Vol 13 No 6, June 2004
1009-1963/2004/13(06)/0850-05

Chinese Physics

© 2004 Chin. Phys. Soc.
and IOP Publishing Ltd

Dielectronic recombination rate coefficient for Cu-like Au^{50+} ion*

Yang Tian-Li(杨天丽), Jiang Gang(蒋 刚)†, and Zhu Zheng-He(朱正和)

Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, *China*

(Received 25 February 2003; revised manuscript received 19 December 2003)

The rate coefficients $\alpha^{\rm DR}$ of dielectronic recombination (DR) for Cu-like Au^{50+} ion collided with the incident free electron are calculated based on the quasi-relativistic multi-configuration Hartree–Fock theory. The results clearly show that the $\alpha^{\rm DR}$ of all recombination channels exhibits resonance characters with electron temperature. At lower temperatures, the recombination for electrons caused by 4s excitation is dominant through outer electron radiative transitions among the intermediate doubly excited autoionizing levels, in which the most components come from $3d^{10}5pns$ states, whereas with increasing electron temperature, DR caused by 3d excitation turns out to be dominant, and the contribution from the $3d^94s4fnf$ state to the total rate coefficient of electron 3d is the largest with $\alpha^{\rm DR} = 1.15 \times 10^{-11}\,{\rm cm}^3{\cdot}{\rm s}^{-1}$ at an electron temperature of $T_{\rm e}$=0.35 keV. Under this condition, there exists a strong competition between the two types of recombination channels.

Keywords: Cu-like Au^{50+}ion, dielectronic recombination
PACC: 3480L, 3150

1. Introduction

Dielectronic recombination (DR), one of the electron–ion inelastic collision processes, plays an important role in the non-local thermodynamic equilibrium (non-LTE) plasma with mid-high electron temperature and mid–low electron density. DR is also an important mechanism of population inversion in laser materials for the research of soft x-ray laser.[1] Recent researches [2,3] indicate that, in high-temperature and high-density inertial confinement fusion (ICF) plasma, DR can greatly affect the behaviour of plasmas and the transform of x-rays. Because of its larger absorption from laser and higher transform of x-rays, gold is taken as a good ICF target material, and then the charge state distribution (CSD) and the average ionization degree of the gold plasma are given much emphasis in the research. Using the atomic collision–radiative model and fully considering the effect of dielectronic recombination process on the population of excited states in the non-LTE plasma, Foord *et al*[4] have theoretically simulated the two parameters with the Cu-like Au^{50+} ion at the peak of the curve of CSD.

Up to now, very few DR calculations have been reported for highly ionized gold ions,[5,6] especially for ions with more than 18 electrons.[7,8] In this paper, the DR rate coefficients of Au^{50+} ion at different electron temperatures have been calculated on the basis of the quasi-relativistic multi-configuration Hartree–Fock theory.[9] At the same time, the rules of variation of $\alpha^{\rm DR}$ with electron temperature, intermediate doubly excited autoionizing states, the recombination types and orbital angular momentum l have been studied. The present work is not only helpful to the study of the interaction between the laser and target material and the structure of doubly excited states, but also to the supply of large amounts of atomic data for astrophysics, plasmas, and x-ray laser studies.

2. Theory

The DR is considered as a two-step process:

$$e + A^{q+} \Leftrightarrow (A^{(q-1)+})^{**}, \tag{1}$$

$$(A^{(q-1)+})^{**} \Rightarrow (A^{(q-1)+})^{*} + h\nu. \tag{2}$$

Equation (1) represents a resonant radiationless dielectronic capture (DC) of a free electron by an A^{q+} ion into an intermediate doubly excited autoionizing state $(A^{(q-1)+})^{**}$. The DR process is completed if

*Project supported by the National High Technology Development Programme of China (Grant No 2002AA84TS12).
†Corresponding author. Tel: 86-28-85405234, E-mail: gjiang@pridns.scu.edu.cn

the intermediate doubly excited state decays radiatively to a state below the autoionization threshold (Eq.(2)). Under the conditions of complete thermodynamic equilibrium, the populations of the ground or steady-excited levels of all ions satisfy the Boltzmann and Saha equations, and the free electrons have a Maxwell–Boltzmann velocity distribution corresponding to a certain electron temperature. By means of the principle of detailed balance, the capture rate can be evaluated in terms of the inverse process (autoionization), i.e.

$$\beta_{id} = \frac{4\pi^{3/2}a_0^3}{(kT_\mathrm{e})^{3/2}}\frac{g_d}{g_i}\mathrm{e}^{-E_{di}/kT_\mathrm{e}}A^\mathrm{a}_{di}, \tag{3}$$

where $|i\rangle$ and $|d\rangle$ are the initial and intermediate doubly excited autoionizing states respectively. In a low-density plasma, the collision de-excitation processes are negligible, and the decay probability for transit to the final state f is given by the branching ratio. Then the state–state recombination rate coefficient via the path $i \to d \to f$ is

$$\alpha^\mathrm{DR}_{idf}(T_\mathrm{e}) = \frac{4\pi^{3/2}a_0^3}{(kT_\mathrm{e})^{3/2}}\frac{g_d}{g_i}\mathrm{e}^{-E_{di}/kT_\mathrm{e}}\frac{A^\mathrm{a}_{di}A^\mathrm{r}_{df}}{\sum\limits_i A^\mathrm{a}_{di} + \sum\limits_f A^\mathrm{r}_{df}}, \tag{4}$$

where T_e is electron temperature, E_{di} is an energy level interval (in Rydberg units) between $|d\rangle$ and $|i\rangle$ states, k is the Boltzmann constant, a_0 is the Bohr radius, g_d and g_i are the statistical weights of $|d\rangle$ and $|i\rangle$ states respectively, and A^a_{di} and A^r_{df} are the autoionization and spontaneously radiative transition rates of the doubly excited autoionizing state. The total DR rate coefficient α^DR should be the sum of all the state–state recombination rate coefficients,

$$\alpha^\mathrm{DR}(T_\mathrm{e}) = \frac{1}{n_N}\sum_d\sum_f\sum_i \alpha^\mathrm{DR}_{idf}(T_\mathrm{e}). \tag{5}$$

For a high-Z multi-electron atomic system, the relativistic effect cannot be ignored in calculating its energy levels. In this work, the energy level, autoionization rate, and spontaneous radiative transition rate have been calculated by using the Cowan's multi-configuration Hartree–Fock code with our developed software to calculate DR rate coefficients, which includes the relativistic mass-velocity, spin-orbit coupling correlation, Darwin term, Breit correction and retardation energies. The continuum orbital wavefunction can be found with the distorted wave theory (DWT) and the independent resonance approximation. The purpose of this paper is to find the basic rules of the DR process about the high-Z multi-electron atom (ion) system.

3. Results and discussion

3.1. DR from 4s electron excitation

The electron temperature is a reflection of the kinetic energy of free electrons. If T_e is low, the valence electron of an ion can be easily excited by the simultaneous radiationless capture of a free electron with small kinetic energy. Here the calculation of α^DR on valence electron 4s excitation ($\Delta n_\mathrm{c} = 1$) is performed, and the recombination channels are chosen as follows:

$$3\mathrm{d}^{10}4\mathrm{s} + \mathrm{e} \Leftrightarrow 3\mathrm{d}^{10}5\mathrm{p}nl \to 3\mathrm{d}^{10}5\mathrm{p}4l' + h\nu, \quad (0 \le l' \le 3), \tag{A}$$

$$3\mathrm{d}^{10}4\mathrm{s} + \mathrm{e} \Leftrightarrow 3\mathrm{d}^{10}5\mathrm{p}nl \to 3\mathrm{d}^{10}4\mathrm{s}nl + h\nu, \quad (0 \le l \le 3), \tag{B}$$

where type A represents the DR with outer electron nl decay of intermediate doubly excited autoionizing state, and type B is the DR with inner electron 5p decay.

All levels of configuration $3\mathrm{d}^{10}5\mathrm{s}6\mathrm{s}$ are above the ionization threshold of Cu-like gold ion. The main quantum number n varies in the range of 6–16. Figure 1 shows the regularities of α^DR about type A recombination of outer electrons radiative decay with electron temperature T_e. It can be seen that the α^DR of type A have different regularities with increasing T_e when the active electron (i.e. outer electron) is located in different orbits. At lower temperatures, the recombination of intermediate doubly excited states $3\mathrm{d}^{10}5\mathrm{p}n\mathrm{s}$ tends to be dominant when its active electron is located in s orbit. The value of α^DR increases sharply with the increase of T_e and the peak of the curve has a value $8.54 \times 10^{-12}\,\mathrm{cm^3{\cdot}s^{-1}}$ at T_e= 0.018 keV, and then the α^DR decreases rapidly with increasing T_e and displays an asymptotic behaviour. The full width at half maximum of this curve is narrow. The recombination of active electron in d orbit is weaker than that in s orbit. After reaching the maximum point, the α^DR then decreases smoothly with increasing T_e. At about 0.25 keV the α^DR values of the two channels are the same. In the range of $T_\mathrm{e} > 0.25$ keV, the α^DR of recombination for d active electrons is larger than that for s active electrons. For the other two recombinations of intermediate doubly excited states with even parity $3\mathrm{d}^{10}5\mathrm{p}n\mathrm{p}$ and $3\mathrm{d}^{10}5\mathrm{p}n\mathrm{f}$, the values

of $\alpha^{\rm DR}$ are smaller than those of the former two channels. This indicates that, in the whole temperature range, the major contribution to the total DR rate coefficient of type A comes from the recombination in which the active electrons are in s and d orbits, and there is a strong competition between the two channels. That is to say, in the range of 0.006 keV $\leq T_{\rm e} \leq$0.25 keV, the recombination of intermediate doubly excited state $3d^{10}5pns$ is larger than that of $3d^{10}5pnd$; and at 0.25 keV $\leq T_{\rm e}$, the latter tends to be dominant. Figure 2 shows the variation of type B $\alpha^{\rm DR}$ with $T_{\rm e}$. It shows that the recombination of intermediate doubly excited state $3d^{10}5pns$ preponderates over the other recombinations in the entire temperature range, which has a maximum value of $6.27 \times 10^{-12}\,{\rm cm^3 \cdot s^{-1}}$ at $T_{\rm e}$=0.018 keV; and the relationship between $\alpha^{\rm DR}$ and $T_{\rm e}$ is similar to that of type A. However, there is not a cross between the two curves of $3d^{10}5pns$ and $3d^{10}5pnd$. For the other two channels of $3d^{10}5pnp$ and $3d^{10}5pnf$, the recombination rate coefficients are also very small.

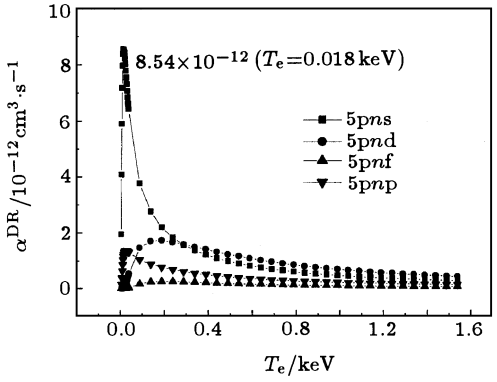


Fig.1. Theoretic values of $\alpha^{\rm DR}$ for type A recombination.

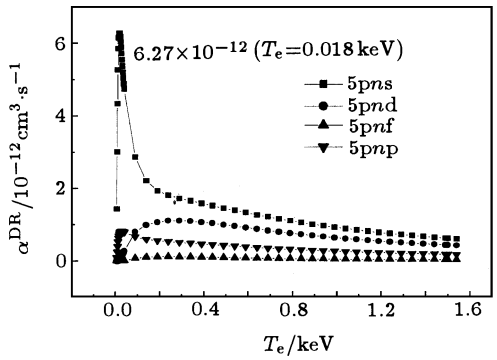


Fig.2. Theoretic values of $\alpha^{\rm DR}$ for type B recombination.

Meanwhile, the results also show that the rate coefficient of the type A recombination is greater than that of the type B recombination at lower temperatures. However, with the increase of $T_{\rm e}$, the dominance of type A recombination becomes weaker and weaker, and type B recombination turn out to be dominant when the electron temperature $T_{\rm e}$ is equal to 0.45 keV. In other words, there is a great competition between types A and B. From formula (4), there are many factors for determining the DR rate coefficient $\alpha^{\rm DR}$. For the recombinations of types A and B with the same intermediate doubly excited state, the spontaneously radiative probability, transition energy and electron temperature are the direct impact factors. The final states of type B belong to Rydberg states, whose levels are higher than those of type A, and the corresponding transition energies ΔE are much less than those of type A. In the light of the definition of spontaneous radiative transition probability,[10] the fact that $A^{\rm r}_{df}$ is directly proportional to $\Delta E^3 (A^{\rm r}_{df} \propto \Delta E^3)$ makes the $A^{\rm r}_{df}$ larger with larger ΔE, so at lower temperatures, the dielectronic recombination rate coefficient $\alpha^{\rm DR}$ is mainly determined by ΔE, not by electron temperature $T_{\rm e}$. When the temperature rises to a certain value, there is a cross-over between A and B curves, indicating that the type A recombination is comparable to type B recombination. With the temperature increasing further, the effect of $T_{\rm e}$ on $\alpha^{\rm DR}$ becomes gradually stronger and the type B recombination tends to be dominant. In addition, for different outer electrons, the temperature for peak values of DR rate coefficient $\alpha^{\rm DR}$ becomes higher and higher with the increase of orbital angular momentum l.

The contributions of other intermediate doubly excited states have also been taken into account in the study of the total DR rate coefficients, like $3d^{10}4pnl$ ($\Delta n_{\rm c} = 0$)and $3d^{10}6pnl$ ($\Delta n_{\rm c} = 2$). For the case of $\Delta n_{\rm c} = 0$, the DR rate coefficient $\alpha^{\rm DR}$ takes on the monotropic degression with electron temperature $T_{\rm e}$, and no resonant peak appears in the whole temperature range. Taking the configuration $3d^{10}4p16s$ as an example, though its average energy is above the ionization threshold by 64.6 eV, the $^3P_{0,1,2}$ levels of this configuration split by orbital-spin coupling are below the level of $3d^{10}4s$ ($^2S_{1/2}$). For this reason, the DR process for this case cannot actually occur. Therefore, the rate coefficients obtained are unreasonable for $\Delta n_{\rm c} = 0$. In the case of $\Delta n_{\rm c} = 2$, the $\alpha^{\rm DR}$ of the intermediate doubly excited state $3d^{10}6pnl$ is only one-tenth as much as the $\alpha^{\rm DR}$ of recombinations with $\Delta n_{\rm c} = 1$, and thus its contribution on the total $\alpha^{\rm DR}$ of Cu-like gold ions can be neglected in the study of DR process.

3.2. DR from 3d electron excitation

As far as the gold plasma in laboratory is concerned, many of the 3d–4f dielectronic satellite lines [11] have been measured with strong intensities, which predicates that the population of excited state $3d^{10}4snl$ has undergone a redistribution under the effect of relative dynamic processes including dielectronic recombination. Thus, it is necessary for us to study DR processes for core electron 3d excitation. The channels of recombination are chosen as follows:

$$3d^{10}4s + e \Leftrightarrow 3d^{9}4s4fnl \rightarrow 3d^{10}4snl + h\nu,$$
$$(0 \le l \le 3, \quad 5 \le n \le 9). \qquad (C)$$

Figure 3 shows the variation of α^{DR} of type C DR with electron temperature T_e. It shows that the recombination curves of intermediate doubly excited states with different spectator electrons have resonance, full width at half maximum and convergence in common, while they show different regularities. Obviously, at lower temperatures, the DR of intermediate doubly excited state $3d^{9}4s4fnf$ prevails over others. The α^{DR} increases fast with increasing T_e and reaches the largest value $1.15\times10^{-11}\,cm^3\cdot s^{-1}$ at T_e=0.35 keV, and the α^{DR} of the state $3d^{9}4s4fnd$ peaks at 0.95 keV with $9.45\times10^{-12}\,cm^3\cdot s^{-1}$. At about 0.75 keV, the α^{DR} of the two channels are comparable, yet in the range of $T_e > 0.75$ keV, the α^{DR} of $3d^{9}4s4fnf$ decreases while the recombination of state $3d^{9}4s4fnd$ becomes dominant. In the case that the spectator electrons are in s and p orbits, their rate coefficients α^{DR} are always smaller than those of the former two recombinations. For instance, the maximum values of the latter two DR are only one-third as much as those of $3d^{9}4s4fnf$ and $3d^{9}4s4fnd$. That is to say, the main components of the total α^{DR} of type C come from the recombinations of intermediate doubly excited states $3d^{9}4s4fnf$ and $3d^{9}4s4fnd$. This result indicates that the free electrons have been likely captured into intermediate doubly excited states with high energy for type C recombination. A comparison between the total DR rate coefficients of types A, B and C is given in Fig.4. At lower temperatures, type A has a larger rate coefficient than types B and C have; when T_e is greater than 0.09 keV, the α^{DR} of type C is almost three times as large as those of types A and B. So the DR process from the core electron 3d excitation is dominant at higher temperatures, and the increasing amount of population of excited states $3d^{10}4snl$ comes from the DR process of type C, not type B recombination.

In addition, in the course of calculating the α^{DR} of type C, we have not considered the case of $3d^{9}4s5fnl$ ($\Delta n_c = 2$), because the α^{DR} is one order of magnitude smaller than that of state $3d^{9}4s4fnl$ ($\Delta n_c = 1$), and its contribution to the total recombination of Cu-like gold ion is tiny.

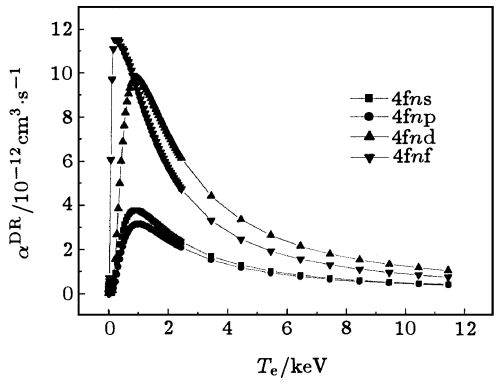


Fig.3. Theoretic values of α^{DR} of type C recombination.

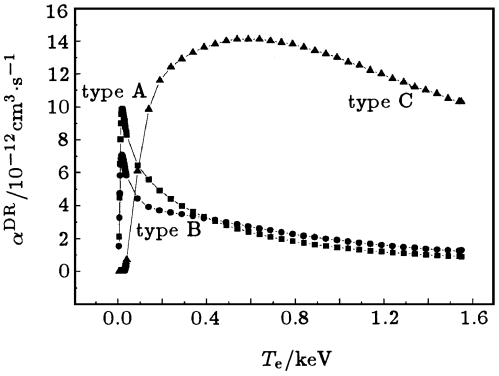


Fig.4. Comparison of α^{DR} between types A, B and C recombinations.

4. Conclusion

In summary, the recombination of type A with valence electron 4s excitation tends to be dominant at lower temperatures, and the major contribution comes from $3d^{10}5pns$, whereas in the middle- and high-temperature ranges, the DR of type C excited from core electrons 3d is superior to others, in which the largest contribution comes from the α^{DR} of intermediate doubly excited states of spectator electrons with orbital angular momentum f that greatly affects the population of ions.

References

[1] Dasgupta A 1995 *J. Quant. Spectrosc. Radiat. Transfer* **54** 737

[2] Gu P J, Wang J G and Chang T Q 1999 *High Power Laser And Particle Beams* **11** 78 (in Chinese)

[3] Glenger S H *et al* 1999 *Phys. Rev. Lett.* **82** 97

[4] Foord M E *et al* 2000 *J. Quant. Spectrosc. Radiat. Transfer* **65** 231

[5] Chen B, Zheng Z J and Zhu Z H 1999 *High Power Laser and Particle Beams* **11** 454 (in Chinese)

[6] Ye A P and Ma M Z 1997 *Acta Sci. Natur. Univ. Pekin.* **33** 632 (in Chinese)

[7] Yan J *et al* 2001 *Chin. Phys.* **12** 1124

[8] Jiao R Z and Chen X L 2002 *Acta Phys. Sin.* **51** 1755 (in Chinese)

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

[10] Grant I P 1974 *J. Phys. B* **7** 1458

[11] Zhang J Y, Yang G H and Zhang B H 2001 *High Power Laser and Particle Beams* **13** 186 (in Chinese)