present DR rate coefficients through $(3s^23p^63d^{10})^{-2}4l4l'$ configurations and those in Ref.[5] is good. It should be noted that the configuration-interaction, NRS and DAC transitions are not taken into account in Ref.[5]. The DR contributions through $(3s^23p^63d^{10})^{-2}4l4l'$ dominate the present total DR rates at electron temperatures below 100 eV and are about 90%–20% of the total rates in the range of 100 eV–100 keV. It could be concluded that the calculations in Ref.[5] underestimated significantly the effective total DR rate coefficients for the ground state of Co-like tantalum at electron temperatures above 100 eV.

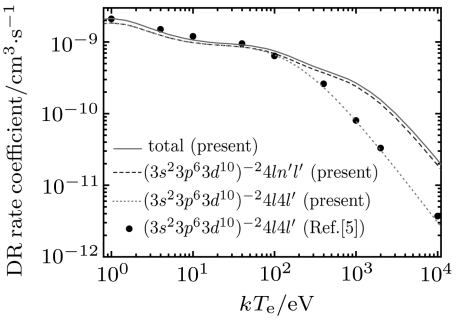



**Fig.4.** Comparison of the present DR rate coefficient with those from Ref.[5].

# 5. Conclusion

The level-by-level calculations of the DR rate coefficients for the ground state of Co-like tantalum have been performed using the relativistic configuration-interaction program FAC. The dependences of the partial DR rate coefficients on the orbital angular momentum $l'$ and primary quantum number $n'$ of the captured electron are investigated. The two complex series $3s^23p^63d^84ln'l'$ and $3s^23p^53d^94ln'l'$ give the main contributions to the total DR rate coefficients. Comparison of the present results with other works shows that the previously published data underestimate significantly the DR rates of Co-like tantalum.

# References

[1] Dubau J and Volante S 1980 *Rep. Prog. Phys.* **43** 199

[2] Whitten B L, Hazi A U, Chen M H and Hagelstein P L 1986 *Phys. Rev.* A **33** 2171

[3] Apruzese J P, Davis J, Blaha M, Kepple P C and Jacobs V L 1985 *Phys. Rev. Lett.* **55** 1877

[4] Sasaki A and Kawachi T 2003 *J. Quart. Spectrosc. Radiat. Transfer* **81** 411

[5] Yan J, Li P, Liu C L, Qiu Y B and Fang Q Y 2001 *Chin.*

*Phys.* **10** 1124

[6] Yan J, Li Y M and Yao J H 2003 *Nucl. Instrum. Methods Phys. Res.* B **205** 382

[7] Zhang H, Li Y M, Yan J and Wang J G 2005 *Phys. Rev.* A **71** 042705

[8] Gu M F 2003 *Astrophy. J.* **582** 1241

[9] Gu M F 2003 *Astrophys. J.* **589** 1085

[10] Gu M F 2003 *Astrophys. J.* **590** 1131

[11] Bar-Shalom A, Klapisch M and Oreg J 1988 *Phys. Rev.* A **38** 1773

[12] Shen T M, Chen C Y, Wang Y S, Zou Y M and Gu M F 2007 *Phys. Rev.* A **76** 022703

[13] Shen T M, Chen C Y, Wang Y S, Zou Y M and Gu M F 2007 *J. Phys.* B **40** 3075

[14] Shi X H, Chen C Y, Wang Y S and Gu M F 2004 *Chin. Phys. Lett.* **21** 1937

[15] Meng F C, Chen C Y, Shi X H, Wang Y S, Zou Y M and Gu M F 2007 *J. Phys.* B **40** 4269

[16] Peleg A , Behar E , Mandelbaum P and Schwob J L 1998 *Phys. Rev.* A **57** 3493

[17] Hahn Y 1985 *Adv. At. Mol. Phys.* **21** 123