Fundamentals of X-ray Interaction with Matter

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ABSTRACT

X-rays have become an essential tool for probing the atomic and molecular structure of materials. This chapter explores the fundamental principles governing the interaction of X-rays with matter. Starting with the discovery of X-rays and their use in material characterization, it delves into the basic physics behind their interaction with atoms, including absorption, scattering, and diffraction phenomena. These interactions are key in various technological fields, from medical diagnostics to materials science and crystallography. This review also covers advancements in X-ray technology, such as synchrotron sources and their applications in diverse industries.

Keywords— X-ray interaction, absorption, scattering, diffraction, synchrotron sources, photoelectric effect, Compton scattering, X-ray fluorescence, material characterization

# INTRODUCTION

X-ray spectroscopy relies on the interaction of X-rays with matter to provide valuable information about the composition and structure of materials. Understanding these interactions is important for interpreting spectroscopic data accurately.

When an atom becomes unstable or is bombarded with high-energy particles, its electrons undergo transitions between energy levels. During these transitions, the atom absorbs and emits high-energy X-ray photons in a manner characteristic of its chemical element. X-ray spectroscopy detects these energy changes, enabling scientists to identify elements and understand the atomic interactions within various materials.

There are two primary techniques in X-ray spectroscopy: wavelength-dispersive X-ray spectroscopy (WDXS) and energy-dispersive X-ray spectroscopy (EDXS). WDXS measures X-rays of a single wavelength diffracted by a crystal. EDXS, on the other hand, measures X-ray radiation emitted by electrons stimulated by a high-energy source of charged particles. In both methods, the distribution of the radiation reveals the material's atomic structure and, consequently, the components of the object under study.

X-rays have as ionizing radiation a number of other unique properties beyond their very short wavelength. One important property for our science is their element selectivity. By choosing and investigating the spectra of particular elements that are placed at unique places in complex molecules we have a localized "atomic sensor". By investigating these atoms at different times after the structure was excited with light we can trace the development of electronic and structural changes even in very complex systems or in other words follow the electron through the molecule and over interfaces.

**X-ray Absorption Spectroscopy (XAS)**

In x-ray absorption spectroscopy (XAS) the energy of the absorbed photon raises an electron from a deeply bound state into unoccupied bound states or it gains enough energy to escape the atom. The absorption spectrum thus contains detailed information about the density of empty states and allows conclusions about coordination, oxidation state and many more information about the local structure. If the energy of the the photon is sufficient to overcome the binding potential the electron the absorption probability is influenced by a electron scattering process from the local environment of the surrounding atoms. This technique called EXAFS and can be used to determine the local structure around the absorbing atoms.

**X-ray Emission Spectroscopy**

The electrons filling the core hole that is generated during the absorption process emit x-ray photons whose energy can be analyzed. The fine structure of this x-ray emission (XES) give detailed information on the density of filled states and can be used due to the influence of spin-orbit coupling to track the oxidation and total spin state of the emitting atom.

**X-ray diffuse scattering (XDS) / X-ray wide angle scattering (WAXS)**

Photons that are not absorbed can be elastically scattered. Since our interest lays primarily in the dynamics of molecules in solution this process can be used to study the relation of points of high electron density to each other. With other words we can use wide angle x-ray scatter (WAXS) also named x-ray diffuse scattering (XDS) to study structural dynamics in materials. This technique does, like the techniques above, not require that there is a relation between different molecules. Since we are missing the coherent amplification of crystals we can primarily study changes in structures with this technique.

**Combination of techniques**

XAS, XES and XDS give complementary information and are used in combination depending on the capabilities of the instruments. Many of our studies use large scale research facilities like synchrotron- and free-electron-laser facilities. With these techniques we have successfully traced the electron transfer in complex molecules like the shown Ruthenium - Platinum complex with very high time-resolution. We are investigating novel iron-carbene complexes for solar light sensitization, light activated catalysts, novel polymer structures combining light sensitization and catalytic properties and novel nano dots for light sensitization and catalysis.

**Other techniques e.g. x-ray photo electron spectroscopy (XPS)**

We also support the development of local facilities at the MaxIV laboratories and at the Lund Laser Center by e.g. advising and designing the experimental spectroscopy end-station at FEMTOMAX.

In support of many other groups we also use x-ray photo electron spectroscopy to analyze the binding energy of electrons directly. The surface sensitivity of this technique makes it very suitable to investigate the binding and e.g. sensitization of surfaces or catalytic activities of materials. Figure 1 show the X-ray image of skeleton. The passage refers to a significant observation made by Professor Wilhelm Conrad Roentgen following his discovery of X-rays. It explains how Roentgen expanded on the earlier work of Philipp Lenard, who had investigated cathode rays which is streams of electrons in vacuum tubes and how they interacted with different materials. Lenard had used an aluminum window to allow cathode rays to pass out of a vacuum tube while still maintaining its integrity, as glass was believed to block these rays. However, Roentgen showed that a part of the cathode rays, now known as X-rays, could pass through the glass walls of the tube without needing an aluminum window. This was important because it demonstrated that X-rays could travel through materials that were not typically transparent to visible light. Roentgen’s discovery that these rays could affect photographic plates, even without direct exposure to air, was groundbreaking. X-rays could penetrate materials and leave an impression on photographic plates, which became an essential tool for non-invasive imaging.

The passage also highlights one of Roentgen’s most striking discoveries: bones are much less transparent to X-rays than soft tissues like flesh and muscle. This difference in transparency is the basis for X-ray imaging, where the bones appear clearly on a radiograph (an X-ray photograph) due to their higher density. When Roentgen placed a living human hand between the Crookes tube (which generated the X-rays) and a photographic plate, the resulting image (or shadow photograph) clearly showed the bones, with the flesh and muscle being less visible. This discovery had an immediate impact, particularly in medicine, as it enabled physicians to see inside the human body without invasive surgery, and it captured the imagination of the public. The ability to "see" the bones inside a living person was perceived as extraordinary and paved the way for the development of modern medical imaging.

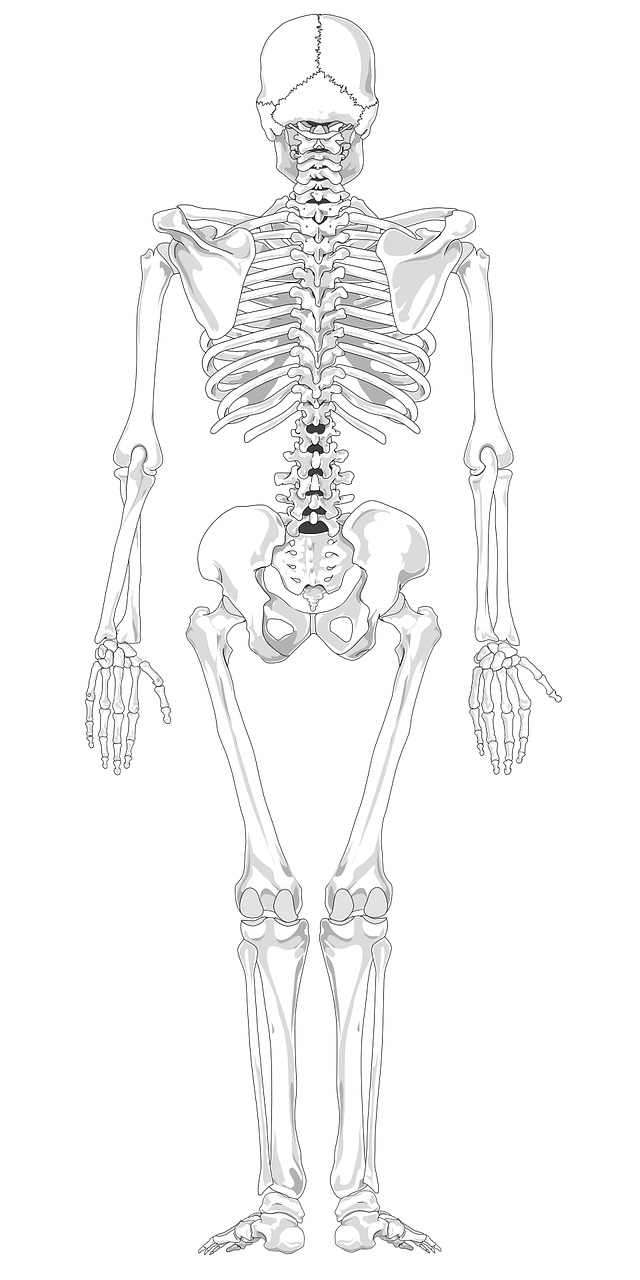


Figure 1. X-ray image of Skeleton taken from https://pixabay.com/vectors/skeleton-human-skeletal-anatomy-41548/

# HISTORY OF X-RAY SPECTROSCOPY

German physicist Wilhelm Conrad Röntgen received the first-ever Physics Nobel Prize in 1901 in recognition of his 1895 discovery of X-rays. According to the SLAC National Accelerator Laboratory, other scientists and doctors immediately adopted his novel method.

Between 1906 and 1908, British physicist Charles Barkla conducted research that resulted in his discovery that X-rays might be characteristic of specific substances. He was also awarded a physics Nobel Prize for his efforts, but that was in 1917.

In 1912, a father-and-son pair of British physicists named William Henry and William Lawrence Bragg actually started using X-ray spectroscopy. They investigated the interactions between X-ray radiation and crystallographic atoms using spectroscopy. Subsequent advances in X-ray technology, including the development of synchrotron sources in the 1940s, have dramatically expanded the use of X-rays in research and industry. These powerful sources allow for the generation of highly intense X-ray beams, making it possible to probe materials with unprecedented resolution and sensitivity.

**How X-ray spectroscopy works**

When an atom is unstable or is bombarded with high-energy particles, its electrons transition from one energy level to another. As the electrons adjust, the element absorbs and releases high-energy X-ray photons in a way that's characteristic of atoms that make up that particular chemical element. X-ray spectroscopy measures those changes in energy, which allows scientists to identify elements and understand how the atoms within various materials interact.

There are two main X-ray spectroscopy techniques: wavelength-dispersive X-ray spectroscopy (WDXS) and energy-dispersive X-ray spectroscopy (EDXS). WDXS measures the X-rays of a single wavelength that are diffracted by a crystal. EDXS measures the X-ray radiation emitted by electrons stimulated by a high-energy source of charged particles.

In both techniques, how the radiation is dispersed indicates the atomic structure of the material and therefore, the elements within the object being analyzed.

**Multiple applications**

Today, X-ray spectroscopy is used in many areas of science and technology, including archaeology, astronomy, engineering and health.

Anthropologists and archaeologists are able to discover hidden information about the ancient artifacts and remains they find by analyzing them with X-ray spectroscopy. For example, Lee Sharpe, associate professor of chemistry at Grinnell College in Iowa, and his colleagues, used a method called X-ray fluorescence (XRF) spectroscopy to identify the origin of obsidian arrowheads made by prehistoric people in the North American Southwest. The team published its results in October 2018 in the Journal of Archaeological Science: Reports.

X-ray spectroscopy also helps astrophysicists learn more about how objects in space work. For example, researchers from Washington University in St. Louis plan to observe X-rays that come from cosmic objects, such as black holes, to learn more about their characteristics. The team, led by Henric Krawczynski, an experimental and theoretical astrophysicist, plans to launch a type of X-ray spectrometer called an X-ray polarimeter. Beginning in December 2018, the instrument will be suspended in Earth's atmosphere by a long-duration, helium-filled balloon. Yury Gogotsi, a chemist and materials engineer at Drexel University in Pennsylvania, creates spray-on antennas and water-desalination membranes with materials analyzed by X-ray spectroscopy. The invisible spray-on antennas are only a few dozen nanometers thick but are able to transmit and direct radio waves. A technique called X-ray absorption spectroscopy (XAS) helps ensure that the composition of the incredibly thin material is correct and helps determine the conductivity. “High metallic conductivity is required for good performance of antennas, so we have to closely monitor the material,” Gogotsi said.

Gogotsi and his colleagues also use X-ray spectroscopy to analyze the surface chemistry of complex membranes that desalinate water by filtering out specific ions, such as sodium. The use of X-ray spectroscopy can also be found in several areas of medical research and practice, such as in modern CT scan machines. Collecting X-ray absorption spectra during CT scans (via photon counting or spectral CT scanner) can provide more detailed information and contrast about what is going on inside the body, with lower radiation doses from the X-rays and less or no need for using contrast materials (dyes), according to Phuong-Anh T. Duong, director of CT at Emory University Department of Radiology and Imaging Sciences in Georgia.

**Fluorescence spectroscopy**

Fluorescence spectroscopy is a powerful technique that can be used for a variety of applications, including life detection. It is based on the principle of fluorescence, which is the emission of light by a substance after it has absorbed photons of a higher energy.

When it comes to life detection, fluorescence spectroscopy can be employed to study biological molecules, such as proteins, nucleic acids, and metabolites. These molecules often possess intrinsic fluorescence or can be labeled with fluorescent probes to enable their detection.

Here's how fluorescence spectroscopy can be used as a life detection technique:

**Protein and Enzyme Analysis:** Many proteins exhibit intrinsic fluorescence due to the presence of aromatic amino acids (such as tryptophan and tyrosine) in their structures. By analyzing the fluorescence properties of proteins, researchers can gain insights into their structure, folding, conformational changes, interactions with other molecules, and enzymatic activity. Changes in the fluorescence characteristics of proteins can indicate alterations in their function or the presence of certain conditions, such as disease states.

**Cellular Imaging:** Fluorescent dyes or probes can be used to label specific cellular components or biomolecules of interest, allowing their visualization and tracking within cells or tissues. This technique, known as fluorescence microscopy, enables researchers to study cellular processes, localization of molecules, and the dynamics of cellular events. For example, fluorescent dyes can be used to stain DNA, RNA, or specific proteins within cells, aiding in the detection of genetic material or protein expression.

**Metabolic Analysis:** Fluorescent probes can be used to monitor metabolic activities within cells. Certain fluorescent dyes can selectively bind to specific metabolites or indicators of metabolic processes. By measuring the fluorescence intensity or lifetime of these dyes, researchers can assess metabolic activities, such as the levels of reactive oxygen species (ROS), pH changes, or calcium ion concentrations. These measurements can provide valuable information about cellular health, energy production, and metabolic alterations associated with diseases.

**DNA/RNA Analysis:** Fluorescence spectroscopy can also be employed to study nucleic acids. DNA and RNA can be labeled with fluorescent dyes or intercalating agents that bind specifically to these molecules. By analyzing the fluorescence emission or changes in fluorescence upon binding, researchers can investigate DNA or RNA structures, study gene expression, perform DNA sequencing, detect mutations, and monitor nucleic acid interactions with other molecules.

Overall, fluorescence spectroscopy offers a versatile and sensitive approach for life detection, enabling the study of biological molecules and processes at the molecular, cellular, and tissue levels. Its applications span various fields, including biochemistry, cell biology, biophysics, and medical research, contributing to our understanding of life and its mechanisms In addition to this it has been concluded that at present the quantitative potentiality of soft and ultrasoft X-ray fluorescence analysis depends decisively on the efficiency of the end window X-ray tube with a thin beryllium window and a rhodium target as well as on the high reflectivity of the SML analyzer. In figure 2. development of X-ray fluorescence spectrometers has been shown.

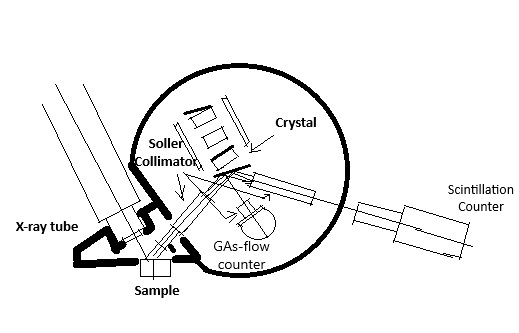


Figure 2. The development of X-ray fluorescence spectrometers

# LITERATURE REVIEW

**3.1. X-ray Absorption and Scattering**

X-ray absorption occurs when an X-ray photon transfers its energy to an electron within an atom, resulting in ionization or excitation of the atom. The probability of X-ray absorption is strongly dependent on the atomic number and the energy of the incident X-rays. The photoelectric effect, first described by Albert Einstein (1905), explains the absorption of low-energy X-rays by inner-shell electrons.

Compton scattering, discovered by Arthur H. Compton (1923), occurs when X-rays interact with loosely bound outer-shell electrons, leading to a shift in the wavelength of the scattered X-rays. The phenomenon is most significant at higher X-ray energies and provides insight into the dual particle-wave nature of X-rays.

Braggs et al (1913) studied that Laue photographs conveniently be interpreted as due to the reflection of X-rays in such planes within the crystal as are rich in atoms. This leads at once to the attempt to use cleavage planes as mirrors, and it has been found that mica gives a reflected pencil from its cleavage plane strong enough to make a visible impression on a photographic plate in a few minutes’ exposure. It has also been observed that the reflected pencil can be detected by the ionization method.

**3.2. X-ray Fluorescence (XRF)**

The foundation of modern atomic structure theory began with the discovery of X-rays in 1895. This discovery was further advanced by the realization of the presence of electrons within atoms, which was confirmed through the observation of spectral line splitting under the influence of an external magnetic field in 1896, and by the scattering of alpha particles by the atomic nucleus in 1910. Over the past several decades, X-ray physics has not only driven research and development in various fields of natural science but has also significantly contributed to medical advancements. In today's world, X-ray technology remains crucial for progress in material science.

Watson and Crick proposed the structure of DNA based on insights from both biological data and structural chemistry, including X-ray crystallography. Wilkins contributed significantly by precisely analyzing the crystal structure of DNA using the rotating crystal method. The integration of their research ultimately led to the discovery of the double helix, a three-dimensional structure resembling a twisted ladder with the four nucleotide bases—adenine, thymine, guanine, and cytosine—regularly arranged between the two strands.

The high transparency of the human body to X-rays, combined with their growing application in medicine, significantly advanced the field of medical imaging. In 1960, Oldendorf envisioned developing a relevant imaging device, and in 1963 and 1964, Cormack introduced a mathematical framework for three-dimensional imaging, laying the groundwork for further innovations.

X-ray fluorescence is a process in which an X-ray photon excites an electron from an inner orbital, causing it to be ejected from the atom. As the atom returns to its ground state, it emits characteristic secondary (fluorescent) X-rays. XRF is widely used for elemental analysis in fields like geology, archaeology, and material science (Lachance and Traill, 1966).

**3.3. X-ray Diffraction (XRD)**

The diffraction of X-rays by crystalline materials was first explained by Max von Laue (1912) and later refined by William L. Bragg and his father, William H. Bragg (1913). XRD has since become a key tool for determining the atomic and molecular structure of materials. The technique is based on the constructive interference of X-rays scattered by atoms in a crystal lattice, revealing the spacing between planes of atoms.

Radiography began without a clear understanding of the radiation involved, as the true nature of X-rays wasn't uncovered until 1912. In that year, the discovery of X-ray diffraction by crystals not only confirmed the wave nature of X-rays but also introduced a new technique for examining the fine structure of matter. While radiography is an essential tool with a broad range of applications, it is typically limited in the resolution of internal details, only revealing structures down to about 10⁻³ mm. In contrast, diffraction can indirectly expose much finer details, down to 10⁻⁷ mm, making it a powerful method for exploring the internal structure of materials.

**3.4. Advances in Synchrotron X-ray Sources**

Synchrotron radiation, first observed by Ginzburg and Frank (1947), has transformed X-ray research. Synchrotron sources generate highly intense, tunable X-ray beams that can be used for various applications, including phase-contrast imaging and microtomography. Their ability to provide brilliant X-rays with narrow energy bandwidths has opened new frontiers in materials characterization (Huang et al., 2014).

Advances in synchrotron X-ray sources have revolutionized the field of X-ray science, offering unprecedented capabilities for material analysis and imaging. Synchrotron radiation is produced when charged particles, typically electrons, are accelerated to near-light speeds and forced to travel in a circular path by powerful magnetic fields. This process generates highly intense, collimated beams of X-rays that can be finely tuned across a wide range of wavelengths. Synchrotron sources provide X-rays with much higher brightness and brilliance compared to conventional X-ray tubes, enabling more detailed and sensitive measurements. Over the years, technological improvements, such as the development of third- and fourth-generation synchrotrons, have enhanced the coherence, focus, and energy tunability of the X-rays. This has led to a broad spectrum of applications, from phase-contrast imaging and high-resolution crystallography to time-resolved studies and nanotomography. These advances have opened new possibilities in diverse fields, including materials science, biology, chemistry, and even environmental science, allowing researchers to investigate atomic and molecular structures, study dynamic processes in real-time, and perform element-specific analyses with remarkable precision.

# OBSERVATION AND RESULTS

This section summarizes key experimental and theoretical findings from the study of X-ray interactions with matter:

* **Absorption Edges:** At specific energies, known as absorption edges, X-rays are more readily absorbed by a material. These edges correspond to the binding energies of electrons in different atomic orbitals, providing insight into the electronic structure of materials.
* **Compton Shift:** The wavelength shift observed in Compton scattering experiments confirms the quantum nature of X-rays, with the magnitude of the shift dependent on the scattering angle and the energy of the incident X-rays.
* **Bragg’s Law:** X-ray diffraction patterns can be analysed using Bragg’s Law, nλ=2dsinθ, to determine the interplanar spacing in crystalline materials. This equation forms the basis of X-ray crystallography, enabling the determination of atomic structures with high precision.
* **Fluorescence Yield:** XRF studies have demonstrated that the intensity of the emitted fluorescent X-rays is directly proportional to the concentration of the element within a sample, making XRF a powerful tool for quantitative elemental analysis.

An X-ray photon can interact with an atom in two primary ways: it can either be scattered or absorbed. We will discuss these processes individually. When X-rays pass through a dense material composed of a large number of atoms or molecules, it can sometimes be more practical to treat the material as a continuous medium with a defined boundary between it and the surrounding vacuum (or air). At this boundary, the X-ray beam undergoes refraction and reflection, providing an alternative framework for discussing the interaction. The scattering and refraction models are fundamentally equivalent. In Chapter 3, we will derive the equations governing X-ray reflectivity and use this equivalence to connect reflectivity with the microscopic properties of the material under study.

# CONCLUSION

The interaction of X-rays with matter is rooted in the foundational principles of quantum mechanics and electromagnetic theory. These interactions occur primarily through processes such as absorption, scattering, and diffraction, each offering unique insights into the atomic and molecular structures of materials. Absorption occurs when X-rays transfer their energy to the electrons within an atom, while scattering involves the deflection of X-rays by the electrons, leading to valuable information about material density and structure. Diffraction, on the other hand, provides a way to probe the arrangement of atoms in crystalline materials by analyzing the interference patterns created when X-rays are scattered by a lattice of atoms. These mechanisms form the basis for several powerful techniques, such as X-ray crystallography and spectroscopy, which have become indispensable in fields ranging from materials science to biology. Moreover, advancements in X-ray technology, particularly with the advent of synchrotron sources, have significantly expanded the scope and precision of these analyses. Synchrotron radiation generates highly intense and tunable X-ray beams, enabling detailed studies of complex systems with enhanced resolution. Consequently, X-rays play a crucial role in both fundamental research, such as studying atomic structures, and practical applications, including medical imaging and material characterization. This chapter emphasizes the importance of X-rays in advancing knowledge and technology across diverse scientific and industrial domains.

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