Multiple photoionization for the K shell in the Fe atom[★]

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ABSTRACT

Multiple photoionization for the K shell in the Fe atom is studied for all levels of the ground configuration. The study shows that sextuple-photoionization cross sections dominate for all levels of the $3d^6 4s^2$ configuration. The cross sections strongly depend on the initial level for which the photoionization is investigated. The partial photoionization cross sections to the configurations of the produced ions are determined. The main sequences of the radiative and Auger cascade following the photoionization of the K shell in the Fe atom are identified. Presented ion yields for subconfigurations and levels are compared with the previous calculations for configuration averages, revealing that they strongly overestimate ion yields for the Fe^{7+} – Fe^{10+} ions.

Key words. atomic data – atomic processes

1. Introduction

The secrets of the universe are mostly revealed to us from the interaction of the electromagnetic radiation with matter. Emission spectra deliver crucial information regarding environments in the remote celestial objects. The relative intensities of the spectral lines are determined by the charge-state distribution in plasma. Photoionization and recombination processes define charge-state distribution in the photoionized plasmas. The photoionized plasmas were observed in diffuse sources (stellar or interstellar gas, supernova remnants) and around compact objects (black holes, neutron stars) (see, e.g., [Watanabe et al. 2006](#); [Temple et al. 2020](#); [Schulz et al. 2020](#)). Lasers or magnetic pinch machines also provided ideal opportunities to study photoionized plasmas in laboratories (see, e.g., [Foord et al. 2006](#); [Hall et al. 2014](#); [Saber et al. 2017](#); [Loisel et al. 2017](#); [White et al. 2018](#)).

Interaction of atoms and ions with high-energy photons can produce excited atomic systems with removed electrons from any inner shell. The energies of the photons define how deep the inner-shell vacancies can be created. Even the lowest electron shells of atoms and ions can be reached in the photoionization process. For example, spectra from the active galactic nuclei show absorption lines from the K shells in the Fe ions ([Iwasawa et al. 2012](#); [Fukazawa et al. 2016](#)). Decay of the inner-shell vacancy leads to radiative and Auger cascades. The ions in various charge states can be produced in the cascade. This determines a multiple-photoionization process by a single photon.

Studying the radiative and Auger cascade is more complicated for vacancies in the deep electronic shells than in the shallow shells. Previous studies of the radiative and Auger cascades mainly dealt with the shells close to the valence electrons (see, e.g., [Verhoef et al. 2011](#); [Palaudoux et al. 2015](#); [Khalal et al. 2017](#)). This can be explained by the complexity of a problem

when thousands or even millions of transitions have to be evaluated for the deep shell decays ([Kučas et al. 2020b](#)). The problem can be overcome by considering the transitions among configuration averages ([Opendak 1990](#); [Kaastra & Mewe 1993](#); [Jonauskas et al. 2000, 2003](#)). Previously, the average characteristics of the configurations ([Kučas & Karazija 1993](#)) and Auger transitions ([Kučas et al. 1995](#)) were used to calculate cascades in Eu ([Jonauskas et al. 2000](#)) and Xe ([Jonauskas et al. 2003](#)). However, the decay of the inner-shell vacancy leads to many overlapping energy levels of the configurations for neighboring ions. A similar situation occurs for configurations connected by radiative transitions. Therefore, level-to-level studies are often required to provide more reliable data for the multiple-photoionization processes produced by high-energy photons.

The aim of this paper is to study multiple-photoionization process for the levels of the Fe atom by considering a creation of the K-shell vacancy. The multiple photoionization obtained for the K-shell vacancy was studied previously in the Fe^{2+} ion ([Kučas et al. 2020b](#)). The study demonstrated that ions up to Fe^{8+} can be produced by interactions with photons. The previous studies for the K-vacancy states in the iron ions analyzed atomic data, such as energy levels, wavelengths, A-values, Auger rates, radiative and Auger widths, fluorescence yields, and ion yields (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](#)). Furthermore, calculations of the photoabsorption and photoionization cross sections were performed using the Breit-Pauli R-matrix method ([Bautista et al. 2004](#)). Emission and absorption spectra of the K lines were investigated for equilibrium photoionized plasmas ([Kallman et al. 2004](#)). The charge-state distribution produced by the photoionization was taken from configuration average calculations ([Kaastra & Mewe 1993](#)). Recent studies of atomic characteristics for the K lines of the iron ions were extended by analyzing plasma-environment effects ([Deprince et al. 2019, 2020](#)).

In the past all steps of the radiative and Auger cascade following the K-shell vacancy creation in the Fe atom were

[★] The photoionization cross sections tables 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/654/A74>

analyzed only by considering transitions among average energies of configurations (Kaastra & Mewe 1993). The fluorescence yield and charge distribution were calculated with the energy levels of the subshells taken from data provided by Lotz (Lotz 1967, 1968). However, the energies of the subshells were modified to account for the effective charges experienced by electrons due to presence of the vacancies (Kaastra & Mewe 1993). This often led to overestimated ion yields for the higher ionization stages (Kučas et al. 2020a,b; Schippers et al. 2021). In this paper, we give results obtained via more consistent calculations.

The paper is organized as follows. Section 2 presents a brief outline of the theoretical approach. In Sect. 3, the obtained results are discussed. Finally, we end with the conclusions from the present investigation in Sect. 4.

2. Theoretical approach

The flexible atomic code (FAC) (Gu 2008), which implements the Dirac–Fock–Slater (DFS) approach, is used to calculate energy levels, and radiative and Auger transition probabilities in the single-configuration approximation. Multiple-photoionization cross sections are studied for all levels of the ground configuration of the Fe atom.

The interaction of photons with the Fe atom leads to the K-shell vacancy:

The study of the multiple-photoionization process includes 293 configurations (Fe⁺: 5, Fe²⁺: 22, Fe³⁺: 52, Fe⁴⁺: 75, Fe⁵⁺: 51, Fe⁶⁺: 53, Fe⁷⁺: 28, and Fe⁸⁺: 7 configurations). The total number of energy levels is 257 301 in this study.

The multiple-photoionization process is evaluated by considering single-photoionization with the following transfer of population from the levels of configuration with vacancy in the K shell (Eq. (1)). Multiple-photoionization cross sections from state i of the Fe atom to the final state j of the Fe ^{q +} ion are expressed as

$$\sigma_{ij} = \sum_k \sigma_{ik}^{\text{PI}} B_{kj}. \quad (2)$$

Here, summation runs through all 63 states of the 1s3d⁶4s² configuration for the Fe⁺ ion. The branching ratios B_{kj} are obtained by solving equations for every k and j state. The single-photoionization cross sections are defined as

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

where S is the generalized line strength, 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 expressed by the matrix element of the electric dipole operator $\mathbf{D} = \sum_i \mathbf{r}_i$ (the sum is over the number of electrons):

$$S = \sum_{\kappa J_T} |\langle \Psi_i || \mathbf{D} || \Psi_f, \kappa; J_T \rangle|^2. \quad (4)$$

Here κ is the relativistic quantum number of the continuum electron, J_T is the total angular momentum, and Ψ_i and Ψ_f are the wavefunctions for the atom and ion bound states, respectively.

The decay of the configuration with K-shell vacancy leads to radiative and Auger cascades. The partial gain of population n_{if} for the level f from the level i is determined by radiative and Auger transitions

$$n_{if} = n_i \frac{A_{if}}{\sum_k A_{ik}^r + \sum_m A_{im}^a}, \quad (5)$$

where n_f (n_i) is the population of the level f (i), A_{if} is a probability of the radiative or Auger transition, and A_{ik}^r and A_{im}^a are respectively the probabilities of the radiative and Auger transitions. The denominator in Eq. (5) corresponds to the total probability of the level i to decay through the radiative and Auger transitions. An inverse of this quantity corresponds to the lifetime of the level i . The total population n_f gained for the level f is obtained by taking the sum over the levels i in Eq. (5). The sequence of the radiative and Auger cascade ends in the states which cannot decay through radiative or Auger transitions. These states are below the single-ionization threshold of the corresponding ion. The same approach was previously used to study transfer of population in the radiative and Auger cascades for various elements (Jonauskas et al. 2000, 2003, 2011; Palaudoux et al. 2010; Kučas et al. 2019, 2020b). It should be noted that the current analysis evaluates an influence of the radiative transitions on the cascade, while the previous calculations for the Eu (Jonauskas et al. 2000), Xe (Jonauskas et al. 2003), and Kr (Palaudoux et al. 2010; Jonauskas et al. 2011) ions omitted the radiative transitions due to the low values for the fluorescence yields. Therefore, the multiple photoionization is expressed by the single-photoionization cross section for the primary K-shell electron ejection multiplied by the branching ratio determined from the radiative and Auger cascades.

3. Results

3.1. Photoionization cross sections

Photoionization of the K shell for the Fe atom requires 7122.66 eV of energy. The energy of the Fe⁺ 1s3d⁶4s² configuration is above the energy of the ground configuration of the Fe¹⁸⁺ ion (2p⁴ – 5961.48 eV); however, it is below the energy of the ground configuration of the Fe¹⁹⁺ ion (2p³ – 7418.20 eV). On the other hand, only states of the Fe⁸⁺ ion are reachable in the current study.

The energy levels for the ground configuration of the Fe atom are compared to the values provided by the National Institute of Standards and Technology (NIST) (Kramida et al. 2021) in Table 1. In addition, the energy levels calculated using the pseudo-relativistic Hartree–Fock (PRHF) approximation (Cowan 1981) are presented for comparison. The indexes of levels presented in Table 1 are also used in the text. It can be seen that the DFS values are in better agreement with the NIST data than the PRHF calculations are. It should be noted that scaling of integrals was not used in the PRHF calculations. The largest discrepancy among the DFS and NIST energy levels is obtained for the level with index $i = 23$ (0.465 eV). The PRHF values are above the DFS and NIST data for all presented levels except for the ground term where DFS is slightly above PRHF.

The multiple-photoionization cross sections for the ground level of the Fe atom are presented in Fig. 1. The photoionization cross sections to the Fe⁶⁺ ion dominate compared to other multiple-photoionization cross sections. The photoionization cross sections to the states of the Fe⁴⁺ ion are ~42% lower than to the levels of the Fe⁶⁺ ion. The sextuple-photoionization

Table 1. Comparison of theoretical energy levels (in eV) to the available NIST values for the Fe $3d^6 4s^2$ configuration.

<i>i</i>	Level	Term	NIST	PRHF	DFS
0	$3d_{3/2}^3 3d_{5/2}^3 (9/2)4$	5D	0.000	0.000	0.000
1	$3d_{3/2}^3 3d_{5/2}^3 (9/2)3$	5D	0.052	0.052	0.060
2	$3d_{3/2}^2 (2)3d_{5/2}^4 (4)2$	5D	0.087	0.089	0.102
3	$3d_{3/2}^1 3d_{5/2}^5 1$	5D	0.110	0.113	0.129
4	$3d_{3/2}^2 (2)3d_{5/2}^4 (2)0$	5D	0.121	0.125	0.142
5	$3d_{3/2}^3 3d_{5/2}^3 (9/2)6$	3H	2.404	2.687	2.381
6	$3d_{3/2}^2 (2)3d_{5/2}^4 (4)5$	3H	2.433	2.715	2.413
7	$3d_{3/2}^2 (2)3d_{5/2}^4 (4)4$	3H	2.453	2.736	2.436
8	$3d_{5/2}^2$	3P	2.279	2.943	2.599
9	$3d_{5/2}^2 4$	3F	2.559	3.082	2.733
10	$3d_{3/2}^3 3d_{5/2}^3 (3/2)3$	3F	2.588	3.110	2.768
11	$3d_{3/2}^1 3d_{5/2}^5 1$	3P	2.424	3.097	2.781
12	$3d_{3/2}^3 3d_{5/2}^3 (3/2)2$	3F	2.609	3.132	2.793
13	$4s_{1/2}^2 0$	3P	2.484	3.163	2.854
14	$3d_{3/2}^3 3d_{5/2}^3 (9/2)5$	3G	2.949	3.402	3.030
15	$3d_{3/2}^1 3d_{5/2}^5 4$	3G	2.990	3.450	3.087
16	$3d_{3/2}^2 (2)3d_{5/2}^4 (2)3$	3G	3.018	3.473	3.112
17	$3d_{3/2}^2 (2)3d_{5/2}^4 (4)6$	1I	3.634	4.049	3.595
18	$3d_{3/2}^2 (2)3d_{5/2}^4 (2)4$	1G	3.695	4.272	3.801
19	$3d_{3/2}^2 (2)3d_{5/2}^4 (2)1$	3D	3.635	4.411	3.942
20	$3d_{5/2}^2$	3D	3.640	4.414	3.944
21	$3d_{3/2}^3 3d_{5/2}^3 (9/2)3$	3D	3.642	4.429	3.964
22	$3d_{3/2}^3 3d_{5/2}^3 (3/2)0$	1S	–	4.974	4.432
23	$3d_{3/2}^1 3d_{5/2}^5 2$	1D	4.294	5.334	4.759
24	$3d_{3/2}^3 3d_{5/2}^3 (3/2)3$	1F	–	6.177	5.512
25	$3d_{5/2}^2 0$	3P	–	7.295	6.492
26	$3d_{3/2}^2 (2)3d_{5/2}^4 (0)2$	3F	–	7.297	6.509
27	$3d_{3/2}^3 3d_{5/2}^3 (5/2)3$	3F	–	7.306	6.528
28	$3d_{3/2}^2 (0)3d_{5/2}^4 (4)4$	3F	–	7.303	6.530
29	$3d_{3/2}^3 3d_{5/2}^3 (5/2)1$	3P	–	7.345	6.553
30	$3d_{3/2}^2 (0)3d_{5/2}^4 (2)2$	3P	–	7.446	6.675
31	$3d_{3/2}^3 3d_{5/2}^3 (5/2)4$	1G	–	8.250	7.361
32	$3d_{3/2}^2 (0)3d_{5/2}^4 (2)2$	1D	–	11.163	9.978
33	$3d_{3/2}^2 (0)3d_{5/2}^4 (0)0$	1S	–	14.427	12.884

Notes. Energies are given relative to the ground energy. DFS – current calculations, PRHF – data calculated using the pseudo relativistic approximation of Cowan (1981).

cross sections from the ground level of the Fe atom are slightly lower than the triple-photoionization cross sections. The double-photoionization cross sections are below the septuple cross sections.

The multiple-photoionization cross sections are sensitive to the initial level of the Fe atom from which the photoionization process is investigated. For example, the septuple-photoionization cross sections from the level with index $i = 33$ (Fig. 2) are ~8% higher than those from the ground level of the Fe atom. Furthermore, the quadruple-photoionization cross sections are above the pentuple-photoionization cross sections from the level $i = 33$, while the pentuple-photoionization cross

Fig. 1. Multiple-photoionization cross sections for the ground level of the Fe atom. **Fig. 2.** Multiple-photoionization cross sections from the level with index 33 of the Fe atom.

sections are above the quadruple ones in the case of the photoionization from the ground level. The octuple-photoionization cross sections are lower than sextuple-photoionization cross sections by two orders of magnitude for the presented levels. There are no Fe^+ ions produced by the K-shell photoionization. The relative strength of the double, triple, and septuple photoionizations is also different from the level with the index $i = 33$ compared to the ground level. The triple-photoionization cross sections are the lowest of these cross sections from the excited level, and the strongest from the ground level.

The partial photoionization cross sections can be important in plasma modeling. The partial photoionization cross sections from the ground level of the Fe atom to configurations of the Fe^{6+} and Fe^{7+} ions are presented in Fig. 3. The cross sections to the ground configuration dominate for the Fe^{6+} and Fe^{7+} ions. The contribution of the excited configurations of the Fe^{6+} ion is negligibly small. On the other hand, the photoionization to the levels of the Fe^{7+} excited $3p^5 3d^2$ configuration is only ~50% lower compared to the photoionization cross sections to levels of the Fe^{7+} $3d$ configuration.

The strongest partial photoionization cross sections from the ground level of the Fe atom to the levels of the ground configuration of the Fe^{6+} ion are shown in Fig. 4. The largest cross sections correspond to the ground level of the Fe^{6+} ion. The cross

Fig. 3. Partial photoionization cross sections from the ground level of the Fe atom to the configurations of the (a) Fe^{6+} and (b) Fe^{7+} ions.

Fig. 4. Partial photoionization cross sections from the ground level of the Fe atom to the long-lived levels of the Fe^{6+} ion. The cross section to the ground level of the Fe^{6+} ion is shown as a solid line.

Fig. 5. Main branches of radiative and Auger cascades following decay of the $\text{Fe}^+ 1s^3d^64s^2$ configuration. The decay branches are presented for the configurations of the Fe^+ ion. The initial population of the levels is proportional to their statistical weights. The numbers near the arrows indicate the branching ratios in percent. Black arrows correspond to Auger transitions, green arrows to radiative transitions. Even configurations are shown in red, odd configurations in blue.

Fig. 6. Same as Fig. 5, but for configurations of the Fe^{2+} ion.

sections to the first excited level are $\sim 36\%$ lower compared to the ground level. It should be noted that our study includes only electric-dipole radiative transitions, while many of the produced configurations are the subject of the higher multipole radiative transitions.

3.2. Radiative and Auger cascades

The main decay branches (sequences) of the cascade for the $\text{Fe}^+ 1s 3d^6 4s^2$ configuration are presented in Figs. 5–10. The initial populations of the levels of the $\text{Fe}^+ 1s 3d^6 4s^2$ configuration are taken to be proportional to the statistical weights of the level to demonstrate the decay paths of the radiative and Auger cascades. The theoretical ionization thresholds are compared to the NIST values in Table 2. It can be seen that all ionization thresholds

Fig. 7. Same as Fig. 5, but for configurations of the Fe^{3+} ion.

calculated using the DFS approach are below the NIST results. For example, the theoretical single-ionization threshold for the Fe atom is 6.21 eV, while the NIST (Kramida et al. 2021) recommended value is 7.90 eV. The theoretical value is below the NIST value by 1.69 eV. The similar tendency for the FAC ionization thresholds compared to the NIST data was previously obtained for other ions (Jonauskas et al. 2015, 2019; Kynienė et al. 2015; Koncevičiūtė et al. 2018). The differences between the FAC and NIST ionization thresholds increase with increasing charge state. For Fe^{8+} it reaches a value of 13.59 eV; however, it is only $\sim 1.7\%$. The energy levels of the Fe^+ $1s3d^64s^2$ configuration are shown in Table A.1. The same indexes of levels presented in Table A.1 are used in the tables available at the CDS.

Fig. 8. Same as Fig. 5, but for configurations of the Fe^{4+} ion.

The strongest branch of the cascade leads to states of the Fe^{4+} ion: $\text{Fe}^+ 1s3d^64s^2 \xrightarrow{33.5\%} \text{Fe}^+ 2p^53d^64s^2$ (Fig. 5) $\xrightarrow{15.5\%} \text{Fe}^{2+} 3p^43d^64s^2$ (Fig. 5) $\xrightarrow{14.2\%} \text{Fe}^{3+} 3p^53d^44s^2$ (Fig. 6a) $\xrightarrow{13.2\%} \text{Fe}^{4+} 3d^34s$ (Fig. 7a). The final configuration cannot decay through electric dipole radiative transitions. The states of this configuration accumulate in the main part of the population residing in the Fe^{4+} ion (15.0%). This branch is started by the radiative decay of the configuration having the 2p subshell vacancy. The strong branch from the $\text{Fe}^+ 2p^53d^64s^2$ configuration also leads to the ground configuration of Fe^{3+} : $\text{Fe}^+ 2p^53d^64s^2 \xrightarrow{8.4\%} \text{Fe}^{2+} 3p^53d^54s^2$ (Fig. 5) $\xrightarrow{7.0\%} \text{Fe}^{3+} 3d^5$ (Fig. 6a). The second strongest branch ends in the states of the Fe^{6+} ion: $\text{Fe}^+ 1s3d^64s^2 \xrightarrow{32.7\%} \text{Fe}^{2+} 2p^43d^64s^2$ (Fig. 5) $\xrightarrow{14.1\%} \text{Fe}^{3+} 2p^53p^43d^64s^2$ (Fig. 6b) $\xrightarrow{3.1\%} \text{Fe}^{4+} 2p^53p^53d^44s^2$ (Fig. 7b) $\xrightarrow{2.1\%} \text{Fe}^{5+} 3p^33d^44s^2$ (Fig. 8a) $\xrightarrow{2.1\%} \text{Fe}^{6+} 3p^43d^34s$ (Fig. 9a). The $3p^43d^34s$, $3p^43d^4$, $3p^53d^24s$, and $3p^53d^3$ configurations of Fe^{6+} decay mainly radiatively to the lower lying states. The total population of the states of the Fe^{6+} ion amounts to 32.0%. The states of the Fe^{7+} ion are mainly populated from the Fe^{6+} $3s3p^53d^34s$, $3p^33d^44s$, $3p^43d^24s^2$, $3s3p^43d^44s$, and $3p^33d^34s^2$ configurations (Fig. 10).

The population of the states for the Fe^{8+} ion reaches $\sim 0.41\%$, while the final population for the states of the Fe^{7+} ion amounts to $\sim 8.2\%$. The main population resides in the Fe^{8+} $3p^53d$ configuration (0.32%). The states of the Fe^{8+} ion are mainly populated from the Fe^{7+} $3s3p^43d^34s$ (0.15%), Fe^{7+} $3s3p^33d^44s$ (0.11%), and Fe^{7+} $3s3p^53d^24s$ (0.04%) configurations. It should be noted

Fig. 11. Ion yields for radiative and Auger cascades following decay of the $\text{Fe}^+ 1s^1 3d^6 4s^2$ configuration: a (yellow) Data from previous calculations (Kaastra & Mewe 1993), b (green) Subconfigurations with the initial population proportional to statistical weights, c (red) and d (blue) Initially populated by only the lowest and the highest levels of the $\text{Fe}^+ 1s^1 3d^6 4s^2$ configuration, respectively.

of 0.55%. The total population amounts to 0.12% for the $\text{Fe}^{7+} 3s 3p^3 3d^4 4s$ configuration. The main part of the population (0.11%) leads to the $\text{Fe}^{8+} 3p^3 3d^3$ configuration. The $\text{Fe}^{7+} 3s 3p^3 3d^2 4s$ configuration decays to $\text{Fe}^{8+} 3p^3 3d$ by transferring 0.04% out of 0.06%. Therefore, there are mainly three configurations (i.e., $3p^3 3d^3$, $3p^4 3d^2$, and $3p^5 3d$) of the Fe^{8+} ion populated in the radiative and Auger cascades following the creation of the $\text{Fe}^+ 1s 3d^6 4s^2$ configuration by the photoionization of the Fe atom.

The ion yield produced by radiative and Auger cascades following the K shell photoionization is shown in Fig. 11. A comparison with the previous calculations by Kaastra & Mewe (1993) that considered transitions among configuration averages is also presented. In addition, the results of the study for subconfigurations are shown. The highest population for the decay of the lowest level of the $\text{Fe}^+ 1s 3d^6$ configuration corresponds to the Fe^{6+} ion (~31.2%). The cascade produced by the decay of the highest level of the $\text{Fe}^+ 1s 3d^6$ configuration leads mainly to states of the Fe^{6+} ion (~34.7%). However, the radiative and Auger cascades studied for the levels and subconfigurations demonstrate large differences for the ion yields of the Fe^{5+} and Fe^{6+} ions. It should be noted that the results from configuration averages provide the highest ion yield for Fe^{7+} (Kaastra & Mewe 1993). Even the population of the Fe^{8+} ion is quite large (17.3%) compared to the data obtained using more detailed calculations. This can be explained by the fact that additional artificial channels are opened in the calculations of the ion yield by modifying subshell energies (Kaastra & Mewe 1993). The similar situation was obtained for the radiative and Auger cascades following the photoionization from the 1s, 2s, and 2p subshells in the Fe^{2+} ion (Kučas et al. 2019, 2020b; Schippers et al. 2021). The study of the subconfigurations is more detailed than that of the configuration averages, but the highest population is produced for the Fe^{5+} ions in the first case. Furthermore, the analysis of the cascade by considering transitions among energy levels is more accurate compared to the study for the subconfigurations. This leads to the higher maximum ion yield (Fe^{6+}) compared to the investigation using the subconfiguration averages (Fe^{5+}). It should be

noted that the calculations for the configuration averages reach the Fe^{10+} ion, while the highest ionization stage of the Fe^{8+} ion is obtained in the current study. The calculations of the radiative and Auger cascades for the highest level of the $\text{Fe}^+ 1s 3d^6 4s^2$ configuration produce a slightly higher ion yield starting from the Fe^{6+} ion compared to the study for the lowest level since a larger number of energy levels of the higher ionization stages is covered by the energetically higher initial level compared to the lowest one. It should be noted that the ion yield for the Fe^{2+} ion is larger than for Fe^{3+} and the ion yield for the Fe^{4+} ion is larger than for Fe^{5+} in the study for configuration averages (Kaastra & Mewe 1993). The same tendency for the ion population is obtained for the decay from the highest level of the $\text{Fe}^+ 1s 3d^6 4s^2$ configuration. A similar situation for the cascade was obtained in the case of the K-shell vacancy for subconfigurations and the lowest level (Fe^{4+} versus Fe^{5+}) of the $\text{Fe}^{3+} 1s 3d^6$ configuration (Kučas et al. 2020b).

It should be noted that the calculations that considered transitions among configuration averages show a contribution of the Fe^+ ion (0.47%). This ion is produced by radiative transitions to the $\text{Fe}^+ 2p^5 3d^6 4s^2$ and $3p^5 3d^6 4s^2$ configurations. Our study demonstrates that the produced configurations are the subject of further decay mainly through Auger transitions to states of the Fe^{2+} ion (Fig. 5). The negligible population in the states of the Fe^+ ion is determined in our study.

The previous study of multiple photoionization for the K shell of the Fe^{2+} ion determined that the Fe^{6+} ions are produced with the highest probability. However, the states of the ion were reached in the third step of the Auger cascade, while it requires five steps for the decay of the $\text{Fe}^+ 1s 3d^6 4s^2$ configuration to Fe^{6+} , which accumulates the highest population in the current study.

As mentioned above, the single-configuration approximation is used in the current study. The configuration interaction (CI) method can be important in the analysis of multiple-photoionization cross sections. The previous studies demonstrated that correlation effects incorporated in calculations have a crucial effect obtaining higher ionization stages in the cascade process and explaining measurements (Jonas et al. 2008, 2011; Palaudoux et al. 2010). However, these calculations require large computational resources and efforts since the CI basis set has to include many admixed configurations (Kučas et al. 1997) that are important for the investigated configurations in the multiple-photoionization process. Furthermore, the CI basis must be extended by including configurations having the highest mixing with the admixed configurations. However, such calculations are hardly feasible at the moment. Nevertheless, the present study provides important results that can be used in the analysis of the charge-state distribution in the photoionized plasmas.

4. Conclusions

The multiple-photoionization cross sections from the K shell of the Fe atom are investigated for all levels of the $3d^6 4s^2$ configuration. The partial photoionization cross sections to the configurations of the Fe^{6+} and Fe^{7+} ions are also analyzed. The study demonstrates that the ground configurations of the produced ions are mainly populated in the photoionization process with the ground levels of the ions mostly being reached. The sextuple-photoionization cross sections dominate compared to other multiple-photoionization cross sections for levels of the Fe atom. The sextuple cross sections for the ground level are ~33%

and ~42% higher compared to quintuple and quadruple, respectively. The main decay branches for the K-shell vacancy in the Fe^+ ion are identified for the statistical distribution of the initial levels. The strongest branches lead to states of the Fe^{4+} and Fe^{6+} ions. The ion yields presented for the study among subconfigurations and energy levels show large variation. The largest ion yield for subconfigurations corresponds to Fe^{5+} , while investigation for the levels leads to Fe^{6+} . The highest ionization stage reached in the photoionization process amounts to Fe^{8+} .

Finally, the multiple-photoionization cross sections are available at the CDS. The partial photoionization cross sections to the configurations of the produced ions are also tabulated.

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Appendix A: Additional table

Table A.1. Energy levels for the $\text{Fe}^+ 1s3d^64s^2$ configuration. Energies are given relative to the ground energy of the $\text{Fe } 3d^64s^2$ configuration. The levels are identified by the largest weight in the expansion of wave function. Closed subshells are omitted in the notations of the levels. J is the total angular momentum quantum number.

Index	Configuration	J	Energy (eV)
34	$1s3d_{3/2}^3[4]3d_{5/2}^3(9/2)$	9/2	7122.664
35	$1s3d_{3/2}^3[4]3d_{5/2}^3(9/2)$	7/2	7122.719
36	$1s3d_{3/2}^2(2)[5/2]3d_{5/2}^4(4)$	7/2	7122.772
37	$1s3d_{3/2}^2(2)[3/2]3d_{5/2}^4(4)$	5/2	7122.805
38	$1s3d_{3/2}^2(2)[5/2]3d_{5/2}^4(4)$	5/2	7122.830
39	$1s3d_{3/2}^2(2)[5/2]3d_{5/2}^4(4)$	3/2	7122.841
40	$1s3d_{3/2}^2(2)3[1/2]3d_{5/2}^4(2)$	1/2	7122.858
41	$1s3d_{3/2}^2[2]3d_{5/2}^5$	3/2	7122.867
42	$1s3d_{3/2}^2(2)[5/2]3d_{5/2}^4(2)$	1/2	7122.887
43	$1s3d_{3/2}^3[2]3d_{5/2}^3(9/2)$	13/2	7125.117
44	$1s3d_{3/2}^3[1]3d_{5/2}^3(9/2)$	11/2	7125.167
45	$1s3d_{3/2}^3[2]3d_{5/2}^3(9/2)$	11/2	7125.179
46	$1s3d_{5/2}^2(4)$	9/2	7125.183
47	$1s3d_{5/2}^2(4)$	7/2	7125.202
48	$1s3d_{3/2}^3[2]3d_{5/2}^3(9/2)$	9/2	7125.210
49	$1s3d_{5/2}^2(2)$	5/2	7125.312
50	$1s3d_{5/2}^2(2)$	3/2	7125.342
51	$1s3d_{5/2}^2(4)$	9/2	7125.449
52	$1s3d_{5/2}^2(4)$	7/2	7125.488
53	$1s3d_{3/2}^3[2]3d_{5/2}^3(3/2)$	7/2	7125.534
54	$1s3d_{3/2}^3[1]3d_{5/2}^3(3/2)$	5/2	7125.555
55	$1s3d_{3/2}^3[2]3d_{5/2}^3$	3/2	7125.567
56	$1s3d_{3/2}^3[2]3d_{5/2}^3(3/2)$	5/2	7125.576
57	$1s3d_{3/2}^3[1]3d_{5/2}^3(3/2)$	3/2	7125.580
58	$1s3d_{3/2}^3[2]3d_{5/2}^3$	1/2	7125.580
59	$1s$	1/2	7125.600
60	$1s3d_{3/2}^2(2)[5/2]3d_{5/2}^4(4)$	11/2	7125.792
61	$1s3d_{3/2}^2(2)[3/2]3d_{5/2}^4(4)$	9/2	7125.840
62	$1s3d_{3/2}^2[2]3d_{5/2}^5$	9/2	7125.865
63	$1s3d_{3/2}^2[1]3d_{5/2}^5$	7/2	7125.895
64	$1s3d_{3/2}^2(2)[5/2]3d_{5/2}^4(2)$	7/2	7125.913
65	$1s3d_{3/2}^2(2)[3/2]3d_{5/2}^4(2)$	5/2	7125.925
66	$1s3d_{3/2}^2(2)[5/2]3d_{5/2}^4(4)$	13/2	7126.381
67	$1s3d_{3/2}^2(2)[3/2]3d_{5/2}^4(4)$	11/2	7126.426
68	$1s3d_{3/2}^2(2)[5/2]3d_{5/2}^4(2)$	9/2	7126.586
69	$1s3d_{3/2}^2(2)[3/2]3d_{5/2}^4(2)$	7/2	7126.618
70	$1s3d_{5/2}^2(2)$	5/2	7126.711
71	$1s3d_{3/2}^2(2)[3/2]3d_{5/2}^4(2)$	3/2	7126.729
72	$1s3d_{3/2}^2(2)[3/2]3d_{5/2}^4(2)$	1/2	7126.747
73	$1s3d_{3/2}^3[1]3d_{5/2}^3(9/2)$	7/2	7126.747
74	$1s3d_{3/2}^2(2)[5/2]3d_{5/2}^4(2)$	3/2	7126.749
75	$1s3d_{3/2}^3[2]3d_{5/2}^3(9/2)$	5/2	7126.784
76	$1s$	1/2	7127.211
77	$1s3d_{3/2}^3[2]3d_{5/2}^3(3/2)$	5/2	7127.559
78	$1s3d_{3/2}^3[1]3d_{5/2}^3(3/2)$	3/2	7127.576
79	$1s3d_{3/2}^3[2]3d_{5/2}^3(3/2)$	7/2	7128.324
80	$1s3d_{3/2}^3[1]3d_{5/2}^3(3/2)$	5/2	7128.348

Continued on next page

Table A.1. continued

Index	Configuration	J	Energy (eV)
81	$1s\ 3d_{5/2}^2(0)$	1/2	7129.261
82	$1s\ 3d_{5/2}^2(2)[5/2]\ 3d_{5/2}^4(0)$	5/2	7129.355
83	$1s\ 3d_{5/2}^3[2]\ 3d_{5/2}^3(5/2)$	7/2	7129.362
84	$1s\ 3d_{5/2}^2(0)[1/2]\ 3d_{5/2}^4(4)$	9/2	7129.362
85	$1s\ 3d_{5/2}^2(2)[3/2]\ 3d_{5/2}^4(0)$	3/2	7129.366
86	$1s\ 3d_{5/2}^3[1]\ 3d_{5/2}^3(5/2)$	3/2	7129.381
87	$1s\ 3d_{5/2}^3[1]\ 3d_{5/2}^3(5/2)$	5/2	7129.392
88	$1s\ 3d_{5/2}^3[2]\ 3d_{5/2}^3(5/2)$	1/2	7129.397
89	$1s\ 3d_{5/2}^2(0)[1/2]\ 3d_{5/2}^4(4)$	7/2	7129.405
90	$1s\ 3d_{5/2}^2(0)[1/2]\ 3d_{5/2}^4(2)$	5/2	7129.531
91	$1s\ 3d_{5/2}^2(0)[1/2]\ 3d_{5/2}^4(2)$	3/2	7129.562
92	$1s\ 3d_{5/2}^3[2]\ 3d_{5/2}^3(5/2)$	9/2	7130.217
93	$1s\ 3d_{5/2}^3[1]\ 3d_{5/2}^3(5/2)$	7/2	7130.247
94	$1s\ 3d_{5/2}^2(0)[1/2]\ 3d_{5/2}^4(2)$	5/2	7132.888
95	$1s\ 3d_{5/2}^2(0)[1/2]\ 3d_{5/2}^4(2)$	3/2	7132.906
96	$1s\ 3d_{5/2}^2(0)[1/2]\ 3d_{5/2}^4(0)$	1/2	7135.847