EFFECT OF *L*- AND *M*-SUBSHELL IONIZATION ON THE *K* X-RAY DIAGRAM AND HYPERSATELLITE LINES OF CADMIUM*

J. Rzadkiewicz, D. Chmielewska, Z. Sujkowski
The Andrzej Sołtan Institute for Nuclear Studies, 05-400 Świerk, Poland

M. Berset, J.Cl. Dousse, Y.-P. Maillard
O. Mauron, P.-A. Raboud
Physics Department, University of Fribourg, 1700 Fribourg, Switzerland

J. Hoszowska
European Synchrotron Radiation Facility
6 Jules Horowitz, 38043 Grenoble, France

M. Polasik, K. Słabkowska
Faculty of Chemistry, Nicholas Copernicus University
Grudziądzka 5, 87-100 Toruń, Poland

and M. Pajek
Institute of Physics, Akademia Świetokrzyska
Świetokrzyska 15, 25-405 Kielce, Poland

(Received January 7, 2002)

The $K\alpha_{1,2}$ X-ray spectrum of $_{48}$Cd bombarded with 22.5 MeV/amu ^{16}O ions was measured with a bent crystal spectrometer. The diagram and hyper satellite $K\alpha_1$ and $K\alpha_2$ lines were resolved from their corresponding L-shell satellites. The experimental data are compared with the theoretical $K\alpha_{1,2}$ and $K^h\alpha_{1,2}$ spectra based on the multi-configuration Dirac–Fock calculations. The influence of the additional M-subshell ionization on the diagram and hyper-satellite lines is discussed.

PACS numbers: 32.30.Rj, 32.70.Jz, 32.80.Hd

* Presented at the XXVII Mazurian Lakes School of Physics, Krzyże, Poland, September 2–9, 2001.

1. Introduction

The study of complex K X-ray spectra provides rich and valuable information about the properties of the singly and multiply ionized atoms produced for *e.g.* in high-temperature plasma [1] or in heavy-ion atom collisions [2]. The $K\alpha_{1,2}$ diagram lines result from $1s^{-1} \rightarrow 2p^{-1}$ transitions in an atom with one hole in the $1s$ state. If the initial state of an atom is doubly ionized in the K-shell, the $1s^{-2} \rightarrow 1s^{-1}2p^{-1}$ transitions correspond to the so-called hyper-satellite X-ray lines ($K^h\alpha_{1,2}$). Atoms doubly ionized in the K-shell can be considered as He-like hole state atoms [3]. The energies of the K X-ray transitions in such atoms can be compared to those in one- and two-electron systems (H- and He-like atoms). The high accuracy of the hyper-satellite data permits to determine with high precision the Breit term (the magnetic interaction) and to discuss the QED corrections on a level comparable with that of the present day measurements with H- and He-like heavy atoms [3–5]. This accuracy can be further improved by the proper taking into account the effect of the accompanying outer shell ionization. While the presence of n-spectator L-shell vacancies results in resolved satellite lines, labeled $K\alpha_{1,2}L^n$, the M-shell ionization produces distortions of the line shapes as well as slight shifts of the centroids of the lines. The present paper presents such composite spectra for cadmium measured with a high resolution spectrometer and calculated with the state-of-the art multi-configuration Dirac–Fock method. The results can be used to deduce corrections for energies of all the resolved lines resulting from the presence of additional M-shell vacancies.

2. Experiment and data analysis

The measurements of the $K\alpha_{1,2}$ spectrum of $_{48}$Cd induced by ^{16}O beam were carried out at the Paul Scherrer Institute (PSI) in Villigen, Switzerland. The X-ray spectrum was recorded with a bent crystal spectrometer in the DuMond slit geometry. The (110) reflecting planes of a 1.0 mm thick quartz lamina were used in first order of reflection. The crystal was bent to a radius of 3.13 m. More details concerning the experimental setup can be found in [6]. A self-supporting metallic foil of natural $_{48}$Cd with a thickness of 51.9 mg/cm^2 was used as a target. The ^{16}O ions of energy 360 MeV were obtained from the PSI variable energy cyclotron. The beam intensity of about 130 nA was monitored by a Si–PIN photodiode. The measured spectrum was analyzed by means of a least-square fit program using a single Voigt function resulting from the convolution of Lorentzian and Gaussian line shapes. The natural X-ray line shape was represented by the Lorentzian function, whereas the Gaussian function accounted for the instrumental response of the spectrometer and the additional ionization in the M- and N-shells.

The natural line widths for the X-ray lines were approximated by the sum of the one K and one L level widths ($\Gamma_K + \Gamma_L$) and by the sum of the three K and one L level widths ($3\Gamma_K + \Gamma_L$) for the diagram and hyper-satellite lines, respectively. For each resolved line the energy, the intensity and the Gaussian width were fitted. The additional M-shell ionization during an ion–atom collision causes a broadening and induces energy shifts of the diagram and hyper-satellite lines. However, the advantage of using heavy ions rather than X-rays to produce He-like hole states (doubly ionized in the K-shell) lies in the higher statistics of the hyper-satellite lines.

3. Theoretical calculations

The theoretical energies and intensities of the $K\alpha_{1,2}$ diagram, satellite and hyper-satellite transitions were obtained using the relativistic Multi-Configuration Dirac–Fock (MCDF) method. This method has been described in many papers [7–11]. Therefore, only some basic ideas are briefly presented below. The effective Hamiltonian for an N-electron atom is expressed by

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

where $h_{\mathrm{D}}(i)$ is the Dirac operator for i-th electron and the terms C_{ij} account for electron–electron interactions and are based on the one-photon exchange processes. These interactions are the sum of the Coulomb (due to longitudinally polarized photons) and the Breit interaction (due to transversely polarized photons) operators. The atomic state functions with the total angular momentum J and parity p are assumed to have the multi-configurational 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), $c_m(s)$ are the configuration mixing coefficients for the state s and γ_m represents all the information needed 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 those described in earlier publications [10, 11].

4. Results

The influence of additional ionization in the L- and M-shell on the $K\alpha_{1,2}$ and $K^h\alpha_{1,2}$ lines in the theoretical spectra of ${}_{48}\mathrm{Cd}$ is illustrated in figures 1 and 2. The line shapes of these theoretical spectra were constructed by using the Voigt profile. The intensities of the hyper-satellite lines were obtained

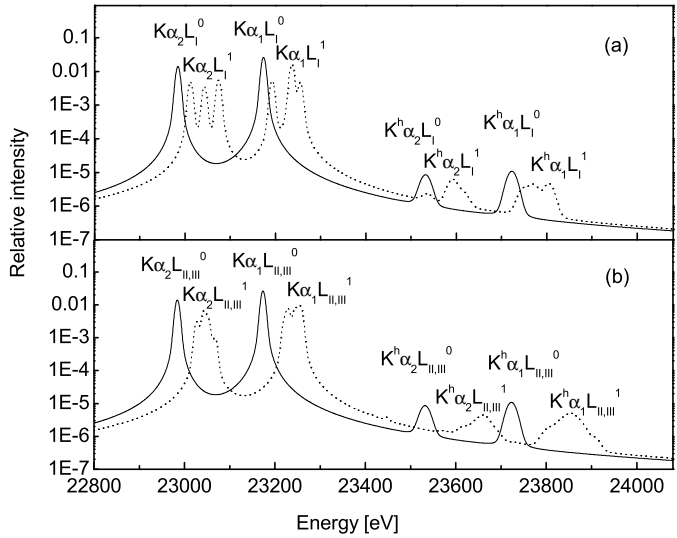

Fig. 1. Theoretical K X-ray spectra of Cd with (dashed line) and without (solid line) vacancy in the $2s$ (a) and $2p$ (b) subshells.

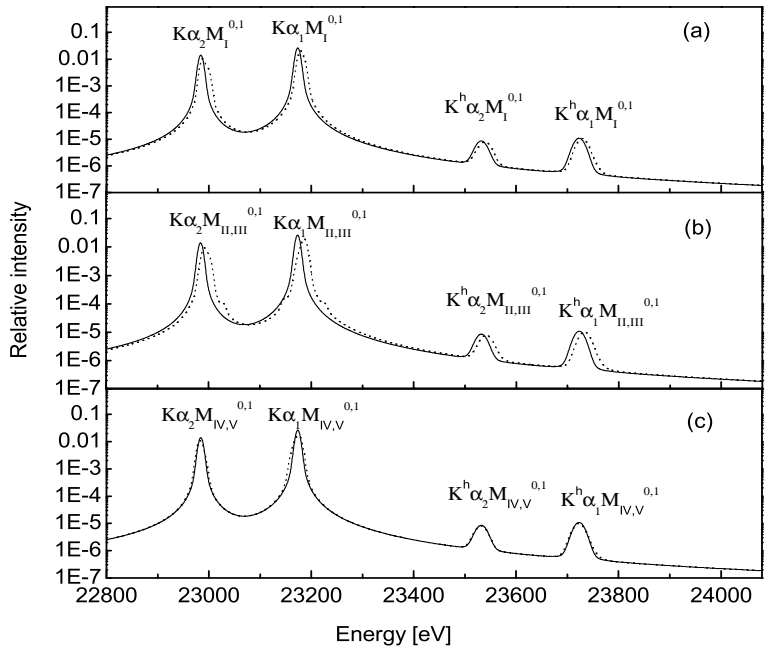

Fig. 2. Theoretical K X-ray spectra of Cd with (dashed line) and without (solid line) vacancies in the $3s$ (a), $3p$ (b) and $3d$ (c) subshells.

assuming a binomial distribution. All satellite lines were constructed separately with the probability for single ionization $P(L_i)$=1 and $P(M_i)$=1 for the L_i- and M_i-subshells, respectively. More details about the construction procedure can be found in [10–12]. Fig. 1 shows the influence of removing one electron from the $2s$ (Fig. 1(a)) and $2p$ (Fig. 1(b)) subshells on the $K\alpha_{1,2}$ and $K^h\alpha_{1,2}$ lines. One can see that the $2s$ and $2p$ additional holes shift noticeably the $K\alpha$ lines in energy and change the line shapes. Especially an additional $2s$ hole strongly modifies the shapes of the $K\alpha_{1,2}$ lines (upper part of Fig. 1).

Fig. 2 presents the influence of the presence the $3s$, $3p$ and $3d$ holes on the K X-ray spectrum. The changes in shapes and energy shifts of the $K\alpha$ lines are smaller than for the L-shell, but noticeable. Fig. 3 shows the $_{48}$Cd $K\alpha_{1,2}$ X-ray spectrum induced by ^{16}O measured on the left side of reflection. The peaks labeled $K\alpha_{1,2}L^1$ are the well resolved satellite lines originating from initial states having one K-shell and one L-shell vacancy. A detailed comparison of the experimental energies of the $K\alpha_{1,2}L^{0,1}$ and $K^h\alpha_{1,2}L^{0,1}$ in ^{16}O-induced X-ray spectrum with theoretical predictions is given in Table I. The theoretical values have been obtained by taking into account the weighted averages of all the transition probabilities multiplied by the degeneracies of the initial states. One can see that the $2p$ hole states are more effective in producing the $K\alpha_1L^1$ energy shifts than the $2s$ ones, while

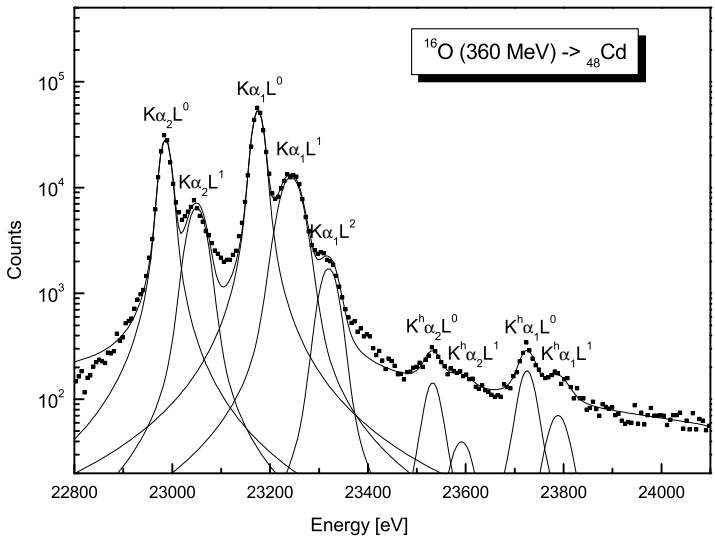

Fig. 3. Crystal spectrometer $K\alpha_{1,2}$ X-ray spectrum induced by 22.5 MeV/amu ^{16}O. The spectrum was fitted with 9 components (solid lines) corresponding to the diagram ($K\alpha_{1,2}L^0$), satellite ($K\alpha_{1,2}L^1$) and hyper-satellite ($K^h\alpha_{1,2}L^{0,1}$) transitions.

TABLE I

Theoretical and experimental $K\alpha$ transition energies of $_{48}$Cd for different L-shell hole configurations.

L-shell	$E(K\alpha_1)$	$E(K\alpha_2)$	$E(K^h\alpha_1)$	$E(K^h\alpha_2)$
L^0	23173.3	22984.0	23722.6	23531.7
$2s^{-1}$	23230.4	23043.8	23778.4	23589.4
$2p^{-1}$	23241.9	23042.9	23792.2	23592.4
L^{-1*}	23238.7	23043.2	23788.3	23591.5
Exp. †	23242.6(0.2)	23049.9(0.2)	23788.6(2.5)	23591.4(1.2)

† Experimental values.
* The average theoretical results for the whole L-shell.

in the case of the $K\alpha_2$ the differences in average values of energy shifts are rather small. The experimental values are in satisfactory agreement with the calculated ones, though some are slightly higher. These small differences might result from the Coster–Kronig transitions, which transfer the hole from the $2s$ shell to $2p$ shell and produce an extra M-shell hole.

The experimental positions of $K\alpha_{1,2}$ and $K^h\alpha_{1,2}$ peaks and the theoretical energies of the $K\alpha_{1,2}M^{0,1}$ and $K^h\alpha_{1,2}M^{0,1}$ lines are given in Table II. The theoretical calculations predict the highest shift for an additional $3p$ hole for all kind of transitions. In the case of the $3d$ hole all transitions are slightly shifted towards lower energies. These calculations are consistent with previous data for the other mid-Z atoms [13]. The $K\alpha_{1,2}$ and $K^h\alpha_{1,2}$ lines are shifted towards higher energies from 0.6 to 2.6 eV due to the additional M-shell ionization. From the energy shifts of the $K\alpha_{1,2}$ lines the probability of the M-shell ionization can be estimated between 46% and 65% per shell.

In conclusion it has been shown that additional M-shell holes cause not only energy shifts but also change the shapes and consequently the relative intensities of the K X-ray lines of cadmium. The influence on the K X-ray lines of the additional M-shell holes is much less than for L-shell, but it is not negligible. Therefore, in an accurate analysis of the diagram and hypersatellite K X-ray lines both the L- and M-shell additional ionization effects must be taken into account.

TABLE II

Theoretical and experimental $K\alpha$ transition energies of $_{48}$Cd for different M-shell hole configurations.

M-shell	$E(K\alpha_1)$	$E(K\alpha_2)$	$E(K^h\alpha_1)$	$E(K^h\alpha_2)$
M^0	23173.3	22984.0	23722.6	23531.7
$3s^{-1}$	23179.6	22990.1	23729.1	23538.0
$3p^{-1}$	23184.5	22993.5	23733.3	23541.2
$3d^{-1}$	23172.9	22983.1	23722.3	23531.0
M^{-1*}	23177.6	22987.4	23726.7	23535.2
Exp.†	23175.3(0.2)	22986.2(0.2)	23725.2(1.1)	23532.3(1.5)

† Experimental values.
* The average theoretical results for the whole M-shell.

The authors believe that the results of this study will be helpful in obtaining precise experimental data for the $K\alpha_{1,2}$ and $K^h\alpha_{1,2}$ X-ray lines and so enable deeper insight in the structure of the single (H-like) and doubly ionized states (He-like hole states) in the K-shell.

This work was supported by the Polish State Committee for Scientific Research (KBN), grants no. 5 P03B 077 20 and 2 P03B 019 16.

REFERENCES

[1] R.L. Kauffman, P. Richard, *Methods of Experimental Physics 13A*, edited by D. Williams, Academic, New York 1993, p. 148.

[2] I.A. Sellin, *Structure and Collision of Ions and Atoms*, Springer, Berlin 1978.

[3] J. Rzadkiewicz, D. Chmielewska, T. Ludziejewski, P. Rymuza, Z. Sujkowski, J. Hoszowska, D. Castella, D. Corminboeuf, J.-Cl. Dousse, B. Galley, Ch. Herren, J. Kern, M. Polasik, M. Pajek, *Phys. Lett.* **A264**, 186 (1999).

[4] T. Stoehlker *et al.*, *Comments At. Mol. Phys.* **33**, 271 (1997).

[5] K. Widmann *et al.*, *Phys. Rev.* **A53**, 2200 (1996) and references therein.

[6] B. Perny, J.-Cl. Dousse, M. Gasser, J. Kern, Ch. Rhême, P. Rymuza, Z. Sujkowski, *Phys. Rev.* **A36**, 2120 (1987).

[7] I.P. Grant, B.J. McKenzie, P.H. Norrington, D.F. Mayers, N.C. Pyper, *Comput. Phys. Commun.* **21**, 207 (1980).

[8] K.G. Dyall, I.P. Grant, C.T. Johnson, F.A. Parpia, E.P. Plummer, *Comput. Phys. Commun.* **55**, 425 (1989).

[9] M. Polasik, *Phys. Rev.* **A39**, 616 (1989).

[10] M.W. Carlen, M. Polasik, B. Boschung, J.-Cl. Dousse, M. Gasser, Z. Halabuka, J. Hoszowska, J. Kern, B. Perny, Ch. Rhême, P. Rymuza, Z. Sujkowski, *Phys. Rev.* **A46**, 3893 (1992).

[11] M. Polasik, *Phys. Rev.* **A52**, 227 (1995).

[12] M. Polasik, *Phys. Rev.* **A39**, 5092 (1989).

[13] M. Polasik, *Phys. Rev.* **A40**, 4361 (1989).