Dielectronic recombination coefficient for Ni-like gadolinium

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Dielectronic recombination (DR) coefficients for the ground-state ion of Ni-like $_{64}$Gd have been calculated in the isolated-resonance approximation for temperatures in the range of $0.05 \leq T \leq 3$ keV. The Auger and radiative rates of each doubly excited state were evaluated explicitly by using the multiconfiguration Dirac-Fock model. The calculations were carried out in the intermediate coupling. The effect of the configuration interaction was also included for the low-lying doubly excited states. The intermediate autoionizing states included in the present work are the states from the $3d^{-1}4lnl'$ ($n \leq 10$), $3p^{-1}4lnl'$ ($n \leq 5$), and $3s^{-1}4lnl'$ ($n \leq 5$) configurations. The dielectronic recombination coefficients for Ni-like $_{64}$Gd from the present calculations are 1.33×10^{-10} and 1.08×10^{-10} cm^3/sec for $T = 500$ and 800 eV, respectively. The semiempirical Burgess-Merts formula has been found to overestimate the dielectronic recombination coefficients for the Ni-like $_{64}$Gd by a factor of 5 for $T \geq 250$ eV.

I. INTRODUCTION

Nickel-like ions in the vicinity of gadolinium ($Z = 64$) have been suggested as possible candidates to achieve amplification in the soft-x-ray regime by an electron collisional excitation scheme.[1,2] This laser scheme is analogous to the Ne-like one which has been successfully demonstrated recently.[3] In order to correctly model the high-temperature plasmas, one needs many atomic data such as energy levels, radiative rates, collisional rates, and recombination rate coefficients. Dielectronic recombination (DR) is a very important recombination process for high-temperature plasmas. Knowledge of DR coefficients is essential in the determination of the ionization balance. Furthermore, DR process has been found to be an important mechanism populating the upper laser state in Ne-like ions.[4] To the best of my knowledge, there exist no *ab initio* calculations of DR rate coefficients for the ground state of Ni-like ion. In this paper we report on the relativistic calculations of DR rate coefficients for the ground-state ion of Ni-like $_{64}$Gd. The calculations were carried out in the isolated-resonance approximation for temperatures in the range of $0.05 \leq T \leq 3$ keV. The Auger and radiative rates for each doubly excited state were evaluated explicitly in intermediate coupling by using the multiconfiguration Dirac-Fock (MCDF) model.[5] The effect of configuration interaction was also included for the low-lying, doubly excited states. This MCDF model has previously been used to calculate the DR coefficients for the He-, F-, and Ne-like ions.[6–8] The present MCDF results for Ni-like $_{64}$Gd are compared with the predictions from the Burgess-Merts[9–10] semiempirical formula.

II. THEORETICAL METHOD

The theory of dielectronic recombination has recently been reviewed by Seaton and Storey[11] and by Dubau and Volante.[12] An earlier paper[6] has also detailed the theoretical treatment of the DR process and the calculational scheme based on the MCDF model. Here we shall simply outline the working formulas. The dielectronic recombination coefficients, in the isolated-resonance approximation, can be written as[11]

$$\alpha_{\mathrm{DR}}(i;\mathrm{total}) = \frac{1}{2g_i}\left[\frac{4\pi R}{kT}\right]^{3/2} a_0^3 \sum_{\kappa_2}\sum_{d}\sum_{f} \exp(-e_2/kT) g_d A_a(d \rightarrow i, e_2\kappa_2) A_r(d \rightarrow f)/[\Gamma_r(d)+\Gamma_a(d)] \ . \quad (1)$$

Here g_d and g_i are the statistical weights for intermediate state d and initial state i, respectively. R is the Rydberg energy and a_0 is the Bohr radius; $A_r(d \rightarrow f)$ is the radiative rate from state d to f; $A_a(d \rightarrow i, e_2\kappa_2)$ is the Auger rate with the free electron characterized by energy e_2 and relativistic quantum number $\kappa_2 = (l_2 - j_2)(2j_2 + 1)$; $\Gamma_r(d)$ and $\Gamma_a(d)$ are the total radiative and Auger widths for the intermediate autoionizing state d, respectively. In the present work, the free electrons are assumed to have a Maxwellian distribution.

The atomic energy levels and wave functions were calculated by the use of the MCDF model.[13,14] In this model an atomic state function for a state i with total angular momentum JM is expanded in terms of the n configuration state functions (CSF):

$$\Psi_i(JM) = \sum_{\lambda=1}^{n} C_{i\lambda}\Phi(\Gamma_\lambda JM) \ . \quad (2)$$

Here, the configuration state function $\Phi(\Gamma_\lambda JM)$ is obtained by a linear combination of the Slater determinants constructed from the Dirac central-field spinors;[13] $C_{i\lambda}$ are the mixing coefficients.

The Auger transition rate from the intermediate autoionizing state d to the initial state i of the recombining ion is given in perturbation theory by[5]

$$A_a(d\rightarrow i,e_2\kappa_2)=\left|\sum_{\lambda,\lambda'} C_{i\lambda}C_{f\lambda'}\left\langle \Phi(\Gamma_{\lambda'},J'M')e_2\kappa_2;JM\left|\frac{1}{2}\sum_{\substack{\alpha\beta\\ \alpha\neq\beta}}\frac{e^2}{r_{\alpha,\beta}}\right|\Phi(\Gamma_\lambda JM)\right\rangle\right|^2 . \tag{3}$$

The continuum wave function $e_2\kappa_2$ is normalized to represent one ejected electron per unit of time.

The radiative transition probability for a discrete transition $d\rightarrow f$, from the MCDF model, is given by[5,15]

$$A_r(d\rightarrow f)=\frac{1}{2J_d+1}\sum_L\frac{2\pi}{2L+1}\left|\sum_{\alpha,\beta}C_{i\alpha}C_{f\beta}\sum_{p,q}d^L_{pq}(\beta,\alpha)\langle p||T_L||q\rangle\right|^2 , \tag{4}$$

where $d^L_{pq}(\beta,\alpha)$ are the angular factors and the one-electron reduced matrix elements $\langle p||T_L||q\rangle$ for the Lth multipole are defined in Ref. 15.

III. NUMERICAL CALCULATIONS

Dielectronic recombination from a Ni-like ground state to a state of a Cu-like ion can be represented by

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

The intermediate autoionizing states included in the present work are $3d^{-1}4lnl'$ ($n\leq 10$), $3p^{-1}4lnl'$ ($n\leq 5$), and $3s^{-1}4lnl'$ ($n\leq 5$). The notation $3l^{-1}$ indicates that an electron is missing in the $3l$ subshell.

The atomic energy levels and bound-state wave functions were obtained by minimizing the average energy of all the levels in the MCDF method.[13] The effects of the intermediate coupling and the configuration interaction from the same complex were included in the present calculations.

The detailed Auger and electric dipole radiative rates for each autoionizing state were evaluated according to Eqs. (3) and (4), respectively. The angular factors of the Auger and radiative matrix elements were calculated by using the modified general angular-momentum subroutines.[13,14] The continuum wave functions were generated by solving the Dirac-Fock equations for the final state without including the exchange interaction between the bound and continuum electrons. The term-dependent transition energies and rates from the MCDF model were then used to calculate the DR rate coefficients according to Eq. (1). In the present work only the electric dipole radiative transitions filling the M subshell vacancy were included. The effect of radiative cascade was neglected.

IV. RESULTS AND DISCUSSION

The total dielectronic recombination coefficients for the ground state of the Ni-like $_{64}$Gd have been calculated for the electron temperature $0.05\leq T\leq 3$ keV by using the MCDF model. The results are listed in Table I.

The partial dielectronic recombination coefficients for the $3d^{-1}4lnl'$, $3p^{-1}4lnl'$, and $3s^{-1}4lnl'$ intermediate autoionizing states are compared in Fig. 1. The contributions from the lowest-lying doubly excited configuration (i.e., $3d^{-1}4l4l'$) to the total DR coefficients for $T>0.5$ keV are quite moderate due to the fact that more than half of the doubly excited states from this configuration are not autoionizing. The DR coefficients for the $3d^{-1}4l4l'$ states peak at very low temperature ($\sim$30 eV) because of the small Auger transition energies. For $T\leq 0.5$ keV, the total DR coefficient is dominated by the contribution from the $3d^{-1}4l4l'$ configuration while, for $T>0.5$ keV, the $3d^{-1}4lnl'$ ($5\leq n\leq 10$) configurations become the most important ones. The contributions from $3p^{-1}4lnl'$ ($n\leq 5$) and $3s^{-1}4lnl'$ ($n\leq 5$) configurations to the total coefficient have been found to be less than 10% and 2%, respectively. Furthermore, the Coster-Kronig transitions such as $3p^53d^{10}4lnl'\rightarrow 3p^63d^94l+e$ become energetically possible for $n>6$. These extra Auger channels to the excited states of the recombining ion further reduce the DR coefficients from the high-n states.[16] Therefore, the contributions from $3p^{-1}4lnl'$ and $3s^{-1}4lnl'$ with $n\geq 6$ were neglected in the present work. For the $3d^{-1}4lnl'$ doubly excited states, we only included

TABLE I. Dielectronic recombination coefficients for Ni-like $_{64}$Gd in the ground state.

kT (keV)	Rate coefficient (10^{-11} cm^3 sec)
0.05	17.6
0.10	15.5
0.20	14.3
0.30	14.2
0.40	13.9
0.50	13.3
0.60	12.5
0.70	11.7
0.80	10.8
1.00	9.29
1.50	6.50
2.00	4.84
2.50	3.75
3.00	3.02

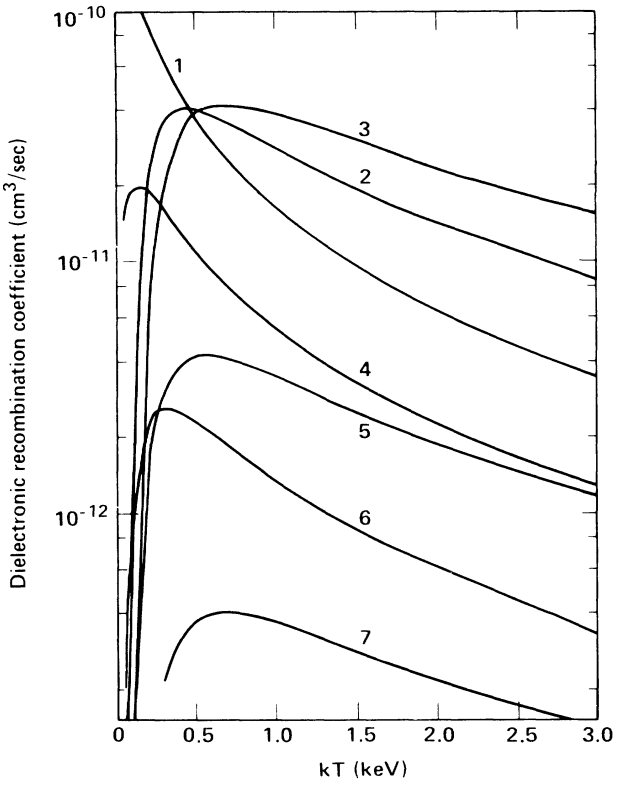

FIG. 1. Partial dielectronic recombination coefficients for the various intermediate autoionizing states as functions of the electron temperature. The legends are as follows: curve 1, $3d^{-1}4l4l'$; curve 2, $3d^{-1}4l5l'$; curve 3, $3d^{-1}4fnl'$ $(6 \leq n \leq 10)$; curve 4, $3p^{-1}4l4l'$; curve 5, $3p^{-1}4l5l'$; curve 6, $3s^{-1}4l4l'$; and curve 7, $3s^{-1}4l5l'$.

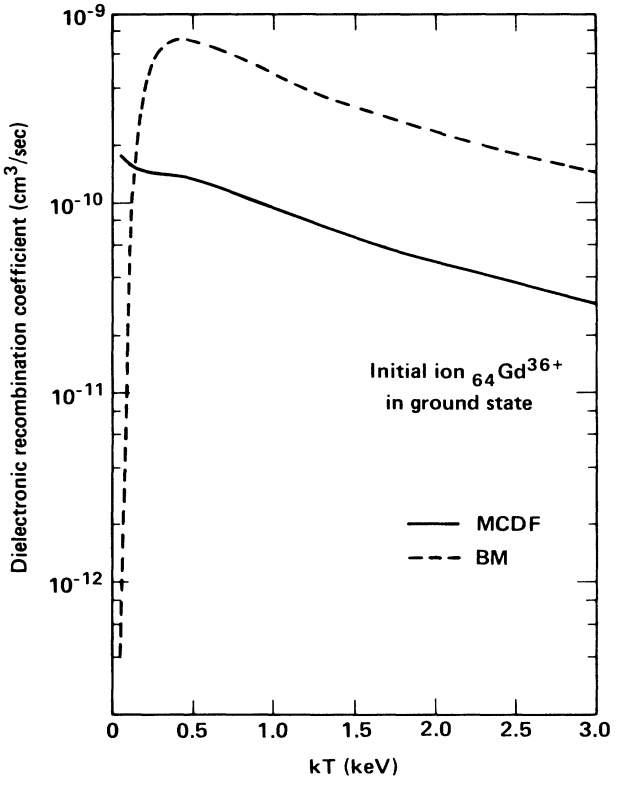

FIG. 2. Total dielectronic recombination coefficients as functions of the temperature. The solid curve represents the results from the present MCDF calculations and the dashed curve indicates the predictions from the Burgess-Merts formula.

the contributions from $n \leq 10$. The contributions from $n > 10$ would be drastically diminished because of the opening of the strong Coster-Kronig channels to the excited states of the recombining ion (e.g., $3d^9 4fnl' \rightarrow 3d^9 4d + e$). The contributions from high-n Rydberg states would be further reduced by electron collisional ionization in dense plasmas.

In Fig. 2, the total DR rate coefficients from the present MCDF model are compared with the predictions from the Burgess-Merts semiempirical formula with hydrogenic oscillator strengths and excitation energies. The Burgess-Merts formula has been found to overestimate the DR rate coefficients by as much as a factor of 5 for $T \geq 250$ eV.

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