Vol 10 No 12, December 2001
1009-1963/2001/10(12)/1124-05
Chinese Physics
© 2001 Chin. Phys. Soc.
and IOP Publishing Ltd

DIELECTRONIC RECOMBINATION OF Co-LIKE Ag AND Ta IONS*

YAN JUN(颜 君)[a,b], LI PING(李 萍)[a], LIU CHUN-LEI(刘春雷)[a],
QIU YU-BO(邱玉波)[a], and FANG QUAN-YU(方泉玉)[a]
[a] *Institute of Applied Physics and Computational Mathematics, Beijing* 100088, *China*
[b] *Centre of Atomic and Molecular Sciences, Tsinghua University, Beijing* 100084, *China*

(Received 27 June 2001; revised manuscript received 21 August 2001)

Ab initio calculations of the rate coefficients for dielectronic recombination (DR) of Co-like Ag and Ta ions are performed based on Cowan's quasi-relativistic multi-configuration Hartree–Fock code. Co-like $(3s^23p^63d^{10})^{-1}$ configurations and Ni-like $(3s^23p^63d^{10})^{-2}4l4l'$ autoionization configurations are included in the present calculation. Because of the extensive distribution of autoionization state energy levels, the DR rate coefficients cannot be reproduced or interpolated by a simple analytical formula, such as the Burgess–Merts formula, or the Hagelstein approximation. We propose to use multi-set Hagelstein parameters, which is convenient in practice and can reproduce well the *ab initio* calculated DR rate coefficients.

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

I. INTRODUCTION

Knowledge of the accurate recombination rates of heavy ions is essential for the study of the ionization balance of highly-ionized elements in hot plasmas.[1] This knowledge is also important for the research of x-ray lasers, specifically for calculating the population of lasing levels.[2,3] The most important recombination process in highly-ionized plasmas is the dielectronic recombination (DR).[4–6] However, due to the complexity of the calculations, very few *ab initio* level-by-level DR calculations have been published for highly-ionized elements, especially for Co-like elements.

In this paper, we focus on the level-by-level calculation of DR rates for Co-like Ag and Ta ions. The present calculation is based on Cowan's non-relativistic multi-configuration Hartree–Fock code, including the relativistic mass-velocity and Darwin corrections.[7] Five Co-like states from configurations $3s^23p^63d^9$, $3s^23p^53d^{10}$ and $3s^13p^63d^{10}$ (denoted by $(3s^23p^63d^{10})^{-1}$), 107 Ni-like singly-excited states from configurations $3s^23p^63d^94l$, $3s^23p^53d^{10}4l$ and $3s^13p^63d^{10}4l$ (denoted by $(3s^23p^63d^{10})^{-1}4l$), and all the autoionization states from Ni-like configurations $3s^23p^63d^84l4l'$, $3s^23p^53d^94l4l'$, $3s^23p^43d^{10}4l4l'$, $3s^13p^63d^94l4l'$, $3s^13p^53d^{10}4l4l'$, $3s^03p^63d^{10}4l4l'$ (denoted by $(3s^23p^63d^{10})^{-2}$ $4l4l'$) are included in the present calculations. It is found that the energy levels of autoionization states lie in an extensive region. As a result, the total net rate coefficients, as functions of electron temperatures, are very interesting: (1) there are more than one 'peak' in the region of interest (from 0.1eV to several keV); (2) at low electron temperatures, especially for the DR of Co-like Ta ions, the rate coefficients are very large. Therefore, such DR rate coefficients cannot be reproduced by a simple analytical formula, such as the Burgess–Merts formula,[8,9] or the Hagelstein approximation.[10] We propose to use the multi-set Hagelstein parameters, which are convenient in practice and can well reproduce the *ab initio* calculated DR rate coefficients.

II. THEORETICAL METHOD AND RESULTS

Dielectronic recombination can be regarded as a resonant radiative recombination process.[4–6] As a free electron with a specific kinetic energy collides with an ion A^{q+} in a state m, one of the bound electrons in the ion A^{q+} is excited and the free electron is captured. Then a resonant doubly-excited state j is formed, and subsequently the resonant doubly-excited state can decay into a non-autoionizing state k through the radiative transition process. In this pa-

*Project supported by the National Natural Science Foundation of China (Grant Nos. 10074062 and 19974006), the National High-Tech ICF Committee of China, and the Science and Technology Funds of the China Academy of Engineering Physics (Grant No. 20010218).

per, the DR process can be represented by

$$[\text{Ne core}]\,(3s^2 3p^6 3d^{10})^{-1} + e^- \rightleftharpoons [\text{Ne core}]\,(3s^2 3p^6 3d^{10})^{-2} 4l4l', \quad (1)$$

$$[\text{Ne core}]\,(3s^2 3p^6 3d^{10})^{-2} 4l4l' \rightarrow \begin{cases} [\text{Ne core}]\,3s^2 3p^6 3d^{10} + h\nu \\ [\text{Ne core}]\,(3s^2 3p^6 3d^{10})^{-1} 4l'' + h\nu' \end{cases}, \quad (2)$$

where [Ne core] represents the full $1s^2 2s^2 2p^6$ electronic inner shell, e^- is the interacting free electron and $h\nu$ denotes the emitted photon. The first process is the electron capture which is reversible via autoionization. The second process is the radiative stabilizing transition. Thus the DR rate coefficient can be defined by

$$\alpha^{DR}_{mjk}(T) = \frac{h^3}{2(2\pi m_e k_B T)^{3/2}} \exp(-E_{jm}/k_B T) \cdot \frac{g_j}{g_m} \frac{A^a_{jm} A^r_{jk}}{\sum_{m'} A^a_{jm'} + \sum_{k'} A^r_{jk'}}, \quad (3)$$

where k_B is the Boltzmann constant, and m_e and T are electron mass and temperature. E_{jm} is the energy difference between level j and level m; g_j and g_m are weight factors of levels j and m respectively; A^a_{jm} is the autoionization rate from the autoionization state j to a low-lying Co-like level m; and A^r_{jk} is the radiative decay rate from the autoionization state j to the stabilizing state k.

In this paper, the energy levels, the Auger rates, the absorption oscillator strengths and wavelengths are calculated using Cowan's codes,[7] which have been described in detail in his book. These codes are used extensively, and are developed for studying other atomic processes, for example, collisional excitation processes between electron and ions, and good results are obtained.[11,12] Since there are too many open shells for the doubly-excited states, we do not take into account the configuration interaction effects in this paper; we only calculate the energy levels of these states and the corresponding parameters within the single-configuration frame. Figure 1 displays the calculated configuration average energy of Co-like and Ni-like Ag and Ta ions. Obviously, some doubly-excited states lie below the ionization limit and cannot be involved in the DR processes as the autoionization states j, but they can be treated as the radiative stabilizing states k obtained from the decay of the autoionization states with opposite parity, lying above the ionization limit. For simplicity, their effect on the DR rates will not be discussed in this paper. The autoionization state can also decay radiatively to another autoionization state lying above the ionization limit and ultimately finish the DR process through several consecutive radiative transitions (cascades). Due to their extreme complexity, the cascades are also not considered in the present calculation. In Fig.1, there are many autoionization states lying very close to the ionization limit, which have a significant effect on the DR processes, as will be seen in the discussion.

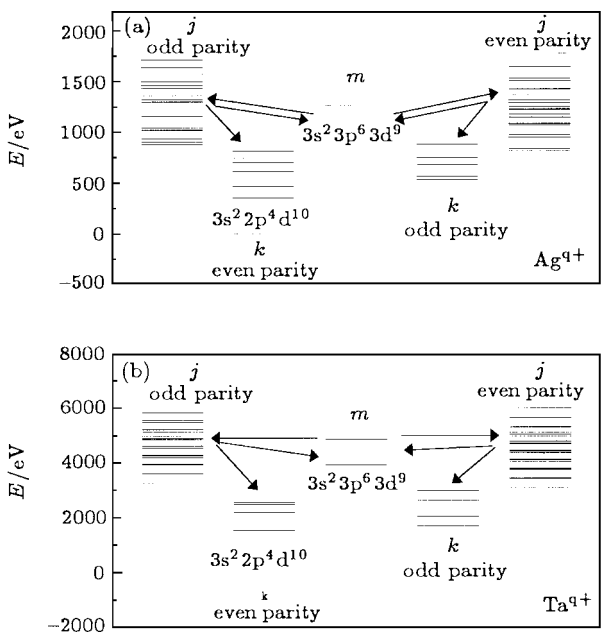


Fig.1. Configuration average energies of Co-like and Ni-like Ag and Ta ions.

With the energy levels, the Auger rates, the absorption oscillator strengths and wavelengths are calculated using Cowan's codes, and the net DR rate coefficient via the path $m \rightarrow j \rightarrow k$ can be obtained using Eq.(3). The total net rate coefficient for all paths is given by

$$\alpha^{DR}(T) = \frac{1}{n} \sum_m \sum_j \sum_k n_m \alpha^{DR}_{mjk}(T), \quad (4)$$

where n_m is the density of ions in level m, and $n = \sum_m n_m$. Here we suppose that $n_m/n = g_m/G_m$ and $G_m = \sum g_m$. Since, to our knowledge, no work on the DR processes of Co-like heavy ions have been published, we first calculate the DR rate coefficients of Ni-like Ta ions. The result is shown in Fig.2, together with the theoretical results of Behar *et al.*[13] for comparison. The results in Ref.[13] have been calculated based on the semi-relativistic distorted-wave approximation for the autoionization coefficients, and the multi-configuration relativistic method for level

energies and radiative coefficients. Good agreement has been obtained between our results and those of Behar *et al.*, indicating the reliability of the present calculations. Figure 3 displays our calculated total net rate coefficients for the DR of Co-like Ag and Ta ions through the whole Ni-like $(3s^2 3p^6 3d^{10})^{-2} 4l4l'$ complex. In Fig.3, the shapes of the DR rate coefficients for Co-like Ag and Ta ions are quite different from those of Ni-like Ta ions in Fig.2: (1) there are more than one 'peak' in the region of interest; (2) at low electron temperatures, especially for the DR of Co-like Ta ions, the rate coefficients are very large.

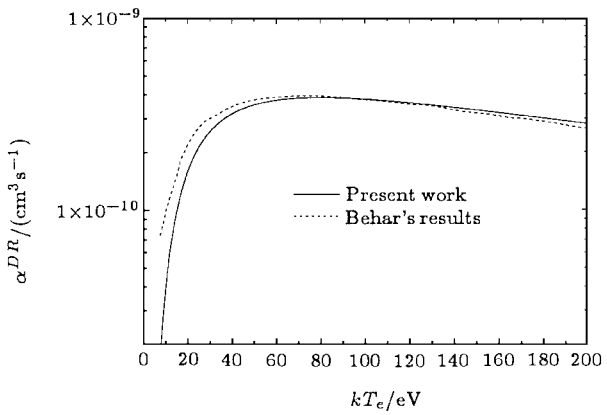


Fig.2. Rate coefficients for DR of Ni-like Ta ions through the Cu-like $3d^9 4l4l'$ complex as a function of the electron temperature: solid line, the present work; dotted line, results from Ref.[13].

In order to make the calculation easy in practice, we often use some simple formulae to describe the DR rate coefficient, such as the general semi-empirical Burgess–Merts formula,[8,9] the numerically fitted formula which was used by Hagelstein and co-workers[14] when treating the DR process of Ne-like ions. Another kind of approximation, also proposed by Hagelstein, is that based on the statistical method, in which a set of parameters is used to describe the DR process, namely the average absorption strength and the average wavelength defined, as in Ref.[10], as

$$\overline{f}_{mk} = \sum_j f_{kj} \frac{A^a_{jm}}{\sum_{m'} A^a_{jm'} + \sum_{k'} A^r_{jk'}}, \qquad (5)$$

$$\overline{\lambda}_{mk} = \sum_j \lambda_{kj} f_{kj} \frac{A^a_{jm}}{\sum_{m'} A^a_{jm'} + \sum_{k'} A^r_{jk'}} \cdot \left(\sum_j f_{kj} \frac{A^a_{jm}}{\sum_{m'} A^a_{jm'} + \sum_{k'} A^r_{jk'}} \right)^{-1}, \qquad (6)$$

where f_{kj} and λ_{kj} are the absorption oscillator strengths and transition wavelengths from level j to k, respectively. The net DR rate coefficient from a level m to a final stable ground or single-excited state k through all possible intermediate states j can be expressed approximately as

$$\alpha^{DR}_{mk}(T) = \sum_j \alpha^{DR}_{mjk} \approx \frac{g_k}{g_m} \frac{1}{2} \left(\frac{h^2}{2\pi m_e k_B T} \right)^{3/2} \times \frac{8\pi^2 e^2}{m_e c \overline{\lambda}^2_{mk}} \overline{f}_{mk} \exp\left(-\frac{\overline{\Delta E}_{km}}{k_B T} \right), \qquad (7)$$

with

$$\overline{\Delta E}_{km} = \frac{12398.5}{\overline{\lambda}_{mk}} + E_k - E_m \quad (in\ \mathrm{eV}), \qquad (8)$$

which can be regarded as the average energy of the captured electrons.

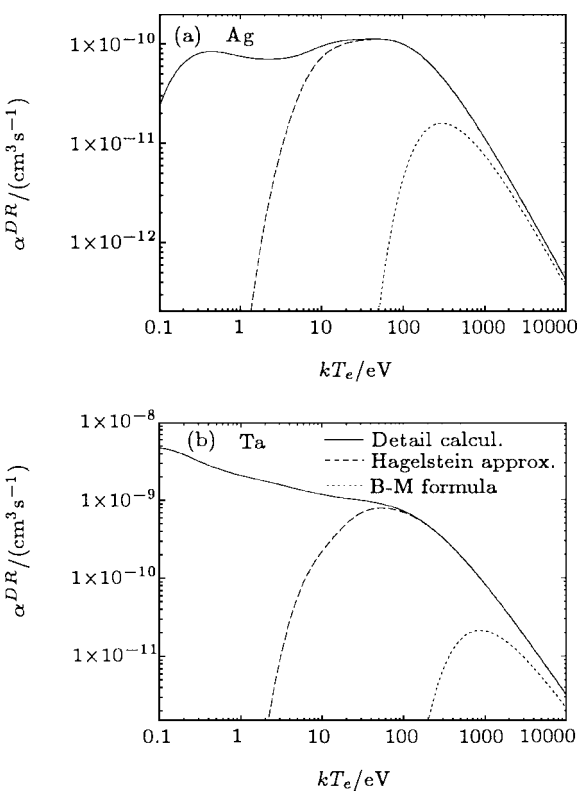


Fig.3. Rate coefficients for the DR of Co-like Ag and Ta ions: solid line, detailed results calculated level-by-level; dashed line, calculated using the Hagelstein approximation; dotted line, calculated using the Burgess–Merts formula.

The abbreviated form of the Hagelstein approximation has made it very convenient in practice and it has been used extensively in past years. Hagelstein's approximation can reproduce the net DR rate coefficient in the DR processes in which the autoionization

states lie in a small energy range, for example, the DR process of Ne-like ions via the $3l3l'$ manifold. Whereas for the DR processes in which the energy levels of the autoionization states lie in an extended range, the simple Hagelstein approximation, as shown in Fig.3, cannot reproduce the net DR rate coefficient. Figure 3 also shows the DR rate coefficients calculated using the semi-empirical Burgess–Merts formula. It is very clear that neither the Hagelstein approximation nor the Burgess–Merts formula can fully reproduce the *ab initio* calculated results.

Ⅲ. DISCUSSION

As pointed out above, there are more than one 'peak' in the total net rate coefficients for the DR of Co-like Ag and Ta ions, and at low electron temperatures, especially for the DR of Co-like Ta ions, the rate coefficients are very large. As a function of the electron temperature, the behaviour of the DR rate coefficients depends mainly on $T^{-3/2}$ and $\exp(-E_{jm}/k_BT)$ in Eq.(3), i.e. it is determined by E_{jm}. As can be seen in Fig.1, the energy levels of the autoionization lie in a fairly wide range, and some lie very close to the ionization limit. This means that E_{jm} is very small. It can be easily understood from Eq.(3) that it is just these states that strongly enhance and even dominate the whole DR process at low electron temperatures. It should be pointed out that such peculiar levels are of special interest in the research of x-ray lasers, since the strong capture to particular autoionization states may lead to a population inversion and a lasing process.

Because of their interesting structure, the DR rate coefficients cannot be well reproduced neither by the Hagelstein approximation nor by the Burgess–Merts formula. In order to make it easy to use, for example, in calculating the occupations of the lasing level in x-ray laser research, a parameterized formula is necessary. Since the simple Hagelstein approximation cannot be adopted for the DR rate of Co-like ions, an easy method is to use the multi-set of Hagelstein parameters

$$\alpha_{mk}^{DR}(T) \approx \sum_i \frac{g_k}{g_m}\frac{1}{2}\left(\frac{h^2}{2\pi m_e k_B T}\right)^{3/2} \times \frac{8\pi^2 e^2}{m_e c \overline{\lambda}_{mk,i}^2}\overline{f}_{mk,i}\exp\left(-\frac{\overline{\Delta E}_{km,i}}{k_BT}\right), \quad (9)$$

where the summation and averaging are carried out for those autoionization state with energy levels close to each other. We find that, for the DR rate of Co-like Ag ions and Co-like Ta ions, five and six sets, respectively, of Hagelstein parameters are good enough to reproduce the *ab initio* calculated DR rate coefficients. The results are plotted in Fig.4.

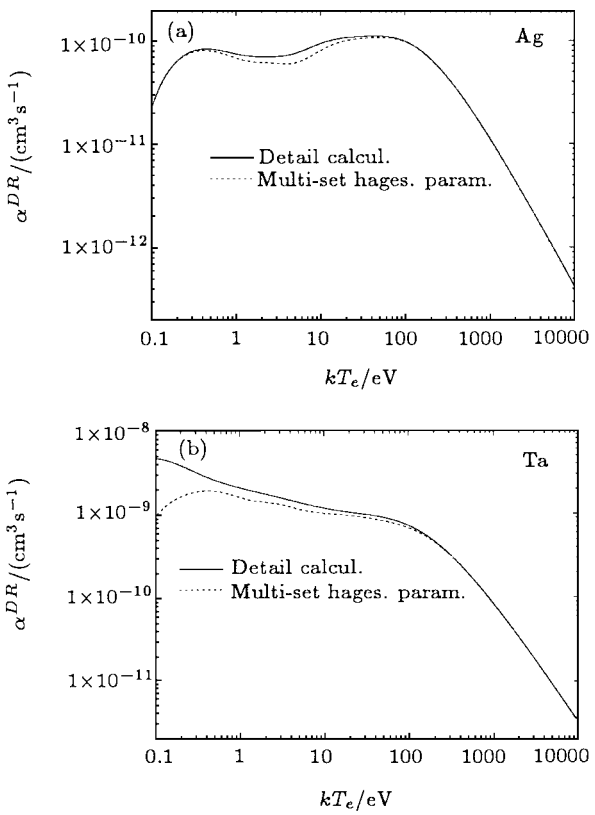


Fig.4. Rate coefficients for the DR of Co-like Ag and Ta ions: solid line, detailed results calculated level-by-level; dotted line, calculated by multi-set Hagelstein parameters.

Finally, we would like to conclude by making the following comments. Because of the extensive distribution of the autoionization state energy levels, especially some energy levels lying very close to the threshold of the Co-like ions, the DR rate coefficient of the Co-like ions are very interesting. There are more than one 'peak' in the region of interest of electron temperatures, and at low electron temperatures, especially for the DR of the Co-like Ta ion, the rate coefficients are very large. Such DR rate coefficients cannot be reproduced using a simple analytical formula, such as the Burgess–Merts formula, or the Hagelstein approximation. We suggest the use of a multi-set of Hagelstein parameters. This method is convenient in practice and can well reproduce the *ab initio* calculated DR rate coefficients. Because of the large number of complete sets of rate coefficients and related atomic data, we only present some of our results and the total net DR rate coefficients in this paper. The detailed data

are available from the authors on request. Further studies, such as those taking into account the configuration interaction effects and the radiative transition between doubly-excited states, and the search for a more suitable parameterized formula to describe such complicated rate coefficients, are underway and will be reported elsewhere. Theoretical calculations based on other methods, such as the relativistic multichannel theory[15,16] and the R-matrix method,[17] are also needed for further studies.

References

[1] Arnaud M and Rothenflug R 1985 *Astron. Astrophys. Suppl. Ser.* **60** 425

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

[3] Yan J and Li J M 2000 *Chin. Phys. Lett.* **17** 194

[4] Dong C Z, Zou Y, Wang J G and Li J M 1995 *Acta Phys. Sin.* **44** 1712 (in Chinese)

[5] Wang J G, Zou Y and Chang T Q 1997 *Acta Phys. Sin.* **46** 2146 (in Chinese)

[6] Dong C Z, Wang J G and Qu Y Z 1998 *Acta Phys. Sin.* **47** 277 (in Chinese)

[7] Cowan R D 1981 *The Theory of Atomic Structure and Spectra* (Berkeley, CA: University of California Press)

[8] Burgess A 1964 *Astrophys. J* **139** 776
Burgess A 1965 *Astrophys. J* **141** 1588

[9] Merts A L, Cowan R D and Magee N H Jr 1976 *Los Alamos Scientific Laboratory Report No. La-6220-MS* (unpublished)

[10] Hagelstein P L 1987 *J. Phys. B: At. Mol. Phys.* **20** 5785

[11] Fang Q Y *et al* 1995 *Acta Phys. Sin.* **44** 383 (in Chinese)

[12] Fang Q Y, Cai W, Zou Y and Li P 1998 *Acta Phys. Sin.* **47** 1612 (in Chinese)

[13] Behar E, Mandelbaum P, Schwob J, Bar-Shalom A, Oreg J and Goldstein W H 1995 *Phys. Rev.* A **52** 3770

[14] Dalhed S, Nisen J and Hagelstein P 1986 *Phys. Rev.* A **33** 264

[15] Yan J, Zhang P H, Tong X M and Li J M 1996 *Acta Phys. Sin.* **45** 1978 (in Chinese)

[16] Zou Y, Zhao L B and Fang Q Y 1999 *Phys. Rev.* A **60** 4510

[17] Yan J, Qu Y Z, Voky L and Li J M 1998 *Phys. Rev.* A **57** 997