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Theory of X-ray Phase-Contrast Imaging

Daniele Pelliccia, Marcus J. Kitchen, and Kaye S. Morgan

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49.1 Introduction

Before making his discovery of “a new kind of rays” public, W.C. Röntgen spent 6 weeks of uninterrupted work in his laboratory, meticulously experimenting on the properties of the new phenomenon he had just discovered. At the end of that 6-week period he made his first public communication at the Würzburg Physico-Medical Society (Röntgen 1895, 1896a,b) (see Section II, Chapter 17). The discovery of the new rays and their ability to make photographic images of bones inside the body was arguably the first truly global media hit by a scientific discovery. Promptly amplified by the media, the new “photography” was soon adopted by physicians and surgeons in their practice (Assmus 1995) (see Section II, Chapter 18).
The astounding new medical applications of X-rays obscured other results that were contained in Röntgen’s first account. X-rays shared with visible light the ability to imprint photographic plates, and, therefore, Röntgen set out to search for other effects, such as diffraction, refraction, or focusing, in analogy with visible light. Using a modern terminology, Röntgen was looking for phase effects in the X-ray beam. Experimenting with conventional (at the time) optical elements, he could find no conclusive evidence of reflection or refraction of X-rays, concluding that X-rays cannot be deviated by ordinary optical elements.

The very nature of the new rays was obviously obscure at the time of their discovery, but evidence of the electromagnetic nature of X-rays began accumulating, starting with the work of Dutch physicists Haga and Wind (1899), who found evidence of X-ray diffraction from a slit, and eventually became clear with the discovery and interpretation of X-ray diffraction from crystals (Bragg and Bragg 1913; Friedrich et al. 1913; von Laue 1913).

Today, a multitude of experimental techniques are based on the wave nature of the X-ray fields (Als-Nielsen and McMorrow 2011). Specifically, with the advent of powerful synchrotron sources (see Section I, Chapter 8), and more recently of innovative X-ray laboratory sources, refraction and interference phenomena of X-ray fields can be routinely observed and used for experiments. The classical diffraction theory, describing wave propagation and image formation through optical systems, can, therefore, be rigorously applied to X-ray waves, just as it is commonly done for light waves. As a consequence, X-ray phase effects in imaging (X-ray phase-contrast imaging) can be confidently used alongside attenuation effects.

This chapter will present the wave optical formulation of X-ray phase-contrast imaging and the different ways phase-contrast can be used to generate image contrast with and without optical elements.

### 49.2 Wave Equations and Paraxial Fields

The propagation of scalar fields is the basic tool of the electromagnetic theory we will need to describe the foundations of phase-contrast X-ray imaging. In this section, we shall introduce the basic ideas upon which all the understanding of phase-contrast X-ray imaging, in its different forms, is based.

#### 49.2.1 Spectral Decomposition of a Wave Function and the Helmholtz Equation

In this paragraph, we shall introduce the basic optical formalism of wave propagation and describe the approximation of paraxial field that is commonly employed to describe X-ray wave propagation.

Let us begin with a scalar field function, \( \Psi(x, y, z, t) \), of three spatial coordinates, \( x, y, z \), and time, \( t \). \( \Psi(x, y, z, t) \) is the solution of the d’Alembert equation in vacuum:

\[
\left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \right) \Psi(x, y, z, t) = 0. \quad (49.1)
\]

In Equation 49.1, \( c \) is the speed of light in vacuum, and \( \nabla^2 = (\partial^2/\partial x^2) + (\partial^2/\partial y^2) + (\partial^2/\partial z^2) \) is the Laplacian operator. Following the approach adopted in Paganin (2006), we spectrally decompose \( \Psi(x, y, z, t) \) into monochromatic components using the Fourier integral:

\[
\Psi(x, y, z, t) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \psi_\omega(x, y, z) e^{-i\omega t} d\omega, \quad (49.2)
\]

where each monochromatic component of the field with angular frequency, \( \omega \), has been written as the product of a spatial part, \( \psi_\omega(x, y, z) \), and a harmonic time-dependent term. By direct substitution of Equation 49.2 into Equation 49.1, one can verify that each (monochromatic) time-independent spatial wave function, \( \psi_\omega(x, y, z) \), must satisfy the equation:

\[
(\nabla^2 + k^2)\psi_\omega(x, y, z) = 0, \quad (49.3)
\]

with \( k = \omega/c \) and, again, the equation is valid in vacuum. Equation 49.3 is called the Helmholtz equation and is the key equation underpinning most of the results in X-ray phase-contrast imaging.

Describing an imaging process by means of the Helmholtz equation usually suffices when the X-ray beam is monochromatic (or quasi monochromatic), a situation commonly encountered in synchrotron-based X-ray imaging. However, most of the radiological imaging is done with polychromatic X-ray generated by X-ray tubes with non-trivial spectral properties. In this case the spectral decomposition of the wave function into monochromatic components has a huge practical importance: it enables the description of imaging processes with a time-independent approach for each monochromatic component, which can then be combined to obtain the complete description of the polychromatic process.

#### 49.2.2 Paraxial Fields

From a theoretical perspective, the very nature of electromagnetic waves precludes the possibility of perfectly confined light transport across free space, that is to say we cannot generate waves with zero angular spread without confinement. However, under certain conditions, one can generate waves with small angular spread, a situation that is commonly referred to as “light beam” (Saleh and Teich 1991). A beam is an electromagnetic wave propagating in free space with small divergence. In a beam, the electromagnetic energy is concentrated within a small region about the beam axis, with small spread compatible with the wave nature of light.

An electromagnetic field with such properties is called a paraxial field. A common example of a paraxial field is a laser beam, whose paraxial nature is defined by the resonating cavity in which the beam is generated (Svelto and Hanna 1976). Importantly, in most situations involving phase-contrast imaging, X-ray fields also behave as paraxial fields. This interesting aspect, which we shall discuss in detail in the next sections, enables one to apply the mathematical formalism of paraxial fields to phase-contrast imaging. Using paraxial fields is a great advantage because it not
only simplifies the equations involved in the theoretical description of phase-contrast imaging, but, more importantly, enables simple algorithms for phase retrieval.

Let us introduce here the mathematical formalism of paraxial fields and discuss the approximations implicit in the paraxial assumption. Let us consider the monochromatic spatial scalar wave function $\psi(x, y, z)$ solution of the Helmholtz equation. In the following, we shall drop the subscript $\omega$, tacitly assuming the wave field to be monochromatic, unless otherwise specified. Such a field is said to be paraxial when

$$
\psi(x, y, z) = \Phi(x, y, z)e^{ikz}, \tag{49.4}
$$

and the variations of the complex envelope, $\Phi(x, y, z)$, with the longitudinal position, $z$, are much smaller than its variation in a transverse plane $(x, y)$. In this way, $\psi(x, y, z)$ displays beam-like propagation properties along the $z$-axis, so that its slowly varying complex envelope, $\Phi(x, y, z)$, is modulated by a carrier plane wave, $e^{ikz}$. This situation is graphically depicted in Figure 49.1, which shows a 2D paraxial wave for simplicity. The carrier wave (oscillating) is shown in black, and the slowly varying envelope $\Phi$ is shown in gray.

The paraxial Helmholtz equation

$$
\nabla^2 \Phi(x, y, z) + 2ik \frac{\partial \Phi(x, y, z)}{\partial z} = 0. \tag{49.8}
$$

In Equation 49.8, $\nabla^2 \Phi$ is the transverse Laplacian $\nabla^2 \Phi = (\partial^2 / \partial x^2) + (\partial^2 / \partial y^2)$. The paraxial Helmholtz equation is the approximation of the Helmholtz equation under the condition of slowly varying envelope.

A notable solution of the paraxial Helmholtz equation is the Gaussian beam, a key concept in the theory of optical resonators and lasers (Svelto and Hanna 1976). Another very important class of solution—central to our discussion about phase-contrast X-ray imaging—is the parabolic wave front, a concept heavily used when studying the near-field diffraction of X-rays after interacting with a sample.

### 49.3 Inhomogeneous Equations and the Refractive Index

The previous section was devoted to the propagation of scalar fields across empty space. All equations we derived are rigorously valid in vacuum. Obviously, any phase-contrast imaging effect requires the interaction of the X-ray wave with a sample, and, therefore, the equations must be generalized to the presence of media.

In this section, we shall briefly introduce the interaction mechanism of X-rays with matter, describing the basic equations and the commonly used approximations in the study of the interaction of X-rays with macroscopic objects.

#### 49.3.1 Inhomogeneous Equations

Our task for this section is to generalize the wave propagation equations to account for the presence of materials. In optics, this is commonly accomplished by introducing a macroscopic, position-dependent, and frequency-dependent (but time-independent) quantity called the refractive index. We shall indicate the refractive index with the symbol $n(x, y, z)$, again omitting its explicit dependence on the frequency, $\omega$. The refractive index is defined as the square root of the ratio between the electrical permittivity of the material, $\varepsilon(x, y, z)$, and the electrical permittivity of the vacuum, $\varepsilon_0$:

$$
n(x, y, z) = \left(\frac{\varepsilon(x, y, z)}{\varepsilon_0}\right)^{1/2}. \tag{49.9}
$$

The d’Alembert equation in the presence of non-magnetic media takes the form:

$$
\left(\frac{n^2(x, y, z)}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2\right)\psi(x, y, z, t) = 0. \tag{49.10}
$$

Before proceeding further, a clarification is in order. The d’Alembert (Equations 49.1 and 49.10), and indeed all subsequent equations, are valid for a scalar field (i.e., for a single component
of the electric or the magnetic field. This is indeed already an approximation: in general, the wave function is a vector quantity, describing the evolution of both electric and magnetic field components and their mixing. Therefore, a single scalar wave equation is in principle not sufficient when polarization effects must be taken into account, as is common practice in visible light optics. Nevertheless, for most cases in hard X-ray imaging, the variations in the optical density of any media are sufficiently slowly varying over length scales comparable to the wavelength, that the electric and magnetic field components can be considered effectively decoupled (see Paganin 2006). This justifies our tacit initial approximation of using a scalar theory to study X-ray wave propagation.

Having briefly discussed this issue, we can resume our discussion on the wave propagation in the presence of media. Following the same procedure we discussed for the propagation in vacuum, the complex field obeying the d’Alembert (Equation 49.10) can be written as superposition of monochromatic fields using the Fourier integral in Equation 49.2. In turn, each monochromatic component obeys the inhomogeneous Helmholtz equation (again the explicit frequency dependence has been omitted):

\[
(\nabla^2 + n^2(x,y,z)k^2)\psi(x,y,z) = 0. \tag{49.11}
\]

Further, since we can almost always assume the paraxiality conditions to be valid, we can write the paraxial inhomogeneous Helmholtz equation for the complex envelope which, following the treatment of the previous paragraph, takes the form:

\[
\nabla_i^2\Phi(x,y,z) + 2i\kappa\frac{\partial\Phi(x,y,z)}{\partial z} + k^2(n^2(x,y,z) - 1)\Phi(x,y,z) = 0. \tag{49.12}
\]

With the paraxial inhomogeneous equation, we now have all the mathematical tools to study X-ray phase-contrast effects in imaging, as well as the different methods to extract quantitative information about the sample from phase-contrast data.

### 49.3.2 More on the Complex Refractive Index

The inhomogeneous equations written above are very general, and can be applied to any electromagnetic wave, not just X-ray waves. The refractive index has peculiar characteristics in the X-ray region of the spectrum that can be used to simplify the solution of the inhomogeneous equation.

It is well known that the refractive index of optical materials for visible light is significantly larger than 1, where 1 is by definition the refractive index of vacuum. Moreover, for most visible optical elements, at least in the first approximation, the absorption can be neglected. For X-rays, on the other hand, the difference in the refractive index from unity is extremely small (of the order of \(10^{-6}\) for hard X-rays), and the attenuation effects are always non-negligible. The X-ray refractive index is usually expressed as

\[
n = 1 - \delta + i\beta. \tag{49.13}
\]

The real part, \(\delta\), is related to the refraction (dispersion), and the imaginary part, \(\beta\), to the absorption.

Figure 49.2 shows the calculated values of \(\delta\) and \(\beta\) for three representative human tissues, using density and composition as reported in White et al. (1989), in the energy range between 10 and 200 keV. It is evident that the real part of the refractive index is always about two orders of magnitude larger than the imaginary part.

We will see in Section 49.5 that conventional radiology is based on attenuation imaging, related to the imaginary part of the complex refractive index. Phase-contrast, on the other hand, yields a quantity that is related to the real part, \(\delta\). It is often said that, since in the spectral region of interest for radiology it is always \(\delta \gg \beta\), phase-contrast is always stronger than the attenuation contrast. While this statement is true in principle, it does not hold true in practice, given the fundamental difference between the measurement of attenuation and phase. Therefore, justifying the development of X-ray phase-contrast imaging solely on the comparison between \(\delta\) and \(\beta\) is too simplistic and does not take into account the actual ways in which the measurements are performed.

A more interesting and sensible comparison can be made when considering the difference in contrast between similar tissues. With reference again to Figure 49.2, we can observe that the cortical bone refractive index is well separated from soft tissues refractive index (hence, the good quality of bone imaging in conventional radiology), but the difference between adipose and skeletal muscle tissue is extremely small. Nevertheless, when we compare the differences \(\Delta\delta = \delta_{\text{max}} - \delta_{\text{adip}}\) and \(\Delta\beta = \beta_{\text{max}} - \beta_{\text{adip}}\) between the real and imaginary parts of skeletal muscle and adipose tissue, respectively (as in Figure 49.3), we notice that \(\Delta\delta \gg \Delta\beta\). This is a more significant figure of merit to compare attenuation and phase-contrast: phase-contrast methods enable tiny differences in the real part of the refractive index to be more readily measured over attenuation contrast. In other words, phase-contrast may offer an advantage when one needs to distinguish between different types of soft tissues.
we can consider the “ray path” as the trajectory defined by the direction of the wave vector at that location in absence of the sample (dashed arrow). Given the negligible scattering that takes place within the sample, we can assume that the presence of the sample has a negligible effect on the local direction of the ray paths. All scattering within the sample can then be described by an exit wave, defined at a plane $z = z_0$ immediately downstream of the object. Transverse changes in the amplitude and phase, accumulated by the unscattered wave front when traversing the sample, are imprinted in the exit wave. Neglecting the scattering effects within the sample is equivalent to discarding the Laplacian term in the inhomogeneous paraxial Helmholtz (Equation 49.12), so that, in the projection approximation, we have

$$2ik \frac{\partial \Phi(x, y, z)}{\partial z} + (n^2(x, y, z) - 1)\Phi(x, y, z) = 0, \quad (49.14)$$

This approximation describes the passage of rays through an object, by defining a nominal exit-surface, immediately “downstream” of the irradiated object, at which transverse phase and intensity changes are imprinted. The projection approximation assumes that all scattering within the object is fully described by this exit wave, with negligible diffraction within the scattering volume.

### 49.5 Visualizing X-ray Phase-Contrast

#### 49.5.1 Attenuation, Phase, and Refraction

The boundary value problem for the differential in Equation 49.14 can be solved using standard procedures (Paganin 2006), yielding the wave field at the position $z = z_0$ as

$$\Phi(x, y, z_0) = \exp \left[ \frac{k}{2\pi} \int_0^{z_0} (1 - n^2(x, y, z))dz \right] \Phi(x, y, 0). \quad (49.15)$$

The complex refractive index is usually written as in Equation 49.13, where the real and imaginary part $\delta$, $\beta \ll 1$ are related to the microscopic scattering coefficients of the interaction of X-rays with matter (Als-Nielsen and McMorrow 2011). Given the small value of $\delta$ and $\beta$ compared to unity, $n^2 \approx 1 - 2\delta + 2i\beta$ and, therefore,

$$\Phi(x, y, z_0) = \exp \left[ -ik \int_0^{z_0} \left( \delta(x, y, z) - i\beta(x, y, z) \right)dz \right] \Phi(x, y, 0). \quad (49.16)$$

The previous formula gives us an expression for the phase shift and attenuation an X-ray wave undergoes when crossing a sample, in the projection approximation. The phase shift is given by the imaginary part of the exponent, $\Delta \phi = -k \int_0^{z_0} \delta(x, y, z)dz$, and the attenuation by its real part, $-k \int_0^{z_0} \beta(x, y, z)dz$. To gain a more solid physical understanding of the previous expressions, let us assume to have a single homogeneous material. In this case,
δ and β are independent of the position, and the transmitted wave field can be written in a simple form:

\[ \Phi(x, y, z_0) = \exp[-k(\delta + \beta)(x, y)]\Phi(x, y, 0), \]  
(49.17)

where \( t(x, y) \) is the projected thickness of the sample along the ray path. The intensity transmitted after the sample is simply the square modulus of the transmitted complex wave field:

\[ I(x, y, z_0) = \exp[-\mu(x, y)]I(x, y, 0). \]  
(49.18)

Equation 49.18 is the well known Beer–Lambert law of attenuation, where we have defined the attenuation coefficient as \( \mu = 2k\beta = 4\pi\beta/\lambda \).

### 49.5.2 Paraxial Fields and the Transport of Intensity Equation

One of the interesting features of the treatment we have just developed is that it is not possible to measure phase-contrast from a conventional radiograph of the sample, thus, an intensity measurement taken immediately downstream of the sample. Any conventional detector will produce an intensity measurement that is proportional to the square modulus of the complex wave field, and the information about the phase shift produced by the sample is lost. Fortunately, there are other ways to access the phase information.

Let us assume that a plane wave has interacted with a sample, and the complex wave field after the sample is \( \Phi(x, y, z_0) \). In the projection approximation, \( \Phi(x, y, z_0) \) is given by Equation 49.16. Let us also assume that, after the sample, the wave field propagates in vacuum. Therefore, at any position, \( z > z_0 \), the field can again be described by the paraxial homogeneous Helmholtz equation.

To make a step forward, let us rewrite the complex envelope as

\[ \Phi(x, y, z_0) = \sqrt{I(x, y, z_0)}e^{i\phi(x, y, z_0)}, \]  
(49.19)

where we have explicitly written the intensity and phase related to the complex envelope. If we substitute the above expression (Equation 49.19) into the paraxial homogeneous Helmholtz (Equation 49.14), and we equate to zero the imaginary part of the resulting expression, we obtain the so-called Transport of Intensity equation (TIE) (Teague 1983):

\[ \nabla_T \cdot [I(x, y, z_0)\nabla_T \varphi(x, y, z_0)] + k \frac{\partial I(x, y, z_0)}{\partial z} = 0. \]  
(49.20)

Now, recalling that the only measurable quantity is the intensity, the TIE has a huge practical importance: it provides a relation between the (measurable) intensity of a slowly varying envelope and the corresponding phase, in the paraxial approximation. We see then a way to measure the phase shift imparted by the sample to an incident wave, by measuring the intensity of the transmitted and propagated wave field.

A clarification is now in order: as it is clear from the Beer–Lambert’s law of attenuation, the phase shift imparted by the sample cannot be extracted by conventional radiography (i.e., a contact intensity measurement). The discussion leading to the TIE, however, suggests that intensity measured after letting the beam propagate further downstream in empty space does contain phase information in it. This information is generally encoded, thus, it cannot be directly recovered during imaging. The way of decoding this information into something useful for imaging is the topic of the next section.

### 49.6 Introduction to Phase Retrieval

At first glance, one might think that a proper use of the TIE written in Equation 49.20 is sufficient to gain information about X-ray phase-contrast from samples. All that is needed is to let the wave field propagate in free space, and this will guarantee the appearance of phase-contrast in the image. While this is certainly true from a qualitative perspective—and indeed phase-contrast is extremely useful to visualize weak samples in hard X-rays—there is a significant caveat when quantitative analysis is required.

It turns out that measuring X-ray phase by means of the TIE is not quite straightforward: the phase cannot be measured directly relying on the TIE, only phase derivatives are accessible.* Let us take another look at Equation 49.20, this time let us expand the derivatives on the first term:

\[ \nabla_T I(x, y, z_0) \cdot \nabla_T \varphi(x, y, z_0) + I(x, y, z_0)\nabla_T^2 \varphi(x, y, z_0) + k \frac{\partial I(x, y, z_0)}{\partial z} = 0. \]  
(49.21)

Since the longitudinal variation of the complex envelope is small compared to the transverse variation, at any position \( z > z_0 \) we can approximate

\[ \frac{\partial I(x, y, z_0)}{\partial z} \approx \frac{I(x, y, z_0) - I(x, y, z_0)}{z - z_0}, \]  
(49.22)

where \( I(x, y, z_0) \) is the intensity that is measurable right after the sample, given by Equation 49.18 for a uniform sample. With some algebraic manipulation, we arrive at the expression:

\[ I(x, y, z) = I(x, y, z_0) - \frac{z - z_0}{k} [\nabla_T I(x, y, z_0) \cdot \nabla_T \varphi(x, y, z_0) + I(x, y, z_0) \nabla_T^2 \varphi(x, y, z_0)]. \]  
(49.23)

Equation 49.23 states that the measurable intensity at any position \( z > z_0 \) downstream of the samples contains three contributions. The first contribution, \( I(x, y, z_0) \), contains only the sample attenuation and, in the case of a weakly interacting object, this term would produce poor image contrast. The second and third terms in Equation 49.23 contain the phase derivatives. These are the ones used in all phase-contrast imaging techniques.

* The X-ray phase can indeed be directly measured with an X-ray crystal interferometer. We shall briefly discuss this type of interferometer later in Section 49.10.
49.6.1 Propagation-Based Phase-Contrast

Propagation-based phase-contrast comes primarily from the third term appearing on the right-hand side of Equation 49.23, namely
\[-(z - z_0)k J(x, y, z_0) \nabla^2 \phi(x, y, z_0).\]
This term grows with the distance from the sample (so long as the distance \(z > z_0\) is not too large), and contains the Laplacian of the phase that modulates the attenuation image. The Laplacian of the phase is responsible for the characteristic edge-enhancement effect in propagation-based phase-contrast imaging. It is worth noting that edge-enhancement is nothing else than Fresnel diffraction in the near-field regime (Paganin 2006).

The edge-enhancement is generated because, in most cases, the transverse phase profile of a sample \(\phi(x, y, z_0)\) is smooth and slowly varying and, therefore, its Laplacian is negligible everywhere, except at the sample edges, where the phase profile changes abruptly.

An example of propagation-based phase-contrast imaging is shown in Figure 49.5, showing the head of a bumblebee. The image has been acquired using synchrotron light at the SYRMEP beamline at Elettra (Trieste, Italy) using 25 keV X-rays and a distance of 60 cm between sample and detector. The propagation distance enables the appearance of the sharp fringe at the boundaries between features of different refractive index.

49.6.2 Differential Phase-Contrast

The second term appearing on the right-hand side of Equation 49.23 can be used to measure a different type of phase-contrast, this time depending on the first derivative of the phase (transverse gradient). This is usually referred to as differential phase-contrast imaging, and it generally requires X-ray optical elements of sorts, or a focused X-ray beam, to be visualized.

The reason for that can be appreciated again in Equation 49.23. The relevant term contains the dot product, \(\nabla I(x, y, z_0) \cdot \nabla \phi(x, y, z_0)\), of the intensity gradient and the phase gradient. This means that, when a sufficiently strong intensity gradient is generated with an optical system before or after the sample, the phase gradient can be recovered with a suitable procedure that depends on the optical element used. We shall see several examples of differential phase-contrast imaging, and related phase retrieval techniques, in the following sections.

The connection between intensity gradient and phase gradient can be made more intuitive when noting that the phase gradient is proportional to the refraction angle that X-rays experience when crossing an interface between two media. With reference to Figure 49.6, let us assume a plane X-ray wave propagating in the \(z\)-direction, incident on a wedge of uniform, non-absorbing material with refractive index \(n = 1 - \delta\).

The phase difference between the wave fronts impinging at the positions \(y\) and \(y + \Delta y\) is \(\Delta \phi = \delta k \Delta t\), where \(\Delta t\) is the difference in thickness between the two positions. For small displacements, it is \(\Delta t \approx \alpha \Delta y / \delta\), where \(\alpha\) is the refraction angle (i.e., the change of the direction of the wave vector after the wave has traversed the wedge). To appreciate this point, we must recall Snell’s law at the exit interface between the medium and the vacuum:

\[(1 - \delta) \sin \theta_1 = \sin \theta_2.\] (49.24)

Now we can use the fact that, for hard X-rays, the refraction angle is small: \(\alpha = \theta_1 - \theta_2 \ll 1\), and, therefore, Snell’s law can be rearranged in the form

\[\alpha \approx \delta \tan \theta_1.\] (49.25)

By looking again at Figure 49.6, we have \(\Delta t = \Delta y \tan \theta_1 \approx \alpha \Delta y / \delta\). Therefore, \(\Delta \phi / \Delta y = k \alpha\), which, for very small displacements, can be written as

\[\frac{\partial \phi}{\partial y} = k \alpha.\] (49.26)

Equation 49.26 links the refraction angle \(\alpha\) to the differential phase in the same direction. We shall see in the following that all differential phase-contrast techniques are realized by introducing an angular sensitivity in the imaging setup, so that small deviation of the wave front direction caused by the sample can

![FIGURE 49.5](image1)

**FIGURE 49.5** Free-space propagation X-ray image of the head of a bumblebee. The image has been acquired using 25 keV synchrotron X-rays at the SYRMEP beamline at Elettra (Trieste, Italy). The distance sample-detector was 60 cm and the detector pixel size was 14 μm.

![FIGURE 49.6](image2)

**FIGURE 49.6** Diagram used to calculate the relation between the refraction angle and the differential phase experienced by an X-ray beam after traversing a wedge-shaped sample.
be readily visualized. The measurement of the refraction angle in any given direction yields the differential phase in the same direction.

In closing this section, we note that, since both propagation-based phase-contrast and refraction contrast require a non-zero propagation distance, \( z \) (see Equation 49.23), it is normal to observe both effects concurrently during the same measurement. Depending on the system used to measure differential phase-contrast (see the following sections for details on that), one can extract both kinds of signal from the same experiment. An example is shown in Figure 49.7, showing experimental X-ray images of a portion of an ant. Figure 49.7a shows the propagation-based phase-contrast imaging. Figure 49.7b,c shows the differential phase-contrast imaging in the horizontal and vertical direction, respectively.

**49.7 Introduction to Visualizing X-ray Scattering**

It is well known that, in the interaction with materials, X-rays can be scattered. Both elastic and inelastic processes can occur, where elastic processes are predominant at low X-ray energy (i.e., below about 30 keV), while inelastic scattering (Compton scattering) is the predominant mechanism at higher X-ray energy.

Compton scattering is an incoherent process in that X-rays are scattered in all directions, regardless of the direction of the incoming wave. Compton scattering is a nuisance in medical imaging, since the halo associated with the incoherent scattering degrades the imaging contrast. Increasing the propagation distance and employing anti-scatter grids are the typical countermeasures that are taken to minimize the deleterious effects of Compton scattering in medical imaging.

The situation for elastic scattering is different. Elastic processes are “coherent”; thus, the direction of the scattered X-rays is related to the incident direction and the sample morphology. Widely-used techniques of small-angle X-ray scattering (SAXS) exploits this kind of idea. SAXS or USAXS (ultra-small-angle X-ray scattering) are extremely powerful to obtain information from samples that are not resolvable in conventional imaging, for instance nanoparticles and nano-structures. By measuring the angular distribution of the scattered X-rays, information about the size, shape, and distribution of the nano-structures can be obtained.

The physics of formation of SAXS/USAXS and phase-contrast imaging is essentially the same; however, phase-contrast is generally measured on a microscopic (or macroscopic) length scale and results from the coherent contribution of extended interfaces, whereas SAXS is the result of a very large number of scattering events happening at the nanoscale. Therefore, in a conventional imaging experiment, SAXS and USAXS can generally degrade the image contrast, just as Compton scattering does. The notable difference is that SAXS/USAXS are coherent processes, and it turns out that differential phase-contrast techniques are generally not able to resolve sub-micron features individually, the scatter imaging modalities are extremely useful in distinguishing regions within the sample where such features are present, by looking at the overall scattering originated therein. For instance, macroscopic regions of increased porosity within a sample, or regions composed of fibrils, can be singled out by measuring the scattering contrast. Scatter imaging techniques are often referred to as “dark field” imaging. It is also possible to extract directional dark field information that arises when there are many scattering features aligned in a certain direction (Jensen et al. 2010).

We will only briefly describe this signal in the following sections, as a detailed treatment of scatter imaging techniques can be found in the following chapters.

**49.8 Propagation-based Phase-Contrast X-ray Imaging**

Whilst phase-contrast can aid in visualizing objects that weakly absorb radiation; phase-contrast can be considered as an aberration to an imaging system, insofar as the image no longer truly represents the object. For this and other reasons it is often considered important to quantitatively recover information about the sample from the images. The exit-surface wavefield provides a true image of the object, free of phase-contrast aberrations, and can reveal quantitative information about the object’s composition. However, it is currently impossible to directly recover this information, as X-ray detectors have only ever been capable of measuring the intensity (amplitude squared) and not the phase information. Recovery of this lost phase information from intensity data alone is a ill-posed problem, and is commonly known as phase retrieval.

Many phase retrieval algorithms have been derived for propagation-based phase-contrast, all of which have required multiple
approximations to be made, and many of them are based on the TIE. Often the approximations are quite restrictive, for example limiting the sample to so-called “weak” or “pure phase” object approximations that limit their use with samples that minimally interact with X-rays. Others require that the sample is composed of a single monomorphous material (sometimes described as homogenous, or single material object). Here we describe a phase retrieval algorithm that falls into the latter category before extending the discussion to more general or multi-material samples.

Using the projection approximation (Paganin et al. 2002) showed that it is possible to accurately recover the projected thickness of a monomorphous object from just a single propagation-based phase-contrast (PB) image. This algorithm requires a priori knowledge of the object’s energy-dependent attenuation coefficient, \( \mu \), and refractive index decrement, \( \delta \). Ideally, the bandwidth of the radiation should be minimal, to ensure a quantitative reconstruction. Upon substitution of the projection approximation for the phase and intensity in the TIE and making use of the following identity

\[
\delta \nabla_T \cdot \{ \exp[-\mu T(x,y)] \nabla_T T(x,y) \} = -\frac{\delta}{\mu} \nabla_T^2 \exp[-\mu T(x,y)]
\]

(49.27)

yields

\[
-\frac{\delta}{\mu} \nabla_T^2 \exp[-\mu T(x,y)] = \frac{\partial}{\partial z} I(x,y,z = 0).
\]

(49.28)

The derivative on the right-hand side can be approximated as the intensity difference between the contact plane and that of the phase-contrast divided by the distance between the planes, \( \Delta \) (see Equation 49.22). Paganin et al. (2002) solved this differential equation via use of the Fourier derivative theorem to yield the projected object thickness as

\[
T(x,y) = \frac{1}{\mu} \ln \left[ F^{-1} \left\{ \frac{F[I(x,y,z = \Delta)]|I_0|}{\Delta |k_T| |\mu + 1|} \right\} \right].
\]

(49.29)

Here, \( F \) is the Fourier transform and \( k_T \) is the Fourier space coordinates dual to \( (x, y) \). Whilst this example may seem somewhat contrived due to the requirement of a monomorphous sample, this algorithm has proven to be extremely successful as it is highly robust against noise, unlike many alternative phase retrieval algorithms. Instability is often created by division-by-zero type artefacts. Here we see that the denominator of this Fourier space filter will never likely be zero, hence its stability. It also depends on the ratio between \( \delta \) and \( \mu \), both of which are proportional to the density of the medium, hence changes in material density throughout the material are permitted. Finally, this algorithm is limited by the TIE, and so should only be valid when a single interference fringe is visible upon free space propagation. However, it has been found to accurately recover the projected thickness of materials when the propagation distance is outside the limit of the TIE, as the “smoothing” properties of this algorithm wash away the fine fringes due to Fresnel diffraction (Mayo et al. 2003).

Wu et al. (2005) have devised an algorithm that is essentially identical to that presented above, but, rather than starting from the requirement of a monomorphous material, they showed that at sufficiently high energy (>60 keV) the attenuation coefficient of soft tissues is dominated by Compton scattering. In that limit, the attenuation is proportional to the electron density, \( \rho_e \), with minimal dependence on the atomic number, \( Z \); hence the soft tissue all have approximately the same attenuation coefficient. Since the real part of the refractive index decrement \( \delta \) is also proportional to the electron density, the ratio of \( \delta \) and \( \mu \) is approximately the same for all such materials. The significance of this discovery for medical imaging comes from the need for relatively high energies (often >60 keV) for penetration through many centimeters of tissues. Based on the paraxial Fresnel-Kirchhoff diffraction theory, their formalism (under plane wave illumination) enables the recovery of the object’s projected electron density as

\[
\rho_e(x,y) = -\frac{1}{\sigma_{KN}} \ln \left[ F^{-1} \left\{ \frac{F[I(x,y,z = \Delta)]|I_0|}{2\pi \left( \frac{\lambda^2 r_0^2}{\sigma_{KN}|k_T|} \right) + 1} \right\} \right].
\]

(49.30)

Here, \( \sigma_{KN} \) is the total cross-section for Compton scattering from a single free electron derived from the Klein–Nishina formula, and \( r_0 \) is the classical electron radius (for biomedical imaging applications, see Section IV, Chapters 50 to 52).

Yan et al. (2008) extended the work of Wu et al. (2005) to apply at all energies for multi-material samples. This method uses an iterative framework to reconstruct the exit-surface phase information using two images, one absorption contrast image and one phase-contrast image. Their attenuation-partition based (iterative phase retrieval) algorithm (APBA) begins with the initial assumption that the attenuation is purely due to Compton scattering. This enables a simple estimate of the attenuation information to be made, which must be corrected for the photoelectric absorption contribution to attenuation. The algorithm uses the attenuation-partition method of Wu et al. (2005) to estimate the amplitude and phase of the exit-surface wavefield using the phase-contrast image as the initial input. Two virtual objects are created, one being the object that will create the image when the attenuation-partition approximation holds, the other being the virtual object being responsible for the differences between the true phase-contrast image and that estimated using the initial virtual object. The measured attenuation contrast image is employed to measure the difference between this and the current estimate of the exit-surface amplitude. A phase-contrast image of the second virtual object is created to account for differences between the estimated and measured phase-contrast intensities. This procedure is repeated until changes in the amplitude of the second virtual object change negligibly between iterations.

Beltran et al. (2010) later extended the phase retrieval algorithm of Paganin et al. (2002), enabling the application of the algorithm to multi-material samples, but without the restriction of high energies as per the work of Wu et al. (2005). This approach requires just a single phase-contrast projection, and enables the user to focus on a material of interest \( (a) \) embedded in an encasing medium \( (b) \). The complex refractive index of all
materials needs to be known \textit{a priori}, as does the total projected thickness of the sample, \( A(x, y) \). Using a similar chain of logic to Paganin et al. (2002) for a two-material sample under the projection approximation, and neglecting spatial derivatives of the encasing material, the projected thickness of the target material can be isolated as

\[
T_s(x, y) = -\frac{1}{\mu_b - \mu_a} \ln \left\{ \frac{1}{\Delta (\delta_b - \delta_a)/(\mu_b - \mu_a) |k_T|} + 1 \right\}. 
\]

(49.31)

Here the difference between real and imaginary components of the refractive index of the material of interest and the encasing medium are of primary importance. This algorithm is of particular utility for computed tomographic applications, as the total projected thickness, \( A(x, y) \), can readily be determined from reconstructed data. Importantly, multiple materials embedded within the same encasing medium can be isolated separately, and the results spliced together provided the internal materials are spaced by at least \( \sqrt{\delta_b \Delta / \mu_b} \), as detailed in Beltran et al. (2010). Like the previously described algorithms, this formalism is generally highly stable in the presence of noise. For tomographic reconstruction, Beltran et al. (2011) demonstrated improvements in the signal-to-noise ratio of phase retrieved data over absorption contrast data of up to 200-fold. Figure 49.8 shows such an example.

### 49.9 Analyzer-Based Phase-Contrast X-ray Imaging

An alternative phase-contrast technique that requires only a single post-object crystalline optical element is called analyzer-based phase-contrast imaging (ABI) (Suortti et al. 2013) (see Section IV, Chapter 53). Alternative names include the X-ray Schlieren method (Förster et al. 1980) and diffraction-enhanced imaging (DEI) (Chapman et al. 1996). For ABI, a near-perfect crystal analyzer is mounted between the object and detector (see Figure 49.9). The crystal is aligned with the beam incident upon atomic planes where the Bragg condition is satisfied for a specific X-ray wavelength, \( \lambda \), at the Bragg angle, \( \theta_B \), namely

\[
2d_{\text{hkl}} \sin \theta_B = \lambda. 
\]

(49.32)

Here, \( hkl \) are the Miller indices of the chosen atomic planes of the analyzer. Reflection from the analyzer only occurs for X-rays within a narrow angular range of the Bragg reflection. The resulting angularly dependent reflectivity is called the “rocking curve” (see Figure 49.9). The width of this curve is dependent upon the incident energy spectrum, the divergence of the incident wavefield, and variations in thickness across the crystal (Zhong et al. 2000; Rigon et al. 2002).

The analyzer crystal serves as an angular filter, selectively reflecting those photons that best satisfy the Bragg condition and rejecting most of those that do not. The rocking curve reveals the reflectivity expected for a given photon angle of incidence upon passing through the sample. Variations in phase gradients within a sample, therefore, lead to variable spatial intensity distributions in the final image. Strong phase-contrast is obtained when the width of the rocking curve is comparable to the maximum deflection of the beam due to the phase gradients. For the \( \mu \text{rad} \) refraction angles typical for biomedical samples in the diagnostic energy regime, a narrow energy bandwidth is required to minimize the rocking curve width and provide strong phase-contrast. High temporal coherence and low beam divergence is, therefore, essential for this modality. Narrower rocking curves provide greater intensity changes (and, hence, contrast) for smaller refraction angles, which mean the contrast is tunable by an appropriate choice of analyzer reflection and energy (Zhong et al. 2000; Lewis et al. 2003).

The orientation of the analyzer’s Bragg planes with respect to the incident beam determines the plane of diffraction, in
which the incident and reflected beams lie (here labeled as the y-z plane; see Figure 49.9). This plane determines the direction along which changes in beam direction will produce a change in contrast. In essence, ABI is only sensitive to phase-contrast in one-dimension, parallel to the diffraction plane. For diffraction vectors aligned in the y-z plane, phase gradients in that direction will alter the incident beam angle and change the intensity in a manner dictated by the shape of the rocking curve.

Herein we explore the formalism of ABI from a geometrical optics perspective. For early works on this topic, see Gureyev and Wilkins (1997) and Bushuev et al. (1998). This provides an intuitive understanding of how the modality provides image contrast, and is the basis of the majority of successful phase retrieval procedures to date. For an in-depth explanation of this modality from a wave-based perspective see, for example, Bushuev et al. (1998) and Paganin (2006). In the geometric limit, we consider waves as rays that can refract or scatter through an object. Recall that, for small scattering angles, the change in angle of the beam, here denoted with $\Delta \theta$, is directly proportional to the phase gradient of the wavefield, as per Equation 49.26.

We define the Bragg angle peak to be located at angle $\theta_B = 0$. The working point, $\theta_A$, of the crystal can be chosen to control the contrast, which depends on the local gradient of the rocking curve. For an incident beam traveling in the z-direction, refraction by the sample deflects the X-ray beam by an angle $\Delta \theta_{ref}$ in the x-y plane. Following Suhonen et al. (2007), we see that the beam’s local angle of incidence, $\theta$, on the analyzer is

$$\theta = \theta_A - \Delta \theta_{ref} \cos \alpha = \theta_A - \Delta \theta_L.$$ (49.33)

Here $\alpha$ is the azimuthal angle of the refracted beam, but the crystal is only sensitive to the component of the refracted beam parallel to the diffraction plane, $\Delta \theta_L$. Figure 49.10 shows the geometry of the scattering vectors in the x-y plane.

Rays scattered by the object outside the angular range of the rocking curve (in the plane of diffraction) will produce negligible intensity at the detection plane. Effectively this provides

**Figure 49.9** Schematic of analyzer based phase-contrast imaging showing the geometrical optics construction for imaging a cylindrical object. The inset shows the analyzer rocking curve for the Si(333) Bragg reflection, as measured experimentally at 33 keV with a double bounce Si(311) monochromator at beamline 20B2 (SPring-8). Experimental data have been fit with a theoretical curve that incorporates beam divergence. $\theta_0$ and $\theta_f$ show the low and high angle points, respectively, where the reflected intensity is half the peak intensity at the Bragg angle, $\theta_B$. (From Kitchen, M.J. et al. 2005. Phase contrast X-ray imaging of mice and rabbit lungs: A comparative study. British Journal of Radiology 78:1018–27.)

**Figure 49.10** Refraction and scattering of a pencil beam in the scattering vector scale, $q = 2 \sin(\theta) / \lambda$. Refraction of the beam within the sample deflects it from point O to A. Radiation scattered about the central beam by small-angle scattering of vector $q$ creates a halo around the beam, as indicated by the circle. The horizontal lines indicate the “long receiving slit” of the analyzer crystal rocking curve (RC) centered at $q = 2 \theta_L / \lambda = 2 \Delta \theta / \lambda + s$. (Adapted from Suhonen, H. et al. 2007. Refraction and scattering of X-rays in analyzer based imaging. Journal of Synchrotron Radiation 14:512–21, Reproduced with permission of the International Union of Crystallography.)
images virtually free of radiation scattered by more than a few μradians in the diffraction plane. The narrow rocking curve thus acts as a near ideal anti-scatter grid (Figure 49.9) with a very low scatter-to-primary ratio. The rejection of rays refracted (or scattered) outside the rocking curve also produces additional image contrast, sometimes called “extinction contrast” (Chapman et al. 1997; Zhong et al. 2000), that can actually dominate both phase and absorption contrast (Kiss et al. 2003).

Microscopic structures smaller than the resolution of the X-ray detector can coherently scatter radiation to small angles, of the order of mrad or less. The analyzer crystal can be highly sensitive to this small (and ultra-small) angle X-ray scattering (SAXS and USAXS). For a pencil beam traversing the sample, this scattered radiation will form a halo about the beam, as indicated in Figure 49.10, which has been assumed to be axially symmetric. Using terminology common in the SAXS community, the analyzer crystal is considered to be a Bonse–Hart camera in the “long slit” geometry (Bonse and Hart 1965; Suhonen et al. 2007). This considers that the angular slit is “open” in the direction τ, perpendicular to the diffraction plane. Hence, scattering at a fixed position s, parallel to the diffraction plane is integrated in the lateral direction τ, as seen in Figure 49.10. The projection of the scattering vector along the diffraction plane is given by

\[ s = \frac{2 \sin \theta}{\lambda} \approx \frac{2(\theta_A - \Delta \theta_A)}{\lambda}. \]  

(49.34)

\( \theta \) indicates the component of the scattering vector, \( q_z \), perpendicular to the diffraction plane along the “slit” opening, whilst the parallel component is denoted by \( u \). It has been shown (Feigin and Svergun 1987) that the detected intensity integrated over the lateral opening of the detector is

\[ I(s) = \int \int R(u)I_{I}(1 + (s - u)^2)^{1/2} \, dr \, du. \]  

(49.35)

Here, \( R(u) \) is the rocking curve reflectivity in the scattering vector scale. Solving for the “long slit” intensity requires integration over \( \tau \) at \( s - u \), denoted \( I_{\infty}(s - u) \), giving

\[ I(s) = \int R(u)I_{\infty}(s - u) \, du = R(s) \ast I_{\infty}(s), \]  

(49.36)

where * denotes the convolution operation.

Photoelectric absorption by the sample, combined with the loss of intensity from photons scattered beyond the extent of the rocking curve, contribute to the attenuation. Measuring the ratio of the integral of the rocking curve with and without the sample yields, under the projection approximation, the net attenuation factor as

\[ \exp(-\mu T) = \frac{\int I(\theta_A) \, d\theta_A}{\int I_0R_{int}(\theta_A) \, d\theta_A}. \]  

(49.37)

Here, \( I_0 \) is the intensity incident on the sample, and \( R_{int}(\theta_A) \) is the intrinsic rocking curve measured without the sample.

X-ray scattering within the sample produces an angular distribution, \( f(\theta) \), of radiation incident on the crystal. When the rocking curve is measured with the sample in the beam, the resulting reflectivity is the convolution of the \( R_{int}(\theta_A) \) with \( f(\theta) \) (Pagot et al. 2003; Wernick et al. 2003)

\[ R(\theta_A) \equiv I(\theta_A)I_0 = \exp \left( -\int \mu \, dz \right) \int f(\theta)R_{int}(\theta - (\theta_A - \Delta \theta_A)) \, d\theta, \]  

(49.38)

where \( f(\theta) \) has been normalized to unity. As a result of the convolution, the rocking curve measured with the sample is broader and flatter than \( R_{int}(\theta) \). Alternatively, when the width of \( f(\theta) \) is negligible, Equation 49.38 simplifies to

\[ I(\theta_A) = I_0 \exp \left( -\int \mu \, dz \right) R_{int}(\theta_A - \Delta \theta_A). \]  

(49.39)

Here, \( R(\theta) \) we see that the image contrast is directly related to the angle of refraction by the sample; hence, ABI is sensitive to the phase gradient (i.e., the middle term on the right-hand side of Equation 49.23).

49.9.1 Analyser-Based Phase Retrieval

As has been shown in Section 49.9, ABI can record information about a sample’s attenuation, refraction, and ultrasmall-angle scattering (USAXS) properties. Herein, we show some of the main results found for producing an increasing level of information from analyzer-based phase-contrast (AB) images. The first section looks at reconstructing the projected thickness of a monomorphous material using just a single AB image in the absence of USAXS. We then look at recovering the intensity and phase of the wavefield passing through an arbitrary object, that produces negligible USAXS, using two AB images. Finally, we look at methods for recovering all three X-ray interaction parameters using multiple AB images. We restrict the discussion to those methods utilizing a geometrical optics approximation (GOA)-based formalism (see Equation 49.39).

49.9.1.1 Monomorphous Material Reconstruction

Paganin et al. (2004) developed a series of phase retrieval algorithms for extracting phase and amplitude information from AB images using wave-optics formalism. The simplest of these requires only a single AB image to reconstruct the projected thickness of a monomorphous (sometimes called a homogenous, or single material) object. The object’s energy-dependent attenuation coefficient, \( \mu \), and refractive index decrement, \( \delta \), must be known a priori. Here the authors assume negligible USAXS from the sample, and assume the projection approximation to be satisfied. Briedis et al. (2005) simplified their formalism under the GOA, couching it in terms of the readily measurable rocking curve, \( R_{int} \). This approach requires the rocking curve to be approximated by a linear function, hence the best results are achieved on the half intensity points on the rocking curve.
where the gradient is steepest and the curve approximately linear (see Figure 49.9). We begin by making a first-order Taylor series approximation of Equation 49.39 at point \( A \) on the curve for every point on the image in the \( x, y \)-plane, yielding

\[
I(\theta_A; x, y) = I_0(x, y) \left[ R(\theta_A) + [dR(\theta_A)/d\theta] \Delta \theta_A(x, y) \right]
\]

(49.40)

Here \( I_0(x, y) = I_o \exp(-\mu(x, y) dz) \) (projection approximation for attenuation), and we have dropped the “int” subscript from \( R_{\text{int}} \) for clarity. \( I_o \) is called the “apparent absorption,” since the attenuation coefficient \( \mu \) has a larger than normal contribution from radiation lost from photon scattering beyond the narrow angular extent of the rocking curve. Making use of the projection approximation for the phase of a single material, \( \varphi(x, y) = -k\delta T(x, y) \), the relation between phase gradient and refraction angle (Equation 49.26) and the following identity

\[
\exp[-\mu T(x, y)] \frac{\partial}{\partial y} T(x, y) = -\frac{1}{\mu} \frac{\partial}{\partial y} \exp[-\mu T(x, y)],
\]

(49.41)

yields the following relation:

\[
I(\theta_A; x, y) = I_0 \left[ R(\theta_A) - \frac{\delta R'_A}{\mu} \frac{\partial}{\partial y} \exp[-\mu T(x, y)] \right]
\]

(49.42)

This differential equation can be solved for the projected thickness using the Fourier derivative theorem as

\[
T(x, y) = \frac{1}{\mu} \ln \left[ \frac{\mathbf{F}^{-1} \left\{ \mathbf{F}(I_0(x, y)) / I_0 \right\}}{R(\theta_A) - i \delta R'_A k / \mu} \right].
\]

(49.43)

### 49.9.1.2 Phase and Amplitude Reconstruction

For recovery of the phase and amplitude information from arbitrary materials that produce negligible USAXS, Chapman et al. (1997) developed one of the first phase retrieval algorithms. In their seminal work, they recorded two images of the sample, one at either side of the rocking curve on the steepest part of the slope. At these angles, the rocking curve is approximately linear over a narrow range of angles, whence the intensity is approximately proportional to the phase gradient in the \( x \)-direction. Typically, images are acquired with the analyzer tilted to the half-maximum reflectivity points, labelled as \( L \) and \( H \) in Figure 49.9. This early method employed a first-order Taylor series approximation of the rocking curve (see Equation 49.40) at each of these points. With two images acquired at two working points on the rocking curve there is sufficient information to mathematically separate the “apparent absorption image,” \( I_0(x, y) \), from the refraction angle image, \( \Delta \theta_j(x, y) \). Solving these simultaneous equations yields

\[
\begin{align*}
I_H(x, y) &= [I_L(x, y) R''_H - I_H(x, y) R'_H] / [R(\theta_L) R'_H - R(\theta_H) R''_H], \\
\Delta \theta_j(x, y) &= [I_H(x, y) R(\theta_H) - I_L(x, y) R(\theta_L)] / [I_L(x, y) R'_H - I_H(x, y) R'_L].
\end{align*}
\]

(49.44)

When the refraction by the sample is comparable to the width of the intrinsic rocking curve, which can be quite common, the linear approximation fails to accurately reconstruct the phase and amplitude information. As such, several authors have developed various non-linear curve fitting techniques to analytically reconstruct these parameters. Variants include using higher order Taylor series expansions (Chou et al. 2007; Rigon et al. 2007) and curve fitting using Gaussian (Pavlov et al. 2001; Nesterets et al. 2006), Voigtian (Suohon et al. 2007), and Pearson type VII functions (Kitchen et al. 2007, 2010). Naturally the Taylor series approximation will have limited accuracy far from the chosen working points, but, due to the “long slit” geometry of ABI, the tails of the rocking curve are typically very broad, hence a Gaussian function often does not suffice either. Voigtians are the convolution between a Gaussian and Lorentzian and, hence, offer a flexible fitting solution. However, the Pearson VII function offers a simple formalism that is highly flexible with limits of the Gaussian, Lorentzian, and modified Lorentzian; hence, we employ this formalism here.

The Pearson VII function has long been known to provide excellent fitting to diffraction peaks (Hall Jr. et al. 1977) and has the form

\[
y = c(1 + (\theta - \theta_0)^2/(ma)^2)^{-m}.
\]

(49.45)

Here \( c, a, \) and \( m \) are all positive, real constants, and \( \theta_0 \) is the centroid of the distribution. Applying this form to Equation 49.39 across the detection plane with the Bragg angle set to zero yields

\[
I(\theta_A; x, y) = c I_0(x, y) [1 + (\theta_A - \Delta \theta_j(x, y))^2/(ma)^2]^{-m}.
\]

(49.46)

Acquiring images at two different crystal orientations \( \theta_A = \theta_{A, L} \) and dividing \( I(\theta_j) \) by \( I(\theta_L) \) enables the refraction angle image to be reconstructed as

\[
\Delta \theta_j(x, y) = \frac{\theta_L - \theta_H \pm \sqrt{[\theta_H - \theta_L]^2 - ma^2(B - 1)^2}/B}{1 - B}.
\]

(49.47)

Here, \( B = \sqrt{I_L/I_H} \) and the negative sign outside the square root in Equation 49.47 provides the physically meaningful solution. Finally, the apparent absorption image can be reconstructed by substituting Equation 49.47 into Equation 49.46, giving

\[
I_L(x, y) = \frac{I_{L, H}}{c} \left[ 1 + \frac{(\theta_{L, H} - \Delta \theta_j(x, y))^2}{ma^2} \right]^{-m}.
\]

(49.48)

Thus far, we have only considered using the analyzer as a mirror that selectively reflects X-rays from the surface of a crystal in the so-called Bragg geometry (see Figure 49.9). An alternative is to use the Laue geometry, whereby Bragg reflection occurs from planes approximately perpendicular to the surface of the crystal, and the diffracted beam exits to the back surface of the crystal. With a sufficiently thin crystal (typically \(<1\ mm) \) it is possible to yield two beams simultaneously, namely the diffracted and transmitted beams. The intensity of the transmitted beam is
maximum when the crystal is aligned far from a Bragg condition and, by conservation of energy, is minimum when the diffracted beam is aligned to the Bragg peak (see Figure 49.11). Rocking the crystal through the Bragg peak, therefore, yields approximately equal and opposite intensity gradients between the two beams. Therefore, it is possible to simultaneously record the two images required for performing phase retrieval via either of the formalisms described above. We note, though, that the algorithms are slightly altered to account for the different shapes of the two opposing rocking curves. A potential challenge with the Laue geometry is that, under plane wave illumination, the rocking curve is highly oscillatory, and the period of oscillation depends upon the thickness of the crystal. This phenomenon is known as the Pendellösung effect, and can be explained using dynamical diffraction theory, as described in Authier (2006), and has been used in so-called Dark Field Imaging experiments (see e.g., Sanaguchi et al. 2010). The downside to the Pendellösung effect for phase retrieval is that a simple bell-shaped curve cannot be fit to the rocking curve, and Taylor expansion becomes impractical. However, imperfections in the imaging system readily remove these effects, restoring the rocking curves to bell-curves. Imperfections are readily achieved using a weakly divergent beam (milliradians), increasing the energy bandwidth, or imperfections in the crystal surface. Under these conditions, Kitchen et al. (2010, 2011) showed that the ratio of the diffracted to transmitted rocking curves is also a bell-shaped curve that can be accurately fit using a Pearson VII function, thereby making the phase retrieval process similar to that shown above.

### 49.9.1.3 Multiple Image Radiography

When USAXS makes a significant contribution to the image, a two-image reconstruction will yield considerable artefacts. Equation 49.38 reveals that the width of the rocking measured with the sample increases as the USAXS distribution, \( f(\theta) \), increases. Furthermore, the centroid is seen to shift compared to \( R_{\text{int}}(\theta) \) by the amount \( \Delta \theta_y \). By measuring rocking curves with the sample present compared to that without enables one to reconstruct the attenuation (see Equation 49.37), refraction, and USAXS information by measuring respective changes in the integral, centroid, and width of the curve compared with \( R_{\text{int}}(\theta) \) (see Figure 49.12). In the language of statistics, these are the zeroth-, first-, and second-order moments (Pagot et al. 2003). Solving for the second moment is generally done by subtracting the full-width half-maxima of the rocking curves in quadrature, which yields an exact solution for Gaussian curves. Solving for all three moments requires multiple images of the object to be acquired at multiple orientations of the analyzer. This procedure is commonly known as Multiple Image Radiography (Wernick et al. 2003). Various authors have provided solutions to this problem using Taylor series expansions (Chou et al. 2007; Rigon et al. 2007), curve fitting using Gaussian (Oltulu et al. 2003; Pagot et al. 2003; Nesterets et al. 2006), Voigtian (Suhonen et al. 2007), and Pearson type VII functions (Kitchen et al. 2007, 2010), and

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**FIGURE 49.11** Measured rocking curves (RCs) for the transmitted and diffracted beams through a Si(1 1 1) Laue analyzer using 26 keV X-rays. This plot shows the intrinsic rocking curves measured with no sample in the beam and with the beam transmitted through the lung of a mouse. The rocking curves measured through the lung show reduced intensity due to absorption; a shift in peak position due to refraction; and broadening by USAXS within the sample. Each curve is measured using a single pixel from 260 angular measurements in 0.1 arc second angular steps. (From Kitchen, M.J. et al. 2010. X-ray phase, absorption and scatter retrieval using two or more phase contrast images. Optics Express 18:19994–20012.)

**FIGURE 49.12** Multiple image radiography of an adolescent mouse thorax. Left: Absorption image. Middle: Small-angle scattering map. Right: Refraction angle image. FOV: 21 × 21 mm\(^2\). X-ray energy: 26 keV. (Adapted from Kitchen, M.J. et al. 2010. X-ray phase, absorption and scatter retrieval using two or more phase contrast images. Optics Express 18:19994–20012.)
an iterative approach using maximum-likelihood expectation-maximization (Wernick et al. 2003). The accuracy of each method is primarily limited by how well the rocking curves can be modeled or fit.

### 49.10 Bonse–Hart X-ray Interferometry

Interferometric methods of phase-contrast X-ray imaging began with the Crystal Interferometer designed by Bonse and Hart (1965). This interferometer, shown in Figure 49.13, uses three crystals cut from a perfect single-crystal block to split, recombine, and interfere the beam. The first crystal splits the beam into two by way of a symmetrical Laue reflection (see Section 49.9.1.2), and the second reflects these two beams back toward each other. In order to render the phase interference effects visible at the pixel scale, the beams are combined at the third crystal, with the detector placed soon after.

The phase depth of the sample can then be extracted from the detector image using one of several different methods. Typically, a wedge-shaped phase shifter is placed in the reference beam (Momose and Fukuda 1995). This reference beam, with a ramp in phase, will interfere with the constant phase of the sample beam, and result in periodic straight interference fringes at the detector. When a sample is introduced, these fringes will be distorted according to the phase depth of the sample. If these fringes are of sufficiently high spatial frequency, a Fourier method may be used to extract the phase depth, as described by Takeda et al. (1982). Given the Fourier transform of the output image \( I_{\text{out}}(x,y) \) is well described by

\[
\mathcal{F}[I_{\text{out}}(x,y)] = 4\pi\delta + \frac{1}{2\pi} \int \int e^{-ik_yy}e^{-i(k_1-k_y(0)y+x+k_y(0)x)}\,dx\,dy + \frac{1}{2\pi} \int \int e^{ik_yy}e^{-i(k_1+k_y(0)y+x+k_y(0)x)}\,dx\,dy, \tag{49.49}
\]

the region around the Fourier peak at the fringe frequency (corresponding to the third term of Equation 49.49) can be extracted and the phase retrieved by taking angle of the inverse Fourier transform of that region, utilizing

\[
\phi_{\text{sh}}(x,y) = \tan^{-1} \left\{ \frac{\text{Im}(e^{i\phi_{\text{sh}}}(x,y))}{\text{Re}(e^{i\phi_{\text{sh}}}(x,y))} \right\}. \tag{49.50}
\]

Alternatively, a series of exposures can be captured while the phase shifter is stepped so that the interference fringes slide across the sample, in a process known as “fringe scanning” (Bruning et al. 1974; Momose and Fukuda 1995). This enables better reconstruction of fine and quickly-varying phase features in the sample.

The retrieved signal will be modulo \( 2\pi \), a problem known as “phase wrapping.” In the case of strong phase features, whose magnitude is larger than \( 2\pi \), it is, therefore, necessary to “unwrap” this phase (Ghiglia and Pritt 1998).

Crystal Interferometry is the most sensitive technique to date, directly detecting the phase of the incident wavefield, rather than derivatives of the wavefield phase. The technique can also be combined with Computed Tomography for highly sensitive 3D structural characterization (Momose et al. 1996).

However, the wider adoption of a three-crystal interferometer has been somewhat limited by transmitting only a low energy bandwidth, as well as difficulties in manufacturing perfect crystals of sufficient size and keeping these crystals stable with time.

One solution to these obstacles is a “Grating Bonse–Hart” interferometer, where high frequency gratings are used in place of the crystals, as recently shown by Wen et al. (2014). Here, three identical high frequency phase gratings (e.g., 200 nm period) are used, providing a large diffraction angle, so that the regime is like that of a crystal interferometer. The second grating is stepped perpendicular to both the grating lines and the direction of wave propagation. This will slide the interference fringes across the sample (analogous to stepping the phase shifter in a crystal interferometer), so that around six exposures can be captured to retrieve the phase (modulo \( 2\pi \)). This highly sensitive setup increases the efficiency of the Bonse–Hart interferometry system, reducing the strict requirements on spatial and temporal coherence.

### 49.11 Talbot/Grating Interferometry

Talbot/Talbot-Laue Interferometry (Momose et al. 2003) or Grating Interferometry (David et al. 2002) is a technique that has been widely adopted in research, and is promising as a future clinical imaging tool. This is in large part due to the robustness of the setup to low spatial and temporal coherence (Pfeiffer et al. 2006) and the ability to extract three different imaging modes—attenuation contrast, differential phase-contrast (David et al. 2002, 2007; Momose et al. 2003) (e.g., Figure 49.7b,c), and dark field contrast (Pfeiffer et al. 2008).

#### 49.11.1 Talbot Effect

The Talbot effect (Talbot 1836; Rayleigh 1881; Cloetens et al. 1999) is central to the operation of the Talbot interferometer, and so we will first present this effect before moving onto the theoretical basis of the grating interferometry setup. The Talbot effect is seen in the propagation of a monochromatic wavefield through and beyond a grating structure, as shown in Figure 49.14.

Diffraction of the X-ray beam will result in a pattern that evolves with propagation, with the micro-beams self-interfering and eventually interfering with each other after significant
According to the Talbot effect, this pattern will repeat at distance $z$ from the absorption grating,

$$z_{\text{Talbot}} = \frac{2T^2}{\lambda},$$  

(49.51)

where $T$ is the period of the original grating, and $\lambda$ is the wavelength of the light (where $\lambda \ll T$). This pattern will repeat at integer multiples of this distance (with decreasing visibility depending on the coherence of the source, not modeled in Figure 49.14), and periodic patterns of higher frequency will also occur at fractions of this distance, as seen in Figure 49.14.

Since the Talbot distances will not change significantly for light of a slightly different wavelength, the Talbot effect can still be observed using a polychromatic X-ray source of limited bandwidth.

This effect is also seen with a phase grating, where the features in the grating alter the phase of the wavefield instead of altering the intensity. In the case of a phase grating of phase shift $\pi$, a rectangular intensity pattern of period $T/2$ will be seen at

$$z_{\text{Talbot}} = (n - 0.5)\frac{T^2}{4\lambda},$$  

(49.52)

where $n = 1, 2, 3 \ldots$

A checkerboard phase grid can be used to generate a two-dimensional “grid” pattern at the same distances. This is a more efficient way of producing a grid pattern, in that almost all of the available flux is utilized, compared to an absorption grating where flux is absorbed according to the duty cycle of the grid and does not make it to the detector.

### 49.11.2 Talbot Interferometry Setup

A Talbot or grating interferometry system makes use of the Talbot effect to realize differential X-ray phase measurements. In a grating interferometry setup at a synchrotron source, two gratings are placed one after the other, as in Figure 49.15 (David et al. 2002; Momose et al. 2003). The first grating, $G_1$, acts to split the wavefield into a large number of small beams, which then pass through the sample. The wavefield will be refracted, scattered, and absorbed by the presence of the sample. After some propagation, a distorted pattern can be observed at a Talbot distance from $G_1$. Because the detector pixels are much larger than the grating period, these effects are not resolvable directly, and an analyzer is required. The second grating acts as the analyzer, rendering the refractive, scattering, and attenuating effects of the sample visible at the detector. Note the sample may alternatively be placed immediately before $G_1$.

In the case of an X-ray source of limited spatial coherence, a third grating, $G_0$, can be added to the setup, upstream of $G_1$ (Pfeiffer et al. 2006). This grating divides the primary beam into an array of smaller sources, increasing the effective spatial coherence of the X-ray wavefield. Since $G_0$ is positioned and designed such that a Talbot image is observed at $G_1$ with the same period and position as $G_1$ itself, this does not significantly change the image formation process. In the case of a divergent laboratory source, the setup must also be adjusted to allow for magnification of the grid images and the sample.

We will begin by considering a setup that uses line gratings, in order to be sensitive to phase gradients in one direction.

Following no sample, the grating pattern created by $G_1$ should be observed at $G_2$, when $G_2$ is placed downstream at a distance that is an integer multiple of $z_{\text{Talbot}}$ according to the Talbot effect (Section 49.11.1). While the setup can be constructed with three absorption gratings, $G_1$ is typically a phase grating to maximize the use of available flux and minimize unnecessary dose. In order to create a pattern of period $T$ at $G_2$, the phase grating $G_1$ will have period $2T$, twice the period of $G_1$. Data collection proceeds by translating $G_2$ in steps through a full period of the grating, recording at least five evenly-spaced images through this cycle.
We can begin by considering the case (Case A) when \( G_2 \) is lined up with the incident grating intensity pattern so that the high intensity regions of the wavefield line up with the grating gaps and maximum flux lands on the detector in the absence of a sample.

If the wavefield is refracted by the sample, this will transversely shift the position of the high intensity regions, so that they no longer line up with the grating gaps, and are instead increasingly absorbed by \( G_2 \), and less flux is recorded on the detector. If the wavefield is scattered by the sample, this will distribute the scattered intensity across \( G_2 \), and, hence, less flux will be recorded. If the wavefield is attenuated by the sample, this will decrease the flux incident on \( G_2 \) and, hence, the intensity recorded at the detector.

We can also consider the case (Case B) where the \( G_2 \) is lined up such that the high intensity regions of the wavefield line up with the grating lines and are absorbed, so that, with no sample, minimum flux is recorded. Refraction will result in the increased flux as the high intensity regions move into the grating gaps, scattering will increase the flux as some scattered photons will now pass through the grating gaps and onto the detector, and attenuation will result in decreased flux at the detector.

The case halfway between Cases A and B is when the high intensity regions of the X-ray wavefield are centered on the edges of the grating lines (as seen in Figure 49.15). In this case, case C, refraction in one direction will shift the high intensity region further into the grating gap and increase the flux, and refraction in the opposite direction will shift the high intensity region further onto the grating line and reduce the flux. Scattering will not have a net effect on the total number of photons landing on the detector, and attenuation will, as always, decrease the intensity detected.

By effectively considering these three cases, the three signals can be extracted—describing refraction, scattering, and attenuation by the sample. In order to ensure the intensity is known for each of these three cases, so that all three effects can be extracted, \( G_2 \) is stepped through a full period to obtain or at least interpolate to these three cases. Another way to consider the problem is that the three signals considered in Section 49.11.2 are shown, and, at the pixel described by this curve, the attenuation is described by the decrease in the mean gray level of that pixel over the scan \( (m) \), the refraction comes from the shift in the relative position of \( G_2 \) when maximum flux is detected \( (\varphi) \), and the scattering is described by the decrease in the amplitude of the curve \( (A) \).

Mathematically, the attenuation is given by

\[
\frac{I_f}{I_i} = \frac{m_{\text{sample}}}{m_{\text{nosample}}}. \tag{49.53}
\]

For a single material sample, the projection approximation (Section 49.4) can then be used to determine the projected sample thickness at every position.

Given Equation 49.26, and taking the angular shift in phase stepping curve of

\[
s = 2\pi \frac{z\gamma}{T}. \tag{49.54}
\]

we can retrieve the differential phase, \((\partial_{\varphi} / \partial x = sT/(\lambda z))\) (for the \( x \) direction in this case). This differential phase can be integrated (with naturally improved results if the phase gradients are obtained in both perpendicular directions, \((\partial_{\varphi} / \partial x)\) and \((\partial_{\varphi} / \partial y)\)) to give the projected phase depth, which can be quantitatively interpreted using the projection approximation (Section 49.4) in a similar way to the attenuation signal.

In the case of very strong phase gradients, there can be an ambiguity in determining the direction of the angular shift in the phase stepping curve and/or if this angular shift is greater than \( 2\pi \). This is the same phase wrapping problem present in the Bonse–Hart interferometer. There are strategies for avoiding it experimentally (e.g., placing a sample in water to reduce strong phase gradients at the sample boundaries) or for dealing with it in reconstruction (see Wen et al. (2013) and references therein) if phase wrapping occurs within the sample internal structure.

The scattering will be described by the decrease in visibility of the stepping curve (Pfeiffer et al. 2008; Yashiro et al. 2010). Michelson’s definition of visibility is

\[
\text{Visibility} = \frac{I_{\text{max}} - I_{\text{min}}}{I_{\text{max}} + I_{\text{min}}}. \tag{49.55}
\]
Therefore, the visibility of a stepping curve (e.g., Figure 49.16) will be

\[
\text{Stepping curve visibility} = \frac{(m + A) - (m - A)}{(m + A) + (m - A)} = \frac{A}{m},
\]

and the decrease in visibility due to the introduction of the sample will be

\[
\text{Dark field signal} = \frac{A_{\text{sample}} - m_{\text{no sample}}}{m_{\text{sample}} - A_{\text{no sample}}}. \tag{49.57}
\]

The ultrasmall-angle X-ray scattering distribution can be extracted by looking at moments of the distribution that results from deconvolving the sample phase stepping curve with the flat field (no sample) phase stepping curve (Modregger et al. 2012).

Grating interferometry with line gratings will only detect phase gradients in one direction; however, either the sample or the gratings can be rotated by 90 degrees to take datasets with sensitivity in perpendicular directions (Kottler et al. 2007). Alternatively, a two-dimensional X-ray grating interferometer can be constructing using checkerboard and grid gratings (Zanette et al. 2010), and scanning the gratings in both directions perpendicular to X-ray propagation. Grating interferometry can also be combined with tomography for lab-compatible high-sensitivity 3D imaging (Momose et al. 2006; Weitkamp et al. 2008).

### 49.12 Edge Illumination

The edge illumination technique uses a custom detector to directly render phase effects visible at the detector (Olivo et al. 2001). As seen in Figure 49.17, an absorption grating is placed before the sample, creating an array of beamlets. A second grid pattern is adhered to the detector, placed in order to reduce the accessible region of each pixel to a half (or some other fraction), with the beamlets falling such that they land half on the detector grid and half on a pixel. This means that if the sample refracts the beam in one direction, the beamlet will fall further onto the pixel and increase the observed intensity at that pixel. If the sample refracts the beam in the opposite direction, the beamlet will shift further onto the detector grid line and the observed intensity at that pixel will be decreased.

A differential phase image (e.g., Figure 49.7b) is observed directly at the detector. One direction of differential phase can be revealed using a line grating on the detector, and two directions of differential phase (e.g., Figure 49.7b,c) can be extracted by placing a two-dimensional arrangement of masks across the pixels (Olivo et al. 2009).

In addition, this method is compatible with conventional X-ray sources (Olivo and Castelli 2011, 2014; Diémoz et al. 2013).

The resulting images can be considered analogous to analyzer-based images, created without the need for a crystal or for a monochromatic X-ray source (Endrizzi et al. 2015).

If two images are acquired, shifting the grating transversely so that the resulting beamlets, in the absence of a sample, first fall on the left side of the detector mask features, and then fall on the right side of the detector mask features, quantitative reconstruction is possible. This is in the same way as seen when capturing analyzer-based images on opposite sides of the rocking curve (Munro et al. 2012). If three images are acquired with different positions of Grating 1 (Endrizzi et al. 2014) or two images are acquired alongside some knowledge of the sample properties (Endrizzi and Olivo 2014), then it is possible to also measure broadening of the beamlets to provide a dark field signal. Further contrast modalities related to small angle X-ray scattering (SAXS) from sub-pixel structures can also be extracted (Modregger et al. 2016, 2017). In addition, the resolution of the final image can be improved by using “dithering,” stepping the sample through sub-pixel displacements and combining images (Olivo et al. 2011). If the sample is well approximated by a single known material, it is also possible to utilize propagation effects, as described by the TIE (Equation 49.20), in the reconstruction (Diémoz et al. 2015, 2016). This means only a single exposure is required for image reconstruction, utilizing a similar approach to that used by Breidis et al. (2005) in analyzer-based imaging (Section 49.9.1.1). This is useful for dynamic imaging and for reducing the number of exposures needed for tomography.

A variant of the edge illumination technique, allowing for quantitative phase reconstruction in a single scan, utilizes the edge of an X-ray mirror in place of an opaque edge (Pelliccia and Paganin 2013, 2014). The mirror is aligned to reflect part of the incoming beam, and both direct and reflected beams are incident on the same detector. The beams now encode complementary refraction information that can be used for quantitative phase retrieval.

A final variation on the edge-illumination technique is to use a “virtual edge” at the detector (Vittoria et al. 2014). The second grating is removed and each beamlet is resolved directly using a high-resolution detector. The detector grating or edge is then implemented in software by multiplication with a heaviside function at any required position, and analysis can be performed in the same way as usual. If resolution at the grid scale is sufficient, only a single exposure will therefore be required (Vittoria et al. 2015). This experimental approach leads us directly into the Section 49.13, where beamlets from a single reference object are directly visualized at the detector.

### 49.13 Single-Grid, Speckle-Tracking, and Speckle-Scanning

There are several other techniques that began development as a kind of Shack-Hartmann interferometer, tracking beams from reference apertures or features to map the wavefront (e.g., see
The two perpendicular phase gradients can be integrated together (e.g., Fourier method, as per Kottler et al. 2007, or an iterative method as per Zanette et al. 2014) to give the phase depth, which, for a single material sample, can provide the sample thickness via the projection approximation (Section 49.4). To retrieve an attenuation image (that may include some propagation-based phase-contrast, Section 49.8), the sample-and-grid image can be divided by a grid image that has effectively been distorted according to the measured local shifts (but is typically performed on a pixel-by-pixel basis. In addition, a kind of visibility or dark field image can extracted by looking at how the reference features are broadened and decreased in visibility, resulting in decreased spatial fluctuations (Zanette et al. 2014), a reduced height local cross-correlation (Morgan et al. 2013), and a smearing of the Fourier peak (extracted by taking the ratio between the Fourier grid frequency region and the Fourier origin region) (Wen et al. 2010).

This technique is well suited to dynamic imaging, in that multiple imaging modes (including differential phase-contrast) can be achieved with a single short exposure. It can also be achieved on a laboratory X-ray source (Wen et al. 2010; Zanette et al. 2014; Zdora et al. 2015; Macindoe et al. 2016). However, in the single-shot mode with conventional detectors, the field of view is limited, as pixels must be sufficiently small to directly resolve distortions to the reference pattern (Macindoe et al. 2016).

In order to somewhat overcome this limitation and increase the spatial resolution of speckle-based images, speckle-scanning methods have been developed that scan the reference object (e.g., sandpaper or a resolvable grid) in front of the sample, in effect capturing a kind of stepping curve for each pixel in the style of Talbot/Grating Interferometry (Section 49.11) (Bérjon et al. 2012a; Bérjon and Ziegler 2015). Because the speckle features do not run in only one direction like a typical Talbot/Grating Interferometer, the “stepping curve” for a given detector pixel can take the form of a 2D raster scan as the reference object is scanned in both transverse directions. This scan, collected with the sample present, can then be deconvolved with a raster scan.
completed without the sample present. The resulting correlation map will have an off-center maximum that can be interpreted using Equation 49.59 (where the shift in pixels $S_s$ should now be multiplied by the step size from the scan) to find the differential phase at the given pixel. In a similar way to the single-exposure method, the attenuation signal for that pixel can be found by dividing the mean of the raster scan with sample present by the mean of the raster scan without the sample present, but taken at the “backwards-shifted” location in order to contain the same region of the reference object. The dark field signal can be extracted using these same two scans (sample-and-reference raster scan and corresponding backwards-shifted reference-only scan), by taking the ratio of the standard deviation in the two scans, and dividing by the attenuation signal for normalization (Bérujon et al. 2012, Bérujon and Ziegler 2015). This simplifies to Equation 49.57 in that it is the ratio of the size of the variations in the sample-and-reference/reference stepping curves, divided by the ratio of the mean values of those two stepping curves (in the speckle case making sure to use the same part of the sandpaper for both curves by examining the “preshifted” location in the reference image).

In order to reduce the number of required exposures, hence the dose and imaging time, sparse sampling schemes can be used, both in projection and tomography (Bérujon and Ziegler 2017). Other schemes scan the sample in just one direction (Wang et al. 2016) or scan the reference pattern more finely than the sample-and-reference to reduce the number of sample exposures required (Bérujon and Ziegler 2016).

A recent approach titled unified modulated pattern analysis (UMPA) uses minimization of cost functions to retrieve image modalities while rotating a single grid or stepping a speckle pattern (Zdora et al. 2017).

49.14 The Effect of Polychromaticity and Source Size on Phase-Contrast Imaging

So far, we have always considered the interaction of a monochromatic wave with a sample. In almost all cases concerning medical imaging, however, one has to deal with polychromatic X-ray sources. In most cases the treatment we have developed so far for the various phase-contrast methods still retains its validity, as one can always identify an average (or median) energy value for the incident X-rays for which the monochromatic treatment is approximately correct.

Nonetheless, the effect arising for the beam polychromaticity cannot be neglected if one is interested in quantitative analysis, and in some important cases that we are going to discuss.

We mentioned in the introductory section that, using the spectral decomposition of the incident wave, the problem of imaging with a polychromatic source can be always decomposed in a number of monochromatic interactions that can subsequently be incorporated into the bigger picture. In saying that we deliberately simplified the problem; in this section we shall discuss the idea in more detail, and give some criteria on how the elementary monochromatic imaging problems can be actually incorporated to describe the polychromatic image formation.

A second problem that we have so far ignored, resides in the physical size of the X-ray sources used for imaging. Most of the discussion above was developed by assuming plane wave illumination of the sample. That is obviously never the case in real systems; the finite dimension of the source always produces image blurring, and must be taken into account when analyzing experimental data.

In fact, the effect of polychromaticity and finite source size are two aspects of the same phenomenon: X-ray sources—just as many other light sources such as lamps for instance—produce “thermal radiation” that means an emission that is random in space and time. Blurring and polychromaticity are the consequence of this randomness in space and time, respectively.

The formal treatment of randomness in light fields belongs to the branch of optics called “statistical optics.” It is outside the scopes of this introductory chapter to describe the details of the theory; we will limit ourselves to introduce only one key concept: the so-called partial coherence.

49.14.1 Introduction to Partial Coherence

Optical coherence is the effective ability of a radiation beam to interfere when interacting with an object or with itself, thus producing interference fringes. That is to say, a coherent source produces a highly correlated wavefield in space and time. The model beams we used in the theoretical description of phase-contrast phenomena are coherent beams. A laser is the prototype of a coherent light source. The stimulated emission process responsible for the laser emission generates photons that are highly correlated in space and time; the result is an almost monochromatic beam with minimal divergence. Conventional sources like lamps, stars, or X-ray tubes do not work that way. In these cases, the emission of photons is a random process in both space and time.

For the sake of simplicity, the spatial and temporal random effects are often treated separately. The usual terminology is that of “spatial coherence” and “temporal coherence,” respectively. Even though a clear-cut distinction between the two is not completely correct, it represents a good approximation in many cases, and it has the advantage of a simplified treatment. For an entry level introduction to the concept of partial coherence, see Van der Veen and Pfeiffer (2004) or Hecht and Zajac (1974). Advanced texts are Mandel and Wolf (1995), Born and Wolf (1999), Wolf (2007), and Goodman and Haupt (2015).

49.14.2 Spatial Coherence and Finite Source Size

It is well known that, to obtain a sharp radiograph, one must place the detector as close as possible to the sample. With reference to Figure 49.19, it is clear that, given that the source is not a point, any finite sample-detector distance $z_2$ will cause any feature of the sample to be blurred at the screen plane. The amount of blurring, $b$, thus the extent over which the image a “point” feature on the sample is spread at the detector plane (the image point-spread function), is proportional to the source size $s$ and the sample-detector distance $z_2$ (Pogany et al. 1997):

$$b = s \frac{z_2}{z_1}.$$  \hspace{1cm} (49.60)

The blurring is ideally zero when the sample is in contact with the detector screen. On the other hand, we have discussed at
length how measuring phase-contrast typically requires a free space propagation distance between sample and detector. That is the practical reason why X-ray phase-contrast imaging could initially only be measured at synchrotrons (Cloetens et al. 1996) and with very specialized X-ray micro-focus sources (Wilkins et al. 1996; Pogany et al. 1997).

For conventional X-ray sources, the blurring introduced by increasing the distance sample-detector is so significant that the phase-contrast effects are washed away in practical cases. In synchrotron experiments the distance \( z_1 \) (source-sample) can be made very large, of the order of tens of meters, in practice \( z \gg z_1 \) and the blurring is greatly reduced. In the case of a micro-focus source, it is the extremely small source size (of the order of few microns) that enables visualization of phase-contrast fringes with acceptable contrast.

The physical origin of the blurring is in the spatial partial coherence of the X-ray beam generated by an extended source. Since the nature of the source is chaotic—there is little or no correlation between electrons bombarding different positions of an anode—X-rays emitted at different positions along the source are uncorrelated (i.e., they in general have a random emission direction).

This means that, if one wants to calculate the effects that the finite extent of the source has on the measured image, it is sufficient to perform the calculation with an ideal point-like source, and then convolve the result over the source intensity distribution, as seen by the sample. The source intensity distribution, in many practical cases, can be approximated by a Gaussian function:

\[
I(x, y) = I_0 \exp \left( -\frac{x^2 + y^2}{2\sigma_s^2} \right). \tag{49.61}
\]

where \( I_0 \) is the maximum intensity, and the variance of the Gaussian \( \sigma_s^2 \) is associated with the source size.

Therefore, by calling \( I_0(x, y) \) the “ideal” image of a sample produced by a point-like source at infinite distance (see Equation 49.23), the blurred image due to the source size can be calculated as

\[
I(x, y) = I_0(x, y) \otimes B(x, y). \tag{49.62}
\]

In the previous equation, \( B(x, y) \) is the blurring kernel given by the source intensity distribution projected on the sample (Pogany et al. 1997):

\[
S(x, y) = I_0 \exp \left( -\frac{x^2 + y^2}{2\sigma_s^2} \right). \tag{49.63}
\]

with \( \sigma^2 \approx \frac{z_1^2 + z_2^2}{z_1 + z_2}, \)

In closing this section, we note that in all practical cases one needs to accounts for the detector resolution as well. Clearly, phase-contrast fringes can be unobservable if the detector resolution is poor. The convolution approach we just described can be extended to include the detector resolution as well by redefining the blurring kernel to include the detector resolution. In practice, one has to redefine the variance (Wilkins et al. 2014):

\[
\sigma^2 \approx (1 - 1/M)^2 \sigma_s^2 + M^{-2}\sigma_D^2 \tag{49.64}
\]

In Equation 49.64 we introduced \( M = (z_1 + z_2)/z_1 \) as the geometrical magnification of the setup, and \( \sigma_D^2 \) as the variance associated with the detector point-spread function, linked to the detector pixel size by the properties of the imaging systems.

### 49.14.3 Temporal Coherence and Polychromaticity

Equation 49.64 provides a realistic description of the blurring effects due to the finite source size and detector resolution, for a monochromatic illumination. Extending the result to a polychromatic beam requires the knowledge of the spectrum of the X-ray source. Denoting by \( w(\lambda) \) the normalized spectrum of the source, the effect of the polychromaticity can be modeled as the superposition

\[
I_\mu(x, y) = \int w(\lambda) I_\lambda(x, y) d\lambda. \tag{49.65}
\]

The monochromatic term \( I_\lambda(x, y) \) is calculated with Equation 49.62.

The source spectrum at the sample can be obtained by either measurement or calculation, considering the source parameters and the filtration, if present. A number of tools exists both for synchrotron sources (Tanaka and Kitamura 2001; del Río and Dejus 2011) and for conventional X-ray tubes (Poludniowski 2007; Poludniowski and Evans 2007).

Once the spectrum is known, the superposition integral in Equation 49.65 enables the calculation of the effect of the polychromaticity on the image. It is outside of the scope of our introductory chapter to describe in detail the effect that polychromaticity has on phase-contrast images obtained with different methods. Nevertheless, some general considerations can be discussed by exploring the link between the polychromaticity and the temporal coherence.

Temporal partial coherence is related to stochastic emission times of different photons from a source, caused by randomness in the arrival times of the electron on the target. Coherent
sources such as lasers displays can display a very narrow bandwidth, reflecting the fact that the photon emission in different positions of the source is simultaneous. A random emitter, such as an X-ray source, will always display a broader spectrum. This is especially the case for the bremsstrahlung radiation.

The energy (or wavelength) spread of the incoming beam has a different effect on the image formation, depending on which method is employed to measure phase-contrast. The use of specific optical elements (or free-space propagation)—as well as the different physical information that can be extracted (phase or phase derivatives)—makes the various techniques sensitive to a different degree to partial coherence.

Besides their difference, there is one aspect that is common when partial coherence effects—and specifically polychromaticity—are introduced in the X-ray optical system. Attenuation and phase response of the sample (i.e., the sample refractive index) is energy dependent. This dependence is called dispersion. The value of the real part $\delta$ of the refractive index, or the attenuation coefficient $\mu$, are well defined for a single incident wavelength. With polychromatic radiation one needs to redefine effective values for $\delta$ and $\mu$, averaged upon the incident spectrum (Arhatari et al. 2008):

$$\bar{\delta}(x, y) = \int w(\lambda)\delta(x, y) d\lambda,$$

$$\bar{\mu}(x, y) = \int w(\lambda)\mu(x, y) d\lambda. \quad (49.66)$$

With the new definitions, one can meaningfully extract quantitative information (if the spectrum is known) from attenuation and phase-contrast data obtained with polychromatic X-rays.

An exhaustive overview of the influence of polychromaticity on the different phase-contrast imaging techniques can be found in Wilkins et al. (2014). In the following we shall review the most important facts about the effects that partial coherence has in general on the incoming photon energy because of the dispersion. The sharp variations in intensity is caused by sharp fringes at the boundaries between regions of different optical density. The sharp variations in intensity is caused by the X-rays deviated from their original path by the sample, as depicted in Figure 49.20. The amount of the deviation depends in general on the incoming photon energy because of the different response of the material refractive index with energy (dispersion). However, the “loss line” depicted in Figure 49.20 is independent of the energy of the X-rays, always producing a relative sharp fringe. Therefore, in-line phase-contrast imaging can be easily visualized with a polychromatic X-ray source, as first demonstrated by Wilkins et al. (1996).

On the other hand, the in-line setup is quite sensitive to spatial coherence. To visualize sharp fringes, the blurring due to finite size of the source must be small. Synchrotrons and micro-focus X-ray sources meet the requirements of in-line phase-contrast X-ray imaging. Conventional X-ray tubes, with focal spot sizes of the order of a few hundred microns or more are generally not suited for the free-space propagation method.

### 49.14.4 Free-Space Propagation

Free-space propagation phase-contrast images are characterized by sharp fringes at the boundaries between regions of different optical density. The sharp variations in intensity is caused by the X-rays deviated from their original path by the sample, as depicted in Figure 49.20. The amount of the deviation depends in general on the incoming photon energy because of the different response of the material refractive index with energy (dispersion). However, the “loss line” depicted in Figure 49.20 is independent of the energy of the X-rays, always producing a relative sharp fringe. Therefore, in-line phase-contrast imaging can be easily visualized with a polychromatic X-ray source, as first demonstrated by Wilkins et al. (1996).

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### 49.14.5 Analyzer-Based Imaging

ABI techniques are very sensitive to minute phase gradients, due to the exquisite angular sensitivity of crystals in Bragg diffraction. On the other hand, the requirements on the incoming beam coherence also tend to be higher. ABI produces maps of the phase gradient by measuring the refraction angle X-rays experience after passing through the sample.

Both divergence and wavelength spread broaden the width of the rocking curve of the analyzer crystal (Zhong et al. 2000; Rigon et al. 2002), thus reducing the sensitivity. In practice, ABI setups are mostly used at synchrotrons, when the incoming beam has already been prepared by a primary monochromator (Rigon et al. 2002; Suortti et al. 2013), which reduces both divergence and energy spread to maximize the sensitivity of the ABI scheme. It is worth noting, though, that modern high power X-ray sources such as rotating anodes offer the possibility of implementing ABI schemes with crystals (Vine et al. 2007; Vagović et al. 2015), but usually with a reduced field of view.

### 49.14.6 Grating-Based and Other Techniques

Grating interferometry works, in the first approximation, with the same principle as ABI, such as detecting maps of the refraction angle experience by the X-ray beam in crossing the sample. That is actually also true for other techniques, such as edge illumination, coded apertures, and speckle-tracking. In all cases, using gratings, grids, or other structures to analyze the beam poses less restrictions on the coherence properties of the incoming beam.

Talbot interferometry requires good spatial coherence to produce high contrast fringes. In laboratory systems, this is usually achieved by using a primary grating (source grating) (Weitkamp et al. 2006) to spatially fractionate the primary source into an array of smaller sources, thus increasing the effective spatial coherence.

Coded apertures and speckle-tracking rely on producing a sort of structured illumination, so that the deviation of the
49.15 Phase-Contrast Tomography

Conventional X-ray computed tomography (CT) is the method to recover the 3D distribution of the attenuation coefficient of a sample, from a series of 2D projections, taken at different relative orientations of the sample (Kak and Slaney 1988). The starting point is again the Lambert’s law of absorption that we here rewrite as

\[ I(x, y) = I_0 \exp \left\{ -\int \mu(x, y, z) \, dz \right\}. \quad (49.67) \]

In the previous expression, \( \mu \) is the attenuation coefficient for a monochromatic illumination or the effective attenuation coefficient for a polychromatic incident beam, as defined in Equation 49.66. The results discussed here are valid in both cases. In Equation 49.67 and all subsequent equations, an integral without integration limit is intended to be a line integral.

In tomography, a rotated reference frame is typically defined. The rotation angle, \( \theta \), is defined to be about the vertical axis, \( y \), and the new coordinates are defined as: \( \xi = x \sin \theta + z \cos \theta \), \( \eta = x \cos \theta - z \sin \theta \), as in Figure 49.21. The generic projection, measured at the rotation angle, \( \theta \), can be defined as (Kak and Slaney 1988)

\[ p_\phi(\xi, \theta, y) = -\ln \left( \frac{I(\xi, y)}{I_0} \right) = \int \mu(\xi, \eta, y) \, d\eta. \quad (49.68) \]

The one-dimensional Fourier transform (FT) of the generic projection, calculated with respect to the coordinate \( \xi \) is

\[ P_\phi(u, \theta, y) = \int_{-\infty}^{\infty} p_\phi(\xi, \theta, y) e^{-2\pi i u \xi} \, d\xi. \quad (49.69) \]

The Filtered Back Projection (FBP) algorithm (Kak and Slaney 1988) is commonly used to reconstruct the 3D distribution of the linear absorption coefficient:

\[ \mu(x, y, z) = \int_{0}^{\pi} \int_{-\infty}^{\infty} F(u) P_\phi(u, \theta, y) e^{2\pi i u \xi} \, du \, d\theta. \quad (49.70) \]

\( F(u) \) is the Fourier representation of the filter function that, for ordinary absorption tomography, can be defined as (Kak and Slaney 1988)

\[ F(u) = \begin{cases} \frac{1}{|u|} & \text{if } |u| < 1/(2\Delta \eta) \\ 0 & \text{if } |u| > 1/(2\Delta \eta). \end{cases} \quad (49.71) \]

Physically realizable projections are sampled at finite steps, \( \Delta \eta \). Therefore, the filter function is truncated at the Nyquist frequency, \( u_N = 1/(2\Delta \eta) \).

The formalism developed for attenuation tomography can be extended without changes when the projection of the sample-induced phase shift is measured for each angle. As we have seen, phase projections can be measured with a Bonse–Hart interferometer, or using a phase retrieval method. In all cases, the individual phase projections are given by the line integrals of the real part of the refractive index:

\[ p_{\rho\phi}(\xi, \theta, y) = \varphi(\xi, \theta, y) = -k \int \delta(\xi, \eta, y) \, d\eta. \quad (49.72) \]

The 3D distribution of the real part of the refractive index can be obtained by a similar FBP:

\[ \delta(x, y, z) = \int_{0}^{\pi} \int_{-\infty}^{\infty} F(u) P_{\rho\phi}(u, \theta, y) e^{2\pi i u \xi} \, du \, d\theta. \quad (49.73) \]

where \( P_{\rho\phi}(u, \theta, y) \) is the one-dimensional FT of \( p_{\rho\phi}(\xi, \theta, y) \) with respect to the coordinate \( \xi \) (see Equation 49.69).

Phase-contrast X-ray methods that are sensitive to the phase gradient offer another avenue to phase tomography that does not require phase retrieval. The idea was first demonstrated with hard X-rays using a Talbot interferometry setup (Pfeiffer et al. 2007), exploiting the concept of refraction tomography that dates back to 1988 (Faris and Byer 1988). As we have seen, the refraction

\[ \int \]
angle experienced by X-rays when propagating through samples is proportional to the transverse gradient of the phase, that is, the gradient in the directions orthogonal to the beam propagation direction. The refraction projection is given by (Faris and Byer 1988)

$$\alpha(\xi, \theta, y) = \frac{1}{k} \frac{\partial \varphi(\xi, \theta, y)}{\partial \xi} = -\int \frac{\partial \delta(\xi, \eta, y)}{\partial \xi} \, d\eta. \quad (49.74)$$

In the further approximation of a straight optical path, the horizontal and vertical deviations are independent from one another, and the derivative operator can be taken outside the integral (Faris and Byer 1988):

$$\alpha(\xi, \theta, y) = -\frac{\partial}{\partial \xi} \int \delta(\xi, \eta, y) \, d\eta. \quad (49.75)$$

Within these approximations, the 3D distribution of the real part of the refractive index can be obtained by FBP:

$$\delta(x, y, z) = \int_{-\infty}^{\infty} d\theta \int_{-\infty}^\pi H(u) A(u, \theta, y) e^{2\pi i u y} \, du. \quad (49.76)$$

where, in analogy to the previous treatment, $A(u, \theta, y)$ is the 1D FT of $\alpha(\xi, \theta, y)$ with respect to the coordinate $\xi$, and the filter function is (Faris and Byer 1988)

$$H(u) = \begin{cases} 
\text{sgn}(u)/(2\pi) & |u| < 1/(2\Delta \eta) \\
0 & |u| > 1/(2\Delta \eta)
\end{cases}. \quad (49.77)$$

$H(u)$ is called the Hilbert filter.

Refractive tomography based on Equation 49.76 is extremely powerful, as it removes altogether the need for phase retrieval, thus speeding up the process of 3D reconstruction. The general formula in Equation 49.76 can be applied to all techniques that are sensitive to the phase gradient, to provide a fast and reliable tomographic reconstruction.

Performing the phase retrieval before the FBP is, however, still preferable for extremely weak contrast samples. It was recently shown in Gasilov et al. (2014) and Pelliccia et al. (2015), using different approaches, that calculating the phase projections and using an ordinary FBP yields better performances than using a Hilbert FBP on differential phase projections.

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