INTERPRETATION OF $\boldsymbol{K}$ X-RAY SPECTRA FROM HIGHLY IONIZED SULPHUR PROJECTILES PASSING THROUGH THIN CARBON FOILS*

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(Received November 8, 1999)

The $K\alpha$ and $K\beta$ energy shifts and $K\beta/K\alpha$ intensity ratios of highly ionized sulphur projectiles passing through carbon foils have been measured. Comparing these data with the results of single-configuration Dirac-Fock calculations it has been found that the average number of holes in the L shell of sulphur projectile strongly increases with its energy.

PACS numbers: 32.30.Rj, 32.70.Fw, 32.70.Jz, 34.50.Fa

1. Introduction

During ion-atom collisions in solids the heavy ion-projectile suffers successive collisions with target atoms, whereas a target atom interacts only once with a projectile. In the first collision with a small impact parameter one K hole and multiple L holes can be produced in the projectile. After that the projectile can collide with other target atoms with larger impact parameter before its original K-hole is filled by outer electrons. The competition between ionization, excitation, capture, losses and decay processes quickly leads to an equilibrium distribution of excited states in the moving projectile. Experimentally observed K X-ray spectra emitted from the projectiles

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

passing through solid targets reflect all these processes, which depend on the kind of the projectile, its energy, and on the kind of target atoms. Most of systematic experimental works have been reported on measurements of K or (and) L X-ray spectra from various projectiles in different solid targets [1–5]. In this paper we present the interpretation of K X-ray spectra parameters of highly ionized sulphur projectiles passing through thin carbon foils, basing on the results of detailed single-configuration Dirac-Fock (DF) calculations of the similar kind as published earlier [6]. For the methodological details see our complementary paper [7].

2. Experiment and data analysis procedure

Sulphur ion beams (of 9.6–38.4 MeV energy) obtained from the tandem accelerator at the Institute of Physics of the Erlangen-Nürnberg University were used to bombard carbon foils of two thicknesses (16.5 and 30 μg cm^{-2}). The experimental set-up used in present experiment was the same as that described earlier [8]. The measured X-ray spectra were analysed by means of a least-squares-fitting program employing Gaussian form of X-ray peak. In this way integrated intensities, transition energies and width (FWHM) of the peaks for all the transitions were obtained. Measured energies of $K\alpha$ and $K\beta$ lines were compared to diagram energy for a single ionized atom [9] and finally the energy shifts of $K\alpha$ and $K\beta$ lines were determined.

3. Results and discussion

The measured values of $K\beta$ and $K\alpha$ energy shifts and $K\beta/K\alpha$ intensity ratios, of highly ionized sulphur projectiles passing through carbon foils of two thicknesses are presented in Table I. As can be seen from this table the $K\alpha$ and $K\beta$ energy shifts are significant and generally increase with increasing beam energy (however, in the case of carbon foil of 16.5 μg cm^{-2} thickness the $K\beta$ energy shift increase is not monotonical). This indicates that the ionization of L and M shells of sulphur projectiles (at the time of emission of the K X-ray spectra) increases with the increase of their incident energy, what is confirmed by the increase of average equilibrium charge state of projectiles with the increase of their incident energy (see the second column of Table I).

As has been shown in the complementary paper [7] to interpret our experimental K X-ray spectra parameters of sulphur it is neccessary to perform theoretical calculations which take into account the simultaneous multiple ionization of L and M shells. The results of our very detailed single-configuration DF calculations for electronic configurations corresponding to various distributions of holes in $2s$, $2p$, $3s$, and $3p$ subshells of sulphur are

TABLE I

The parameters of K X-ray spectra from highly ionized sulphur projectiles passing through thin carbon foils (at different incident energies). For a given projectile energy the upper values correspond to 16.5 μg cm^{-2} thickness of carbon foil, while the lower values to 30 μg cm^{-2} thickness. The theoretical value of $K\beta/K\alpha$ ratio for singly ionized sulphur atom is 0.0658 (see our complementary paper [7]).

Projectile energy (MeV)	Average equilibrium charge state [10]	$K\beta$ energy shift (eV)	$K\alpha$ energy shift (eV)	$K\beta/K\alpha$ intensity ratio
9.6	7.8 ± 0.1	175.5 ± 22.3	45.4 ± 9.1	0.0349 ± 0.0149
		175.3 ± 14.7	45.0 ± 8.9	0.0595 ± 0.0068
16.0	9.1 ± 0.1	240.4 ± 11.0	64.1 ± 8.4	0.0266 ± 0.0015
		228.8 ± 13.1	60.9 ± 8.5	0.0295 ± 0.0008
22.4	9.9 ± 0.1	251.9 ± 10.4	75.8 ± 8.5	0.0374 ± 0.0010
		232.7 ± 10.2	71.4 ± 8.4	0.0366 ± 0.0008
32.0	10.8 ± 0.1	226.6 ± 11.5	82.4 ± 8.4	0.0758 ± 0.0024
		251.7 ± 10.9	87.8 ± 8.3	0.0574 ± 0.0012
38.4	11.3 ± 0.1	292.2 ± 13.5	100.3 ± 8.7	0.0716 ± 0.0025
		298.0 ± 11.0	101.9 ± 8.5	0.0771 ± 0.0016

presented in Table II. From the comparison of these results with the experimental parameters of the measured K X-ray sulphur spectra (Table I) it is possible to estimate the average number of holes in M shell (accompaning the L-shell holes). It seems that only those configurations of sulphur in which the average number of M-shell holes is between 4–5 can play an important role in the measured K X-ray spectra. This average number of M-shell holes slightly increases with the sulphur projectile energy.

It is very important to note that the $K\alpha$ energy shift strongly depends on the ionization of $2p$ and $2s$ subshells while the influence of removal of one electron from $3p$ subshell on the $K\alpha$ shift is 28 times smaller than from $2p$ subshell and the influence of removal of one electron from $3s$ subshell is 40 times smaller than from $2s$ subshell. However, in the case of the $K\beta$ energy shift and $K\beta/K\alpha$ intensity ratio there is not so large difference between the effects of L- and M-shell ionization (see [7]). Therefore, to reliably determine the average number of holes in L shell of sulphur projectile for its given incident energy (at the presence of approximately 4–5 holes in M shell) we decided to base not on all three paremetrs of the measured K X-ray sulphur spectra but only on the $K\alpha$ energy shift.

To determine the average number of holes in L shell of sulphur (for given incident energy) one must subtract the influence of multiple M-shell

TABLE II

Shifts of average $K\beta$ and $K\alpha$ transition energies (in eV) and the values of $K\beta/K\alpha$ X-ray intensity ratios for different sulphur ions with various electronic configurations. The electronic ground state configuration of neutral sulphur atom is $1s^2 2s^2 2p^6 3s^2 3p^4$.

Charge state	Initial hole configuration	$K\beta$ energy shift	$K\alpha$ energy shift	$K\beta/K\alpha$ intensity ratio
8+	$1s^{-1}2s^{-2}3s^{-2}3p^{-3}$	103.8	34.0	0.0374
	$1s^{-1}2s^{-1}2p^{-1}3s^{-2}3p^{-3}$	110.1	35.8	0.0434
	$1s^{-1}2p^{-2}3s^{-2}3p^{-3}$	117.3	38.0	0.0514
	$1s^{-1}2p^{-3}3s^{-1}3p^{-3}$	154.0	54.6	0.0679
	$1s^{-1}2s^{-2}3s^{-2}3p^{-4}4p^{1}$	170.9	36.2	0.0136
	$1s^{-1}2s^{-1}2p^{-1}3s^{-2}3p^{-4}4p^{1}$	177.5	38.0	0.0159
	$1s^{-1}2p^{-2}3s^{-2}3p^{-4}4p^{1}$	185.4	40.2	0.0191
9+	$1s^{-1}2s^{-2}2p^{-1}3s^{-2}3p^{-3}$	148.9	52.1	0.0469
	$1s^{-1}2s^{-1}2p^{-2}3s^{-2}3p^{-3}$	156.3	54.4	0.0566
	$1s^{-1}2p^{-3}3s^{-2}3p^{-3}$	164.5	57.1	0.0719
	$1s^{-1}2p^{-4}3s^{-1}3p^{-3}$	202.9	75.0	0.1046
	$1s^{-1}2s^{-2}2p^{-1}3s^{-2}3p^{-4}4p^{1}$	228.1	54.6	0.0175
	$1s^{-1}2s^{-1}2p^{-2}3s^{-2}3p^{-4}4p^{1}$	236.1	56.9	0.0213
	$1s^{-1}2p^{-3}3s^{-2}3p^{-4}4p^{1}$	244.9	59.7	0.0274
10+	$1s^{-1}2s^{-2}2p^{-2}3s^{-2}3p^{-3}$	196.5	71.8	0.0603
	$1s^{-1}2s^{-1}2p^{-3}3s^{-2}3p^{-3}$	205.0	74.6	0.0777
	$1s^{-1}2p^{-4}3s^{-2}3p^{-3}$	214.2	77.9	0.1094
	$1s^{-1}2s^{-2}2p^{-2}3s^{-2}3p^{-4}4p^{1}$	288.6	74.6	0.0231
	$1s^{-1}2s^{-1}2p^{-3}3s^{-2}3p^{-4}4p^{1}$	297.7	77.5	0.0300
	$1s^{-1}2p^{-4}3s^{-2}3p^{-4}4p^{1}$	307.4	80.8	0.0430
11+	$1s^{-1}2s^{-2}2p^{-3}3s^{-2}3p^{-3}$	246.6	93.1	0.0825
	$1s^{-1}2s^{-1}2p^{-4}3s^{-2}3p^{-3}$	256.1	96.5	0.1181
	$1s^{-1}2s^{-2}2p^{-3}3s^{-2}3p^{-4}4p^{1}$	352.1	96.2	0.0323
	$1s^{-1}2s^{-1}2p^{-4}3s^{-2}3p^{-4}4p^{1}$	362.2	99.7	0.0468

ionization (which accompanies the L-shell ionization) on the $K\alpha$ energy shift. Evaluating this influence we have subtracted from theoretical $K\alpha$ energy shifts (Table II) for configuration with n holes in L shell and 5 (or 4) holes in M shell (which can play an important role in the measured K X-ray spectra) the theoretical $K\alpha$ energy shifts for configuration with n holes in L shell and no holes in M shell (Table 1 in [7]). From this comparison it can be found that although the average number of holes in M shell is about 4–5, and does not change much with the projectile energy, the influence of the M-shell ionization (which accompanies the L-shell ionization) on the $K\alpha$ energy shift is much stronger than in the case of absence of L-shell holes and significantly increases with the projectile energy increasing (see the third column of Table III). This increase is mainly caused by the effect of nonadditivity of removal of electrons from L and M shells, which strongly increases with the increase of projectile energy. This is a result of the increase of the average number of L-shell holes with the projectile energy increasing. After subtracting the effect of M-shell ionization on the $K\alpha$ energy shift we have obtained (the fourth column of Table III) the $K\alpha$ energy shift value which corresponds purely to the average number of holes in L shell.

TABLE III

The dependence of average L- and M-shell ionization on the sulphur beam energy. In the third column the influence of multiple M-shell ionization on the $K\alpha$ energy shifts is presented. For a given beam energy the upper values correspond to 16.5 μg cm^{-2} thickness of carbon foil, while the lower values to 30 μg cm^{-2} thickness.

Sulphur beam energy (MeV)	Measured $K\alpha$ energy shift (eV)	Influence of M-shell ionization (eV)	Pure effect of L-shell ionization (eV)	Average number of L-shell holes	Average number of M-shell holes
9.6	45.4 ± 9.1	9.0 ± 1.0	36.4 ± 9.2	2.4 ± 0.6	4.4 ± 0.6
	45.0 ± 8.9		36.0 ± 9.0	2.4 ± 0.5	4.4 ± 0.6
16.0	64.1 ± 8.4	10.0 ± 1.0	54.1 ± 8.5	3.4 ± 0.5	4.6 ± 0.5
	60.9 ± 8.5		50.9 ± 8.6	3.3 ± 0.5	4.8 ± 0.5
22.4	75.8 ± 8.5	11.0 ± 1.0	64.8 ± 8.6	4.0 ± 0.4	4.9 ± 0.4
	71.4 ± 8.4		60.4 ± 8.5	3.8 ± 0.4	5.1 ± 0.4
32.0	82.4 ± 8.4	13.0 ± 1.0	69.4 ± 8.5	4.2 ± 0.4	5.6 ± 0.4
	87.8 ± 8.3		74.8 ± 8.4	4.5 ± 0.4	5.3 ± 0.4
38.4	100.3 ± 8.7	15.0 ± 1.0	85.3 ± 8.8	5.0 ± 0.4	5.3 ± 0.4
	101.9 ± 8.5		86.9 ± 8.6	5.1 ± 0.4	5.2 ± 0.4

The average number of holes in L shell of sulphur (at different incident energies) have been determined by comparing the $K\alpha$ energy shifts (the fourth column of Table III) obtained in the way described above with the theoretical $K\alpha$ energy shift values calculated for different number of holes in $2p$ subshell of sulphur (Table I in [7]). We considered only $2p$ and not $2s$ subshell ionization because the effects of ionization of $2s$ and $2p$ subshells on the $K\alpha$ energy are very similar, so not differentiating between them does not provide a significant error. This possible error is practically negligible because the ionization of $2s$ subshell plays a little role at the time of emission of the K X-ray lines (because the number of electrons in $2s$ subshell is three times smaller than in $2p$ subshell). The determined numbers of holes in L shell of sulphur corresponding to the measured $K\alpha$ energy shifts (at different incident energies of sulphur projectile for two carbon foil thicknesses) are presented in the fifth column of Table III. As can been seen from this table the average number of holes in L shell of sulphur projectile strongly increases with its incident energy increasing (from about 2.4 to about 5.1).

Additionally, we have evaluated the average number of M-shell holes by subtracting (for a given energy of sulphur projectile) the average number of L holes and one K hole from the values of average equilibrium charge state (see the second column of Table I). The determined average number of holes in M shell changes from about 4.4 to about 5.6 (the seventh column of Table III). This confirms that our initial assumption of about 4–5 M-shell holes not changing much with the sulphur projectile energy was resonable and could not provide any significant errors in determining average number of L-shell holes. Comparing our experimental data (Table I) with the results of our calculations (Table II) for electronic configurations corresponding to singly occupied $3p$ subshell and various distributions of holes in $2s$, $2p$, and $3s$ subshells of sulphur ions and similar configurations with singly occupied $4p$ subshell (instead of $3p$ subshell) we have found that the initial states having one electron in $4p$ subshell can play an important role at the time of emission of the K X-ray spectra from sulphur projectiles. This is very interesting since $4p$ subshell is empty in the ground states of neutral sulphur atom.

This work was supported by the Federal Ministry for Research and Technology, Germany, under Contract No. POL–017–98 and by the Polish State Committee for Scientific Research under Grants No. 2 P03B 019 16 and No. 2 P03B 06514.

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