Dielectronic recombination coefficients for Ni-like tantalum

Mau Hsiung Chen
University of California, Lawrence Livermore National Laboratory, Livermore, California 94550
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Dielectronic-recombination (DR) rate coefficients for the ground state of Ni-like Ta^{45+} have been calculated for the electron temperatures in the range $0.02 < T < 10$ keV. The calculations were carried out in the isolated resonance approximation using the multiconfiguration Dirac-Fock model in intermediate coupling with configuration interaction. The total DR rate coefficients were obtained by including the contributions from the 3s, 3p, and 3d excitations. The rate coefficients are found to peak at very low temperature ($\sim$80 eV) with a value of 3.58×10^{-10} cm^3/sec and reduce to 1.48×10^{-10} cm^3/sec at $T=1$ keV.

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I. INTRODUCTION

Nickel-like Ta ($Z=73$) has recently been demonstrated to achieve amplification in the soft-x-ray regime by an electron collision excitation scheme [1]. The lasing transition with a wavelength of 44.83 Å is well suited for probing biological specimens. In order to correctly model the high-temperature plasmas, one needs vast amounts of high quality atomic data such as energy levels, radiative rates, collisional rates, and recombination rate coefficients. Dielectronic recombination (DR) is an important recombination process for high-temperature plasmas [2]. Knowledge of DR coefficients is essential in the determination of ionization balance and level population [2,3]. Very few *ab initio* calculations of DR rate coefficients for the Ni-like ion exist in the literature. For the plasma modeling applications, one relies heavily on the Burgess-Merts [4,5] semiempirical formula. However, our previous theoretical study for Ni-like $_{64}$Gd using the multiconfiguration Dirac-Fock (MCDF) model [6] revealed that the Burgess-Merts formula overestimates the rate coefficients by a factor of 5 for the electron temperature $T > 250$ eV. To remedy this deficiency, we have carried out the relativistic calculations of DR rate coefficients for the ground state of Ni-like $_{73}$Ta in the isolated-resonance approximation for temperatures in the range of $0.02 < T < 10$ keV. The Auger and radiative rates for each autoionizing state were evaluated explicitly in intermediate coupling with configuration interaction using the MCDF method [7,8]. As in the case of Gd, the rate coefficients are dominated by the contributions from the $3d^{-1}4lnl'$ doubly excited states. Here, $3d^{-1}$ indicates an electron is missing from the 3d shell. The total recombination rate coefficients are found to have a peak value of 3.58×10^{-10} cm^3/sec at $T=80$ eV and decrease to 1.48×10^{-10} cm^3/sec at $T=1000$ eV.

II. THEORETICAL METHOD

Dielectronic recombination from a Ni-like ground state to a state of a Cu-like ion with M-shell excitation can be schematically represented by

$$(\text{Ne core})3s^23p^63d^{10}+e\leftrightarrow(\text{Ne core})3l^{-1}n'l'n''l''$$
$$\rightarrow(\text{Ne core})3s^23p^63d^{10}nl+h\nu\ . \quad (1)$$

In the isolated-resonance approximation and a Maxwellian distribution of plasma electrons, the total dielectronic-recombination coefficients from the initial states i can be written as [9]

$$\alpha_{\rm DR}(i;\text{total})=\frac{1}{2g_i}\left[\frac{4\pi R}{kT}\right]^{3/2}a_0^3\sum_{\kappa_2}\sum_d\sum_f \exp(-e_2/kT)g_d A_A(d\to i,e_2\kappa_2)A_r(d\to f)/[\Gamma_r(d)+\Gamma_A(d)]\ . \quad (2)$$

Here g_d and g_i are the statistical weights for the intermediate states d and initial state i, respectively. R is the Rydberg energy and a_0 is the Bohr radius; $A_r(d\to f)$ is the radiative rate from state d to f; $A_A(d\to i,e_2\kappa_2)$ is the Auger rate with the free electron characterized by energy e_2 and relativistic quantum number $\kappa_2=(l_2-j_2)(2j_2+1)$; and $\Gamma_r(d)$ and $\Gamma_A(d)$ are the total radiative and Auger widths for the intermediate autoionizing state d, respectively.

The Auger and radiative rates required for the calculations of the DR rate coefficients [Eq. (2)] were computed from the perturbation theory using the MCDF model [7,8]. In this model, an atomic state function for a state i with total angular momentum JM is expressed as a linear combination of the configuration state functions $\phi(\Gamma_\lambda JM)$:

$$\psi_i(JM)=\sum_{\lambda=1}^{n}C_{i\lambda}\phi(\Gamma_\lambda JM)\ , \quad (3)$$

where $C_{i\lambda}$ are the mixing coefficients. The Auger transition rate from state d to i is given by [7]

$$A_A(d \rightarrow i, e_2\kappa_2) = 2\pi \left| \sum_{\lambda,\lambda'} C_{i\lambda} C_{f\lambda'} \times \left\langle \phi(\Gamma_{\lambda'} J'M') e_2\kappa_2; JM \right| \times \frac{1}{2} \sum_{\substack{\alpha,\beta \\ \alpha \neq \beta}} \frac{e^2}{r_{\alpha\beta}} \left| \phi(\Gamma_\lambda JM) \right\rangle \right|^2 . \quad (4)$$

The continuum wave function $e_2\kappa_2$ is normalized in energy. The electric dipole radiative transition rate can be written as [7,10]

$$A_r(d \rightarrow f) = \frac{2\pi}{3(2J_d+1)} \left| \sum_{\alpha,\beta} C_{i\alpha} C_{f\beta} \sum_{p,q} d^1_{pq}(\beta,\alpha) \times \langle p \| T_1 \| q \rangle \right|^2 , \quad (5)$$

where $d^1_{pq}(\beta,\alpha)$ are the angular factors and the one-electron reduced dipole matrix elements $\langle p \| T_1 \| q \rangle$ are defined in Ref. [10].

III. NUMERICAL CALCULATION

We carried out detailed calculations of Auger and radiative rates for the intermediate autoionizing states $3d^{-1}4lnl'$ ($n<10$), $3p^{-1}4lnl'$ ($n<10$), and $3s^{-1}4lnl'$ ($n<7$). The atomic energy levels and bound-state wave functions were obtained by minimizing the average energy of all the levels in the MCDF method [8]. The effects of the intermediate coupling and the configuration interaction from the same complex were included in these calculations. These atomic data were then used to compute the DR rate coefficients according to Eq. (2). The contributions from the high-n states were taken into account for the first two cases by using the n^{-3} scaling rule applied to the Auger transition rates. In the present work only the electric dipole radiative transitions filling the M-shell vacancy were included. The effects of radiative cascade were neglected.

As the principal quantum number n increases along the autoionizing Rydberg series, the Coster-Kronig transitions to the excited states of the recombining ion (e.g., $3p^5 3d^{10} 4lnl' \rightarrow 3p^6 3d^9 4l + e$) can become energetically allowed for n greater than a certain critical value n_0. In the present work, the Coster-Kronig transitions $3p^5 3d^{10} 4lnl' \rightarrow 3p^6 3d^9 4l + e$ were taken into account. However, the Coster-Kronig transitions filling the $n=4$ vacancy (e.g., $3d^{-1}4dnl \rightarrow 3d^{-1}4p + e$) were ignored.

IV. RESULTS AND DISCUSSION

The total DR rate coefficients for Ta^{45+} for $0.02 < T < 10$ keV are listed in Table I. Although there is no $\Delta n = 0$ DR transition (i.e., the DR process with no change of principal quantum number in the major radiative stabilizing decay) for the Ni-like ground state, the DR rate coefficients peak at very low temperature of 80 eV with a value of 3.58×10^{-10} cm^3/sec and decrease to 1.48×10^{-10} cm^3/sec at $T = 1000$ eV. The reason for the strong DR rates at low temperatures can be traced to the energy-level structures of the low-lying $3d^{-1}4l4l'$ and $3p^{-1}4l4l'$ configurations. For these two doubly excited configurations, the thresholds for the Auger decay occur in the middle of the manifolds. As a result, near 30% of the $3p^{-1}4l4l'$ and more than half of the $3d^{-1}4l4l'$ states are not autoionizing. In addition, the Auger energies of some strong Auger states are only a few tens of electron volts. These low-energy Auger transitions dominate the low-temperature behavior of the DR rate coefficients.

The partial DR rates for the $3d^{-1}4lnl'$, $3p^{-1}4lnl'$, and $3s^{-1}4lnl'$ states are compared in Fig. 1. One can see that the rate coefficients are dominated by the contributions from the $3d$ excitation. The $3s$ excitation contributes amount less than 2% to the total DR rate coefficients. Hence, the contributions from the high-n states of the

TABLE I. Dielectronic-recombination coefficients for Ni-like $_{73}$Ta in the ground state.

Temperature (keV)	Rate coefficient (10^{-11} cm^3/sec)	Temperature (keV)	Rate coefficient (10^{-11} cm^3/sec)
0.02	16.7	1.50	10.9
0.05	32.7	2.00	8.40
0.08	35.8	2.50	6.69
0.10	35.6	3.00	5.46
0.20	29.5	3.50	4.57
0.30	25.2	4.00	3.89
0.40	22.5	4.50	3.37
0.50	20.7	5.00	2.95
0.60	19.3	6.00	2.33
0.70	18.0	7.00	1.90
0.80	16.8	8.00	1.59
0.90	15.8	9.00	1.35
1.00	14.8	10.00	1.17

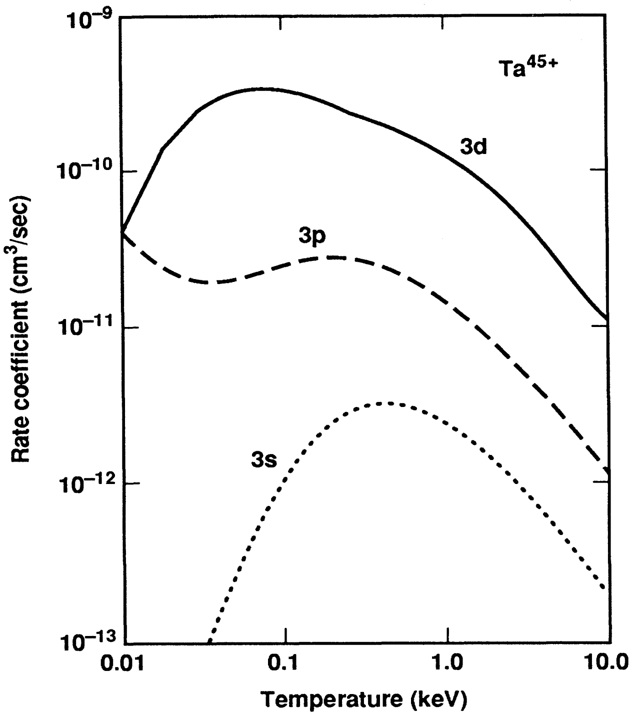

FIG. 1. Partial DR rate coefficients for Ta^{45+} as functions of electron temperature. The solid, dashed, and dotted curves represent the rate coefficients from $3d$, $3p$, and $3s$ excitations, respectively.

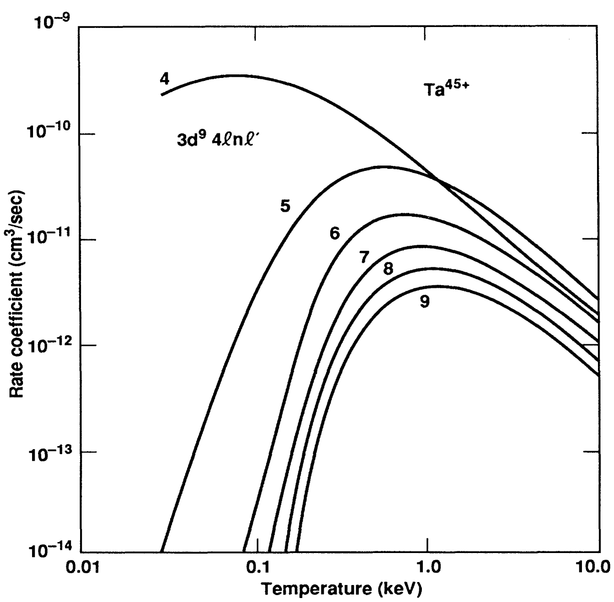

FIG. 2. Partial DR rate coefficients for the $3d^{-1}4lnl'$ intermediate states. The curves are labeled by the principal quantum number n.

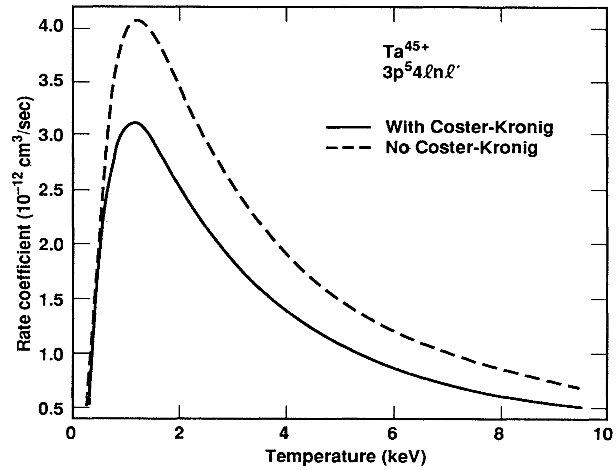

FIG. 3. DR rate coefficients for the $3p^{-1}4lnl'$ intermediate states. The solid curve indicates the values including the Coster-Kronig transitions. The dashed curve represents the results without the Coster-Kronig transitions.

$3s^{-1}4lnl'$ $(n>6)$ were ignored.

In Fig. 2, the n dependence of the DR rate coefficients for the $3d^{-1}4lnl'$ intermediate states is displayed. For $T<200$ eV, the contributions from the intermediate $3d^{-1}4l4l'$ states are several orders of magnitude larger than those from the other high-n states. For $T>1$ keV, the $3d^{-1}4l5l'$ becomes the most important one. As n increases to 9, the DR rate coefficient is reduced by a factor of 10. The contributions from $3d^{-1}4lnl'$ $(n>9)$ to the total DR rate coefficients are about 4% at the peak temperature and 11% at $T=1$ keV.

The effects of the Coster-Kronig transitions to the excited states of the recombining ion on the DR rate coefficient are also investigated in the present work. For the $3p^{-1}4lnl'$ intermediate states, the onset of the $3p$-$3dnl$ Coster-Kronig transitions occurs at $n>5$. The inclusion of these transitions reduces the DR rate coefficients for the $3p^{-1}4ln'l$ states by 25% (see Fig. 3). The N-shell Coster-Kronig transitions (e.g., $4s$-$4pnl$) can become energetically possible for $n>10$. A sample calculation for the $3d^{-1}4l15l'$ states reveals that the DR rate coefficients of these high-n states are reduced by 20% due to the inclusion of the N-shell Coster-Kronig transitions. Therefore, the omission of the N-shell Coster-Kronig transitions is expected to cause less than 2% errors in the total DR rate coefficients for $T<1$ keV and no more than 4% for higher temperatures.

In summary, we have carried out *ab initio* calculations of the DR rate coefficients for the ground state of Ni-like Ta^{45+} using the MCDF model. As in the case of Gd^{36+}, we found that the DR rate coefficients peak at very low temperature and are dominated by the contributions from the $3d$ excitation.

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