Dielectronic recombination coefficient for F-like selenium

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Total dielectronic recombination coefficients from F-like to Ne-like selenium have been calculated for three F-like initial states for electron temperatures in the range $0.01 \leq T \leq 6$ keV/k_B. The detailed Auger and radiative rates were evaluated by using the multiconfiguration Dirac-Fock model. Including additional autoionization channels to the excited states of the recombining ion in calculations of the stabilization fluorescence yields leads to a reduction of the total dielectronic coefficients by an amount less than 15%. The peak total dielectronic recombination coefficients are 3.2×10^{-11}, 4.2×10^{-11}, and 3.7×10^{-11} cm^3/sec for the initial $^2S_{1/2}$, $^2P_{1/2}$, and $^2P_{3/2}$ states, respectively.

I. INTRODUCTION

Dielectronic recombination (DR) is a most important recombination process for ions in hot plasmas.[1,2] It can significantly affect the ionization balance[3] and the plasma kinetics.[4]

Recently, selenium has been used successfully to demonstrate lasing in soft-x-ray regions based on the Ne-like scheme.[5,6] Dielectronic recombination becomes an important issue in the analysis of these experimental data. Dielectronic recombination has been shown to be a significant process for populating the upper laser levels and should be included in the modeling of the excited-state kinetics of the neonlike ion.[4] The total dielectronic recombination rate coefficient for F-like selenium employed in the original analysis[6] is an order of magnitude larger than the value used by Apruzese *et al.*[7] in their interpretation of the Livermore experiments.[5] To resolve these discrepancies, we have extended our earlier calculations for low-lying states[4] to include the contributions from high-n states to obtain the total dielectronic recombination coefficients. The detailed Auger and radiative rates of the intermediate autoionizing states were calculated by using multiconfiguration Dirac-Fock (MCDF) model.[8,9] The results from the present work were compared with the predictions from the other theoretical calculations and with the values from the semiempirical formula.[10,11]

II. ATOMIC MODEL

In the isolated resonance approximation, the dielectronic recombination coefficient for ions in low-density plasmas can be obtained by the use of the following equation:[1,2]

$$\alpha_{\rm dr}(i;\ \text{total}) = \frac{1}{2g_i}\left[\frac{4\pi R}{k_B T}\right]^{3/2} a_0^3 \times \sum_{\kappa_2}\sum_{d}\sum_{f} \exp(-e_2/k_B T) g_d A_a(d\rightarrow i,e_2\kappa_2)\omega_d \ , \tag{1}$$

where

$$\omega_d = A_r(d\rightarrow f)/[\Gamma_a(d)+\Gamma_r(d)] \ . \tag{2}$$

The dielectronic capture of a free electron with energy e_2 and relativistic quantum number $\kappa_2=(l_2-j_2)(2j_2+1)$ from initial state i of the recombining ion to the intermediate state d is related to the inverse Auger process $A_a(d\rightarrow i,e_2\kappa_2)$ by detailed balance. The radiative transition from the intermediate state d to the stabilized final bound state f is denoted by $A_r(d\rightarrow f)$. Γ_r and Γ_a are the total radiative and Auger rates, respectively. g_d and g_i are the statistical weight factors for ionic states d and i, respectively. a_0 is the Bohr radius and R is the Rydberg energy. The plasma electronic temperature is denoted by T. A Maxwellian distribution is assumed for the plasma electrons. The total dielectronic rate is obtained by summing over all possible initial continuum, intermediate autoionizing, and final bound states.

The detailed Auger and radiative rates and transition energies for each autoionizing state were calculated by using the MCDF model.[9] No averaging procedure has been employed in the present work. The relativistic Auger transition probability is calculated from perturbation theory. The transition rate in a frozen-orbital approximation is given in atomic units by[9]

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

Here, the $C_{d\lambda}$ are the mixing coefficients and $\phi(\Gamma_\lambda JM)$ are the configuration state functions.[8] The continuum wave function, characterized by (e_2,κ_2), is normalized in energy.

The spontaneous electric dipole radiative transition probability is given in perturbation theory by[9,12]

$$A_r(i\rightarrow f)=\frac{2\pi}{3(2J_i+1)} \times\left|\sum_{\lambda}\sum_{\lambda'} C_{i\lambda}C_{f\lambda'}\sum_{p,q} d^1_{pq}(\lambda',\lambda)\langle p||T_1||q\rangle\right|^2 . \quad (4)$$

Here, the one-electron reduced matrix elements $\langle p||T_1||q\rangle$ are defined by Grant.[12] The $d^l_{pq}(\lambda',\lambda)$ are the angular factors.

The atomic energy levels and bound-states wave functions were calculated using the MCDF model in the average-level scheme (AL).[8] The continuum wave functions were obtained by solving the Dirac-Fock equations for the final state without including the exchange interaction between bound and continuum electrons.

III. NUMERICAL CALCULATIONS

In the present work, dielectronic recombination coefficients for the three F-like initial states, namely, $1s^22s^22p^5\,^2P_{1/2}$, $1s^22s^22p^5\,^2P_{3/2}$ and $1s^22s\,2p^6\,^2S_{1/2}$, have been calculated by using the MCDF model. The intermediate autoionizing states included in the present calculations are

$1s^22s^22p^43lnl'$,

$1s^22s\,2p^53lnl'$,

$1s^22p^63lnl'$,

and

$1s^22s\,2p^6nl$.

For the initial $1s^22s^22p^5\,^2P$ states, dielectronic recombination involves not only $\Delta n\neq 0$ transitions but also $\Delta n=0$ transitions. Here, Δn refers to the change of the principal quantum number of the main radiative stabilizing transitions. These two classes of transitions can exhibit quite different convergence properties. The contributions from $4lnl'(n\geq 4)$ and $nln'l'(n,n'\geq 5)$ states are quite small. Hence, they were neglected in the present calculations.

The low-lying $2p^43lnl'(n\leq 4)$, $2s\,2p^53lnl'(n\leq 4)$ and $2p^63lnl'(n\leq 4)$ configurations have approximately 3400 coupled states. They were calculated explicitly in intermediate coupling with configuration interaction by using the MCDF-AL scheme.[8] For the high-lying doubly excited $3lnl'$ states, explicit calculations were performed in intermediate coupling for $n\leq 10$ and $l'\leq 5$. For states with $n>10$, DR coefficients were obtained by using an n^{-3} extrapolation to the DR coefficient. In the present work, the additional autoionization channels to the excited states of the recombining ion were included in the calculation of stabilizing fluorescence yields.

For the $\Delta n=0$ transitions with intermediate states of the $2s\,2p^6nl$ configurations, the autoionizing transitions become energetically possible for $n\geq 7$. Explicit calculations for $\Delta n=0$ transitions were performed for $n\leq 15$ and $l\leq 8$ including all the possible stabilizing radiative transitions. For the high-lying states with $n>15$, the n^{-3} extrapolation procedure was employed to estimate the autoionization rates.

In the present work, we included only the electric dipole stabilizing radiative transitions. The higher multipole radiative transitions and transitions leading to other autoionizing states were neglected.

IV. RESULTS AND DISCUSSION

Dielectronic recombination coefficients for the F-like $_{34}Se^{25+}$ ion were calculated for the electron temperatures in the range $0.01\leq k_BT\leq 6$ keV using the MCDF model. The results for the $\Delta n\neq 0$ and $\Delta n=0$ transitions for the three initial states of the recombining ion are listed in Table I.

For the $\Delta n=0$ transitions, the dielectronic recombination coefficient converges quite slowly (Fig. 1). In the present work, the contributions from $n\leq 150$ were included in the calculations. Certainly, for ions in a plasma environment, collisional ionization will limit the contributions from the high-n Rydberg states. These cases will not be treated here. Radiative stabilizing transitions can come from either the less-excited inner electron or the higher-excited Rydberg electron in the case of $\Delta n=0$ transitions. For the $_{34}Se^{25+}$ ion, the dielectronic recombination coefficient for $\Delta n=0$ transitions has been found to increase by as much as a factor of 2 (Fig. 2) because of the inclusion of the radiative stabilizing transitions from the outer Rydberg electron (e.g., $2s\,2p^68f\rightarrow 2s\,2p^6nd$, $n<6$).

The effect due to the autoionization to the excited states of the recombining ion on the dielectronic rate coefficient has been found to be very important for low-Z ions.[13–15] For the $_{34}Se^{25+}$ ion, the Coster-Kronig transitions $2p^43dnl\rightarrow 2p^43l(l=0,1)\epsilon l$ become energetically possible

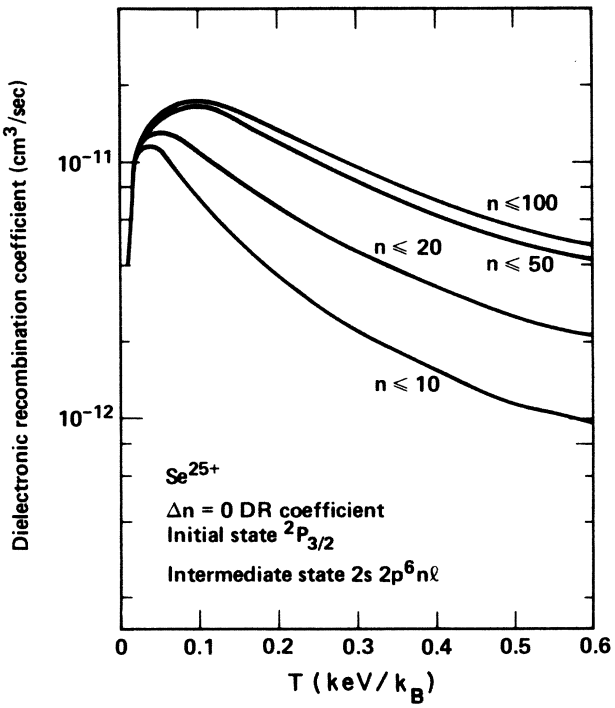

FIG. 1. Dielectronic recombination coefficients for the $\Delta n=0$ transitions from the initial $^2P_{3/2}$ state for several different maximum n, as functions of temperature.

TABLE I. Dielectronic recombination coefficient (in 10^{-12} cm^3/sec) for the F-like $_{34}Se^{25+}$ ion.

	Dielectronic recombination coefficient				
	$^2S_{1/2}$	$^2P_{1/2}$		$^2P_{3/2}$	
Temperature (keV/k_B)	$\Delta n \neq 0$	$\Delta n = 0$	$\Delta n \neq 0$	$\Delta n = 0$	$\Delta n \neq 0$
0.01		2.97		3.89	
0.02		8.60		10.30	
0.04		16.88		14.08	
0.06	0.108	21.88	0.0697	16.53	0.0547
0.10	1.76	22.90	1.55	17.93	1.28
0.20	12.64	15.74	13.11	13.69	11.19
0.30	22.71	10.79	24.62	9.83	21.25
0.50	31.12	6.04	36.14	5.74	31.64
0.80	29.66	3.32	37.15	3.23	32.84
1.0	27.62	2.46	34.45	2.42	30.55
1.5	20.59	1.41	26.81	1.39	23.90
2.0	16.13	0.935	20.92	0.933	18.70
3.0	10.47	0.521	13.73	0.523	12.30
4.0	7.43	0.342	9.80	0.345	8.79
5.0	5.60	0.247	7.42	0.249	6.66
6.0	4.35	0.189	5.87	0.190	5.27

for $n \geq 9$. Since the contribution from the $2p^4 3lnl (n \geq 9)$ states is only $\sim 8\%$ of the total DR coefficient at temperature $T = 1$ keV, the total DR coefficient is reduced by only a few percent after including the autoionization to the excited states. For the intermediate states of the $2s\,2p^5 3lnl'$ configurations, the $2s\,2p^5 3lnl' \rightarrow 2s^2 2p^4 3l\epsilon l$ and $2s\,2p^5 3dnl' \rightarrow 2s\,2p^5 3l (l = 0,1)\epsilon l'$ transitions become energetically possible for $n \geq 7$ and $n \geq 9$, respectively.

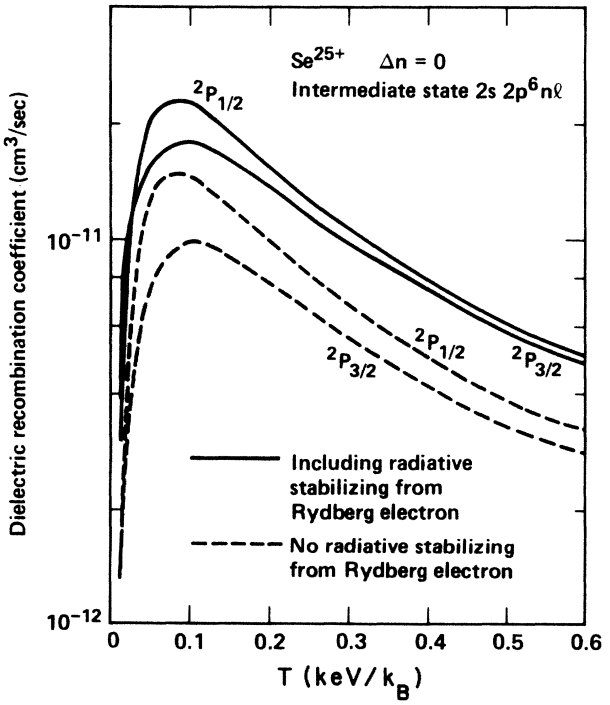

FIG. 2. Dielectronic recombination coefficient for $\Delta n = 0$ transitions as functions of temperature. Solid and dashed curves display the results with and without including radiative stabilizing transitions from outer Rydberg electron, respectively.

The total DR coefficient for the initial $^2S_{1/2}$ state of the recombining ion has been found to decrease by 5—15% due to the inclusion of the Coster-Kronig rate in calculations of the fluorescence yield.

The effect of radiative cascade[16] was not included in the present calculations. In the present work, the radiative transitions leading to the other autoionizing states were neglected both in A_r and Γ_r of Eq. (2) (i.e., the truncated approximation).[16] For Ne-like $_{42}Mo^{32+}$, the DR coefficients from this truncated approximation have been found to agree with the values obtained by including full cascade effect to within 2%.[16] Furthermore, the cascade effect has been shown to reduce the total DR coefficients from the truncated approximation by an amount less than 3% for the He-like isoelectronic sequence.[17] Therefore, the truncated approximation used in the present calculations is a reasonable approximation.

In Fig. 3, we compare the partial DR rate coefficients for the initial $^2P_{3/2}$ state from the $\Delta n = 0$ and $\Delta n \neq 0$ transitions. For the electron temperature $T < 200$ eV, the $\Delta n = 0$ transition is the dominant DR process. For higher temperature, the contributions to the total DR rate coefficient mostly come from the intermediate states $3lnl' (n \leq 10)$ of the $\Delta n \neq 0$ transitions.

In Fig. 4, the total DR rate coefficients for the three initial states are compared with the results from the semiempirical formula,[10,11] and the theoretical prediction quoted by Apruzese *et al.*[7] In the application of the semiempirical formula, the original Burgess formula[10] was used for $\Delta n = 0$ transitions while the Burgess-Merts formula was employed for the $\Delta n \neq 0$ transitions. The oscillator strengths and excitation energies from the Dirac-Fock model were used in the semiempirical calculations. For the temperature $T < 500$ eV, the semiempirical formula underestimates the DR coefficient by 50% to a factor of 10. For higher temperatures, the results from sem-

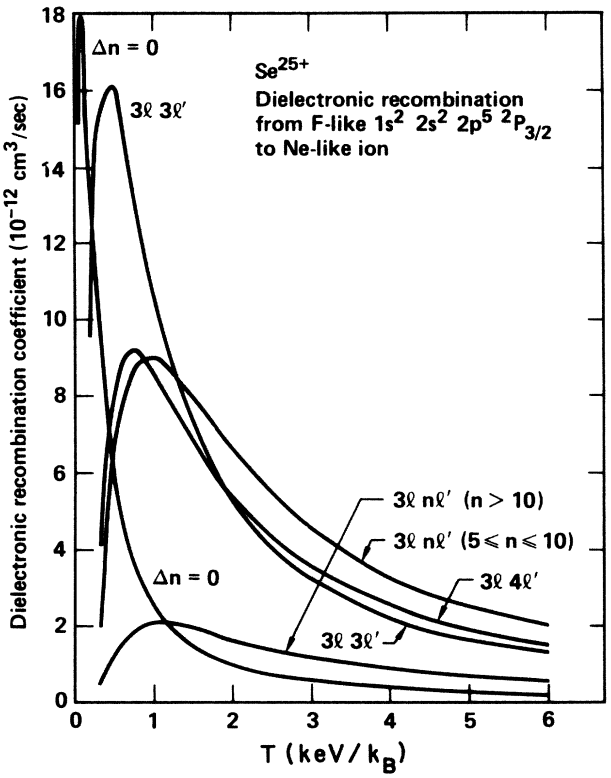

FIG. 3. Partial dielectronic recombination coefficients for $\Delta n=0$ and $\Delta n\neq 0$ transitions as functions of temperature.

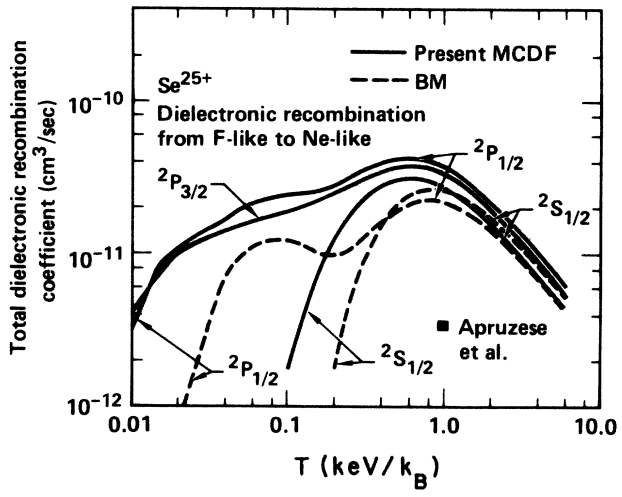

FIG. 4. Total dielectronic recombination coefficients for F-like selenium as functions of temperature. Solid curves are the results from the present MCDF calculations. Dashed curves indicate the predictions from the Burgess-Merts formula. The square represents the value quoted by Apruzese *et al.* (Ref. 7).

iempirical formula agree with the values from the present MCDF calculations within 50%.

The DR rate coefficient for $_{34}Se^{25+}$ at $k_BT=1000$ eV used by Apruzese *et al.*[7] in the reanalysis of the Livermore experiment[5] is a factor of 10 smaller then the present result. The discrepancy is most probably due to the assumption made in Refs. 7 and 13 that the Coster-Kronig transition is energetically allowed for all values of n. This assumption would grossly underestimate the DR rate coefficients for medium-Z and heavy ions. Furthermore, the dielectronic rate coefficient from Ref. 7 were obtained by using autoionization rates derived from extrapolation of calculated electron-impact excitation cross sections.[13,14] The extrapolation procedure and the use of dipole approximation have been found to introduce large errors in calculations of the Auger rates for the low-lying doubly excited states.[18] Similar large discrepancies have also been found for Li-like[19] and Ne-like ions.[15,18]

The peak total DR rate coefficients for the initial $^2S_{1/2}$, $^2P_{1/2}$, and $^2P_{3/2}$ states from the present MCDF calculations are 3.2×10^{-11}, 4.2×10^{-11}, and 3.7×10^{-11} cm^3/sec, respectively. Similar results have recently been obtained by Hagelstein.[20] The average total DR rate coefficient of F-like selenium from the present work for $\Delta n\neq0$ transitions at $T=1000$ eV is 3.08×10^{-11} cm^3/sec. The theoretical total DR coefficients for Ne-like iron,[21] selenium,[15] and molybdenum[22] at $k_BT=1000$ eV are 1.4×10^{-11}, 2.95×10^{-11}, and 2.19×10^{-11} cm^3/sec, respectively. Hence, the present DR coefficients for F-like selenium are consistent with the results for Ne-like isoelectronic sequence.

The effect of the plasma density on the dielectronic recombination coefficient can be approximately taken into account by cutting off the sum over the principal quantum number n of the Rydberg electron in the doubly excited Rydberg series at some n_c.[13,18] The value of n_c is determined by the plasma condition. For the plasmas of F-like selenium with electron density of 5×10^{20} cm^{-3} and (1 keV)/k_B temperature, the value of n_c is about 7.[18] With the cutoff value $n_c=7$, the DR rate coefficient for the $\Delta n=0$ transitions is reduced to zero while the DR rate coefficient for $\Delta n\neq0$ transitions is only decreased by 21%. Since the total DR coefficient at $k_BT=1$ keV is dominated by the $\Delta n\neq0$ transitions, the total DR coefficient for the initial ^2P state is reduced by $\sim$27% due to the plasma electronic collisional ionization.

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