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X-Ray Diffraction Imaging

Technology and Applications

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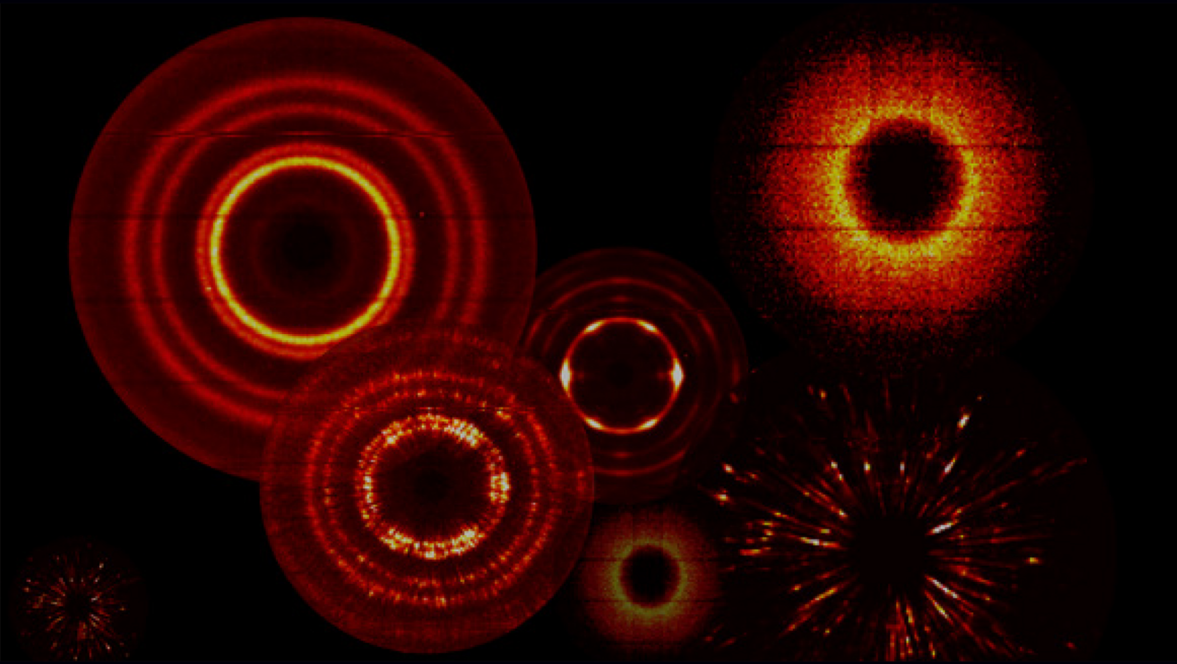

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Technology and Applications

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Introduction to X-Ray Diffraction Imaging

X-rays have been used for an array of sensing, imaging, and detection tasks for well over 100 years. The birth of radiographic imaging followed mere months after Röntgen's "discovery" of the X-ray in 1895, and X-ray diffraction (XRD) was already in use for aiding in the determination of crystalline structure by 1912. The pioneering work of Max von Laue and the father–son team of W. L. and W. H. Bragg provided both demonstrations and interpretations of the physics behind XRD and have enabled a variety of refinements, generalizations, and simplifications of the method. As a result, XRD is now a quantitative, versatile, and ubiquitous tool that has been used across science and engineering.

The most common X-ray diffraction systems, however, measure only the XRD signal from a single location on the surface of a sample (i.e., they do not perform imaging). Thus, despite the commercial and scientific success of X-ray diffraction in general, its implementation as a non-imaging modality limits its applicability to the analysis of thin samples and/or surfaces only. As a consequence, many industries have historically not been able to use XRD for performing meaningful material characterization; instead, they have had to settle for transmission-based X-ray imaging, which provides the required spatial information but insufficient material specificity. The inadequacy of this approach is particularly apparent in cases in which both the shape and composition of a sample must be analyzed or in which the material of interest is concealed or otherwise obfuscated. Important examples of these scenarios arise in the diagnosis and detection of cancer in medical imaging and the detection of explosives and/or contraband items for security applications.

Various schemes for transforming XRD into an imaging modality have been proposed, dating back to the late 1980s. While these approaches were successful in demonstrating the capacity for realizing spatially resolved XRD analysis, they were prohibitively slow, expensive, and complicated, typically requiring some combination of a synchrotron X-ray source, cryogenically cooled, high-purity Germanium detectors, and minimal computational resources. As a result, X-ray diffraction imaging was regarded as an interesting prospect but went several decades without significant advancement or adoption for commercial application.

Over the last decade, though, two key technological innovations have revolutionized X-ray diffraction imaging. The first centers around the role and capabilities of computers in imaging systems today. The incredible growth of CPU and GPU performance in combination with theoretical insights in information and sensing theory have led to a paradigm shift in the approach to imaging system design in general. Alternative physical measurement architectures combined with novel post-processing algorithms allow for smarter, faster, cheaper, and more optimized imaging and detection systems. As an example of a computationally centric X-ray architecture, Chapter 1 of this book discusses a coded aperture approach to XRD imaging that leverages compressed sensing and machine learning techniques for improved performance. Similarly, Chapter 6 describes the newly developed XRD focal construct technology for performing fast, robust, depth-resolved XRD imaging. Finally, Chapter 7 introduces new measurement and data processing approaches that enable high-resolution XRD imaging with reduced scan times and dose, as well as methods to efficiently image textured, crystalline materials. Together, these techniques allow one to extract more information about a sample given a fixed set of resources, thus allowing XRD imaging to be realized at lower dose, shorter acquisition times, and lower cost, using inexpensive, off-the-shelf components.

The second technological innovation that has enabled practical XRD imaging is the development of efficient, multi-pixel spectroscopic detector arrays with shot-noise-limited performance. These components build on critical advances in the growth of high-quality, high-yield semiconductor materials, such as CdTe and CZT, as well as the development of low-noise electronics and attachment schemes. Such detectors are critical to XRD imaging, as the measurable XRD signal is generally weak, diffuse, and both energy- and angle-dependent; high-quality imaging therefore requires high signal-to-noise ratio measurements of the X-ray signal over each of these dimensions. The topics of semiconductor detector development and the associated integrated circuits are discussed in Chapters 2 and 3, respectively. Chapter 8 extends this discussion in the context of airport security systems by describing the specifications and design tradeoffs for such detectors as part of the inverse fan beam XRD imaging architecture.

Having established the tools and methods that have given rise to the recent renaissance in XRD imaging, this book continues by exploring a range of areas in which XRD imaging is currently having or could have a significant impact. Chapter 4 discusses applications of XRD imaging in medicine, including topics such as cancer detection, analysis of brain tissue, and bone mineral analysis. Chapter 5 discusses broadly the impacts and opportunities for XRD imaging in materials science, with a particular focus on processing–structure–property relationships and implications to security applications. In addition, Chapters 1, 6, 7, and 8 touch on other uses of XRD imaging, including explosives detection in aviation security, inspection of mail and cargo, process control in various industries, environmental monitoring, and food inspection.

This is the first book to focus on XRD imaging and is well-timed to capture both the remarkable recent progress and potential impact of this new and exciting field. All of the discussions in this book are based on the most state-of-the-art methods and results in the field and are written by leading international researchers who are performing groundbreaking work. Despite the cutting-edge nature of the content, the book is written to provide a self-contained historical and technical introduction to the topic so that experts and newcomers alike can understand and appreciate this powerful technology.

Thank you to all of our collaborators and colleagues that contributed to the content of this book. We hope that the readers will be as excited about the prospects for XRD imaging as we are, and that this book serves as a teaching tool and reference for the next generation of X-ray diffraction imaging scientists.

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Coded Aperture X-Ray Diffraction Tomography

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CONTENTS

1.1 Introduction

X-ray photons, with wavelengths of 0.01 to 10 nm, reside in a unique place within the electromagnetic spectrum, in that they can investigate samples at two disparate length scales. On the one hand, X-rays can pass through centimeters of most materials and, in so doing, map out an object's properties at this macroscopic length scale. On the other hand, the fact that X-ray wavelengths are comparable to the atomic and/or molecular spacing of different materials means that one can determine the microscopic structure of a material. The interaction that makes the structural analysis possible, known as coherent scatter, underlies the mechanism of X-ray diffraction (XRD). X-ray diffraction is a well-established technique that represents a gold standard in materials analysis. Taken together, the capacity for X-rays to both penetrate the entirety and interact at the microscopic scale with a target object make possible non-destructive, volumetric imaging of the molecular structure of objects that are not transparent at conventional optical wavelengths. We refer to this imaging method as X-ray diffraction tomography (XRDT).

X-ray diffraction tomography has been explored since the 1980s as a method to provide spatially resolved information about the molecular structure of materials.[1,2] This technique has the potential to greatly complement existing tomographic imaging modalities, such as computed tomography (CT),[3] ultrasound,[4] and magnetic resonance imaging (MRI),[5] by providing orthogonal material information and enhanced contrast. However, traditional XRDT approaches have typically required excessively long scan times and/or large doses and specialized or expensive components.[6] As a result, XRDT has not yet emerged as a practical imaging modality, despite the extensive literature supporting the rich and relevant information contained within the XRD signal itself.[7]

A new approach to XRDT, known as coded aperture XRDT, was developed in the early 2010s and has been shown to reduce scan times by several orders of magnitude and requires only conventional, off-the-shelf X-ray components.[8,9] The technique uses a combination of physical coding (i.e., modulation of the XRD signal in real space) and computational processing to optimally extract information from the measured X-rays. This technique has been made possible by the exponential growth of computing power over recent decades, the development of advanced and compressive sensing algorithms, and the availability of simple and high-performing detectors and sources. The resulting CA-XRDT architecture is highly flexible and can be customized to a particular application and associated set of constraints. In this chapter, we introduce CA-XRDT in the context of previously developed XRDT methods, describe specific instantiations of the method (including practical considerations), and discuss areas in which the CA-XRDT approach provides distinct benefits. Examples of scenarios in which CA-XRDT is particularly well-suited to the problem space include bottle and luggage inspection for aviation or border security, the diagnosis and/or detection of cancer, food inspection, and environmental monitoring.

1.2 Overview of X-Ray Diffraction Tomography

1.2.1 Tomographic Imaging

Tomography involves the estimation of a higher dimensional object from the measurement of one or more lower dimensional projections of the object. The fact that the measurement dimension is usually smaller than the object's embedding dimension (i.e., dimension in which the object physically exists) implies that tomographic imaging involves multiplexed measurements.[10] Through a combination of measurement design and computational data processing techniques, one can invert (i.e., demultiplex) the acquired data and recover an estimate of the object. The mechanism for contrast in the image depends on the physics of the interaction between the X-rays and the sample which, in turn, strongly influences the overall measurement architecture.

A well-known example of tomographic imaging is X-ray computed tomography (CT), in which a multitude of transmission-based projection images of an object are acquired from different perspectives around the object (see Figure 1.1a). While each projection image multiplexes attenuation from all points along the direction of propagation, the measurement diversity includes many different multiplexing instantiations, which allows for an accurate and unique determination of the underlying object. For the case of single-energy CT, the contrast mechanism is based on photoelectric absorption, and the resulting image is a map of the electronic density throughout the measured object volume. Alternatively, one can perform multi-energy (or spectral) CT,[11] which enables one to recover a volumetric mapping of both the effective atomic number and electron density (or photoelectric and Compton interaction strengths) throughout the object.

While this scheme has the advantage that the measured X-ray signal is typically bright and highly focused, it has several drawbacks. For example, the requirement that one make many different measurements to estimate a single voxel renders imaging dynamic scenes challenging.[12] In addition,

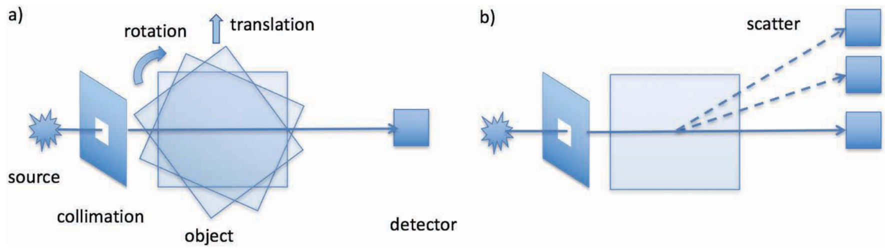

FIGURE 1.1
Schematic for tomographic measurement using (a) transmission and (b) scatter measurements. For transmission tomography, the requirement that each voxel be measured from multiple orientations implies that the rotation and/or translation of the object must occur. For scatter tomography, the angular spread of the scatter signal relegates the need for rotation and enables snapshot operation.

this leads to unnecessarily high-object exposure (including the exposure of unwanted regions of the sample), which is particularly undesirable for the case of medical imaging.[13] Finally, the contrast produced by attenuation alone may be insufficient for distinguishing particular features of interest.[14] In general, these contrast, dose, and speed-related issues stem from the fact that transmission-based imaging is sensitive only to X-rays that did not interact with the sample. As a result, all object-specific information is indirect, and the system makes poor use of the photons passing through the object because all directly interacting, or scattered, X-rays are blocked. While proposed methods, such as hyperspectral CT,[15] promise the potential for chemical sensitivity via transmission imaging, they still do not provide the molecular specificity often required in a variety of diagnosis- and/or analysis-focused tasks.

Rather than using the non-interacting, directly transmitted X-rays to perform tomography, one can instead produce an image of the object by measuring the scattered X-rays. While the underlying physics varies between scatter mechanisms, the fact that the scattered X-rays interact with the material means that their properties will have changed in a material-specific way. For example, the wave vector, energy, and/or polarization of the scattered photons represent new measurement degrees of freedom in scatter tomography that can provide additional contrast mechanisms (i.e., reveal additional information about the object of interest). Furthermore, these additional degrees of freedom result in a wide range of possible scattering tomography architectures (as will be discussed below in the context of XRDT), which open the door to novel tomographic capabilities. For example, the finite deflection of the scattered X-rays effectively lifts the degeneracy inherent in transmission tomography and makes snapshot (i.e., single measurement) scatter tomography possible (see Figure 1.1b). Alternatively, one can structure the illumination and measurement components to enable compressive tomography, in which the object dimensionality exceeds the measurement dimensionality.[10]

A challenge of scatter tomography, however, stems from the fact that the scatter signal is weak compared to the transmitted signal. This disparity in signal strengths arises from two distinct mechanisms: first, the scatter interaction strength is small. As a result, the total scattered X-ray flux is usually only a few percent of the incident beam flux. Second, the scatter signal is spatially diffuse (i.e., the signal originating at any point within the object can be emitted into a large angular range) and decays with distance much more rapidly than the incident beam. While the discussion to this point has been general, the focus of the remainder of the chapter is on the specific case of XRDT and discusses methods for its successful implementation.

1.2.2 X-Ray Diffraction

X-ray diffraction is well-understood and can be interpreted in terms of coherent X-ray scatter from a phase-sensitive, multibody system. More specifically, the electric field of an incident X-ray creates an oscillation of the electron charge distribution within the target object. This, in turn, causes the atoms to re-radiate X-rays at the same energy but spread out over a range of angles. This elastic scattering process, known as Rayleigh scatter, occurs for all atoms illuminated by the incident X-ray beam. For electrons located within the coherence volume of X-ray beam, the scattered fields have a well-defined phase relationship and can therefore interfere with one another. The resulting scattered X-ray distribution depends sensitively on the structure of the illuminated material and can therefore be used for material analysis (as discussed in more detail below).

The probability for an X-ray with energy E to undergo coherent scatter into a solid angled Ω is given by the differential scatter cross section

$$\frac{d\sigma_{coh}(E)}{d\Omega} = \frac{{r_e}^2}{2}\left[1+\cos^2(\theta)\right] f(q) \tag{1.1}$$

where r_e is the classical electron radius and θ is the X-ray deflection angle (relative to the incident wave vector, see Figure 1.2a). The function $f(q)$ is the square of the coherent scatter form factor (or structure factor), which modifies the free electron Thomson cross section by taking into account both intra-atomic and interatomic interference effects. This form factor is related to the Fourier transform of the electron density of an object and is therefore unique to each material. Furthermore, because it combines both chemical and structural information, $f(q)$ provides molecular specificity that allows one to go beyond standard chemical identification (as in fluorescence[16] or hyperspectral transmission imaging[15]). For example, diamond and graphite can be easily distinguished via XRD, despite having identical chemical compositions. In this way, XRD provides a fingerprint that is material-specific and enables one to determine the molecular structure of a material and/or identify the type and class of an unknown substance. Figure 1.3a shows