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Electron impact double ionization of Fe^{+} and Fe^{3+}

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Abstract. Electron impact double ionization cross-sections for Fe^{+} and Fe^{3+} have been calculated in the modified binary encounter model incorporating the effects of the Coulombic field of the target on the incident electron. Accurate expression of cross-section for energy transfer ΔE given by Vriens and Hartree-Fock velocity distributions for the target electrons have been used throughout the calculations. The present results show satisfactory agreement with experimental observations. It is concluded that the discrepancy in the high energy region observed in the present calculations may be attributed to non-inclusion of indirect ionization processes arising from the L-shell.

PACS. 34.80.Dp Atomic excitation and ionization by electron impact

1 Introduction

Electron impact ionization of ions is one of the fundamental atomic collision processes. It plays an important role in hot astrophysical plasmas and in controlled nuclear fusion research. Cross-sections of electron impact ionization are required for modelling structure and dynamics of all kinds of high temperature plasmas. In the case of nuclear fusion research, knowledge concerning the behaviour of impurities in the plasma is important. If neutrals or ions in low charge states are suddenly exposed to high electron temperature, multiple ionization processes strongly influence the charge state evolution. Knowledge of single and multiple ionization cross-sections for ions by electron impact finds wide applications in plasma kinematics problems, mass spectrometry, gas lasers, upper atmosphere physics and astrophysics. From an applied viewpoint multiple ionization processes are important in moderate and high temperature plasmas and in all gaseous environments with an abundance of energetic electrons [1]. Among different multiple ionization processes the double ionization is the most important and hence experimental and theoretical studies of these processes are considered to be valuable.

In the last decade experimental work on multiple ionization of ions by electron impact has received much attention. However, there are several difficulties in determination of ionization cross-sections in case of metals. Therefore, ionization cross-sections in such cases have been measured only by very few experimental groups and for a limited number of targets. Among different investigations an interesting work on experimental measurements of cross-sections for electron impact double ionization of Fe^{q+} ions in charge states $q = 1$–6 (except 2) has been carried out by Stenke et al. [2] using the crossed-beams technique. These measurements are important because iron is a major constituent of a fusion reactor chamber. To the best of our knowledge, no other experimental work is available in the literature for comparison with the above mentioned measurements. The experimental data of cross-sections for iron ions have been compared only with the results obtained by using the scaling laws of Fisher et al. [3] and semi-empirical formula published by Shevelko and Tawara [4] (see also Belenger et al. [5]). It has been seen that the calculated results do not show satisfactory agreement at all with the experimental data.

The theoretical description of electron impact multiple ionization of ions/atoms remains a relatively unexplored domain. Due to extreme complexities there have been no theoretical attempts to calculate triple and higher multiple ionization cross-sections. Electron impact integrated double ionization cross-sections of atoms and ions in the Born approximation have been reported for a few light targets e.g. H^{-}, He and Li^{+} (see Tweed [6,7] and McGuire [8]). Rigorous theoretical calculation of double ionization cross-sections becomes extremely difficult as it is related with consideration of four charged particles in the final channel interacting through the long range Coulomb potential [9]. Sophisticated calculations of the integrated double ionization cross-section of atoms and ions by electron impact are not available in literature. Due to this reason semi-empirical formulae and scaling laws

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have been developed for calculation of multiple ionization cross-sections. These formulae are deduced on the basis of experimental data on multiple ionization cross-sections σ_n of atoms and ions by electron impact and on the assumption of the Born-Bethe dependence of σ_n on the incident electron energy where n is the number of ejected electrons (see Stenke et al. [2]).

Theoretical studies of electron impact double ionization cross-sections are considered to be of much significance because contributions from different mechanisms e.g. simultaneous ejection of two electrons, inner shell ionization followed by autoionization, resonant excitation-autoionization etc. can be separately estimated at different impact energies. Gryzinski [10] reasonably considered the process of direct double ionization to be a two-step interaction and proposed a double binary encounter model to describe charged particle impact direct double ionization of atoms/ions. According to this model the double ionization may proceed via two processes. In the first process the two electrons may be ejected from the atom/ion by two successive interactions of the incident particle with the target electrons. Alternatively the incident particle may knock out only one atomic/ionic electron and the second electron is removed by the first ejected electron. The corresponding double ionization cross-sections are denoted by Q_{sc}^{ii} and Q_{ej}^{ii} respectively. Gryzinski made some unrealistic assumptions and unjustified approximations to obtain analytical expressions for double ionization cross-sections. Later on Vriens [11] detected errors in Gryzinski's work and obtained an accurate expression for $\sigma_{\Delta E}$ (cross-section for energy transfer ΔE) which is used frequently in calculations of single and double ionization cross-sections.

The simplifications and unrealistic features in Gryzinski's mathematical formulation have been discussed in detail by Roy and Rai [12]. However, the idea of the two binary encounter processes proposed by Gryzinski corresponds to the existence of the correlation between the electrons of atoms and to the finite probability of the second Born process (see Vriens [13]). Roy and Rai modified the mathematical framework of Gryzinski's theory of electron impact double ionization suitably incorporating the necessary corrections. Later on this modified model for calculation of direct double ionization cross-section was used in case of several atomic/ionic targets and encouraging results were obtained. In these calculations Hartree-Fock (HF) and hydrogenic velocity distributions were used while considering the ejection of the first and the second electron respectively.

Recently Jha and Roy [14] have calculated electron impact double ionization cross-sections for magnesium in the modified double binary encounter model and the results obtained show reasonably good agreement with experimental observations. Nearly at the same time using the above mentioned model Jha [15] has reported calculations of electron impact double ionization cross-sections for singly charged positive ions. In these calculations focusing action of the target ion on the incident electron has been incorporated along the line suggested by Thomas and Garcia [16]. The calculated results for the ions considered show satisfactory agreement with experimental data. In the above mentioned calculations for Mg and ionic targets, accurate expression for $\sigma_{\Delta E}$ and HF velocity distributions for the target electrons have been used throughout the calculations. Encouraged by the success achieved in previous calculations we considered it worthwhile to carry out calculations of electron impact double ionization cross-sections for Fe^+ and Fe^{3+} ions in the modified double binary encounter model in order to compare our results with the experimental data and to analyse the direct double ionization cross-sections involving ejection of electrons from different shells. The choice of the above mentioned ions for theoretical investigation has been made because structures in double ionization cross-section curves due to indirect ionization mechanisms have not been observed in these cases.

Here we would like to mention that consideration of correlation is desirable in calculation of direct double ionization cross-sections. In this context, it may be noted that calculation using correlated wave function would become very complicated particularly for heavier targets and the aim of adopting simplified binary encounter approach will not be achieved. Jha et al. [17] have discussed that the study of direct double ionization process in double binary encounter model using HF wave functions for target electrons partly takes into account the effect of correlation and hence such studies may be considered to be reasonable.

2 Method of calculation

The theoretical methods for calculating electron impact double ionization cross-sections of positive ions have been described by Jha [15]. Keeping in view the convenience for the reader we consider it worthwhile to discuss briefly the ideas and method of calculation used in the present work.

Thomas and Garcia [16] have modified the binary encounter model for ionization by charged particle impact to evaluate the cross-section for ionization of positive ions by electron impact. In vicinity of the positive ion, the Coulombic field has been considered to cause an increase in kinetic energy and decrease in impact parameter of the incident electron. It has been shown that the ionization cross-section incorporating the two effects can be obtained using the relation.

$$\sigma_I(E_1) = \sigma_I(E_1') \left[\frac{1}{2} + \frac{1}{2}\left(1 + Z'e^2/E_1\xi\right)^{1/2}\right]^2 . \qquad (1)$$

In the above expression the symbols E_1, $Z'e$ and $\sigma_I(E_1')$ denote incident energy, charge on the target ion and ionization cross-section at increased electron energy E_1' ($E_1' = E_1 + Z'e^2/\xi$). Here ξ is the collision radius whose value depends upon the ionic radius and the electron-electron separation.

In order to obtain direct double ionization cross-section at increased energy E_1' we have integrated the expression for Q_{sc}^{ii} and Q_{ej}^{ii} numerically over energy transfer and the HF momentum distribution for ejection of the two electrons and they take the form (see Jha [15])

$$Q^{ii}_{sc} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2}\int\limits_{t=0}^{\infty}\int\limits_{U_i}^{E_1'-U_{ii}} \sigma_{\Delta E} \times \left[\int\limits_{t=0}^{\infty}\int\limits_{U_{ii}}^{E_1'-\Delta E} \sigma_{\Delta E'} f(t) U_{ii}^{1/2} d(\Delta E')dt\right] \times f(t) U_i^{1/2} d(\Delta E)dt \times 8.797\times 10^{-17}(\pi a_0^2) \quad (2)$$

and

$$Q^{ii}_{ej} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2}\int\limits_{t=0}^{\infty}\int\limits_{U_i+U_{ii}}^{E_1'} \sigma_{\Delta E} \times \left[\int\limits_{t=0}^{\infty}\int\limits_{U_{ii}}^{\Delta E-U_i} \sigma_{\Delta E'} f(t) U_{ii}^{1/2} d(\Delta E')dt\right] \times f(t) U_i^{1/2} d(\Delta E)dt \times 8.797\times 10^{-17}(\pi a_0^2). \quad (3)$$

Using dimensionless variables s and t introduced by Catlow and McDowell [18] $\sigma_{\Delta E}$ is given by (see Jha [15])

$$\sigma_{\Delta E} = \frac{2}{(s^2+t^2+1)u}\left[\left(\frac{1}{\Delta E^2}+\frac{4t^2u}{3\Delta E^3}\right) + \left(\frac{1}{(s^2u+u-\Delta E)^2}+\frac{4t^2u}{3(s^2u+u-\Delta E)^3}\right) - \frac{\phi}{\Delta E(s^2u+u-\Delta E)}\right] \quad (4)$$

where $\phi = \cos\{(s^2u+u)^{-1/2}\ln s^2\}$.

In terms of the above mentioned variables the factor connecting the cross-sections at incident and increased electron energies becomes $(s+s')^2/4s^2$, s and s' corresponding to E_1 and E_1' respectively. To obtain the values of Q^{ii}_{sc} and Q^{ii}_{ej} at incident energy E_1 the expression corresponding to increased energy E_1' should be multiplied by the above mentioned factor (see Jha [15]). Due to indistinguishability of electrons in the symmetrical model of Vriens [11], Q^{ii}_{sc} and Q^{ii}_{ej} are exactly equal at all incident energies (see Kumar and Roy [19]) and hence in order to obtain double ionization cross-section either of the cross-sections should be multiplied by two. In equation (2) u and s^2 have been replaced by U_i and E_1'/U_i in the expression for $\sigma_{\Delta E}$. In case of $\sigma_{\Delta E'}$ the corresponding replacements have been made by U_{ii} and $(E_1'-\Delta E)/U_{ii}$.

The momentum distribution function $f(t)$ appearing in equations (2, 3) is given by (see Catlow and Mc Dowell [18])

$$f(t) = 4\pi t^2 u \rho_{nl}(tu^{1/2}). \quad (5)$$

Here $\rho_{nl} = (2l+1)^{-1}\sum\limits_{m=-l}^{m=+l}|\psi_{nlm}(\mathbf{x})|^2$ where $\psi_{nlm}(\mathbf{x}) = (2\pi)^{-3/2}\int \phi_{nlm}(\mathbf{r})e^{i\mathbf{x}\cdot\mathbf{r}}d\mathbf{r}$ is the Fourier transform of the one electron orbital $\phi_{nlm}(\mathbf{r}) = N_{nl}R_{nl}(r)Y_{lm}(\Omega)$ in which $R_{nl}(r)$ is the Hartree-Fock radial function. $f(t)$ has been constructed replacing u by U_i and U_{ii} for the ejection of the first and the second electron respectively.

We have considered total cross-section for electron impact direct double ionization as given by

$$Q^{ii}_D = Q^{ii}_D(4s,\,3d) + Q^{ii}_D(4s,\,3p) + Q^{ii}_D(4s,\,3s) \quad (6)$$

and

$$Q^{ii}_D = Q^{ii}_D(3d,\,3d) + Q^{ii}_D(3d,\,3p) + Q^{ii}_D(3d,\,3s) \quad (7)$$

for Fe^{+} and Fe^{3+} respectively. Here $Q^{ii}_D(4s,\,3p)$ denotes the double ionization cross-section corresponding to one electron ejected from the $4s$ shell and the other from the $3p$ shell. The factor $n_e(n_e-1)/4\pi\bar{r}^2$ has been suitably modified for considering the modes of ionization in which electrons are ejected from different shells. $n_e(n_e-1)$ has been replaced by $n_e1 \times n_e2$ where these two stand for the number of electrons in shells under consideration. We have used the binding energies of the shells of ions as given by Clementi and Roetti [20]. The ionic radii reported by Fraga et al. [21] have been used in the present calculations. The momentum distribution function has been calculated using Hartree-Fock radial wave functions given by Clementi and Roetti [20].

3 Results and discussion

Experimental measurements of electron impact double ionization cross-sections for Fe^{+} and Fe^{3+} have been carried out in the energy regions from the respective thresholds to 900 eV. First of all we would like to discuss the degree of agreement of the results calculated using scaling laws of Fisher et al. [3] and semi-empirical formula of Shevelko and Tawara [4] with the experimental data. In case of Fe^{+} both the calculations underestimate the cross-sections beyond 100 eV impact energy. At 900 eV (the highest energy considered) the calculations using the semi-empirical formula of Belenger et al. [5] and the scaling laws of Fisher et al. underestimate the cross-sections by about 40% and 45% respectively. The agreement of the calculations with the experimental data is much worse in case of Fe^{3+}. The calculation using the semi-empirical formula of Belenger et al. severely underestimates the cross-sections at all impact energies and the cross-section curve is almost flat in the region of maximum cross-section. The results obtained by scaling law underestimate the cross-sections at low impact energies but they show overestimation beyond 200 eV. The overestimation becomes much pronounced in the energy region 500–900 eV and the calculated cross-sections are found to differ from the experimental data by a factor more than 2 and at 900 eV the factor becomes 2.7. The position of the calculated peak is found to be shifted by about 200 eV on the higher energy side as compared to its experimental counterpart. A discussion on the present investigation for Fe^{+} and Fe^{3+} is given below.

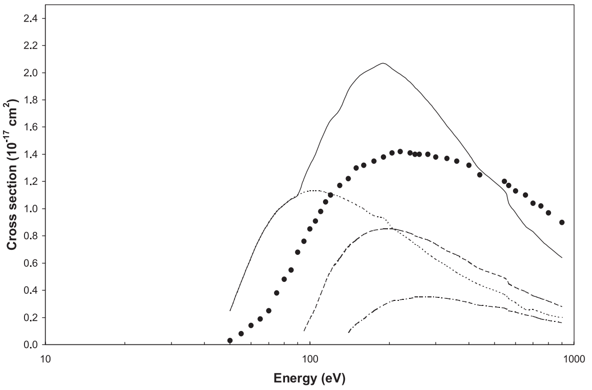

Fig. 1. Electron impact double ionization cross-sections of Fe$^+$: (----) contributions of $(4s, 3d)$; (– – –) contributions of $(4s, 3p)$; (–·–) contributions of $(4s, 3s)$; (——) total; (●●●) experimental data [2].

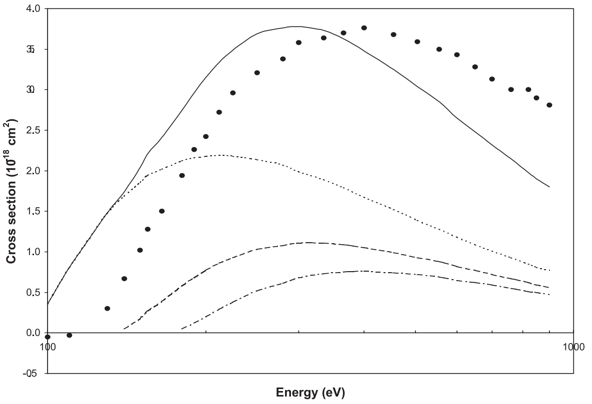

Fig. 2. Electron impact double ionization cross-sections of Fe^{3+}: (----) contributions of $(4s, 3d)$; (– – –) contributions of $(4s, 3p)$; (–·–) contributions of $(4s, 3s)$; (——) total; (●●●) experimental data [2].

Our results of double ionization cross-sections along with the experimental data obtained by Stenke et al. [2] have been presented in Figures 1, 2 and Tables 1, 2. The contributions to direct double ionization of Fe$^+$ from ejection of $(4s, 3d)$, $(4s, 3p)$, and $(4s, 3s)$ electrons have been shown separately in Figure 1 and Table 1. Similarly Figure 2 and Table 2 for Fe^{3+} contain separate contributions from ejection of $(3d, 3d)$, $(3d, 3p)$ and $(3d, 3s)$ electrons. We have not presented the calculated cross-sections using scaling laws and semi-empirical formula, as they do not show satisfactory agreement at all with the experimental data. We have carried out calculations of double ionization cross-section from the ground state configurations $3s^2 3p^6 3d^6 4s$ and $3s^2 3p^6 3d^5$ for Fe$^+$ and Fe^{3+} respectively.

The calculated results for Fe$^+$ overestimate the double ionization cross-sections at low impact energies but at 85 eV the theoretical result becomes within a factor of 2 of the experimental value. Beyond this energy our results show closer agreement with experiment and the calculated results are found to be within a factor of 1.5 of the experimental values in the energy region 115–200 eV. At still higher energies the calculated results are found to be closer and closer to experimental values and at 440 eV they are almost identical. Beyond this energy value the experimental cross-sections become larger than the calculated ones but they remain within a factor of 1.25 up to 600 eV. At still higher energies the ratio of experimental to theoretical cross-sections increases with increase in energy and becomes 1.4 at 900 eV. It is seen that the present calculation underestimates the cross-section by 29% at the highest energy considered. Stenke et al. have observed a peak of magnitude 1.42×10^{-17} cm^2 at about 220 eV impact energy whereas a peak of magnitude 2.07×10^{-17} cm^2 at 190 eV is obtained in the present calculation. Thus the position of the theoretical cross-section maximum is shifted by about 30 eV on low energy side. In the region of maximum experimental cross-section the theoretical result is found to be 1.4 times larger than the observed value and can be considered to be satisfactory.

The theoretical results of double ionization cross-section for Fe^{3+} also are found to overestimate the cross-sections at low impact energies. However, the calculated cross-section becomes within a factor of 2 of the experimental result at 150 eV impact energy and beyond this energy the experimental and theoretical cross-sections become closer rapidly. It is seen that at impact energies 180 and 212 eV the theoretical cross-sections are within a factor of 1.5 and 1.25 of the experimental data. This trend continues at still higher energies and the theoretical cross-sections become closer and closer to experimental data till they become almost identical at 335 eV. Beyond this energy the experimental cross-sections become larger and larger than theoretical values with increase in energy. The theoretical cross-sections differ from experimental data within a factor of 1.25 up to 555 eV impact energy. Finally the experimental cross-section is found to be 1.56 times larger than the calculated value at 900 eV. It is seen that the present calculations underestimate the cross-section by 35.3% at the highest energy considered. In the experimental investigation cross-section maximum of magnitude 3.76×10^{-18} cm^2 is observed at 400 eV impact energy whereas the theoretical calculation predicts a peak of magnitude 3.78×10^{-18} cm^2 at 300 eV. Thus the magnitude of the calculated peak is almost identical to that found in experiment, but its position is shifted by about 100 eV towards low energy side. In the region of maximum experimental cross-section the theoretical result is found to be about 92% of the observed value showing good agreement with experiment.

Now we would like to discuss the common features of the calculated double ionization cross-sections of Fe$^+$ and Fe^{3+}. It is found that the theoretical results overestimate the cross-sections at low impact energies. In this context, it may be noted that overestimation at low energies is a usual feature of calculations of ionization cross-sections in the BEA. The shift in position of the calculated peaks towards low energy side may be attributed to overestimation of cross-sections at low impact energies. The magnitudes of the cross-sections in general (above 85 eV for Fe$^+$ and 150 eV for Fe^{3+}) show a satisfactory agreement with experimental data but there is some

Table 1. Electron impact double ionization cross-sections of Fe^+in units of 10^{-17} cm^2.

Energy (eV)	Contributions of $(4s, 3d)$	Contributions of $(4s, 3p)$	Contributions of $(4s, 3s)$	Total	Experiment [2]
50	0.25			0.25	0.03
55	0.46			0.46	0.08
60	0.64			0.64	0.14
65	0.79			0.79	0.19
70	0.90			0.90	0.25
75	0.98			0.98	0.38
80	1.03			1.03	0.48
85	1.07			1.07	0.55
90	1.10			1.10	0.68
95	1.12	0.10		1.22	0.76
100	1.13	0.19		1.32	0.85
105	1.13	0.27		1.40	0.91
110	1.13	0.37		1.50	0.98
115	1.12	0.46		1.58	1.05
120	1.11	0.54		1.65	1.10
130	1.09	0.64		1.73	1.17
140	1.06	0.72	0.09	1.87	1.22
150	1.03	0.77	0.15	1.95	1.30
160	1.00	0.81	0.19	2.00	1.32
175	0.95	0.84	0.25	2.04	1.35
190	0.93	0.85	0.29	2.07	1.38
205	0.86	0.85	0.32	2.03	1.41
220	0.82	0.84	0.33	1.99	1.42
240	0.77	0.82	0.34	1.93	1.41
250	0.74	0.80	0.35	1.89	1.40
260	0.72	0.79	0.35	1.86	1.40
280	0.67	0.77	0.35	1.79	1.40
300	0.63	0.74	0.35	1.72	1.38
330	0.58	0.69	0.34	1.61	1.37
360	0.53	0.66	0.33	1.52	1.35
400	0.48	0.61	0.31	1.40	1.32
440	0.44	0.56	0.29	1.29	1.25
545	0.37	0.49	0.27	1.13	1.20
565	0.34	0.45	0.25	1.04	1.17
600	0.31	0.42	0.24	0.97	1.13
655	0.26	0.39	0.22	0.87	1.10
700	0.26	0.36	0.21	0.83	1.04
750	0.24	0.34	0.19	0.77	1.02
800	0.22	0.32	0.18	0.72	0.97
900	0.20	0.28	0.16	0.64	0.90

discrepancy in the high energy region where the calculated cross-sections are found to be smaller and smaller as compared to experiment with increase in energy. This discrepancy reflects the possibility of some other physical processes contributing to double ionization. Structures in experimental double ionization cross-section curves of Fe^{4+}, Fe^{5+}, Fe^{6+} in high energy region have been attributed to indirect ionization processes arising from inner shells (see Stenke et al. [2]). However, there are no clear indications of structures in the double ionization cross-section curves for Fe^+ and Fe^{3+} but the decrease in experimental cross-section is rather slow in the energy region 220–900 eV for Fe^+ and 400–900 eV for Fe^{3+}. Experimental data of Fe^+ and Fe^{3+} at 900 eV show decrease of about 37% and 25% respectively as compared to maximum cross-sections. This is not in accordance with the usual trend of direct double ionization cross-sections which show a faster decrease in high energy region after attaining the maximum value.

In case of double ionization of Fe^{4+}, Fe^{5+} and Fe^{6+} ions a second rise of cross-section is experimentally observed which is correlated to inner shell effects (excitation

Table 2. Electron impact double ionization cross-sections of Fe^{3+}in units of 10^{-18} cm^2.

Energy (eV)	Contributions of $(3d, 3d)$	Contributions of $(3d, 3p)$	Contributions of $(3d, 3s)$	Total	Experiment [2]
100	0.36			0.36	−0.05
110	0.81			0.81	−0.03
130	1.48			1.48	0.30
140	1.69	0.05		1.74	0.67
150	1.86	0.18		2.04	1.02
155	1.94	0.27		2.21	1.28
165	2.02	0.39		2.41	1.50
180	2.12	0.58	0.05	2.75	1.94
190	2.16	0.68	0.12	2.96	2.26
200	2.18	0.77	0.20	3.15	2.42
212	2.19	0.86	0.29	3.34	2.72
225	2.18	0.93	0.38	3.49	2.96
250	2.14	1.03	0.52	3.69	3.21
280	2.07	1.08	0.61	3.76	3.38
300	1.99	1.11	0.68	3.78	3.58
335	1.89	1.11	0.73	3.73	3.64
365	1.79	1.09	0.75	3.63	3.70
400	1.67	1.05	0.76	3.48	3.76
455	1.52	0.99	0.74	3.25	3.68
505	1.39	0.93	0.72	3.04	3.59
555	1.28	0.88	0.69	2.85	3.50
600	1.18	0.82	0.65	2.65	3.43
650	1.09	0.77	0.62	2.48	3.28
700	1.01	0.72	0.59	2.32	3.13
760	0.93	0.67	0.55	2.15	3.00
820	0.85	0.62	0.51	1.98	3.00
850	0.81	0.59	0.50	1.90	2.90
900	0.77	0.56	0.47	1.80	2.81

double autoionization) and becomes stronger with increasing charge state. Besides contributions from excitation double autoionization processes, a remarkable number of structures arising from resonant excitation – triple – autoionization are observed [2]. Employing the multiconfigurational Dirac-Fock code of Grant et al. [22], Stenke et al. [2] have calculated and presented the ionization thresholds of inner shell electrons and excitation energies of some configurations relative to $3s^2 3p^6 3d^4$, $3s^2 3p^6 3d^3$ and $3s^2 3p^6 3d^2$ ground state configurations of Fe^{4+}, Fe^{5+} and Fe^{6+} ions respectively. With the help of these results they have attempted to identify the observed structures in case of the above mentioned ions. However, they have not presented such calculations for Fe^+ and Fe^{3+}. The above mentioned discussion prompts us to think about the possibility of indirect ionization processes arising from the L-shell with moderate contribution to double ionization of Fe^+ and Fe^{3+} at high impact energies. Thus, it is expected that inclusion of the contributions of inner shell effects would improve the theoretical results at high energies leading to better agreement with experiment. Unfortunately it is not possible to calculate excitation-autoionization cross-section in the BEA. However, our calculations show significant improvement over the results obtained by using the scaling law of Fisher et al. and semi-empirical formula of Shevelko and Tawara [4]. It is found that the present theoretical study gives a reasonable prediction of the experimental data, position and height of the maximum cross-section as well as the shape of the cross-section. It is expected that this work would stimulate other theoretical workers to take up further study of the problem.

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References

1. H. Deutsch, K. Becker, T.D. Mark, J. Phys. B: At. Mol. Opt. Phys. **29**, L497 (1996)
2. M. Stenke, U. Hartenfeller, K. Aichele, D. Hathiramani, M. Steidl, E. Salzborn, J. Phys. B: At. Mol. Opt. Phys. **32**, 3641 (1999)
3. V. Fisher, Yu. Ralchenko, A. Goldgirsh, D. Fisher, Y. Maron, J. Phys. B: At. Mol. Opt. Phys. **28**, 3027 (1995)
4. V.P. Shevelko, H. Tawara, Semi-empirical formulae for multiple ionization cross-sections of atoms and ions by electron impact, *11th Coll. on UV and X-ray Spectroscopy of Astrophysical and Laboratory Plasmas* (Nagoya) Abstracts, p. 109 (1995)

5. C. Belenger, P. Defrance, E. Salzborn, V.P. Shevelko, H. Tawara, D.B. Uskov, J. Phys. B: At. Mol. Opt. Phys. **30**, 2667 (1997)
6. R.J. Tweed, J. Phys. B **5**, 256 (1973)
7. R.J. Tweed, J. Phys. B **6**, 270 (1973)
8. J.H. McGuire, Phys. Rev. Lett. **49**, 1153 (1982)
9. J. Berakdar, Phys. Lett. A **220**, 237 (1996)
10. M. Gryzinski, Phys. Rev. A **138**, 336 (1965)
11. L. Vriens, Proc. Phys. Soc. **89**, 13 (1966)
12. B.N Roy, D.K. Rai, J. Phys. B: At. Mol. Phys. **6**, 816 (1973)
13. L. Vriens, *Case studies in atomic collision physics* (North Holland Publishing Company, Amsterdam, 1969), Vol. 1, p. 358
14. L.K. Jha, B.N. Roy, Eur. Phys. J. D **20**, 5 (2002)
15. L.K. Jha, Phys. Scripta, **66**, 228 (2002)
16. B.K. Thomas, J.D. Garcia, Phys. Rev. **179**, 94 (1969)
17. L.K. Jha, S.N. Chatterjee, B.N. Roy, Pramana J. Phys. **43**, 169 (1994)
18. G. Catlow, M.R.C. Mc Dowell, Proc. Phys. Soc. **92**, 875 (1967)
19. A. Kumar, B.N. Roy, Can. J. Phys. **56**, 1255 (1978)
20. E. Clementi, C. Roetti, At. Data Nucl. Data Tables **14**, 237 (1974)
21. S. Fraga, J. Karwowski, K.M.S Saxena, *Handbook of Atomic Data* (Elsevier, Amsterdam, 1976), pp. 465–473
22. P.M. Grant, B.J. Kenzie, P.H. Norrington, D.F. Mayers, N.C. Pyper, Comput. Phys. Commun. **21**, 207 (1980)