Multiple photoionization cross sections for Fe²⁺ K shell[★]

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ABSTRACT

Multiple photoionization cross sections from the K shell are studied for all levels of the Fe²⁺ 3d⁶ configuration. The study shows that the quadruple photoionization leads to the largest cross sections. A large variation in the multiple photoionization cross sections is determined among the levels of the Fe²⁺ 3d⁶ configuration. Main decay branches of radiative and Auger cascades, following the photoionization of the K shell for the ground configuration of the Fe²⁺ ion, are identified. The radiative and Auger cascade is studied by considering transitions among energy levels and subconfigurations. The obtained data for ion yields are compared with previous calculations produced for configuration averages.

Key words. atomic data – atomic processes

1. Introduction

The study of emission spectra provides valuable information regarding the environment of astronomical objects. The relative intensities of spectral lines depend on the charge state distribution in the emitting environment. The ionization balance is regulated by photoionization and recombination processes in the photoionized plasmas. The photoionized plasmas were identified in stellar gas, supernova remnants, around compact objects such as black holes and neutron stars (see, e.g., Watanabe et al. 2006; Lee et al. 2009; Kallman et al. 2019). Furthermore, laboratory-generated photoionized plasmas were studied using power lasers and fast magnetic pinch machines (see, e.g., Foord et al. 2006; Hall et al. 2014; White et al. 2018).

Inner shell ionization by a photon leading to multiple ionization is an important mechanism producing higher ionization stages of atoms in photoionized plasmas. The inner shell vacancy that is created decays through the cascade of radiative and Auger transitions. The Auger transition emits an electron from the atomic system, while the radiative transition produces a photon. The process ends when the ground or metastable states of the ion are reached. The radiative and Auger cascades were widely studied theoretically (Kaastra & Mewe 1993; Jonauskas et al. 2000, 2003, 2008, 2011; Kučas et al. 2019) and experimentally (Palaudoux et al. 2010; Rudek et al. 2012; Schippers et al. 2017; Beerwerth et al. 2019). The theoretical study included the analysis of transitions among average energies of configurations (Jonauskas et al. 2000; Kaastra & Mewe 1993) or energy levels (Jonauskas et al. 2008, 2011; Kučas et al. 2019). The extension of the level-to-level study by including correlation effects are often necessary to explain measurements (Palaudoux et al. 2010; Jonauskas et al. 2011). On the other hand, this leads to extremely heavy calculations.

The K-vacancy states for the Fe ions were studied previously (see, e.g., Jacobs & Rozsnyai 1986; Opendak 1990;

Kaastra & Mewe 1993; Bautista et al. 2003, 2004; Palmeri et al. 2003; Kallman et al. 2004; Deprince et al. 2019, 2020). Those studies included energy levels, radiative and Auger widths, fluorescence yields, electron impact excitation, and photoabsorption cross sections. Branching ratios for the K-vacancy states were presented by considering transitions among the average energies of configurations (Kaastra & Mewe 1993). The Fe K spectra were modeled using atomic data of the entire Fe isonuclear sequence (Kallman et al. 2004). The multiple photoionization contribution was incorporated in the model by multiplying the Auger widths of the upper level of the configuration with the K-vacancy by the branching ratios calculated using configuration average energies (Kaastra & Mewe 1993). However, no level-resolved studies for the multiple photoionization of the K shell were previously presented for the Fe ions.

The aim of the current work is to study the radiative and Auger cascade produced by the K-shell photoionization in the Fe²⁺ ion by considering the transitions among the energy levels. Recently, the radiative and Auger cascades in Fe³⁺ have been investigated for the L-shell vacancies (Kučas et al. 2019, 2020). However, an analysis of the K shell decay in Fe³⁺ was not previously investigated. The study of energy levels is more complicated since a number of transitions drastically increase compared to a study using configuration averages. However, the level-to-level study is often needed since it provides more reliable results.

The rest of the paper is structured as follows. In Sect. 2, an overview of the theoretical approach is given; photoionization cross sections, branching ratios, and ion yields are presented in Sect. 3; and a brief summary with some final conclusions are provided in Sect. 4.

2. Theoretical approach

Energy levels, photoionization cross sections, and radiative as well as Auger transition probabilities are studied using the Flexible Atomic Code (FAC), where the Dirac-Fock-Slater approximation is implemented (Gu 2008). The relativistic *jj*-coupling scheme is utilized in the code. The single-configuration

[★] Data are only available at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via <http://cdsarc.u-strasbg.fr/viz-bin/cat/J/A+A/643/A46>

approximation is employed in this work. The potentials of the ground configurations of the corresponding ions are used to calculate bound and continuum wavefunctions. The Auger transition probabilities are obtained from the nonorthogonal wavefunctions of different neighboring ionization stages. The nonorthogonality of the wavefunctions for the different ionization stages is expected to only have a small influence on such calculations (Cowan 1981). The study of a multiple photoionization process includes 150 configurations (Fe^{2+} : 1, Fe^{3+} : 5, Fe^{4+} : 15, Fe^{5+} : 25, Fe^{6+} : 39, Fe^{7+} : 23, Fe^{8+} : 25, and Fe^{9+} : 17 configurations) with a total number of 113629 energy levels.

The single photoionization cross section is proportional to the generalized line strength:

$$\sigma_{\text{PI}} = \frac{2}{3} \pi \alpha \frac{\omega}{g_i} S, \quad (1)$$

where α is the fine structure constant, g_i is the statistical weight of the initial bound state, and ω is the photon energy. The generalized line strength is

$$S = \sum_{\kappa J_T} |\langle \Psi_i | \mathbf{D} | \Psi_f, \kappa; J_T \rangle|^2, \quad (2)$$

where $\mathbf{D} = \sum_i \mathbf{r}_i$ is an electric dipole operator and the sum is over the number of electrons, κ is the relativistic quantum number of the free electron, J_T is the total angular momentum, and Ψ_i and Ψ_f are the wavefunctions for the initial and final bound states, respectively.

Multiple photoionization cross sections are obtained by considering the population transfer from the excited states. The transfer of population is investigated in every step of the radiative and Auger cascade:

$$n_f = \sum_j n_j \frac{A_{jf}}{\sum_k A_{jk}^r + \sum_m A_{jm}^a}. \quad (3)$$

Here, n_j is the population of level j , which can decay further, n_f is a part of the population of level f that is reached from level j , A_{jf} is the probability of a radiative or Auger transition, and A_{jk}^r and A_{jm}^a are the probabilities of radiative and Auger transitions, respectively. Only electric dipole transitions are used in the study of the cascade. The summation in Eq. (3) is over the j levels; the transitions from which lead to level f . The same approach was previously used to obtain populations of the levels in the radiative and Auger cascades (Jonauskas et al. 2000, 2003, 2011; Palaudoux et al. 2010; Kučas et al. 2019). It should be noted that studies for Eu (Jonauskas et al. 2000), Xe (Jonauskas et al. 2003), and Kr (Palaudoux et al. 2010; Jonauskas et al. 2011) omitted the radiative transitions. The configuration average transitions (Kučas et al. 1995) were previously used to investigate Auger cascades in Eu (Jonauskas et al. 2000) and Xe (Jonauskas et al. 2003). The main branches of the cascade in Xe were determined using configuration averages and level-to-level studies were performed for the configurations on these branches (Jonauskas et al. 2003).

Our study of the cascade omits double- and triple-Auger transitions since the probabilities of these processes are lower compared to single-Auger transitions (Müller et al. 2015, 2018; Zhou et al. 2016; Jonauskas & Masys 2019). It should be noted that double- and triple-Auger transitions can be modeled by considering sequential ionization by the electron produced in the single-Auger transition (Zhou et al. 2016; Jonauskas & Masys

2019). The same approach was used to study the direct double ionization by the electron impact (Jonauskas et al. 2014; Koncevičiūtė et al. 2018, 2019).

The K-shell vacancy in the Fe^{2+} ion is produced by photon

The resulting $\text{Fe}^{3+} 1s^1 3d^6$ configuration decays through radiative and Auger transitions. For every ionization stage, the configurations with populations exceeding 0.01% are considered for further decay. Furthermore, the configurations with total summed populations lower than 0.1% are not included in the further decay calculations. As a result of this, a large number of configurations with a negligible contribution to the population transfer in the cascade have been discarded in the study. Therefore, the error of calculations is lower than 0.6% for the ion yield and the population of configurations of Fe^{9+} . However, this error is much lower since many omitted configurations cannot decay further through Auger transitions.

3. Results

The multiple photoionization cross sections for the ground and first excited levels of the ground $\text{Fe}^{2+} 3d^6$ configuration are presented in Figs. 1 and 2, respectively. The energy levels of the $\text{Fe}^{2+} 3d^6$ configuration are shown in Table 1. Theoretical values are compared with data provided by the National Institute of Standards and Technology (NIST; Kramida et al. 2019). The difference in the theoretical energy levels compared to the NIST recommended values is lower than 0.7 eV. The NIST values are mainly above the theoretical data. The order of the energy levels is different in both datasets. All of this can be explained by the correlation effects that are missing in the current study. The quadruple photoionization corresponds to the largest values of cross sections. For the ground level, the single photoionization cross sections are lower than the quadruple photoionization cross sections by two orders of magnitude. For the first excited level, the single photoionization cross sections are lower than the quadruple photoionization cross sections by three orders of magnitude. This shows that multiple photoionization cross sections are sensitive to the level of the initial configuration for which the process is studied.

The multiple photoionization mainly leads to the ground configurations of the corresponding ions. However, there are still populations residing in the long-lived states of the excited configurations. The partial photoionization cross sections from the ground level of Fe^{2+} to the configurations of the Fe^{6+} and Fe^{7+} ions are shown in Fig. 3. It can be seen that multiple photoionization to the ground configurations of the presented ions dominate. However, the excited configurations provide an important contribution to the multiple photoionization cross sections. This fact can be important in the modeling of the radiative spectra in plasma since radiative and dielectronic recombination, photoionization, and electron-impact ionization rates depend on the configuration for which processes are studied. Therefore, the modeling of the ionization balance in the plasma has to take the population of the configurations produced by multiple photoionization into account.

The decay of the K-vacancy state populates long-lived levels of the ions since the current modeling only includes electric dipole transitions. The partial photoionization cross sections to levels of the ground configuration having the strongest populations for the Fe^{6+} and Fe^{7+} ions are shown in Fig. 4. It should be

Fig. 1. Multiple photoionization cross sections for the ground level of the Fe²⁺ ion.

Fig. 2. Multiple photoionization cross sections for the first excited level of the Fe²⁺ ion.

noted that the excited levels of the ground configurations accumulate the main part of populations in the multiple photoionization process.

The branching tree for the radiative and Auger cascade following a creation of the K shell vacancy in the Fe²⁺ ion is shown in Figs. 5–9. The Auger transitions occur from states that are above the single ionization threshold of the corresponding ion. The single ionization threshold for the Fe³⁺ ion is 52.78 eV, while the NIST recommended value is slightly higher (54.91 eV). The double ionization threshold is 126.33 eV and the NIST value equals 129.91 eV. The triple ionization threshold amounts to 224.04 eV when NIST presents a value of 228.90 eV. It needs 347.84 eV (NIST – 353.87 eV) and 497.68 eV (NIST – 504.93 eV) to reach the ground states of the Fe⁷⁺ and Fe⁸⁺ ions, respectively, from the ground state of the Fe³⁺ ion. The energy levels of the Fe³⁺ 1s¹3d⁶ configuration span the energy range from 7115.31 to 7130.44 eV.

The initial populations of levels for the Fe³⁺ 1s¹3d⁶ configuration are taken to be proportional to the statistical weights of the levels to demonstrate the decay branching tree of the cascade (Figs. 5–9). Only the strongest branches of the cascade ($\geq 1\%$) are shown. Fluorescence yields for energy levels of the Fe³⁺

Table 1. Energy levels of the Fe²⁺ 3d⁶ configuration.

Index	Level	<i>J</i>	FAC (eV)	NIST (eV)
0	3d ³ _{3/2} (3/2)3d ³ _{5/2} (9/2)	4	0.000	0.000
1	3d ³ _{3/2} (3/2)3d ³ _{5/2} (9/2)	3	0.062	0.054
2	3d ² _{3/2} (2)3d ⁴ _{5/2} (4)	2	0.104	0.092
3	3d ¹ _{3/2} (3/2)3d ⁵ _{5/2} (5/2)	1	0.132	0.116
4	3d ² _{3/2} (2)3d ⁴ _{5/2} (2)	0	0.145	0.127
5	3d ³ _{3/2} (3/2)3d ³ _{5/2} (9/2)	6	2.481	2.486
6	3d ² _{3/2} (2)3d ⁴ _{5/2} (4)	5	2.515	2.517
7	3d ² _{3/2} (2)3d ⁴ _{5/2} (4)	4	2.539	2.539
8	3d ² _{5/2} (2)	2	2.713	2.710
9	3d ² _{5/2} (4)	4	2.849	2.661
10	3d ³ _{3/2} (3/2)3d ³ _{5/2} (3/2)	3	2.885	2.690
11	3d ¹ _{3/2} (3/2)3d ⁵ _{5/2} (5/2)	1	2.896	2.565
12	3d ³ _{3/2} (3/2)3d ³ _{5/2} (3/2)	2	2.911	2.406
13	3d ⁶ _{5/2} (0)	0	2.969	2.629
14	3d ³ _{3/2} (3/2)3d ³ _{5/2} (9/2)	5	3.156	3.045
15	3d ¹ _{3/2} (3/2)3d ⁵ _{5/2} (5/2)	4	3.214	3.092
16	3d ² _{3/2} (2)3d ⁴ _{5/2} (2)	3	3.240	3.117
17	3d ² _{3/2} (2)3d ⁴ _{5/2} (4)	6	3.746	3.764
18	3d ² _{3/2} (2)3d ⁴ _{5/2} (2)	4	3.961	3.829
19	3d ² _{3/2} (2)3d ⁴ _{5/2} (2)	1	4.105	3.809
20	3d ² _{5/2} (2)	2	4.106	3.808
21	3d ³ _{3/2} (3/2)3d ³ _{5/2} (9/2)	3	4.126	3.825
22	3d ³ _{3/2} (3/2)3d ³ _{5/2} (3/2)	0	4.618	4.316
23	3d ¹ _{3/2} (3/2)3d ⁵ _{5/2} (5/2)	2	4.957	4.439
24	3d ³ _{3/2} (3/2)3d ³ _{5/2} (3/2)	3	5.740	5.319
25	3d ² _{5/2} (0)	0	6.764	6.094
26	3d ² _{3/2} (2)3d ⁴ _{5/2} (0)	2	6.779	6.222
27	3d ² _{3/2} (0)3d ⁴ _{5/2} (4)	4	6.797	6.233
28	3d ³ _{3/2} (3/2)3d ³ _{5/2} (5/2)	3	6.797	6.236
29	3d ³ _{3/2} (3/2)3d ³ _{5/2} (5/2)	1	6.825	6.147
30	3d ² _{3/2} (0)3d ⁴ _{5/2} (2)	2	6.946	6.250
31	3d ³ _{3/2} (3/2)3d ³ _{5/2} (5/2)	4	7.665	7.095
32	3d ² _{3/2} (0)3d ⁴ _{5/2} (2)	2	10.386	
33	3d ² _{3/2} (0)3d ⁴ _{5/2} (0)	0	13.414

Fig. 3. Partial photoionization cross sections from the ground level of the Fe²⁺ ion to the configurations of the (a) Fe⁶⁺ and (b) Fe⁷⁺ ions.

Fig. 4. Partial photoionization cross sections from the ground level of the Fe^{2+} ion to the long-lived levels of the (a) Fe^{6+} and (b) Fe^{7+} ions. The cross sections to the ground levels of the Fe^{6+} and Fe^{7+} ions are shown by solid lines.

Fig. 5. Main branches of radiative and Auger cascade following decay of the $\text{Fe}^{3+} 1s^1 3d^6$ configuration. The decay branches are presented for the configurations of the Fe^{3+} ion. The initial population of the levels is proportional to their statistical weights. The numbers near the arrows indicate the branching ratios in percent. Even configurations are shown with a red color, and odd configurations are shown with a blue color.

$1s^1 3d^6$ configuration amount to ~ 0.38 . It is in a close agreement with the value of 0.37 from the previous studies (Palmeri et al. 2003) obtained using the HFR package by Cowan (1981). It can be seen that the strongest branch corresponds to the radiative decay from $\text{Fe}^{3+} 1s^1 3d^6$ to $2p^5 3d^6$ ($\sim 33.4\%$). The main part of population from the $\text{Fe}^{3+} 2p^5 3d^6$ configuration is transferred further through the Auger transitions ($\sim 33.3\%$). Part of the population even reaches the states of the Fe^{5+} ion (Fig. 6). The second strongest radiative branch corresponds to the $\text{Fe}^{3+} 1s^1 3d^6 \rightarrow \text{Fe}^{3+} 3p^5 3d^6$ transition ($\sim 4.1\%$). The produced $\text{Fe}^{3+} 3p^5 3d^6$ configuration decays further to $\text{Fe}^{4+} 3d^4$ ($\sim 4.0\%$). The second strongest branch of the cascade is produced by the Auger transition from $\text{Fe}^{3+} 1s^1 3d^6$ to $\text{Fe}^{4+} 2p^4 3d^6$ ($\sim 32.4\%$). The $\text{Fe}^{4+} 2p^4 3d^6$ configuration decays further through the Auger transitions to $\text{Fe}^{5+} 2p^5 3p^4 3d^6$ (12.9%), $\text{Fe}^{5+} 2p^5 3p^5 3d^5$ (9.4%), $\text{Fe}^{5+} 2p^5 3d^4$ (5.9%), and $\text{Fe}^{5+} 2p^5 3s^1 3p^5 3d^6$ (3.6%). Only $\sim 0.2\%$ of the population is transferred from $\text{Fe}^{4+} 2p^4 3d^6$ by radiative transitions to the lower configurations of the Fe^{4+} ion.

Fig. 6. Same as Fig. 5, but for configurations of the Fe^{4+} ion.

Fig. 7. Same as Fig. 5, but for the lower group of configurations of the Fe^{5+} ion.

The produced configurations of the Fe^{5+} ion with the largest population transferred from $\text{Fe}^{4+} 2p^4 3d^6$ have a vacancy in the 2p shell (Fig. 6). All of these configurations are subject to the further decay through Auger transitions since their energy levels are above the single ionization threshold of the Fe^{5+} ion. The decay of these configurations mainly ends in the states of the Fe^{6+} ion with vacancies in the 3s or 3p shells (Fig. 7).

Many of transitions are responsible for the formation of the Fe^{7+} ion. The population of the Fe^{7+} ion is initiated by the $\text{Fe}^{3+} 1s^1 3d^6 \rightarrow \text{Fe}^{4+} 2s^1 2p^5 3d^6$ (13.2%) and $\text{Fe}^{3+} 1s^1 3d^6 \rightarrow \text{Fe}^{4+} 2s^0 3d^6$ (4.1%) transitions (Fig. 5). The $\text{Fe}^{4+} 2s^1 2p^5 3d^6$ and $\text{Fe}^{4+} 2s^0 3d^6$ configurations mainly decay to $\text{Fe}^{5+} 2p^4 3d^5$ (9.2%), $2p^4 3p^5 3d^6$ (2.1%), and $2s^1 2p^5 3d^5$ (3.6%) (Fig. 6), which lead to $\text{Fe}^{6+} 2p^5 3d^3$, $2p^5 3p^5 3d^4$, $2p^5 3p^4 3d^5$, $2p^5 3s^1 3p^5 3d^5$, $2p^5 3p^3 3d^6$, and $2p^4 3d^4$ (Fig. 7). On the other hand, there is an additional path that ends in these configurations of the Fe^{6+} ion. It is initiated by the Auger transition from $\text{Fe}^{3+} 1s^1 3d^6$ to $\text{Fe}^{4+} 2p^4 3d^6$ (Fig. 5). The $\text{Fe}^{4+} 2p^4 3d^6$ decays to the $\text{Fe}^{5+} 2p^5 3p^4 3d^6$ (12.9%), $2p^5 3p^5 3d^5$ (9.4%), $2p^5 3d^4$ (5.9%), and $2p^5 3s^1 3p^5 3d^6$ (3.6%) (Fig. 6) population, which are transferred to $\text{Fe}^{6+} 3s^1 3p^3 3d^6$ (1.2%) (Fig. 6), $2p^5 3p^5 3d^4$ (0.7%) (Fig. 8), and $3s^1 3p^4 3d^5$ (0.5%) (Fig. 7). There are also other branches that end in the $\text{Fe}^{6+} 3s^1 3p^4 3d^5$, $3s^1 3p^3 3d^6$ (Fig. 7), and $2p^5 3p^5 3d^4$ (Fig. 8) configurations. Therefore, the population for the $\text{Fe}^{6+} 3s^1 3p^4 3d^5$ configuration reaches 4.5%, $2p^5 3p^5 3d^4$ – 4.2%, and $3s^1 3p^3 3d^6$ – 2.7%. Finally, the Fe^{7+} ions are reached from the $\text{Fe}^{6+} 2p^5 3p^4 3d^5$ (5.0%), $2p^5 3p^5 3d^4$ (4.0%), $2p^4 3d^4$ (3.0%), $3s^1 3p^4 3d^5$ (1.7%), $2p^5 3d^3$ (1.7%), $2p^5 3s^1 3p^5 3d^5$ (1.5%), and $3s^1 3p^3 3d^6$ (1.5%)

Fig. 8. Same as Fig. 5, but for the upper group of configurations of the Fe⁵⁺ ion.

Fig. 9. Same as Fig. 5, but for configurations of the Fe⁶⁺ ion.

configurations (Fig. 9). The decay from Fe⁷⁺ 2p⁵3p⁴3d⁴ (1.6%), 2p⁵3p⁵3d³ (0.9%), 2p⁵3s¹3p⁵3d⁴ (0.4%), and 2p⁵3d² (0.4%) reaches the states of the Fe⁸⁺ ion. The branches of the Auger cascade from the configurations of the Fe⁷⁺ ion are not presented in the figure since their branching ratios are lower than 1%. The Fe⁷⁺ 2p⁵3p⁴3d⁴ → Fe⁸⁺ 3p²3d⁴ (0.53%), Fe⁷⁺ 2p⁵3p⁴3d⁴ → Fe⁸⁺ 3p³3d³ (0.50%), and Fe⁷⁺ 2p⁵3p⁵3d³ → Fe⁸⁺ 3p³3d³ (0.43%) transitions are the three strongest ones from the Fe⁷⁺ ion.

The ion yield for different ionization stages of iron is presented in Fig. 10. The current results for transitions among the levels and subconfigurations are compared with calculations for configuration averages (Kaastra & Mewe 1993). The largest ion yield is obtained for the Fe⁶⁺ ion in our study. It can be seen that calculations corresponding to transitions among average energies of configurations provide the higher values for the Fe⁷⁺, Fe⁸⁺, and Fe⁹⁺ ions compared to the current results. This can be explained by the fact that additional decay channels were artificially opened in the Auger cascade process (Kaastra & Mewe 1993). Interestingly, the ion yield for Fe⁸⁺ that was studied using the subconfigurations shows a very good agreement with level-to-level data. The population of the Fe⁸⁺ states is determined by transitions from the Fe⁷⁺ 2p⁵3p⁴3d⁴, 2p⁵3p⁵3d³, 2p⁵3s¹3p⁵3d⁴, and 2p⁵3d² configurations for both applied approaches. What is more, good agreement among our ion yields is obtained for the Fe⁶⁺ ion. On the other hand, the previous calculations that used configuration averages strongly underestimate population

Fig. 10. Ion yields for radiative and Auger cascades following decay of the Fe³⁺ 1s¹3d⁶ configuration: a (yellow) – data from previous calculations (Kaastra & Mewe 1993), b (green) – the subconfigurations with the initial population proportional to statistical weights, c (red) and d (blue) – the lowest and the highest levels of the Fe³⁺ 1s¹3d⁶ configuration, respectively.

of Fe⁶⁺ (Kaastra & Mewe 1993). These calculations showed the largest ion yield for the Fe⁷⁺ ions.

A large variation in ion yields obtained using different approaches is seen for Fe⁴⁺ (Fig. 10). The data obtained for subconfigurations demonstrate the highest ion yield. Since the main decay channels for the Fe³⁺ ion are in a good agreement for data that consider transitions among the subconfigurations and levels, the difference is related to Auger transitions from the configurations of Fe⁴⁺. The main part of the population (14.4%) of the Fe⁴⁺ 3p⁴3d⁶ configuration goes to Fe⁴⁺ 3p⁵3d⁵, which mainly decays further to Fe⁴⁺ 3d⁴ in the study for subconfigurations. For a level-to-level study when an initial population of levels is proportional to their statistical weights, only 6.5% out of 14.5% are transformed to Fe⁴⁺ 3p⁵3d⁵ by radiative transitions. Furthermore, 13.6% out of 15.8% decays from Fe⁴⁺ 3p⁵3d⁵ to Fe⁴⁺ 3d⁴. Our study for energy levels and subconfigurations shows that main populations for the Fe⁴⁺ ion reside in the ground configuration. The differences between data obtained using the different approaches demonstrate the importance of the level-to-level study for the multiple photoionization process.

It should be noted that calculations using the configuration interaction method (CI) may have a crucial effect on the photoionization cross sections and ion yields (Jonaukas et al. 2008, 2011; Palaudoux et al. 2010). However, these types of calculations for the photoionization of the Fe²⁺ K shell are hardly feasible at the present time since they require large computational resources and efforts. As mentioned in Kučas et al. (2020), the CI basis set not only has to include admixed configurations that have the largest weight in the expansion of the intermediate wavefunctions for the configurations considered in the multiple photoionization calculations, but the basis set also has to be extended for the main admixed configurations, from which radiative and Auger transitions have to be studied. Furthermore, the convergence of the radiative and Auger transitions must be ensured. Additional channels for radiative transitions may be opened, leading to a transfer of population to states below the corresponding single ionization threshold. In addition, there are many overlapping configurations that strongly mix together in the neighboring ionization stages and this renders their decay properties sensitive to correlation effects. The increased CI basis

for these overlapping configurations may lead to the diminished transfer of the population through Auger transitions from Fe^{4+} to Fe^{5+} (Fig. 6), from Fe^{5+} to Fe^{6+} (Figs. 7 and 8), and from Fe^{6+} to Fe^{7+} (Fig. 9). But all of this has to be a subject of a separate study engaging more powerful computing machines. Nevertheless, the present single configuration data are important in predicting charge state distribution in photoionized plasmas, whether they are of astrophysical origin or man-made.

4. Conclusions

The multiple photoionization cross sections from the K shell are presented for all levels of the ground $\text{Fe}^{2+} 3d^6$ configuration. The study shows a large variation in the multiple photoionization cross sections on the levels of the initial ion. The photoionization of the K shell leads to radiative and Auger cascades, producing multiple charged ions. The radiative and Auger cascades are studied for all levels of the $\text{Fe}^{3+} 1s^1 3d^6$ configuration. The quadruple photoionization cross sections are the largest ones and they are about 50% and 70% higher compared to double and triple photoionization cross sections, respectively, for the ground level at the peak values. The radiative and Auger cascade leads to Fe^{6+} with the largest ion yield. It should be noted that the Fe^{4+} ion yield is higher compared to Fe^{5+} in the radiative and Auger cascade following the K shell photoionization for the lowest level of the $\text{Fe}^{3+} 1s^1 3d^6$ configuration. On the other hand, the Fe^{5+} ion yield is higher than the one of the Fe^{4+} ion for photoionization from the highest level of the $\text{Fe}^{3+} 1s^1 3d^6$ configuration. The obtained differences show that a level-to-level analysis has to be carried out to obtain reliable data for multiple photoionization. Finally, multiple photoionization cross sections for all levels of the ground configuration and partial photoionization cross sections from the levels of the $\text{Fe}^{2+} 3d^6$ configuration to the configurations of the produced ions and their levels are presented as supplementary data.

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