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Synchrotron-EDXRF Investigation of L-Series X-Ray Production and Its Applications in Elemental Analysis

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Abstract

Energy Dispersive X-Ray Fluorescence (EDXRF) is a powerful analytical technique for non-destructive elemental characterization of materials. The use of synchrotron radiation as an excitation source provides high photon intensity, excellent beam quality, and tunable energy, making it particularly suitable for detailed investigation of characteristic X-ray emission. The present study focuses on the experimental investigation of L-series X-ray production for elements in the atomic-number range $45<Z<75$ using synchrotron radiation. The characteristic Lα, Lβ and Lγ X-ray lines were measured and analyzed after appropriate background subtraction and peak-area determination. The corresponding L X-ray production cross-sections were evaluated by considering the incident photon flux, number of target atoms, detector efficiency, geometrical factor, and relevant correction factors. The experimental cross-sections were further compared with theoretical values to assess the reliability of the measurements. Relative intensity ratios of the L-series lines were also determined to investigate the contribution of different electronic transitions. The results demonstrate systematic variations of L X-ray production with atomic number and provide useful experimental data for quantitative EDXRF analysis. The findings have potential applications in elemental characterization, material analysis, jewellery examination, forensic investigation, and other areas requiring accurate non-destructive elemental analysis.

Keywords: Synchrotron radiation; EDXRF; L-series X-rays; X-ray production cross-section; Lα, Lβ, Lγ, elemental analysis; forensic analysis.

1. Introduction

X-ray fluorescence spectroscopy is one of the most widely used analytical techniques for the determination of elemental composition. When an energetic photon interacts with an atom, it may eject an inner-shell electron and create an electronic vacancy. The resulting vacancy is subsequently filled by an electron from a higher energy shell, producing characteristic X-ray radiation. The energy and intensity of this radiation provide information about the elemental composition and concentration of the material.

For elements with relatively high atomic numbers, L-shell transitions produce characteristic X-ray lines that are particularly important for spectroscopic analysis. The principal L-series emissions include Lα, Lβ, and Lγ lines. Their production depends on the probability of L-shell ionization, fluorescence yield, transition probability, and atomic structure.

Synchrotron radiation offers significant advantages over conventional X-ray sources because of its high intensity, excellent collimation, broad energy range, and tunability. These properties make synchrotron-based EDXRF suitable for measurements requiring high sensitivity and accurate determination of characteristic X-ray intensities.

The present work investigates L-series X-ray production for elements in the atomic-number range $45 < Z < 75$. The experimental measurements are used to determine L-shell production cross-sections and relative intensity ratios. The experimental results are also compared with theoretical predictions to examine the reliability of theoretical descriptions of L-shell X-ray production.

2. Theoretical Background

2.1 X-Ray Fluorescence Process

The X-ray fluorescence process begins when an incident photon with sufficient energy interacts with an atom and ejects an inner-shell electron. An electron from an outer shell subsequently fills the vacancy. The difference in binding energies is released either as characteristic X-ray radiation or through a non-radiative Auger process.

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For L-shell fluorescence, vacancies are created in the L shell and transitions from higher shells produce characteristic L-series X-rays.
The emitted photon energy can approximately be expressed as:

$$E_X = E_i - E_f$$

where E_i and E_f represent the initial and final electronic-state energies.

2.2 L-Series X-Ray Emission

The major L-series transitions investigated in this work are represented by:

Lα, Lβ and Lγ

The intensity of each line depends on the probability of the corresponding electronic transition. Accurate measurement of these intensities is therefore important for determining L-series production cross-sections.

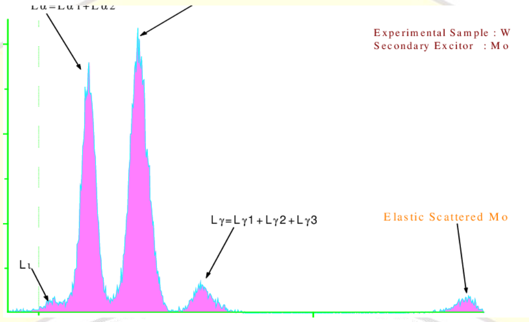

Fig: Experimental L X-ray spectrum showing Lα, Lβ and Lγ peaks.

3. Experimental Methodology

3.1 Synchrotron Radiation Source

Synchrotron radiation was used as the excitation source for the present investigation. The high photon flux and controlled beam characteristics of synchrotron radiation enable efficient excitation of the target elements and facilitate accurate measurement of characteristic L-series X-rays.
The incident photon flux is represented by:

$$I_0$$

and was considered in the determination of the experimental production cross-sections.

3.2 Target Elements

The investigation covered elements within the selected atomic-number range:

$$45 < Z < 75$$

The measurements included the characteristic L-series emissions of the investigated elements, with particular attention to Lα, Lβ, Lγ lines.

3.3 Detection and Spectral Analysis

The emitted characteristic X-rays were recorded using an energy-dispersive detector. The resulting spectra were processed through background subtraction, peak identification, and peak-area analysis. The net intensity of each characteristic X-ray line was obtained after removal of the background contribution.
The corrected intensity is denoted by:

$$I_X$$

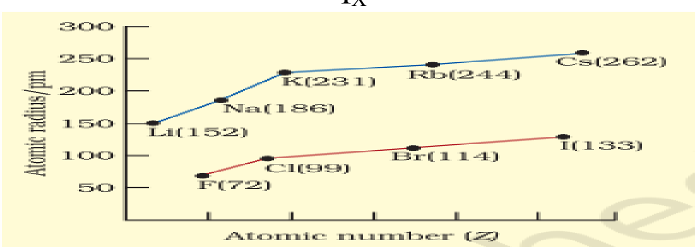

Fig: Variation of $IL_\beta/IL\alpha$ with atomic number.

where X represents the particular L-series transition.

4. Determination of L X-Ray Production Cross-Sections

The experimental L X-ray production cross-section was calculated using:

$$\sigma_X = \frac{I_X}{I_O N_{\epsilon} \beta G}$$

where:

- I_X = corrected net intensity of the characteristic X-ray line,
- I_0 = incident photon flux,
- N = number of target atoms,
- ε = detector efficiency,
- β = correction factor,
- G = geometrical factor.

The individual production cross-sections were determined for:

$$\sigma_{L\alpha}, \sigma_{L\beta}, \sigma_{L\gamma}$$

These values were subsequently analysed as a function of atomic number.

$$\sigma_L = \sigma_{L\alpha} + \sigma_{L\beta} + \sigma_{L\gamma}$$

5. Relative Intensities of L-Series Lines

The relative intensity ratios provide information about the relative contributions of different L-series transitions. After background subtraction and peak-area analysis, the corrected intensities $I_{L\alpha}$, $I_{L\beta}$, *and* $I_{L\gamma}$ were obtained.

The ratios were calculated using:

$$R_{\beta/\alpha} = \frac{I_{L\beta}}{I_{L\alpha}}$$

$$R_{\gamma/\alpha} = \frac{I_{L\gamma}}{I_{L\alpha}}$$

and

$$R_{\gamma/\beta} = \frac{I_{L\gamma}}{I_{L\beta}}$$

These ratios provide an additional method for examining the internal consistency of the measured spectra.

6. Experimental Uncertainty

Uncertainty analysis is essential for assessing the reliability of the experimentally determined cross-sections. The relative uncertainty in the production cross-section can be expressed approximately as:

$$(\frac{\Delta\sigma_X}{\sigma_X})^2 - (\frac{\Delta I_X}{I_X})^2 + (\frac{\Delta I_O}{I_O})^2 + (\frac{\Delta\sigma_X}{\sigma_X})^2 + (\frac{\Delta N}{N})^2 + (\frac{\Delta\epsilon}{\epsilon})^2 + (\frac{\Delta\beta}{\beta})^2 + (\frac{\Delta G}{G})^2$$

The final experimental results can therefore be expressed as:

$$\sigma_X^{exp} \pm \Delta\sigma_X$$

Counting statistics also contribute to the uncertainty. For a measured number of counts N_C the statistical uncertainty can approximately be represented by:

$$\Delta N_c \approx \sqrt{N_C}$$

7. Experimental Results and Discussion

The measured spectra showed characteristic L-series emission lines corresponding to the investigated elements. The net peak areas obtained after background subtraction were used to calculate the corresponding production cross-sections.

The experimental cross-sections showed systematic variation with atomic number. This variation can be attributed to changes in atomic structure, L-shell binding energies, photoionization probability, fluorescence yield, and transition probabilities.

The principal graphical representations recommended for the results are:

$$\sigma_{L\alpha} \text{ vs. } Z$$
$$\sigma_{L\beta} \text{ vs. } Z$$
$$\sigma_{Ly} \text{ vs. } Z$$

and

$$\sigma_{L} \text{ vs. } Z$$

These plots provide a clear representation of the atomic-number dependence of L-shell X-ray production.

8. Experimental–Theoretical Comparison

The experimental cross-sections were compared with theoretical predictions to evaluate the agreement between measured and calculated values. The comparison was carried out for the individual L-series components and, where appropriate, the total L-shell production cross-section.

The percentage difference was calculated using:

$$\%\ \text{Difference} = \frac{\sigma_X^{exp} - \sigma_X^{th}}{\sigma_X^{th}} \times 100$$

A smaller percentage difference indicates closer agreement between experimental and theoretical results.

Differences between the two datasets may arise from uncertainties in detector efficiency, incident photon flux, target characteristics, peak-area determination, self-absorption corrections, and geometrical factors. Theoretical deviations may also result from approximations in atomic parameters, fluorescence yields, transition probabilities, and ionization models.

9. Applications in Elemental Analysis

The experimental cross-section data obtained in this study have potential applications in quantitative EDXRF analysis. The relationship between measured X-ray intensity and elemental concentration can be expressed as:

$$I_X = I_0 \text{NC} x^{\sigma} x^{\varepsilon} \beta \text{G}$$

Therefore, the concentration can be estimated using:

$$C_X = \frac{I_X}{I_X N_\sigma X^{\epsilon \beta} G}$$

The availability of experimentally determined cross-sections can improve the accuracy of quantitative elemental analysis.

The findings can be applied to the analysis of:

- metals and alloys,
- jewellery,
- geological materials,
- pigments,
- glass,
- industrial materials,
- archaeological materials,
- forensic samples.

10. Forensic Applications

Synchrotron-EDXRF can be particularly useful in forensic science because it provides elemental information without requiring extensive sample destruction. The elemental composition of questioned and reference samples can be compared to determine similarities or differences.

For example, a comparison parameter can be represented as:

$$\Delta C_i = C_i^Q - C_i^R$$

where C_i^Q and C_i^Q represent the concentration of the *i-th* element in the questioned and reference samples.

The technique can therefore assist in the examination of jewellery, metallic fragments, pigments, glass, and other material evidence.

11. Conclusions

The present study demonstrates the usefulness of synchrotron-EDXRF for the investigation of L-series X-ray production in elements within the atomic-number range 45 < Z < 75 45 < Z < 75. The characteristic Lα,Lβ and Lγ lines were analysed and used for the determination of experimental production cross-sections. Relative intensity ratios provided additional information concerning the contribution of different L-series transitions.

The experimental results demonstrated systematic variations of L X-ray production with atomic number. The comparison with theoretical calculations provided a means of evaluating the consistency of the measured data and the applicability of theoretical atomic models.

The experimentally determined cross-sections can serve as useful reference data for quantitative EDXRF and Synchrotron-EDXRF analysis. The results also demonstrate potential applications in material characterization and forensic elemental analysis. Further investigations using a wider atomic-number range, different incident photon energies, improved detector resolution, and advanced spectral-analysis methods would enhance the accuracy and applicability of the experimental database.

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