EFFECT OF *L*- AND *M*-SHELL IONIZATION ON THE *K* X-RAY SPECTRA PARAMETERS OF SULPHUR*

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(Received November 11, 1999)

Extensive single-configuration Dirac–Fock (DF) calculations (within the multiconfiguration DF method) have been performed for sulphur to explain the influence of removing electrons from L and M shells on the average $K\beta$ and $K\alpha$ x-ray transition energies and the values of $K\beta/K\alpha$ intensity ratio. Our results can be used for interpreting the measured K X-ray spectra accompanying the ionization of sulphur projectiles or sulphur targets.

PACS numbers: 32.30.Rj, 31.15.Ar, 32.70.Fw, 32.70.Jz

1. Introduction

It is well known that the bombardment of targets by fast moving ions leads to the emission of X-rays, which characterise both the projectile and the target. In the case of the heavy-ion-induced X-ray spectra of targets atoms, the multiple ionization of the M and L shells is extremely likely to occur [1, 2]. Also in the case of the X-ray emission from the projectiles passing through different foils the multiple ionization of projectiles have been reported [3–6]. In recent years, several theoretical models [2, 7, 8] for reliable description of very complex X-ray spectra accompanying the ionization of targets [1, 2] and projectiles [6] in collision processes based on the multiconfiguration Dirac–Fock (MCDF) method have been developed and applied.

2. Theoretical calculations

The methodology of our single-configuration Dirac–Fock (DF) calculations performed within the MCDF method [9, 10] is similar to the one published earlier, in which the systematic study on the simultaneous L- and

* Presented at the XXVI Mazurian Lakes School of Physics, Krzyże, Poland September 1–11, 1999.

M-shell ionization of ^{80}Se target bombarded by various projectiles has been performed [2]. The Hamiltonian for the N-electron atom is taken in the form

$$H = \sum_{i=1}^{N} h_{\mathrm{D}}(i) + \sum_{j>i=1}^{N} C_{ij} \tag{1}$$

where $h_{\mathrm{D}}(i)$ is the Dirac operator for i-th electron and the terms C_{ij} account for electron-electron interactions and come from one-photon exchange process. The latter are a sum of the Coulomb interaction operator and the transverse Breit operator. The atomic state functions with the total angular momentum J and parity p are represented in the multiconfigurational form

$$\Psi_s(J^p) = \sum_m c_m(s)\Phi(\gamma_m J^p), \tag{2}$$

where $\Phi(\gamma_m J^p)$ are configuration state functions (CSF's), $c_m(s)$ are the configuration mixing coefficients for state s, γ_m represents all information required to uniquely define a certain CSF. In the present calculations the energy functional is averaged over all the initial and final states and its form is identical with one published earlier [8].

3. Results and discussion

In order to explain the influence of removing electrons from L and M shells on the average $K\beta$ and $K\alpha$ X-ray transition energies and values of $K\beta/K\alpha$ intensity ratios extensive single-configuration DF calculations have been performed for sulphur within the MCDF method (including the transverse Breit interaction and QED corrections [10]). The results of our calculations for various electronic configurations of sulphur ions are presented in Table I. Performed calculations are of a large scale because there exist dozens or hundreds of initial and final levels corresponding to a certain electronic configuration. Between these levels hundreds or thousands of transitions (see numbers of transitions in the second column of Table I) are possible. For the clarity of the disscusion we have decided to present only a little part of the results of our studies.

It can be seen from Table I that the ionization of the $2p$ subshell causes drastic increase of $K\beta/K\alpha$ intensity ratio (what is natural because $2p$ electrons are directly responsible for the $K\alpha$ transitions) and the largest increase of the average $K\beta$ and $K\alpha$ transition energies. The removal of an electron from $2s$ subshell causes significant increase of the $K\beta/K\alpha$ intensity ratio, strong increase of $K\alpha$ transition energy and very strong (but a bit less than in $2p$ case) increase of $K\beta$ transition energy. The increase of the $K\beta/K\alpha$ intensity ratio is also observed in the case of removing electrons from $3s$

TABLE I

Effect of removing electrons from various subshells on the average $K\beta$ and $K\alpha$ transition energies (in eV) and the values of $K\beta/K\alpha$ intensity ratio for sulphur. The electronic ground state configuration of neutral sulphur atom is $1s^2 2s^2 2p^6 3s^2 3p^4$.

Initial hole configuration	Number of transitions	$K\beta$ energy shift	$K\alpha$ energy shift	$K\beta/K\alpha$ intensity ratio
$1s^{-1}$	164	0.0	0.0	0.0658
$1s^{-1}2s^{-1}$	575	31.7	12.2	0.0833
$1s^{-1}2s^{-2}$	164	64.9	25.5	0.0988
$1s^{-1}2p^{-1}$	2123	38.2	13.6	0.0924
$1s^{-1}2p^{-2}$	7636	77.9	29.0	0.1224
$1s^{-1}2p^{-3}$	10102	121.6	45.8	0.2293
$1s^{-1}2p^{-4}$	5163	166.3	64.7	0.3512
$1s^{-1}2p^{-5}$	907	213.9	84.9	0.7390
$1s^{-1}3s^{-1}$	575	5.1	0.3	0.0747
$1s^{-1}3s^{-2}$	164	11.0	0.8	0.0839
$1s^{-1}3p^{-1}$	239	3.7	0.5	0.0563
$1s^{-1}3p^{-2}$	143	8.5	1.3	0.0431
$1s^{-1}3p^{-3}$	32	14.6	2.3	0.0253
$1s^{-1}2s^{-2}2p^{-5}$	907	293.5	120.8	0.8659
$1s^{-1}3s^{-2}3p^{-3}$	32	30.4	4.8	0.0300
$1s^{-1}2s^{-2}2p^{-5}3s^{-2}3p^{-3}$	60	358.7	144.0	0.2019

subshell. The $K\beta$ transition energy increases slightly by the ionization of $3s$ subshell. The $K\alpha$ transition energy is almost not changed by the ionization of $3s$ subshell — the increase of this energy is 40 times smaller than in the case of $2s$ subshell. The ionization of the $3p$ subshell causes a dramatic decrease of $K\beta/K\alpha$ intensity ratio, what is natural because $3p$ electrons are directly responsible for the $K\beta$ transitions. The removal of an electron from $3p$ subshell causes the smallest shift of $K\beta$ energy (one order smaller than in $2p$ case). The $K\alpha$ energy is very slightly increased by the ionization of $3p$ subshell (28 times less than in the case of $2p$ subshell).

Generally, the ionization of each sulphur subshell, besides $3p$ subshell, causes the increase of the $K\beta/K\alpha$ intensity ratio (see Table I). This ratio is influenced, first of all, by the ratio of the number of electrons in $3p$ and $2p$ subshells, and, secondly, by ionization degree of $2s$ and $3s$ subshells. Moreover, the ionization of each sulphur subshell causes the increase of $K\beta$ and $K\alpha$ transition energies. However, the very large shifts of $K\beta$ and $K\alpha$ energies are only in the case of the ionization of the $2p$ and $2s$ subshells.

It is very important to note (see Table I) that the effects of removal of electrons from the subshells on the $K\beta$ and $K\alpha$ transition energies and values of the $K\beta/K\alpha$ intensity ratio are strongly nonadditive. Especially, the $K\beta$ and $K\alpha$ transition energies increase much faster than lineary with the number of holes in a given subshell. Moreover, in the case of projectiles passing through various foils [3–6] (and also in the case of targets bombarded by fast heavy ions [1, 2]) the ionization of K shell is always accompanied by simultaneous multiple ionization of L and M shells. It can be seen from the last three rows of Table I that the effects of removal of electrons from L and M shells on the K X-ray spectra parameters are also strongly nonadditive. Therefore to apply our results for theoretical interpretation of experimental K X-ray spectra of sulphur it is neccessary to perform more detailed single-configuration DF calculations (than presented in Table I) which take into account the simultaneous multiple ionization of L and M shells.

Very good example of the application of these studies is our complementary paper [11], in which (see Table II of that paper) we present the results of very detailed single-configuration DF calculations performed within the MCDF method for electronic configurations corresponding to various distributions of holes in $2s$, $2p$, $3s$, and $3p$ subshells and used for interpreting the experimental parameters of the K X-ray spectra of highly ionized swift sulphur projectiles passing through carbon foils at different incident energies. The presented studies can also be helpful in interpreting various sulphur target K X-ray spectra bombarded by different light and heavy projectiles.

This work was supported by the Polish Committee for Scientific Research (KBN), Grant No. 2 P03B 019 16.

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