Electron-impact excitation for F-like selenium

Chen Guo-xin and Qiu Yu-bo
Institute of Applied Physics and Computational Mathematics, P.O. Box 8009-57, Beijing 100088, China
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Electron-impact excitation cross sections from the low-lying $1s^2 2s^2 2p^5$ state of F-like selenium to singly excited states have been calculated. Our relativistic distorted-wave Born procedures have been used for the present calculations. Instead of atomic structure code GRASP, the latest version GRASP^2 code is used as multiconfiguration Dirac-Fock atomic structure calculations. The present results have been comprehensively compared with earlier calculations. One of the motivations for the present work is that there are some discrepancies between our results and those of others. [S1050-2947(97)10611-4]

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I. INTRODUCTION

The cross sections of highly stripped ions impacted by electrons are of interest for developing lasers in the extreme-UV (XUV) and soft-x-ray regimes. One perplexing consequence of the observation of Co-like analog lasers in Ni-like lasers is the absence of F-like lasers in Ne-like x-ray laser plasmas. The absence of any measurable gain on F-like lines is currently a mystery [1,2]. This mystery stimulates us to calculate extensively electron-impact excitation of F-like selenium. Investigations have been made recently by Hagelstein [1] but the cross sections he obtained are in poor agreement with ours. Considering the accuracy and elaboration of our calculation, Hagelstein's results seem to be incorrect. Comprehensive relativistic distorted-wave Born (RDWB) calculations of collision strengths for different F-like ions have also been published by Sampson *et al.* [3]. They modified Cowan's atomic structure code to calculate a fully relativistic case [4] and used the energy-independent Dirac-Fock-Slater (DFS) potential to evaluate continuum orbitals. Comparison of their results with ours indicates that the agreement of cross sections are generally good for relatively large excitation processes, but differences exist.

In Sec. II the calculation procedures are outlined. A discussion of the present results is given in Sec. III. Finally, we give a brief summary to outline the main points.

II. CALCULATION PROCEDURES

The present calculation is fulfilled by using the rapid fully RDWB electron-impact excitation procedures. Most of the theory and procedures for the calculations of the present cross sections were described in detail in Ref. [5], except that some modifications have been made in order to use the atomic structure code GRASP^2 [6]. The GRASP^2 code was completed in 1992. Atomic orbitals are taken to be four-component spinors. Multiconfiguration (MC) self-consistent-field (SCF) calculations are based on the Dirac-Coulomb Hamiltonian. The nuclear potential is modeled as a spherically symmetric distribution of nuclear charge. The one-body operator is based upon the Dirac kinetic-energy operator. The transverse photon interaction is added to the two-body operator. It is calculated perturbatively in the atomic structure part. Ion atomic-state functions (ASFs) are a linear combination of configuration state functions (CSFs) sharing common values of parity, and total target angular momentum J. The mixing coefficients are obtained by diagonalizing the Hamiltonian. Low-order QED modifications due to transverse electromagnetic interaction and the radiative corrections are treated via perturbation theory [7,8].

The theory of atomic structure is outlined above. In the collision dynamic part, to compare with Hagelstein's results, we performed some approximations to calculate the continuum orbitals as Hagelstein. These approximations are (a) using a fictitious configuration with fraction occupation numbers given by Hagelstein and (b) calculating the continuum orbitals without exchange potential. When an exchange potential is added there is some influence on the cross sections. So, a local semiclassical exchange (SCE) [9] potential that is energy dependent and has more physics than the DFS exchange potential is used in some of our calculation models. Comparison of the results of single excitation to the M shell involving the 113-level MCDF configuration expansion (CE) and single excitation to both M and N shells involving the 279-level MCDF CE from the ground state has also been done. The comparison indicates that calculation with the 279-level MCDF CE is necessary especially for the excitations to the high-lying levels because the principal quantum number $n=3$ shell with holes in the $2s$ or $2p$ subshells overlaps in energies the $n=4$ shell with holes in the $2s$ or $2p$ subshells. To our knowledge, the present work is the first publication of a fully relativistic calculation of cross sections for excitation of F-like selenium with singly excited M and N shells involving the 279-level MCDF CE.

III. RESULTS AND DISCUSSION

In Table I we compare the values of the resonance transition energies obtained by different authors. The level designations are the same as those in Table I of Ref. [1], except that some minor errors should be corrected: level 74 should be exchanged with 75, level 106 should be exchanged with level 107, levels 78, 79, and 100 should be $[2s2p_{1/2}^2 2p_{3/2}^3]_1 3p_{3/2}$, $[2s2p_{1/2}2p_{3/2}^4]_0 3p_{1/2}$, and $[2s2p_{1/2}^2 2p_{3/2}^3]_1 3d_{5/2}$, respectively. The entry of ''Present 1'' is obtained by the 113-level MCDF CE (referred to as mode A), which is the total-energy-level number of the singly excited M shell plus the ground state. The entry of

TABLE I. Comparison of selected resonance transition energies ΔE (in eV) from various calculations. J is the total angular momentum. The entry labeled ''Hagel.'' is obtained from Ref. [1] and the entry labeled ''Samp.'' is from Ref. [3].

		ΔE (eV)						ΔE (eV)			
Level	J	Present 1	Present 2	Hagel.	Samp.	Level	J	Present 1	Present 2	Hagel.	Samp.
1	3/2	0	0	0	0	59	5/2	1687.42	1688.23	1688.9	1687.8
2	1/2	42.74	42.87	42.8	42.8	67	1/2	1735.73	1736.45	1737.2	1736.2
3	1/2	212.95	213.20	212.4	213.0	74	3/2	1765.33	1766.12	1766.8	1765.6
4	5/2	1498.59	1499.34	1500.5	1499.2	75	5/2	1765.46	1766.29	1766.7	1765.8
5	3/2	1503.28	1504.02	1505.2	1504.0	76	3/2	1766.38	1767.18	1767.7	1766.8
11	5/2	1552.12	1552.87	1554.2	1552.8	78	1/2	1772.29	1773.03	1773.6	1772.6
12	3/2	1553.49	1554.23	1555.5	1554.2	79	1/2	1784.23	1784.88	1785.4	1784.5
17	3/2	1570.16	1570.85	1571.9	1570.8	80	3/2	1789.82	1790.62	1791.2	1790.3
18	3/2	1575.66	1576.43	1577.4	1576.2	88	3/2	1809.98	1810.81	1811.3	1810.1
22	5/2	1597.29	1598.07	1599.1	1597.9	91	1/2	1819.53	1820.35	1820.8	1819.7
23	1/2	1598.02	1598.74	1599.9	1598.7	94	3/2	1823.43	1824.29	1824.7	1823.6
33	3/2	1613.95	1614.34	1615.4	1614.6	99	1/2	1826.94	1827.16	1827.7	1826.9
45	1/2	1655.23	1655.74	1656.9	1656.0	113	5/2	2045.14	2045.68	2045.6	2044.9

''Present 2'' is obtained with the 279-level MCDF CE (referred to as mode B), which is the total-energy-level number of the singly excited M shell and N shell plus the ground state. The relaxation effect (nonorthogonal orbitals used in obtaining the ground and excited energy levels [1]) is partly included in the ''Present 2'' calculations. The difference in calculation mode A and mode B is less than 1.0 eV. The entry labeled ''Hagel'' is the results from Ref. [1]. ''Samp'' is the results calculated by Sampson *et al.* [3] who also used a mean configuration. This is somewhat the same as the work of Hagelstein. The calculations of Sampson *et al.* were different from the present calculations in two points: (a) the present results are obtained with a more accurate MCDF potential to determine the radial wave functions instead of a mean configuration in determining the central potential used in calculating the radial wave functions, namely, the GRASP[2] code is used in the present calculation; (b) the relaxation effect is partly included in the present results. The former difference made the energies of Sampson *et al.* [3] generally exceed the present value by about 1 eV, but the latter difference made his results generally lower than the present calculation by about 1 eV. So the present results are in good agreement with those of Sampson *et al.* [3] except for some high-lying excitational levels in which the differences are about 1 eV.

We have tabulated the cross sections in cm^2 in Table II for 2-3 transitions from the $2s^22p^{52}P_{3/2}$ state at three energies above threshold. In Table II, in the interest of space, five calculational models are only tabulated at 1000 eV above threshold. The entry ''Present 1'' is obtained with the 113-level MCDF CE. Also, the continuum orbitals are computed without the exchange potential. The purpose of this calculation model is to make a comparison with the work of Hagelstein [1]. The entry ''Present 2'' is obtained with the same approximations as the entry ''Present 1,'' except that the SCE exchange potential is added. So, we can see how the exchange potential influences the final values of the cross sections. The entry ''Present 3'' is obtained with the 279-level MCDF CE. The SCE exchange potential is also added. The entry ''Hagel.'' is the results calculated by Hagelstein [1]. The entry ''Samp.'' is the results calculated by Sampson *et al.* [3], but the energy above threshold is about 1016.8 eV, which is slightly different from 1000 eV in the present calculations. The detailed comparisons among the abovementioned five entries will be given in the following paragraph. The entry ''Present'' at energies 200 and 4000 eV above threshold is also tabulated. Their calculation models are the same as the entry ''Present 3'' at energy 1000 eV above threshold.

Inspecting Table II, we can get the following comparisons: (1) comparisons of the entry ''Present 1'' and the entry ''Present 2,'' which is referred to as ''Comparison A,'' reveal generally very good agreement with each other. This indicates that an exchange potential has only a little influence on the calculation. Most of the discrepancies are less than 1%. (2) ''Comparison B'': comparisons of the entry ''Present 2'' and the entry ''Present 3'' do show some differences. The transitions that have large discrepancies ($>5\%$) are 9% for transition 1-27, 6% for 1-33, 7% for 1-79, 5% for 1-98, 10% for 1-99, 14% for 1-105, 19% for 1-106, 39% for 1-109, 7% for 1-110, 23% for 1-111, 11% for 1-112, and 6% for 1-113. About one-fourth of the total transitions have discrepancies of more than a few percent. This indicates the necessity of the calculation with the 279-level MCDF CE, because the $n=3$ shell with holes in the $2s$ or $2p$ subshells overlaps in energy the $n=4$ shell with holes in the $2s$ and $2p$ subshells, i.e., $2s^22p^44l,2s2p^54l,l=s,p,d,f$. This conclusion was also drawn by Chen [5] for Ni-like highly charged ions, where the $n=4$ shell overlaps in energy the $n=5$ shell. (3) ''Comparison C'': perusal of Table II shows generally very good agreement between the entry ''Present 2'' and the entry ''Samp.'' However, some differences exist. These transitions are 1-67, 1-76, 1-78, 1-79, 1-80, 1-88, 1-91, 1-94, 1-99, 1-107, 1-109, 1-110, 1-111, 1-112, and 1-113. The collision strengths for these transitions are very small ($<10^{-3}$ or even $<10^{-4}$). The largest three discrepancies are 41% for transition 1-99, 59% for 1-109, and 76% for 1-113. (4) ''Comparison D'': when the comparisons of the entry ''Present 1'' and the entry ''Hagel.''

TABLE II. Electron collisional cross sections (cm^2) for selected 2-3 transitions from the $2s^2 2p^5\ ^2P_{3/2}$ state in F-like selenium. The cross sections are tabulated at three different energies (in eV) above threshold. Three different calculation models at present are tabulated and compared with that of Hagelstein [1] and Sampson *et al.* [3] at energy 1000 eV. The level indices for transition are given under the heading levels: I, F, where I stands for the initial level and F for the final level. $[n]$ means $\times 10^n$.

Levels		200.0 eV	1000.0 eV					4000.0 eV
I	F	Present	Present 1	Present 2	Present 3	Hagel.	Samp.	Present
1	2	2.638[−20]	4.792[−21]	4.761[−21]	4.806[−21]		4.73[−21]	8.594[−22]
1	3	1.176[−19]	4.655[−20]	4.645[−20]	4.725[−20]		4.98[−20]	1.762[−20]
1	4	3.548[−22]	2.027[−22]	2.017[−22]	2.040[−22]	1.922[−22]	1.95[−22]	8.768[−23]
1	5	3.939[−22]	4.126[−22]	4.127[−22]	4.216[−22]	4.521[−22]	3.93[−22]	4.349[−22]
1	11	2.991[−22]	2.970[−22]	2.970[−22]	3.038[−22]	3.344[−22]	2.83[−22]	2.996[−22]
1	12	1.155[−22]	6.878[−23]	6.840[−23]	6.882[−23]	8.016[−23]	6.64[−23]	3.273[−23]
1	17	2.577[−21]	1.883[−21]	1.892[−21]	1.863[−21]	1.125[−21]	1.80[−21]	9.384[−22]
1	18	1.067[−21]	6.983[−22]	6.991[−22]	6.815[−22]	3.592[−22]	6.86[−22]	2.905[−22]
1	22	3.193[−22]	1.447[−22]	1.420[−22]	1.424[−22]	4.362[−22]	1.34[−22]	2.248[−23]
1	23	1.316[−22]	7.215[−23]	7.140[−23]	7.190[−23]	1.373[−22]	6.78[−23]	2.478[−23]
1	33	9.415[−21]	7.314[−21]	7.362[−21]	6.923[−21]	1.267[−20]	7.08[−21]	3.495[−21]
1	45	2.285[−23]	1.180[−23]	1.162[−23]	1.070[−23]	1.451[−23]	1.12[−23]	2.009[−24]
1	59	1.765[−22]	7.692[−23]	7.566[−23]	7.650[−23]	6.275[−23]	7.16[−23]	1.156[−23]
1	67	2.801[−24]	1.509[−24]	1.490[−24]	1.514[−24]	1.321[−23]	1.76[−24]	5.460[−25]
1	74	4.230[−22]	3.257[−22]	3.277[−22]	3.229[−22]	6.174[−22]	3.38[−22]	1.735[−22]
1	75	2.384[−22]	2.581[−22]	2.585[−22]	2.633[−22]	2.776[−22]	2.75[−22]	2.854[−22]
1	76	9.947[−23]	9.087[−23]	9.087[−23]	9.184[−23]	1.117[−22]	1.01[−22]	8.802[−23]
1	78	2.335[−23]	1.644[−23]	1.640[−23]	1.605[−23]	1.374[−23]	1.96[−23]	1.045[−23]
1	79	1.642[−23]	1.678[−23]	1.679[−23]	1.565[−23]	1.171[−23]	2.14[−23]	1.556[−23]
1	80	2.288[−24]	1.643[−24]	1.640[−24]	1.594[−24]	1.163[−24]	1.47[−24]	8.981[−25]
1	88	2.955[−23]	2.483[−23]	2.481[−23]	2.510[−23]	2.174[−23]	2.88[−23]	2.266[−23]
1	91	8.909[−24]	5.298[−24]	5.269[−24]	5.280[−24]	5.529[−24]	5.83[−24]	2.425[−24]
1	94	2.716[−23]	2.323[−23]	2.319[−23]	2.277[−23]	2.655[−23]	2.98[−23]	2.060[−23]
1	99	1.419[−23]	8.398[−24]	8.357[−24]	7.601[−24]	7.401[−24]	1.18[−23]	1.965[−24]
1	113	1.280[−23]	1.082[−23]	1.083[−23]	1.021[−23]	2.879[−23]	1.91[−23]	7.257[−24]

are made, the agreement is often very poor. This conclusion was also drawn by Sampson *et al.* [3]. About half of the total transitions have more than a 10% discrepancy. In about one-third of the total transitions discrepancies are greater than 30%. For transitions from level 1 to levels 18, 22, 23, 24, 61, 62, 74, 77, 82, 83, 84, 102, 105, 112, and 113, the discrepancies are about an order of magnitude or even more. One reason for the differences in ''comparison *D*'' is some approximations made in the collision dynamic part in Ref. [1]. For example, a summation cutoff in the product of the expansion coefficients and no more than 30 partial collision strengths were used in obtaining the total collision strengths. Also, Hagelstein may use a different spherically averaged potential in calculating the continuum orbitals as opposed to the bound orbitals. Then the continuum orbitals are not orthogonal to the bound orbitals in his calculations and an additional correction is necessary when calculating the exchange collision matrix elements, but he omitted it. However, the main reasons for the discrepancies in ''comparison *D*'' as well as in ''comparison *C*'' may be due to the different atomic structure used in the calculations. This can be seen from the energy values and the oscillator strengths. It is interesting to note that some of the transitions that have large differences in ''comparison *C*'' are in good agreement or have fewer discrepancies in ''comparison *D*.'' One reason for this is that the atomic structure used in the three calculational codes are more or less different from each other.

To obtain electron-impact excitation cross sections, adequate treatment of the atomic structure part is very important when the collision dynamic part is properly calculated. Although most of the correlation effects in energies were obtained by Hagelstein's calculations [1], he used the mean configuration in determining the potential instead of the MCDF potential in his atomic structure calculations, as did Sampson *et al.* [3]. These approximations should be consulted, especially for small transition rates that are sensitive to the influence of bound wave functions. Because the GRASP[2] code is now used to calculate the atomic structure part and because there are several detailed considerations in the present calculational procedures of the collisional dynamics part, the present cross sections should be reliable and more accurate than previous calculations.

Monopole excitations (ME) play a key role in the gain calculation for x-ray laser research [1,10]. Transition 1-33 is the largest monopole transition ($J=3/2$-$3/2$) in the present calculation, which has a near-threshold cross section of 9.415×10^{-21} cm^2 at 200 eV above threshold. This cross section is larger than the dipole cross section for 1-55 but slightly less than that for 1-56. Level 33 is expected to be the upper $3p$ state of ME $3p$-$3s$ inversion driven from the

ground state $^2P_{3/2}$. The cross section for transition 1-33 calculated by Hagelstein [1] differ by about a factor of two from ours. The present cross section for 1-33 is more reasonable than that of Hagelstein according to the viewpoint of Ref. [10]. In most of the monopole transitions (from level 1 to levels 9, 17, 18, 20, 24, 27, 33, and 46) the cross sections obtained by the present calculations and by Hagelstein are greatly different. This may be due to the strong correlation effect for monopole transitions. With the reliable and accurate cross sections here, the intensities of $n=2$-3 lines and the gains of $3p$-$3s$ and $3d$-$3p$ transitions for F-like selenium should be recalculated as done in Ref. [1]. Very recently Dasgupta *et al.* [11] extended their previously developed model by using the more accurate fully relativistic atomic data developed by Sampson *et al.* [3] and others in self-consistent, analyzing and diagnosing a selenium plasma. Decreasing the ME cross section can greatly influence the gain calculation [10,11], so using accurate atomic data, especially accurate ME cross sections and other cross sections of transitions coupled with ME, can greatly improve the ability to diagnose a selenium plasma. Excitation cross sections play a crucial role in the diagnosis. Because there are some different physics and numerical considerations in the present calculations when compared with those of Hagelstein [1] and Sampson *et al.* [3], the gain coefficient prediction in Refs. [10, 11], line ratio and total emitting power isocontour plots in temperature and density space could be somewhat changed when the more sophisticated cross sections of the present calculations are used.

IV. SUMMARY

In conclusion, the inclusion of $n=4$ states and accurate and elaborate atomic structure such as using the strict MCDF potential instead of the mean configuration potential play a very important role in electron-impact excitation calculations when a detailed collision dynamic part is considered in RDWB procedures. In addition to the dynamic part, the main reason for the differences among the present results and others is due to the different atomic structure used. ME cross sections directly and greatly influence the gain coefficient prediction. The present cross section for excitation 1-33 is about half the value of Hagelstein [1] and in good agreement with that of Sampson *et al.* [3] However, as reascertained in the summary of Ref. [10], the ME cross sections in various theoretical calculation models including the RDWB method, relativistic or nonrelativistic R-matrix methods are too large by several times. This may be due to the curious behavior of $3p$ orbital in the upper state of ME. We will continue this interesting and important subject on the research of accurate calculation of ME cross sections.

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[1] P. L. Hagelstein, Phys. Rev. A **34**, 92 (1986).
[2] B. J. MacGowan, L. B. Da Silva, D. J. Fields, C. J. Keane, J. A. Koch, R. A. London, D. L. Matthews, S. Maxon, S. Mrowka, A. L. Osterheld, J. H. Scofield, G. Shimkaveg, J. E. Trebes, and R. S. Walling, Phys. Fluids B **4**, 2326 (1992).
[3] D. H. Sampson, H. L. Zhang, and C. J. Fontes, At. Data Nucl. Data Tables **48**, 25 (1991).
[4] D. H. Sampson, H. L. Zhang, A. K. Mohanty, and R. E. H. Clark, Phys. Rev. A **40**, 604 (1989).
[5] Chen Guo-xin, Phys. Rev. A **53**, 3227 (1996).
[6] F. A. Parpia, I. P. Grant, and C. F. Fischer (unpublished).
[7] K. G. Dyall *et al.*, Comput. Phys. Commun. **55**, 425 (1989), and references therein.
[8] Chen Guo-xin, Chin. Phys. Lett. **11**, 533 (1994); Chin. J. Comput. Phys. **13**, 153 (1996).
[9] M. E. Riley and D. G. Truhlar, J. Chem. Phys. **63**, 2182 (1975).
[10] A. Dasgupta, K. G. Whitney, M. Blaha, and M. Buie, Phys. Rev. A **46**, 5973 (1992).
[11] A. Dasgupta, K. G. Whitney, H. L. Zhang, and D. H. Sampson, Phys. Rev. E **55**, 3460 (1997).