Effects of Coster-Kronig transitions on electron-impact excitation rates for fluorinelike ions in their ground states

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The contributions of Coster-Kronig resonances to the electron-impact excitation rate coefficients have been calculated for six F-like ions with $Z=26$, 34, 42, 47, 54, and 63. The calculations are carried out using the relativistic distorted-wave approximation and the multiconfiguration Dirac-Fock model. We found that resonance excitation via Coster-Kronig transitions is the dominant excitation mechanism at low temperatures for $Z \leq 34$ and is as important as the direct excitation for heavier ions. In addition, we found that the effects of relativity can reduce the rate coefficients by more than an order of magnitude at electron temperatures $T < 100$ eV.

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I. INTRODUCTION

Cross sections for electron-impact excitation of multiply charged ions are important for studies of astrophysical and laboratory produced plasmas. In these applications, cross sections for many transitions and for several ion stages are usually required. To meet these heavy demands, the distorted-wave approximation is frequently employed to calculate electron collision cross sections for highly charged ions [1]. In general, the electron collision excitation can proceed through a direct excitation channel or via autoionizing resonances. It has been shown that the autoionizing resonances can significantly enhance the calculated rates for electron collision excitation of some transitions in light positive ions [1] as well as in highly charged ions [2–7]. For example, it was found that the $2p^5 3lnl'$ resonances increased the excitation rates for the $2p^6\,{}^1S \rightarrow 2p^5 3s\,{}^3P$ transition of Ne-like krypton by a factor of 2 near the threshold region [4]. Similar large enhancements have also been found for Li-like [2,5], Be-like [7], O-like [8], and F-like ions [9].

For the F-like isoelectronic sequence, nonresonant electron collisional excitation cross sections for the $n=2$ to $n=3$ transitions in Fe^{17+} [10,11] and in Se^{25+} [12] have been calculated using the distorted-wave method. Cross sections for the $n=2$ to $n=2$ transitions in Ti^{13+} and Kr^{27+} have also been reported by Bhatia and coworkers [13,14]. In our previous work on F-like ions [9], we calculated rates for electron-impact excitation of $n=2$ to $n=2$ transitions including the contributions from the autoionizing resonances. However, the effects of the Coster-Kronig-type capture and decay processes on the rate coefficients from the ground state to the first excited state were not taken into account in our earlier calculations. A Coster-Kronig transition is a radiationless transition in which the initial hole and one of the final holes reside at the same shell. For the other $n=2$ to $n=2$ transitions, there are no Coster-Kronig contributions. In this paper, we report calculations of resonance enhancement of the electron-impact excitation rates from the ground state to the first excited state in the $n=2$ manifold made possible by the Coster-Kronig transitions. We find that these Coster-Kronig transitions are the dominant excitation mechanism for $Z \leq 34$ with electron temperatures $T \leq 100$ eV. We also investigated the effects of relativity on the rate coefficients via Coster-Kronig transitions by comparing the results from the relativistic and nonrelativistic calculations. The nonrelativistic results were obtained by repeating the calculations with the velocity of light increased by a thousandfold to simulate the nonrelativistic limit.

II. CALCULATIONAL PROCEDURE

The excitation of a F-like ion from the ground state to the first excited state in the $n=2$ manifold by electron impact can be schematically represented by

$$2s^2 2p_{1/2}^2 2p_{3/2}^3 + e \rightarrow 2s^2 2p_{1/2}^1 2p_{3/2}^4 + e \ , \tag{1a}$$

$$2s^2 2p_{1/2}^2 2p_{3/2}^3 + e \rightarrow 2s^2 2p_{1/2}^1 2p_{3/2}^3 nln'l' \ , \rightarrow 2s^2 2p_{1/2}^1 2p_{3/2}^4 + e \ , \tag{1b}$$

and

$$2s^2 2p_{1/2}^2 2p_{3/2}^3 + e \rightarrow 2s 2p_{1/2}^2 2p_{3/2}^4 nl \ , \rightarrow 2s^2 2p_{1/2}^1 2p_{3/2}^4 + e \ . \tag{1c}$$

Here, Eq. (1a) indicates the direct or background excitation process; Eq. (1b) and Eq. (1c) represent the excitations via Auger and Coster-Kronig resonances, respectively. As in our previous work [8,9], we use intermediate coupling to describe the initial, final, and intermediate states.

As indicated in Eqs. (1b) and (1c), the resonances are produced when the incoming electron excites the F-like ion and is simultaneously captured to form a doubly excited state of a Ne-like ion. The subsequent decay of the doubly excited state to an excited state of the F-like ion by emission of an Auger electron results in a contribution to the excitation cross section.

The procedures for calculating the direct excitation

TABLE I. Direct electron-impact excitation rate coefficients (D) and resonance contributions (R) in cm^3/sec for the $e+2s^22p_{1/2}^2 2p_{3/2}^3 \rightarrow 2s^22p_{1/2}^1 2p_{3/2}^4 + e$ transition in F-like ions. Numbers in square brackets denote powers of 10.

Electron	$Z=26$		$Z=34$		$Z=42$	
temp. (eV)	D	R	D	R	D	R
30	9.68[−11]	2.07[−10]	1.83[−11]	3.60[−11]	1.22[−12]	9.96[−13]
50	8.79[−11]	1.66[−10]	2.52[−11]	4.11[−11]	4.08[−12]	4.28[−12]
80	7.56[−11]	1.20[−10]	2.73[−11]	3.87[−11]	7.31[−12]	8.07[−12]
100	6.95[−11]	1.07[−10]	2.71[−11]	3.54[−11]	8.57[−12]	9.22[−12]
500	3.34[−11]	4.63[−11]	1.64[−11]	2.03[−11]	8.72[−12]	7.97[−12]
1000	2.38[−11]	2.37[−11]	1.19[−11]	1.30[−11]	6.65[−12]	6.15[−12]
1500	1.94[−11]	1.48[−11]	9.81[−12]	8.90[−12]	5.54[−12]	4.61[−12]
2000	1.68[−11]	1.03[−11]	8.53[−12]	6.52[−12]	4.84[−12]	3.56[−12]
2500	1.51[−12]	7.68[−12]	7.65[−12]	5.02[−12]	4.35[−12]	2.84[−12]
3000	1.38[−11]	6.01[−12]	6.99[−12]	4.01[−12]	3.98[−12]	2.33[−12]
4000	1.19[−11]	4.04[−12]	6.07[−12]	2.77[−12]	3.46[−12]	1.66[−12]
6000	9.74[−12]	2.28[−12]	4.96[−12]	1.61[−12]	2.83[−12]	9.95[−13]

cross sections and the resonance contributions have been described in details in Ref. 9. Here, we only outline the essential points. Following Cowan's procedure [15], separate calculations are carried out for the direct and resonance excitation cross sections. The interference between these two processes is neglected and the resonance contribution is calculated in the isolated resonance approximation.

The direct excitation cross sections without resonances were calculated using a relativistic multiconfiguration distorted-wave code [16]. In the calculations of F-like target wave functions, states from the $1s^22l^7$ and $1s^22l^63l'$ configurations were included in the configuration-interaction expansion. For the dipole-forbidden transition [Eq. (1a)], partial waves up to $l=12$ were sufficient to converge the cross sections.

The resonance excitation is treated as a two-step process: dielectronic capture followed by Auger decay to a singly excited state. Assuming a Maxwellian distribution for the plasma electrons at temperature T, the total resonance contribution to the excitation rate from state i to state j is obtained by multiplying the capture rate $C_{id}^{\rm cap}$ by the Auger branching ratio B_{di}^A and summing over all intermediate states d,

$$C_{ij}^{\rm res}=\sum_d C_{id}^{\rm cap}B_{dj}^A \ , \tag{2}$$

where

$$C_{id}^{\rm cap}=(2g_i)^{-1}\left[\frac{4\pi R}{kT}\right]^{3/2} a_0^3 \exp(-E_{di}/kT) g_d A_{di}^A \ , \tag{3}$$

and

$$B_{dj}^A=\frac{A_{dj}^A}{\sum_m A_{dm}^A+\sum_n A_{dn}^r} \ . \tag{4}$$

Here, g_i and g_d are the statistical weights of the states i and d, respectively, R is the Rydberg energy and a_0 is the Bohr radius, A_{di}^A and E_{di} are the rate and energy of the autoionizing transition d to i, and A_{dn}^r is the radiative rate for the transition $d \rightarrow n$.

In our work, the detailed Auger and electric-dipole ra-

TABLE II. Direct electron-impact excitation rate coefficients (D) and resonance contributions (R) in cm^3/sec for the $e+2s^22p_{1/2}^2 2p_{3/2}^3 \rightarrow 2s^22p_{1/2}^1 2p_{3/2}^4 + e$ transition in F-like ions. Numbers in square brackets denote powers of 10.

Electron	$Z=47$		$Z=54$		$Z=63$	
temp. (eV)	D	R	D	R	D	R
50	7.57[−13]	1.38[−12]	2.50[−14]	2.65[−14]		
80	2.31[−12]	3.70[−12]	2.43[−13]	2.57[−13]	2.63[−15]	1.35[−15]
100	3.24[−12]	4.79[−12]	5.01[−13]	5.11[−13]	1.25[−14]	6.49[−15]
500	5.86[−12]	4.98[−12]	3.14[−12]	1.95[−12]	1.13[−12]	3.77[−13]
1000	4.76[−12]	3.96[−12]	2.99[−12]	1.99[−12]	1.51[−12]	5.67[−13]
1500	4.03[−12]	3.09[−12]	2.65[−12]	1.78[−12]	1.50[−12]	6.06[−13]
2000	3.54[−12]	2.46[−12]	2.37[−12]	1.52[−12]	1.42[−12]	5.78[−13]
2500	3.19[−12]	2.00[−12]	2.16[−12]	1.30[−12]	1.33[−12]	5.31[−13]
3000	2.92[−12]	1.66[−12]	1.99[−12]	1.12[−12]	1.25[−12]	4.81[−13]
4000	2.55[−12]	1.21[−12]	1.74[−12]	8.56[−13]	1.11[−12]	3.92[−13]
6000	2.09[−12]	7.43[−13]	1.43[−12]	5.50[−13]	9.27[−13]	2.71[−13]

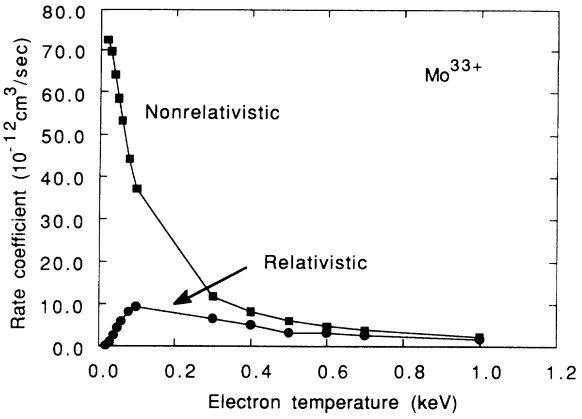

FIG. 1. Excitation rate coefficients via Coster-Kronig transitions for the $2p_{1/2}$-$2p_{3/2}$ transition for Mo^{33+} as functions of electron temperature. The squares indicate the nonrelativistic results. The circles represent the relativistic values. The lines are drawn to guide the eyes.

diative rates were calculated in intermediate coupling from perturbation theory using the multiconfiguration Dirac-Fock (MCDF) model [17,18]. The energy levels and wave functions for the bound states were evaluated explicitly in intermediate coupling including configuration interaction within the same complex by using the MCDF model in the average-level scheme [18].

III. RESULTS AND DISCUSSION

The rate coefficients for direct excitation [Eq. (1a)] and the resonance excitation rates via the Auger resonances [Eq. (1b)] have been obtained in our previous work [9]. For completeness, they are included in the results given in Tables I and II. In the calculations of resonance contributions through the Coster-Kronig resonances [Eq. (1c)], we include autoionizing states $2s2p^6nl$ with $n \leq 20$ and $l \leq 6$. The results for six ions with $Z=26$, 34, 42, 47, 54, and 63 and for electron temperatures in the range $30 \leq T \leq 6000$ eV are listed in Tables I and II. Here, the resonance contributions to the excitation rates (columns labeled R) include contributions both from Auger and Coster-Kronig transitions. From these comparisons, we can see that resonance excitation is more important than the direct excitation at low temperatures. As the temperature increases, the resonance contributions decrease gradually. For Fe^{17+}, autoionizing resonances contribute about 20% to the total rate coefficients even for electron temperature as high as 6000 eV. As a function of atomic number Z, resonance contributions diminish as Z increases to higher values due to the increasing importance of the radiative decay relative to the autoionization. Specifically, the average L-shell fluorescence yields for the $3l3l'$ doubly excited states of Ne-like ions increases from 0.18 at $Z=26$ to 0.8 at $Z=54$ [9]. Hence the radiative damping can reduce the resonance contributions by more than a factor of 2 for Xe^{45+}.

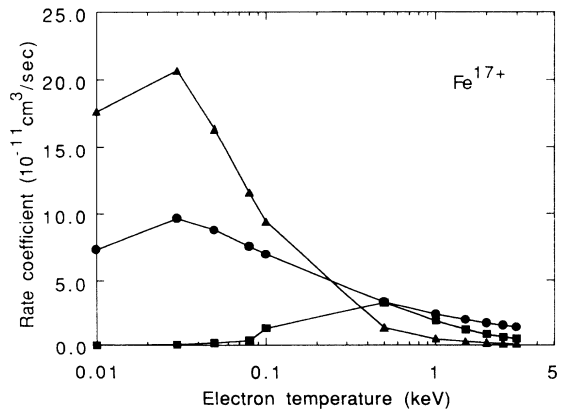

FIG. 2. Partial excitation rate coefficients for the $2p_{1/2}$-$2p_{3/2}$ transition for Fe^{17+} as functions of electron temperature. The circles indicate the rates for direct excitation. The squares represent the resonance contributions through Auger resonances and the triangles display the resonance contributions via the Coster-Kronig transitions. The lines are drawn to guide the eyes.

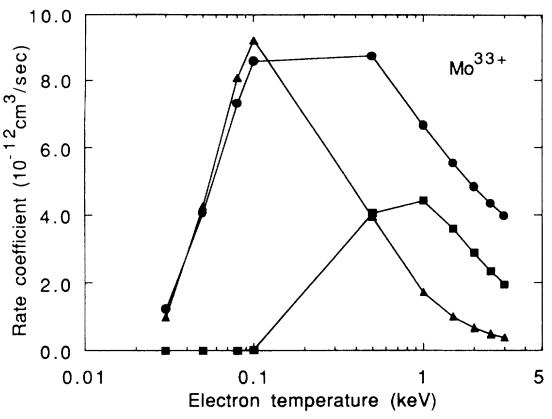

FIG. 3. Partial excitation rate coefficients for Mo^{33+}. The symbols are the same as in Fig. 2.

In Fig. 1, the rate coefficients via Coster-Kronig transitions for Mo^{33+} from the relativistic and nonrelativistic calculations are compared. The effects of relativity reduce the rate coefficients by as much as two orders of

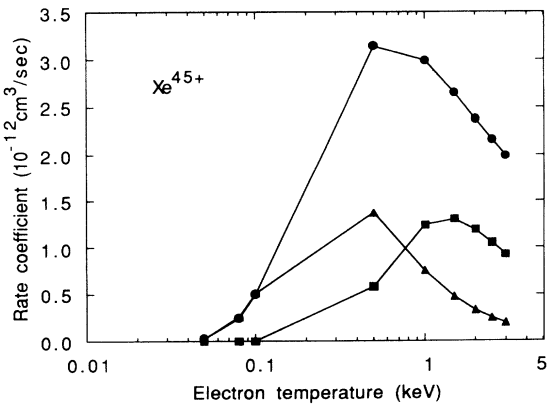

FIG. 4. Partial excitation rate coefficients for Xe^{45+}. The symbols are the same as in Fig. 2.

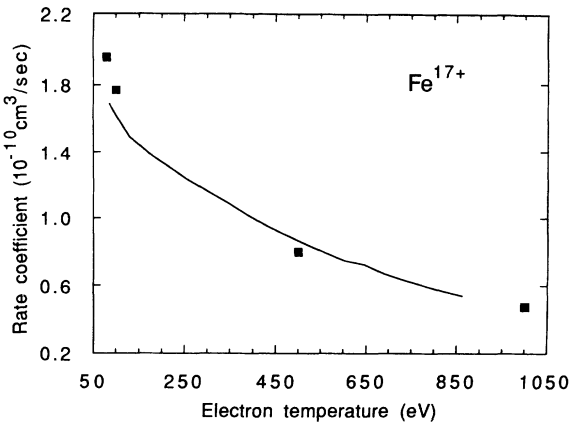

FIG. 5. Comparison of our distorted-wave results (squares) with R-matrix results from Ref. [19] (solid curve) for the $2p_{1/2}$-$2p_{3/2}$ transition for Fe^{17+}.

magnitude for $T<100$ eV. This large reduction is caused by an increase of the Coster-Kronig resonance energies by 120 eV due to the relativistic effects.

In Figs. 2–4, the direct excitation rates and the resonance contribution through Auger and Coster-Kronig resonances are compared. For $T\leq 100$ eV and $Z\leq 34$, the total rates are dominated by the Coster-Kronig contributions. For the other heavier ions, the Coster-Kronig contributions are as important as the direct excitation. The contributions of the Coster-Kronig resonances decrease to 10% and 16% at $T=1000$ eV for Fe^{17+} and Mo^{33+}, respectively.

Excitation rate coefficients for Fe^{17+} have also been calculated using the R-matrix method [19,20]. In these calculations the J-dependent energies were obtained by diagonalizing the Hamiltonian matrix arising from the nonrelativistic and Breit-Pauli terms. In Fig. 5, we compare the rate coefficients for the $2p_{1/2}$-$2p_{3/2}$ transition for Fe^{17+} from our distorted-wave calculations to those obtained in the R-matrix calculation [19]. Our results differ from the R-matrix results by only 10%, 6%, and 4% at $T=100$, 500, and 860 eV, respectively. This close agreement indicates that relativistic effects other than the shift in energy are not very important for Fe^{17+}. It also indicates that interference between the direct and indirect processes is not significant. Similar good agreement between the results of distorted-wave calculations and R-matrix calculations has been observed for other $n=2$ to $n=2$ transitions [20,21].

In summary, we have calculated the resonance contribution via Coster-Kronig transitions to the excitation rates for transition from the ground state ($^2P_{3/2}$) to the $n=2$ first excited ($^2P_{1/2}$) state in F-like ions. These rates together with previously calculated direct excitation rates and rates from Auger resonances yield the total excitation rate coefficients. We found that the resonance excitation by way of Coster-Kronig transition is the dominant excitation mechanism at low temperatures for $Z\leq 34$. Furthermore, the relativistic increase in Coster-Kronig energies plays a crucial role in determining the magnitude of the excitation rate coefficients at low temperatures and must be included in calculations to obtain accurate results.

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