

K_α X-ray satellite spectra of Ti, V, Cr and Mn induced by photons

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Abstract. K X-ray emission spectra of Ti, V, Cr and Mn generated by photon excitation have been studied with a crystal spectrometer. The measured energy shifts of K_α satellite relative to the diagram line are compared with values obtained by electron excitation and with different theoretical estimates. The present experimental values of $K_\alpha L^1/K_\alpha L^0$ relative intensities are compared with values obtained by electron excitation.

Keywords. K X-ray satellites; crystal spectrometer.

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1. Introduction

When an atom ionized simultaneously in different shells de-excites, X-ray satellites are produced. If some holes are present in the L-shell along with a hole in the K-shell, the transitions to the K-shell from the higher shells give rise to K X-ray satellites, with the holes in the L-shell acting as spectators. These satellites are usually denoted as KL^n , where n stands for the number of holes in the L-shell. In the absence of any such L-holes, the diagram line KL^0 is emitted. The transitions originating from the L and M shells give rise to K_α and K_β satellites respectively.

In the present work, energies and relative intensities of K_α satellites of Ti, V, Cr and Mn are measured. The experimental energy shifts are compared with different theoretical estimates and with those obtained by electron excitation.

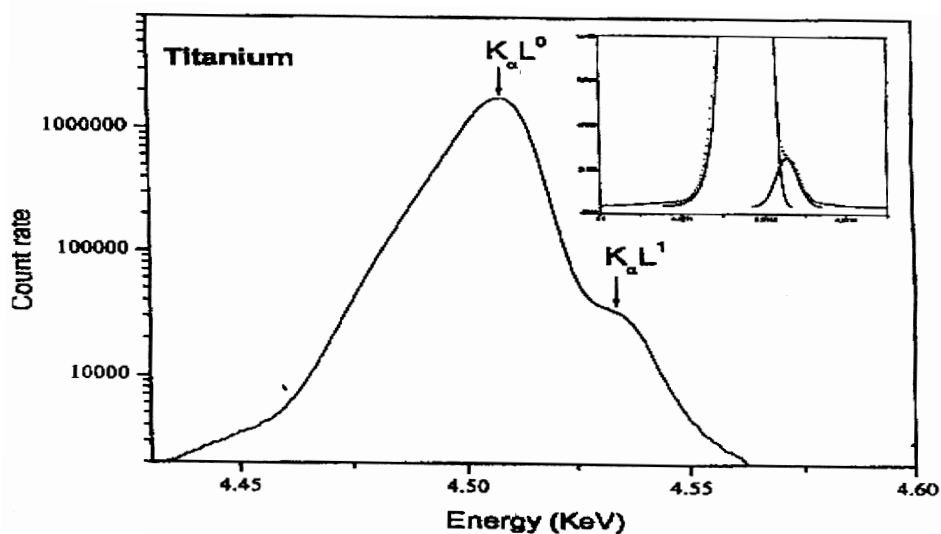


Figure 1. K_{α} satellite spectrum of titanium.

2. Experimental details

The principle involved, general experimental details and procedure have already been reported by [1]. In the present study, a Philips 2404 model wavelength dispersive crystal spectrometer was employed. LiF (200) plane crystal ($2d = 4.07 \text{ \AA}$) was used for Ti whereas LiF (220) plane crystal ($2d = 20848 \text{ \AA}$) was used for V, Cr and Mn. The energy calibration was done taking $K_{\alpha}L^0$ lines of Sc, Ti and V for LiF (200) crystal and V, Ni and Zn for LiF (220) as the reference lines and assuming their energies reported by Bearden [2].

3. Results and discussion

The collected data were first smoothed using sliding least square fitting and then the spectra were corrected for background using 'CORSPC' programme. The deconvolution of the peaks and estimation of areas under different peaks was carried out by 'PEAKFIT' software version 4.11 as detailed in the previous report [3]. The full spectrum in the log scale along with the deconvoluted $K_{\alpha}L^1$ satellite peak in the inset for each of the four elements Ti, V, Cr and Mn are presented in figures 1–4. The intensities of the diagram line $K_{\alpha}L^0$ and its satellite $K_{\alpha}L^1$ are determined from the areas under the respective peaks.

K_{α} X-ray satellite spectra

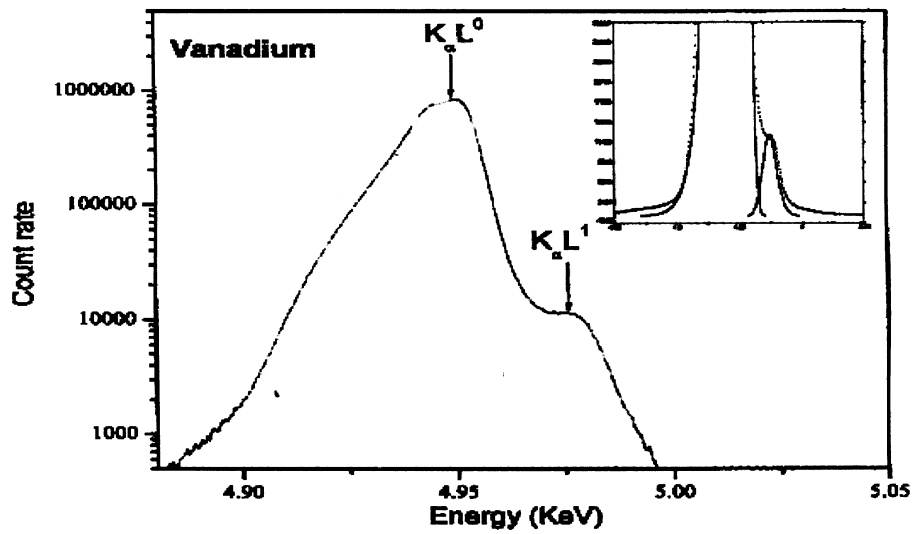


Figure 2. K_{α} satellite spectrum of vanadium.

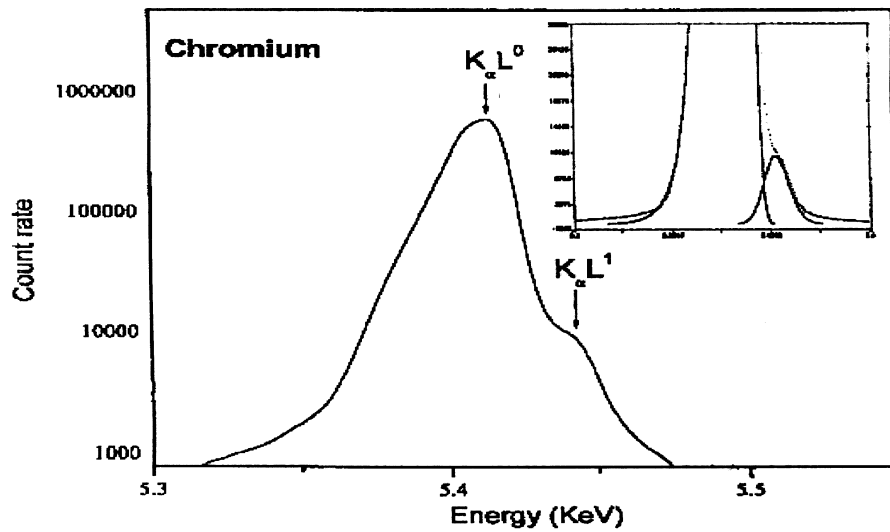


Figure 3. K_{α} satellite spectrum of chromium.

4. Satellite energy shifts

The energies of the diagram line $K_{\alpha}L^0$ and its satellite $K_{\alpha}L^1$ are determined for the four elements using appropriate calibration constants and the energy shifts of the satellite line relative to the diagram line is computed for the four elements (table 1). Deutch [4] has computed this energy shift using several theoretical models available:

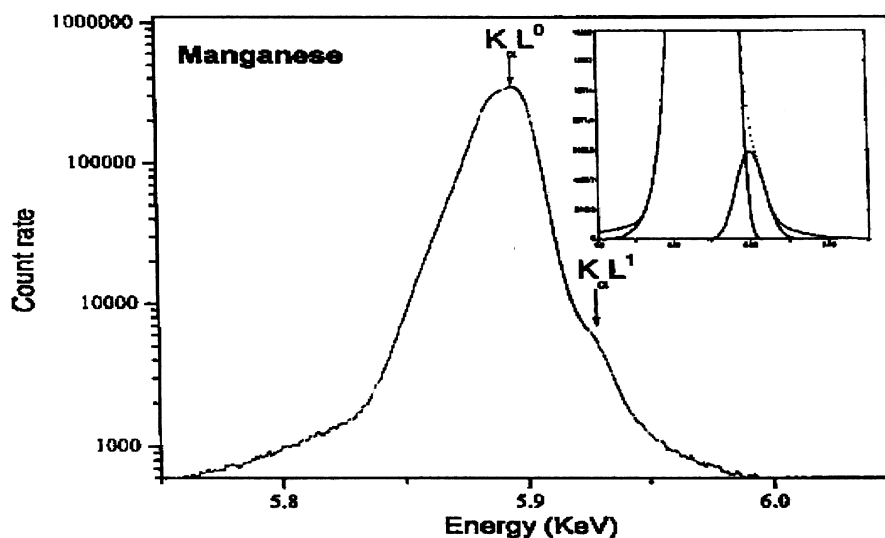


Figure 4. K_{α} satellite spectrum of manganese.

Table 1. $K_{\alpha}L^1$ X-ray satellite energy shifts (eV).

Z	Present	Electron	HF [4]	BS [4]	B-HF [4]	SCF [4]	SE [7]
	expt. value	excitation [8]					
22	25.3 ± 1.0	28.7 ± 2.0	22.0	29.6	28.7	26.3	23.2
23	26.2 ± 1.0	28.3 ± 2.0	23.5	31.3	30.3	28.0	24.7
24	27.9 ± 1.0	29.6 ± 2.0	25.1	33.0	31.9	29.7	26.3
25	29.6 ± 1.0	31.4 ± 2.0	26.4	34.6	33.5	31.4	27.8

- (a) *HF*: The non-relativistic Hartree–Fock calculations with the intermediate coupling scheme using MCHF 78 programme of Froese Fischer [5].
- (b) *BS*: The simple analytical model of Burch *et al* [6].
- (c) *B–HF*: Modified model of the previous model of Burch, where relativistic effects were included.
- (d) *SCF*: Further improved version of Burch’s model where analytic self-consistent field wave functions were employed.
- (e) *SE*: Semi-empirical formula proposed by Torok *et al* [7].

It can be seen in table 1 that the present experimental values of the $K_{\alpha}L^1$ energy shifts are in agreement within experimental errors with those obtained by Parrat [8] by electron excitation. Among the theoretical estimates, those obtained by Bhattacharya *et al* [9] are in good agreement with the experimental values. While BS and B–HF values overestimate the shifts, HF values underestimate them. The semi-empirical formula of Torok *et al* [7] also slightly underestimates the $K_{\alpha}L^1$ energy shifts.

5. The $K_\alpha L^1$ relative intensity ratios

The measured values of the $K_\alpha L^1$ intensity ratio relative to that of the diagram line of the $K_\alpha L^0$ obtained for Ti, V, Cr and Mn are supplemented with the previous data on K, Ca and Sc and compared with the value obtained by electron excitation [8].

The general trend observed (table 2) is that the values obtained by electron excitation are higher than those obtained by photon excitation, but the difference goes on decreasing with Z and the values are equal by the time Z value reaches 24. This is in consonance with the findings in the previous works [10,11].

As has already been explained, $K_\alpha L'$ X-ray satellites are produced when an atom ionized simultaneously in K and L shells decays. The mechanism by which the initial double ionization takes place may be different in the two modes of ionization, viz. electron and photon excitation modes. In the case of electron mode of excitation, it is very difficult for an electron to knock out K and L shell electrons simultaneously in a single impact as the electron should have an energy $E \geq E_K + E_L$, where E_K and E_L are the binding energies of the K and L shell electrons respectively. Besides, the density of the electrons in the cathode beam is small compared to the density of the electrons in the atom.

Hence it is thought that after single ionization produced by direct impact in the relaxation process from the perturbed state second ionization is produced either by shake-up or shake-off mechanism in the relaxation process from the perturbed state. In the shake-up process the electron jumps to an unoccupied higher level and in the shake-off process a valance electron is ejected to the continuum (Auger effect).

In the case of photon excitation there are two possibilities. Either double ionization may occur in a manner similar to the one described, i.e., single ionization followed by Auger transition or sufficient energy is absorbed by the atom in the photon impact making it possible for the production of simultaneous ionization in the K and L shells.

Thus, though the edge energies and consequently satellite energies are not affected by the mode of excitation, the double ionization cross-section appears to be dependent to some extent on the mode of excitation, resulting in some difference in the relative intensity of the satellites. As Z increases this difference is found to decrease and finally at some limiting value it is assumed to tend to zero. No experimental values are available to check this fact at higher Z values in both modes of excitation.

6. Summary

The energy shifts and relative intensities of $K_\alpha L^1$ X-ray satellite line relative to the diagram line $K_\alpha L^0$, measured for the elements Ti, V, Cr and Mn by photon excitation using a plane crystal spectrometer are reported. Among theoretical estimates those based on analytical SCF model of Bhattacharya *et al* are found to be in good agreement with the experimental shifts. While BS and B-HF models overestimate the shifts, HF calculations underestimate them. The semi-empirical

Table 2. $K_{\alpha}L^1$ X-ray satellite relative intensity (%).

Element	Present expt. value	Electron excitation value [8]
K	$2.61 \pm 0.13^*$	3.90 (± 0.2)
Ca	$2.31 \pm 0.12^*$	3.36 (± 0.17)
Sc	$1.80 \pm 0.09^*$	2.78 (± 0.13)
Ti	1.66 ± 0.08	2.20 (± 0.11)
V	1.54 ± 0.08	1.80 (± 0.09)
Cr	1.36 ± 0.07	1.37 (± 0.07)
Mn	1.07 ± 0.05	1.10 (± 0.05)

*Ref. [12].

formula of Torok underestimates the shifts. The relative intensity of K_{α} X-ray satellite is found to be dependent on the mode of excitation being higher for electron excitation at least for low Z elements but the energy shift of the satellites is independent of the mode of excitation.

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