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Atomic Relaxation Dynamics and X-Ray Fluorescence Cross-Sections of Heavy Elements under Monochromatic Synchrotron Excitation

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Abstract

When a high-energy photon from a synchrotron source strikes a heavy atom and removes an electron from an inner shell, the atom is left in an excited and unstable state. It returns to a stable, lower-energy configuration either by emitting a characteristic X-ray photon, a process called X-ray fluorescence, or by ejecting a second electron, known as the Auger effect or, for transitions within the same shell, the Coster–Kronig effect. This paper explains, in simple physical terms, how this atomic relaxation process works and how it is studied experimentally using monochromatic synchrotron radiation. We describe how an inner-shell vacancy is created, how the competition between radiative and non-radiative decay is captured by the fluorescence yield, and how X-ray fluorescence cross-sections are defined, measured, and calculated. A representative experimental methodology for synchrotron-based X-ray fluorescence studies of heavy elements (high atomic number Z) is presented, together with the typical trends seen in fluorescence yield and cross-section with increasing atomic number, and a comparison with established theoretical predictions.

Keywords: atomic relaxation, X-ray fluorescence, fluorescence yield, photoionization cross-section, Auger effect, Coster–Kronig transitions.

1. Introduction

Every atom is built around a nucleus surrounded by electrons arranged in shells, labelled K, L, M, N and so on, moving outward from the nucleus. Electrons in the inner shells, especially the K and L shells, are held very tightly because they sit close to the positively charged nucleus. In heavy elements, those with a large atomic number Z such as gold, lead, tungsten, or uranium, these inner-shell electrons are bound by energies ranging from a few keV to over a hundred keV. To remove one of these electrons, a photon must carry at least as much energy as the binding energy of that shell.

Synchrotron radiation facilities can produce X-ray beams of extremely high intensity, and, after passing through a crystal monochromator, these beams can be tuned to a single, well-defined photon energy. When such a monochromatic beam is directed at a sample containing heavy atoms, photons with energy above a particular shell's binding energy can knock out an electron from that shell. This process is called photoionization, and it leaves behind an atom with a hole, or vacancy, in an inner shell.

An atom with an inner-shell vacancy is not in its lowest energy state, so it does not stay that way for long. Within a very short time, typically of the order of 10^{-14} to 10^{-16} seconds, an electron from a higher shell falls down to fill the vacancy. The energy released in this process can leave the atom in one of two ways: as a photon of characteristic X-ray radiation (fluorescence), or by transferring the energy directly to another electron in the atom, which is then ejected (the Auger or Coster–Kronig effect). Which of these two outcomes happens, and how often, depends strongly on the atomic number of the element and on which shell the original vacancy was in.

Understanding this relaxation process matters for several reasons. X-ray fluorescence is widely used as an analytical technique to identify and quantify elements in a sample, from art conservation to environmental monitoring to materials science. Auger electron spectroscopy is used to study surfaces. Inner-shell vacancy production and decay are also important in radiation physics, nuclear medicine, and astrophysics, where similar processes occur in stellar and interstellar environments. Heavy elements are of particular interest because their fluorescence

yields are high and their characteristic X-ray energies are large enough to be cleanly separated from background signals, making them convenient test cases for precise cross-section measurements.

This paper has three goals. First, to explain in plain language the physics of atomic relaxation following inner-shell ionization, covering the basic theory of fluorescence yield and Coster–Kronig transitions. Second, to describe how X-ray fluorescence cross-sections are defined and related to the more fundamental photoionization cross-section. Third, to describe how monochromatic synchrotron radiation is used in practice to measure these cross-sections for heavy elements, including a representative experimental methodology, typical results, and a comparison with theoretical models. The treatment is kept at an introductory research level, suitable for a reader who is familiar with basic atomic physics but who wants a clear, self-contained account of this particular topic.

2. Theoretical Background

2.1 Creating an Inner-Shell Vacancy

Photoionization is the starting point of the complete process. An incoming photon of energy hν is absorbed by an atom and if hν is greater than the binding energy E_B of an electron in a certain shell, that electron can be expelled as a free photoelectron. The surplus energy over the binding energy is taken away as the kinetic energy of this photoelectron:

$$E_{kinetic} = h\nu - E_B$$

The binding energies of inner shells are substantially larger than those of outer shells, therefore a photon must have enough energy to overcome the binding energy of the shell it ionizes. This is why photoionization cross sections have dramatic jumps termed absorption edges at photon energies equal to the binding energy of each shell. A photon with energy below the K - edge energy cannot ionize the K shell at all, no matter how powerful the beam is. Just above the K - edge, K - shell photoionization suddenly becomes conceivable, and the absorption cross - section jumps upward. Here monochromatic synchrotron radiation is particularly beneficial as the photon energy may be precisely regulated above or below a specified absorption edge, allowing the investigator to analyze one shell at a time selectively. The K and L shells of heavy elements are most routinely examined because their binding energies are in a convenient X-ray range (a few keV to around 100 keV) and their fluorescence yields are substantial enough to provide a strong, quantifiable signal.

2.2 Radiative versus Non-Radiative Relaxation

If an inner shell becomes vacant, the atom relaxes and an electron from a higher shell falls down to fill the void. Where does the energy differential between the two shell levels go? There are two competing channels.

The first potential channel is radiative decay, i.e. X-ray fluorescence. The electron falls in to fill the vacancy, and the excess energy is expelled as a photon. The photon energy is equal to the difference between the two atomic energy levels involved and so is characteristic of the element and the particular transition for example K_α, K_β, L_α etc. Each element has its own unique energies. X-ray fluorescence can therefore be used as a fingerprint to determine which elements are present in a sample.The second pathway is a nonradiative decay. Rather than emitting a photon, the atom transfers the transition energy directly to another electron, which is then ejected from the atom. If the expelled (Auger) electron originates in a shell further out than that of the shell providing the filling electron, this is called the Auger effect. If the vacancy is filled by an electron from a sub-shell of the same primary shell, e.g. an L_1 vacancy filled by an L_3 electron with another L-shell electron ejected, the process is called a Coster–Kronig transition. Coster-Kronig transitions are essential because they can move a vacancy from one subshell to another inside the same shell before the emission of an X-ray, therefore affecting the total fluorescence yield of that shell.Both radiative and non-radiative decay leaves the atom with a new vacancy, this time in a less tightly bound shell, and the entire relaxation process

can cascade through several subsequent steps until all vacancies have moved out to the outermost shells, where they are filled by capturing free electrons from the surrounding medium.

2.3 Fluorescence Yield

The most essential metric describing the competition between radiative and non-radiative decay is the fluorescence yield, generally denoted as ω. The fluorescence yield for a given shell is the likelihood that a vacancy in a certain shell will be filled by the emission of a distinctive X-ray photon in preference to the ejection of an Auger electron:

$$\omega K \frac{number\ of\ K-shell\ vacancies\ filled\ radiatively}{total\ number\ of\ K-shell\ vacancies}$$

Equivalently, if Γ_R is the radiative decay rate (the rate of X-ray emission) and Γ_A is the non-radiative (Auger) decay rate, the fluorescence yield can be written as:

$$\omega = \Gamma_R / \Gamma_R + \Gamma_A$$

The yield of fluorescence is quite sensitive to atomic number. For light elements like carbon or oxygen the Auger process is almost fully dominant and the K-shell fluorescence output is barely a few percent. The radiative decay rate increases as approximately Z^4 while the Auger rate is almost independent of Z. This means that the fluorescence yield of the K shell is considerable for heavy materials such as gold (Z=79), lead (Z=82), or uranium (Z=92), typically greater than 0.9, suggesting that more than 90 percent of the vacancies in the K shell are filled by X-ray emission, and not by the Auger effect. This is one of the reasons why heavy elements have strong easily quantifiable X-ray fluorescence signals and are convenient objects for cross-section research. The fluorescence yields for the L- and M-shell are often smaller than the K-shell yield for the same element. thus is due to the smaller energy differences between levels in the outer shells, and thus favours the (relatively energy-independent) Auger process. The L shell is further complicated by the fact that there are three sub-shells, L_1, L_2, and L_3, each of which has its own fluorescence yield and its own set of probable Coster-Kronig transitions between them.

2.4 Coster–Kronig Transitions and Their Effect

Coster–Kronig transitions make the straightforward picture of a single fluorescence yield per shell complicated. Since a L_1 vacancy may be transferred to a L_2 or L_3 sub-shell via a Coster-Kronig transition before any photon is emitted, the effective (or average) fluorescence yield observed for the L shell as a whole depends not only on the individual sub-shell yields but also on the Coster-Kronig transition probabilities, usually denoted f_{ij} for a transition from sub-shell i to sub-shell j. Thus, a full description of L-shell or M-shell relaxation needs a modest set of coupled equations connecting the sub-shell fluorescence yields, the Coster-Kronig probability and the initial distribution of vacancies formed by photoionization. The main physical point for the purpose of this paper is simple: Coster-Kronig transitions redistribute vacancies between sub-shells of the same principal shell and because different sub-shells have different fluorescence yields the overall measurable intensity of the different fluorescence lines is changed. Therefore, accurate measurements of XRF cross-sections on heavy components, in particular in the L-shell area, must use Coster-Kronig effects instead of treating each sub-shell separately.

3. X-Ray Fluorescence Cross-Sections

3.1 From Photoionization to Fluorescence

In a synchrotron XRF experiment, what is measured is not the fluorescence yield but the X-ray fluorescence production cross-section. This cross-section tells us, with a beam of photons of a specific energy impinging on a sample, the probability of producing a particular characteristic x-ray line (e.g., K_α) per atom. It combines two pieces of physics: how likely the incoming photon is to create a vacancy in the relevant shell in the first place (the photoionization cross-

section) and how likely that vacancy is to be filled radiatively rather than through the Auger effect (the fluorescence yield) – together with the relative probability that the emitted photon belongs to the particular line being measured (the radiative transition probability, or branching ratio).

The K-shell fluorescence cross-section for a particular line such as Kα is, in the simplest example, given by:

$$\sigma_{K\alpha}(E) = \sigma_K(E)\omega_K f_{K\alpha}$$

Here $\sigma_K(E)$ is the K-shell photoionization cross-section at incident photon energy E, ω_K is the K-shell fluorescence yield introduced earlier, and $f_{K\alpha}$ is the fractional radiative transition probability that, given a radiative K-shell decay occurs, the emitted photon is specifically a K_α photon rather than a K_β or other K-line photon. This last factor is sometimes called the emission rate or branching ratio for that line.

3.2 The Photoionization Cross-Section

The photoionization cross-section $\sigma_K(E)$ itself is a function of the input photon energy E and of the atomic number Z of the absorbing atom. The cross-section is largest near and just above the absorption edge and then falls off smoothly as the photon energy is increased further above the edge. The dependence is approximately a power-law: $\sigma \propto E^{-n}$ where n is usually in the range 2.5-3 for K-shell photoionization in the few-keV to few-hundred-keV range of interest for heavy elements. Tabulated photoionization cross sections calculated within the framework of relativistic atomic structure calculations are available for all elements and have been frequently used as reference values for the comparison of experimental fluorescence cross-section observations. The situation for L-shell and M-shell ionization is more complicated, because each principal shell contains multiple sub-shells with their own absorption edges and their own photoionization cross sections, and, as discussed in Section 2.4, Coster-Kronig transitions mix the vacancies between these sub-shells before the final X-ray emission occurs.

3.3 Why Heavy Elements and Monochromatic Excitation

The nature of this type of investigation is determined by the choice of two experimental parameters: the use of heavy elements as samples and the use of a tunable, monochromatic synchrotron beam as excitation source. Heavy components are favored for a variety of reasons. Their K and L binding energies are conveniently placed to coincide with the photon energies accessible to most synchrotron beamlines (about 5 to 100 keV). Their fluorescence yields are substantial, as indicated in Section 2.3, which gives a bright, easily recognized signal over background. Their characteristic x-ray energies are well separated from one another and from common background and scattering lines, such that identification of peaks in the observed spectrum is straightforward. Finally, there is a strong practical reason to measure cross-section data accurately for applications such as elemental analysis of geological and archaeological artifacts, nuclear forensics and radiation shielding estimates.

On the other hand, monochromatic synchrotron radiation has a number of advantages over traditional X-ray tube sources. A crystal monochromator can be used to set the photon energy to great precision so that the experimenter can stimulate a given shell cleanly, just above its absorption edge, without also stimulating neighboring shells or causing undesired background. The beam intensity is quite strong and good counting statistics are obtained even for elements or transitions with small cross-sections. The beam can be focussed to a small spot size which is advantageous for analyzing small or non-uniform samples. The incident photon energy is known exactly and hence the measured fluorescence cross-section may be directly compared with theoretical values at the same energy, which is critical in testing the atomic structure calculations.

4. Synchrotron Radiation as an Excitation Source

Origin of Synchrotron Radiation

Charged particles, usually electrons, are accelerated to near the speed of light in a huge storage ring and forced to change direction by magnetic fields, producing synchrotron radiation. When a relativistic charged particle is accelerated it radiates electromagnetic radiation. This includes when it changes direction (not speed). This occurs continuously in a storage ring as the electron beam circulates and at relativistic speeds the radiation is strongly beamed forward in the instantaneous direction of motion. The result is an extremely intense, narrow cone of radiation covering a broad range of photon energies from infrared through visible light to hard X-rays. Modern synchrotron facilities also have insertion devices such as wigglers and undulators in straight areas of the storage ring. These devices wiggle the electron beam back and forth with a periodic series of magnets, generating radiation of even higher intensity and, in the case of undulators, with the intensity concentrated into narrow energy bands through constructive interference of the radiation from successive magnetic periods. The high flux combined with the tunability makes synchrotron beamlines especially well-suited for atomic and X-ray physics investigations such as those detailed in this study.

Monochromatization

The radiation that comes straight out of a synchrotron source even after going through an insertion device still spans a range of photon energies (this is frequently called "white" or "pink" beam). The beam is transmitted via a crystal monochromator, usually a pair of silicon crystals in what is called a double-crystal monochromator, to produce a single well-defined photon energy sufficient for the selective excitation of a particular absorption edge. The principle of a crystal monochromator is Bragg diffraction. When the Bragg condition is satisfied, X-rays of a certain wavelength λ are significantly reflected from a crystal lattice:

$$n_\lambda = 2d\ sin\theta$$

where d is the spacing between crystal lattice planes, θ is the angle of incidence on the crystal, and n is an integer (the diffraction order). For a crystal set at a specific angle θ, only the photons satisfying the Bragg condition at that angle are significantly reflected; other energies are largely rejected. The use of two crystals in series fixes the direction of the outgoing beam when the angle (and, consequently, the energy selected) is varied, which is beneficial for the further optics of the beamline and the experimental setup downstream.

The monochromatic beam obtained in this way generally has an energy resolution (ΔE/E) of about 10^{-4}, which is much less than the natural width of most absorption edges. This allows the experimenter to set the incident photon energy just above a chosen absorption edge, e.g. just above the K-edge of a heavy element, so that in this configuration only K-shell photoionization contributes to the observed fluorescence signal and not L-shell or other competing processes at higher energy. The photoionization cross-section itself can also be mapped as a function of energy by stepping the monochromator through an energy range around an edge.

Practical Advantages for Heavy-Element XRF Studies

In view of the aforesaid qualities, monochromatic synchrotron radiation is a useful source for the determination of x-ray fluorescence cross-sections in heavy elements for three reasons. The first is selective excitation: by adjusting the photon energy slightly above a selected absorption edge it is possible to ionize a single shell with little interference from the other shells, which simplifies the interpretation of the ensuing spectrum. Secondly, large flux: while the monochromator selects only a narrow energy band, the underlying synchrotron beam is so intense that the monochromatic flux achieved is still many orders of magnitude higher than that from a conventional X-ray tube, allowing precise measurements even for weak fluorescence lines. Third, known incident energy and flux: both the photon energy and the number of incident photons can be measured accurately (the latter by using calibrated ionization chambers or photodiodes placed before the sample). Therefore, from the data the absolute fluorescence cross-section can be extracted, not only relative intensities, allowing a direct comparison with theoretical predictions.

5. Experimental Methodology

5.1 Beamline Setup: The synchrotron based XRF experiment is performed on a hard X-ray beamline equipped with a monochromator to provide monochromated beam. The beam traverses slits and ionization chambers that measure the incident photon flux. The sample is positioned at 45° to the incident beam, and is prepared as a thin foil, pellet or film. To minimize scattering, an energy dispersive detector such a Silicon Drift Detector (SDD) or High Purity Germanium (HPGe) detector is positioned at 90° to the incident beam to detect the fluorescence X-rays emitted.

5.2 Sample Preparation: To limit self-absorption effects and simplify cross-section computations, thin target samples are created. Heavy element samples are usually made up as evaporated thin films, pressed pellets with low-Z binders or dried solutions on polymer backings. The areal density of the sample is separately assessed as it is needed for the proper cross-section determination.

5.3 Measurement Procedure: The incident photon energy is tuned by a monochromator just above the absorption edge (K-edge or L-edge) of the element of interest. The monochromatic beam is then used to irradiate the sample and the detector is used to record the fluorescence spectrum. The spectrum includes recognizable peaks like K_α, K_β, L_α, L_β lines and background radiation. Energy calibration and background correction are performed before data analysis complete cross-section data were obtained by repeating the measurements for some heavy elements and at varying incidence energy.

5. 4 Data Analysis : The fluorescence cross-section is then determined by subtracting the background to determine the net peak area. The measured count rate is then corrected for detector efficiency, detector solid angle and self-absorption. The experimental fluorescence cross-section is determined as:

$$\sigma_F = N/ I_0 N_t \varepsilon(E) \Omega T$$

where:
σ_F = Experimental X-ray fluorescence cross-section
N = Net fluorescence peak counts after background subtraction
I_0 = Incident photon flux
N_t = Number of target atoms per unit area
$\varepsilon(E)$ = Detector efficiency at fluorescence energy E
Ω = Solid angle subtended by the detector
T = Correction factor for self-absorption and transmission effects

6. Results and Discussion

Trends in K-Shell Fluorescence Yield with Atomic Number

As can be seen in Section 2.3, the K-shell fluorescence yield ω K increases sharply with atomic number Z. This is because the radiative decay rate increases roughly as Z^4, whereas the Auger decay rate is almost constant with Z. Table 1 shows this trend with typical, widely referenced values for K-shell fluorescence yield for elements ranging from a light element for comparison to several heavy elements common in synchrotron XRF studies.

Table 1. Representative K-shell fluorescence yield (ω_K) and approximate Kα energy for selected elements, illustrating the increase of fluorescence yield with atomic number Z

Element	Z	Kα Energy (keV)	ω_K (approx.)
Aluminium (Al)	13	1.49	0.04
Iron (Fe)	26	6.40	0.34

Element	Z	Kα Energy (keV)	ω_K (approx.)
Copper (Cu)	29	8.05	0.44
Silver (Ag)	47	22.16	0.83
Tungsten (W)	74	59.32	0.96
Gold (Au)	79	68.80	0.96
Lead (Pb)	82	74.97	0.97
Uranium (U)	92	98.43	0.98

Values are representative figures compiled from standard atomic data compilations (e.g. Bambynek et al., Krause) and are intended to illustrate the trend rather than serve as precision reference data.

The tendency is unmistakable: ω_K climbs from a mere few percent for light elements such as aluminium to almost unity for the heaviest elements such as uranium. This is the main reason why heavy elements are favoured for XRF cross-section studies. A vacancy in the K shell of uranium is almost always filled radiatively, giving a strong, clean fluorescence signal, whereas the same vacancy in aluminium is overwhelmingly more likely to be filled by the (experimentally less convenient) Auger process.

K-Shell versus L-Shell Behaviour

The L-shell fluorescence yields show the same qualitative increase with Z but are systematically lower than the corresponding K-shell yields for the same element. This is because the L-shell sub-levels are less tightly bound and the energy released in an L-shell transition is smaller, again favouring the (roughly Z-independent) Auger rate over the (Z-dependent) radiative rate. For the heaviest elements investigated at synchrotron facilities, such as the actinides, L-shell fluorescence yields are typically in the range 0.3 to 0.6, far below the K-shell values of 0.9 or more seen in Table 1 for similarly heavy elements. Also, the measurements of the L-shell cross-sections are more sensitive to Coster-Kronig effects (Section 2.4), as the vacancies formed in the L_1 or L_2 sub-shells can be transported to L_3 before any photon is released. This means that a proper treatment of the L-shell XRF data for heavy elements generally requires the complete set of the sub-shell photoionization cross-sections and Coster-Kronig transition probabilities instead of a single, effective L-shell yield. This is particularly the case when the incident photon energy is tuned just above the L_1 or L_2 edges rather than above all three L edges simultaneously.

Energy Dependence near the Absorption Edge

By setting the monochromator to a number of energies across an absorption edge, the photoionization cross-section (and thus fluorescence) can be plotted as a function of incident photon energy. The overall pattern that appears is a steep increase in cross section at the edge energy itself, and then a smooth fall down as photon energy is taken to higher energies above the edge, consistent with the power law behaviour $\sigma \propto E^{-n}$ outlined in Section 3.2. This behavior is consistent with the idea that once a photon has enough energy to ionize a given shell, the probability of additional excess energy passing through the atom (or ionizing the shell through some other, higher-energy, less-probable interaction) becomes larger than the probability of further ionization of that shell. Small but measurable deviations from the simple power law trend, related to fine details of the atomic potential, and to multi-electron effects, are sometimes observed close to the edge. These deviations themselves are of theoretical interest, providing a sensitive test of more detailed relativistic atomic structure calculations than the simpler tabulated cross-sections capture.

Comparison to Theoretical Predictions

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Experimental fluorescence cross-sections obtained as described in Section 5.4 are usually compared to theoretical values constructed from tabulated photoionization cross-sections (usually from relativistic Dirac–Hartree–Slater or Dirac–Fock calculations), combined with evaluated fluorescence yields and radiative transition probabilities from standard compilations. The synchrotron-based experimental cross sections are in good agreement with theory for K-shell measurements on heavy elements, with differences typically within 5 to 10 percent, similar to the combined experimental uncertainty from detector efficiency calibration, solid-angle determination, and self-absorption corrections. For L-shell and M-shell measurements, the agreement is, in general, somewhat less good, reflecting the increased complexity of multiple sub-shells and Coster–Kronig mixing discussed above, and measurements of this kind continue to provide useful tests and refinements of the underlying atomic structure calculations, especially for the heaviest elements where relativistic effects are most pronounced.

Table 2: Representative L-Shell Fluorescence Yield ((\omega_L)) for Selected Heavy Elements

Element	Z	Lα Energy (keV)	L-Shell Fluorescence Yield (ω_L)
Silver (Ag)	47	2.98	0.12
Tungsten (W)	74	8.40	0.38
Gold (Au)	79	9.71	0.42
Lead (Pb)	82	10.55	0.45
Uranium (U)	92	13.61	0.55

Source: Representative values adapted from Bambynek et al. (1972), Krause (1979), and standard atomic data compilations.

Table 2 gives representative L-shell fluorescence yields for some heavy metals. The data reveal the fluorescence yield grows gradually with the atomic number in a manner comparable to the K-shell behavior. However, the L-shell fluorescence yields are still much smaller than the comparable K-shell values, as Auger and Coster-Kronig transitions compete more strongly with radiative decay in the L shell. For uranium the L-shell fluorescence yield is about 0.55 and the K-shell fluorescence yield is about 0.98. This discrepancy illustrates the higher complexity of analysis of L-shell fluorescence spectra and underscores the necessity of careful consideration of sub-shell photoionization and vacancy transfer processes for accurate measurements of L-shell cross sections.

Table 3: Typical Variation of K-Shell Fluorescence Cross-Section with Incident Photon Energy near the Absorption Edge

Incident Energy (keV)	Normalized Cross-Section (σ/σ_{max})
Edge − 0.5	0.00
Edge + 0.1	1.00
Edge + 1	0.82
Edge + 5	0.58
Edge + 10	0.42
Edge + 20	0.28

Values are normalized to the maximum cross-section at the absorption edge and are intended to illustrate the general trend.

Table 3 shows the fluctuation of K-shell fluorescence cross-section with incident photon energy near the absorption edge. The cross section increases rapidly for incoming energies above the absorption edge and reaches a maximum just above the threshold. The cross-section slowly declines for higher photon energy, with a power-law dependence, approximately, σ∝

E^{-n}. This behaviour is caused by the lower probability of photoionization at high photon energy. Near the edge, small deviations from this smooth trend might arise from fine atomic structural effects, electron correlations and relativistic interactions. Measurements of these deviations with synchrotron radiation give critical tests of sophisticated atomic models and relativistic computations for heavy elements.

7. Applications

Accurate knowledge of atomic relaxation dynamics and fluorescence cross-sections for heavy elements has a practical significance far beyond fundamental atomic physics. These cross sections are the essential input to the conversion of a measured fluorescence intensity to an elemental concentration in quantitative X-ray fluorescence analysis, a technique used routinely in mineral exploration, environmental monitoring of heavy-metal contamination, cultural-heritage and art-conservation studies (identification of pigments and alloys in a non-destructive way), and quality control of industrial materials.
Fluorescence yields and cross-sections of heavy elements such as uranium, thorium and plutonium are needed in nuclear science and radiation physics for nuclear forensics (identifying the origin or processing history of nuclear materials from their characteristic X-ray signatures) , for radiation shielding and dosimetry calculations, and for the interpretation of X-ray emission in studies of nuclear reactions and decay. Inner-shell ionization followed by fluorescence also happens in hot, X-ray irradiated plasmas in astrophysics, like the neighbourhood of accreting black holes or stellar coronae. Fluorescence cross section measurements for heavy elements in the laboratory provide important benchmarks for the modelling of such astrophysical environments. Finally, in medical physics, knowledge of inner-shell ionization in heavy elements serves as a basis for the use of contrast agents and the interpretation of dose enhancement effects in radiotherapy with high-Z materials.

8. Conclusion

A high energy photon from a synchrotron source hits a heavy atom and knocks an electron out of an inner shell. This leaves the atom in an excited state and unstable. It relaxes by generating an or it relaxes into a stable lower energy form by In this study we have discussed in an approachable way the physics of atomic relaxation after inner-shell photoionization and its relation to X-ray fluorescence cross-sections, in particular for heavy metals examined with monochromatic synchrotron radiation. Photoionization produces a vacancy in the inner shell which is then relaxed radiatively, and a characteristic X-ray photon is emitted, or non-radiatively, through the Auger or Coster Kronig effect. The relative importance of the two pathways is described by the fluorescence yield which increases strongly with atomic number. The measurable fluorescence cross-section is the product of the photoionization cross-section, fluorescence yield and the radiative branching ratio for a specific line. Monochromatic synchrotron radiation is particularly suited for the measurement of these cross-sections, since it permits selective, energy-tunable activation of a selected shell with very high photon flux and a well-defined incident energy. A representative experimental methodology, based on a monochromatized beamline, thin-target sample preparation, energy-dispersive detection and careful correction for detector efficiency and self-absorption, allows the extraction of absolute fluorescence cross-sections for direct comparison with theoretical predictions. K-shell fluorescence yields for heavy elements tend to unity, and K-shell cross section measurements generally compare well with theory. L-shell and M-shell measurements are more susceptible to Coster-Kronig effects, and remain an important ongoing test of relativistic atomic structure calculations. These measurements can usefully be extended in future work to less studied heavy and superheavy elements, to higher order satellite and hypersatellite transitions from multiple simultaneous vacancies, and to chemical environment effects on fluorescence parameters, all of which remain active and productive areas of atomic and X-ray physics research.

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