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# Investigation of Lα, Lβ and Lγ X-Ray Production Cross-Sections Using Synchrotron Radiation

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## Abstract

The present study investigates the production cross-sections of characteristic L-series X-rays, namely Lα, Lβ and Lγ, produced following photoionization of L-shell electrons by monochromatic synchrotron radiation. Measurements are proposed/performed for selected medium- and high-Z elements using an energy-tunable synchrotron X-ray beam. The incident photon energy is varied across the L-shell ionization thresholds while the emitted characteristic X-rays are recorded using an energy-dispersive semiconductor detector. The measured spectra are processed to determine net peak areas after background subtraction, detector-efficiency correction, geometrical correction and incident-photon normalization. The experimental Lα, Lβ and Lγ production cross-sections are obtained from the corrected fluorescence intensities. The results are compared with theoretical predictions based on L-subshell photoionization cross-sections, fluorescence yields, Coster–Kronig transition probabilities and fractional radiative emission rates. Particular attention is given to the energy dependence of the cross-sections near the L1, L2 and L3 absorption thresholds and to the relative contributions of different L-subshell vacancies to the observed Lα, Lβ and Lγ groups. The investigation provides experimental information relevant to atomic relaxation parameters, fundamental-parameter databases and quantitative X-ray fluorescence analysis. The results can also be used to assess the accuracy of theoretical atomic models and available fluorescence-yield and Coster–Kronig data.

**Keywords: Synchrotron radiation; X-ray fluorescence; L-shell; Lα; Lβ; Lγ; production cross-section; fluorescence yield; Coster–Kronig transition; photoionization.**

## 1. Introduction

Characteristic X-ray emission following inner-shell photoionization is an important atomic process with applications in X-ray fluorescence (XRF), elemental analysis, radiation physics, astrophysics, plasma diagnostics and the development of fundamental atomic databases. When an atom is irradiated by photons having energy greater than an inner-shell binding energy, photoionization can produce a vacancy in one of the atomic subshells. The subsequent rearrangement of the atomic electrons results in the emission of characteristic X-rays or Auger electrons.

For medium- and high-Z elements, L-shell X-ray emission is particularly important. The L shell consists of the L1, L2 and L3 subshells, corresponding approximately to the 2s and 2p subshells. Radiative transitions involving these subshells produce groups of characteristic lines conventionally designated as Lα, Lβ and Lγ. The measured intensity of each group depends not only on the probability of initial photoionization but also on fluorescence yields, Coster–Kronig transitions and the radiative transition probabilities associated with the individual lines. The L-shell X-ray production cross-section can therefore be considered a sensitive quantity for testing the consistency of the different atomic parameters entering the fluorescence process. In general, theoretical production cross-sections are calculated from L-subshell photoionization cross-sections together with fluorescence yields, Coster–Kronig probabilities and fractional emission rates.

Synchrotron radiation is particularly advantageous for such measurements because it provides intense, highly collimated and energy-tunable X-ray beams. By tuning the incident photon energy around the L-shell absorption edges, the individual contributions of the different L subshells can be investigated with considerably greater control than is generally possible using conventional laboratory X-ray sources.

Previous synchrotron investigations have demonstrated the feasibility of measuring line-resolved L-shell production cross-sections. Measurements for Sn and Sb using 6–14 keV synchrotron radiation included Lα, several Lβ groups and Lγ groups and compared the measured cross-sections with calculations using different combinations of photoionization cross-sections, emission rates, fluorescence yields and Coster–Kronig probabilities. Differences of up to approximately 25% were found between calculated values obtained from different atomic-parameter datasets.

Other synchrotron investigations have measured L-series production cross-sections by tuning the photon energy through the L1, L2 and L3 ionization thresholds. Such measurements demonstrate that the experimental cross-section can be expressed in terms of the detected characteristic-X-ray yield, incident photon fluence, detector efficiency, geometrical factors and target areal density. The objective of the present work is therefore to investigate experimentally the production cross-sections of Lα, Lβ and Lγ X-rays induced by synchrotron radiation and to compare the experimental results with theoretical predictions. Particular emphasis is placed on the energy dependence of the cross-sections and on the role of L-subshell ionization and subsequent atomic relaxation.

## 2. Theoretical Background

### 2.1 L-shell photoionization

The incident photon can remove an electron from one of the L subshells when

$$E_O > E_{L_i}$$

where $E_O$ is the incident photon energy and $E_{L_i}$ is the binding energy of the $L_i$ subshell, with $I$ = 1,2,3.

The corresponding photoionization cross-sections are represented by

$$\sigma_{L_1}(E_O), \qquad \sigma_{L_2}(E_O), \qquad \sigma_{L_3}(E_O),$$

When a vacancy is created in an L subshell, the vacancy may be filled through radiative or non-radiative transitions.

### 2.2 Fluorescence yield

The fluorescence yield ωi represents the probability that an L-subshell vacancy is filled through an X-ray-emitting radiative transition rather than an Auger or related non-radiative process. Thus,

$$W_i = \frac{Number\ of\ Radiative\ Transitions}{Total\ number\ of\ Vacancy\ Decays}$$

The fluorescence yield generally increases with atomic number and differs for the L1, L2 and L3 subshells.

### 2.3 Coster–Kronig transitions

An L-subshell vacancy can migrate between L subshells through Coster–Kronig transitions. The corresponding transition probabilities are commonly denoted by

$$f_{12}, \quad f_{13}, \quad f_{23},$$

For example, an L1 vacancy can undergo an L1→L2 or L1→L3 Coster–Kronig transition. Consequently, the observed Lα, Lβ and Lγ intensities may contain contributions originating from more than one initial L-subshell.

### 2.4 Lα production cross-section

Using the standard fundamental-parameter formalism, the Lα production cross-section can be represented as

$$\sigma_{L_\alpha} = [\ \sigma_{L_1} f_{13} + \sigma_{L_1} f_{12}\ f_{23} + \sigma_{L_2} f_{23} + \sigma_{L_3}]\ w_\ni\ F_{3\alpha},$$

where F3α is the fractional radiative emission rate for the Lα group.

This expression demonstrates that Lα emission is strongly associated with L3 vacancies, including vacancies transferred to L3 through Coster–Kronig transitions.

### 2.5 Lβ production cross-section

The Lβ group contains transitions involving several subshells. A generalized expression is

$$\sigma_{L\beta} = \ \sigma_{L_1} w_1\ F_{1\beta} + (\sigma_{L_2} + \sigma_{L_1} f_{12})\ w_2 F_{2\beta} + (\sigma_{L_1} f_{13} + \sigma_{L_1} f_{12}\ f_{23} + \sigma_{L_2} f_{23} + \sigma_{L_3}) w_\ni F_{\ni\beta}$$

Thus, the measured Lβ cross-section contains contributions from multiple L subshells.

### 2.6 Lγ production cross-section

Similarly,

$$\sigma_{L\gamma} = \sigma_{L_1}\omega_1 F_{1\gamma} + (\sigma_{L_2} + \sigma_{L_1} f_{12})\omega_2 F_{2\gamma} + (L_3\text{-vacancy contribution})$$

The exact expression should be expanded according to the individual Lγ lines included in the experimental peak group.

These fundamental-parameter relationships are consistent with formulations used in recent synchrotron L-shell XRF studies.

## 3. Experimental Method

### 3.1 Synchrotron radiation source

The experiment is performed at a synchrotron X-ray fluorescence beamline providing a monochromatic and tunable photon beam.

The incident photon energy is selected using a double-crystal monochromator. A Si(111) monochromator is commonly employed for this purpose. For example, previous L-shell measurements at the ELETTRA XRF beamline used a Si(111) double-crystal monochromator with an energy range extending to approximately 14 keV and high energy resolution

For the present experiment, the photon energy should be selected according to the absorption edges of the investigated element:

$$E_{L1} < E_0 < E_K,$$

unless measurements above the K edge are specifically required.

The exact beamline, photon-energy range, beam size, monochromator resolution and storage-ring operating conditions should be reported from the actual experiment.

### 3.2 Target preparation

Thin, homogeneous targets of the selected elements are prepared or obtained in a form suitable for XRF measurement.

The target thickness should be sufficiently small to minimize self-absorption while maintaining adequate fluorescence intensity.

The target areal density is given by

$$m = \frac{M}{A},$$

where M is the target mass per unit area.

The target is positioned at a known angle relative to the incident beam and detector.

### 3.3 Detection system

The characteristic X-rays emitted by the target are measured using an energy-dispersive X-ray detector, such as a silicon drift detector (SDD) or another calibrated semiconductor detector.

The detector energy calibration is established using reference X-ray lines with accurately known energies. The detector efficiency,

$\in(E)$,

must be known over the energy range containing the Lα, Lβ and Lγ lines.

The detector should be placed at a well-defined angle with respect to the incident beam in order to minimize background and scattering contributions.

### 3.4 Measurement procedure

For each incident photon energy $E_O$, an X-ray emission spectrum is recorded.

The measurement sequence consists of:

1. Setting the synchrotron photon energy.
2. Measuring the incident photon intensity.
3. Irradiating the target for a known acquisition time.
4. Recording the emitted X-ray spectrum.
5. Repeating the measurement at each selected photon energy.
6. Measuring background/scattering contributions where required.
7. Performing detector calibration and efficiency corrections.

The photon energy should be scanned across the L-shell ionization thresholds where feasible. Such measurements allow changes in L-subshell photoionization contributions to be directly investigated.

## 4. Spectral Analysis

The recorded spectrum contains characteristic L-series peaks together with continuum background and scattered radiation.

The net number of counts associated with an individual L line is obtained from

$$N_{L_K} = N_{Peak} - N_{background},$$

where k represents the relevant L-series line or line group.

Peak fitting may be performed using Gaussian or experimentally appropriate response functions together with a suitable background function.

For unresolved or partially resolved lines, the complete line group should be fitted consistently at all photon energies.

The fitted peak areas should be corrected for dead time, detector efficiency and other instrumental effects.

**5. Determination of X-Ray Production Cross-Sections**

The experimental production cross-section may be determined from

$$\sigma_{L_K}(E_O) = \frac{N_{L_K}\ (E_O)}{Q_O(E_O)\ G\ \epsilon_{L_K}\ \beta_{L_K}\ m},$$

where:

- NLk = net number of detected Lk X-ray counts;
- Q0 = integrated incident photon fluence;
- G = geometrical/solid-angle factor;
- ϵLk = detector efficiency at the Lk photon energy;
- βLk = attenuation and related correction factor;
- m = target areal density.

The integrated incident photon fluence is

$$Q_0\ (E_O) = \int_0^t I_0(E_0, t)\ dt,$$

where I0 is the incident photon flux and t is the measurement time.

This type of normalization has been used in synchrotron measurements of L-shell X-ray production cross-sections

**6. Corrections**

Several corrections are required to obtain reliable absolute cross-sections.

**6.1 Detector efficiency correction**

The energy-dependent detector efficiency is applied according to

$$N'_{L_K} = \frac{N_{L_K}}{\epsilon\ (E_{L_K})}$$

**6.2 Geometrical correction**

The detector subtends a finite solid angle Ω. For a detectoΩr at distance r,

$$G \simeq \frac{\Omega}{4\pi},$$

for the appropriate experimental geometry.

**6.3 Self-absorption correction**

The attenuation of both incident and emitted photons inside the target should be considered. For a sufficiently thin target the correction may be close to unity. For thicker targets, the correction must be calculated from the appropriate mass attenuation coefficients and experimental geometry.

**6.4 Dead-time correction**

If the detector operates with non-negligible dead time, the observed count rate must be corrected using the detector's live-time information.

**6.5 Incident-beam normalization**

Because synchrotron beam intensity may vary with time, each spectrum should be normalized to the integrated incident photon fluence rather than simply to acquisition time.

**7. Theoretical Calculations**

The theoretical production cross-sections are calculated from

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Type equation here.

$$\sigma_{L_K}^{th} = \sum_{i=1}^{3} p_i(E_0)\omega_i F_{ik},$$

represents the effective population of the Li vacancy after accounting for direct photoionization and Coster–Kronig redistribution.

The direct photoionization contribution is obtained from

$$P_i(E_0) = \sigma_{L_i}(E_0)$$

After inclusion of Coster–Kronig transitions, the effective populations become combinations of $\sigma_{L_i}$ and the transition probabilities $f_{ij}$

Several theoretical parameter sets can be tested. These may include:

- Hartree–Fock–Slater photoionization cross-sections;
- Dirac–Fock radiative transition rates;
- Dirac–Hartree–Slater fluorescence and Coster–Kronig parameters;
- semi-empirical fluorescence-yield values;
- experimentally determined atomic parameters.

Recent experimental work on Sn and Sb demonstrated that the calculated L-shell production cross-section can depend significantly on which combination of these atomic parameters is used.

## 8. Uncertainty Analysis

The uncertainty in the experimental cross-section is obtained by propagating the uncertainties of all significant quantities:

$$\sigma_{L_K} = \frac{N_{L_K}}{Q_0 G \in \beta m}$$

The relative uncertainty can be approximated by

Type equation here.

$$\left(\frac{\Delta\sigma}{\sigma}\right)^{2} = \left(\frac{\Delta N}{N}\right)^{2} + \left(\frac{\Delta Q_O}{Q_0}\right)^{2} + \left(\frac{\Delta G}{G}\right) 2^{+}\left(\frac{\Delta\in}{\in}\right) 2^{+}\left(\frac{\Delta\in}{\in}\right) 2^{+}\left(\frac{\Delta\beta}{\beta}\right) 2^{+}\left(\frac{\Delta m}{m}\right)$$

Statistical uncertainty in the measured peak area should be combined with systematic uncertainties arising from detector efficiency, target thickness, incident-photon normalization, geometrical factors and spectral fitting.

As an example of the scale achievable in synchrotron L-shell experiments, a previous Sn/Sb investigation reported overall experimental uncertainties of approximately 7–9%

The uncertainty reported for the present experiment must, however, be calculated from the actual experimental parameters.

## 9. Results and Discussion

### 9.1 X-ray emission spectra

Representative X-ray emission spectra should be presented for each investigated target.

Representative synchrotron-induced X-ray emission spectrum of [element] at an incident photon energy of [XX] keV, showing the Lα, Lβ and Lγ emission groups.

The spectra should demonstrate the characteristic peaks and their evolution with incident photon energy.

The Lα group is generally among the most intense L-series features, whereas the Lβ and Lγ groups may have lower intensities and can contain several unresolved or partially resolved transitions.

### 9.2 Energy dependence of Lα cross-section

The measured Lα production cross-section should be plotted as a function of incident photon energy. Experimental Lα X-ray production cross-section as a function of incident photon energy.

Above the relevant L-shell absorption threshold, the production cross-section is expected to exhibit a characteristic energy dependence reflecting the underlying L-subshell photoionization cross-section.

The experimental points should be compared with the calculated values using the selected atomic parameter sets.

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The comparison should be discussed in terms of:

- agreement below and above the absorption edge;
- magnitude of the experimental cross-section;
- slope with incident photon energy;
- possible discrepancies between theory and experiment.

**9.3 Lβ production cross-section**

The Lβ production cross-section should be analyzed similarly.

Because Lβ emission may receive contributions from more than one L subshell, its energy dependence can provide information about the relative importance of L1, L2 and L3 vacancy production and Coster–Kronig redistribution.

**9.4 Lγ production cross-section**

The Lγ lines generally have lower intensity than the dominant Lα group, making accurate background subtraction and detector-efficiency correction particularly important.

Agreement or disagreement between the measured and calculated Lγ cross-sections should be discussed with particular attention to the radiative transition rates and fluorescence yields used in the theoretical calculation.

**9.5 Comparison with theory**

The deviation between experimental and theoretical cross-sections can be quantified using

$$R = \frac{\sigma_{exp} - \sigma_{th}}{\sigma_{th}} \times 100$$

Alternatively,

$$R = \frac{\sigma_{exp}}{\sigma_{th}}$$

may be reported.

A table should be constructed as follows:

| Photon energy (keV) | σLα(exp) | σLα(th) | σLβ(exp) | σLβ(th) | σLγ(exp) | σLγ(th) |
|---|---|---|---|---|---|---|
| 4.0 | 1.20 | 1.15 | 0.82 | 0.78 | 0.34 | 0.32 |
| 4.1 | 1.38 | 1.32 | 0.91 | 0.87 | 0.39 | 0.37 |
| 4.2 | 1.56 | 1.49 | 1.02 | 0.97 | 0.44 | 0.42 |
| 4.3 | 1.73 | 1.65 | 1.12 | 1.07 | 0.49 | 0.47 |
| 4.4 | 1.91 | 1.82 | 1.23 | 1.17 | 0.54 | 0.52 |
| 4.5 | 2.08 | 1.98 | 1.34 | 1.27 | 0.59 | 0.56 |
| 4.6 | 2.24 | 2.14 | 1.44 | 1.37 | 0.64 | 0.61 |
| 4.7 | 2.40 | 2.29 | 1.54 | 1.47 | 0.69 | 0.66 |
| 4.8 | 2.55 | 2.44 | 1.64 | 1.56 | 0.74 | 0.71 |
| 4.9 | 2.70 | 2.58 | 1.74 | 1.66 | 0.79 | 0.76 |
| 5.0 | 2.84 | 2.72 | 1.83 | 1.75 | 0.84 | 0.81 |

The final numerical values must be populated using the measured experimental data rather than estimated or fabricated values.

**10. Lα/Lβ and Lα/Lγ Intensity Ratios**

In addition to absolute production cross-sections, intensity ratios provide useful information because several systematic factors cancel partially when the same measurement conditions are used.

The ratios are defined as

$$R_{a/\beta} = \frac{\sigma_{La}}{\sigma_{L\beta}}$$

AND

$$R_{a/y} = \frac{\sigma_{La}}{\sigma_{Ly}}$$

Their energy dependence can be investigated experimentally.

Changes in these ratios near L-shell absorption thresholds may provide information concerning the changing contributions of different L subshells.

Recent synchrotron studies have likewise used L-shell X-ray intensities and fundamental-parameter calculations to investigate the relative emission behavior of Lα, Lβ and Lγ groups.

## 11. Discussion

The experimental investigation of Lα, Lβ and Lγ production cross-sections provides a direct test of the atomic parameters used in theoretical X-ray emission calculations.

The measured cross-section is not determined solely by the photoionization probability. Instead, it is the result of a sequence of processes:

photoionization→L-subshell vacancy→Coster–Kronig redistribution→radiative/non-radiative decay→characteristic X-ray emission.

Consequently, discrepancies between experiment and theory can originate from uncertainties in photoionization cross-sections, fluorescence yields, Coster–Kronig probabilities or radiative transition rates.

The Lα group is particularly sensitive to the population of the L3 subshell because of the strong contribution from transitions terminating in L3. The Lβ and Lγ groups provide additional sensitivity to L1 and L2 vacancy populations and their redistribution through Coster–Kronig transitions.

The use of tunable synchrotron radiation provides an important advantage because the incident photon energy can be selected with respect to individual L-subshell thresholds. This makes it possible to distinguish effects that would be difficult to separate using a conventional broadband X-ray source.

Previous measurements on Sn and Sb have shown that different theoretical parameter combinations can produce differences of up to approximately 25% in predicted L-shell production cross-sections. This demonstrates the importance of obtaining reliable experimental benchmarks for atomic databases.

The present measurements can therefore contribute to improving fundamental-parameter datasets used in quantitative XRF and related spectroscopic applications.

## 12. Conclusions

The production cross-sections of Lα, Lβ and Lγ X-rays induced by synchrotron radiation provide valuable information about the photoionization and subsequent relaxation of L-shell vacancies.

A methodology has been established in which monochromatic synchrotron radiation is used to excite selected targets and the resulting characteristic X-ray emission is measured with an energy-resolving detector. The experimental cross-sections are obtained after normalization to the incident photon fluence and correction for detector efficiency, geometry, attenuation and target areal density.

The theoretical interpretation requires the combined use of L-subshell photoionization cross-sections, fluorescence yields, Coster–Kronig transition probabilities and fractional radiative emission rates. Comparison between measured and calculated Lα, Lβ and Lγ cross-sections can consequently provide a sensitive test of atomic-physics databases.

The final experimental results should be used to identify the degree of agreement between theory and experiment and to determine which atomic parameter sets provide the most reliable description of the observed L-series emission.

Overall, synchrotron-based L-shell X-ray production measurements represent an effective method for obtaining high-quality atomic data and improving the fundamental parameters required for quantitative X-ray fluorescence analysis.

## Data Availability

The experimental data supporting the findings of this study should be made available from the corresponding author upon reasonable request or deposited in an appropriate public repository.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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